



MultiMat 2026

12th International Conference on
Numerical Methods for Multi-Material Fluid Flow

Abstract Booklet

Biarritz, France — Monday 7 to Friday 11 September 2026
Centre de Congrès Bellevue – Salle des Vagues



The Centre de Congrès Bellevue overlooking the Grande Plage of Biarritz

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The organizers of MultiMat 2026 gratefully acknowledge the generous support of the official sponsors of the conference:



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The conference also benefits from the support of the **LRC ANABASE**, a joint research laboratory between the Institut de Mathématiques de Bordeaux and CEA-CESTA devoted to the development of innovative numerical methods for the simulation of complex fluid flows.

The organizers would like to thank Webkomomai webkomomai.fr/ for the professionalism in developing the website and posters, and ADERA adera.fr/ for their diligence in managing the financial aspects of this conference.

Welcome to MultiMat 2026 in Biarritz!

The Atlantic ocean, the Casino, the animated area and the famous French cuisine from the South-West and Basque country associated to the agreeable weather provide a perfect incubator for exceptional science here at MultiMat 2026 in Biarritz.

The 12th International Conference on Numerical Methods for Multi-Material Fluid Flow (MultiMat 2026) will push forward the state-of-the-art in the field of compressible multi-phase and multi-material flow problems. Researchers from academic and/or national institutions will focus their discussions on relevant numerical methods, including the analysis of such methods as well as the modeling of complex multi-material flows, which is essential for the investigation and development of new sources of energy, including inertial confinement fusion.

The MultiMat conference series

MultiMat 2026 is the twelfth edition of a conference series that has, for almost a quarter of a century, gathered the international community working on numerical methods for multi-material fluid flows. It follows the previous MultiMat conferences held in Breckenridge (CO, U.S.A., 2024), Zürich (Switzerland, 2022), Trento (Italy, 2019), Santa Fe (NM, U.S.A., 2017), Würzburg (Germany, 2015), San Francisco (CA, U.S.A., 2013), Arcachon (France, 2011), Pavia (Italy, 2009), Prague (Czech Republic, 2007), Oxford (UK, 2005) and Paris (France, 2002).

This 2026 edition is held at the **Centre de Congrès Bellevue – Salle des Vagues** in Biarritz, from Monday 7 to Friday 11 September 2026. About 100 persons are on-site, and about 60 presentations and 35 posters are scheduled.

Scientific topics

The scientific program covers the following themes, which also structure the abstracts gathered in this booklet:

- 1 **Lagrangian and Arbitrary-Lagrangian-Eulerian Methods**
- 2 **Numerical Methods for Fluid Mechanics**
- 3 **Multiphase Flows**
- 4 **Inertial Confinement Fusion, Plasma physics, Radiative transfer**
- 5 **Mesh Adaptation and Interface Methods**
- 6 **High-Performance Computing (HPC) and Mesh optimization**
- 7 **Solid Mechanics, Materials and Industrial applications**

Local organization

Alessia Del Grosso, Vincent Delmas, Pierre-Henri Maire, Raphaël Loubère and François Vilar.

Practical information

Venue	Centre de Congrès Bellevue – Salle des Vagues Place Bellevue, Biarritz, France
GPS	43.483, -1.562
Website	multimat-2026.eu
Contact	contact@multimat-2026.eu

Biarritz and the Pays Basque

Biarritz lies on the shore of the Bay of Biscay, in the Basque province of Labourd, at the extreme south-west of France and less than 25 kilometres from the Spanish border. Along its four kilometres of coastline, sandy coves and beaches – the Grande Plage below the conference venue, the Port Vieux, the legendary Côte des Basques – alternate with cliffs and rocky promontories such as the famous Rocher de la Vierge, all under the mild oceanic climate of the Basque coast, with the foothills of the Pyrénées and the silhouette of La Rhune closing the horizon to the south.



*The Grande Plage of Biarritz, with the Hôtel du Palais
and the lighthouse of the Pointe Saint-Martin in the background*

The town has a long maritime past: for centuries it lived from whale hunting, with lookouts posted on the Atalaye plateau scanning the ocean for the tell-tale spout, before its sailors turned to deep-sea fishing and privateering. Its destiny changed radically in the 19th century with the fashion of sea bathing. The **Empress Eugénie**, who loved the place, persuaded her husband **Napoléon III** to make it their imperial summer residence: the Villa Eugénie – today the Hôtel du Palais – was built for her in 1854, and in their wake the crowned heads and high society of all Europe flocked to what became “the queen of beaches and the beach of kings.” Queen Victoria, King Alfonso XIII of Spain and the Russian aristocracy – to whom Biarritz owes its Orthodox church – were among its faithful visitors.

During the Belle Époque and the Roaring Twenties the promenades around the Bellevue belvedere saw the greatest couturiers of the time open their boutiques, Coco Chanel among them. This prestigious past has left the town an eclectic architectural heritage of villas, palaces and follies of every style. More recently, Biarritz hosted the G7 summit in 2019.

Biarritz is also the European capital of **surf**: introduced from California in the late 1950s, the sport found on the Côte des Basques some of the finest waves of the Atlantic, and the town has been the cradle of French surfing ever since. Add to this the Basque traditions of pelota and rugby, the mountains at the doorstep, and a gastronomy nourished by the ocean and the hinterland – from the stalls of the Halles market to the great tables of the coast – and one understands why science should thrive here so naturally.

Social events: great science in a magnificent place

MultiMat has always cultivated the conjunction of an outstanding scientific program with venues that inspire it, and Biarritz is no exception. Perched above the Grande Plage, the Centre de Congrès Bellevue offers, between two sessions on Lagrangian schemes and multiphase flows, an uninterrupted view of the Atlantic ocean and of the surfers riding the waves that gave the *Salle des Vagues* its name. The social program of the conference has been designed in the same spirit: to bring the participants together, in the most emblematic places of the city, and let scientific discussions continue well beyond the lecture room.

Icebreaking cocktail – Marché couvert des Halles

The conference opens with an icebreaking cocktail held at the **Marché couvert des Halles**, the covered market at the heart of Biarritz. Surrounded by the stalls that every morning showcase the best of Basque and South-West gastronomy, participants will get to know each other – or renew longstanding MultiMat friendships – over local delicacies, in the warm and lively atmosphere that only a true market hall can offer. Let us meet on Monday evening starting at 19:30 (7:30PM), at location "Halles Centrale, Rue des Halles".



The Marché couvert des Halles of Biarritz, host of the icebreaking cocktail

Gala dinner – Rooftop of the Hôtel Talaia

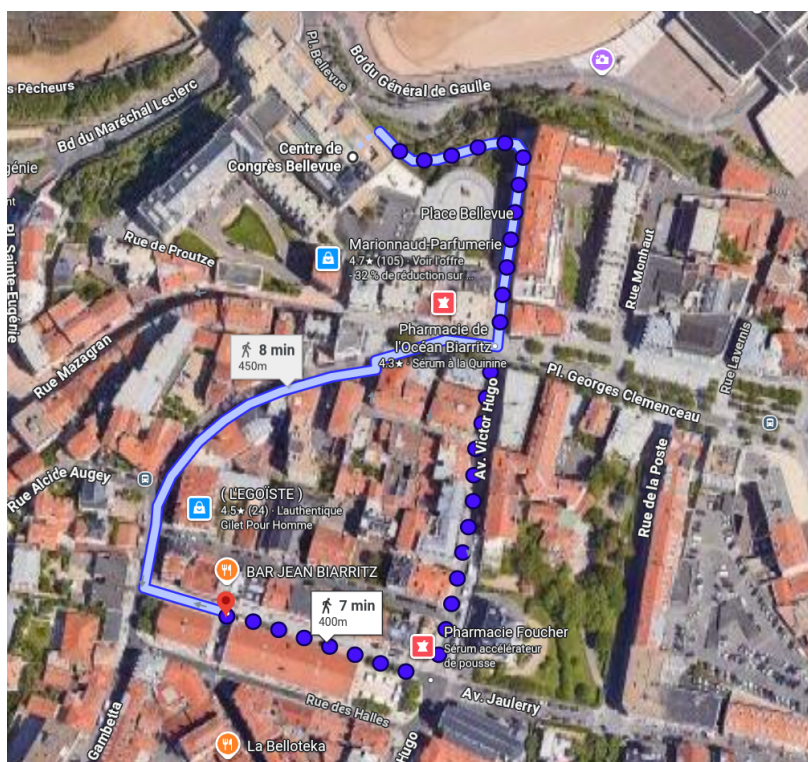
The traditional MultiMat gala dinner takes place on the **rooftop of the Hôtel Talaia**. Facing the ocean, with the sunset over the Bay of Biscay as a backdrop, the gala dinner celebrates the community and the collaborations – past, present and future – that the MultiMat series has nurtured since 2002. We expect the gala dinner to start with a welcome drink around 19:30 (7:30PM) on Wednesday evening.



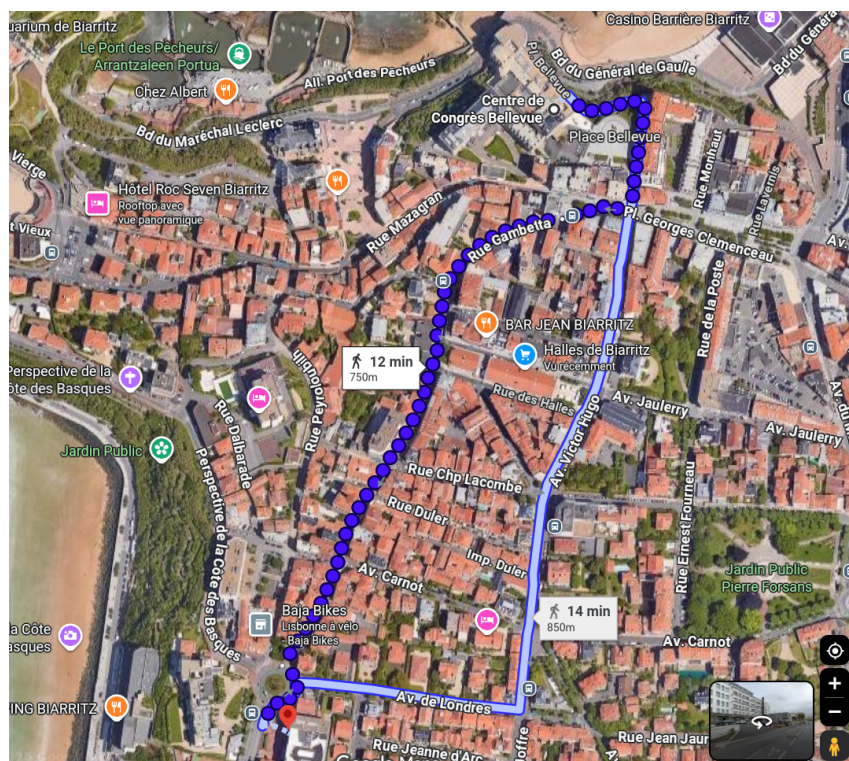
Dinner above the ocean: the rooftop terrace by day and at sunset

May the beauty of the Basque coast inspire, once again, great science: we wish all participants an excellent MultiMat 2026 in Biarritz!

Maps to the “Halles” and “Talaia restaurant”



Map from the "Centre de congrès Bellevue" to "The Marché couvert des Halles" of Biarritz, host of the icebreaking cocktail



Map from the "Centre de congrès Bellevue" to "Talaia Hôtel & Spa Biarritz", host of the gala diner on its rooftop restaurant

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Program at a glance (see this web-link for the most updated version)

Program	Monday	Tuesday	Wednesday	Thursday	Friday
8h00-8h30	Intro	Gil	Droniou	Livescu	Orlando
8h30-9h00	Rider	Aubram	Lee	Del-Rio Martin	Favrie
9h00-9h30	Hajduk	Kozhanova	Lyon	Dhaouadi	Mahy
9h30-10h00	Owen	Dobrev	Sementilli	Olson	Haegeman
10h00-10h30	PAUSE	PAUSE	PAUSE	PAUSE	PAUSE
10h30-11h00	Semplice	Winters	Jung	Chipman	Collis
11h00-11h30	Tallois	Labourasse	Baumgard	Kuzmin	Haines
11h30-12h00	Chiochetti	Maire	Hoch	Tovar	Bassett
12h00-13h30	PAUSE	PAUSE	PAUSE	PAUSE	PAUSE
14h00-14h30	Villedieu	Delmas	PAUSE	Milcent	Talamini
14h30-15h00	Ndanou	Preda	Monasse	Harmon	Dumbser
15h00-15h30	Liberman	Pandare	Shashkov	Gaburro	Mossier
15h30-16h00	Heuze	Vilar	Delpino	Evrard	Korner
16h00-16h30	PAUSE	PAUSE	PAUSE	PAUSE	PAUSE
16h30-17h00	Xu	Guisset	Poster	Whetstone	Uminski
17h00-17h30	Vaughn-kukura	Tomov	Poster	Boscheri	Closure
17h30-18h00	Poster	Poster	Poster	Poster	
19h00-	Ice Breaking Diner		Gala Diner		

More than 100 participants on-site

Academics are referred to by the name of the city where their university is located, while researchers and engineers are identified by their company name:

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“Shashkov Mikhail, *shashkov@lanl.gov* LANL, USA” from the Los Alamos National Laboratory, NM, USA.

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Presentations

Key Themes in the presentations

- | | |
|---|--|
| 1 Lagrangian and ALE Methods | 5 Mesh Adaptation and Interface Methods |
| 2 Numerical Methods for Fluid Mechanics | 6 High-Performance Computing (HPC) and Optimization |
| 3 Multiphase Flows | 7 Solid Mechanics, Materials and Industrial applications |
| 4 Inertial Confinem. Fusion, Plasma, Radiative transfer | |
-

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Technische Universität Berlin, Germany
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Lawrence Livermore National Laboratory, USA
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Laboratoire de Mathématiques UMR 5127 CNRS, Université Savoie Mont Blanc, France
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Institute of Mathematics, University of Cologne, Germany
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Bordeaux INP, France; University of Trento, Italy; Aix-Marseille University, France
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J. Droniou

Institute of Mathematics Alexander Grothendieck, CNRS, France

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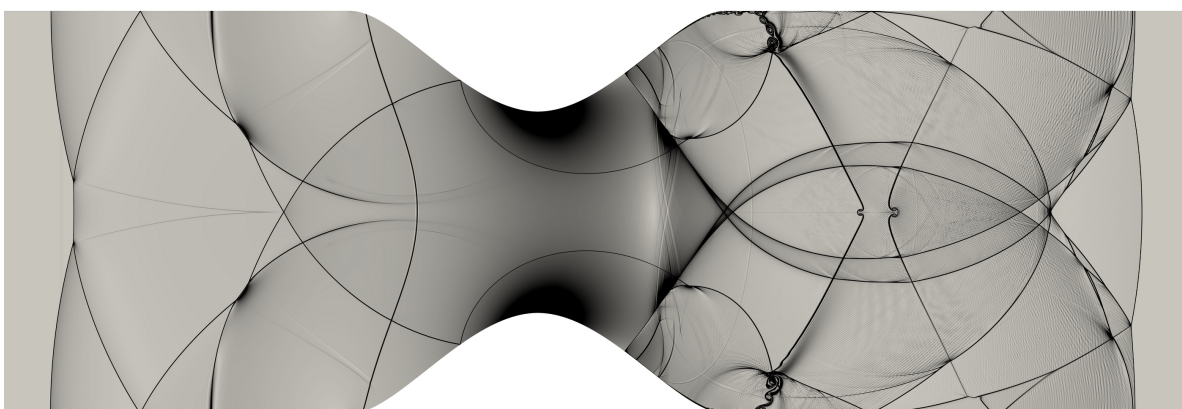
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A MULTI-MATERIAL ALE METHOD WITH IMPLICIT LAGRANGIAN STEP FOR APPLICATIONS IN GEOMECHANICS

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ABSTRACT

In this work, an Arbitrary Lagrangian-Eulerian (ALE) method is presented in which multiple materials (solids, fluids, or gases) and their interfaces may move relative to the computational mesh. The objective is to simulate very large deformations, shear and vorticity in the context of geomechanics and geotechnical engineering. Each ALE solution step is subdivided into a Lagrangian step, rezone step, and remap step, in which the implicit time integration employed in the Lagrangian step represents a unique feature. Numerical examples concerned with benchmark problems are presented which highlight the capabilities of the method.

INTRODUCTION

The simulation of large-deformation phenomena and material flow has become an increasingly important topic in geomechanics and geotechnical engineering. Representative applications include debris flows, the post-failure response of slopes, and pile driving. These problems are typically characterized by interactions among multiple physically distinct materials on different spatial scales [1, 2]. Throughout the process, material interfaces may continuously evolve, form, or merge. Furthermore, because of its multiphase composition and intricate internal structure, soil can exhibit either solid-like or fluid-like behavior depending on the prevailing flow regime. In such cases, the traditional Lagrangian finite element method (FEM) often suffers from reduced accuracy or even simulation failure, as it enforces the tracking of material interfaces through the computational mesh. In this work, a multi-material Arbitrary Lagrangian-Eulerian (ALE) formulation is introduced, allowing materials and their interfaces to move independently of the computational mesh; see [3, 4, 1] for a review of related formulations and methods.

OVERVIEW OF ALE METHOD

The implementation of the ALE method follows the approach of Benson [5] and decomposes each solution step into three stages: a Lagrangian step, a rezoning step, and a remapping step. During the Lagrangian step, a formulation closely aligned with standard FEM procedures is employed, combined with implicit time integration. Elements intersected by material interfaces are treated as multi-material cells, where each constituent is governed by its own constitutive model. The interfaces are reconstructed and tracked using the volume-of-fluid (VOF) method [3, 5], ensuring sufficient accuracy in the flux-based, conservative remapping procedure.

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EXAMPLE APPLICATION

As an example application we consider the retrogressive failure of a long slope made of sensitive clay. The model contains 92160 two-dimensional elements including void elements, which are empty elements covering the remaining domain of interest without clay. The sensitive clay material is modeled with a von Mises elastoplastic constitutive equation including linear softening and residual shear strength. Figure 1 above shows the initial model configuration with vertical stress contours and boundary conditions. The process of retrogressive failure at different time steps is shown in Figure 1 below, where the equivalent plastic strain contours highlight shear zones and sliding surfaces.

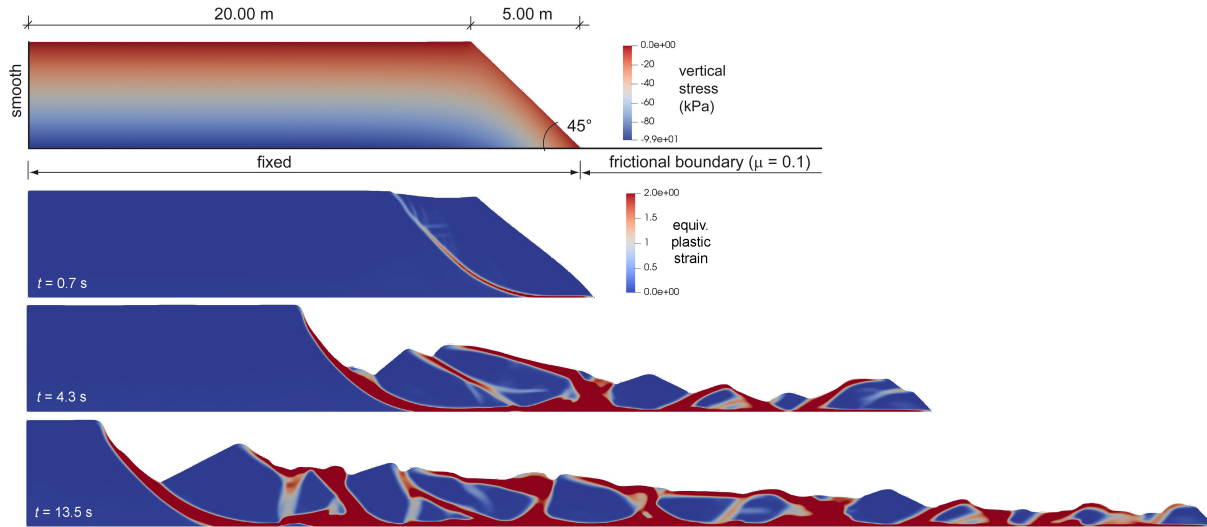


FIGURE 1: Initial model configuration and boundary conditions (above), and simulated process of retrogressive slope failure at different time steps (below).

ACKNOWLEDGMENT

This work was partially funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) – Project no. 76838227 – in the context of DFG Research Unit FOR 1136.

The author is particularly grateful to Prof. David J. Benson for stimulating discussions and for the opportunity to join his team at UC San Diego as a postdoc in 2015.

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SMOOTHED PARTICLE RADIATION HYDRODYNAMICS IN A VACUUM

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ABSTRACT

Approximations to the radiation diffusion equations are presented that permit mixed hydrodynamics and vacuum regions in a smoothed particle hydrodynamics code. The radiation diffusion equations are discretized in time with backward Euler and accelerated using nonlinear elimination. Challenges including flux limiting, zero-density opacities, vacuum particle management via Voronoi tessellations with Lloyd iterations, and the isotropic limitation of diffusion in the free-streaming regime are discussed. Results include validation of radiation propagation through a vacuum at the speed of light and a 2D foil ablation problem comparing the vacuum treatment against an ideal gas substitute.

INTRODUCTION

In this abstract, approximations to the radiation diffusion equations are presented that permit mixed hydrodynamics and vacuum regions in a smoothed particle hydrodynamics code. For recent reviews on radiation in smoothed particle hydrodynamics and astrophysics, see Refs. [1, 2, 3]. The radiation diffusion equations provide a good approximation to the radiation transport equation in the diffusion limit, which occurs when the photon mean free path is much smaller than other characteristic length scales in the problem. In this limit, the radiation is nearly isotropic and the approximations that (1) the specific (angularly-dependent) photon intensity can be truncated at the first spherical harmonic and (2) the time dependence of the photon current can be neglected are correct. As the opacities decrease, the problem shifts toward the free-streaming limit where the photon mean free path is considerable compared to other problem features, which presents a few challenges.

CHALLENGES

The first problem is that the standard diffusion coefficient describes bulk propagation with a velocity that can be greater than the speed of light [4]. The flux-limited diffusion approximation [5] limits the propagation speed of the diffusion equation to the speed of light where needed. The results in this paper use the Larsen flux limiter [6].

The second problem is that the diffusion coefficient contains a $1/\sigma_t$ term and $\sigma_t \propto \rho$ (the density), which is zero in a vacuum region. The approximation made here is that the total opacity σ_t contains only a scattering component σ_s , which is constant spatially and independent of density.

The third problem is specific to the integration of diffusion into a Lagrangian hydrodynamics code and is especially pronounced in smoothed particle hydrodynamics: the resolution follows mass, not volume. To

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allay this, extra, vacuum-specific particles are added to the simulation and are evolved to fill gaps between the hydrodynamic particles using a Voronoi tessellation with Lloyd iterations.

The final problem with diffusion in the free-streaming limit is that diffusion is isotropic, while the specific intensity can be strongly directional or even monodirectional. This problem is left untreated here and is the largest source of potential error in the continuous equations.

THEORY

The radiation diffusion equations are discretized in time with backward Euler and accelerated using non-linear elimination [7]. The material energy equation is solved using Newton iteration, while the multigroup radiation diffusion equation is solved implicitly,

$$\frac{1}{\Delta t} E_g - \nabla \cdot D_g \nabla E_g + c \sigma_{a,g} E_g = \frac{1}{\Delta t} E_g^{n-1} + c \sigma_{a,g} B_g,$$

where E_g is the radiation energy, D_g the diffusion coefficient, $\sigma_{a,g}$ the absorption opacity, and B_g the per-group emission. The diffusion derivative is discretized in space using a simple diffusion derivative approximation [8] and the coupling to hydrodynamics is detailed for grey diffusion in Refs. [9, 10]. In a vacuum, the material energy equation disappears and the diffusion equation becomes $\frac{1}{\Delta t} E_g - \nabla \cdot D_g \nabla E_g = 0$, with D_g calculated using only a chosen scattering opacity $\sigma_{s,g}$ as mentioned previously. The solve for the material energy and its coupling to the radiation diffusion equation disappear and the grey acceleration equation collapses to be a simple sum of the diffusion equations for each group.

The radiation diffusion here is implemented in Spheral, which optionally creates a pseudo-Voronoi tessellation. When vacuum points are active, these relax to the center of the Voronoi cells at the end of each time step before the radiation diffusion performs its implicit update. This effectively fills the space between the hydrodynamic particles. During a hydrodynamics update, the vacuum nodes are ignored entirely and do not contribute to the hydrodynamic derivatives except that the radiation energy in the vacuum nodes is used together with that in the hydrodynamic nodes to compute the radiation energy gradient used in the radiation pressure term in the velocity equation. The volume change equation remains the same for the vacuum and hydrodynamics particles as they are compressed or rarefied, $E_{i,g} = \left(\frac{V_i^{n-1}}{V_i} \right)^{4/3} E_{i,g}^{n-1}$.

RESULTS

Radiation through a vacuum

This problem simulates radiation flowing from a boundary source on the left through a vacuum. The radiation source is held at 0.3 keV (3.481×10^6 K) and the length of the problem is 1.0 cm. Three energy groups are used with upper energy group bounds of [0.0464, 2.154, 100] keV and a constant scattering opacity for all groups of 0.001 cm^{-1} .

Figure 1 shows the position of the half-max magnitude radiation energy with time for problems run with a varying number of points across the vacuum. As expected, the speed of the wave converges to the speed of light with an increasing number of points, with an error of 5 percent in the estimated wave speed with 512 points.

Ablation of a foil

This problem is similar to the first, but is run in 2D with a 0.09 keV (1.044×10^6 K) radiation source on the left and a 0.1 cm slab of material on the right separated by a 0.4 cm vacuum region. The second dimension has a height of 0.1 cm and periodic boundaries. The vacuum has a constant opacity of 0.1 cm^{-1} , while the slab uses 11-group opacities from TOPS and a $\gamma = 5/3$ gamma law gas equation of state with an initial density of 2.7 g/cm^3 .

Results are included in Fig. 2 for three cases: Spheral with a vacuum, Spheral with a diffuse ideal gas, and FLASH [11] with a diffuse ideal gas. Spheral and FLASH agree reasonably well when run with similar parameters and an ideal gas substitute for the vacuum. In Fig. 1a, it appears that Spheral has a hydrodynamic instability between the slab and ideal gas. Because the radiation struggles to transport past this first ablated layer of particles, the velocity inside the problem is lower. With the vacuum treatment, the vacuum particles intersperse between the hydrodynamic particles and permit continuous ablation without the hydrodynamic shock seen in the ideal gas cases. The results later in time (Fig. 1b) show a larger inward velocity in the vacuum case. The particles are freely ablating without the resistance provided by mocking up the vacuum as an ideal gas.

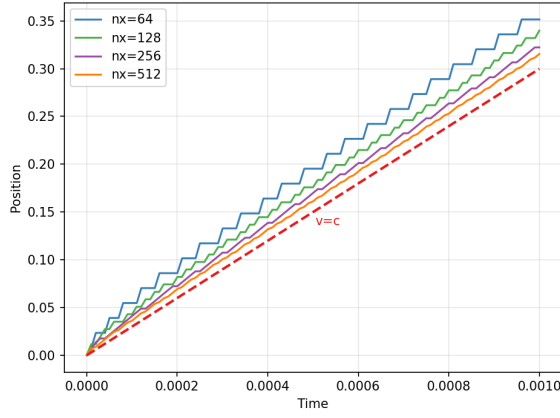


FIGURE 1: Position of half-max magnitude in radiation energy for the vacuum problem. The radiation propagation speed converges to the speed of light as the number of points increases.

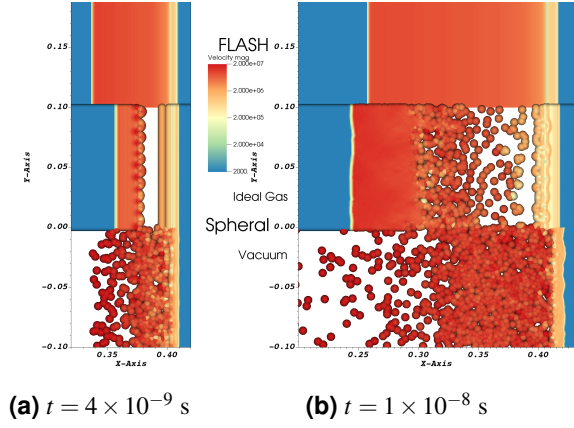


FIGURE 2: Comparison of velocity for FLASH with an ideal gas (top), Spheral with an ideal gas (middle), and Spheral with the novel vacuum treatment (bottom) for the foil problem.

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DYNAMIC SUBGRID-SCALE EDDY VISCOSITY WITH ADAPTIVE MESH REFINEMENT

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ABSTRACT

This work leverages adaptive mesh refinement for computing a dynamic subgrid-scale eddy viscosity. The approach is demonstrated for the large eddy simulation of the Richtmyer-Meshkov instability.

INTRODUCTION

Large eddy simulation (LES) is a useful framework for reducing the computational cost of turbulent flows. By solving the spatially-filtered Navier-Stokes equations, the smallest flow scales do not need to be resolved; many models exist for closing these subgrid scale terms. One such model, dynamic subgrid scale eddy viscosity, derives from relating subgrid scale stresses at the “grid filter” scale to those at a larger “test filter” scale.

For practical large scale simulations, adaptive mesh refinement (AMR) is beneficial for maintaining fine resolution around important flow features, allowing for coarser resolution elsewhere. However, an adaptive mesh results in local grid and test filter scales that evolve during the simulation, posing a challenge for explicit test filter stencils. This work aims to leverage the AMR hierarchy directly in the test filter operation.

METHODOLOGY

The spatially-filtered momentum equation is

$$\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial}{\partial x_j} (\bar{u}_i \bar{u}_j) = -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial \bar{\sigma}_{ij}}{\partial x_j} - \frac{\partial}{\partial x_j} (\tau_{ij}), \quad (1)$$

with the subgrid-scale stress,

$$\tau_{ij} = \overline{u_i u_j} - \bar{u}_i \bar{u}_j. \quad (2)$$

A common approach to closing τ_{ij} is through a subgrid-scale eddy viscosity model, such as that of Smagorinsky,

$$\tau_{ij} - \frac{\delta_{ij}}{3} \tau_{kk} = -2\nu_t \bar{S}_{ij} = -2C\Delta^2 |\bar{S}| \bar{S}_{ij}. \quad (3)$$

To close τ_{ij} , Germano et al. [1] introduced a dynamic subgrid-scale eddy viscosity. In this model, two subfilter-scale stresses are considered. First, the subgrid-scale stress (as in Eq. (3)) where the filter width Δ corresponds to the grid size; second, the subfilter-scale stress corresponding to a larger test filter, indicated by $\hat{\cdot}$,

$$T_{ij} = \widehat{\overline{u_i u_j}} - \hat{u}_i \hat{u}_j, \quad T_{ij} - \frac{\delta_{ij}}{3} T_{kk} = -2C\hat{\Delta}^2 |\hat{S}| \hat{S}_{ij}, \quad (4)$$

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where $\hat{\Delta}$ is the test filter length scale. The difference between the subtest-scale stress and subgrid-scale stress is

$$L_{ij} - \frac{\delta_{ij}}{3} L_{kk} = 2C(\hat{\Delta}^2 |\hat{S}| \hat{S}_{ij} - \Delta^2 |\widehat{S}| \widehat{S}_{ij}) = 2CM_{ij}. \quad (5)$$

During the simulation, the coefficient C is the only unknown in Eq. (5); the grid-filtered velocity components $\bar{u}_i$ are the transported quantities, and are used to compute $\bar{S}_{ij}$. The test filter operation is calculated explicitly. This enables the dynamic calculation of the eddy viscosity coefficient as

$$C = -\frac{1}{2} \frac{\langle L_{ij} \bar{S}_{ij} \rangle}{\langle M_{ij} \bar{S}_{ij} \rangle} \quad \text{or} \quad C = -\frac{1}{2} \frac{L_{ij} M_{ij}}{M_{ij} M_{ij}}. \quad (6)$$

The angle brackets indicate spatial averaging in homogeneous directions. The latter form was introduced by Lilly [2] to improve the numerical stability of the denominator.

In the present work, two test filters are investigated. The first is an explicit box filter. The second test filter leverages the AMR hierarchy, taking the coarser solution and refining it to the finer level. This allows the AMR communication framework to be used, improving the robustness of the test filter operation.

1 RESULTS

Dynamic large eddy simulation of a Richtmyer-Meshkov instability with reshock is performed. AMR is used for maintaining fine resolution around the shock and mixing layer, so this problem is a good demonstration of the AMR-based test filtering approach. Compared with the constant Smagorinsky model in Fig. 1, the dynamic eddy viscosity model captures the evolution of key quantities including turbulent kinetic energy. The AMR-based test filter is found to be more robust compared to the box filter.

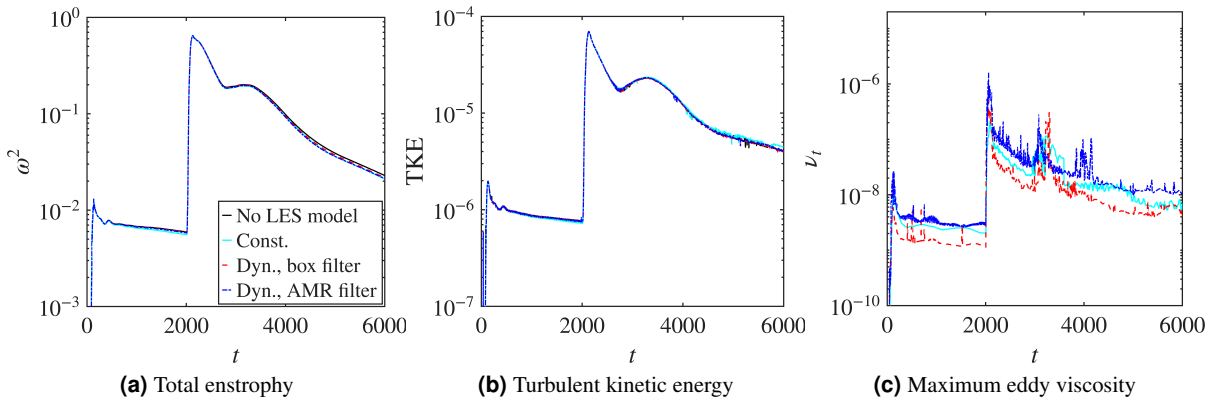


FIGURE 1: Time evolution of the Richtmyer-Meshkov problem for each model.

ACKNOWLEDGMENT

This work was preformed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract No. DE-AC52-07NA27344, release number LLNL-ABS-2017954.

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A STRUCTURE-PRESERVING AND THERMODYNAMICALLY COMPATIBLE CELL-CENTERED LAGRANGIAN FINITE VOLUME SCHEME FOR CONTINUUM MECHANICS

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ABSTRACT

In this talk we present a novel structure-preserving scheme for the discretization of the Godunov-Peshkov-Romenski (GPR) model of continuum mechanics written in Lagrangian form. This model admits an extra conservation law for the total energy (first principle of thermodynamics) and satisfies the entropy inequality (second principle of thermodynamics). Furthermore, in the absence of algebraic source terms, the distortion field of the continuum and the specific thermal impulse satisfy a curl-free condition, provided the initial data are curl-free. Last but not least, the determinant of the distortion field is related to the density of the medium, i.e. the system is also endowed with a nonlinear algebraic constraint. The objective of this work is to construct and analyze a new semi-discrete thermodynamically compatible cell-centered Lagrangian finite volume scheme on moving unstructured meshes that satisfies the following structural properties of the governing PDE exactly at the discrete level: i) compatibility with the first law of thermodynamics, i.e. discrete total energy conservation; ii) compatibility with the second law of thermodynamics, i.e. discrete entropy inequality; iii) exact discrete compatibility between the density and the determinant of the distortion field; iv) exact preservation of the curl-free property of the distortion field and of the specific thermal impulse in the absence of algebraic source terms. We show that it is possible to achieve all above properties simultaneously. Unlike in existing schemes, we choose to directly discretize the entropy inequality, hence obtaining total energy conservation as a consequence of an appropriate and thermodynamically compatible discretization of all the other equations.

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ADER SCHEMES GO FASTER AND FASTER

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ABSTRACT

The higher efficiency of ADER numerical schemes [1] with respect to similar semi-discrete methods is often cited as one of their main benefits, and attributed to their communication-avoiding properties. Since 2006-2008 [2, 3], thanks to the introduction of a local DG predictor step replacing the Cauchy–Kovalevskaya procedure, these numerical methods offer greater versatility, making them well suited for applications to general PDE systems. This talk focuses on the algorithmic performance of the schemes on the node-level and simplifying their implementation.

We discuss how numerical methods of the ADER family can be pushed to the extreme for applications in fluid flow. We show how some appropriate choices of basis functions can be used to construct very simple and efficient space-time evolution operators that are valid on arbitrary geometries. We show how partial orthogonalization of the basis functions and sparsity patterns and in the space-time operators, initially studied in this work as a purely implementation-level optimization, can explicitly guide the construction of the scheme, where the implementer can choose the “preferable” option depending on hardware-level considerations like minimizing storage requirements or minimizing floating point operations in the DG predictor step which constitutes the core of the scheme. The talk tries to give some insights on the co-design process of these numerical methods where implementation takes a central role. We also try to compare with even simpler numerical schemes, where optimization has been pushed even further.

ACKNOWLEDGMENT

The Authors acknowledge financial support from the European Union under Marie Skłodowska-Curie Post-doctoral Fellowship (European Union’s Horizon Europe Research and Innovation Programme, grant agreement No. 101109532) and from the Deutsche Forschungsgemeinschaft under the excellence cluster EXC 3037, Unser dynamisches Universum (Dynaverse).

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MULTI-MATERIAL THERMAL CONDUCTION SOLVERS FOR INERTIAL CONFINEMENT FUSION SIMULATIONS

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ABSTRACT

Indirectly driven inertial confinement fusion (ICF) experiments compress layered hydrogen-isotope capsules to thermonuclear conditions by converting high-energy laser energy into radiation within a high-Z hohlraum. Multi-material radiation-hydrodynamic codes such as xRAGE, developed at Los Alamos National Laboratory, are employed for the design, modeling, and analysis of ICF experiments [1]. Accurate modeling of laser-to-radiation energy conversion in the hohlraum is essential for predictive simulations. Early in the pulse, laser energy is deposited in thin, optically-dense regions, producing steep temperature gradients that strain the nonlinear thermal-conduction solvers. The resulting unconverged hotspots can lead to unphysical behavior or simulation crashes.

The nonlinear thermal-conduction equations are solved implicitly, using a linearization of the temperature-dependent conductivity. This approximation works for smooth gradients but fails when coupled to laser physics. The accelerated pseudo-transient (APT) method [2, 3] introduces a dual-time iteration in physical and pseudo-time, mitigating the limitations of the linearization. We describe the development and implementation of this solver in xRAGE and demonstrate that it improves both runtime performance and physical fidelity of fully integrated hohlraum-capsule simulations.

ACKNOWLEDGMENT

This work was supported by the U.S. Department of Energy through the Los Alamos National Laboratory. Los Alamos National Laboratory is operated by Triad National Security, LLC, for the National Nuclear Security Administration of U.S. Department of Energy (Contract No. 89233218CNA000001). Released under LA-UR-26-22641.

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EFFICIENTLY ACHIEVING CONVERGENCE IN MAGLIF SIMULATIONS WITH THINC

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ABSTRACT

Modeling multi-material flows requires numerical representations of interfaces that robustly capture materials with differing physical properties. Traditional Eulerian methods rely on numerical diffusion to stabilize interfaces, but often require prohibitively fine mesh resolution to counteract numerical material mixing and achieve convergence. Lagrangian approaches avoid interface mixing, but struggle when large deformations lead to highly distorted meshes. Arbitrary Lagrangian–Eulerian (ALE) methods attempt to balance these approaches by remapping fields from a Lagrangian mesh to an Eulerian mesh, but introduce additional complexity and can reintroduce diffusion when remapping is frequent. As a result, ALE methods are widely used in inertial confinement fusion (ICF) simulations, yet are computationally expensive, algorithmically complex, and still struggle with controlling material mixing.

In this work, we demonstrate that a purely Eulerian interface-capturing approach—Tangent Hyperbola Interface Capturing (THINC)—can achieve yield-converged MagLIF implosion simulations at substantially reduced cost compared to standard upwind-biased Eulerian schemes. THINC provides a high-resolution, low-dissipation representation of material interfaces by incorporating sharpening directly within the finite-volume reconstruction, maintaining interface thicknesses of approximately 2–3 computational cells. As a result, grid convergence can be achieved with a purely Eulerian solver at practical resolution, without requiring the complexity of an ALE formulation.

Moreover, the inherent interface sharpening provided by THINC enables a delayed-refinement strategy as an additional benefit for the liner-fuel interface in MagLIF. When studying clean implosions, simulations may be initialized on relatively coarse meshes and refined later in time. The numerical re-sharpening from the THINC reconstruction can sharpen the planar fuel-liner interface following refinement and recover the converged solution by effectively canceling out early time numerical diffusion errors. This allows convergence to be achieved without requiring high resolution around material interfaces throughout the simulation, providing further reductions in computational cost. All simulations are performed using the FLASH multi-physics framework with block-structured adaptive mesh refinement (AMR).

BACKGROUND

We solve the multi-species 3T (rad-hydro) extended MHD equations through the FLASH multi-physics solver for modeling ICF MagLIF implosions [1]. In the hydrodynamics solve, Total-Variational-Diminishing

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(TVD) limiters are used to interpolate fields in the finite volume reconstruction. TVD limiters use numerical diffusion to avoid oscillations caused by dispersion errors. The diffusive mechanism keeps oscillations from occurring around sharp gradients in fields. Material interfaces are not self-sharpening, and the added numerical diffusion from a TVD limiter results in increasing the spatial extent of the mixing zone separating material interfaces over time. Existing approaches for restricting this diffusion include using less dissipative limiters and increasing spatial resolution around material interfaces. Instead, the THINC interpolation offers a balance of compressive and diffusive characteristics to keep interface thickness bounded in time, while avoiding adding spurious oscillations. The appropriate application of THINC around material interfaces reduces the need to increase spatial resolution to only restrict the negative effect of the numerical diffusion from TVD limiters. THINC uses hyperbolic tangent profiles to interpolate variables from a cell-center to a cell-face. The function is defined as

$$Q_i(x) = \frac{\bar{q}_{i-1} + \bar{q}_{i+1}}{2} + \frac{\bar{q}_{i+1} - \bar{q}_{i-1}}{2} \tanh\left(\beta\left(\frac{x - x_i}{\Delta} - d_i\right)\right)$$

where $(\bar{\cdot})$ indicates an averaging operator over a cell, β is a user parameter to determine the interface thickness, and the location of the center of the hyperbolic tangent function within each cell, d_i , is determined by satisfying the following conservation condition,

$$\frac{1}{\Delta} \int_{x_{i-1/2}}^{x_{i+1/2}} Q_i(x) dx = \bar{q}_i.$$

The evaluation of this condition has been derived and algebraically formulated to strictly preserve the spatial-symmetry property of the numerical solution [2]. Although THINC works well for capturing sharp gradients, it can produce numerical artifacts (e.g. grid-alignment) when used in smooth zones. To produce accurate solutions in both smooth zones and around interfaces, THINC is hybridized with an existing TVD limiter to activate only around sharp gradients. The hybridization function used in this work is based on a boundary-variation-diminishing (BVD) condition [2].

RESULTS

In Table 1 the fusion yield is reported for both TVD and THINC reconstructions for simulations of a high-gain MagLIF target. Table 1 reports the yield using a static maximum refinement level around the fuel-liner interface, as well as a time-varying interface refinement level. In the static refinement case the THINC scheme is able to surpass the max yield produced using the TVD scheme at a 4x coarser resolution – 1.5 microns vs 0.375 microns. Additionally, THINC can recover the full yield with a late-in-time refinement strategy.

TABLE 1: Yield comparison for the delayed refinement in time approach (2D) and a static refinement approach (1D) with using a traditional TVD scheme and THINC

	TVD yield (2D)	THINC yield (2D)	TVD yield (1D)	THINC yield (1D)
Max refinement	time-based refinement	time-based refinement	static refinement	static refinement
	(MJ/cm)	(MJ/cm)	(MJ/cm)	(MJ/cm)
3 μm	180	2005	1207	2003
1.5 μm	351	2349	1870	2371
0.75 μm	380	2443	2154	2463
0.375 μm	380	2509	2265	2505

Figure 1 shows the application of THINC to the mass-fraction profile of deuterium-tritium fuel (blue) profile during a 2D periodic extension of a 1D MagLIF implosion using the late-in-time refinement approach (first two columns of Table 1). The left shows the mass-fraction profile when a traditional TVD-limiter is used to capture the fuel-liner interface and the right shows the THINC reconstruction. For these simulations the mesh refinement starts at 12 microns and is increased around the interface over time. The THINC reconstruction sharpens the interface to the scale of the local grid resolution for each refinement level, whereas the TVD limiter only presents an interface at the scale of the original 12 micron mesh. The difference in the liner-fuel

mixing region length-scales results in a large degradation of performance of the TVD scheme compared to THINC scheme, even though the wall-time for both simulations are comparable.

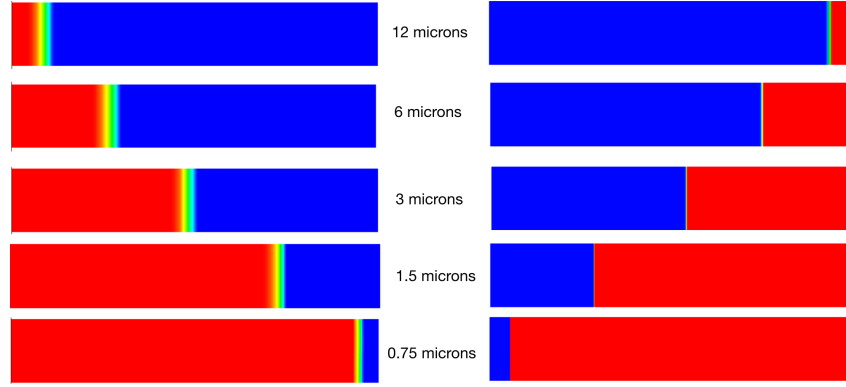


FIGURE 1: Comparison of fuel (blue) mass fraction in a 2D periodic MagLIF simulation when using a late-in-time refinement strategy around the liner-fuel interface for tradition TVD reconstruction (left) and the THINC interface capturing reconstruction (right). Both simulations are initialized with 12 micron mesh resolution and refinement around the liner interface is increased during the implosion.

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TRIANGULAR-BASED AMR AND APPLICATION TO FLUID-STRUCTURE INTERACTION

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ABSTRACT

We present a triangular-based mesh adaptation method to deal with fluid-structure interaction in shock dynamics.

Since their introduction, cell-centered semi-Lagrangian schemes [3, 8] have proved their efficiency. They have been extended to high-order accuracy, to solid mechanics or to MHD for instance. Nevertheless one of their major strengths is their natural compatibility with remeshing techniques (such as indirect-ALE for instance). Indeed, their finite-volume nature and their total energy formulation simplify the writing of a conservative remapping. Beyond classical rezoning-remapping approaches, connectivity changes have been investigated in [5, 7, 1, 2] for instance.

On the other hand, if providing a conservative method to deal with fluid-structure interaction remains an issue, in a large part of the literature, the extension of cell-centered schemes treats it naturally. Indeed, semi-Lagrangian schemes developed in [6, 4] provide natural conservative coupling at the interface since (in those cases) the hyperelastic solvers naturally degenerate to Euler solvers.

We shall present how the use of conformal remeshing techniques can lead to efficient and robust solvers to treat fluid-structure interaction in presence of shocks.

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A NOVEL TWO-PHASE FLOW FORMULATION THROUGH DISPERSIVE REGULARIZATION

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ABSTRACT

In this talk, we describe a novel symmetric-hyperbolic two-phase flow model derived from variational principles. The key novelty lies in the introduction of a dispersive regularization term via the material derivative of the volume fraction, ensuring hyperbolicity and energy conservation. The resulting system, which can be interpreted as a consistent approximation of the classical two-velocity one-pressure model, overcomes the well-known hyperbolicity issues of the classical two-fluid formulations, such as the Baer-Nunziato model, in regimes where standard pressure-equilibrium formulations fail. To handle the stiff relaxation source terms efficiently without restrictive time-step constraints, an IMEX Runge-Kutta time integrator is employed. Numerical simulations illustrate the validation of the proposed model on several benchmark test cases, including smooth solutions, Riemann problems and strong shocks.

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DESIGN AND DEVELOPMENT OF INNOVATIVE NUMERICAL METHODS TO SOLVE THE 3D NAVIER-STOKES EQUATIONS IN THE HYPERSONIC REGIME ON HYBRID MESHES

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ABSTRACT

The objective of this presentation is to develop robust and accurate numerical methods for the simulation of three-dimensional hypersonic flows around vehicles with complex geometries [1, 2, 3, 4]. The flow regimes considered correspond to flight altitudes at which the continuum hypothesis remains valid, and the fluid behavior is governed by the compressible Navier–Stokes equations, expressing the conservation of mass, momentum, and energy.

Hypersonic flows, characterized by velocities far exceeding the speed of sound, involve extreme physical phenomena. In particular, strong detached shock waves generate abrupt discontinuities in the flow variables, leading to a significant conversion of kinetic energy into internal energy and, consequently, to very high temperatures. Additionally, a very thin boundary layer develops along the vehicle surface, where steep velocity and temperature gradients normal to the wall induce intense momentum and energy transfers. These combined effects result in severe aerodynamic and aerothermal loads. Their accurate numerical prediction—especially of wall heat fluxes—remains a major challenge in the design of thermal protection systems for hypersonic and space vehicles.

This work focuses on the development of a robust and accurate surface-based, cell-centered finite volume method for solving the three-dimensional compressible Navier-Stokes equations in hypersonic regimes on hybrid unstructured meshes [1, 4]. While unstructured grids are essential for handling complex geometries, they impose stringent requirements in terms of robustness, stability, and accuracy. A key difficulty lies in the simultaneous resolution of strong bow shocks ahead of the vehicle and thin flow structures developing along its potentially non-smooth surface. Sufficient numerical dissipation is required to stabilize shock waves, whereas excessive dissipation deteriorates the resolution of small-scale features. One of the central objectives of this work is therefore to achieve a careful balance between these competing requirements.

Concerning the discretization of the 2D/3D Euler equations, a novel positivity-preserving cell-centered finite volume discretization of the is proposed. The method relies on a partitioning of each cell face into subfaces associated with mesh nodes. Subface fluxes are computed using an approximate Riemann solver based on the mean states of adjacent cells and on a nodal velocity projected onto the subface normal. Global conservation is enforced by requiring that the sum of subface fluxes around each node vanishes, which uniquely determines the nodal velocities. This approach eliminates classical numerical instabilities such as odd–even decoupling and the carbuncle phenomenon. With a suitable design of the Riemann solver and an appropriate explicit CFL condition, both positivity and entropy preservation can be established.

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The resulting first-order subcell-based finite volume scheme is further extended to second-order accuracy using a piecewise-linear limited reconstruction combined with a MUSCL–Hancock time discretization [2, 1, 4]. Several second-order reconstruction strategies have been assessed on both academic and more challenging test cases (see, e.g., the ARD test in Figure 1). Combined with a monolithic flux limiting procedure, the overall scheme demonstrates strong robustness and stability, even for demanding configurations. Finally, the performance of the proposed overall numerical schemes is demonstrated on a range of three-dimensional hypersonic test cases, highlighting both their robustness and accuracy.

Due to time constraints, we will not detail the discretization of the diffusion term. Instead, we will present the general underlying approach and evaluate the performance of the overall simulation code for the Navier–Stokes equations on unstructured 3D meshes by analyzing the heat flux around reentry objects [4].

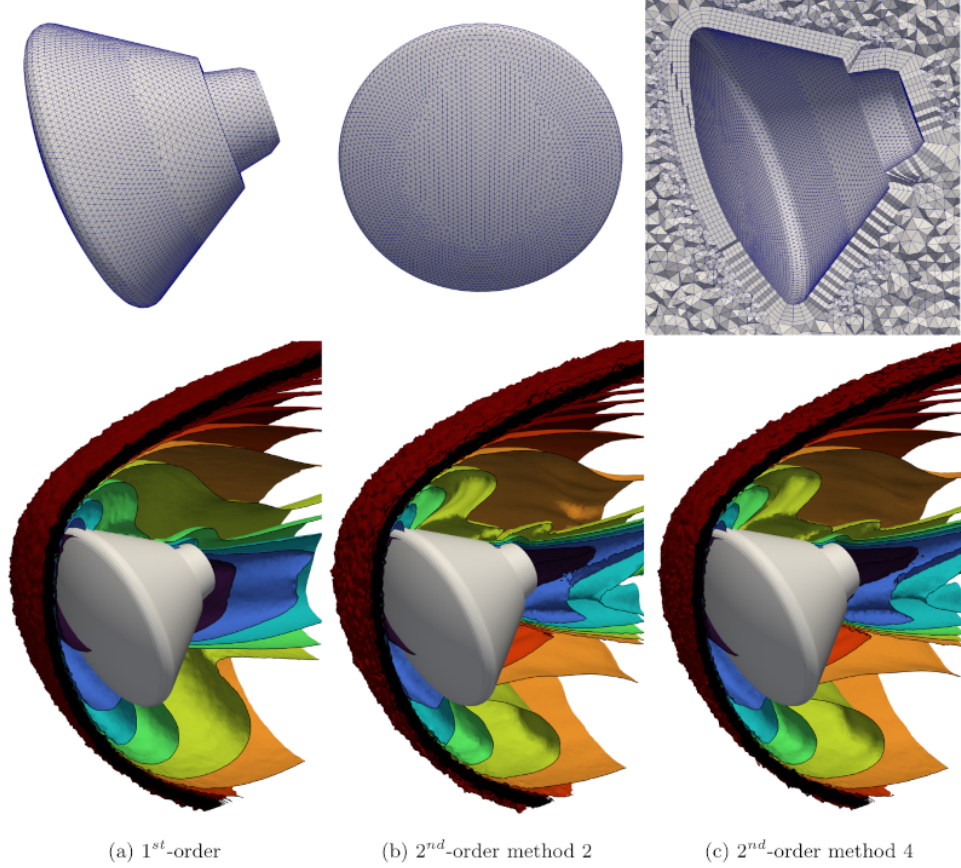


FIGURE 1: Atmospheric reentry demonstrator at Mach 24. Top: Mesh using only tetrahedra in the far-field and triangular basis prisms near the surface. Bottom: Mach isosurfaces for different schemes.

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A FIRST-ORDER HYPERBOLIC REFORMULATION OF THE CAHN-HILLIARD EQUATION

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ABSTRACT

We present a new first-order hyperbolic reformulation of the Cahn-Hilliard equation [1]. The model is obtained from the combination of so-called augmented Lagrangian techniques with a classical Cattaneo-type relaxation that allows to reformulate diffusion equations as augmented first order hyperbolic systems with stiff relaxation source terms. The proposed system is proven to be hyperbolic and to admit a Lyapunov functional, in accordance with the original equations. A new numerical scheme is proposed to solve the original Cahn-Hilliard equations based on conservative semi-implicit finite differences, while the hyperbolic system was numerically solved by means of a classical second order MUSCL-Hancock-type finite volume scheme. The proposed approach is validated through a set of classical benchmarks such as spinodal decomposition, Ostwald ripening and exact stationary solutions.

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IMPLICIT LAGRANGIAN HYDRODYNAMICS WITH HIGH-ORDER FINITE ELEMENTS

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ABSTRACT

In this talk we present implicit time discretizations of the high-order curvilinear finite element methods for Lagrangian hydrodynamics introduced in [1]. We use singly diagonal implicit Runge-Kutta (SDIRK) methods which require the solution of a nonlinear system, involving the time-dependent operator of the spatially discretized hydrodynamics equations, at each time stage. To solve these systems using gradient based methods like Newton's method, we construct the operator gradient using the ∂ FEM framework of MFEM [5], based on the Enzyme automatic differentiation (AD) tool [2]. We discuss the general discretization approach and modifications that were required to ensure smooth differentiability of the discrete operators including artificial viscosity smoothing similar to the one presented in [3]. Finally, we demonstrate the behavior of the methods, implemented in the Laghos miniapp [4], and their performance on a suite of hydrodynamics benchmarks including Sedov's blast, the triple-point, and the smooth Taylor-Green vortex problems. Prepared by LLNL under Contract DE-AC52-07NA27344.

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POLYTOPAL SCHEMES FOR CONTACT PROBLEMS IN FRACTURED MEDIA

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ABSTRACT

We present two numerical schemes for contact mechanics with various contact models (Tresca, Coulomb). Both schemes are applicable on meshes made of generic polyhedra, and differ by their order of approximation: one is low order and is enriched with “bubbles” for stabilisation purposes, the other is of higher order and naturally stable as well as locking-free. Convergence of these schemes is rigorously obtained, and their efficiency is compared through numerical tests.

INTRODUCTION

We present two schemes, applicable on polyhedral meshes, for a mechanical model of fractured media. The displacement of the porous matrix is subjected to linear elasticity, but can be discontinuous across fractures. Different contact models, possibly allowing for friction, can be considered along the fractures. The representation of the contact conditions is done by the introduction of Lagrange multipliers, representing normal tractions along the fractures.

MODEL

We consider a domain $\Omega \subset \mathbb{R}^3$ with a fracture network Γ , represented by a union of portions of planes; along each of these portions we arbitrarily fix a positive and negative side of the fracture. The contact problem with Tresca friction reads

$$\begin{aligned} -\operatorname{div} \sigma(\mathbf{u}) &= \mathbf{f} & \text{on } \Omega \setminus \Gamma, & T_n(\mathbf{u}) \leq 0, \llbracket \mathbf{u} \rrbracket_n \leq 0, \llbracket \mathbf{u} \rrbracket_n T_n(\mathbf{u}) = 0 & \text{on } \Gamma, \\ \sigma(\mathbf{u}) &= \frac{E}{1+\nu} \left(\varepsilon(\mathbf{u}) + \frac{\nu}{1-2\nu} (\operatorname{tr} \varepsilon(\mathbf{u})) I_3 \right) & \text{on } \Omega \setminus \Gamma, & |\mathbf{T}_\tau(\mathbf{u})| \leq g & \text{on } \Gamma, \\ \gamma_n^+ \sigma(\mathbf{u}) + \gamma_n^- \sigma(\mathbf{u}) &= \mathbf{0} & \text{on } \Gamma, & \mathbf{T}_\tau(\mathbf{u}) \cdot \llbracket \mathbf{u} \rrbracket_\tau + g |\llbracket \mathbf{u} \rrbracket_\tau| = 0 & \text{on } \Gamma, \end{aligned}$$

where $\mathbf{u} : \Omega \setminus \Gamma \rightarrow \mathbb{R}^3$ is the displacement, $g \geq 0$ is the Tresca threshold, ν and E are the Poisson ratio Young's modulus E , I_3 is the 3×3 identity matrix, and the normal and tangential surface tractions are $T_n(\mathbf{u}) = \gamma_n^+ \sigma(\mathbf{u}) \cdot \mathbf{n}^+$ and $\mathbf{T}_\tau(\mathbf{u}) = \gamma_n^+ \sigma(\mathbf{u}) - T_n(\mathbf{u}) \mathbf{n}^+$ ($\gamma_n^\pm$ represents the trace on the positive/negative fracture side).

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SCHEMES

To account for the contact conditions along the fractures, we introduce a Lagrange multiplier λ representing the negative normal traction, and the model can then be recast as a variational inequality with a saddle point form: Find $\mathbf{u} \in \mathbf{H}_0^1(\Omega \setminus \Gamma)$ and $\lambda \in \mathcal{C}_f$ (the cone translating the contact conditions)

$$\begin{aligned} \int_{\Omega} \boldsymbol{\sigma}(\mathbf{u}) : \boldsymbol{\varepsilon}(\mathbf{v}) + \langle \lambda, \llbracket \mathbf{v} \rrbracket \rangle_{\Gamma} &= \int_{\Omega} \mathbf{f} \cdot \mathbf{v} & \forall \mathbf{v} \in \mathbf{U}_0, \\ \langle \mu - \lambda, \llbracket \mathbf{u} \rrbracket \rangle_{\Gamma} &\leq 0 & \forall \mu \in \mathcal{C}_f. \end{aligned} \quad (1)$$

The lowest-order scheme [2, 1] (LO) has unknowns at all the mesh nodes, as well as on the fracture faces. Each node outside Γ is associated with one displacement while, to account for the possibly discontinuity of $\mathbf{u}$ across fractures, each node on Γ is associated with as many displacement as there are fracture sides at this node

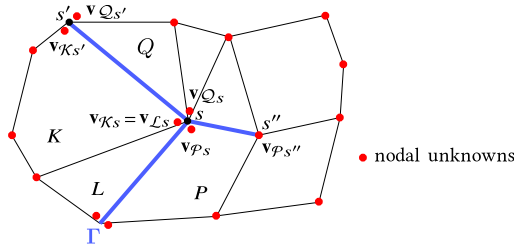


FIGURE 1: Unknowns for the low-order scheme (Γ in blue)

(see Figure 1). The fracture face displacements, which represent “bubbles”, have a stabilising role: they ensure the inf-sup property between the displacement space and the Lagrange multiplier space (made of piecewise constant tractions). Using the displacement unknowns, local operators (symmetric gradients, traces, jumps) can be constructed and used to write a scheme for (1).

The higher order scheme [3] (HO) is built on a richer space, including the same nodal unknowns, but also edge, face and element unknowns (edge and face unknowns are also multiplied on each side of the fractures). These allows

to naturally define quadratic approximation of displacements and, due to the presence of face unknowns and the choice of a suitable interpolator, also yield the inf-sup condition as well as a locking-free method.

RESULTS

Error estimates (H^1 in the displacement, $H^{-1/2}$ for Lagrange multipliers) been proved for both schemes:

$\mathcal{O}(h)$ for (LO), $\mathcal{O}(h^{3/2})$ for (HO) without friction ($g = 0$), and $\mathcal{O}(h)$ for (HO) with friction ($g \neq 0$); (HO) is moreover locking-free, in the sense that the constants in the error estimates do not depend on the Poisson ratio. Numerical evidence shows that (HO) seems to actually achieve an $\mathcal{O}(h^2)$ convergence (with or without friction). The improved behaviour of (HO) over (LO) is also illustrated on qualitative measures, in better approximation of the Lagrange multiplier (see Figure 2).

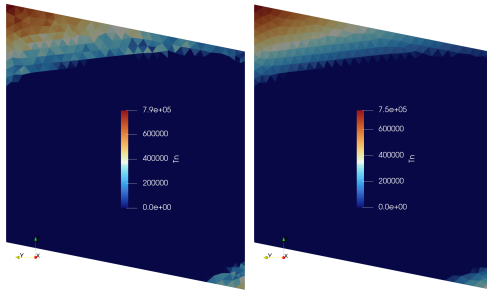


FIGURE 2: Normal component of Lagrange multiplier. Left: (LO), right: (HO).

(LO) has also been coupled in full poroelastic models, including for Coulomb friction, and displayed a good behaviour in this case [1]. The adaptation of (HO) in such a model is an ongoing work.

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A SIMPLE AND GENERAL FRAMEWORK FOR THE CONSTRUCTION OF EXACTLY DIV-CURL-GRAD COMPATIBLE DISCONTINUOUS GALERKIN FINITE ELEMENT SCHEMES ON UNSTRUCTURED SIMPLEX MESHES

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ABSTRACT

We introduce a new family of discontinuous Galerkin (DG) finite element schemes for the discretization of first order systems of hyperbolic partial differential equations (PDE) on unstructured simplex meshes in two and three space dimensions that respect the two basic vector calculus identities exactly also at the discrete level, namely that the curl of the gradient is zero and that the divergence of the curl is zero. The key ingredient here is the construction of two compatible discrete nabla operators, a primary one and a dual one, both defined on general unstructured simplex meshes in multiple space dimensions. Our new schemes extend existing cell-centered finite volume methods based on corner fluxes to arbitrary high order of accuracy in space. An important feature of our new method is the fact that only two different discrete function spaces are needed to represent the numerical solution, and the choice of the appropriate function space for each variable is related to the origin and nature of the underlying PDE. The first class of variables is discretized at the aid of a discontinuous Galerkin approach, where the numerical solution is represented via piecewise polynomials of degree N and which are allowed to jump across element interfaces. This set of variables is related to those PDE which are mere consequences of the definitions, derived from some abstract scalar and vector potentials, and for which involutions like the divergence-free or the curl-free property must hold if satisfied by the initial data. The second class of variables is discretized via classical continuous Lagrange finite elements of approximation degree $M = N + 1$ and is related to those PDE which can be derived as the Euler-Lagrange equations of an underlying variational principle. The primary nabla operator takes as input the data from the FEM space and returns data in the DG space, while the dual nabla operator takes as input the data from the DG space and produces output in the FEM space. The two discrete nabla operators satisfy a discrete Schwarz theorem on the symmetry of discrete second derivatives. From there, both discrete vector calculus identities follow automatically. We apply our new family of schemes to three hyperbolic systems with involutions: the system of linear acoustics, in which the velocity field must remain curl-free and the vacuum Maxwell equations, in which the divergence of the magnetic field and of the electric field must remain zero. In our approach, only the magnetic field will remain exactly divergence free. As a third model we study the Maxwell-GLM system of Munz et al., which contains a unique mixture of curl-curl and div-grad operators and in which the magnetic field may be either curl-free or divergence-free, depending on the choice of the initial data. In all cases we prove that the proposed schemes are exactly total energy conservative and thus nonlinearly stable in the L^2 norm.

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A MOMENT-OF-FLUID METHOD USING PIECEWISE-QUADRATIC INTERFACE RECONSTRUCTIONS

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ABSTRACT

The volume-of-fluid (VOF) and moment-of-fluid (MOF) methods are widely used to track the evolution of interfaces in numerical simulations of multi-material flows due to their inherent ability to conserve volume with machine precision. State-of-the-art VOF and MOF algorithms rely on piecewise-linear interface calculations (PLIC) to construct local geometric approximations of the material interface. However, the linear nature of these reconstructions limits volume-fraction transport to second-order accuracy, while interface curvature estimation is at best zeroth-order accurate. Recent advancements in interface reconstruction algorithms for MOF schemes have significantly improved the ability to capture complex subgrid-scale interfacial structures by leveraging local geometric moments of the fluid. Interfaces can be represented by combinations of multiple planes and/or curved surfaces, motivating the use of higher-order phasic moments beyond the traditional zeroth- and first-order quantities. Piecewise-parabolic interface calculations (PPIC) provide a natural high-order extension to local interface representation. In this work, we propose a PPIC-based MOF framework transporting the phasic moments of inertia and reconstructing parabolic interfaces through a nonlinear moment-matching minimization procedure. A challenge in this approach is the need for sufficiently accurate initial guesses, so as to ensure scalability and robust convergence. To overcome this limitation, we further propose volume-fraction-based reconstruction algorithms that produce reconstruction guesses with satisfactory accuracy and robustness at relatively low computational cost.

INTRODUCTION

The volume-of-fluid (VOF) and moment-of-fluid (MOF) methods provide a volume-conservative framework for capturing the evolution of interfaces between immiscible materials in numerical simulations. In unsplit geometric VOF and MOF schemes, the preimage of a computational cell is constructed by tracing its faces backward in time along the velocity field. The transported fluid moments are subsequently evaluated by intersecting this preimage with the reconstructed interface and the underlying computational mesh. In conventional implementations, the preimage is typically approximated by a polyhedral volume, and the interface is represented using a piecewise-linear interface calculation (PLIC). Current MOF frameworks have been limited to the transport of zeroth- and first-order fluid moments, namely the phasic volume fractions and barycenters. In the present work, we extend the MOF methodology to include second-order moments of fluid and employ piecewise-parabolic interface calculations (PPIC) for interface reconstruction.

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TRANSPORT OF HIGH-ORDER MOMENTS OF FLUID IN INCOMPRESSIBLE FLOW [1]

The evolution of the second moment tensor of the phase indicator χ over a material region $\Lambda(t)$, e.g., the preimage, follows the Reynolds transport theorem

$$\frac{d}{dt} \int_{\Lambda(t)} \chi \mathbf{x} \mathbf{x}^\top d\mathbf{x} = \int_{\Lambda(t)} \chi \left(\mathbf{x} \mathbf{u}^\top + \mathbf{u} \mathbf{x}^\top \right) d\mathbf{x}. \quad (1)$$

Using a Taylor series expansion of the fluid velocity $\mathbf{u}(\mathbf{x}, t)$ inside $\Lambda(t)$ about $\mathbf{u}(\mathbf{x}_l, t)$, where $\mathbf{x}_l = \mathcal{M}_{1,\ell}/\mathcal{M}_{0,\ell}$ is the liquid centroid and $\mathcal{M}_{n,\alpha}$ denotes the n th-order moment of phase α , the rate of change of the second moments of liquid can be approximated as

$$\frac{d\mathcal{M}_{2,\ell}}{dt} = \mathcal{M}_{0,\ell} \left(\bar{\mathbf{x}}_l \mathbf{u}_l^\top + \mathbf{u}_l \bar{\mathbf{x}}_l^\top - \bar{\mathbf{x}}_l \bar{\mathbf{x}}_l^\top \nabla \mathbf{u}_l^\top - \nabla \mathbf{u}_l \bar{\mathbf{x}}_l \bar{\mathbf{x}}_l^\top \right) + \mathcal{M}_{2,\ell} \nabla \mathbf{u}_l^\top + \nabla \mathbf{u}_l \mathcal{M}_{2,\ell}^\top. \quad (2)$$

PIECEWISE-PARABOLIC INTERFACE RECONSTRUCTION

The piecewise-parabolic reconstruction of the interface is obtained by solving a constrained optimization problem in which the interface parameters $\mathcal{P}$ are chosen to minimize the mismatch in the phasic moments inside a supercell $\mathcal{S}$, while constraining the zeroth-moment in the target cell $\mathcal{C} \subset \mathcal{S}$,

$$\begin{aligned} \min_{\mathcal{P}} \quad \mathcal{J}(\mathcal{P}) &= \sum_{\alpha \in \{\ell, g\}} \left(\mathcal{M}_{0,\alpha}^{S_\star} \right)^{-8/3} \left\| \mathcal{M}_{1,\alpha}^{S_\star} - \mathcal{M}_{1,\alpha}^{S_\mathcal{P}} \right\|^2 + \left(\mathcal{M}_{0,\alpha}^{S_\star} \right)^{-10/3} \left\| \widehat{\mathcal{M}}_{2,\alpha}^{S_\star} - \widehat{\mathcal{M}}_{2,\alpha}^{S_\mathcal{P}} \right\|^2 \\ \text{subject to:} \quad \mathcal{M}_{0,\ell}^{C_\star} &= \mathcal{M}_{0,\ell}^{C_\mathcal{P}}. \end{aligned} \quad (3)$$

Here, $\mathcal{M}_{n,\alpha}^{\square_\star}$ denotes the reference moments, $\mathcal{M}_{n,\alpha}^{\square_\mathcal{P}}$ refers to the moments computed from the reconstructed interface and $\widehat{\square}$ corresponds to moments that have been recentered about their barycenter. In the present work, an initial guess can be obtained using one of the following relatively low-cost volume-fraction-based approaches: (1) by fitting a paraboloid to minimize volume mismatch within a local neighborhood of PLIC reconstructions [3]; (2) by blending neighboring interface representations to extract a level-set isosurface whose derivatives are sampled to reconstruct a paraboloid; or (3) by estimating the local directional curvatures from the PLIC neighborhood and using them to reconstruct the principal directions and curvatures of a paraboloid [2].

The performance of the proposed method is demonstrated with the transport of a spherical interface subjected the steady velocity field $\mathbf{u} = \boldsymbol{\omega} \times \mathbf{x}$. The PLIC-MOF¹ reconstruction is obtained by matching the zeroth- and first-order phasic moments, while the PPIC-MOF² reconstruction additionally accounts for second-order phasic moments. Figure 1 shows that the PPIC-MOF² method preserves the spherical geometry far more effectively, so that the final interface remains much closer to the initial configuration than in the PLIC-MOF¹ case.

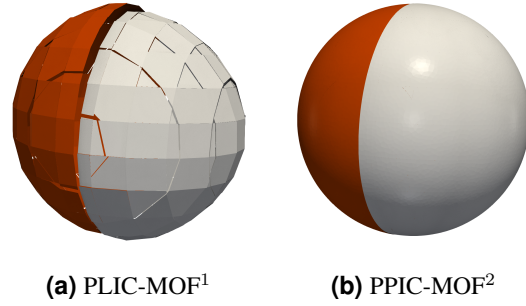


FIGURE 1: Initial (orange) and final (gray) interface reconstructions for the rigid-body rotation of a sphere.

ACKNOWLEDGMENT

This work was supported by the U.S. National Science Foundation under Award #2438854.

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A UNIFIED DIFFUSE-INTERFACE MODEL FOR COMPRESSIBLE MULTIPHASE FLOWS WITH ELASTO-VISCOPLASTIC SOLIDS AND IRREVERSIBLE COMPACTION

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ABSTRACT

The interaction between compressible fluids, dense solids and porous materials under dynamic loading is involved in many applications such as impacts, shock to detonation transition or cavitation near propeller. These problems are characterized by strong shock waves, large deformations and complex multiphase interactions. While diffuse-interface methods have proven to be efficient for compressible multi-material flows, existing approaches remain limited when dealing simultaneously with shear effects, plasticity and irreversible compaction in porous media.

In this work, we propose a unified diffuse-interface multiphase model capable of describing fluids, dense solids and porous materials within a single Eulerian framework [1]. The formulation relies on a thermodynamically consistent construction based on the generalised-standard-material framework. The total energy is written in a separable form combining hydrodynamic, elastic and compaction contributions. A key ingredient of the model is the introduction of a configuration variable governing the compaction state of the porous matrix, allowing the description of both reversible and irreversible compaction mechanisms. Finite-rate relaxation processes are introduced to model pressure disequilibrium, plastic flow and compaction, ensuring compatibility with the first and second laws of thermodynamics.

The resulting system is hyperbolic in the reversible limit and is solved using a Godunov-type finite-volume method based on a reduced HLLC Riemann solver and operator splitting for the relaxation terms. The model naturally recovers classical limits such as pure fluids or purely elastic solids.

The approach is assessed on a series of one- and two-dimensional configurations including impacts and spallation in porous metals, with or without fluid-filled pores. The simulations demonstrate the ability of the model to capture key physical mechanisms such as shock propagation, wave attenuation, pore collapse, plastic deformation and fragmentation.

Figure 1 illustrates a two-dimensional impact configuration in a porous metal. The color map represents the solid volume fraction and highlights the irreversible compaction of the material. One can observe the propagation of the shock wave, followed by a progressive collapse of the pores in the compressed region. The attenuation of the wave is clearly visible as it propagates through the porous medium, while strong gradients reveal localisation of deformation and the onset of damage. This example demonstrates the ability of the model to consistently capture the coupled effects of compressibility, plasticity and compaction within a unified framework.

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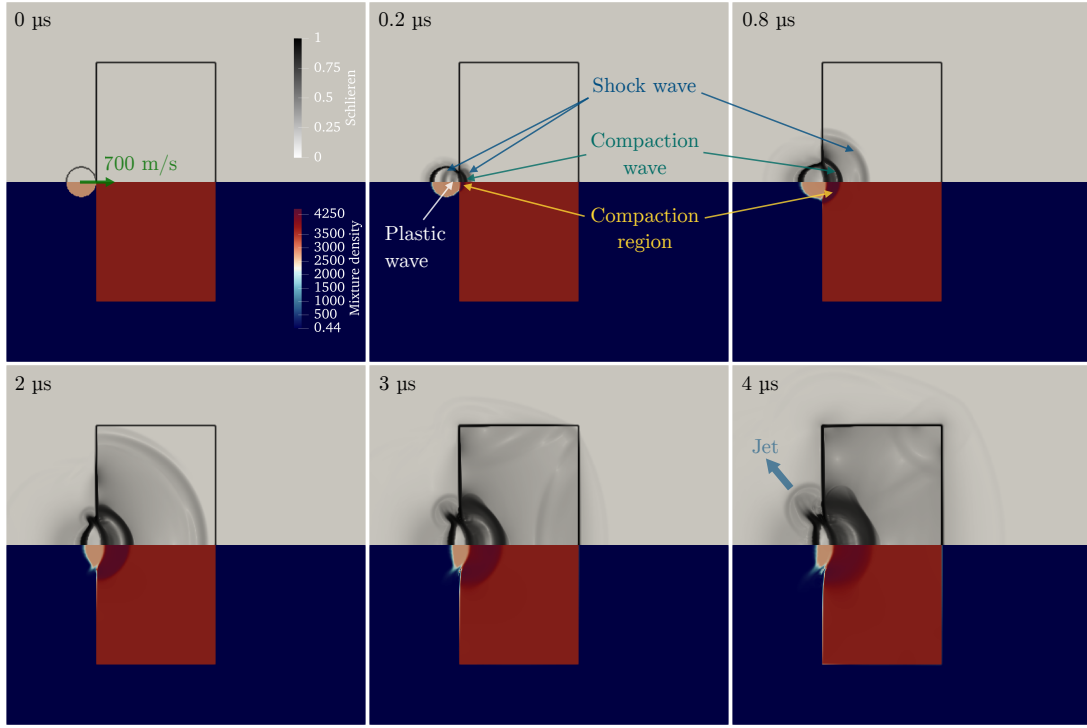


FIGURE 1: Two-dimensional impact of an aluminum cylinder (diameter 2 mm, velocity 700 ms^{-1}) on a porous titanium plate (20% initial porosity). The titanium target has dimensions $8 \text{ mm} \times 16 \text{ mm}$ and is embedded in a $24 \text{ mm} \times 24 \text{ mm}$ computational domain with non-reflecting boundary conditions. Initial pressure is 10^5 Pa and densities are $\rho_{\text{air}} = 1.2 \text{ kg m}^{-3}$, $\rho_{\text{alu}} = 2700 \text{ kg m}^{-3}$ and $\rho_{\text{tit}} = 4527 \text{ kg m}^{-3}$. Both materials follow a GTN plasticity model. The simulation is performed on a 400×400 Cartesian grid using a second-order finite-volume scheme with van Leer limiter [2]. Top: numerical Schlieren visualisation highlighting wave structures. Bottom: mixture density showing compaction. Snapshots are shown at $t = 0.2, 0.8, 2, 3$ and $4 \mu\text{s}$. After impact, strong shock and compaction waves propagate in both materials. While compaction in aluminum remains limited, the porous titanium undergoes rapid pore collapse, leading to a nearly fully compacted state. Wave attenuation is observed in the aluminum due to multiple reflections, whereas the compaction front in titanium remains well defined and propagates through the plate. At later times, the shock reaches the rear surface, generating transmitted and reflected waves and complex interactions inside the target. The aluminum cylinder experiences severe plastic deformation and flattening, accompanied by lateral jetting and a leading shock in the surrounding air. This test case illustrates the ability of the model to capture large deformations, shock interactions and irreversible compaction of porous materials within a unified framework.

ACKNOWLEDGMENT

This work was partially supported by ANR; ANR-ASTRID project SNIP ANR-19-ASTR-0016-01 and ANR-24-CE51-0508-01. Simulations presented in this paper were carried out using the PlaFRIM experimental testbed, supported by Inria, CNRS (LABRI and IMB), Université de Bordeaux, Bordeaux INP and Conseil Régional d'Aquitaine (see <https://www.plafrim.fr>).

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ON THE TREATMENT OF TOPOLOGY CHANGES ON MOVING 3D POLYHEDRAL MESHES VIA 4D SPACE-TIME HOLE-LIKE ELEMENTS IN DIRECT ALE ADER-DG METHODS

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ABSTRACT

This talk introduces a high-order ADER Discontinuous Galerkin (ADER-DG) method for hyperbolic systems on 3D moving polyhedral meshes. Operating within a *direct* Arbitrary-Lagrangian-Eulerian (ALE) framework, the scheme, which is based on PDE integration over 4D space-time control volumes, effectively handles also topology changes. This capability is obtained thanks to the introduction of degenerate 4D objects, termed *hole-like* elements, which allow for a complete covering of the space-time domain, thus ensuring the conservation properties and the high-order accuracy of the scheme. In this talk, we provide a detailed description of the occurrence, construction, and management of these *hole-like* elements in a 4D (3D+time) setting. Furthermore, we demonstrate through a von Neumann stability analysis, performed in 1D+time, by introducing a fictitious sliver-like element, that these degenerate objects do not restrict the global timestep size. We conclude the talk by presenting a set of 3D numerical benchmarks that prove the effectiveness of our 4D *hole-like* strategy. The results confirm that the method is fully conservative, satisfies the Geometric Conservation Law (GCL), and maintains the expected order of accuracy even under frequent topology changes.

CONTEXT AND MOTIVATION

In the simulation of complex vortical and high shear flows, traditional Lagrangian methods often suffer from severe mesh distortion, which limits their applicability to short-term evolutions. To preserve high mesh quality, a robust framework must allow for dynamic connectivity changes during the mesh evolution.

In this talk, we present a 3D extension of the direct Arbitrary-Lagrangian-Eulerian (ALE) strategy proposed in the works of Gaburro et al. [4, 3], where the governing hyperbolic equations are evolved in a single high-order step directly from one mesh to the subsequent one, without the need for any projection-reconstruction or remapping strategy. By adopting a space-time formulation, we perform the numerical integration over 4D control volumes that connect even two potentially different tessellations. This approach ensures a naturally conservative treatment of the PDEs and the exact satisfaction of the Geometric Conservation Law (GCL) by construction.

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4D HOLE-LIKE ELEMENTS: A NOVEL APPROACH TO HANDLING TOPOLOGY CHANGES

The transition between different mesh topologies, which manifests on a polyhedral mesh when 2-3, 3-2, or 4-4 flips occur on the underlying dual tetrahedralization, is managed by introducing *hole-like* elements.

These are unique 4D geometries that, despite having zero 3D volume at both the beginning and the end of the timestep, provide the necessary space-time shape to fill the gaps that would otherwise occur in the space-time during a flip. We provide here a rigorous geometric description of these elements, showing that they are well-defined and can be easily incorporated into the high-order solver. This approach results in a manageable implementation that avoids expensive mechanisms, such as the mesh-intersection operations typically required in indirect ALE schemes.

STABILITY ANALYSIS OF DEGENERATE GEOMETRIES

Another point that will be treated during this talk is the numerical stability of the proposed approach. We address the potential concern that degenerate elements might dictate a smaller timestep through a von Neumann stability analysis. By testing a 1D configuration containing a fictitious *sliver* element which mimics the hole-like behavior, we have demonstrated that our ALE ADER-DG scheme maintains the same CFL stability limit regardless of the presence of these elements [2]. This ensures that the global timestep size is governed by the standard mesh resolution rather than the topological transitions.

NUMERICAL VALIDATION

The framework is validated through a set of 3D tests. We first perform a series of *sanity checks* on elementary mesh flips, designed to generate a single *hole-like* element. These tests confirm that the scheme is fully conservative and satisfies the Geometric Conservation Law (GCL) to machine precision. Moreover, we show that stationary initial conditions represented by polynomials of degree N are exactly preserved. We then concentrate on rotational benchmarks to demonstrate the robustness, conservativity, and high order of accuracy of the method under frequent mesh deformations, also providing statistics on the generation of *hole-like* elements and on the evolution of the timestep size over time.

ACKNOWLEDGMENT

The authors gratefully acknowledge the support received from the European Union with the ERC Starting Grant *ALcHyMiA* (grant agreement No. 101114995). Views and opinions expressed are however those of the author only and do not necessarily reflect those of the European Union or the European Research Council Executive Agency. Neither the European Union nor the granting authority can be held responsible for them.

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A VARIATIONALLY CONSISTENT FIRST-ORDER CONSERVATION LAW FORMULATION IN ARBITRARY LAGRANGIAN EULERIAN FRAMEWORK FOR LARGE STRAIN SOLID DYNAMICS

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ABSTRACT

This work will introduce a novel computational framework for nonlinear solid dynamics based on a first-order hyperbolic Arbitrary Lagrangian Eulerian (ALE) conservation law formulation. In addition to the usual material and spatial configurations, a fixed referential configuration will be introduced to separate material motion from mesh kinematics. Within isothermal hyperelasticity, the governing system will be formulated on this reference configuration and will consist of the conservation of mass and linear momentum, together with evolution equations for the material and spatial deformation gradients. In the ALE setting, mesh motion will be treated as an independent kinematic field, which will naturally lead to an extended variational (Lagrangian) structure in which a conjugate configurational momentum arises. At the continuum level, the standard Lagrangian formulation and the extended ALE variational formulation will provide exactly equivalent representations of the same underlying variational structure. However, the introduction of independent mesh motion will lead, at the semi-discrete level, to incompatible numerical representations of the physical and configurational momentum balances, resulting in a loss of variational consistency, which must therefore be monitored and controlled. To assess this effect, a *constrained Hamiltonian* energy density will be introduced, combining kinetic energy, elastic strain energy, and a constraint enforcing consistency between linear and configurational momenta. This formulation will require solving an additional conservation law for the configurational momentum, providing a consistent set of conservation variables. The resulting Hamiltonian structure will then be used to quantify and control variational inconsistencies introduced by numerical discretisation. Mesh motions will be explored either to enforce strict variational consistency or, alternatively, to introduce controlled numerical dissipation through relative motion between mesh and material, in a manner consistent with the second law of thermodynamics. Extensions to include thermal effects will also be presented, requiring the introduction of a *constrained Ballistic* energy. Exploiting the hyperbolic structure of the governing equations, together with appropriate wave speed estimates, will ensure stability under explicit time integration. For spatial discretisation, both vertex-centered finite volume and Smoothed Particle Hydrodynamics (SPH) schemes will be implemented and assessed. A variety of benchmark problems will demonstrate the robustness and applicability of the framework for solids experiencing large deformation.

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FIRST-ORDER CONSERVATION LAW FRAMEWORK

Building on References [1, 2], the motion of a deformable solid undergoing non-thermal processes will be described by a system of first-order conservation laws formulated within an ALE framework as follows

$$\frac{\partial}{\partial t} \Big|_{\chi} p_{\chi} - \text{DIV}_{\chi} [(P + p_X \otimes W) H_{\Psi}] = f_{\chi}; \quad (1a)$$

$$\frac{\partial}{\partial t} \Big|_{\chi} F_{\Phi} - \text{DIV}_{\chi} (\hat{v} \otimes I) = 0; \quad (1b)$$

$$\frac{\partial}{\partial t} \Big|_{\chi} F_{\Psi} - \text{DIV}_{\chi} (W \otimes I) = 0; \quad (1c)$$

$$\frac{\partial}{\partial t} \Big|_{\chi} J_{\Psi} - \text{DIV}_{\chi} (H_{\Psi}^T W) = 0; \quad (1d)$$

$$\frac{\partial}{\partial t} \Big|_{\chi} q_{\chi} - \text{DIV}_{\chi} [(Q + q_X \otimes W) H_{\Psi}] = g_{\chi}. \quad (1e)$$

Here, the kinematics are defined by $\hat{v} = v + FW$ with $F = F_{\Phi} F_{\Psi}^{-1}$. The quantities $p_{\chi} = \rho_{\chi} v$ and $p_X = \rho_R v$ denote the linear momentum per unit reference and material volume, respectively, with $\rho_{\chi} = J_{\Psi} \rho_R$. The tensor P is the first Piola-Kirchhoff stress, and f_{χ} is the body force per unit reference volume. The operator DIV_{χ} denotes divergence with respect to the reference configuration. The system (1a)-(1d) comprises the balance of linear momentum, geometric conservation laws, and mass conservation (assuming uniform material density). In addition, a configurational momentum balance [3] will be introduced through the Eshelby stress, $Q = -(F^T P + \mathcal{L}_X I)$, where $\mathcal{L}_X$ denotes the material Lagrangian. The variable q_{χ} represents the configurational (material) momentum per unit reference volume and g_{χ} is its source term. This equation represents the balance of configurational momentum in ALE form, driven by the divergence of the Eshelby stress. It is the configurational counterpart of the ALE linear momentum balance (1a) and is formulated on the same reference configuration, ensuring consistency between the linear and configurational momentum balances. Although equation (1e) is decoupled and redundant, it will be retained to assess the variational consistency of the ALE formulation. When the material mesh motion W is treated as an independent variable, the *constrained Hamiltonian* of the system will be defined as

$$\mathcal{H}_{\chi}(\chi, t) = \hat{\mathcal{H}}_{\chi}(p_{\chi}, F_{\Phi}, F_{\Psi}, J_{\Psi}, W, q_{\chi}) = \frac{1}{2} \frac{1}{J_{\Psi} \rho_X} p_{\chi} \cdot p_{\chi} + J_{\Psi} \Psi(F_{\Phi}, F_{\Psi}) + W \cdot (q_{\chi} + F^T p_{\chi}). \quad (2)$$

The first term represents the kinetic energy per unit reference volume, the second term is the strain energy density, and the third enforces a constraint linking physical and configurational momenta. Although this constraint is exactly satisfied at the continuum level, it is generally violated in semi-discrete formulations, resulting in a non-zero residual. It will therefore serve as a consistency measure to monitor and potentially enforce variational consistency of the numerical scheme. An extension to include thermal effects is also possible by introducing a *constrained Ballistic energy* [5]. In this presentation, both vertex-centred finite volume and SPH [4] schemes will be presented. Several numerical examples will be provided to compare the performance of both schemes.

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NON-REFLECTING BOUNDARY CONDITIONS FOR UPDATED LAGRANGIAN HYDRODYNAMICS SIMULATIONS

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ABSTRACT

This presentation deals with a non-reflecting boundary condition (NRBC) strategy specifically designed for compressible flow simulations within an updated Lagrangian hydrodynamic framework. The method is grounded in the characteristic decomposition of the linearized Euler equations, extending the approach pioneered by Giles [1]. By analyzing the local eigenstructure of the system, incoming and outgoing waves are precisely identified at the domain boundaries. This identification enables the selective suppression of incoming waves, effectively preventing unwanted reflections. A key advantage of this NRBC approach is its full compatibility with all standard updated Lagrangian schemes, whether staggered or cell-centered. The practical implementation of the NRBC is discussed. Numerical experiments conducted on one-dimensional and two-dimensional problems demonstrate the method's effectiveness in absorbing outgoing disturbances, confirming its non-reflecting properties [2].

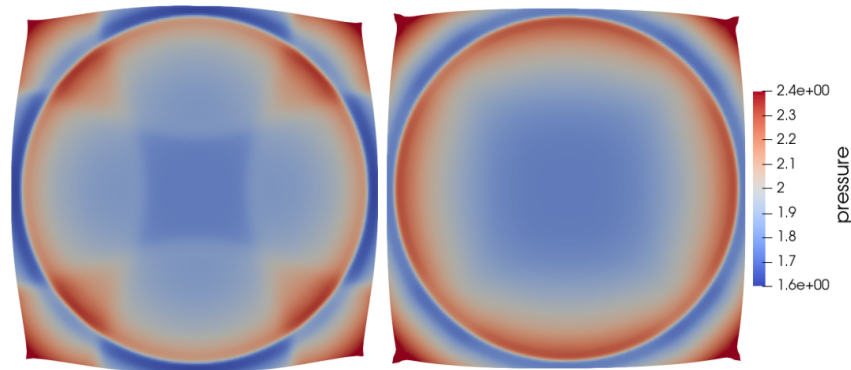


FIGURE 1: 2D diverging shock wave: Neumann boundary conditions (left) and NRBC (right).

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AN ALL-TOPOLOGY TWO-FLUID MODEL FOR TWO-PHASE FLOWS DERIVED FROM THE STATIONARY ACTION PRINCIPLE

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ABSTRACT

We propose a novel two-fluid model allowing for full non-equilibrium and derived from a two-trajectory Stationary Action Principle [1]. All interfacial quantities have physically sound closures that are directly provided by the variational principle and a new interfacial quantities is introduced. The model is shown to be hyperbolic, symmetrizable, and to admit an entropy conservation law; moreover, in one dimension, its non-conservative products yield uniquely defined jump conditions.

INTRODUCTION

Two-phase flows play a key role in many natural and engineering systems. Multi-fluid models are widely used owing to their ability to capture different topological regimes. Among these, the class of Baer–Nunziato models has become quite popular [2]. However, it requires closure relations for the interfacial velocity and pressure to be provided, which impact both the physical validity of the model, and its mathematical structure.

A common choice for the interfacial quantities is to take the interfacial velocity as one of the phasic velocities and the interfacial pressure as that of the other phase. Such closures, while simple, are adapted to specific types of flows and may not be sufficiently general to treat complex flow configurations.

In order to develop *all-topology* models valid over a wide range of flow configurations, more versatile choices for the interfacial velocity are necessary. When aiming for uniquely defined jump conditions and a well-posed Riemann problem, one has to consider the barycentric (mixture) velocity for the interfacial velocity, and an interfacial pressure which is an average pressure with weights depending explicitly on the phasic temperatures [3]. From a physical standpoint, the interfacial pressure is not expected to depend explicitly on the phasic temperatures, and several studies rely on closures obtained by physical arguments [4]. These closures do not guarantee an entropy inequality, and do not allow to properly define shocks. Alternatively, the Godunov-Peshkov-Romenski framework provides several two-fluid models which satisfy a supplementary conservation law and are closely related to Baer-Nunziato models in the barotropic case [5]. However, the proposed extensions to non-barotropic flows involve artificial heat exchanges proportional to the relative velocity.

Consequently, for the models that allow the description of complex flow topologies, there remains a gap between those retaining the necessary mathematical properties to handle shocks, and those that have been used in practice and derived through physical considerations. In this contribution, we present a novel *all-topology* two-fluid model derived by variational principles and which overcomes previously identified limitations [1].

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PRESENTATION OF THE MODEL

The model is derived by the Stationary Action Principle with two families of trajectories [1]. The physical Lagrangian is the difference between the kinetic energies of the phases and their internal energies. The interfacial velocity is imposed as a constraint in the variational principle, which then provides the remaining interfacial quantities, including a new one which is the interfacial work. The resulting model reads,

$$\begin{aligned} \partial_t \alpha_1 + \mathbf{u}_I \cdot \nabla \alpha_1 &= 0, \\ \partial_t (\alpha_k \rho_k) + \nabla \cdot (\alpha_k \rho_k \mathbf{u}_k) &= 0, \quad k = 1, 2, \\ \partial_t (\alpha_k \rho_k \mathbf{u}_k) + \nabla \cdot (\alpha_k \rho_k \mathbf{u}_k) - p_I \nabla \alpha_k &= \mathbf{0}, \quad k = 1, 2, \\ \partial_t (\alpha_k \rho_k E_k) + \nabla \cdot (\alpha_k (\rho_k E_k + p_k) \mathbf{u}_k) - (p \mathbf{u})_I \cdot \nabla \alpha_k &= 0, \quad k = 1, 2. \end{aligned}$$

Here α_k denotes the volume fraction of the k^{th} phase, while ρ_k , p_k , $\mathbf{u}_k$ and E_k respectively denote its density, pressure, velocity and total energy. Denoting Y_k the mass fraction of the k^{th} phase, the interfacial velocity is set to $\mathbf{u}_I = Y_1 \mathbf{u}_1 + Y_2 \mathbf{u}_2$, while the closures $p_I = Y_1 p_2 + Y_2 p_1$ and $(p \mathbf{u})_I = Y_1 p_2 \mathbf{u}_1 + Y_2 p_1 \mathbf{u}_2$ are provided by the variational principle. The model admits a supplementary conservation law for the entropy. Its mathematical analysis in the one-dimensional setting shows that it is hyperbolic and symmetrizable under a classical non-resonance condition. Moreover, owing to the linearly degenerate character of the interfacial wave, its non-conservative products are uniquely defined through discontinuities, and shocks are unambiguously defined.

NUMERICAL RESULTS

Adapting the numerical method for the Baer-Nunziato model proposed in [6], we illustrate the model on a series of Riemann problems such as the one shown in Figure 1. Moreover, a comparison with classical Baer-Nunziato models allows to demonstrate the strengths of the newly derived model.

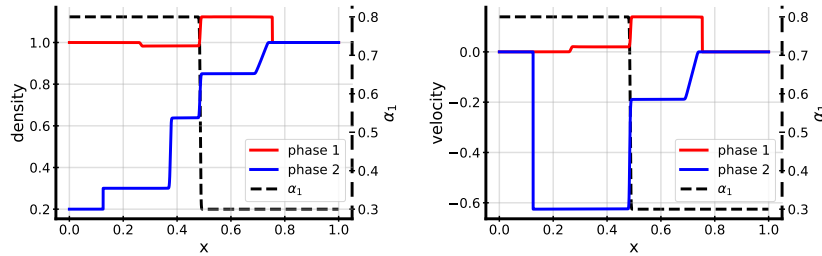


FIGURE 1: Density (left) and velocity (right) profiles for a Riemann problem with the proposed model. The right axis and dashed line shows the volume fraction and indicates the interface location.

CONCLUSIONS

A new *all-topology* two-fluid model is derived using variational principles. It is both physically consistent and possess the required mathematical structure to properly describe shock-type solutions, allowing it to overcome the limitations of previously derived models.

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PLASMA TRANSPORT MODELING FOR LASER-DRIVEN HOHLRAUMS

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INTRODUCTION

Hohlraums are high-Z (Au, depleted U) cylinders that are used to convert laser energy into a uniform X-ray bath to drive high yield capsule implosions on the National Ignition Facility. As hohlraum and capsule material ablate into the interior of the hohlraum (a low density He-filled cavity), the material in the cavity achieve high temperature, low density conditions where the Knudsen number Kn , the ratio of the ion mean free path to a representative fluid lengthscale, can reach values $Kn > 10$ [1], while the wall and capsule exhibit $Kn < 1$. Recent experiments have demonstrated that it is important to account for the non-hydrodynamic behavior of the ablated Au bubbles to correctly predict the evolution of material distributions in the hohlraum [2].

Detailed models have been developed [3, 4] for multi-species hydrodynamics that have shown to improve agreement with experiment when implemented in radiation-hydrodynamics codes [5, 2]. Nevertheless, such models introduce substantial complexity and expense beyond the hydrodynamics solvers typically used in radiation-hydrodynamics codes for physics that is important for a fairly small region of hohlraums. Simpler diffusion approximations to this physics [6] offer a potential compromise, modeling plasma viscosity and plasma transport processes seeded by gradients in species concentrations as well as gradients in electron and ion pressures and temperatures.

We will discuss the plasma transport algorithm introduced in [6], details of its implementation into the xRAGE code [7, 8, 9], and applications to recent hohlraum science experiments [2, 10].

PLASMA TRANSPORT MODEL

Our plasma transport model [6] adds a viscous stress Π to the equations for momentum and energy solved by xRAGE,

$$\Pi_{mn} = \eta_0 \left(\nabla u + \nabla^T u - \delta_{mn} \frac{2}{3} \nabla \cdot u \right),$$

where η_0 is the viscosity and u is the fluid velocity. In addition, we allow each ion species i to have a drift velocity $w_i := u_i - u$, calculated as

$$\rho_i w_i = - \frac{P_{\text{ion}} \alpha_i (\chi_i) \sum_{j \neq i} \rho_j}{\rho \sum_{j \neq i} v_{ij}} \left(\nabla \chi_i + (\chi_i - c_i) \frac{\nabla P_{\text{ion}}}{P_{\text{ion}}} + (z_i - c_i) \frac{\nabla P_{\text{electron}}}{P_{\text{ion}}} + \chi_i \alpha_{\text{electron}} \frac{\nabla T_{\text{electron}}}{T_{\text{ion}}} + \chi_i \frac{\nabla T_{\text{ion}}}{T_{\text{ion}}} \right),$$

where ρ_i is the mass density, χ_i is the number fraction, c_i is the mass fraction, z_i is the charge fraction, v_{ij} is the collision rate between species, and α are coefficients. The equation for w_i is solved explicitly due to the high level of nonlinearity in the equations, but the viscous component can be solved implicitly.

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IMPACT ON HOHLRAUM SIMULATIONS

The plasma transport model changes the evolution of the Au bubble substantially, shown in Figure 1, and leads to better agreement with experiment for the measured X-ray flux and energy coupling to the capsule [10] as well as direct measurements of interpenetration performed in [5, 11].

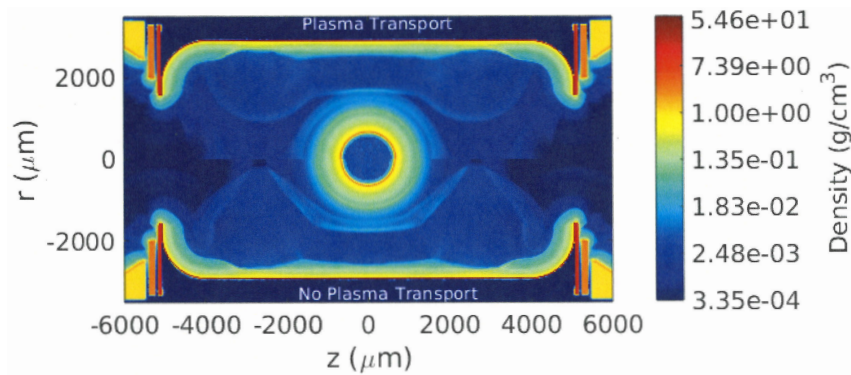


FIGURE 1: Comparison of hohlraum density profile at $t = 3.5$ ns for NIF shot N230105 with and without plasma transport modeling in xRAGE. This demonstrates a substantial difference in Au bubble growth.

ACKNOWLEDGMENT

Los Alamos National Laboratory is operated by Triad National Security, LLC, for the National Nuclear Security Administration of U.S. Department of Energy (Contract No. 89233218CNA000001).

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ALGEBRAIC FLUX CORRECTION SCHEMES FOR COMPRESSIBLE NAVIER–STOKES EQUATIONS

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ABSTRACT

In this work we design algebraic stabilization techniques for compressible gas dynamics. Specifically, the monolithic convex limiting (MCL) framework [1] designed for hyperbolic problems is extended to the viscous case of compressible Navier–Stokes equations (NSE). Compared to hyperbolic conservation laws, for which the MCL technique was first designed, the NSE contain second-order diffusive terms which can be handled by a splitting approach (e. g., Strang) or in a monolithic manner. Pursuing the latter, we generalize the previously mentioned limiting techniques to the parabolic regime. To this end, we make use of semi-implicit time stepping schemes, which were first combined with MCL in [4]. Our target scheme is based on our previously employed dissipation-based WENO-stabilization [3, 2] of standard Galerkin methods. Invoking a shock-detector, these schemes use adaptive dissipation for shock-capturing purposes yielding high-order accurate solutions in smooth regions and resolving discontinuities accurately, too. However, there is no guarantee, that numerical approximations are physically meaningful. To enforce this property, we thus perform failsafe MCL-type limiting on top of WENO-based stabilization to guarantee the validity of nonnegotiable constraints. In the case of the Navier–Stokes equations, these properties are nonnegativity of density and internal energy. In our numerical examples, we apply the newly developed discretizations to common test problems to demonstrate their capabilities. We then draw conclusions and give an outlook to future work.

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A RENOVATION OF THE ELVIRA CONCEPT FOR HIGH-PERFORMANCE MULTIPHYSICS

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ABSTRACT

We consider the partitioning of $N > 1$ materials with vastly different character to fine subcell resolution. An interface reconstruction variant assembled from volume fractional data in neighboring stencils, perhaps hierarchically structured or even unstructured, our method enables sharp preservation of interfaces in otherwise diffusive Eulerian frame discretizations. Based on the ubiquitous Least-squares Volume-of-fluid Interface Reconstruction Algorithm (LVIRA) and Efficient LVIRA (ELVIRA) concepts [1], our scheme, termed the Highly Efficient LVIRA (HELVIRA), adopts a non-iterative, finite candidate strategy suitable, in particular, for finite volume methods under adaptive mesh refinement. Our HELVIRA technology produces comparable interface quality to conventional LVIRA at a fraction of the cost. With LVIRA constrained to the fixed cost of HELVIRA, HELVIRA yields better interfaces according to the L^2 -norm of the reconstruction error. To illustrate the performance of our approach, we consider a series of benchmark multimaterial hydrodynamic and multiphysics problems.

INTRODUCTION

Multiphysics problems of hydrodynamic character, modeled by sophisticated numerical methods, enable the predictive study of many physical phenomena, spanning the mesoscale to astrophysical-scale. In the Eulerian frame, finite volume context, such numerical methods induce, of course, numerical and model error that, particularly in locally multimaterial regimes, can lead to excessive material mixing and diffusion. In the years since the first computational hydrodynamics efforts, many corrective schemes have emerged, among them the *volume-of-fluid* method, which, via appropriate interface reconstruction routines, preserves material sharpness along with physical invariants, *viz.* mass conservation. Such interface reconstruction implies a heavy geometric component, namely the localization of material characteristics, to supply appropriate fluxes to maintain expected intercell multimaterial flow.

In this work, we consider a renovation of the Least-squares Volume-of-fluid Interface Reconstruction Algorithm (LVIRA) and Efficient LVIRA (ELVIRA) concepts [1]. Our technology, denoted by the Highly Efficient LVIRA (HELVIRA), provides a non-iterative, finite candidate scheme that yields higher quality interfaces (as measured by the L^2 -norm of the reconstruction error) than a standard least-squares gradient fit, while remaining

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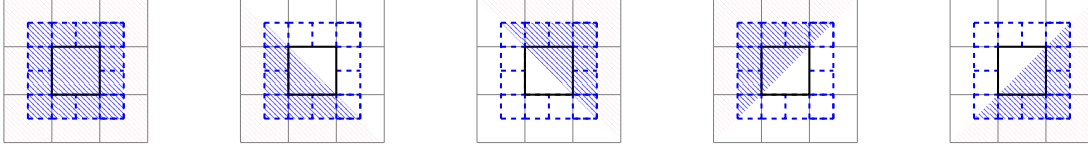


FIGURE 1: Candidate stencils in 2-D. Left: Central stencil. Remaining: Maximally unaligned candidates. The blue region indicates the inclusion of data generated at a finer discretization level than the target control volume, otherwise indicated in red. The approach may be applied identically for unstructured grids.

well below the cost of conventional LVIRA computations. HELVIRA, moreover, remains suitable in the context of unstructured or hierarchical control volumes, such as those obtained by adaptive mesh refinement. Finally, the method is architecturally amenable to GPU parallelization, delivering a high-performance capability for large-scale multiphysics workflows.

OUR APPROACH

We suppose at any given time t we possess a full specification of volume fractions for $M \in \mathbb{Z}^+$ materials associated with control volumes $K \subseteq \mathcal{T}$ over a domain $\mathcal{T} \subset \mathbb{R}^d$, $d = \{2, 3\}$. While tracking material *centroids* in addition to volume fractions enables performant interface reconstruction schemes [2], we restrict ourselves to volume fractions alone (and associated state quantities, densities, internal energies, etc.). We further impose a partition of the M materials in two categories: those immiscible, represented by $\omega^\sharp$, and those miscible, or $\omega^\flat$. For each material of $\omega^\flat$ present in a multimaterial, or mixed, control volume K , we form an artificial, aggregated mixture, which, in the following partitioning, behaves as a single member of the “sharp” materials $\omega^\sharp$. Finally, for control volumes containing mixtures of > 2 materials, we assume there exists an oracle provided ordering.

Unlike in the standard ELVIRA case, which considers a sequence of forward, backward, and central finite difference stencils, with HELVIRA we partition a local neighborhood of volume fractional data for each $\omega^\sharp$ material according to Figure 1. In two dimensions, this procedure yields 5 candidates, as opposed to ELVIRA’s 6, and is entirely agnostic to the arrangement of the set of control volumes in the neighborhood of K . Each candidate yields an estimated interface normal according to a least-squares gradient estimate. All components of this scheme, but particularly the fixed enumeration of candidates, incentivizes GPU parallelization. To document its performance, we will consider a series of hydrodynamic and multiphysics benchmark problems, including the result of Figure 2, which illustrates the potency of HELVIRA. With LVIRA constrained to HELVIRA’s cost, HELVIRA yields quantitatively better interfaces. Our method is implemented in *Tangram* [3].

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FIGURE 2: Material partition for linear advection of a three-material concentric configuration after one period. Left: Employing only the central stencil of Figure 1. Center: Employing all the candidate stencils of Figure 1. Right: Optimization via the LVIRA algorithm [1].



VARIATIONAL CONSTITUTIVE UPDATES FOR DISSIPATIVE SOLIDS AND MULTIPHASE FLOWS IN HYPERBOLIC PROBLEMS

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ABSTRACT

This talk first introduces a variational framework dedicated to thermally-coupled constitutive updates [1], within which various dissipative responses like hyperelastic-plastic or visco-hyperelastic ones can be recast. The variational constitutive update is driven by the updated internal energy density, which allows a natural coupling with the conservation of total energy. Next, this framework is extended to describe the local relaxation process at finite rate of the mechanical states of various co-existing phases in a context of Eulerian compressible multiphase flows. The presentation focuses on a multiphase fluid medium, describing the relaxation over time of an interfacial pressure.

INTRODUCTION

The numerical simulation of impacts on dissipative multi-phase or multi-material media is of great importance for various engineering applications, including potentially solid and/or fluid phases. As examples, we can cite cavitation near blades, lithotripsy, dynamic forming processes, ballistic impacts, or compaction of heterogeneous porous media [2, 3].

A first crucial point is to ensure the thermodynamic consistency of strong thermo-mechanical couplings in the constitutive modeling, both on hydrodynamic and shear effects. The latter can yield e.g. temperature increase due to plastic strains, and thermal softening. Thermal effects in solids are more easily described using the temperature as main thermal unknown [4], essentially because it is a measurable quantity, leading to using Helmholtz's free energy density in constitutive models. The construction of thermo-mechanical constitutive updates, compatible with the conservation of total energy, and efficient for levels of pressure ranging from moderate to high is thus of particular relevance.

Second, the modeling of compressible multiphase flows, including potentially solid and/or fluid phases, often involve high levels of deformation making Eulerian descriptions of the motion suitable. However, such formulation requires the ability to track interfaces over time and to handle mixtures within a fixed computational mesh. Among the various existing approaches, the diffuse interface method [5] allows interfaces and mixtures to be considered with the same model and numerical scheme throughout the computational domain, with interfaces being considered as mixing zones. But, at a microscopic scale, the geometry of the interfaces between phases plays an important role in wave interaction, particularly with waves whose wavelength is of the

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order of the characteristic size of specific shapes such as bubbles and pores. In particular, these local interactions can give rise to dissipative damping and attenuation effects at the macroscopic scale, which are important to account for in multiphase numerical simulations.

This talk aims at presenting a variational framework dedicated for thermomechanical constitutive updates [1], which allows a natural coupling with the conservation of total energy. In the continuous setting, the thermal part of the constitutive update is driven by the rate of the internal energy density, while it is driven by its increment in the discrete setting. Various dissipative constitutive flows can be recast within this framework, which this presentation will first show a succinct tour. As examples, one can cite hyperelastic-plasticity coupled with isotropic [1] or non-linear kinematic hardenings [6], or viscohyperelasticity of Zener-type [7] dedicated to polymeric materials and/or applications in non-linear acoustics. The flow direction is parameterized with the concept of pseudo-stresses [8]. The constitutive updates can be coupled either with Lagrangian or Eulerian conservation laws, which are solved with any favourite shock-capturing numerical scheme.

Next, in the context of the modeling of Eulerian compressible multiphase flows with the diffuse interface method, this variational framework is adapted to describe the local relaxation process at finite rate of the mechanical states of the various co-existing phases. This constitutive relaxation at finite rate is dissipative, and accounts for exchanges of internal energy density between the phases, while it also enforces a unit sum of volume fractions through a Lagrange multiplier, *a posteriori* interpreted as an interfacial pressure. The presentation focuses on a multiphase fluid medium, describing the relaxation over time of an interfacial pressure. This lays some groundwork for future extensions to multiphase solid media or fluid-solid couplings.

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NOVELTIES ON ARBITRARY HIGH-ORDER MULTIDIMENSIONAL COMPOSITE FINITE VOLUME SCHEMES

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ABSTRACT

We deal with extension of the finite volume classical ARS (Approximate Riemann Solver) of conservation laws in dimension $d = 2, 3$:

$$\partial_t \mathcal{U} + \operatorname{div}_{\mathbf{x}} \mathcal{F}(\mathcal{U}) = 0, \quad \mathbf{x} \in \mathbb{R}^d.$$

We consider composite finite volume schemes in the sense that the numerical fluxes are well defined (consistent and locally conservative) at all co-dimension mesh object (nodes and edges here).

First part is devoted to geometrical properties of normals at such locations. For each of these mesh items, we propose an extension in the construction of local normals [1] [2] in such a way to fulfill (some necessary) LSV conditions: Local conservation, Stokes formula and cell Volume formula. The new normal corner vector $\hat{\mathbf{C}}_j^r$ are based on standard $\mathbf{C}_j^r$ (e.g. [1]) and some other complementaries vectors $\mathbf{D}_j^r$. They posses properties that do not break LSV conditions and also show some rotational properties (orthogonality with $\mathbf{C}_j^r$ in each cell and around nodes). Up to our knowledge, this is a new result for finite volume methods on unstructured meshes making a link with discrete Helmholtz-Hodge decomposition. Moreover, they still permits to obtain arbitrary order quadrature (composite) formula.

The second part is devoted to extending classical edge schemes (Roe, VFFC, Rusanov, HLL ..) at node in such a way that consistency and local conservation is obtained. The resulting composite node/edge scheme offer an other way of obtaining a multi-dimensional aware scheme (see also [3]). For Euler equations of compressible gas dynamics, we use arbitrary order composite formula flux and a valid high order spatial reconstruction obtained with an induced limitation process [4]. We will show numerical results to asses the accuracy and robustness of some composite schemes.

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DISCRETE HODGE-HELMHOLTZ DECOMPOSITION AND CURL PRESERVING NUMERICAL SCHEMES. APPLICATION TO LOW MACH NUMBER COMPRESSIBLE FLOWS.

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ABSTRACT

Some hyperbolic systems implicitly involve a curl or a divergence constraint. For example, the wave system ensures the preservation of the vorticity, or the Maxwell system ensures the preservation of the divergence of the magnetic field. These constraints are generally difficult to preserve at the discrete level. To achieve this in practice, it is common to use *staggered schemes*, such as the MAC scheme to satisfy a constraint of the form $\text{div}(\mathbf{u}) = 0$, or more generally, numerical schemes based on Nédélec or Raviart-Thomas finite elements. In this work, we propose finite-volume schemes (for first-order) and discontinuous Galerkin schemes (for high-order), i.e. *colocated schemes*, which preserve a curl constraint at the discrete level. The sense in which this curl is preserved will be defined. We will first discuss the case of a linear wave system, and then the case of compressible flows at low Mach numbers (Euler equations).

WAVE SYSTEM

The linear wave system is

$$\begin{cases} \partial_t p + c_0^2 \text{div}(\mathbf{u}) = 0, \\ \partial_t \mathbf{u} + \nabla p = 0, \end{cases}$$

where p is the pressure and $\mathbf{u}$ the velocity. c_0 is the wave speed. Taking the curl of the velocity equation, we formally obtain $\partial_t(\text{curl}(\mathbf{u}))$ which means that the vorticity $\text{curl}(\mathbf{u})$ is preserved. Using a Hodge-Helmholtz decomposition (which allows to write any vector field $\mathbf{u}$ as the sum of a curl-free component $\mathbf{u}^\varphi$ and a divergence-free component $\mathbf{u}^\psi$), the preservation of the vorticity $\text{curl}(\mathbf{u})$ corresponds to the preservation of the divergence-free component $\mathbf{u}^\psi$. Then, the long time limit of the wave system (under some boundary condition hypotheses) can be identified. At the discrete level, for a given approximation space, does such a decomposition exist?

For piecewise constant vectors, such a decomposition exists on triangular meshes [1, 2]. It explains why the finite volume Godunov scheme preserves vorticity and is long time consistent on triangular meshes. However, this is not the case on quadrangular meshes. Building on our understanding of the triangular case, a discrete Hodge-Helmholtz decomposition is proposed on quadrangular meshes leading to a numerical scheme that preserves vorticity and is long time consistent [3]. The key to obtaining this decomposition on quadrangular meshes is to enrich the approximation space of the velocity field. Instead of having two degrees of freedom per cell, there are now three.

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These results can be extended to high-order discontinuous Galerkin schemes. On triangular meshes, using the classical approximation space (nodal or modal basis for each variable) and a Godunov flux, the numerical scheme preserves vorticity and is long time consistent [4]. This property does not hold on quadrangular meshes, for which the approximation space of the vector field must be adapted [5, 6].

EULER SYSTEM AND LOW MACH NUMBER ACCURACY

The low Mach number behaviour of the Euler system is strongly linked to a linear wave system. More precisely, performing a two time scale asymptotic expansion in powers of the Mach number, the first-order pressure and the zeroth-order momentum satisfy a wave system, so that the low Mach number limit of the Euler system corresponds to the long time solution of this wave system [11, 7].

Based on the results obtained for the wave system, we recover that the Roe/HLLC/Godunov finite volume schemes are low Mach number accurate on triangular meshes [10] and are not on quadrangular meshes [8].

On quadrangular meshes, using the approximation space for vector field proposed for the wave system together with a numerical flux such as Roe, HLLC, Godunov or Osher (without any low Mach number fix), a low Mach number accurate numerical scheme can be obtained [3]. The resulting numerical scheme is stable, allows also the propagation of low Mach number acoustic waves (unlike low Mach number fixes such as [8], as explained in [11]) and is free of checkerboard modes (unlike low Mach number fixes such as [12], as explained in [13]).

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DIFFERENTIABLE HIGH PERFORMANCE HYDRODYNAMIC SIMULATION FOR OPTIMIZATION OF SHOCK DRIVEN FLOWS

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ABSTRACT

Keywords: gradient-based optimization; adjoint methods; shock hydrodynamics; multi-material hydrodynamics; Lagrangian methods; multiphysics simulation.

INTRODUCTION

Recent advances in topology optimization and machine learning have intensified the need for scalable, robust gradient computation in large-scale, time-dependent multiphysics simulations. In inertial confinement fusion (ICF), optimizing shock timing, strength, and stability requires sensitivities of shock-driven objectives with respect to material properties and controllable inputs, often in high-dimensional design spaces. This work targets gradient-based optimization of shock behavior in ICF-relevant simulations using the production multiphysics code MARBL at Lawrence Livermore National Laboratory.

Automatic differentiation (AD) provides a robust way to algorithmically compute derivatives and assemble gradients of complex compositions of functions, enabling rapid, flexible experimentation with sophisticated mathematical models. Frameworks such as JAX and PyTorch have demonstrated that AD can scale to very large problems, but extending these capabilities to high-order finite element discretizations and production shock-hydrodynamics workflows requires additional methodological development, particularly in the presence of shock-capturing nonlinearities and other non-smooth components.

We develop discrete-adjoint equations for the multi-material Euler equations discretized with high-order finite elements, and design AD-enabled sensitivity algorithms that exploit the sequential structure of time integration. The resulting approach computes gradients efficiently with respect to both control and material parameters, supporting topology optimization, material parameter inference, and optimal control of initial-value problems [1]. We further investigate robust gradient treatments for non-smooth operations (for example, min/max and absolute values) via regularization and smoothing strategies.

We discuss practical challenges in making this methodology effective at scale, including heterogeneous compute environments, parallel execution, and checkpointing schemes for long time integrations, as well as the use of just-in-time compilation for user-defined inputs while preserving performance and flexibility. We present preliminary results on shock-driven design optimization, including suppression and enhancement of Richtmyer-Meshkov instabilities via minimization of a quantity of interest measuring jet length, demonstrating efficient optimization in design spaces of ~ 1000 variables and significantly improved performance relative to non-derivative-based strategies.

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ACKNOWLEDGMENT

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344 and Project No. 21-SI-006, 24-ERD-005, and 26-SI-002 and Release No. LLNL-ABS-2015165.

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VARIATIONAL CELL-CENTERED DIRECT ALE SCHEME FOR COMPRESSIBLE MULTIMATERIAL FLOWS: CONSISTENCY AND STRUCTURE PRESERVATION IN THE LAGRANGIAN LIMIT

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ABSTRACT

INTRODUCTION

The simulation of compressible multi-material flows on moving meshes remains challenging due to the need to capture interfaces while preserving conservation and consistency under strong deformation. ALE methods provide a flexible framework, but robustness across regimes remains difficult, particularly for multiple materials. We propose a variational, cell-centered direct ALE formulation within the GEEC framework [2], based on a discrete least-action principle and yielding a structure-preserving scheme.

VARIATIONAL FORMULATION

The method is derived from a variational principle applied to a multi-material action

$$\mathcal{A} = \int_{t_0}^{t_1} \int_{\Omega(t)} \mathcal{L} dV dt,$$

with

$$\mathcal{L} = \sum_{\varphi=1}^N \left[\frac{1}{2} \alpha_{\varphi} \rho_{\varphi} |\mathbf{u}_{\varphi}|^2 - \alpha_{\varphi} \rho_{\varphi} e_{\varphi} + \phi_{\varphi} D_t^{\varphi} (\alpha_{\varphi} \rho_{\varphi}) + \psi_{\varphi} D_t^{\varphi} (\alpha_{\varphi} \rho_{\varphi} \xi_{\varphi}) \right] - \Pi \left(\sum_{\varphi} \alpha_{\varphi} - 1 \right).$$

Here, $D_t^{\varphi} = \partial_t + \mathbf{u}_{\varphi} \cdot \nabla$ denotes the material derivative along phase φ . The Lagrange multipliers ϕ_{φ} enforce phase mass conservation, while ψ_{φ} impose label advection, ensuring isentropic consistency. The multiplier Π enforces the constraint $\sum_{\varphi} \alpha_{\varphi} = 1$ (no void). Stationarity yields Euler–Lagrange equations enforcing single-pressure equilibrium, exact advection of mass and labels, and consistent momentum and energy balances. A semi-discrete ALE formulation preserves this structure, ensuring conservation, geometric compatibility, and entropy consistency. The resulting scheme maintains a coherent coupling between mass transport, pressure forces, and material distribution across all regimes.

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IMPROVEMENTS IN THE LAGRANGIAN LIMIT

Two corrections are introduced to restore geometric and thermodynamic consistency in near-Lagrangian and multi-material regimes [1]. First, antisymmetric definitions of swept face volumes are enforced to satisfy the discrete geometric conservation law (DGCL). The original formulation [2] does not guarantee this property, leading to inconsistencies between volume evolution and transported fluxes. The corrected definition restores exact balance, ensuring preservation of uniform states and robustness under strong deformation.

Second, the off-centering coefficients used in transport and pressure terms are reformulated. While upwinding ensures stability for transport, its direct use in the pressure gradient breaks symmetry near Lagrangian faces and may violate local momentum conservation. A symmetrized, continuous definition is introduced, enforcing pairwise consistency and a partition-of-unity condition. This yields a smooth transition between centered (Lagrangian) and upwind (Eulerian) regimes, removing spurious oscillations.

Together, these modifications restore antisymmetry, geometric conservation, and consistent pressure coupling, ensuring stable behavior across regimes and material interfaces.

NUMERICAL RESULTS

The method is assessed on test cases involving shocks, strong compression, and multi-material interface dynamics. Results demonstrate accurate shock capturing, stable interface evolution, and robustness under large mesh deformation. In particular, improved behavior is observed near the Lagrangian limit compared to previous GEEC-ALE formulations. Figure 1 presents the results for multi-material triple point problem by using direct ALE strategy.

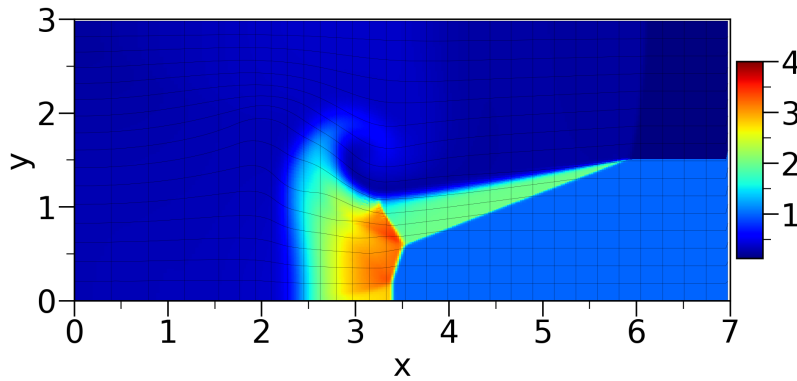


FIGURE 1: 2D triple point shock tube, two materials, density, 300×150 cells.

CONCLUSION

An improved discretization to variational ALE formulation for compressible multi-material flows will be presented. By combining a discrete least-action principle with consistent geometric and pressure coupling, the method provides a robust and structure-preserving framework for compressible multi-material flows on arbitrary moving meshes.

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FINITE ELEMENT SIMULATIONS OF RADIATIVE TRANSFER USING REALIZABLE MOMENT MODELS AND CONVEX LIMITING

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ABSTRACT

We discretize the M_1 model of radiative transfer using continuous finite elements and propose a tailor-made monolithic convex limiting (MCL) procedure for enforcing physical realizability [1, 2]. The M_1 system of nonlinear balance laws for the zeroth and first moments of a probability distribution function is derived from the linear Boltzmann equation and equipped with an entropy-based closure for the second moment. To ensure hyperbolicity and physical admissibility, evolving moments must stay in an invariant domain representing a convex set of realizable states. We first construct a low-order method that is provably invariant domain preserving (IDP). Introducing intermediate states that represent spatially averaged exact solutions of homogeneous Riemann problems, we prove that these so-called bar states are realizable in any number of space dimensions. This key auxiliary result enables us to show the IDP property of a fully discrete scheme with a diagonally implicit treatment of reactive terms. To achieve high resolution, we add nonlinear correction terms that are constrained using a two-step MCL algorithm. In the first limiting step, local bounds are imposed on each conserved variable to avoid spurious oscillations and maintain positivity of the scalar-valued zeroth moment (particle density). The second limiting step constrains the magnitude of the vector-valued first moment to be realizable. The flux-corrected finite element scheme is provably IDP. A series of numerical experiments demonstrate its ability to effectively prevent nonphysical states while avoiding the side effects that were observed in [3]. The practical potential of the proposed method is demonstrated through a numerical study for dose calculation in proton therapy.

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APPROXIMATION OF LAGRANGIAN HYDRODYNAMICS BY A DDFV TYPE METHOD

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ABSTRACT

This work introduces a novel Discrete Duality Finite Volume (DDFV) method [1, 2] for the approximation of the compressible Euler equations in Lagrangian form. The proposed approach relies on a double integration over primal and dual meshes, leading to a consistent discretization of differential operators. This construction enables a natural coupling between kinematic and thermodynamic variables while preserving key structural properties of Lagrangian hydrodynamics.

The resulting scheme is formulated within a finite-volume framework and incorporates pseudo-viscosity terms to ensure stability and entropy consistency in the presence of shocks. A leapfrog-type time discretization is employed, yielding a method that is conservative with respect to mass, momentum, and total energy, while also satisfying the discrete geometric conservation law and preserving angular momentum at the dual level.

The method is assessed on a series of standard benchmark problems. Numerical results demonstrate the robustness of the approach on both Cartesian and highly distorted meshes, as well as its ability to accurately capture shock waves and low-Mach features. Comparisons with a reference Lagrangian scheme (EUCCLHYD [3]) highlight the competitiveness of the DDFV formulation in terms of accuracy and stability.

This work constitutes a first step toward the extension of DDFV techniques to more complex Lagrangian systems, such as magnetohydrodynamics and radiative hydrodynamics.

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SYMMETRISATION AND HYPERBOLICITY OF FIRST-ORDER CONSERVATION LAWS IN LARGE STRAIN VISCOELASTICITY

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ABSTRACT

This paper will present a first-order hyperbolic framework with relaxation (or dissipation) terms for large strain viscoelastic solids. The framework is based on a Maxwell-type viscoelastic model [1, 2] and will incorporate conservation of linear momentum, geometric conservation laws, and evolution equations for internal variables. The viscous relaxation model will first be developed for compressible behaviour. A polyconvex strain energy function, jointly convex in the deformation measures and internal variables, will be introduced. This will then lead to a generalised convex entropy function that symmetrises the hyperbolic system in terms of dual entropy variables. It will be shown that the system is hyperbolic (i.e., admits real wave speeds) under all deformation states, and that the relaxation terms correctly predict viscoelastic dissipation. The framework will then be extended to incompressible viscoelasticity. This will require the introduction of a new polyconvex energy formulation together with a formulation enforcing the incompressibility constraint. Using backward Euler time integration, the resulting update of the internal variables will naturally enforce the incompressibility constraint at the discrete level. For spatial discretisation, a vertex-centred finite volume scheme [3] and a Smoothed Particle Hydrodynamics (SPH) scheme [4] will be presented. Both schemes will enforce the second law of thermodynamics at the semi-discrete level by monitoring the time rate of the generalised convex entropy, providing a mechanism to control numerical dissipation and enhance stability. Finally, the framework will be validated through numerical examples using both algorithms, demonstrating stability, accuracy, and consistent energy dissipation for both compressible and incompressible viscoelastic regimes.

SYMMETRISATION IN FIRST-ORDER CONSERVATION LAWS

Hyperbolicity in first-order conservation laws with relaxation for large strain solids [5] will be ensured by reformulating the system in symmetric hyperbolic form using a convex entropy function. The first-order system for viscoelastic solids with Maxwell-type relaxation can be written as [1]

$$\frac{\partial \mathcal{U}}{\partial t} + \sum_{I=1}^3 \frac{\partial \mathcal{F}_I}{\partial X_I} = \mathcal{S}(\mathcal{U}); \quad \mathcal{S}(\mathcal{U}) = \mathcal{S}_{\text{ext}} + \mathcal{R}(\mathcal{U}); \quad \mathcal{R}(\mathcal{U}) = \sum_{\alpha=1}^{n_M} \mathcal{R}_{\alpha}(\mathcal{U}). \quad (1)$$

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Here, $\mathcal{U}$ denotes the set of conservation variables and $\mathcal{F}_I(\mathcal{U})$ is the flux vector in the material Cartesian direction I . The source term $\mathcal{S}(\mathcal{U})$ can be decomposed into two contributions. Specifically, $\mathcal{S}_{\text{ext}}$ accounts for external sources such as body forces, and $\mathcal{R}$ the relaxation contribution. The relaxation term itself is a sum of branch contributions $\sum_{\alpha=1}^{n_M} \mathcal{R}_\alpha(\mathcal{U})$, each describing the evolution of internal variables associated with Maxwell branch α . The following conditions (summarised from Chen, Levermore, and Liu [6]) will ensure symmetric hyperbolicity [7, 8, 9] of the system (1) and thermodynamically consistent treatment of relaxation (or dissipation) effects:

- (i) Existence of a convex entropy function S , which requires a polyconvex viscoelastic energy density W consistent with thermodynamic equilibrium.
- (ii) Positive definiteness of the Hessian operator $\frac{\partial^2 S}{\partial \mathcal{U} \partial \mathcal{U}}$, ensuring the existence of a suitable symmetriser for the system.
- (iii) Symmetry of the flux Jacobian matrices in entropy variables, expressed by $\mathcal{A}_I \mathcal{A}_0$, with $\mathcal{A}_I = \frac{\partial \mathcal{F}_I}{\partial \mathcal{U}}$ and $\mathcal{A}_0 = \left[\frac{\partial^2 S}{\partial \mathcal{U} \partial \mathcal{U}} \right]^{-1}$.
- (iv) Satisfaction of the dissipation inequality $-\sum_{\alpha=1}^{n_M} \mathcal{V}^T \mathcal{R}_\alpha \geq 0$, where $\mathcal{V} = \frac{\partial S}{\partial \mathcal{U}}$ denotes the conjugate entropy variables, guaranteeing non-negative entropy production during relaxation.

Condition (i) will be addressed by introducing a polyconvex viscoelastic model with evolution equations for internal variables. Building on this, the generalised convex entropy function will then be constructed by combining the polyconvex strain energy density with the kinetic energy, thereby obtaining its conjugate variables and Hessian components (as required by condition (ii)). This structure will then enable the symmetrisation of the hyperbolic system to obtain its dual formulation in terms of entropy conjugate variables (as required by condition (iii)). Finally, we will demonstrate that the source term associated with relaxation effects satisfies the dissipation inequality, as required by condition (iv). Examples of large strain viscoelastic solids will be presented and compared in the oral presentation.

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VERIFICATION OF PLASTIC FLOW MODELING IN HYDRODYNAMIC CODES

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ABSTRACT

We present new exact solutions for performing verification tests on plastic flow modeling for solids in hydrodynamic codes. New exact solutions are derived for the elastic-plastic piston problem incorporating linear and power-law hardening models, whereas previously the problem had only been derived for the case of no hardening [1]. The elastic-plastic piston problem involves an impact on a one-dimensional solid body, producing an elastic precursor wave followed by a slower plastic wave. In the case of linear hardening, we not only derive an exact solution from the general solid dynamics of the problem but also identify a unique additional solution that originates from the particular numerical method implementation of the rate-insensitive plastic flow rule, demonstrating that a different method is needed to produce the proper exact solution. We perform verification tests on multiple plastic flow methods in a Lagrangian hydrodynamic method for the linear hardening solution and show that different methods can converge to different solutions. For the case of power-law hardening only the general exact solution is derived, but verification tests are performed on both Lagrangian and Eulerian hydrodynamic methods and while both methods converge to the proper solution, we show differences that exist in both accuracy and convergence.

INTRODUCTION

Verification is an important tool for ensuring that a hydrodynamic simulation code is both performing correctly in its mathematics of numerical methods and behaving properly in its programming. Such investigation can be achieved via a variety of ways, but the ideal case remains the comparison of simulation results to a known exact solution for a particular problem that exercises as many functions of the hydrodynamic code as possible. There are a large number of problems with exact solutions that feature ideal gases such as Noh, Sod, Sedov, Osher-Shu, and Taylor-Green vortex, just to name a few. There are notably fewer problems that feature solids with plasticity, with the list possibly being as short as Hunter, Bleich-Nelson, Verney and the elastic-plastic piston. All of these problems deal with perfect plasticity, where yield stress is constant for all times and states. As this work will show, adding hardening, which is the increase in yield stress with deformation, is critical to being able to adequately testing the plastic flow behavior of the kinds of models used in these sorts of problems. The problem this work will focus on the elastic-plastic piston problem, which has been derived previously for hypoelastic-perfectly plastic [1] and for hyperelastic-perfectly plastic [2]. This is a one-dimensional problem (1D) in which a piston of constant velocity is impacting one end of a solid material, propagating into that material an elastic precursor wave and a slower plastic wave. We take the derived solution for hypoelasticity and

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expand it to include either linear or power-law hardening. These new solutions are used to perform verification studies with both a Lagrangian staggered-grid hydrodynamic (SGH) method [3] and an Eulerian split lagrange remap hydrodynamic (SLRH) method [4].

LINEAR HARDENING

The first exact solution derived in this work is for the case of linear hardening, in which the yield stress is evolved by

$$Y(\bar{\epsilon}_p) = Y_0 + k\bar{\epsilon}_p \quad (1)$$

where Y_0 is the initial yield stress, k is the linear hardening coefficient and $\bar{\epsilon}_p$ is the equivalent plastic strain. The key derivation to make is to relate plastic strain, which controls yield and thus the deviatoric stress solution, to other fields related to conservation equations. The limitations to fields imposed by the problem being 1D allows for a relationship to be established between plastic strain and density.

$$\epsilon_p = \frac{2G}{3G+k} \ln \left(\frac{\rho_y}{\rho_f} \right) \quad (2)$$

where G is the shear modulus, ρ_y is the density at initial yield and ρ_f is the final density behind all waves. Combining this equation with the Hugoniot jump condition equations allows for a solution to be found for all fields in the presence of plasticity.

However, when compared to Lagrangian SGH simulations there was a large discrepancy in the results compared to the general derived solution. We determined that the discrepancy was caused by the numerical method used to solve the plastic flow behavior, the Wilkins radial return method, was creating fundamental changes to the constitutive equations that must be accounted for in order to find the appropriate solution. In particular, it was that the Wilkins radial return method was being executed in a single step (1-Step RR), which changes the effective elastic modulus as shown in Figure 2a. Thus we actually derive two exact solutions for linear hardening, a general one and one specifically for 1-Step RR as shown in Figure 2b. The Lagrangian SGH simulation is then run with both the 1-Step RR and with an iterative radial return method at multiple mesh resolution and the result converge to the new exact solution and the general solution, respectively.

POWER-LAW HARDENING

The second exact solution derived in this work is for the case of power-law hardening, in which the yield stress is evolved by

$$Y(\bar{\epsilon}_p) = Y_0 + k\bar{\epsilon}_p^n \quad (3)$$

where n is the hardening exponent. A consequence of adding this non-linear hardening behavior is that the problem no longer solely consists of an elastic precursor wave and plastic wave. Now there is a non-linear post-yield flow behavior existing between the two waves, complicating the solution derivation. As before, it is still critical to relate plastic strain and density, which for this hardening law takes the form of

$$\frac{2}{3}k[\bar{\epsilon}_p^n(t_2) - \bar{\epsilon}_p^n(t_1)] + 2G[\bar{\epsilon}_p(t_2) - \bar{\epsilon}_p(t_1)] = -\frac{4G}{3} \ln \left(\frac{\rho_1}{\rho_2} \right) \quad (4)$$

Finding the solution for the post-yield flow and plastic wave still requires the use of the Hugoniot jump condition equations. The post-yield flow becomes a semi-analytic solution through the discretization of particle velocity space, while special criteria are required to determine the state at which post-yield flow is instead dominated by the plastic wave. The solution to the power-law hardening model is compared to both the Lagrangian SGH and Eulerian SLRH simulation results at multiple mesh resolutions in Figure 2a. The resulting convergence behavior from the measured L1 and L2 norms are shown in Figure 2b.

ACKNOWLEDGMENT

Special thanks to Miles Buechler for discussion and input. This work was funded by the Advanced Simulation and Computer program. The Los Alamos release number is LA-UR-26-22062.

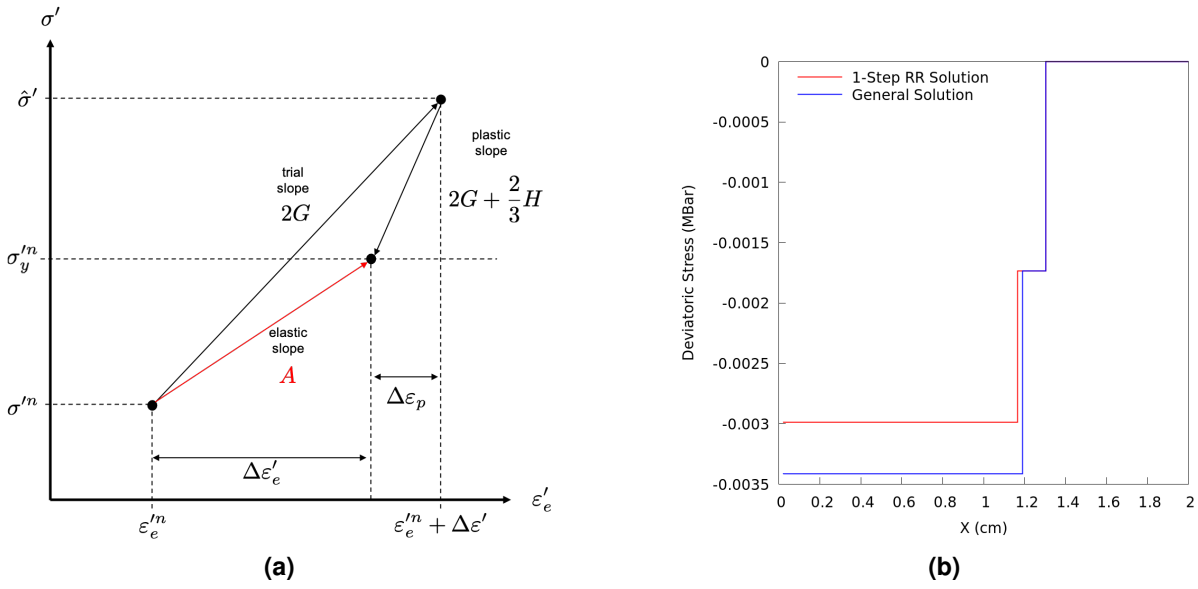


FIGURE 1: The anomalous elastic slope created by the 1-Step RR method is shown in (a). This leads to a new exact solution unique to that method, which is compared to the general solution for linear hardening in (b).

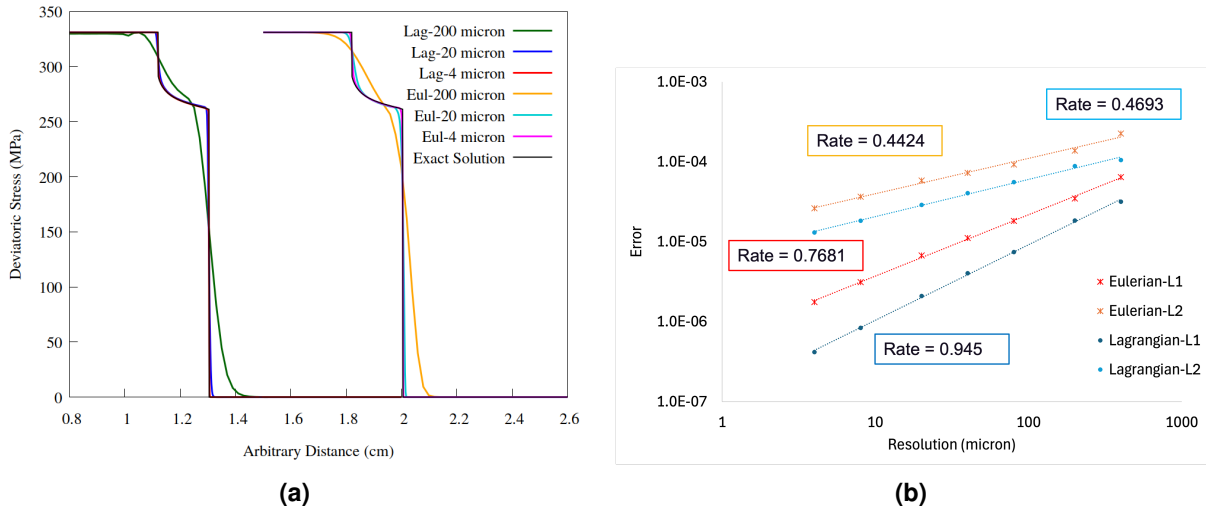


FIGURE 2: Results from the Lagrangian and Eulerian simulations at multiple mesh resolutions are compared to the exact solution for power-law hardening in (a) and the convergence behavior for both methods in (b).

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GENERALIZED CAHN-HILLIARD NAVIER-STOKES SIMULATIONS OF COMPLEX MULTIPHASE FLOWS

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ABSTRACT

In this work, we have developed a generalized set of multi component Cahn-Hilliard Navier-Stokes equations applicable to fluids with arbitrary thermodynamic properties that can undergo compressible flow phenomena, heat transfer, and phase change. The derivation uses general conservation equations for fully compressible multi-component flows and combines Onsager's reciprocal method with the second-law of thermodynamics together with basic thermodynamic relations. Previous formulations can be recovered as limiting cases. The equations are demonstrated for several compressible flow problems, including bubble mergers, bubble collapse, and bubble-shock interaction, relevant to material ejecta.

INTRODUCTION

Flows with immiscible materials occur in many areas, including industrial and natural applications such oil-water separation, ink-jet printing, material ejecta, and so on. In some cases, e.g. in metallurgical applications, the flows are slow and the interfaces do not become excessively corrugated. However, in many other cases, such flows are driven by fluid instabilities (e.g. Richtmyer-Meshkov instability for ejecta) and / or occur in the presence of background turbulence. In this case, the sharp interfaces between immiscible fluids undergo complex morphological changes including mergers, interface breakup and reconnection and phase change, which significantly reduce our abilities to accurately predict such flows. Another challenge pertaining to simulations of multi-component fluid systems is that the fluid properties, such as molar mass and viscosity, change abruptly across the interface making accurate simulations of flows with immiscible materials even more difficult.

Most numerical approaches describing the evolution of sharp interfaces, e.g. front tracking, volume-of-fluid and level-set methods generally use phenomenological models for the interface physics and struggle to maintain mass and momentum conservation. Furthermore, the equations are regularized through the numerical algorithm, which further reduces the accuracy. For example, in the volume-of-fluid method, the piecewise interface reconstruction has limited accuracy and the calculation of interface curvature from the discontinuous volume fraction introduces significant error. On the other hand, diffuse interface approaches, e.g. based on the Cahn-Hilliard (CH) equations, remedy these issues as the conservation laws are naturally satisfied and the interfacial properties arise from first principles, but they introduce their own specific limitations. For example, usual CH-based approaches are derived for the incompressible binary case with Boussinesq and isothermal assumptions. Attempts to generalize the resulting equations to more complex flow or fluid situations are prone

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to failure, as it is difficult to guess the missing terms. Thus, for certain classes of problems, such as the interaction of a shock wave with a gas bubble embedded in a liquid, there are no available CH-type formulations, while sharp interface methods likely also miss important physics and introduce significant numerical errors.

RESULTS

By using basic thermodynamic relations and following Onsager’s reciprocal method, a generalized set of physically consistent Cahn-Hilliard Navier-Stokes equations describing multi component ($N > 2$) compressible flows with arbitrary thermodynamics properties was developed for the first time. Without assuming any "a priori" thermodynamic properties, the derivation starts from the general conservation equations for fully compressible multi-component flows. By using non-local and repulsive components to the Helmholtz free energy as proposed in the original Cahn-Hilliard derivation, and combining Onsager’s reciprocal method with the second-law of thermodynamics together with basic thermodynamic relations, all the transport terms including the Cahn-Hilliard and surface tension terms are directly derived, which leads to the compressible generalized Cahn-Hilliard Navier-Stokes (CGCHNS) equations. The coefficients in the interface free energy expression can, in principle, be derived through expansions of the molecular dynamics (MD) particle pair correlation function. In addition, the Onsager coefficients can be calculated from MD particle trajectories through either a mean square displacement or velocity autocorrelation function, which connects CGCHNS with first principles. For consistency, under certain limiting conditions, e.g. incompressibility and binary mixing, previous results can be recovered. The CGCHNS equations have been implemented into an in-house solver built on ASC’s FleCSI [1] platform that uses different back-ends such as MPI, Legion, or HPX for inter-node communication and KOKKOS for intra-node communication. The spatial differencing is performed with high order central finite differences and time advancement using an adaptive Runge-Kutta-Fehleberg scheme. We demonstrate the equations against several test problems, such as bubble mergers, bubble oscillations, and bubble collapse. Simulations are then performed for the interaction of a shock wave with a gas bubble embedded in a liquid (figure 1). The shock wave can be fully resolved with large enough meshes or a shock capturing scheme [2] can be used. In all cases, mass, momentum and energy are conserved, and mass fractions remain bounded while the interface remains sharp.

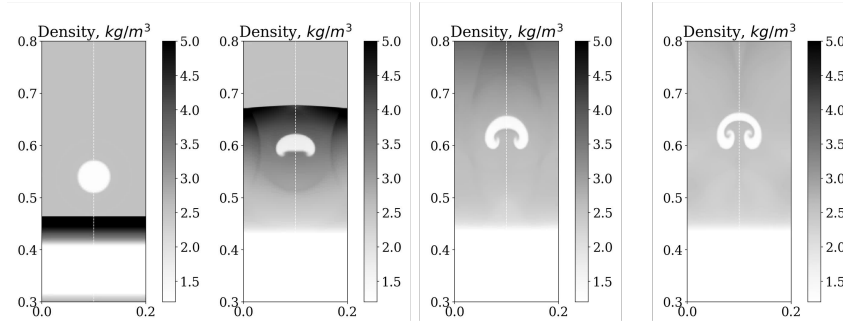


FIGURE 1: The interaction of a Mach 1.5 shock wave with a gas bubble in an ambient liquid at different times.

ACKNOWLEDGMENT

This article has been co-authored by employees of Triad National Security, LLC which operates Los Alamos National Laboratory (LANL) under Contract No.89233218CNA000001 with the U.S. Department of Energy/National Nuclear Security Administration. DL and OC acknowledge funding from ASC’s Mix and Burn Project and LANL’s LDRD program and resources from LANL’s Institutional Computing (IC) program.

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VALIDATING CURVATURE-AWARE HIGH-EXPLOSIVE PROGRAMMED BURN MODELS IN ARC GEOMETRIES

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ABSTRACT

In this work, we validate variations on the FSD programmed burn model compared to established reactive burn models in arc geometries. Experiments performed at Los Alamos National Laboratories' M division of 135° arcs of unconfined and confined high explosives provide a useful case study of high explosive (HE) propagation about a narrow range of curvatures with both HE-air and HE-metal interfaces. The shots were equipped with a variety of diagnostics (Photon Doppler Velocimetry probes, shorting wires, streak camera) making cross validation for high confidence in experimental results possible. The following study seeks to validate these experiments in the adaptive Eulerian finite volume hydrodynamics code xRAGE. Comparison is performed using Arrhenius-Wescott-Stewart-Davis (AWS) reactive burn, Chapman-Jouguet constant velocity programmed burn, and Fast Sweeping Detonation (FSD) programmed burn. The primary motive for this study is to evaluate the accuracy of the curvature-aware FSD programmed burn model, which admits higher timesteps than reactive burn models thereby reducing simulation run time. Additional comparison using the Dynamic Small-Resolved Energy Release (DASHER) velocity-dependent burn rate model will attempt to capture process variable trailing at the detonation burn front.

ARC EXPERIMENTS

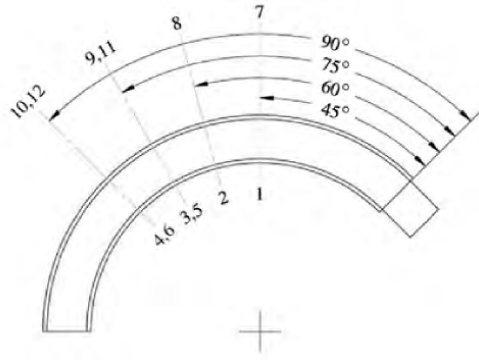
Arc experiments involve a 135° arc of a high explosive (HE) of constant thickness. They may be unconfined [1, 2] or confined by thin copper walls[3], and use insensitive high explosive (IHE)[1, 3] or conventional high explosive (CHE)[2]. The detonation front time-of-arrival (ToA) is measured by Photon Doppler Velocimetry (PDV) probes or shorting wires along the interior and exterior of the arc at fixed angular offsets. All arcs are detonated uniformly on one end of the arc via a wave lens and a small CHE booster charge. The end of the arc opposite the booster has a streak camera to record breakout times as a function of radius from the arc center. See Figure 2 for an example of a confined IHE arc [3].

BURN MODELS

We use the well-validated Arrhenius-Wescott-Stewart-Davis (AWS) reactive burn model as a benchmark for programmed burn models [4]. The Chapman-Jouguet (CJ) constant velocity programmed burn model is used as a point of poor comparison, where the burn velocity is unaffected by the clear curvature inherent in arc geometry. The Fast Sweeping Detonation (FSD) method accounts for HE curvature by downscaling velocity

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(a) PDV probe layout (Figure 2 of [3])



(b) HE arc assembly with copper confining wall, PDV probes (Figure 1 of [3])

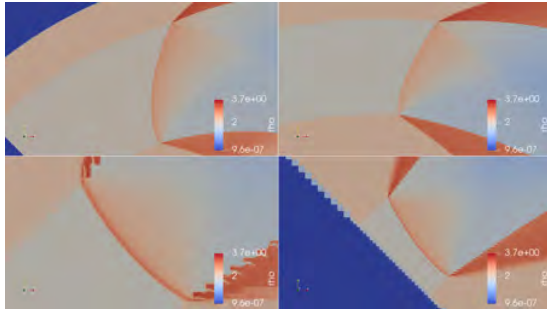
FIGURE 1: Example confined arc experiment from [3]

furthest from the medial axis tree of the 2D HE body [5]. The lower velocity attempts to account for lateral energy losses into the HE-adjacent material for detonation fronts moving parallel to the edge of the HE.

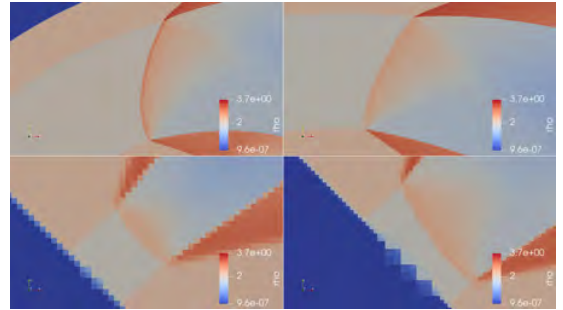
DASHER is a new hybrid burn rate model that can restrict programmed burn progress as a function of detonation velocity in the media, and is a runtime evaluated addendum to programmed burn models [6].

PRELIMINARY RESULTS

The presentation will focus on validation of summary parameters matching between the experimental data, AWSD simulations, and programmed burn simulations. The two datasets to match are interior/exterior angular burn front velocities in steady state and the breakout front shapes. Shown below are Paraview captures showing AWSD and FSD frontshapes for experiments [1, 2] run in Los Alamos National Laboratories' adaptive Eulerian hydrodynamics code xRAGE [7].



(a) Arrhenius-Wescott-Stewart-Davis



(b) Fast Sweeping Detonation

FIGURE 2: Simulated density ρ [g/cm^3] in arcs at steady state. Clockwise from top left: IHE $65mm \times 90mm$ [1], CHE $100mm \times 120mm$ [2], CHE $65mm \times 70mm$ [2], CHE $65mm \times 67mm$ [2].

ACKNOWLEDGMENT

Thanks to Josh McConnell for the extensive introduction to FSD, the LANL EAP xRAGE team, the LANL CMF team, and the experimentalists in M and J divisions for making this all possible.

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A FULLY CONSERVATIVE SIX-EQUATION MODEL WITH SHARP INTERFACE CAPTURING FOR STIFF COMPRESSIBLE MULTIMATERIAL DYNAMICS

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ABSTRACT

We develop a numerical method for the simulation of immiscible compressible multi-material flows within an Eulerian interface-capturing framework. Such flows are characterized by strong discontinuities and complex interface dynamics, whose accurate numerical treatment remains particularly challenging. In conservative finite volume formulations, spurious pressure oscillations are known to arise at material interfaces [1], while non-conservative approaches may lead to incorrect weak solutions.

To address these issues, we derive a novel fully conservative six-equation model based on an extension of the five-equation model of Allaire et al. [2], under the assumption of pressure equilibrium and closed by a stiffened-gas equation of state. The key ingredient of the proposed formulation is the introduction of an additional conservative variable, which enables the construction of a strictly conservative system. A theoretical analysis demonstrates that a consistent numerical treatment of the governing equations prevents the occurrence of spurious pressure oscillations at material interfaces, a property further confirmed by numerical experiments [3].

Particular attention is devoted to the design of a high-order and robust interface-capturing strategy compatible with the fully conservative formulation. The model is discretized using a second-order accurate finite volume scheme in both space and time. A multidimensional MUSCL reconstruction is employed in combination with the MLP-UB limiter [4], ensuring sharp interface resolution while preserving stability, boundedness, and multidimensional consistency. In this context, the consistency of the numerical treatment plays a central role, as the coupling between interface sharpening and conservative transport introduces additional constraints that must be carefully enforced. To ensure robustness, we identify and enforce a set of key properties, including stability conditions on slope reconstruction, consistency between the total energy equation and volume fraction transport, and a dedicated pressure reconstruction procedure ensuring the positivity of thermodynamic variables.

The proposed method is assessed on a series of classical benchmark problems involving compressible multi-material flows. Numerical results demonstrate second-order accuracy on smooth solutions and the ability to sharply capture complex interface dynamics in multidimensional configurations, even in the presence of strong discontinuities and large deformations, while remaining free of spurious pressure oscillations.

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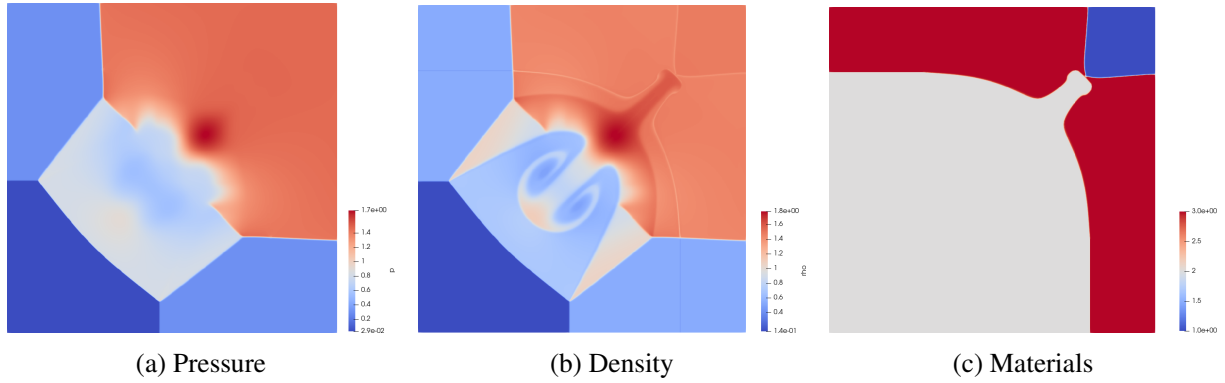


FIGURE 1: Multimaterial 2D-Riemann problem computed on an 800×800 mesh.

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ON NODAL FLUX APPROXIMATIONS FOR MULTIDIMENSIONAL CELL CENTERED LAGRANGIAN HYDRODYNAMICS

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ABSTRACT

The Lagrangian kinematic representation is particularly well suited not only for tracking shock and compression waves, but also for exactly capturing interfaces between distinct materials and for accurately following moving computational domains undergoing large deformations. Among the available numerical approaches [2, 5], the cell-centered Finite Volume discretization of the Lagrangian gas dynamics equations relies on a direct discretization of the conservation laws for volume, momentum, and total energy on a mesh moving with the fluid velocity.

Within this framework, two key ingredients are required. First, a consistent numerical approximation of the interfacial fluxes must be defined in order to update the cell-centered states. Second, an approximation of the nodal velocity must be constructed so as to move the mesh in a manner compatible with the discrete evolution of the volume equation. In addition, the numerical fluxes are designed to satisfy a semi-discrete entropy inequality, thus ensuring the physically consistent conversion of kinetic energy into internal energy in accordance with the second law of thermodynamics. The construction of a robust Lagrangian gas dynamics discretization therefore relies on **genuinely multidimensional** approximations of both the fluxes and the nodal velocity; see [3, 5] for representative examples.

In the present work, we revisit the cell-centered Finite Volume discretization of Lagrangian gas dynamics by exploiting the subface-based Finite Volume formalism introduced in [4] for the Eulerian gas dynamics equations. This approach leads to a novel positivity-preserving and entropy-stable cell-centered Finite Volume discretization for multidimensional Lagrangian gas dynamics, based on a partition of each cell face into subfaces impinging at the nodes [4].

The subface flux approximation is derived from an approximate Riemann solver that incorporates not only the mean values of the cells adjacent to the subface, but also the velocity of the node from which the subface emanates. The projection of the nodal velocity onto the unit normal vector to the subface may be interpreted as a parameter of this Riemann solver. As a consequence, the resulting subface flux is not uniquely defined, which leads to a loss of conservation in the classical sense. Conservation is recovered by imposing that the sum of the subface fluxes around each node vanishes, which determines the nodal velocity through a **nodal solver**. The resulting scheme may thus be interpreted as a **multipoint flux approximation**, thereby providing a formal reinterpretation of the original cell-centered Finite Volume formulation introduced more than twenty years ago [5]. Furthermore, this multipoint flux approximation provides a theoretical framework for establishing the

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positivity and entropy stability of the proposed discretization through a domain-preserving property. This is obtained in two steps. First, given initial states belonging to the domain of definition of the Lagrangian gas dynamics equations, the corresponding approximate Riemann solver also belongs to this domain, provided that the Lagrangian wave speeds of the solver satisfy suitable constraints. Second, the updated cell mean value given by the discrete Finite Volume scheme can be written as a convex combination of the initial and intermediate states attached to each node of the cell under consideration, provided that the time step satisfies a CFL-like condition expressed in terms of the constrained Lagrangian wave speeds. Therefore, the Finite Volume scheme is domain-preserving under an explicit time-step condition.

Moreover, it is worth noting that this node-based conservation condition can be reformulated as a sum of numerical fluctuations, thereby revealing a natural connection with the consistency condition used in the Residual Distribution framework [1].

In a second part, we consider an alternative cell-centered Finite Volume discretization in which the numerical fluxes are uniquely defined at the nodes [6]. By construction, this formulation is conservative. Exploiting its fluctuation form, we derive a node-based condition linking the nodal fluxes [4, 1] in such a way as to satisfy a discrete entropy inequality. We then propose a genuinely multidimensional closure for the nodal fluxes that enforces this entropy condition. These nodal fluxes consist of a centered contribution, interpretable as a node-based average of the physical flux, augmented by a discrete divergence/gradient-type operator. The resulting multidimensional discretization is similar to the formulation obtained by a different route in [7].

Finally, we compare the structure and properties of the above-mentioned discretizations and assess their robustness and accuracy on several representative multidimensional test cases, such as the von Neumann-Taylor-Sedov problem; see Figure 1.

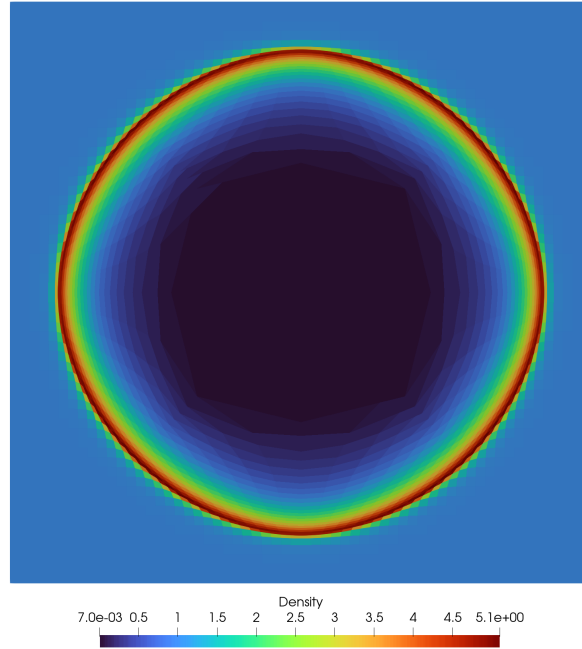


FIGURE 1: Sedov test case: density map at stopping time.

ACKNOWLEDGMENT

This work has been undertaken under the auspice of LRC ANABASE, which is a joined research laboratory between Institut de Mathématiques de Bordeaux and CEA-CESTA devoted to the development of innovative numerical methods for the simulation of complex fluid flows.

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EXACT COMPUTATION OF MOMENTS OF THE CUBOID–ELLIPSOID INTERSECTION WITH APPLICATIONS TO MOF INITIALIZATION

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ABSTRACT

This paper introduces a novel analytical method for computing the moments of the intersection between an ellipsoid and a cube. This approach is then applied to the exact initialization in the Moment-Of-Fluid (MOF) method of an ellipsoid in a cartesian mesh. Numerical results demonstrate that the proposed method is significantly faster (by several orders of magnitude) than numerical integration techniques while achieving higher accuracy (machine precision).

1 INTRODUCTION

Accurate simulation of the evolution of interfaces separating different media is a crucial challenge in many applications (multiphase flows, fluid–structure interaction, etc.). The MOF (Moment-Of-Fluid) method, introduced in [2], is an extension of the classical VOF (Volume-Of-Fluid) method. In addition to volume fractions, MOF uses the centroids of each material, allowing the interface to be reconstructed using only cell information, which is an advantage for parallelization. Moreover, this method provides a simple way to represent $n \geq 2$ materials within a single cell and enables the treatment of filaments [3]. However, these improvements come at the cost of solving a minimization problem involving computationally expensive geometric operations related to the flood algorithm [4]. This reconstruction problem has been improved through an analytical evaluation of the objective function in the case of cubic cells [5] and later extended to tetrahedral cells [6].

This reconstruction step is performed at each time step, after the so-called advection step, which consists in advecting the geometry and then intersecting it with the underlying mesh. This step can be carried out using a Lagrangian remapping method [1]. Before performing the first reconstruction, an initialization step is required, consisting in computing the volume fraction and centroid of the intersection between the initial material and each cell. This computation typically relies on numerical integration methods, which are costly and not precise.

2 IDEA OF THE METHOD AND NUMERICAL RESULTS

In the specific case of initializing an ellipsoid on a Cartesian mesh, we propose a new formula based on the analytical integral computation of indicatrix functions, allowing the moments of the intersection to be computed exactly. The computational times for initializing an ellipsoid on a 50^3 Cartesian mesh using our analytical method and a numerical integration method with a uniform sampling of N points per direction (ppd) are reported in Table 1. Our method achieves machine precision and is significantly faster (by several orders

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of magnitude). Increasing the number of points in the numerical method drastically increases computational cost without significantly reducing the error. The reconstruction associated with this test case on the 50^3 mesh with our analytical method and using 10 points per direction for the numerical one, is shown in Figure 1. The reconstruction is clearly improved with the analytical method, as volumes and centroids are computed exactly. Finally, Table 2 presents the computational times of the analytical method on finer meshes. All cases achieve machine precision, and notably, initializing an ellipsoid on a 200^3 mesh takes only about one second!

Method	Runtime	Error
Analytic	0.026s	$5.0 \cdot 10^{-14}$
Numerical 10 ppd	4.4s	$4.8 \cdot 10^{-5}$
Numerical 20 ppd	28.6s	$1.0 \cdot 10^{-5}$
Numerical 40 ppd	218.0s	$4.5 \cdot 10^{-5}$
Numerical 60 ppd	700.0s	$3.8 \cdot 10^{-5}$

TABLE 1: Runtime and error with analytic and numerical integration with uniform sampling for the initialization of an ellipsoid in the cartesian mesh 50^3 .

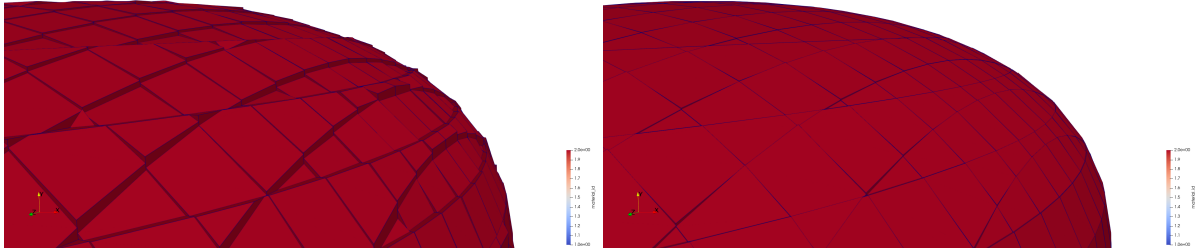


FIGURE 1: Reconstruction of an ellipsoid in the Cartesian mesh $= 50^3$. Numerical method with 10 ppd (left), analytic method (right)

Mesh	Runtime
50^3	0.026s
100^3	0.14s
200^3	1.04s

TABLE 2: Runtime of the analytic method on different meshes.

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CUT-CELL DISCONTINUOUS GALERKIN FOR SHOCK AND CONTACT-DISCONTINUITY FITTING

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ABSTRACT

In this work we develop a space-time cut-cell method for shock and contact-discontinuity fitting with Discontinuous Galerkin methods and ADER time integration.

INTRODUCTION

In compressible multimaterial fluid flows, competing strategies have been adopted to handle discontinuities arising from shock formation or fluid state discontinuities. Successful results have been obtained by high-order Finite Volume methods or Discontinuous Galerkin methods on fixed Eulerian grids with slope-limiting or artificial viscosity, with the inherent drawback of smearing out some physical acoustic waves or requiring adequate fixes in case of stiff materials or large density jumps [1]. Lagrangian methods have been largely used in order to circumvent these issues, with the additional difficulties of large mesh deformation and handling of sliding lines [2, 3]. In this work, we propose the alternative use of a combination of shock-fitting methods [4] with Discontinuous Galerkin cut-cell methods [5]. However, contrary to usual cut-cell methods which focus on space discretization on cut-cells followed by time-integration, we show that space-time geometric integration on cut-cells is able to recover Galilean invariance, while being conveniently combined with an ADER time-integration method for Discontinuous Galerkin.

GENERAL FRAMEWORK

Consider the hyperbolic conservation law as a space-time divergence problem [6]:

$$\partial_t U + \nabla_x \cdot F(U) = \nabla_{(t,x)}(U, F(U)) = 0.$$

If the computational domain is composed of cells Ω , which can be cut by a moving interface Γ_t , we consider the fluid state in the cut-cell Ω_t . The boundary of Ω_t is composed of two parts: the cut faces F_t with fluid neighbours on the same side of the boundary, and the interface Γ_t in cell Ω (see Figure 1). Applying a similar approach to ALE methods on DG schemes [7],

$$\underbrace{\int_{\Omega_t^{n+1}} U^{n+1} \varphi - \int_{\Omega_t^n} U^n \varphi}_{\text{Dynamic term}} + \underbrace{\int_{t^n}^{t^{n+1}} \int_{F_t} F(U) \cdot n \varphi dx dt}_{\text{Fluid numerical fluxes}} + \underbrace{\int_{t^n}^{t^{n+1}} \int_{\Gamma_t} (F(U^*) - U^* V_t) \cdot n \varphi dx dt}_{\text{Interface flux}} - \underbrace{\int_{t^n}^{t^{n+1}} \int_{\Omega_t} F(U) \cdot \nabla \varphi dx dt}_{\text{DG local term}} = 0, \quad (1)$$

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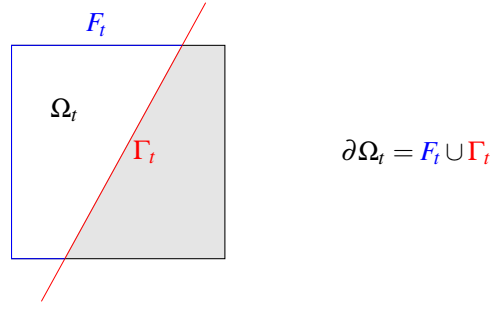


FIGURE 1: Cut-cell and interface

where V_t is the velocity of interface Γ_t . Notice here that the space-time geometric cut-cell approach lies in exact computation of the space-time cut-cell quadratures, while the fluxes $F(U)$ and $F(U^*) - U^*V_t$ can be approximated with an explicit ADER procedure. In the case of an interface Γ_t separating two fluids U_L and U_R , conservation implies equality of fluxes, which translates into a normal Rankine-Hugoniot relation:

$$V_t \cdot n_\Gamma (U_R^* - U_L^*) = (F(U_R^*) - F(U_L^*)) \cdot n_\Gamma.$$

Similarly to [4], it is possible to follow one or several of the waves by solving the local 1D normal multimaterial Riemann problem with U_L and U_R , and setting V_t as the wave velocity.

We will focus in the presentation on some technical aspects of the approach, in particular the high-order quadratures on cut-cells, the stabilization procedure of small cut-cells and the ability to combine the cut-cell approach with a Shifted Boundary method [8].

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FROM MULTI-PHASE TO MULTI-ARCHITECTURE: A PERFORMANCE-PORTABLE PATH TO EXASCALE CFD

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ABSTRACT

This talk presents **PHANTOMS** (**P**ortable **H**p-**A**daptive **N**umerics **T**owards **M**ultiphase **S**imulation), a high-performance framework designed to bridge the gap between advanced multi-phase numerics and next-generation heterogeneous HPC architectures. As the accelerated successor to the multi-phase framework **FLEXI**, **PHANTOMS** addresses the dramatic shift toward GPU-accelerated systems by utilizing the hardware-agnostic portability library Kokkos to decouple numerical algorithms from specific hardware backends. The approach refactors the established hp-adaptive hybrid DG/FV discretization to enable concurrent execution on accelerators, while supporting hybrid OpenMP/MPI parallelization for multi-node systems. The novel code builds on a dynamic memory management to allow for adaptive refinement and narrow band-masking, providing an efficient basis for exascale-ready sharp-interface simulations.

INTRODUCTION

Compressible multi-phase and multi-component flows are central to aerospace and automotive applications, with phenomena ranging from the vaporization and mixing of e-fuels in next-generation aerospace engines to the high-speed injection and turbulent mixing of underexpanded hydrogen jets in H_2 -ready internal combustion engines. Simulating such flows remains highly challenging due to the strongly nonlinear interaction of shock waves, turbulence, material interfaces and interfacial thermodynamics, all of which span a wide range of spatial and temporal scales. To address these challenges, the high-order framework **FLEXI** combined a sharp-interface approach with an interface Riemann solver, enabling the consistent coupling of micro-scale thermodynamics with the compressible continuum bulk flow. The framework exploits the exponential convergence of a p-adaptive Discontinuous Galerkin Spectral Element Method (DGSEM), while ensuring robustness through h-refined Finite-Volume (FV) shock capturing on a sub-grid level. The approach was demonstrated to accurately and efficiently simulate complex droplet dynamics with phase transition (Fig. 1a) [1, 3] as well as supersonic, turbulent multi-component flows (Fig. 1b) [2].

With modern HPC architectures undergoing a dramatic shift towards heterogeneous CPU/GPU systems, the remaining building block for large scale multi-phase simulations - efficient and scalable implementation for current HPC systems - poses significant challenges for existing CFD codes. With the novel code framework **PHANTOMS**, this talk addresses this *missing link* with three core implementation strategies to adapt to heterogeneous HPC architectures:

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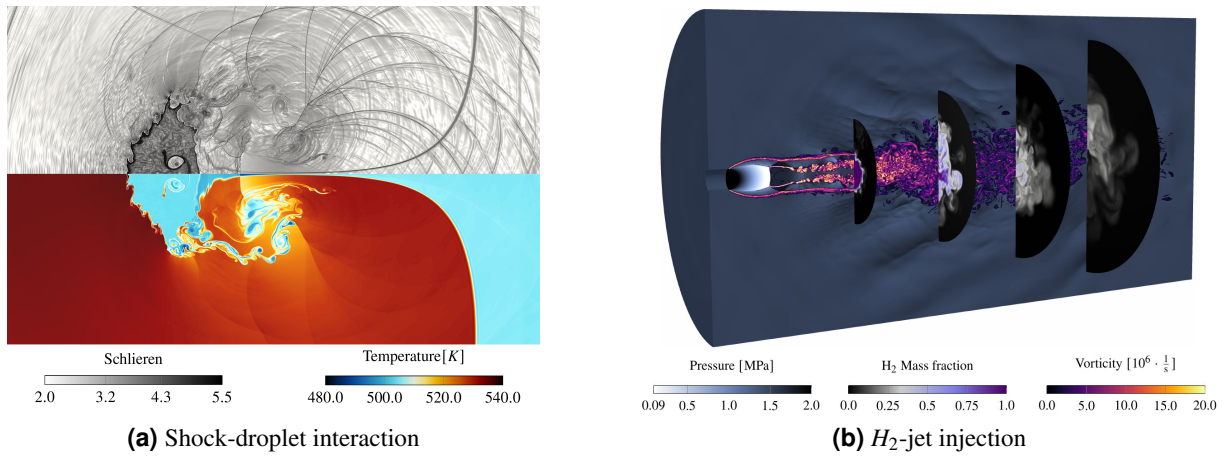


FIGURE 1: Demonstration of the hp-adaptive hybrid DG/FV framework applied to (a) a multi-phase flow with phase transition and (b) a compressible turbulent multi-component flow.

- **Performance Portability:** PHANTOMS utilizes the **Kokkos** library to decouple numerical kernels from specific hardware backends. By abstracting memory management and execution spaces, the framework achieves *write-once, run-anywhere* capability across NVIDIA, AMD, and Intel GPUs, as well as multi-core CPUs, ensuring long-term viability on evolving heterogeneous clusters.
- **Multi-Layered Parallelization:** The hybrid DG/FV algorithms have been refactored to support a sophisticated multi-layered parallelization strategy. PHANTOMS uses **MPI** for inter-node communication while orchestrating intra-node workloads by offloading the simulation loop to accelerators and utilizing **OpenMP** for CPU-based execution of pre- and postprocessing. This allows the framework to exploit the full hardware spectrum on heterogeneous CPU/GPU nodes.
- **Dynamic Resource Management:** On modern heterogeneous systems, memory bandwidth and capacity often become the primary bottleneck. PHANTOMS introduces a novel dynamic memory management system specifically for hp-adaptive refinement and narrow-band interface capturing. By dynamically allocating resources only where needed, the framework drastically reduces the memory footprint and computational overhead for complex phenomena like droplet grouping.

The efficiency of the novel framework PHANTOMS is evaluated through a series of scaling tests and high-fidelity benchmarks for compressible turbulent flows. The results confirm the effectiveness of the multi-layered parallelization strategy on GPU-accelerated clusters and demonstrate the framework's applicability to complex flow phenomena and current HPC hardware.

ACKNOWLEDGMENT

We gratefully acknowledge the support of the German Research Foundation (DFG) for this talk through the project *Droplet Interaction Technologies*, grant GRK 2160/1 and GRK 2160/2, through the grant BE6100/4-1 and the Simtech PN1-11 "*Data Driven Simulation Methods of Multiphase Flow Systems*".

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HYPERELASTIC POWER LAWS

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ABSTRACT

This research presents a new class of hyperelastic laws in the context of large deformations. These laws are mathematically well-posed, regardless of the deformation. They are power laws that satisfy the hyperbolicity criterion. Hyperbolicity, also known as rank-one convexity, is a weaker condition than polyconvexity. Consequently, we have more hyperelastic laws that satisfy the hyperbolicity criterion. These laws can be combined to fit the energy curves of real materials. The Neo-Hookean model, the Yeoh model, and the famous Aruda-Boyce model are derived.

INTRODUCTION

In the article [1], S. Ndanou et al. proposed a new hyperbolicity criterion for the hyperelasticity system of equations, where they considered that the density is a separated variable, free from the elastic variables. We proposed a hyperelastic law W that depends on $J_2 = \mathbf{G} : \mathbf{G}$, where $\mathbf{G} = \mathbf{B}^{-1}$, with $\mathbf{B}$ being the left Cauchy stress tensor. We have shown that this law satisfies the proposed theorem. More importantly, we have shown that this law does not satisfy the polyconvexity criterion of Dacorogna et al. in 3D: [2]. The polyconvexity criterion (global) is a significantly more restrictive condition than the rank-one convexity (local) criterion. Therefore, the objective was to ascertain the hyperelastic law that would render the system of hyperelasticity equations hyperbolic without satisfying the polyconvexity criterion. The new hyperelastic law has the form:

$$\begin{aligned}
 AN_{pqnmos} = & \sum_{k=1}^n \sum_{h=1}^m C_{kh} \left((j_1^2)^k (j_2)^h - (3)^{3kh} \right) \\
 & + \sum_{i=1}^p G_i \left((j_1^2)^i - 9^i \right) + \sum_{j=1}^q H_j \left(j_2^j - 3^j \right) \\
 & + \sum_{i=1}^o Z_i \left[\left(\frac{(j_1^2 - j_2)}{2} \right)^i - 3^i \right] + \sum_{j=1}^s R_j \left(J_1^{jr} - 3^{jr} \right),
 \end{aligned} \tag{1}$$

where r is a rational number, $j_1 = tr(\bar{\mathbf{G}})$ and $j_2 = \bar{\mathbf{G}} : \bar{\mathbf{G}} = tr(\bar{\mathbf{G}}^2)$, $\bar{\mathbf{G}} = \frac{\mathbf{G}}{(\mathbf{G})^{\frac{1}{3}}}$, $\mathbf{G} = \mathbf{B}^{-1}$, where $\mathbf{B}$ is the left Cauchy stress tensor and C_{kh} , G_i , H_j , Z_i , R_j are constants depending on material parameters.

Another proof of the rank-one convexity of W is done. We have achieved an ingenious decomposition of the eigenvalue matrix of the system associated with this energy W into a sum of matrices that are more readily analyzable. These matrices are non-negative and positive definite. This decomposition allowed us to circumvent, in a way, the theorem we established earlier (2014), which is remarkable.

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ACKNOWLEDGMENT

This work was done in homage to the late Professor Philippe Angot, who did remarkable work in teaching hyperbolic PDEs, the group to which belongs the hyperelasticity equations on which this work is based.

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A WELL POSED AND STABLE CANONICAL EVAPORATION MODEL PROBLEM FOR PHASE-CHANGE IN TWO-PHASE FLOWS

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ABSTRACT

We formulate an energy bounded interface formulation for canonical one-dimensional nonlinear evaporation two-phase model problems (the Stefan and/or sucking problem). We focus on the interface between the vapor and the liquid and derive interface conditions leading to well-posedness and energy stability.

INTRODUCTION

We prove energy stability of two important model problems for incompressible two-phase liquid-gas flows. In particular, we consider the evaporation interface between the two phases for the so called Stefan and sucking problems [1]. These stiff model problems are commonly used to validate production codes. Our ambition is to provide a correct mathematical-numerical formulation of the given physical models leading to energy stability.

THE GOVERNING INITIAL BOUNDARY VALUE PROBLEM

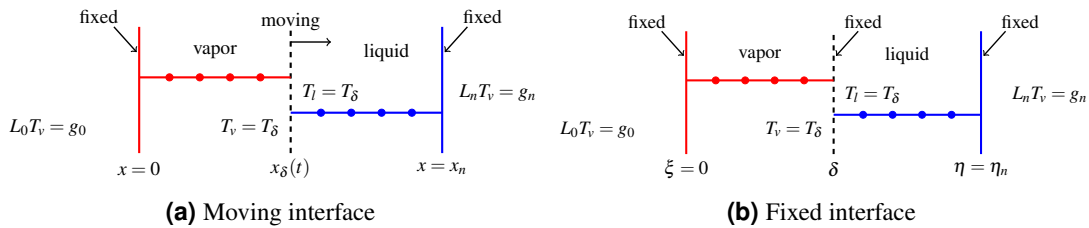


FIGURE 1: Transformation from (x, t) with a moving interface to (ξ, τ) and (η, τ) with a fixed interface.

We consider the temperature distribution close to a moving evaporation interface between an incompressible viscous vapor and liquid in space one dimension. The governing coupled initial boundary value problems (IBVPs) in $\Omega = [x_0, x_n]$ transformed to a fixed interface geometry with metric coefficients, see Figure 1, are

$$\begin{aligned} \beta_v \left((J_v T_v)_\tau + (a_v T_v)_\xi \right) &= k_v (J_v^{-1} T_{v,\xi})_\xi, \quad \xi \in \Omega_v = [\xi_0, \delta], \\ T_v &= T_\delta, \quad \xi = \delta, \end{aligned} \quad (1a)$$

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$$\beta_l \left((J_l T_l)_\tau + (a_l T_l)_\eta \right) = k_l (J_l^{-1} T_{l,\eta})_\eta, \quad \eta \in \Omega_l = [\delta, \eta_n], \quad (1b)$$

$$T_l = T_\delta, \quad \eta = \delta,$$

where T, ρ, C_p, k denotes temperature, density, specific heat at constant pressure and scaled heat conduction coefficient respectively while $\beta = (\rho C_p)$. The subscripts v, l, δ denotes vapour, liquid and evaporation interface respectively. The problems are connected at the fixed interface $\xi = \eta = \delta$ by the externally given evaporation temperature T_δ . We ignore outer boundary and initial conditions in (1) and focus on the interface. Furthermore, $a_v = u_v + J_v \xi_t = u_v - x_\tau = u_v - \tilde{u}_v, a_l = u_l + J_l \eta_t = u_l - x_\tau = u_l - \tilde{u}_l$ are the transformed wave speeds, J_v and J_l are the Jacobians of the transformation and u_v, u_l are the original wave speeds which satisfy the incompressibility constraint. The mesh velocity at the interface where $\tilde{u}_v = \tilde{u}_l = \tilde{u}_\delta$ is given by the interface gradients

$$\rho_v h_{lv} \tilde{u}_\delta = [k_l J_l^{-1} T_{l,\eta} - k_v J_v^{-1} T_{v,\xi}]_\delta. \quad (2)$$

In the talk: By using the continuous energy method on the IBVP (1) with the mesh velocity definition (2) and a strong and weak imposition of the interface conditions $T_v = T_l = T_\delta$, we *prove energy-boundedness*.

SEMI-DISCRETE ENERGY STABILITY

Following [2], we mimic the continuous analysis numerically by using the SBP-SAT framework. We denote $\mathbf{T}_v$ as the numerical approximation of T_v at all grid points and the vectors $D_\xi \mathbf{T}_v = \mathbf{T}_{v,\xi}$ to be the approximation of $T_{v,\xi}$ where $D_\xi = P_\xi^{-1} Q_\xi$ is the differentiation matrix on SBP form [3]. The so called SBP property is

$$Q_\xi + Q_\xi^T = B_\xi = E_N^\xi - E_0^\xi \quad (3)$$

where $E_0^\xi = \text{diag}(1, 0, \dots, 0)$ and $E_N^\xi = \text{diag}(0, 0, \dots, 1)$. The matrix P_ξ is diagonal, positive definite and defines a quadrature formula $\phi^T P_\xi \psi \approx \int \phi \psi dx$, $\phi^T P_\xi \phi = \|\phi\|_{P_\xi}^2$ where ϕ and ψ are vectors with ϕ_i and ψ_i at node ξ_i .

The semi-discrete version of the continuous IBVPs (1) with weak SAT interface conditions are

$$\begin{aligned} \frac{\beta_v}{2} \left((\mathbf{J}_v \mathbf{T}_v)_\tau + \mathbf{J}_v \mathbf{T}_{v,\tau} + D_\xi A_v \mathbf{T}_v + A_v D_\xi \mathbf{T}_v \right) &= k_v D_\xi (\mathbf{J}_v^{-1} \mathbf{T}_{v,\xi}) \\ &+ P_\xi^{-1} \left(\sigma_v^1 E_N^\xi (\mathbf{T}_v - \mathbf{T}_v^\delta) + \sigma_v^2 (E_N^\xi \mathbf{T}_v - E_0^\eta \mathbf{T}_l) + \sigma_v^3 D_\xi^T E_N^\xi (\mathbf{T}_v - \mathbf{T}_v^\delta) \right), \\ \frac{\beta_l}{2} \left((\mathbf{J}_l \mathbf{T}_l)_\tau + \mathbf{J}_l \mathbf{T}_{l,\tau} + D_\eta A_l \mathbf{T}_l + A_l D_\eta \mathbf{T}_l \right) &= k_l D_\eta (\mathbf{J}_l^{-1} \mathbf{T}_{l,\eta}) \\ &+ P_\eta^{-1} \left(\sigma_l^1 E_0^\eta (\mathbf{T}_l - \mathbf{T}_l^\delta) + \sigma_l^2 (E_0^\eta \mathbf{T}_l - E_N^\xi \mathbf{T}_v) + \sigma_l^3 D_\eta^T E_0^\eta (\mathbf{T}_l - \mathbf{T}_l^\delta) \right). \end{aligned} \quad (4)$$

In (4), $\mathbf{T}_v^\delta$ is equal to $\mathbf{T}_v$ except in the last node which contain T_δ and $\mathbf{T}_l^\delta$ is equal to $\mathbf{T}_l$ except in the first node which contain T_δ . Moreover $\mathbf{J}_v, \mathbf{J}_l$ and A_v, A_l are diagonal matrices approximating J_v, J_l and a_v, a_l , respectively.

In the talk: By using the discrete energy method on the semi-discrete approximation (4) of IBVP (1) we determine the penalty coefficients σ_i^k in the SAT terms and *prove energy stability*.

ACKNOWLEDGMENT

J.N was supported by Vetenskapsrådet, Sweden [award no. 2021-05484 VR] and University of Johannesburg Global Excellence and Stature Initiative Funding.

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A SUITABLE SIX-EQUATION MODEL FOR COMPRESSIBLE MULTI-MATERIAL FLOW USING A HIGH-ORDER FINITE DIFFERENCE METHOD

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ABSTRACT

High-order methods offer computational advantages for resolving physical scales of motion, like those associated with turbulence and mixing [1,2]. A structured computational mesh simplifies high-order discretization schemes but creates complexity in how non-grid aligned features are modeled in the flow, such as at solid or material boundaries. A smoothed interface (SI) method and a six-equation model are used to model the interaction between material interfaces and shock waves for arbitrary equations of state. Spurious interfacial pressure errors are greatly reduced for the given method where equilibration methods generate spurious errors and instabilities. The new model is adapted from Saurel [3] and includes an interface sharpening method from Brill [4] which keeps interfaces sharp. A surface tension model is considered for low Weber number flows. Several numerical test problems are used to quantify the accuracy and errors associated with the model.

INTRODUCTION

This work leverages previously developed six-equation multi-material into a high-order finite difference code in order to solve flows with liquid metal-air interfaces while preserving stability and accuracy. A water-droplet impact problem is retained as a baseline verification case, and a liquid-tin Weber-number comparison is used to show sensitivity to surface tension.

Equations of motion

The governing model follows the pressure-relaxation six-equation formulation highlighted in the presentation, evolving species density, species mass, bulk momentum, and species total energy while retaining separate material states in a shared velocity field. The full model and terms will be defined and described in the presentation.

$$\frac{\partial \rho_i}{\partial t} + \nabla \cdot (\rho_i \mathbf{u}) = \nabla \cdot \mathbf{J}_{\rho_i} + C_{\rho} \quad (1)$$

$$\frac{\partial \rho Y_i}{\partial t} + \nabla \cdot (\rho Y_i \mathbf{u}) = \nabla \cdot \mathbf{J}_i, \quad (2)$$

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u} + p \delta) = \nabla \cdot \boldsymbol{\tau} + \nabla \cdot \mathbf{F}, \quad (3)$$

$$\frac{\partial V_i E_i}{\partial t} + \nabla \cdot (V_i E_i \mathbf{u}) = \nabla \cdot (V_i \boldsymbol{\tau}_i \cdot \mathbf{u}) + C_e \quad (4)$$



RESULTS

Qualitative results for two test problems are shown here. The first is the single droplet-impact test problem used to assess interface behavior and shock structure in air. The second is a molten-tin, multi-droplet splash test problem in air at 0.1 km/s, where finite- and infinite-Weber-number calculations illustrate the qualitative impact of surface tension on splash-back structure.

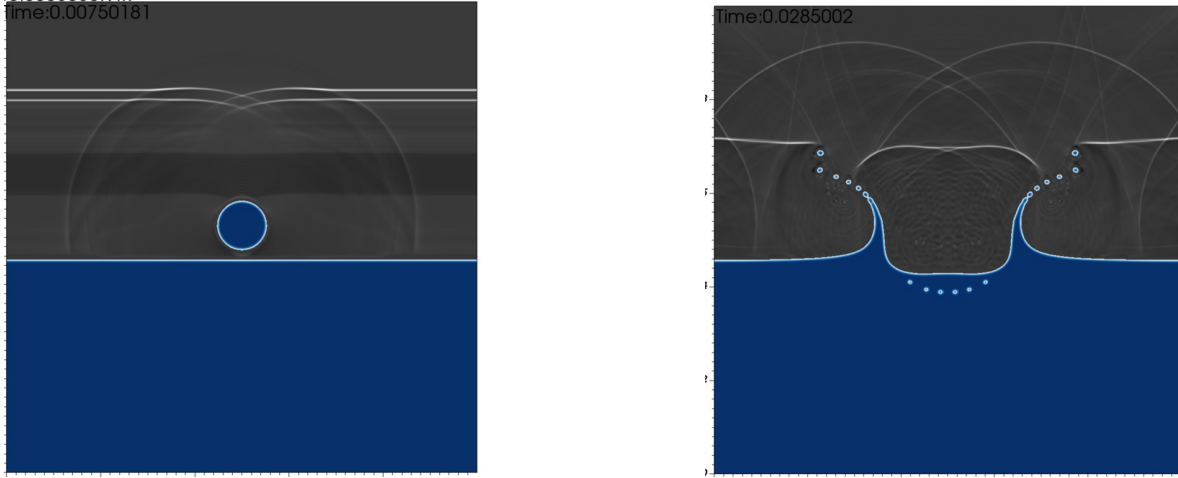


FIGURE 1: Volume fraction of liquid water from a simulation of a droplet impact problem (blue) with numerical schlieren (grayscale) showing the resulting shock wave structure in the air. Left shows initial droplet in motion (Mach= 0.5) just before impact and right shows resulting splash pattern and breakup of the impact.

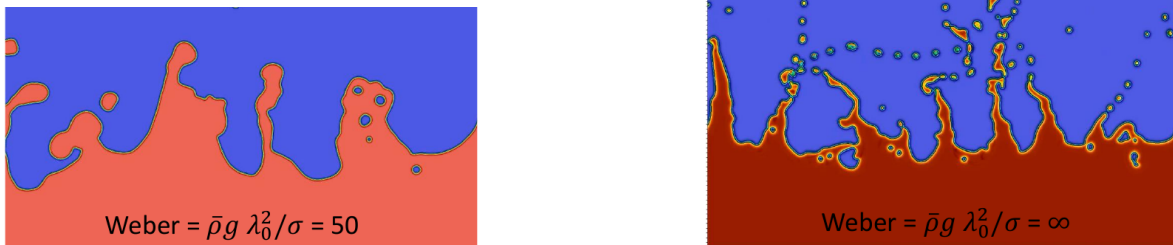


FIGURE 2: Finite Weber number (left) and infinite Weber number (right) droplets impacting a pool of molten tin in air at 0.1 km/s. Weber number effects impact the structure and scale of splash back particles.

CONCLUSION

The current multi-material formulation provides a concrete path toward direct focused-physics calculations of liquid metal-air interfaces.

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Acknowledgements. Lawrence Livermore National Laboratory is operated by Lawrence Livermore National Security, LLC, for the U.S. Department of Energy, National Nuclear Security Administration under Contract DE-AC52-07NA27344.



A TWO-SCALE TWO-PHASE MODEL FOR THE SEPARATED-TO-DISPERSE PHASE TRANSITION BY ATOMIZATION

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ABSTRACT

A novel and unified compressible two-phase model with two scales for the separated-to-disperse transition in atomizing flows is presented [1]. The model accounts for surface tension at both large and small scales and can dynamically transition from a large-scale separated regime to a small-scale disperse regime. The inter-scale mass transfer from the large to the small scale is activated when local kinks in the large-scale interface lead to curvatures that exceed a prescribed threshold. This transfer is local, dissipative and leads to regularization of the large-scale interface and the formation of a spray of droplets. A numerical scheme is proposed and the numerical simulation of a liquid column in a gaseous flow allows to demonstrate the performance and properties of both the model and the numerical scheme.

INTRODUCTION

Two-phase flows of liquid and gaseous phases play an important role in many industrial applications, such as the injection and atomization of a liquid jet in combustion chambers. Several models have been developed for the various regimes (separated phases and disperse phase). For the simulation of atomization processes in industrial applications such models are often coupled numerically, sometimes with mesh-dependent parameters.

In this contribution, we present a two-scale compressible model [1], which provides a unified description of separated-disperse phases, so as to naturally take into account the multi-scale nature of atomization phenomena. The small scale is assumed to be in the disperse regime, made of small liquid inclusions carried in the gaseous phase. An inter-scale mass transfer process from the large scale to the small scale is derived by introducing a length-scale threshold and leads to separation of scales. The mass transfer allows to regularize the large-scale interface consistently with a surface energy balance at both scales. The resulting process is dissipative, in the sense that it satisfies the second law of thermodynamics.

MODELLING APPROACH

The proposed modelling approach follows the one proposed in [3]. However, the model derived in [3] exhibits a thermodynamic mismatch between scales, whereas the present approach allows the model to be thermodynamically consistent across scales [1]. The liquid volume fraction α_{liq} is decomposed into a large-scale contribution α_ℓ and a small-scale one α_d representing droplets. The model is derived using the Stationary

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Action Principle framework presented in [2]. The physical Lagrangian reads

$$\mathcal{L} = \frac{1}{2}\rho|\mathbf{u}|^2 - (m_\ell + m_d)f_{\text{liq}}(\rho_{\text{liq}}) - m_g f_g(\rho_g) - \sigma|\nabla\alpha_\ell| - \sigma\Sigma_d,$$

where $m_b = \alpha_b \rho_b$ ($b = \ell, d$) is the effective mass and where f_b ($b = \text{liq}, g$) is the free energy of each phase. The large-scale surface energy is represented by $\sigma|\nabla\alpha_\ell|$, following the Continuum Surface Stress approach. The sub-scale surface tension is represented using an interfacial area density Σ_d , for which an evolution equation is presented.

The variational principle yields the reversible part of the model. Source terms are then added and include a relaxation towards a modified Laplace law with a curvature threshold. Inter-scale mass transfer source terms are derived to remove large-scale interface kinks which exceed the curvature threshold and generate sub-scale droplets. The resulting process is based on a surface energy balance and is compatible with the second law of thermodynamics. Extension of the model to include thermal non-equilibrium between the phases is also discussed.

NUMERICAL PROOF OF CONCEPT

The proposed numerical approach is based on a finite volume discretization combined with the method of lines. Time integration relies on an operator-splitting strategy, whereby the system is decomposed into three subsystems: a first-order hyperbolic subsystem accounting for convective and acoustic fluxes; a subsystem describing large-scale capillary effects; and a subsystem governing relaxation and inter-scale mass transfer. For the hyperbolic subsystem, the HLLC scheme is used, while for the large-scale capillary subsystem a centered discretization is used. Finally, for the source terms, instantaneous relaxation is considered and the numerical method is based on a dual-time stepping approach enabling the design of a bound-preserving method.

A proof-of-concept test case is presented to illustrate the properties and advantages of the model. In a two-dimensional configuration, a liquid column is deformed by an incident gas flow, leading to the formation of filaments on both sides of the interface. As shown in Figure 1, in the absence of inter-scale mass transfer, the interface continues to stretch and develop increasingly fine structures. Eventually, the interface is no longer closed. In contrast, with the two-scale approach, when the mass transfer mechanism is active, the interface remains well localized and closed, and small-scale droplets are generated (see again Figure 1).

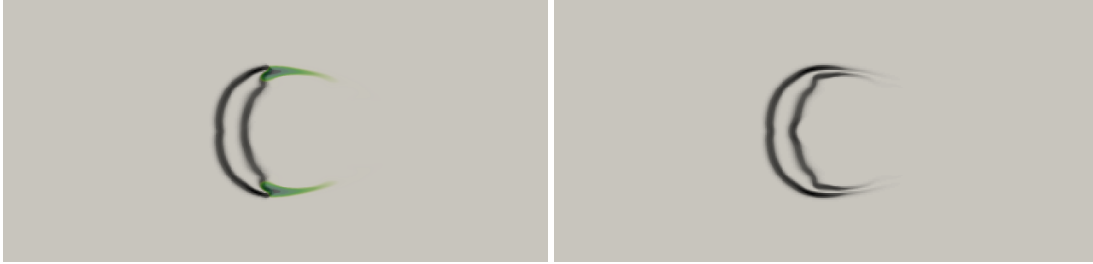


FIGURE 1: Large-scale interface represented by $|\nabla\alpha_\ell|$ (grey scale colormap) and small-scale volume fraction α_d (semitransparent green colormap) for the two-scale model (left) and without two-scale approach (right).

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A NEW APPROACH TO CONSTRUCTING AREA-WEIGHTED AXISYMMETRIC DISCRETIZATIONS FOR SMOOTHED PARTICLE HYDRODYNAMICS

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Axisymmetric (or rz) discretizations are useful for modeling rotationally symmetric problems at a substantial computational savings compared with fully three-dimensional calculations. Examples of problems where this is useful span many disciplines: astrophysics (modeling stars, supernova, planetary bodies, etc); impacts on spherical bodies; inertial confinement fusion capsule modeling; bubble rising models; etc. The challenge of developing such discretizations in any numerical method is that the coordinate system is singular as one approaches the $r = 0$ (or z) axis: the typical error one sees in axisymmetric hydrodynamical models is a deviation from the expected symmetry as this line is approached. Depending on their severity, such errors can render axisymmetric models useless for many problems where the most interesting evolution is occurring near this axis of symmetry (such as crater modeling where the impactor travels along the $r = 0$ line). For mesh based hydrodynamics methods several successful rz discretizations have been developed [14, 2, 1, 4], mostly based on so called area-weighting discretizations (though [4] uses an alternative finite-element approach). Similarly for SPH there have been several studies devoted to developing an axisymmetric smoothed particle hydrodynamics (SPH) discretization, some based on variations on area-weighting ideas [3, 7, 6, 5, 13, 8], while others have used different methods of starting with the 3D SPH equations in (r, z, θ) space and integrating out the θ contributions [11, 9, 12].

In this work we examine a new variation on the use of area-weighting ideas in the SPH framework. Fundamentally area-weighting is the idea of doing the numerics of the discretization in the (r, z) plane as much as possible; i.e. treating the numerics similarly to the 2D (x, y) discretization which does not have the singularity of the axisymmetric coordinate system and attendant numerical difficulties. The advantage of such methods is they are more stable as we approach the $r = 0$ axis and therefore maintain the expected symmetries (such as allowing spherical flows to remain spherically symmetric). However, this stability comes at the expense of rigorous conservation of the hydrodynamic invariants: because area-weighting does not maintain the standard symmetries usually enforced in the momentum equation rigorous conservation of linear momentum is lost. Nonetheless most of the successful mesh-based (r, z) discretizations referenced above are based on area-weighting for the sake of maintaining stability and the expected symmetries in problems such as spherical inflow or outflow.

In our new methodology we are able to treat more of the SPH differencing in a Lagrangian manner in the 2D (r, z) plane compared with prior studies, and find improvements in the stability of our results. We also demonstrate how to extend the compatible energy discretization for SPH [10] for use in axisymmetric coordinates. We will show results for classic hydrodynamics test cases such as the Sedov and Noh problems using planar, cylindrical, and spherical symmetries – i.e., modeled along the z (planar), r (cylindrical), and equally in (r, z) (spherical) cases. These problems are very useful for stressing the discretization in different

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ways and testing how well the expected symmetry is maintained in each case. Additionally the Noh and Sedov cases test two interesting endpoints of strong shock hydrodynamic problems: the Noh problem starts with all the energy in kinetic and progressively converts that to thermal energy via shock processing, while the Sedov problem proceeds in the opposite sense converting thermal to kinetic energy. As an example Fig. 1 shows the outcome for the mass density for the spherical Noh problem. The images in Fig. 1a show the final mass densities for all points modeled using the compatible energy treatment (on top) vs. standard non-compatible on the bottom. The right panel in Fig. 1b shows the final profiles in each case plotted against the analytic solution. We plot the $1 - \sigma$ scatter around these profiles as shaded regions around these plots, which demonstrates there is very little scatter except near the origin where the classic wall heating problem is also evident.

We also derive the solid form SPH using the full stress tensor, and demonstrate results for classic solid test cases such the Verney shell implosion (an analytic test of plastic work).

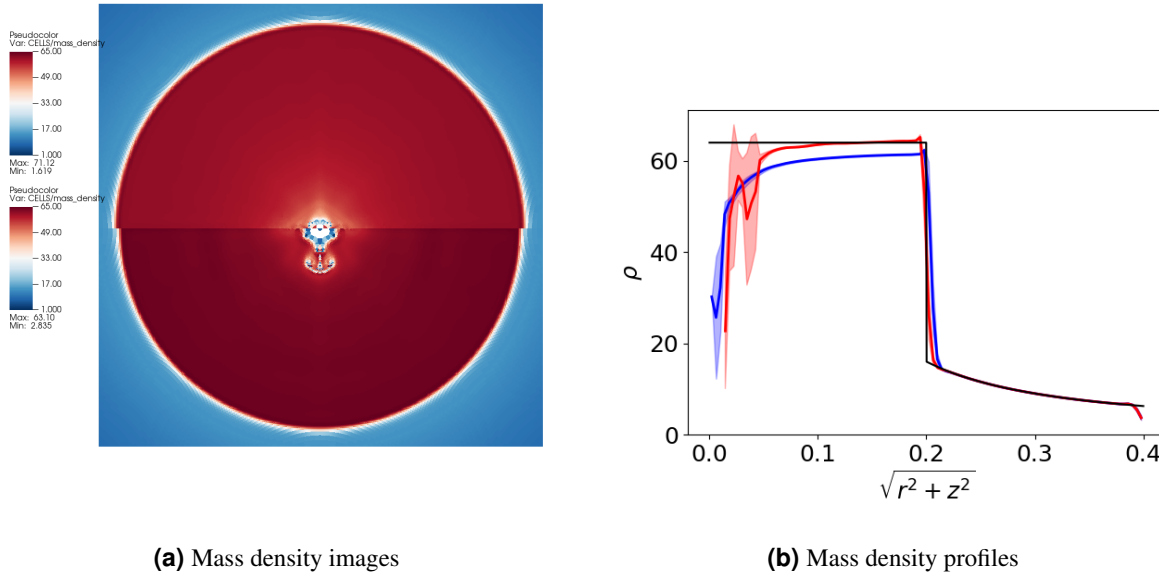


FIGURE 1: Spherical Noh problem at $t = 0.6$. Panel 1a compares the mass density at this time using the compatible energy discretization on top, vs. the standard time evolution for the thermal energy on the bottom. Panel 1b shows the averaged profiles as a function of radius from the origin for both calculations vs. the analytic solution (blue is the compatibly differenced result while red the standard case); shaded regions show the $1 - \sigma$ scatter of the values in each averaged bin about these curves.

ACKNOWLEDGMENT

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. LLNL-ABS-2018130.

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MASSIVELY PARALLEL HIGH-STRAIN-RATE MULTI-MATERIAL SOLID DYNAMICS

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ABSTRACT

We present progress towards incorporating a solid dynamics model into a massively parallel high order multi-material solver. We employ the thermodynamically consistent hyperelastic constitutive models to describe the response of solid materials under large deformations. Plastic behavior is incorporated through the plastic deformation-rate tensor, which introduces additional source terms into the evolution equations for the deformation gradient. These terms are mathematically stiff due to the relatively small plasticity time-scales. We use an Implicit–Explicit (IMEX) Runge–Kutta time-integration strategy to resolve plasticity terms implicitly while the remaining terms are advanced explicitly in time. This mixed treatment mitigates the otherwise severe time-step constraints associated with plasticity, without resorting to low-order approaches (e.g. operator-splitting) and improves the overall accuracy and robustness of the time integration. This work extends an existing multi-material hydrodynamics model, in which each constituent material is allowed to evolve its own thermodynamic state—pressure, temperature, and deformation gradients (i.e. p , T , σ non-equilibrium). This separation of states provides a more faithful representation of the underlying physics than approaches that enforce instantaneous equilibrium across materials with vastly different properties. Initial tests on problems involving multiple solids and fluids demonstrate the robustness and accuracy of the method.

INTRODUCTION

We present a numerical method for multi-material solid dynamics for high-strain-rate problems. The method is built in a previously developed high order multi-material framework [1, 2]. The baseline numerical method combines the following key recipes: (A) High order discontinuous Galerkin spatial discretization; (B) Algebraic interface reconstruction for material interface capturing; and (C) Direct time integration. Details about these can be found in our previous articles [1, 2]. The THINC algebraic interface reconstruction is able to capture material interfaces in 2-3 computational cells [2]. It is important to note that THINC does this without any iterative solvers involving geometric intersection operations, with a trade-off that it cannot capture material interfaces within a single cell. However, the computational savings from a single-step algebraic reconstruction are large, and can be easily put towards AMR in interface regions to obtain a very sharp interface. This can also be combined with p –refinement to result in a highly efficient and accurate multi-material method.

In this work, we extend the above method to solids. We use the hyperelastic-plastic [3] model to obtain Cauchy stresses from the material deformation gradient tensor. Plastic deformation is handled using the plastic

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deformation-rate tensor [4]. Since the time scales of plasticity are very small, this leads to a mathematically stiff system. We use an Implicit-Explicit (IMEX) Runge-Kutta time integrator that allows selective implicitization of these stiff terms while maintaining overall high order accuracy in time. This avoids the need for low order operator-split approaches, therefore improving overall solution accuracy. As a preliminary step to include damage, we use a Johnson–Cook–type model [5]. We are aware of the localization issues (viz. mesh convergence) with this model, and improved damage models will be a topic of future work. The method is implemented in an open source massively parallel hydrodynamics solver, Quinoa[†]. Quinoa is based on Charm++, an asynchronous-parallel task-based runtime system that handles dynamic load balancing. This automatic load balancing capability is instrumental for efficient simulations of heterogeneous multi-material hydrodynamics scenarios.

EXAMPLE PROBLEMS

Example solutions of multi-solid-fluid problems using the presented method are shown in Fig. 1. The presented method shows great potential for application to high-deformation multi-material hydrodynamics applications.

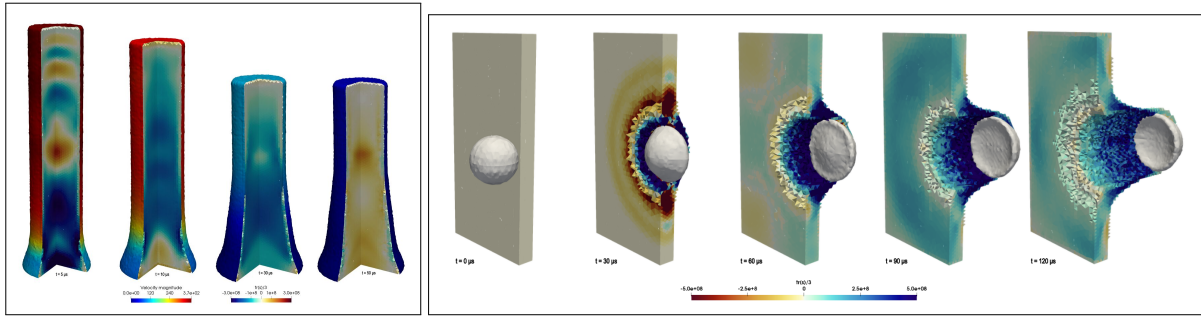


FIGURE 1: Aluminum Taylor anvil problem (left), and Steel sphere impact problem (right).

ACKNOWLEDGMENT

Research presented in this article was supported by the Advanced Simulation and Computing program of Los Alamos National Laboratory. This abstract has been approved for unlimited release and has been assigned LA-UR-26-22042.

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[†]<https://quinoacomputing.github.io/>



A CWENO HIGH-ORDER NODE CONSERVATIVE FINITE VOLUME SCHEME FOR THE 2D EULER EQUATIONS

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ABSTRACT

We present a high-order extension of the surface flux-based Finite Volume (FV) method proposed in [2, 3], for solving the compressible Euler equations on general unstructured grids, based on the seminal work [1]. The underlying multipoint (MP) approach relies on a node-based formulation that enables a genuinely multidimensional treatment of numerical fluxes, addressing the limitations of dimensionally split approximate Riemann solvers. The second order MP-FV scheme of [3] exhibits a reduced sensitivity to pathological instabilities, such as the carbuncle phenomenon, as well as to mesh-induced artifacts like odd–even decoupling, at the price of being slightly more dissipative than classical face-based FV approaches. In this context, the development of a high-order hybrid extension is thus motivated by the need to improve accuracy, while preserving the robustness properties of the original formulation. In particular, we propose a hybrid discretization where the flux integrals are approximated through the Simpson quadrature rule, employing the multipoint surface fluxes at the endpoints (vertices of the grid), and a standard face-based flux at the midpoint (baricenters of the faces). This choice provides a balance between multidimensional consistency and numerical accuracy. Third-order accuracy in space and time is then achieved by employing a Central Weighted Essentially Non-Oscillatory (CWENO) spatial reconstruction and a Strong-Stability Preserving Runge–Kutta time integration scheme. The performance of the proposed method is assessed on a set of benchmark tests, demonstrating improved accuracy while retaining the favorable stability properties of the pure node-based formulation, with reduced sensitivity to typical numerical pathologies of classical face-based FV schemes.

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THE LEGACY OF PETER LAX IN MULTIMATERIAL HYDRODYNAMICS

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ABSTRACT

Peter Lax was a giant of applied mathematics with few equals. Last Spring, he passed away at the age of 99. It is a good time to reflect upon the monumental contributions that he made in his storied career. In honor of his extensive and storied career, it would be good to reflect upon the contributions he made to our chosen field of endeavor. This is but one of his areas of contribution; Lax did even more. To highlight the magnitude of his achievement, he received the 2005 Abel Prize. He was at Los Alamos during the Manhattan Project, right out of high school as a draftee. He rode this momentum, providing mathematical rigor to the birth of computational science, most prominently in hydrodynamics. His contributions to compressible hydrodynamics are foundational. We have summarized some of this recently[1].

The Equivalence Theorem is amongst his most fundamental contributions[2]. It is limited in rigorous applicability, but encapsulates the basic benefits of growth in computing capability. More computing effort yields improved results via convergence toward the correct solution. The theory connects consistent and stable methods to that convergence. These combined expectations are the foundation of verification practice. The difficulty of the theory is highlighted as the theorem only applies to linear equations and methods. Nevertheless, the practice of numerical methods shows that convergence is seen with nonlinear equations and methods of broad interest.

Next is the Lax-Wendroff theorem[3]. This work provides the theoretical basis for choosing a conservation form numerically. The use of conservation form provides the benefit of producing weak solutions of the equations. The problem is the non-uniqueness of those weak solutions. Pairing with the importance of conservation form are entropy conditions[4]. The key to computing weak solutions is choosing the correct physical solution. This admissibility gives rigor to the use of numerical dissipation in methods. High-resolution methods are the lifeblood of modern computing[5]. Lax defined this concept, where high-order elements provide clear benefits computationally. They do so without giving formal high-order accuracy. Nonetheless, these methods are now standard.

He also contributed the Lax-Friedrichs method that continues to strongly influence modern numerical methods[6]. His use of the Riemann problem to test methods is also standard. Below, we demonstrate the method in its simplest setting as a demonstration of verification of a method. We solve the scalar advection equation using Lax-Friedrichs and show the computed results that reflect analytical properties. We can derive the properties of consistency and stability analytically. These are then demonstrated in code verification numerically.

All of this work is combined with a mathematical theory of hyperbolic conservation laws[7]. This theory is extensive and general. It is limited to one dimension and reflects the challenges and reality of the field. Today, the multi-dimensional theory is still beyond our ability to define and remains an active area of research. Lax defined the basis of these studies. His works have provided an inestimable foundation for the work we do today. My goal is to both honor Lax's contributions and also speak to how his key focus has provided a fundamental basis for advances to follow.

ACKNOWLEDGMENT

Thanks to my recent co-authors, and the friendship with Burt Wendroff in particular that allowed me to meet Peter.

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MULTI-VELOCITY FORMULATION FOR MIXED MATERIAL POINT METHOD/EULERIAN SIMULATIONS

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ABSTRACT

In this study, a multi-velocity formulation was developed and implemented for material interaction between Material Point Method (MPM) particles and Eulerian material fields. This formulation allows for improved simulation of fluid-structure interaction by introducing variable material interaction forces between the MPM materials as well as with an averaged Eulerian phase.

Unlike the contact algorithm for a single-velocity formulation where techniques such as penalty functions are used, a multi-velocity formulation is used which calculates the interaction between materials through modeled drag coefficients with relative velocity, which is more physical than simplified penalty functions. Also, the material interface in this formulation is non-diffusive, without the need for any special interface reconstruction treatment. This study proposes a method in which the material interaction force is calculated on the Eulerian grid, with individual velocities for Eulerian materials and MPM materials.

In this method, all Eulerian materials keep a single velocity, which allows those materials to still use interface reconstruction. This is important in simulations where Eulerian materials benefit from interface reconstruction, while large-deformation processes such as crack opening and fragmentation are handled by MPM. The main drawback to this implementation is that it is unable to handle fully mixed debris flow or dispersive flows. The advantages of this method are the savings in computational time in allowing some materials to be Eulerian as well as the flexibility of choosing which materials are modeled with MPM.

The average momentum equation is given by Zhang [1].

$$\frac{\partial}{\partial t}(\theta_i \langle \rho_i^0 \rangle \tilde{\mathbf{u}}_i) + \nabla \cdot (\theta_i \langle \rho_i^0 \rangle \tilde{\mathbf{u}}_i \tilde{\mathbf{u}}_i) = -\theta_i \nabla \langle p \rangle + \nabla \cdot [\theta_i (\langle \boldsymbol{\sigma}_i \rangle - \langle \rho_i^0 \mathbf{u}_i' \mathbf{u}_i' \rangle + \langle p \rangle \mathbf{I})] + \mathbf{f}_i \quad (1)$$

where the phase interaction force $\mathbf{f}_i$ is modeled as a drag or friction force [2],

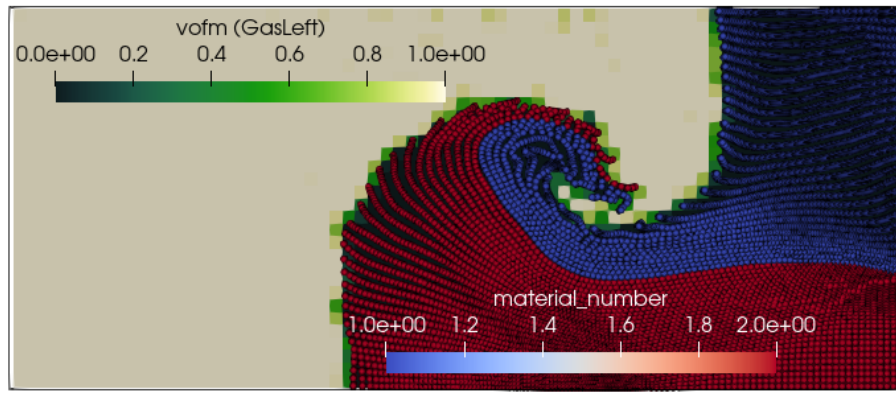
$$\mathbf{f}_i = \frac{3\theta_i\theta_j C_d}{4d} \rho_i^0 |\mathbf{u}_j - \mathbf{u}_i| (\mathbf{u}_j - \mathbf{u}_i) \quad (2)$$

and where subscript i is the current material, subscript j is the other material, C_d is the drag coefficient, d is the characteristic length, θ is the volume fraction, ρ^0 is density, $\mathbf{u}$ is velocity, and the angle brackets denote ensemble material averages. This force is broken into a tangential component and normal component so that separate coefficients can be specified for slip and for penetration/separation.

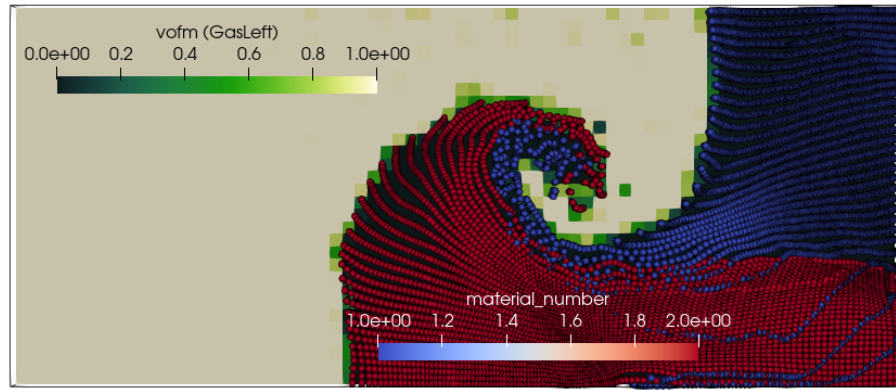
Preliminary results are shown in Fig. 1, demonstrating the ability to control the amount of penetration between the two MPM materials and into the Eulerian fluid on the left of the classic triple point problem.

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(a) No Slip/Penetration



(b) Full Slip/Penetration

FIGURE 1: Triple Point Problem with Eulerian fluid on the left. Results for (a) no slip/penetration and (b) full slip/penetration, showing the effect of the interaction force coefficients on material interface behavior.

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A WHITNEY FORMS MIMETIC SCHEME FOR STOKES' PROBLEM

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ABSTRACT

We present a novel mimetic method based on finite element exterior calculus (FEEC) [1] and Whitney forms. Differently from [2], the method works on simplicial grids and its characterizing feature is the adoption of a novel approach in defining the degrees of freedom. In fact, we replace moments, usually adopted for Whitney forms, with *weights*, linear functionals obtained by integration over appropriate subdomains. This concept encodes the duality between k -differential forms and k -manifolds.

Our construction [3, 4] is based on a specific cell-complex in each element T , whose cells are in duality with an explicitly computable basis for $\mathcal{P}_r^-\Lambda^k(T)$. Thus, the action of the exterior derivative d on this basis can be written in terms of the topological boundary operator ∂C , leading to a very simple assembly of linear system matrices in the Finite Element approach. Another important consequence is that the discrete differential inherits properties from the continuous structure and in particular, our discrete solution satisfies point-wise involution constraints arising from $d^2 = 0$.

This approach is suitable to construct discretizations for systems of partial differential equations in which it is crucial to satisfy involution constraints up to machine precision. We present the general construction and a specific application the VVP formulation of the Stokes’ problem to the language of differential forms. Tests have been conducted up to third order accuracy, and preconditioning techniques have also been studied.

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A VARIATIONAL MIMETIC FINITE DIFFERENCE METHOD FOR ELLIPTIC INTERFACE PROBLEMS ON NON-MATCHING POLYTOPAL MESHES WITH GEOMETRIC INTERFACE INCONSISTENCIES

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ABSTRACT

A new variational mimetic finite difference method for elliptic interface problems with perfect and imperfect thermal contacts on non-matching polytopal meshes with geometric interface inconsistencies is developed and analyzed theoretically and numerically. The method is defined on multiple non-matching submeshes with gaps and overlaps along their interfaces - Fig.1. The discrete equations are derived from a minimization problem for the augmented Dirichlet functional. For a perfect thermal contact, the functional uses a modified mimetic gradient with extended stencil which couples unknowns from both sides of an interface, as well as penalty terms to enforce weak continuity of temperature across the interface. The method leads to a symmetric positive definite matrix for any scaling of the penalty terms. For an imperfect thermal contact, the Dirichlet functional is supplemented with a quadratic jump term along the interface related to the interface thermal resistance. We prove that the method conserves the total heat flux across each interface. The obtained results are verified with numerical experiments showing convergence in the discrete L_2 and L^∞ norms. Some details can be found in [1].

ACKNOWLEDGMENT

This work was carried out under the auspices of the National Nuclear Security Administration of the U.S. Department of Energy at Los Alamos National Laboratory under Contract No. 89233218CNA000001. We acknowledge the financial support from the LANL ASC NUMIC project. We thank M. Kenamond and N. Vaughn-Kukura for discussion related to computation of weights. LA-UR-26-21275

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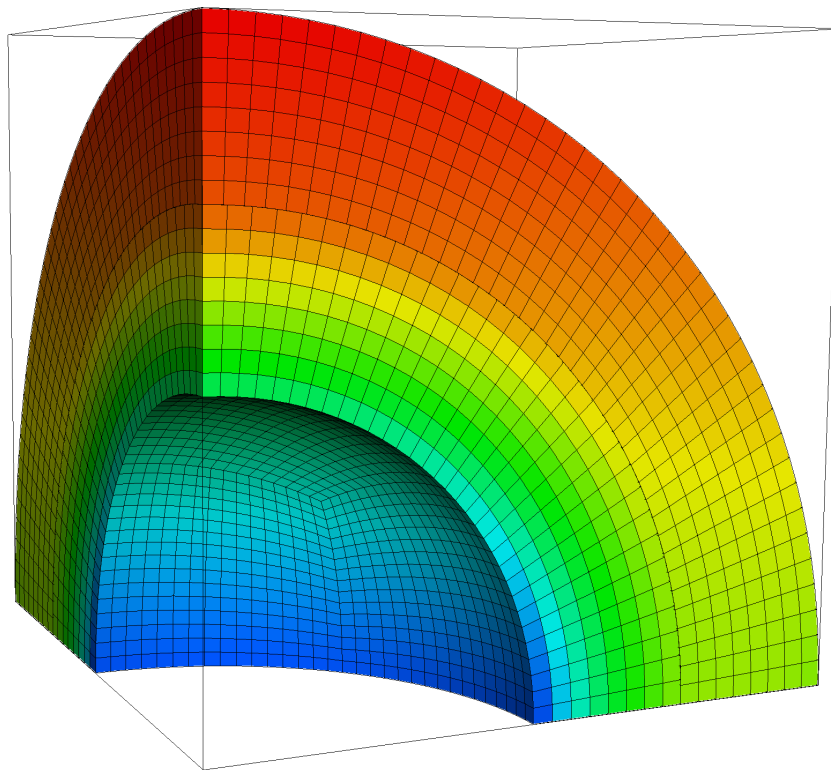


FIGURE 1: Meshes with geometric interface inconsistencies. Color map of the solution - demonstrates continuity of the solution across interface.



GRADIENT-BASED DESIGN OPTIMIZATION FOR UNSTEADY PROBLEMS WITH CONTACT MECHANICS

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ABSTRACT

INTRODUCTION

Adjoint methods for efficiently computing sensitivities of quantities of interest were largely pioneered within the physics simulation community. More recently, machine learning, with its need to train extremely high dimensional models, has driven innovation in these techniques. New theory, algorithms, and software make it an opportune time to take a fresh look at differentiable multi-physics simulation.

This talk describes methods for gradient-based optimization of systems with contact, with a focus on solids undergoing large deformations, inelastic material behavior, and dynamics unfolding over multiple time scales. Gradient-based optimization proceeds by launching simulations in an automated loop, using gradients of objective and constraint functions with respect to the parameters to guide updates. The first challenge in this framework is robustness. In implicit time integration, contact mechanics is infamous for making even a single simulation difficult to solve. We present solution methods that are based on minimization of scalar energy-like potentials. The minimization structure opens the door to methods from mathematical optimization that deliver excellent efficiency and robustness. Using tools such as variational constitutive updates, the minimization structure extends to discrete formulations of dissipative systems.

The second challenge is smoothness. Contact is plainly non-smooth, and closure models may introduce additional non-smoothness, such as elastoplasticity. These non-differentiabilities lead to noisy gradients that retard or even block convergence in design optimization. We describe reformulations of the contact physics and closure models that regularize these behaviors and improve optimization performance. We conclude with design optimization examples that highlight practical strategies, and common pitfalls, in formulating objective and constraint functions to achieve useful outcomes.

ACKNOWLEDGMENT

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344 and was supported by the LLNL-LDRD Program under Project No. 26-SI-002. LLNL-ABS-2017564

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ENTHALPY PRESERVING SIMPLE RIEMANN SOLVERS FOR STEADY HYPERSONIC FLOWS

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ABSTRACT

This work is devoted to the numerical resolution of the stationary Euler equations around vehicles submitted to hypersonic flows. Especially, the question of total enthalpy preservation of Riemann solvers through shocks. It is well known that Rusanov, HLL, HLLC, or Roe schemes do not preserve total enthalpy when solving stationary problems. It makes them less attractive than flux vector splitting schemes for some Navier-Stokes problems, as some algorithms may rely on total enthalpy based criterion to detect the boundary layer, or to consider ablation coupling with solids. The RoeM schemes [1] were developed to solve this issue by modifying the Roe scheme, and total enthalpy is finally preserved. Inspired by the RoeM schemes, a solution is proposed to correct this flaw using Godunov-type schemes based on Simple Riemann solvers [2]. An example of the Mach 20 flow around a cylinder is presented on Figure 1, and shows that this modification effectively preserves enthalpy.

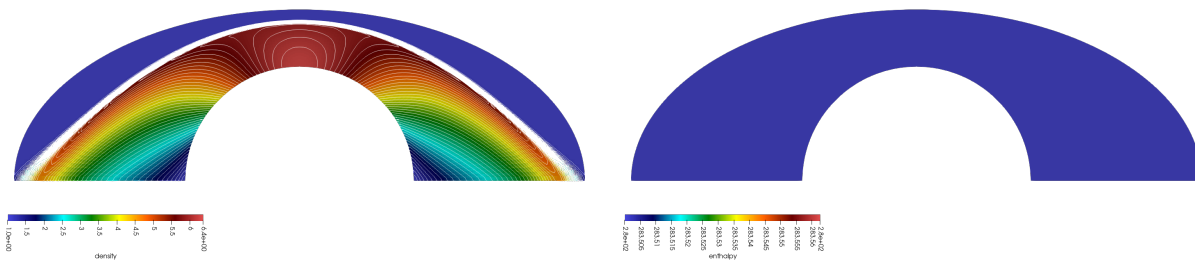


FIGURE 1: Density (left) and total enthalpy (right) for the mach 20 flow around a cylinder. The density field matches the reference solutions of the literature, while the enthalpy field is constant in the whole domain. The correction proposed here preserves enthalpy.

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REMAP FOR MULTI-MATERIAL ALE HYDRODYNAMICS VIA DIRECT INTERPOLATION AND CONSTRAINT OPTIMIZATION

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ABSTRACT

We propose a remap approach for multi-material Arbitrary Lagrangian-Eulerian (ALE) hydrodynamics that simultaneously enforces sharp material resolution, conservation of volume, mass, and total energy (per material), momentum, bounds preservation, and material volume fractions summing to one. Achieving this combination of properties is the central challenge in remap methods. The proposed approach is well-suited for ALE frameworks capable of performing significant purely Lagrangian displacements between consecutive remesh/remap steps. Our discretization is based on high-order finite elements [1]. Given the initial and optimized meshes, we begin by performing a direct interpolation in physical space, bypassing the concept of PDE-based pseudotime advection. This approach is computationally feasible due to recent advancements in parallel, GPU-capable interpolation routines provided by the GSLIB library [2]. The resulting interpolation ensures bounded fields with minimal diffusion but violates conservation. To restore conservation while preserving physical bounds, we employ two alternative optimization techniques. The first leverages interior point methods implemented via the HiOp optimization library [4]. The second technique builds on the recent research on Proximal Galerkin Methods [3], performing optimization in a latent space that inherently avoids the need for explicit bounds constraints. The proposed method produces minimal diffusion for finite element fields of arbitrary order and enables the direct remapping of quantities defined at integration points, eliminating the need to project onto finite element spaces. It circumvents challenges typically associated with synchronization between primal variables and conserved quantities in advection-based remap methods. We show results on standard 2D and 3D remap benchmarks and full multi-material ALE hydrodynamics simulations.

REMAP FORMULATION

For n materials, we evolve volume fractions $\{\eta_k\}_1^n$, densities $\{\rho_k\}_1^n$, specific internal energies $\{e_k\}_1^n$, and a common material velocity v . Starting from an initial mesh Ω_h^0 with fields $(\eta_k^0, \rho_k^0, e_k^0, v^0)$, and an optimized mesh Ω_h , we first perform an interpolation in physical space to obtain the interpolated fields $(\eta_k^*, \rho_k^*, e_k^*, v^*)$. Our optimization problem finds the solution (η_k, ρ_k, e_k, v) by solving:

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$$\min_{\eta_k, \rho_k, e_k, v} \|\eta_k - \eta_k^*\|_{L^2} + \|\rho_k - \rho_k^*\|_{L^2} + \|e_k - e_k^*\|_{L^2} + \|v - v^*\|_{L^2}, \text{ subject to} \quad (1)$$

$$\int_{\Omega_h} \eta_k = \int_{\Omega_h^0} \eta_k^0, \quad k = 1 \dots n, \quad (2)$$

$$\int_{\Omega_h} \eta_k \rho_k = \int_{\Omega_h^0} \eta_k^0 \rho_k^0, \quad k = 1 \dots n, \quad (3)$$

$$\int_{\Omega_h} \sum_k \eta_k \rho_k v = \int_{\Omega_h^0} \sum_k \eta_k^0 \rho_k^0 v^0, \quad (4)$$

$$\int_{\Omega_h} \eta_k \rho_k e_k + \frac{1}{2} \eta_k \rho_k v^2 = \int_{\Omega_h^0} \eta_k^0 \rho_k^0 e_k^0 + \frac{1}{2} \eta_k^0 \rho_k^0 (v^0)^2, \quad k = 1 \dots n, \quad (5)$$

$$\eta_{i,k}^{\min} \leq \eta_{i,k} \leq \eta_{i,k}^{\max}, \quad k = 1 \dots n, \quad (6)$$

$$e_{i,k}^{\min} \leq e_{i,k} \leq e_{i,k}^{\max}, \quad k = 1 \dots n, \quad (7)$$

$$\rho_{i,k}^{\min} \leq \rho_{i,k} \leq \rho_{i,k}^{\max}, \quad k = 1 \dots n, \quad (8)$$

$$v_{i,c}^{\min} \leq v_{i,c} \leq v_{i,c}^{\max}, \quad c = 1 \dots d, \quad (9)$$

$$\sum_k \eta_{i,k} = 1, \quad (10)$$

where the index i goes over all degrees of freedom of the corresponding field. Note that the interpolated solution $(\eta_k^*, \rho_k^*, e_k^*, v^*)$ satisfies all inequality constraints and (10), but not the conservation constraints.

Figure 1 illustrates an example of material-specific density remap, showing the density distribution of one material in the Triple Point benchmark.

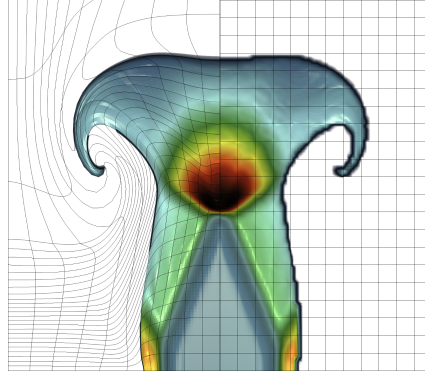


FIGURE 1: Remap of material-specific density in a three-material problem: initial mesh and field (left), optimized mesh and remapped field (right).

This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344 (LLNL-ABS-2002031).

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SECOND-ORDER IDP-ALE APPROXIMATION OF THE NONEQUILIBRIUM GREY RADIATION HYDRODYNAMICS EQUATIONS

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ABSTRACT

In this work we introduce a high-order implicit-explicit (IMEX) invariant-domain preserving (IDP) approximation of the nonequilibrium gray radiation-hydrodynamics equations within an Arbitrary Lagrangian–Eulerian (ALE) framework. Building on the first-order IDP method and the novel three-stage operator split (two hyperbolic, one parabolic) introduced in [1], we construct a method that is at least second-order accurate in both space and time. The explicit hyperbolic stages are advanced using a high-order Runge–Kutta scheme within a direct ALE formulation that allows for an arbitrary mesh velocity field. The parabolic stage, which accounts for radiation diffusion and the stiff radiation–matter energy exchange, is treated implicitly with high-order time stepping. The invariant-domain preserving property of the high-order method is enforced using a locally conservative mass redistribution limiting technique that is non-intrusive and discretization agnostic. The proposed method is proved to be conservative, consistent, and invariant-domain preserving. The performance of the method is illustrated on several benchmark problems.

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A SIMPLE AND SCALABLE HIGH-ORDER DIRECT-ALE METHOD

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ABSTRACT

We present a high-order numerical method for solving conservation laws that allows the computational mesh to move freely (direct Arbitrary Lagrangian–Eulerian, or dALE, approach). The method is designed to work with a wide range of flux functions, source terms, and equations of state, making it suitable for complex physical problems and geometries. We use the Multidimensional Optimal Order Detection (MOOD) method [2], which reduces computational cost and actively eliminates a class of numerical artifacts. All computations rely only on local information from each cell or node and a small, fixed number of neighbouring elements. This locality makes the method efficient and well suited for parallel computing on large distributed memory systems. Overall, the proposed approach combines flexibility, accuracy, and scalability for solving conservation equations in challenging applications.

INTRODUCTION

Most computational fluid dynamics (CFD) methods use either a fixed mesh (Eulerian) or a mesh that moves with the flow (Lagrangian). Arbitrary Lagrangian Eulerian (ALE) methods aim to combine the advantages of both by allowing the mesh to move in an arbitrary, user-prescribed manner. This is done either by using a Lagrangian scheme and then performing a remap onto a new, higher-quality mesh (indirect-ALE), or by incorporating mesh relaxation directly in the scheme (direct-ALE). We focus on the latter approach because it provides a natural way of handling moving boundary conditions.

ALGORITHM

Discretisation

The method has been implemented in the open-source 2D/3D CFD code UCNS3D [4], which employs unstructured, collocated grids. High-order spatial accuracy is achieved through classic (C)WENO non-linear polynomial reconstruction on fixed stencils of neighbouring cells. All mesh motion is included directly in single update step by modifying the fluxes to account for arbitrary face velocity. For temporal discretisation we adopt explicit strong-stability preserving (SSP) Runge-Kutta method. Compared to ADER-based approach [1] this choice simplifies incorporating additional fluxes (e.g. viscosity), source terms (e.g. reactive flows), or different equations of states (including tabulated) easier, since no local space–time predictor problem must be solved. Moreover, it allows nodes to follow more complex trajectories within a time step, which improves following the shape of curved boundaries, and in the future may simplify handling connectivity changes by avoiding space-time slivers.

MOOD

In addition to the classical CWENO polynomial reconstruction, we investigate the Multidimensional Optimal Order Detection (MOOD) method [2] and WENO-MOOD hybrid approaches, which enhance the robustness of the simulation and reduce the computational cost, by reducing the number of stencils and polynomials that need to be constructed. We evaluate a novel MOOD trigger algorithm based on entropy production, which can reliably flag numerical pathologies and physical discontinuities within a single evaluation.

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Mesh relaxation

Mesh relaxation is incorporated directly into nodes' velocities. The aim is to maximise accuracy in key regions by following the material flow as closely as possible and to allow the relaxation to be higher elsewhere to improve the overall mesh quality.

$$\mathbf{v}_{node} = \mathbf{v}_{Eulerian} + r \frac{\mathbf{x}_i^{relaxed} - \mathbf{x}_i^{lagrangian}}{dt} \quad r \in [0, 1]$$

Approximating Voronoi meshes

We consider using Voronoi tessellation for mesh relaxation. In their standard form, Voronoi-based methods require connectivity updates, and the position of each node depends on an unpredictable number of generator points. This leads to significant computational overhead and is incompatible with our objective of designing a fully local algorithm. To address this, we propose an approximation strategy that reproduces key geometric properties of Voronoi nodes while relying solely on strictly local information.

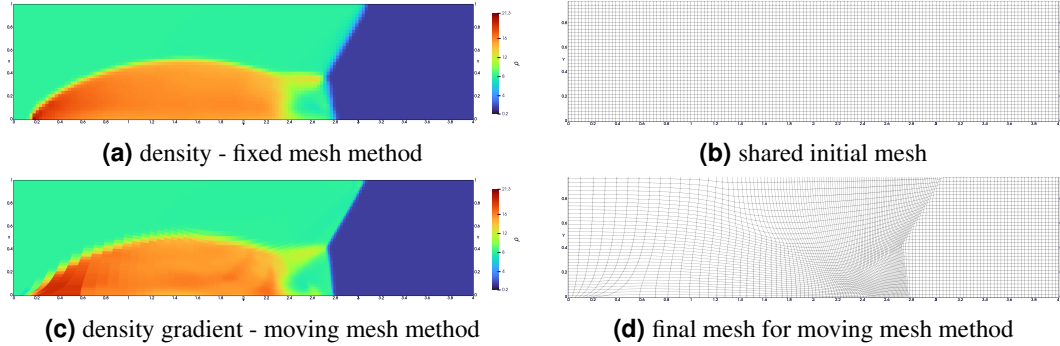
Jacobi matrix based optimisation

The second approach relies on indicators derived from the properties of the Jacobian matrix, such as the condition number or the Oddy's metric, to assess mesh quality and perform iterative local optimisation [3]. We modify the Newton iteration to be capable of robustly handling ill-conditioned mesh configurations.

Modulating mesh relaxation based on normalised density gradient

We vary the mesh-relaxation coefficient based on physical relevance of the region quantified using the normalised density or volume-fraction gradient, which serve as indicators of shock waves and material interfaces, and the local mesh quality evaluated using the selected Jacobian-based mesh quality metric. In our initial tests, the relaxation coefficient r is computed using a simple piecewise-linear function of these two quantities.

PRELIMINARY RESULTS



Results for Double Mach Reflection test obtained with the reference Eulerian method and our ALE.

ACKNOWLEDGMENT

The work is conducted as part of a PhD project funded by AWE plc. The computations are performed on ARCHER2 with resources funded through the UK Turbulence Consortium [EPSRC grant number EP/L000261/1 and EP/R029326/1].

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A SINGLE-MESH MULTI-VELOCITY FORMULATION FOR CONTACT AND SLIDING IN ARBITRARY LAGRANGIAN EULERIAN HYDRODYNAMICS

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INTRODUCTION

Staggered-grid hydrodynamics (SGH) is widely used for Lagrangian simulations of solid dynamics and high-strain-rate phenomena. In the standard SGH formulation, mesh motion is governed by a single nodal velocity that determines the kinematic evolution of the computational mesh. When multiple materials share a node, this formulation enforces velocity continuity across material interfaces. While appropriate for bonded materials, this constraint prevents sliding between contacting solids and limits the ability of SGH to represent contact and slip.

Existing approaches introduce slidelines or multi-mesh discretizations to enable relative motion across interfaces. Although effective, these techniques require conformal mesh interfaces and complicate coupling with multiphysics models that assume a single mesh discretization.

In this work we develop a single-mesh *multi-velocity* extension of SGH that enables sliding and contact while preserving the standard mesh structure and geometric remap infrastructure.

MULTI-VELOCITY FORMULATION

In the classical SGH formulation, mesh motion is governed by a single nodal velocity $\mathbf{v}$. When multiple materials share a node, this velocity determines the motion of all materials locally, enforcing velocity continuity across material interfaces and preventing sliding.

The multi-velocity formulation relaxes this constraint by allowing each material m to evolve its own material velocity $\mathbf{v}^{(m)}$ while the mesh continues to move with the SGH nodal velocity $\mathbf{v}$. The relative motion between material and mesh is characterized by the slip velocity

$$\mathbf{u}^{(m)} = \mathbf{v}^{(m)} - \mathbf{v}. \quad (1)$$

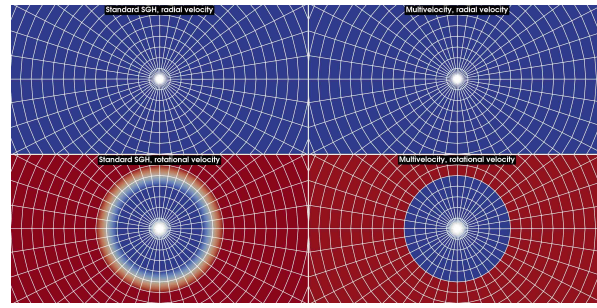
This slip velocity represents motion of material relative to the moving mesh and provides a mechanism for sliding along material interfaces while retaining a single geometric mesh.

At the algorithmic level, the Lagrangian step evolves material-specific nodal velocities using material mass and stress contributions while the mesh continues to move with the SGH nodal velocity. Relative motion between material and mesh is incorporated during the remap stage through additional transport driven by the slip velocity.

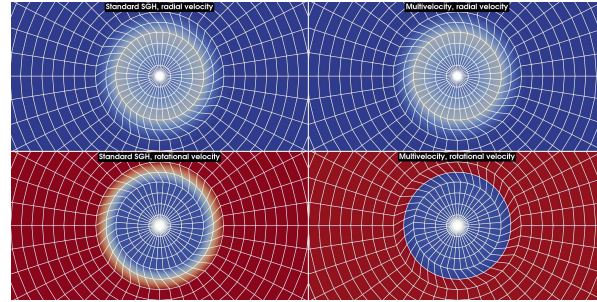
DEMONSTRATION

The following demonstration shows a simulation of two materials, a circle embedded in a ring. The inner circle is given an initial rotational velocity, the outer ring is stationary. SGH treats the materials as bonded, while the multi-velocity scheme can treat them as unbonded and allow them to slide relative to one another. The figures below show the velocity field and the stress field demonstrating the ability of the method to maintain tangential velocity discontinuities and alleviate SGH's artificial shear stresses.

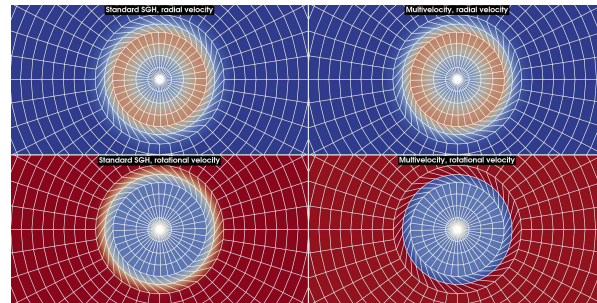
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(a) Initial velocity configuration.



(b) Intermediate time velocity.



(c) Late time velocity.

FIGURE 1: Comparison of SGH to the multi-velocity scheme for a simulation of an embedded rotating circle. The inner material has an initial rotational velocity, the outer material is stationary. In each figure, the left column shows standard SGH, the right shows multi-velocity. The top row shows the radial velocity field, the bottom shows the rotational velocity. By construction, the multi-velocity scheme respects SGH in the normal direction (radial), while maintaining a velocity discontinuity in the tangential direction (rotational), unlike SGH.

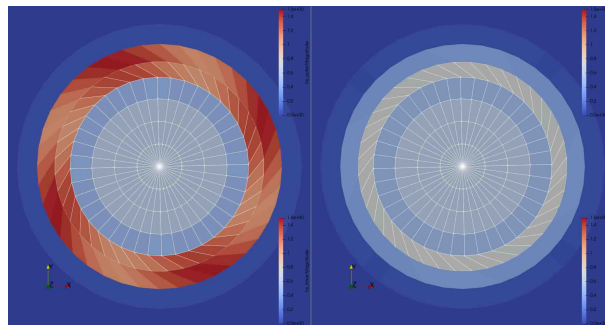


FIGURE 2: The stress fields for the SGH and multi-velocity case show the significant stress on the materials in the SGH case due to the artificial “bonding.” This large stress is alleviated by the multi-velocity method.



ENTROPY CONSERVATIVE/DISSIPATIVE MONOLITHIC SCHEME

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ABSTRACT

In this talk, based on our previous work [1], as well as the technique developed by R. Abgrall in [2], we present an entropy conservative/dissipative positivity-preserving subcell monolithic DG/FV scheme

This talk aims at presenting an entropy conservative/dissipative and convex property preserving subcell monolithic DG/FV scheme, solving system of conservation laws on 2D unstructured grids. This is known that discontinuous Galerkin (DG) method needs some sort of nonlinear limiting to avoid spurious oscillations or nonlinear instabilities which may lead to the crash of the code. The main idea motivating the present work is to improve the robustness of DG schemes, as well as ensuring a conservative/dissipative behavior, while preserving as much as possible its high accuracy and very precise subcell resolution. To do so, a convex blending of high-order DG *entropy conservative* and first-order finite volume (FV) scheme will be locally performed at the subcell scale where it is needed. To this end, by means of the theory developed in [1], we first show that it is possible to rewrite *entropy conservative* DG scheme as a subcell FV scheme on a subgrid provided with some specific numerical fluxes referred to as DG reconstructed fluxes. Then, the monolithic DG/FV scheme will be defined as following: to each face of each subcell will be assigned two fluxes, a 1st-order FV one and a high-order reconstructed one, that will be in the end blended in a convex way. The goal is now to determine, through analysis, optimal blending coefficients to achieve the desired properties. Let us emphasize the *entropy conservative* DG scheme, which is latter reformulated as a subgrid FV scheme, is obtained by adapting the entropic correction, introduced by R. Abgrall in [2], to the frame of subcell reconstructed fluxes technique. Numerical results on various type problems will be presented to assess the very good performance of the design method.

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A MULTIMATERIAL MODEL TO SIMULATE AIRCRAFT IN-FLIGHT ICE ACCRETION

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ABSTRACT

The objective of this article is to propose a new methodology for calculating ice accretion, based on a multimaterial phase-field model rather than on an iterative coupling (with successive remeshing) between a two-phase flow model to calculate the air flow and the droplet impact rate, and a surface solver to calculate the local ice growth rate on the surface of the solid body. Specifically, instead of treating the ice thickness h at each point on the surface as an unknown, we treat the volume fraction of ice α_s at each point in the space outside the solid body. This requires solving a system of coupled equations whose unknowns are the volume fraction of liquid α_l (corresponding to water droplets) and the volume fraction of ice α_s . It is not necessary to explicitly reconstruct the accretion front. It is automatically captured as the region where α_s changes from 0 to 1. Consequently, remeshing at regular intervals is not necessary, and the conservation of the total water mass is guaranteed by the model's construction.

INTRODUCTION

Ice accretion represents a critical concern across multiple engineering domains. Under specific meteorological conditions, super-cooled water droplets can impinge on exposed surfaces, and then freeze upon impact or run-back and solidify downstream. In aerospace applications, in-flight ice accumulation on aircraft components must be carefully considered throughout the design cycle to ensure performance and safety.

The ice accretion process is typically simulated using a multistep workflow [3, 4, 5]. First, a steady-state flow-field is computed around the geometry to get the aerodynamic conditions. Next, the droplet field is solved using either a Lagrangian approach, where individual droplets are tracked, or an Eulerian approach, which treats the droplets as a continuous phase. Once the droplet field is obtained, the surface values are computed using the local droplet impingement mass flux, the convective heat flux, and solving mass and energy balance equations. The solution of these equations provides the local ice growth rates on the surface, which are used to update the surface geometry by displacing the surface nodes to account for ice accretion. The procedure can be repeated iteratively in a semi-coupled

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manner, allowing the flow-field to adjust to the evolving ice shape and enabling the simulation of ice accumulation by layers.

To summarize, all approaches that are currently used in industrial numerical tools for simulating ice accretion on a surface in the presence of a flow rely on an iterative coupling between volume-based solvers to compute the air flow and the droplet trajectories, and a surface-based solver to compute the local ice growth rate. The main limitations of these approaches are, on the one hand, the computational cost and complexity of the remeshing procedure (which can potentially be circumvented using Immersed Boundary Methods (IBM)) and, on the other hand, the risk of mass non-conservation when complex ice shapes are reconstructed from local growth rates, leading to significant numerical errors.

The objective of the method proposed in this paper is to circumvent these two difficulties by modelling ice accretion with a volumetric solver rather than a surface-based solver. Concretely, instead of considering the ice thickness h at each point on the surface as an unknown, we consider the ice volume fraction α_s at every point in space outside the solid body. This requires solving a coupled system of equations - a multimaterial model - with unknowns being the liquid volume fraction α_l (corresponding to water droplets) and the ice volume fraction α_s . It is not necessary to explicitly reconstruct the accretion front. It is automatically captured as the region where α_s changes from 0 to 1. Consequently, remeshing at regular intervals is not necessary, and the conservation of the total water mass is guaranteed by the model's construction. The method still has certain limitations, which will be discussed during the conference. In particular, it currently only applies to cases where droplets freeze on impact, i.e. *rime* conditions. Nevertheless, based on the work currently underway, we are confident that these limitations can be overcome in the near future.

MODEL FORMULATION

In this paper, our aim is not to address the problem of ice accretion simulation in its full generality. We have therefore made simplifying assumptions that can be abandoned at a later stage. In particular, the droplet velocity field is not updated. Only the droplet density field changes, as it necessarily changes in regions where ice forms (through the capture of droplets by ice deposits and the creation of shadow zones downstream of the deposits). In future work, the air and droplet velocity fields will be updated consistently, using a penalization approach based on the ice volume fraction for the airflow and by solving the droplet momentum equation. In the present model, the droplet velocity field is prescribed through a known velocity field $\mathbf{u}$ (that is simply pre-computed around the clean geometry). The second important simplifying assumption is to assume that all droplets freeze upon impact, without any water-film runoff, thereby forming rime ice. In addition, for simplicity, the densities of liquid water ρ_l and solid ice ρ_s are considered constant.

Let us denote by α_l , respectively α_s , the liquid volume fraction (droplets), respectively the solid volume fraction (ice), and by $\alpha_d = \frac{\alpha_l}{1 - \alpha_s}$ the droplet bulk volume fraction (that is, the ratio of the volume of the droplets contained in a given volume to the sum of the volume of the air and the volume of the droplets). Assuming that $\alpha_d \ll 1$ (which is not a restrictive assumption in practice) and the ice being supposed at rest with respect to the reference frame, it can be shown [6] that the mass conservation for both droplets and ice leads to the following system of equations :

$$\partial_t(\rho_l \alpha_l) + \nabla \cdot (\alpha_l \rho_l \mathbf{u}) = -\rho_l \alpha_d \max(\mathbf{u} \cdot \nabla \alpha_s, 0) \quad (1)$$

$$\partial_t(\rho_s \alpha_s) = \rho_l \alpha_d \max(\mathbf{u} \cdot \nabla \alpha_s, 0) \quad (2)$$

Since the masses of the liquid and solid phases are not conserved, it is not surprising that each equation contains a non-conservative term that corresponds to the mass accretion rate. But of course if we sum the two equations, we get the conservation equation :

$$\partial_t(\alpha_d(1 - \alpha_s)\rho_l + \alpha_s\rho_s) + \nabla \cdot (\alpha_d(1 - \alpha_s)\rho_l \mathbf{u}) = 0 \quad (3)$$

which expresses the conservation of total water mass. It is worth mentioning that, since α_d is expected to be continuous across the accretion front, the non-conservative product in the r.h.s. of equation (1) and (2) is mathematically well-defined even if α_s is a discontinuous function (sharp interface limit).

Let us now examine the hyperbolicity of the system (1)-(2) and without loss of generality let us restrict our attention to the domains where $\mathbf{u} \cdot \nabla \alpha_s > 0$ (the other domains corresponding to the shadow areas where the system (1)-(2) is trivial). In such domain, the system (1)-(2) is equivalent (as far as smooth solutions are concerned) to the following one:

$$\partial_t \alpha_l + \mathbf{u} \cdot \nabla \alpha_l + \alpha_d \mathbf{u} \cdot \nabla \alpha_s = -\alpha_l \nabla \cdot \mathbf{u} \quad (4)$$

$$\partial_t \alpha_s - \frac{\rho_l}{\rho_s} \alpha_d \mathbf{u} \cdot \nabla \alpha_s = 0 \quad (5)$$

This clearly shows that the system (1)-(2) is a first order hyperbolic system of partial differential equations with two distinct eigenvalues (in 1d) : $\lambda_1 = u$ and $\lambda_2 = -\frac{\rho_l}{\rho_s} \alpha_d u$, λ_1 corresponding to the droplet velocity and λ_2 corresponding to the accretion front velocity. This is a stiff system since $|\lambda_1| \gg |\lambda_2|$ because $\alpha_d \ll 1$.

Finally, in a cloud of supercooled droplets, not all droplets are generally the same size. To account for the distribution of droplet sizes, the overall spectrum is discretized into a set of diameter bins, where each bin corresponds to a fraction of the total Liquid Water Content (LWC). For each bin, an independent droplet velocity field, $\mathbf{u}_i$, can be pre-computed and (1) can be splitted into a separate transport equation for each droplet class in the distribution. The resulting system of equations to be solved is :

$$\begin{aligned} \partial_t \alpha_{l_1} + \nabla \cdot (\alpha_{l_1} \mathbf{u}_1) &= -\alpha_{d_1} \max(\mathbf{u}_1 \cdot \nabla \alpha_s, 0) \\ \partial_t \alpha_{l_2} + \nabla \cdot (\alpha_{l_2} \mathbf{u}_2) &= -\alpha_{d_2} \max(\mathbf{u}_2 \cdot \nabla \alpha_s, 0) \\ &\vdots \\ \partial_t \alpha_{l_N} + \nabla \cdot (\alpha_{l_N} \mathbf{u}_N) &= -\alpha_{d_N} \max(\mathbf{u}_N \cdot \nabla \alpha_s, 0) \end{aligned} \quad (6)$$

$$\partial_t \alpha_s = \sum_{i=1}^N \frac{\rho_l}{\rho_s} \alpha_{d_i} \max(\mathbf{u}_i \cdot \nabla \alpha_s, 0) \quad (7)$$

NUMERICAL METHOD

The system (1)-(2) was discretized in 2D and 3D using a finite volume method on unstructured grids. Details of the numerical method will be presented at the conference. Particular attention was paid to the time discretization scheme due to the stiffness of the system, as well as to the accuracy of the scheme in order to avoid numerical diffusion of the accretion front.

RESULT EXAMPLES

Figure 1 illustrates the effect of the scheme's spatial order and the choice of slope limiter on the numerical diffusion of the accretion front. As can be seen, using a second-order scheme and a compressible slope limiter yields a very sharp interface, spread over only two rows of cells.

Figure 2 corresponds to the case 241 from the First Ice Prediction Workshop [2]. This configuration was generally well predicted by the workshop participants, providing a reliable benchmark for comparison. The phase field model captures very well the experimental ice shape profile (defined as the maximum envelope of the ice shape obtained by combining multiple parallel cross-section normal to the wing leading edge) and closely matches the ten-layer and 200 sub-iterations surface deformation method solutions.

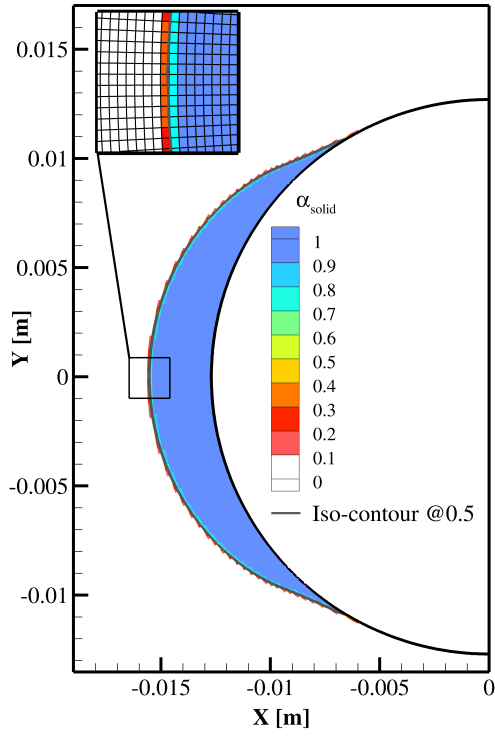
The last case is a three-dimensional test case that corresponds to the mid-span rime accretion case from the Second Ice Prediction Workshop [1]. Figure 3 depicts three-dimensional views of the ice shape by blanking regions where $\alpha_s = 0$. The ice-accretion subdomain is localized around the center of the half-wing, where the experimental measurements were extracted. The mesh resolution is high, with 198,352 cells representing the accreted ice. The full computational mesh contains 8,376,214 cells and required 4.5 h to compute for the seven-bin droplet size distribution. Each time increment was 1.04 s, corresponding to a CFL number of 300,000 based on the droplet velocity, for a total of 1,675 iterations. The simulation was performed on a single node equipped with 192 cores ($2 \times$ AMD EPYC 9655, Zen 5 @ 2.6 GHz).

ACKNOWLEDGMENT

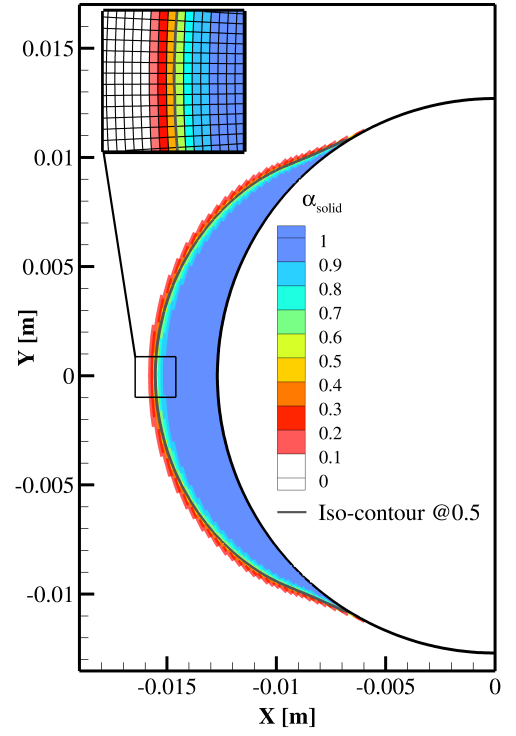
This work was undertaken during a three-month research stay of the second author at Polytechnique Montréal. ONERA and Polytechnique Montréal are gratefully acknowledged for financially supporting this research exchange. This research was enabled in part by support from Calcul Québec, the Digital Research Alliance of Canada and the Canada Research Chair program.

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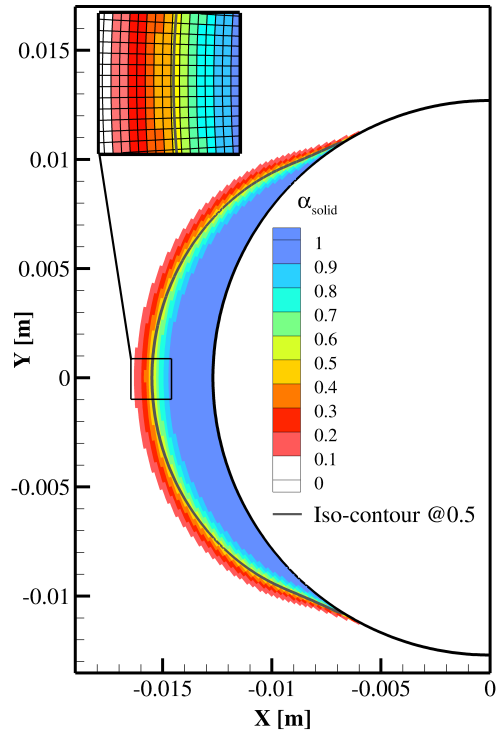
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(a) Second order scheme - Compressible limiter



(b) Second order scheme - Barth-Jespersen limiter



(c) First order scheme

Figure 1: Influence of the choice of the limiter on the numerical diffusion of the accretion front

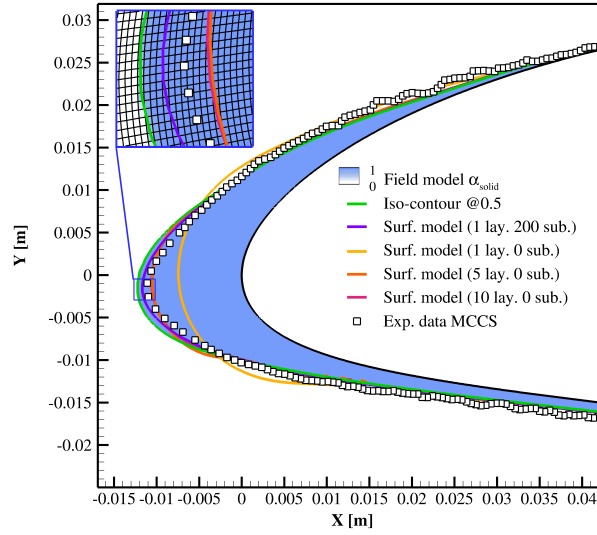


Figure 2: Ice accretion obtained with the phase field model and comparison with a surface deformation model

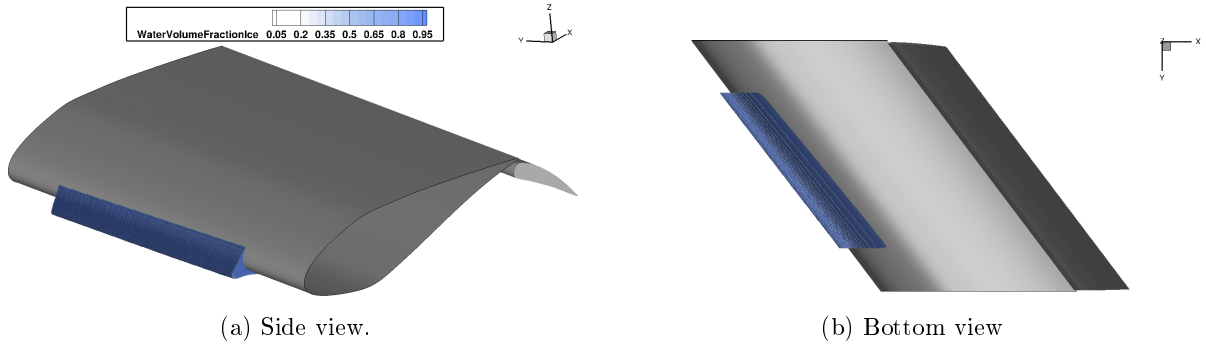


Figure 3: Three-dimensional views of the ice volume fraction on a section of the CRM-65 mid-span



LAGRANGIAN HYDRODYNAMIC KINETIC CONTACT BASED IN NEWTON'S SECOND LAW

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ABSTRACT

We present a novel approach to contact mechanics in Lagrangian hydrodynamics based on kinematic particle pathing within the finite element space, with acceleration expressed through an expression derived from Newton's Second Law. The results shown use linear hexahedral elements; however, the formulation is agnostic to element order, allowing future extension to arbitrary-order elements undergoing contact. We include both qualitative and quantitative demonstrations: qualitative examples highlight contact pairing and resolution in scenarios such as multi-body interactions, while quantitative validation is provided through a Taylor anvil impact comparison against experimental data.

INTRODUCTION

Accurately simulating material behavior under large deformations and contact is critical to diverse applications but challenging. In developing a robust, scalable contact surface method, this research effort enhances simulation accuracy, speed, and robustness. These advancements enable using high-fidelity multi-scale material models—including microstructure-aware models—in simulations for moderately large deformation applications. As such, this research project is vital for the advancement of Lagrangian Hydrodynamic capabilities with contact.

BACKGROUND AND STATEMENT OF THE PROBLEM

In engineered systems subjected to impact events or shocks, materials commonly undergo large deformations, high strain rates, and complex multi-component interactions involving sliding, separation, and collision. Traditionally, Lagrangian methods are the workhorse for solid dynamics simulations because they track the material with a mesh, enabling natural representation of history-dependent material models and clear resolution of material interfaces. However, applying traditional Lagrangian finite element methods in demanding environments exposes fundamental numerical and computational challenges that limit robustness, accuracy, and scalability. The limitations of contact are discussed below here, and finding solutions to these problems aids in the advancement of Lagrangian Hydrodynamics.

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Challenges Arise in Handling Contact

Engineered systems typically consist of multiple components that may slide, separate, or collide. Enforcing non-penetration while conserving momentum and energy requires robust contact algorithms. Contact introduces discontinuities in velocity and stress fields that can destabilize solvers, and the search for interacting surfaces across thousands or millions of elements poses severe scalability challenges in large problems. The challenge grows when multiple bodies come into contact. Advanced contact algorithms are needed to manage mesh-to-mesh interactions among numerous components, enhancing both the accuracy and robustness of simulations.

RESULTS

Three test cases are shown. The first is a comparison to experimental data that shows strong agreement with reality. The initial diameter of each rod was 1.91 cm and the initial length was 7.51 cm. The experimentally observed final diameter was 2.36 cm and the simulation predicted 2.38 cm. The experimentally observed final length was 7.03 cm and the simulation predicted 7.059 cm. The next two test cases are qualitative stress testing of the algorithm dealing with complex geometries, a bunny and a teapot followed by spheres.

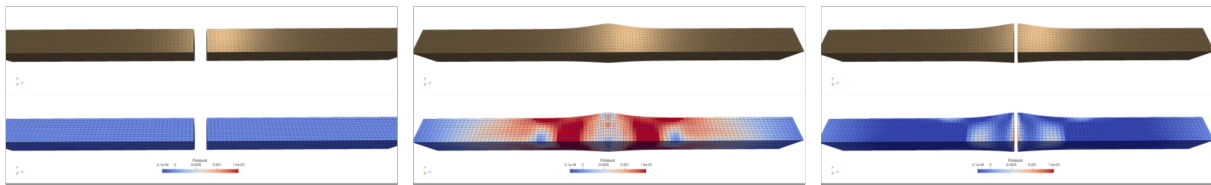


FIGURE 1: Taylor Anvil Impact with 2 copper rods colliding at 0.0083 cm/microsecond. The final diameter and length of the bar is within 0.03 cm of experimental data.

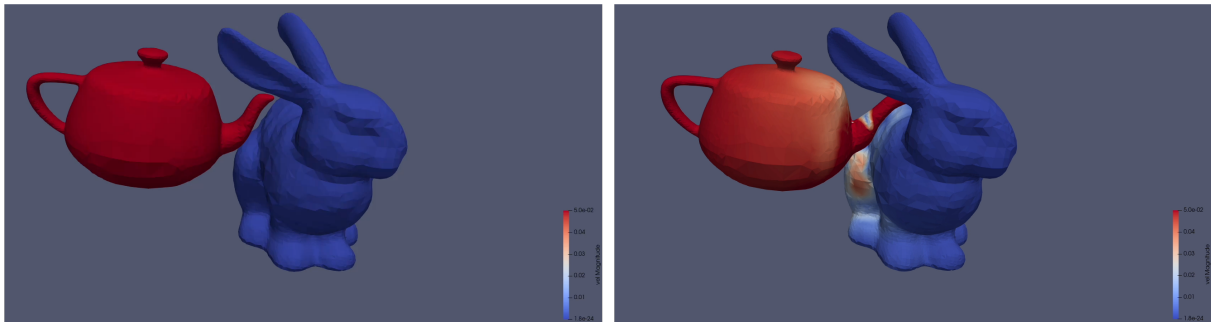


FIGURE 2: A complex geometry test case of a teapot hitting the Stanford bunny.

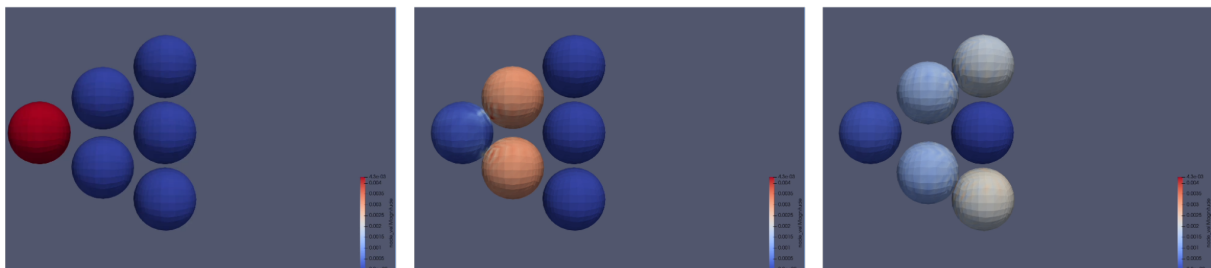


FIGURE 3: Elastic billiards balls with simultaneous impacts on the same body.

ACKNOWLEDGMENT

We acknowledge the support of the LDRD program at Los Alamos National Laboratory.



INFORMATION GEOMETRIC REGULARIZATION: HIGH-ORDER LAGRANGIAN SHOCK HYDRODYNAMICS WITHOUT VISCOSITY

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ABSTRACT

The compressible Euler equations develop nonsmooth solutions in the form of shocks in virtually all smooth initial conditions. Existing remedies, such as artificial viscosity or limiters, can smear fine-scale structures if too much is added or fail to prevent spurious oscillations if too little is added. The recently proposed Information-Geometric Regularization (IGR, [1]) overcomes this problem by introducing the first inviscid shock regularization. Applied to Eulerian CFD, it has recently enabled the first compressible fluid simulation to exceed a quadrillion degrees of freedom [2].

This work extends IGR to Lagrangian fluid dynamics with shocks. The accumulation of mesh points towards shock fronts coupled and the use of an adaptive IGR that shrinks with an element's size allows for sharper shock resolution than in the Eulerian case. We integrate the IGR into Laghos, an MFEM-based high-order Lagrangian discretization of compressible shock hydrodynamics equations using curvilinear finite elements. We show that IGR is able to prevent singular shocks from forming without adding artificial viscosity, enabling the use of high-order discretizations of shock-laden flows in the Laghos framework.

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SIMPLEX SOLVER FOR LAGRANGIAN HYDRODYNAMICS

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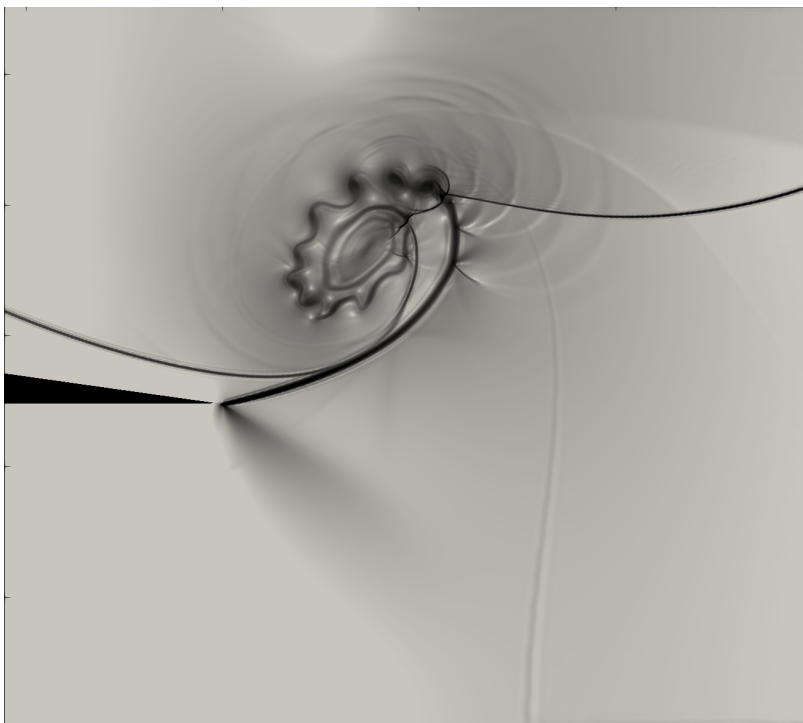
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ABSTRACT

Over the past seven decades, Lagrangian staggered-grid hydrodynamics (SGH) and cell-centered hydrodynamics (CCH) have emerged as two dominant paradigms for solving the compressible Euler equations. Although both approaches are formally derived from the same continuum conservation laws, they differ fundamentally in their discretization strategies and numerical behavior: SGH schemes typically rely on artificial viscosity to capture shocks and dissipate kinetic energy, whereas CCH methods employ Riemann solvers at cell interfaces to convert kinetic energy into internal energy. This talk introduces a novel simplex solver that unifies the treatment of Lagrangian hydrodynamics on both primary and dual meshes. The formulation is rigorously constrained by Newton's three laws of motion, ensuring conservation of mass, momentum, and total energy. Moreover, the discretization satisfies thermodynamic compatibility. The simplex solver requires no empirical parameters, exhibits strong universality, and can be naturally extended to arbitrary 2D polygonal or 3D polyhedral meshes, providing a reliable numerical framework for multiphysics simulations involving complex geometries.

Keywords: staggered-grid hydrodynamics, cell-centered hydrodynamics, artificial viscosity, Riemann solver.

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Abstracts of posters

ranked by presenters' name



BRIDGING FINITE DIFFERENCES AND NEURAL NETWORKS: A VARIATIONAL FRAMEWORK WITH RIGOROUS ERROR ESTIMATES

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ABSTRACT

Physics-informed neural networks (PINNs) are an emerging approach to approximate PDEs solutions. However, the theoretical study of error estimates remains underdeveloped; see [2,3]. Classical PINNs use the strong form of the PDE, namely its residual and boundary conditions/initial data, as the loss function. Hence, the training process for said classical PINNs requires the derivatives present on the PDE operator, typically calculated using Automatic Differentiation (AD), which comes at a substantial cost.

Instead of training the Neural Network (NN) to approximate the classical pointwise residual (classical PINN) or a continuous variational formulation (vPINN), we train it to minimize a discrete energy functional of a finite difference/finite element discretization. This avoids computing the derivatives of the PDE through back-propagation and circumvents Monte Carlo integration. Therefore, we propose a general framework for these discrete variational PINNs (dvPINN) and, assuming the underlying bilinear form is symmetric, coercive and continuous, we prove an error estimate that depends on: (i) the optimization error, (ii) the NN approximation error and (iii) the FDM/FEM classical approximation error.

As a proof of concept, we apply the abstract framework to the one-dimensional Poisson problem, with different types of boundary conditions (Dirichlet, Neumann and Robin). In the Dirichlet case, we cover both the strong imposition as well as a weak enforcement of the boundary data through a Nitsche/Ghost penalty-type method. In all cases, we recover second-order convergence on a suitable discrete version of the H^1 norm, matching the underlying FDM/FEM accuracy [1].

Using a suitable universal approximation theorem for tanh networks, we show that, for all problems, it suffices a number of network parameters that is $\mathcal{O}(h_{\max}^{-1})$ to achieve the same accuracy as the underlying numerical method.

We will illustrate the robustness of the approach through numerical experiments.

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NUMERICAL IMPLEMENTATION FOR PLASMA 3-T TEMPERATURE DIFFUSION IN MULTIMATERIAL SYSTEMS

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ABSTRACT

A numerical method is developed for three-dimensional time-dependent plasma 3-T temperature diffusion in numerical simulations involving mixed cells. The focus of the development is on the formulation for large time steps, the correct treatment of the discontinuity, the conservation of energy, and the nonlinearity in the mathematical equations. The discontinuity in material diffusion coefficient is correctly treated based on governing physics principles. For mixed cells, material interface reconstruction is applied. The nonlinearity is exactly treated. Compared with existing interface-aware methods for plasma 3-T temperature diffusion, the proposed method and implementation are simpler. The correctness and features of the method are demonstrated through numerical examples.

Solving plasma 3-T radiation diffusion equations is often a critical step in numerical simulations of multi-physics. Many of these simulations involve mixed cells. Within a mixed cell there are more than one material. The existence of mixed cells is due to either initial distribution of material or other physics packages, such as hydrodynamics and advection.

For plasma 3-T diffusion equations to resolve the sub-cell structure within mixed cells is important for many problems. The importance is due to three facts. First, materials within a mixed cells are not necessarily in thermal equilibrium with each other. The use of a single value for temperature within a mixed cell is inappropriate. Second, for real physics and engineering problems, tables for equation of state (EOS) are unavailable for a mixture of materials. An averaging procedure of EOS tables cannot describe the mixture well. Third, an operator-splitting technique is used in many multi-physics codes, in which the results of temperature are used as inputs of a subsequent physics package. A subsequent physics could be temperature-sensitive, i.e., the result of subsequent physics could sensitively depend on temperature of each material in mixed cells. If temperatures and material properties within a mixed cell are homogenized through some weighted average, after the homogenized temperature is updated through plasma 3-T radiation diffusion equations there is no physics principle available to separate the temperatures of different materials.

To resolve the sub-cell structure, a mixed cell is decomposed to a set of sub-cells through material interface reconstruction. The sub-cells generated through the reconstruction are general polyhedrons in three dimensions. Therefore, the approach proposed and implemented here is for general polyhedral meshes. The coupling between radiation and electron temperatures is nonlinear. The treatment of the nonlinearity is complete nonlinear in this method and implementation, and no approximation is made for this.

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A ROBUST APPROACH FOR INTERFACE RECONSTRUCTION IN THREE DIMENSIONS AND ITS APPLICATIONS

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ABSTRACT

To resolve subcell structure, material interface reconstruction is often used in numerical simulations with multi-material. We present an approach to approximately reconstruct the interfaces between materials within arbitrary polyhedrons in three dimensions. The approach is simple, accurate, and robust, which includes the orientation and location of each interface. The number of materials in the problem could be more than two. The approach is applicable to both structured and unstructured meshes. The approach could be used in numerical simulations for, such as, hydrodynamics, adaptive mesh refinement, thermal and radiation diffusion, and diffusion of magnetic field. The numerical examples are presented to show the feature of the approach in the applications.

The key step in the material interface reconstruction is to determine the equation of the interface between materials with a mixed cell, in which the normal direction of the interface is first calculated. After that, the plane constant is calculated obtained in a rotated coordinate system in which the z-coordinate is along the normal direction of the interface. We then order the vertices of the polyhedron in the order of their z-coordinates. Finally, for a given volume of the target material within the mixed cell, we find two bounding vertices of the polyhedron, and through bisecting or Newton iteration to find the final the location of the interface.

This approach works for multi-material simulations with mixed cells of more than two-materials and works for the polyhedrons with non-planar faces.



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SYNCHRONISED NUMERICAL METHODS

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ABSTRACT

Discretising partial differential equations can produce numerical errors, and in particular symmetry errors. Symmetry can be fitted into the numerical method [4] based on three approaches. The first is to align the mesh with the underlying symmetry and adapt the numerical method accordingly [1, 8]. A second approach is to use the natural coordinate frame and to use a coordinate transformation from physical to computational space. For this type of strategy, the symmetry is contained within the Jacobian for the transformation and is embedded in a Geometric Conservation Law [9]. Finally, a third approach is to modify the numerical method to reduce the asymmetric errors, inherent within the truncation terms, by using more information from the wider computational mesh stencil [7]. Partial differential equations remain unchanged when certain transformations are performed; these symmetries leave the equations invariant after a given transformation. Lie group theory has been shown to be a general way of determining these symmetries and has been used to find analytic solutions to many partial differential equations, such as the hydrodynamic related equations [3]. However, in general the discretised equations do not preserve these symmetries, unless specifically constructed [2,5]. By extending Lie groups to the discrete system [6] we develop governing principles of SYNChronised numerical methods; SYmmetries of the partial differential equations are Numerically Captured. By introducing the concept of numerical symmetry breaking, we will show why some numerical techniques are more suitable than others for a given application.

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ARBITRARY ORDER SUB-CYCLING STRATEGY APPLIED TO FINITE-VOLUME UPDATED-LAGRANGIAN SECOND ORDER METHOD FOR FLUID-STRUCTURE INTERACTION

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ABSTRACT

We propose a partitioned numerical framework for the simulation of fluid–structure interaction problems in fast transient regimes, where strong compressibility effects and shock waves propagate across moving interfaces and may penetrate the solid domain. The method is designed to combine arbitrary-order time integration, sub-cycling capabilities, and strict discrete conservation properties within a unified formulation.

The coupling strategy is formulated at the algebraic level as a saddle-point problem that enforces the conservation of mass, momentum, and total energy at the fluid–structure interface [5]. Under standard definiteness assumptions inherited from the underlying fluid [1, 3] and solid [2, 4] discretizations, the resulting coupled system is well posed and admits a unique solution. This formulation also naturally accommodates sliding interface conditions.

High-order temporal accuracy is achieved by enforcing the coupling conditions consistently at each Runge–Kutta stage. Sub-cycling enables the fluid and solid solvers to evolve according to their respective stability constraints, without resorting to temporal interpolation at the interface.

The present work focuses on second-order spatial accuracy, which is sufficient to assess the proposed coupling and time-integration strategy and remains independent of the specific spatial discretization. A series of numerical experiments in one, two, and three space dimensions demonstrates that the method preserves the expected order of accuracy in time, maintains conservation up to machine precision, and remains robust in shock-dominated configurations involving strong fluid–structure interactions.

Overall, these results establish a general and systematic framework for the construction of high-order, conservative, partitioned fluid–structure interaction methods suited to fast dynamics and disparate time scales.

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IMPLEMENTATION OF A HOT ELECTRON SOURCE TERM AND ELECTRON CASCADE MODEL TOWARDS SIMULATING LASER-PLASMAS RELEVANT TO INERTIAL CONFINEMENT FUSION

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ABSTRACT

We present a nonlocal heat transport source term and energy cascade algorithm, implemented into the radiation hydrodynamics code `xRAGE`[1, 2], to consider the effect of suprathermal—i.e. “hot”—electrons on heat transport in material conditions relevant to inertial confinement fusion (ICF). These hot electrons are typically generated via parametric instabilities from laser-plasma interactions that preferentially accelerate electrons to high velocities (energies). Both the hot electron source term and energy cascade algorithm are integrated into the multigroup diffusion, nonlocal heat transport convolution “SNB” model first proposed by Schurtz, Nicolai, and Busquet[3]. The hot electron source term models far-reaching pre-heat effects, while the cascade algorithm modifies the hot electron heat transport in a manner consistent with a continuous slowing down approximation. The details of the implementation will be described in this work. In addition, we will show comparisons of simulations with experiment[4], for assessing and benchmarking the model.

Recent progress in inertial confinement fusion experiments demonstrate significant fusion yields that exhibit promise for commercial fusion energy and other scientific applications. But a longstanding challenge in the field of high-energy-density physics is the development of a predictive simulation framework, as these experiments are complex multi-physics systems. One difficulty emerges from laser-plasma-interactions (LPI) at the fusion-relevant laser intensities that can generate hot electrons, which transports heat far from the laser-plasma and can cause deleterious preheating. These hot electrons are generated by LPI such as Stimulated Raman Scattering or Two-Plasmon Decay that decay the light wave into one or two electron-plasma waves which excite electrons to high energies.

In plasmas, where collisions between particles are dominated by Coulombic interactions, thermal heat conduction via electrons scales as $\kappa_e \propto T_e^{5/2}$, where T_e is the plasma (electron) temperature. The thermal conductivity exhibits a much stronger temperature dependency here than in neutral gases, where $\kappa \propto T^{1/2}$. In the laboratory, ICF plasma conditions are typically progenated by high intensity lasers, coupling energy to matter with absorption coefficient $\kappa_{abs} \propto n_e^2$, where n_e is the free electron particle density. This strong scaling of κ_{abs} with n_e means that the laser energy deposition occurs over small spatial extents, leading to high temperatures

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and strong temperature gradients. Thus, energy transport via electron heat conduction is very significant in many ICF systems.

The validity of Fourier-type heat transport requires that the Knudsen number is small, or $\text{Kn} = \lambda_{ei}/L_T \ll 1$, where the electron-ion mean free path λ_{ei} is proportional to T_e^2 , and the temperature gradient scale length $L_T = |T_e/\nabla T_e|$. This is frequently invalid in ICF conditions, where heat-carrying electrons propagate far beyond local temperature gradients. Alternatively, Schurtz, Nicolaï and Busquet proposed a multigroup diffusion convolution approach to represent the *nonlocal* transport present at such conditions. The SNB model has been benchmarked against kinetic calculations, and has been integrated into numerous radiation-hydrodynamic codes used for ICF modeling, including xRAGE.

In this work, the SNB modeling framework is leveraged to model the heat transport effects from high energy—aka hot—electrons via a hot electron source term and electron cascade. An example of these effects is shown in Figure 1 which represents a temperature relaxation problem from a hot, low-density material through a cold, high density material. The temperature relaxation with nonlocal (SNB) transport exhibits longer spatial heating compared to the fourier type conduction, however the transport is attenuated by the cold, dense material. In contrast, the hot electron source term enables substantial long range preheating. The details of the implementation will be described in this talk, and we will present results in experimentally relevant conditions.

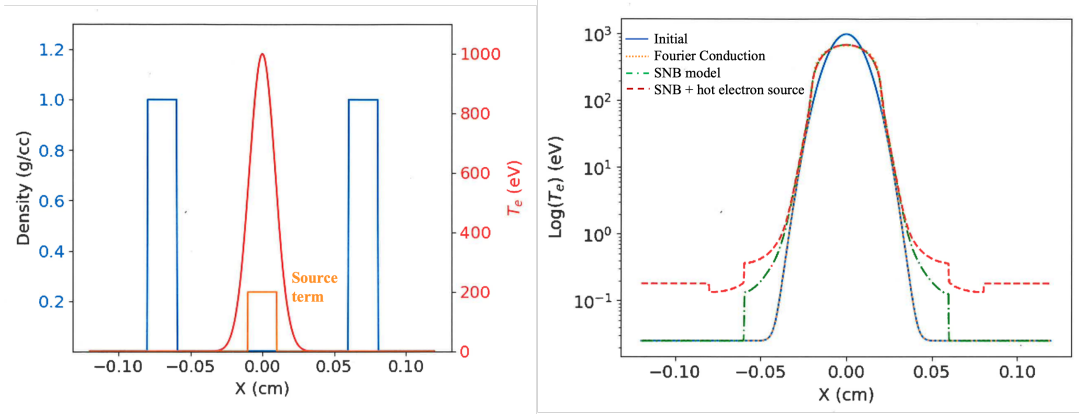


FIGURE 1: Left: Temperature and density conditions for temperature relaxation test. The orange line (dimensionless) indicates the hot electron source. Right: temperature profile after some time from fourier conduction, nonlocal (SNB) conduction, and nonlocal heat conduction with the hot electron source.

ACKNOWLEDGMENT

We would like to thank Gary Kerbel, Marty Marinak, and Mehul Patel from Lawrence Livermore National Laboratory, and Zachary Johnson from Los Alamos National Laboratory.

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LAGRANGE-REMAP SCHEME FOR 3D IDEAL MHD EQUATIONS IN A CARTESIAN AMR HYDROCODE

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ABSTRACT

We present the high-order numerical scheme implemented in the cartesian AMR hydrocode HERA developed at CEA for 3D ideal MHD equations. Our method is based on the theoretical work published by Després in [1]. The cornerstone of this method is a reformulation of the MHD system in which we duplicate the magnetic field: one instance - that we denote $\mathbf{B}$ - is used for conservation purposes while the other - denoted $\mathbf{C}$ - supports the involution equation. From a numerical point of view, $\mathbf{B}$ is cell-centered while $\mathbf{C}$ is face-staggered and advanced separately in time. By doing so, we show that our 8-equation MHD model is conservative and symmetrizable. This allows to design a first-order entropic multidimensional Lagrangian scheme, based on a 7-wave Riemann solver which is an extension to ideal MHD of the two-state acoustic Riemann solver of Godunov for hydrodynamics [2]. High-order is achieved - in the limit of the linearized MHD equations - thanks to an extension to ideal MHD of the GAIA solver of Del Pino *et al.* [3]. The high-order remapping step is similar to the one published in [4] for hydrodynamics.

We will also discuss the coarsening and refinement AMR steps and conclude by presenting numerical results on standard test-cases in 2 and 3 dimensions.

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ADAPTIVE MESH REFINEMENT FOR COMPRESSIBLE MULTIMATERIAL HYDRODYNAMICS SIMULATIONS USING A PERFORMANCE PORTABLE IMPLEMENTATION

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ABSTRACT

Kalypso (Kokkos Applicative LaYer for Parallel and Scalable Solvers on Octrees) is a new software platform, recently introduced [1], implementing octree-based block-structured adaptive mesh refinement (AMR) in a performance portable way. Kalypso is capable of running efficiently large-scale compressible hydrodynamics simulations on a cluster of multicore CPUs or a cluster of graphics processors (GPU), using a single C++ code base, designed with the Kokkos library [2]. Mesh management in distributed memory is implemented with the help of the p4est library, which provides MPI parallel CPU implementation of the forest of octrees AMR algorithms. All application data are allocated on the computing device, either a CPU or a GPU, and managed directly by kalypso. One of the key design choice of kalypso architecture is to use a lightweight hash table based (or dictionary) data structure for exchanging mesh geometry information between p4est, running on the host CPU, and the computational kernels executed on the accelerated device. Using comparable hardware resources and considering a second order MUSCL-Hancock solver for Euler equations with AMR activated, kalypso demonstrates a consistent $\times 5$ speedup for CPU to GPU time to solution. Figure 1 illustrates AMR capabilities on a air-helium shock bubble interaction.

In the present work, we consider two different types of numerical schemes for solving compressible multimaterial hydrodynamics on distributed adaptive meshes. The first one consists in extending the direct approach, solving the so-called 5-equations model [3] with a second order MUSCL-Hancock method and the HLLC Riemann solver. We also use the THINC (Tangent of Hyperbola for Interface Capturing) method for material interface reconstruction in mixed cells [4, 5]. The second numerical scheme uses a Lagrange-Remap approach [6] which is able to handle simulations with a large number of materials by using a new sparse data structure for storing efficiently all material volumic fractions. We will present performance measurements of both numerical schemes on high-end supercomputers.

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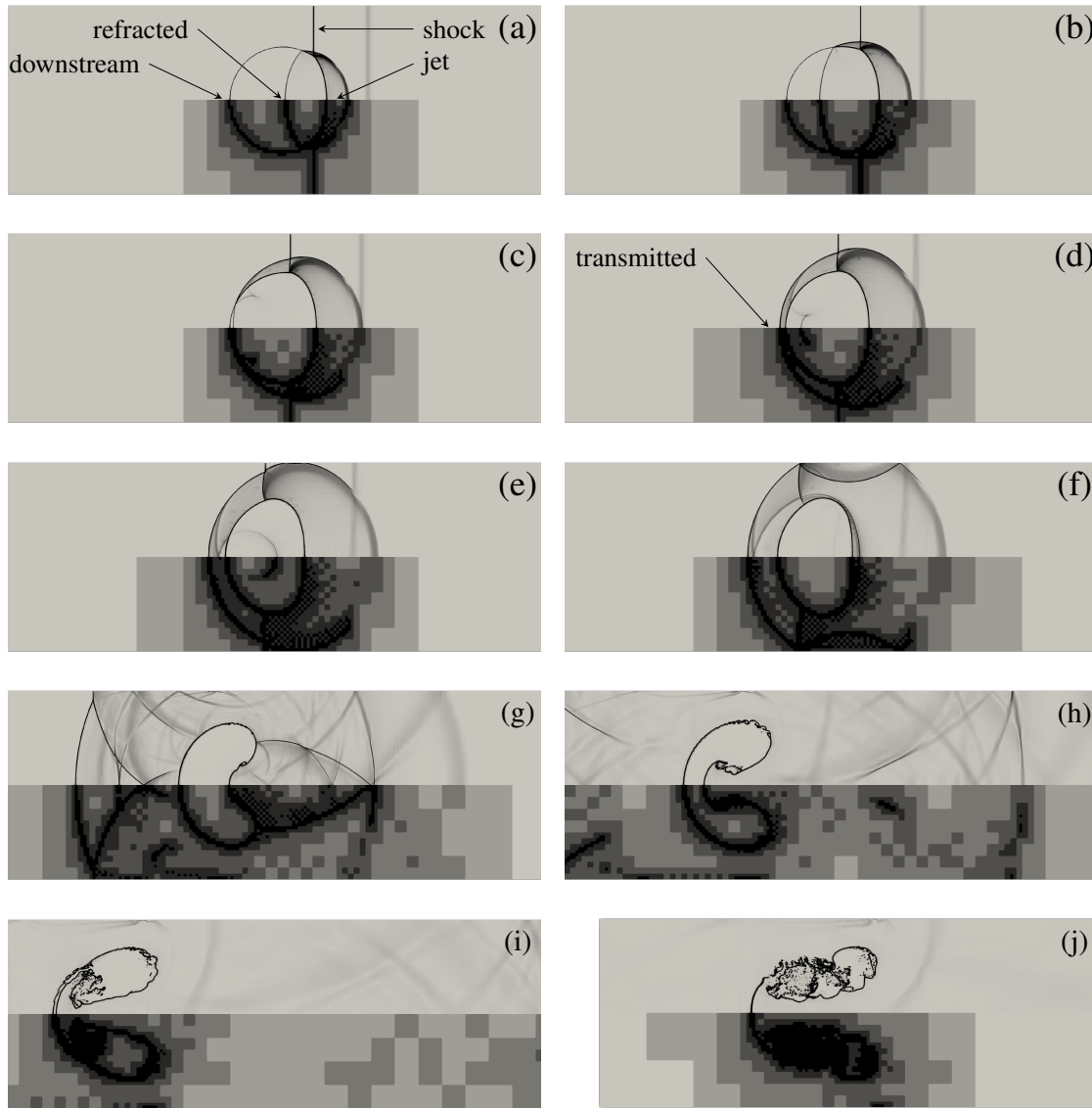


FIGURE 1: Numerical schlieren plots of the air-helium shock-bubble interaction at different times after the shock first hits the bubble: (a) 26, (b) 37, (c) 52, (d) 62, (e) 80, (f) 102, (g) 245, (h) 427, (i) 674 and (j) 983 μs ; those times were chosen to allow direct comparison with experimental data by Haas & Sturtevant (1987) and subsequent numerical works, e.g. Quirk & Karni (1996), Coralic & Colonius (2014), Terashima & Triggvason (2009), Jolgam et al (2024) to name a few. For each snapshot, the upper half shows the numerical schlieren of density and the lower half displays the AMR levels ($l_{\min} = 2$ to $l_{\max} = 7$). Block size is 8^2 , AMR cycle run every 10 time steps. From (a) to (i), all images are drawn using the same frame; (j) was recentered. Numerical scheme is MUSCL-Hancock. This figure is borrowed from [1].

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MODELING OF CONTACT LINE DYNAMICS WITH A VOF/EMBEDDED BOUNDARY METHOD FOR ISOTHERMAL SLOSHING

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ABSTRACT

This work presents a validated numerical framework for simulating isothermal sloshing in complex geometries, developed as part of the HASTA project to support future non-isothermal studies [1]. Utilizing the Basilisk open-source CFD solver [2], the hydrodynamics are modeled using a finite-volume formulation on adaptive quadtree/octree meshes [3]. The liquid-gas interface is captured via a geometric Volume-of-Fluid (VOF) method, while complex tank geometries are represented through an embedded boundary (cut-cell) approach [4].

A key technical contribution of this study is the modification of the contact-line treatment to overcome numerical pinning in small cut cells [5]. By extrapolating the volume fraction from one cell inside the fluid domain, an implicit one-cell slip length is introduced. This approach allows the contact line to slide effectively along the embedded walls without artificial pinning.

The modified scheme is validated against several benchmarks:

- **Sessile Droplet Tests:** Demonstrates improved equilibrium profiles and reduced orientation-dependent spreading errors on inclined planes in both 2D and 3D simulations.
- **Standard Sloshing Benchmarks:** Shows excellent agreement with pressure signals from Rezaei and Ketabdari (2007) [6] and torque loads compared to STARCCM+ simulations [7].
- **Experimental Validation:** Validation against the experimental data of Ángel Martín (2013) [8] covering filling levels of 25%, 50%, and 75% and excitation frequencies ranging from 0.8 to 2.4 Hz, demonstrates the model's capability to predict periodic sloshing-induced loads with a mean nRMSE of 6.5%.

The results confirm that this robust VOF/embedded-boundary framework provides a reliable foundation for the subsequent development of non-isothermal, thermally coupled sloshing simulations involving tank excitation.

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ACKNOWLEDGMENT

This work is part of the HASTA project, which has received funding from the European Union's Horizon Europe research and innovation programme under Grant Agreement No. 101138003. Views and opinions expressed are however those of the authors only and do not necessarily reflect those of the European Union.

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DEVELOPMENT OF A NON-LINEAR MODEL FOR CROSS BEAM ENERGY TRANSFER FOR LASER RAY-TRACING IN RADIATION-HYDRODYNAMICS CODES

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ABSTRACT

Accurate modeling of laser energy deposition is critical for capturing hydrodynamic behavior in laser-driven inertial confinement fusion (ICF) implosions and high energy density (HED) experiments. Cross Beam Energy Transfer (CBET), a laser-plasma instability that resonantly transfers energy between beams, fundamentally alters deposition patterns and subsequent implosion dynamics. While CBET is known to significantly impact ICF experiments and is routinely used as a tool to control implosion symmetry, existing code models do not reproduce behavior observed in experiments [1]. Modeling laser-plasma instabilities in complex HED environments presents significant challenges. The commonly employed linear model is inadequate because CBET nonlinearly influences laser energy transport, altering the plasma conditions that drive the instability itself. Accurately modeling laser-plasma instabilities thus requires a self-consistent co-evolution of both the plasma state and the instabilities themselves. Nonlinear effects lead to deviations of CBET gain from linear theory based on single-Maxwellian distributions and determine the time-dependent nature and magnitude of CBET gain as the system approaches steady state [2]. We discuss the development and implementation of the nonlinear model described in [2] into the xRAGE radiation-hydrodynamics code. This work presents a comparative analysis of nonlinear and linear CBET models to assess their predictive capabilities in capturing CBET. We will present simulations of an experimental platform specifically designed to directly quantify inner beam CBET at peak power, enabling isolated measurement of CBET effects [3]. These results will provide crucial insights into the role of nonlinear physics in CBET modeling and may help resolve discrepancies in current implosion symmetry predictions.

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INCREMENTAL MESH OPTIMIZATION BY RECONNECTIONS FOR 3D DIRECT ARBITRARY-LAGRANGIAN-EULERIAN SIMULATIONS

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ABSTRACT

Moving mesh numerical methods are very useful for representing sharp interface multi-material interactions and naturally adapt the resolution to continuum flow. But after a certain time, ALE computations are prone to mesh overdeformation and potentially catastrophic tangling especially in high shear or vortical flow regions. This can be effectively prevented by mesh optimization consisting of vertex smoothing and reconnection, greatly increasing the robustness of such computations.

We work with the high order ADER-DG numerical scheme on moving Voronoi-like polyhedral meshes determined by Delaunay tetrahedral generator grids. This method is based on a fully-discrete space-time conservation formulation of the governing hyperbolic PDE system, utilizing its weak formulation to integrate a polynomial solution over 4D space-time control volumes [2, 3]. Such control volumes can be determined for moving polyhedra, but also for regions with changing connectivity (creating degenerate space-time *hole-like elements*), given that the reconnections are constrained to transformations with a uniquely definable and continuous geometrical space-time description. This has been employed in two-dimensional setting [2] and is recently investigated also in 3D [1]. Examples of such transformations in three spatial dimensions are the reciprocal 3-2 and 2-3 flips on tetrahedral meshes and their corresponding dual representation (see Figure 1).

Our mesh optimization algorithm makes use of the fact that every transformation of the tetrahedral mesh preserving the number of vertices can be expressed as a sequence of elementary flips. The combination of flip sequences and vertex smoothing is shown to be an effective mesh optimization strategy in practice (eg. [5]). To avoid an indirect remeshing step or mesh intersections, our mesh reconnections are fully embedded within the numerical method, having the same accuracy with no recognizable imprinting of reconnecting operations on the solution. This comes with constraints on the mesh optimization algorithm – the optimal mesh cannot be reached at once, but following *incremental* elementary transformations performed over the course of several successive timesteps.

The available software tools (eg. [4]), although very capable, usually do not offer the option of performing mesh reconnection on a sequential flip-by-flip basis. Therefore we investigate the possibilities of performing the required *incremental* mesh optimization and the properties of such algorithm. We consider its ability to uphold the mesh quality while not further decreasing the time step, its performance in context of preventing or removing *sliver*-type tetrahedra and the interplay of reconnections and mesh smoothing. We study the influence of algorithm parameters such as the various mesh quality indicators available on the resulting mesh time development representing vortex-like flows.

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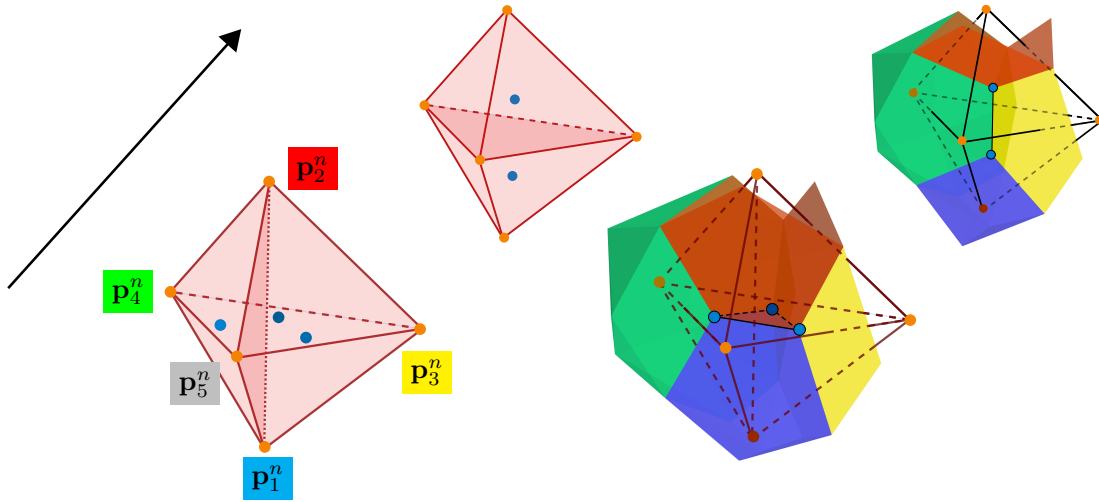


FIGURE 1: Local transformation of a dual mesh (right) corresponding to the 3-2 elementary flip on a tetrahedral mesh (left)

ACKNOWLEDGMENT

M. Klima and E. Gaburro gratefully acknowledge the support received from the European Union with the ERC Starting Grant ALcHyMiA (No. 101114995). Views and opinions expressed are however those of the author only and do not necessarily reflect those of the European Union or the European Research Council Executive Agency. Neither the European Union nor the granting authority can be held responsible for them.

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HOURLASS CONTROL IN STAGGERED-GRID HYDRODYNAMICS USING VIRTUAL ELEMENT STABILIZATION TECHNIQUES

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ABSTRACT

Numerical simulations using the staggered-grid hydrodynamics (SGH) discretization suffer from hourglass instabilities. In this work, we develop a stabilization method to suppress the hourglass instabilities using techniques from the virtual element method (VEM). The stiffness matrix of the VEM consists of two terms: the *consistency matrix* which is rank deficient and the *stability matrix*. We first show that in two dimensions and on general polygons, the stiffness matrix of the SGH is identical to the consistency matrix of the linear VEM for both the diffusion equation and the linear elasticity equation. These analyses explain the origin of the hourglass instabilities of the SGH discretization method, and establish a theoretical foundation for our proposed stabilization method by augmenting the stiffness matrix of the SGH discretization using the VEM stability matrix. Then, we present numerical examples using Lagrangian SGH simulations. The numerical experiments demonstrate that the proposed VEM stabilization method is effective at eliminating hourglass modes in the SGH discretization.

INTRODUCTION

In this work we develop a stabilization method to suppress the hourglass instabilities in the staggered-grid hydrodynamics using techniques from the virtual element method (VEM) [1].

1 LINEAR ELASTICITY

Let $\mathbf{u} : \mathbb{R}^d \rightarrow \mathbb{R}^d$ be the vector-valued displacement field, the linear elasticity equation is given as

$$-\nabla \cdot \boldsymbol{\sigma}(\mathbf{u}) = \mathbf{f}, \quad \text{on } \Omega, \quad (1)$$

where $\boldsymbol{\sigma}$ is the Cauchy stress tensor, and $\mathbf{f}$ is a vector-valued forcing term. The Cauchy stress tensor is given as

$$\boldsymbol{\sigma}(\mathbf{u}) = \lambda (\nabla \cdot \mathbf{u}) \mathbf{I} + \mu (\nabla \mathbf{u} + \nabla \mathbf{u}^T), \quad (2)$$

where λ and μ are the Lamé constants, $\mathbf{I}$ is the second-order identity tensor.

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1.1 Staggered-grid hydrodynamics

Using staggered-grid hydrodynamics (SGH) to discretize the left-hand-side of eq. (1), we arrive at the following:

$$\sum_{j=1}^{N^E} \mathbf{K}_{E,ij}^{\text{SGH}} \mathbf{u}_j, \quad \forall i = 1, \dots, N^E, \quad (3)$$

where N^E is the number of nodes in the element E, $\mathbf{K}_{E,ij}^{\text{SGH}}$ is the element stiffness matrix using SGH, and $\mathbf{u}_j$ is the displacement at node j .

1.2 Virtual element method

Similarly, the stiffness matrix using the virtual element method (VEM) is given by

$$\mathbf{K}_{E,ij}^{\text{VEM}} = \mathbf{K}_{E,ij}^{\text{VEM,C}} + \mathbf{K}_{E,ij}^{\text{VEM,S}}, \quad i, j = 1, \dots, N^E. \quad (4)$$

Herein, $\mathbf{K}_{E,ij}^{\text{VEM,C}}$ and $\mathbf{K}_{E,ij}^{\text{VEM,S}}$ is the consistency and stability matrix, respectively.

1.3 Major results

In this work, we showed that in two-dimension, the stiffness matrix using the SGH is the same as the consistency matrix using the VEM.

$$\mathbf{K}_{E,ij}^{\text{SGH}} = \mathbf{K}_{E,ij}^{\text{VEM,C}}. \quad (5)$$

The matrix $\mathbf{K}_{E,ij}^{\text{VEM,C}}$ is rank deficient. The stiffness matrix of the SGH $\mathbf{K}_{E,ij}^{\text{SGH}}$ is not stable and hourglass instabilities can manifest in the simulation because the SGH discretization does not contain the stability contribution $\mathbf{K}_{E,ij}^{\text{VEM,S}}$ as in the VEM. Our analysis of the SGH and the VEM on the linear elasticity equation is also valid for general polygons.

We propose to stabilize the SGH using the stabilization techniques in the VEM, namely, $\mathbf{K}_{E,ij}^{\text{VEM,S}}$.

1.4 Numerical example

We consider a thick cylinder subjected to a constant internal pressure. The deformed mesh configurations and the stress profiles at $t = 9.3 \mu\text{s}$ using different stabilization techniques are shown in fig. 1.

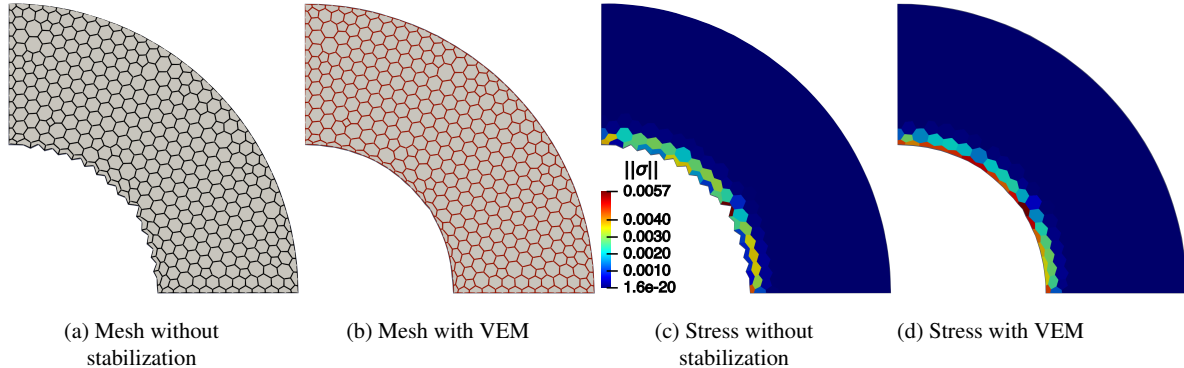


FIGURE 1: Deformed mesh (a-b) and stress in the Frobenius norm (c-d) at $t = 9.3 \mu\text{s}$ using the polygonal mesh with different stabilization techniques.

ACKNOWLEDGMENT

The authors gratefully acknowledge the support of the U.S. Department of Energy through the Advanced Scientific Computing (ASC) program at Los Alamos National Laboratory.

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ASSESSING NUMERICAL SCHEMES FOR MULTI-VELOCITY MULTI-PHASE COMPRESSIBLE MODELS

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ABSTRACT

When simulating multi-velocity multiphase compressible flows, very few comparative studies of numerical schemes exist. This lack is primarily due to intrinsic mathematical difficulties of the total-non-equilibrium model (Baer–Nunziato model without closure laws and relaxations terms). The model generates numerous sub-models due to its underdetermination, requiring assumptions on interfacial quantities, such as u_I and p_I . Moreover, the phase equations for volume fraction, mass, momentum and total energy are non-conservative, and the associated non-conservative products involve ill-defined terms, as they correspond to products of discontinuous functions that cannot be interpreted in the classical sense of derivative.

Consequently, most numerical schemes developed over the past three decades rely on different modelling assumptions, which complicates their comparison. Early work by Saurel and Abgrall introduced the HLL [1], followed by the Discrete Equations Method (DEM) [2], the HLLC of Fufaro & Saurel [3] and the HLLAC of Lochon *et al.* [4].

In this context, we propose to establish a set of discriminating test cases that impose convergence toward a common model, allowing meaningful differentiation between schemes. We aim to assess the discretisation of non-conservative products of existing methods and to recover the expected physical behavior in limiting configurations.

Figure 1 illustrates a shock tube containing two identical phases. Gradients of the volume fraction are non-zero only at the interfaces, resulting in non-zero non-conservative products. Since both phases are identical, this configuration enables the assessment of the discretisation of non-conservative terms independently of any closure effects. It therefore constitutes a particularly discriminating test case for evaluating the ability of numerical methods to recover the single-phase limit.

It is observed that all methods, except the DEM, generate a spurious wave upstream of the shock. A clear hierarchy is observed, with DEM providing the most accurate results, followed by HLLAC, HLLC, and finally HLL, which exhibits the largest deviations.

ACKNOWLEDGMENT

The authors would like to thank Maxime Reynaud and Pierre Graumer for their remarks and support.

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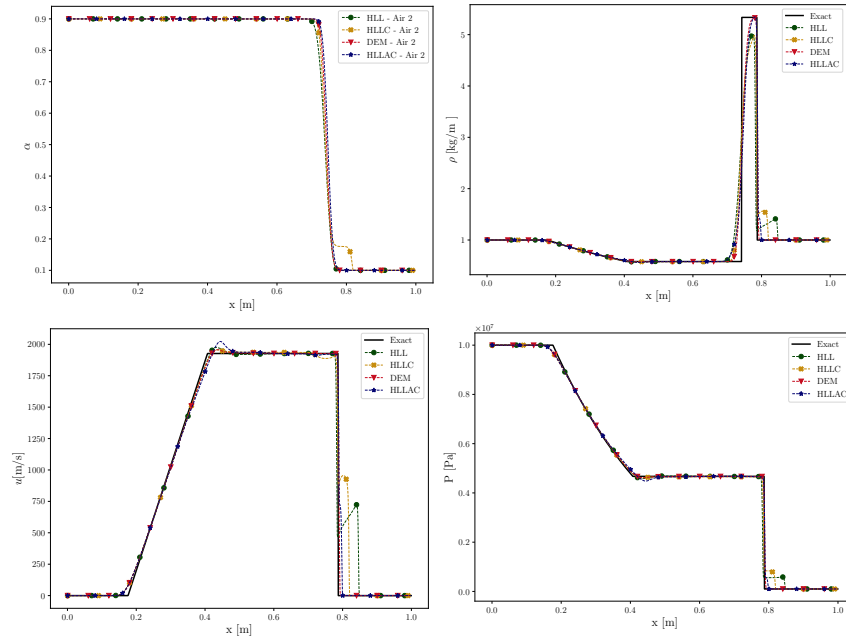


FIGURE 1: Two-phase (air–air) shock tube with non-constant volume fractions – $\alpha = 0.9/0.1$. Air is modelled as a perfect gas, $p = (\gamma - 1)\rho e$, where $\gamma = 1.4$. Uniform densities $\rho_{\text{air}} = 1 \text{ kg m}^{-3}$ and velocities $u_{\text{air}} = 0 \text{ m s}^{-1}$ are imposed on both sides, with a pressure discontinuity defined by $p_{\text{air},L} = 10^7 \text{ Pa}$ on the left and $p_{\text{air},R} = 10^5 \text{ Pa}$ on the right. The computation is carried out in one dimension on a Cartesian mesh of 10^3 cells, using a first-order scheme with non-reflecting boundary conditions. The solution is evaluated at the final time $t = 10^{-4} \text{ s}$ and $\text{CFL} = 0.8$. The reference solution, labeled ‘exact’, is the exact solution of the Euler equations, while the others correspond to the previously mentioned methods.

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VALIDATION OF A HYBRID HIGH-EXPLOSIVES BURN APPROACH IN LANL MULTIPHYSICS APPLICATIONS

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ABSTRACT

In this work, the authors validate a hybrid programmed-reactive high explosives (HE) burn approach against insensitive HE detonation experiments. Three Multiphysics applications are considered: xRAGE, which solves governing equations on an adaptive Eulerian grid, Pagosa, which performs calculations on a fixed Eulerian mesh, and FLAG, which leverages the finite element method on a Lagrangian mesh. The programmed burn models considered are the Fast Sweeping Detonation (FSD) model (xRAGE, Pagosa) and the Detonation Shock Dynamics (DSD) model (FLAG). Both programmed burn approaches are augmented with the Dynamic Small-Resolved Energy Release (DASHER) model to ensure consistency between pre-computed detonation velocities and the local thermodynamic state.

INTRODUCTION

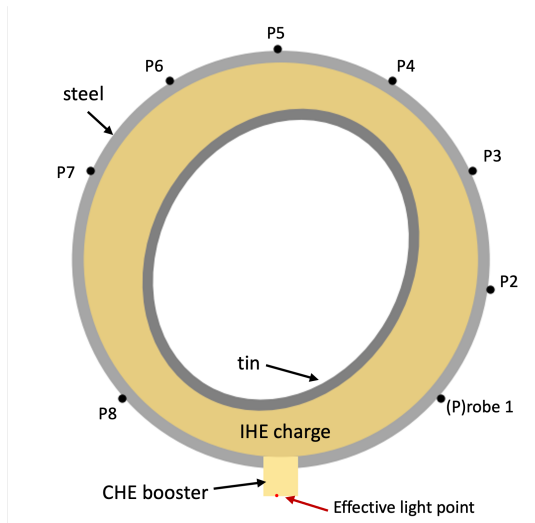
Programmed burn models, such as the Detonation Shock Dynamics (DSD) and Fast Sweeping Detonations (FSD) models, are often used for high explosives (HE) burn calculations due to their computational efficiency compared to reactive burn models. Scenarios in which the pre-computed detonation velocity (D_n) substantially deviates from the Chapman-Jouguet (CJ) velocity of HE material can yield thermodynamically inconsistent states, which can manifest as unphysically-high pressures in the vicinity of reflected shocks in HE burn calculations. This type of scenario is of particular concern for insensitive high explosives (IHEs), whose detonation behavior is sensitive to the boundary conditions of the HE material. The Dynamic Small-Resolved Energy Release (DASHER) model avoids thermodynamic inconsistencies by setting the reaction progress variable at the detonation front to a value consistent with the local detonation velocity [1] then and applying a reactive burn rate law post-detonation. This approach preserves the energy released by conversion of HE reactants to products and creates a reaction zone tail in behind the detonation front when $D_n < D_{CJ}$; this effect can be seen by visualizing computed pressure at the detonation front (Figure 1b)

PRELIMINARY VALIDATION RESULTS

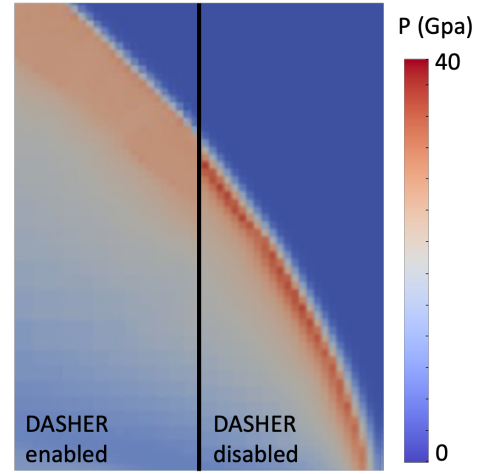
In the work to be presented the authors will validate the programmed burn models augmented with DASHER in xRAGE, Pagosa, and FLAG Multiphysics applications against IHE detonation experiments. One of the experiments to be considered is CYCLOPS I [2], which consists of an IHE main charge confined by an outer cylindrical steel jacket and an inner elliptic tin shell. A booster charge consisting of conventional HE is used to light the main IHE charge. A diagram of the experimental system is given in In Figure 1a. Photon Doppler

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(a) Diagram of the CYCLOPS I experiment. PDV probes point orthogonally at the locations designated by black circles.



(b) Pressure contour from an xRAGE simulation of CYCLOPS I with DASHER enabled (left) and disabled (right).

FIGURE 1

Velocimetry (PDV) data collected during the CYCLOPS I experiments is compared to xRAGE computations with and without DASHER enabled (Figure 2).

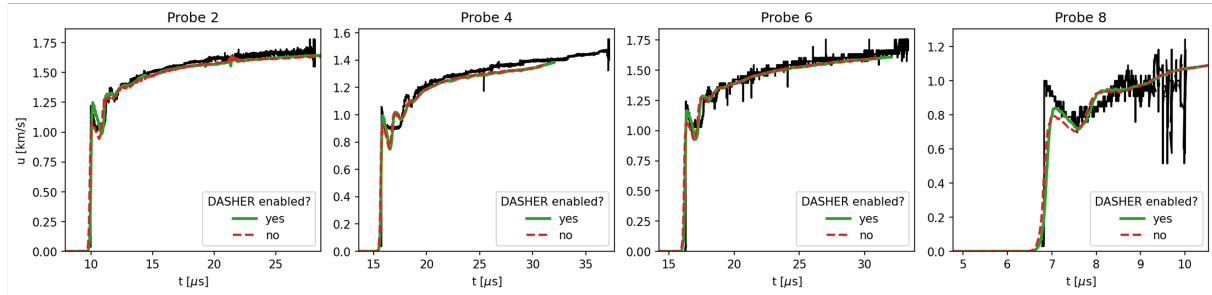


FIGURE 2: Experimental velocity of the steel case (solid black line) compared to xRAGE computations with DASHER enabled (solid green line) and disabled (dashed orange line).

ACKNOWLEDGMENT

This work was supported by the US Department of Energy through the Los Alamos National Laboratory. Los Alamos National Laboratory is operated by Triad National Security, LLC, for the National Nuclear Security Administration of U.S. Department of Energy (Contract No. 89233218CNA000001).

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INTERFACES ON A HIGH-ORDER MESH

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ABSTRACT

We have developed a high-order hydrodynamics kernel for making first assessment of the use of high-order schemes in some of our applications. To make a deeper assessment, we are interested in using the high-order kernel in multi-material problems that require a sharp interface tracking scheme on material boundaries. An existing interface scheme is available [1, 2] but it uses straight edges and is designed for low-order (p_1) cells. It is not obvious how to extend this scheme to capture curved interfaces on high-order meshes. However, it may be possible to utilise it on a refined low-order mesh with volume fractions that have been mapped down from the high-order mesh. A Low-Order Refined (LoR) method [3, 4, 5] is investigated for relevance in this approach.

INTRODUCTION

The current work is concerned with a pure Lagrangian frame in which all mesh nodes move with the fluid velocity. Conserving momentum, energy and mass in this frame gives

$$\begin{aligned}\rho(r) \frac{\partial u(\mathbf{r})}{\partial t} &= -\nabla \cdot \boldsymbol{\sigma}(r), \\ \rho(r) \frac{\partial e(r)}{\partial t} &= -\boldsymbol{\sigma}(r) : \nabla u(\mathbf{r}), \\ \frac{1}{\rho(r)} \frac{\partial \rho(r)}{\partial t} &= -\nabla \cdot u(\mathbf{r}),\end{aligned}$$

where $\rho(r)$, $u(\mathbf{r}) = (\mathbf{u}_x(\mathbf{r}), \mathbf{u}_y(\mathbf{r}))$ and $e(r)$ are defined as the density, velocity and energy at position $r(x, y)$ in the fluid at time t . $\boldsymbol{\sigma}(r) = -\mathbf{I}(EOS(\rho, e)) + \hat{\boldsymbol{\sigma}}$ is a stress tensor in which $\mathbf{I}$ is the identity matrix. $\hat{\boldsymbol{\sigma}}$ is a matrix containing (for example) strength terms or an artificial viscosity tensor. We discretise these equations with a high-order finite element method similar to that introduced in [6, 7]. An initial assessment in some of our applications has shown this approach can improve robustness, stability and fidelity in simple calculations. We are now interested in making a deeper assessment in multi-material problems which require interfaces to be tracked with minimal dissipation and without introducing excessive diffusion. In the approach we consider, a volume fraction field in a multi-material problem is mapped down from the high-order mesh on to a refined low-order mesh (p_1) by applying a LoR transform. This is done after completing a Lagrangian step on the high-order mesh. The low-order mesh is refined such that it has the same number of DoF as the high-order mesh. We assess whether an existing interface scheme can be deployed on the low-order refined mesh and if it

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can use the mapped-down volume fractions to compute volume fluxes. It may be possible to map these back to the original high-order mesh, for example by reversing the LoR transform, where they might be used to attempt an ALE step.

ACKNOWLEDGMENT

The author wishes to acknowledge the support and technical guidance of Dr. Andy Barlow in this work.

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DYNAMIC MATERIAL PRIORITY ASSIGNMENT FOR MULTI-MATERIAL EULERIAN ADVECTION

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ABSTRACT

In multi-material Eulerian simulations, material advection depends on the order in which materials are processed, commonly referred to as material priority. This ordering is typically specified *a priori* by the user based on problem geometry, but simulation results can be highly sensitive to this choice and may exhibit unphysical behavior if priorities are poorly selected. This work introduces a method for dynamically assigning material priorities on a per-cell basis using reconstructed interface geometry and local flow direction. Material centroids are computed from volume fractions and ordered according to their distance from the downwind cell vertex, ensuring consistency with the direction of advection. The method is evaluated on canonical advection problems, including the ball and jacks, and applied to a shaped charge jet impacting a flat plate.

INTRODUCTION

Accurate advection of multiple materials across computational cells is a fundamental component of modern Eulerian hydrocodes. In many multi-material methods, the advection order is prescribed *a priori* by the user based on problem geometry. During interface reconstruction, materials are recursively combined in priority order, reducing an N -material cell to a sequence of two-material problems. This assumes the chosen ordering is consistent with the local material configuration and flow direction.

However, material priority can strongly influence simulation results. If the ordering is non-monotonic with respect to the local flow direction, interface reconstruction may become inconsistent with the flow, leading to non-physical material advection. These errors are often difficult to detect and can degrade solution quality.

To address this, we propose a method for dynamically assigning material priorities locally in each cell. Material centroids are computed from volume fractions, and priorities are assigned by ordering materials according to their distance from the downwind cell vertex. The material closest to the downwind direction is assigned highest priority, aligning the ordering with the local flow.

METHOD

Interface reconstruction from volume fractions is the first step in multi-material advection in the hydrocode Pagosa [1]. The code employs Youngs' method, in which interface normals are computed from volume fraction gradients and planar interfaces are reconstructed within each mixed cell [3].

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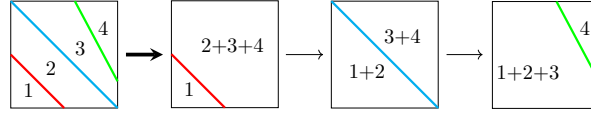


FIGURE 1: Priority Summation Example [1]

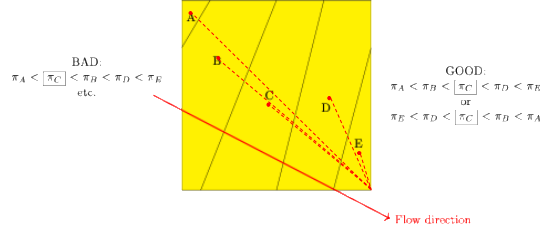


FIGURE 2: Volume Fractions and Flow Direction [1]

For cells containing more than two materials, materials are recursively combined in priority order, reducing the problem to a sequence of two-material reconstructions (Figure 1). The highest priority material is reconstructed first, followed by reconstruction of interfaces between the combined lower-priority materials.

This approach assumes that the prescribed priority ordering is consistent with the local material arrangement and flow direction. If the ordering is non-monotonic with respect to the flow direction, reconstructed interfaces may be inconsistent with the true configuration, leading to errors in material advection.

To address this, we introduce a dynamic priority assignment strategy. Material centroids are computed from volume fractions, and priorities are assigned by ordering materials according to their distance from the downwind cell vertex (Figure 2). The closest material is assigned highest priority, with remaining materials ordered by increasing distance.

This produces a monotonic ordering aligned with the flow direction and improves the consistency of interface reconstruction.

RESULTS

The proposed dynamic priority method is evaluated on canonical advection test problems, including the ball and jacks, where it preserves interface structure under complex deformation.

The method is also applied to a shaped charge jet impacting a flat plate. This problem highlights a key limitation of static priority schemes: priorities that accurately capture jet formation can degrade solution quality during jet–target interaction. The dynamic approach adapts locally to the evolving flow, improving robustness without requiring user intervention.

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AN APITALI APPROACH FOR LAGRANGIAN SCHEMES ENFORCING THE DISCRETE ENTROPY GROWTH FOR EULER EQUATIONS

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ABSTRACT

High-order numerical schemes are increasingly used for simulating compressible flows due to their ability to capture fine-scale features with high accuracy. However, ensuring physical fidelity in these schemes, particularly in the presence of shocks and discontinuities, remains a significant challenge. One critical aspect is the discrete entropy growth which is essential for maintaining the thermodynamic consistency of numerical solutions. Entropy is the nonlinear stability criterion for Euler equations and is generally not used in MOOD and APITALI methods. In this study, we explore the application of the APITALI (A Posteriori ITeRAtive LImiter) method to address entropy variation issues in the GAIA scheme (see [3]) for solving Euler equations in pure Lagrangian coordinates, making our method invariant-domain preserving.

The APITALI method (see [2]) is an a posteriori limiter method. In this work, we use it to enforce entropy stability by adaptively adjusting high-order fluxes based on local entropy growth. This method applies to incomplete equations of state (EOS) by estimating the variation of entropy. The validity of this approach is verified with comparison to complete EOS calculation. This strategy ensures compliance with the second law of thermodynamics and prevents spurious oscillations near discontinuities.

We validate our approach using the challenging Bizarrium test case (see [1]), characterized by non-convex isentropes and complex shock structures. Without APITALI, high-order schemes such as GAIA with TVD or Minmod limiters fail to converge or capture the physical solution. With APITALI the schemes converge robustly, accurately capturing the entropic solution. These results highlight the importance to carefully tune numerical dissipation to achieve a balance between stability and accuracy.

We also apply the method to multi-dimensional Lagrangian schemes as high-order extensions of Glace and Eucclhyd. Relevant test problems show that APITALI also performs well in this framework. This work demonstrates the effectiveness of the APITALI method in ensuring entropy stability for high-order Lagrangian schemes, particularly for non-convex EOS and complex shock interactions.

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SMASH: A NEXT-GENERATION MULTIPHYSICS SHOCK-HYDRODYNAMICS CODE

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ABSTRACT

SMASH is a new multiphysics shock-hydrodynamics code developed at Sandia National Laboratories. It solves the multimaterial compressible Euler equations with material strength using a block structured adaptive mesh refinement (AMR) grid. The Lagrange step uses a staggered finite element spatial discretisation and a midpoint predictor-corrector time integration method with artificial viscosity for shock capturing. Remap is based on the compatible total energy conservation method of Burton et al. [1]. Multiphysics solves use an interface-aware sub-cell integration method in an attempt to approach body-fitted accuracy on a Cartesian grid. Additionally, we use the shifted boundary method to apply Dirichlet boundary conditions on material surfaces inside mixed material elements. SMASH has been designed from the ground up for performance portability and in particular takes advantage of GPUs and SIMD vector instructions on CPUs. We present details of the numerical methods, computational infrastructure, and initial results on terminal ballistics problems and verification results for elliptic solves with the shifted boundary method.

ACKNOWLEDGEMENT

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

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A REGULARISATION KERNEL METHOD FOR INTERFACIAL PHASE CHANGE IN DIFFUSE INTERFACE APPROACHES

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ABSTRACT

INTRODUCTION

The numerical diffusion of the liquid–vapour interface over several mesh cells is inherent to many two-phase modelling approaches, such as Euler–Euler, algebraic Volume Of Fluid (VOF) and phase-field methods. The presence of a diffuse interface complicates the accurate modelling of phase change, which is physically a phenomenon localised at the interface.

To improve the accuracy of phase change modelling in this context, one approach is to first calculate the phase change flux per unit area at the interface position reconstructed via an isocontour. This source term is then redistributed over the thickness of the diffuse interface, yielding a phase change term per unit volume. Hardt and Wondra [1] were the first to introduce this method. It was subsequently adopted in several computational codes, such as OpenFOAM [2] (VOF) and NEPTUNE_CFD [3] (Euler–Euler). Loiseau *et al.* [3] demonstrated that this approach provides significantly improved mesh convergence and accuracy compared to methods that directly compute a volumetric phase change term.

The redistribution method proposed by Hardt and Wondra consists in solving a diffusion equation of the form:

$$\frac{\partial \Gamma}{\partial t} = D \Delta \Gamma, \quad (1)$$

where Γ represents the rate of phase change per unit volume, which is initialised to $\dot{m} \frac{A_i}{V}$. $\dot{m}$ corresponds to the rate of phase change per unit area, and A_i to the interfacial area reconstructed on a control volume of size V . This approach introduces two parameters that control the diffusion thickness: the coefficient D and the resolution time of the partial differential equation. Their calibration is delicate and does not guarantee a distribution of the source term consistent with the thickness of the diffuse interface.

REDISTRIBUTION METHOD

In this work, we propose a new method to redistribute the surface mass flux $\dot{m}$ [kg/m²/s] into a volumetric source term Γ [kg/m³/s]. This approach is inspired by immersed boundary methods used to distribute surface forces [4].

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Let A denote the interfacial area, and let $x_A \in A$ be a point on this surface. Mass conservation then implies:

$$\Gamma(x) = \int_A \dot{m}(x_A) \delta(x - x_A) dA. \quad (2)$$

The Dirac δ distribution is approximated by a regularisation kernel K , which is decomposed into a normal component and a tangential component at the reconstructed interface as follows:

$$K(x - x_A) = K_n(d_n) K_t(d_t), \quad (3)$$

where $d_n = (x - x_A) \cdot \vec{n}$ and $d_t = (x - x_A) \cdot \vec{t}$ are the distances projected along the normal and tangent to the interface, respectively. The normal component K_n is constructed from the volume fraction profile of the diffuse interface and is evaluated at every time step. The tangential component K_t is chosen such that analytical integration is possible on each segment resulting from the reconstruction of the interface.

VALIDATION

The proposed method allows for a more accurate redistribution of the surface source term, in accordance with the geometry of the interface. This strategy has been implemented in a non-thermal-equilibrium Euler-Euler model (in the TRUST code [5]) and validated on the one-dimensional Stefan problem using the properties of liquid water and steam, with a wall temperature set at 125 °C. Figures 1 (a) and (b) show the interface position and the relative error in the interface position, respectively, as a function of time. The proposed method yields a significantly lower error compared to the results obtained by Loiseau using the NEPTUNE_CFD code [6] at the same mesh resolution. Preliminary two-dimensional simulations are ongoing and exhibit encouraging results.

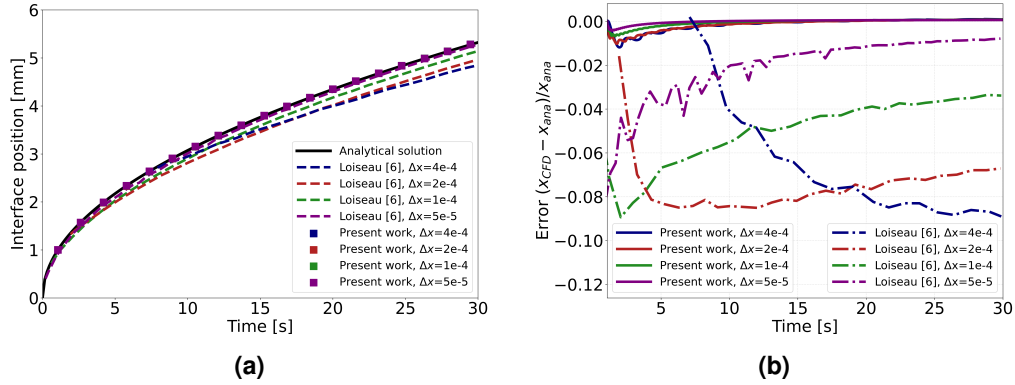


FIGURE 1: Interface position (a) and relative error (b) as a function of time for different meshes, compared with the analytical solution and the results from Loiseau [6].

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MATHEMATICAL AND NUMERICAL STUDY OF OPTIMIZED NAVIGATION IN STRATIFIED WATERS

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ABSTRACT

This work investigates the dead-water phenomenon, a hydrodynamic effect that can slow down ships navigating in stratified fluids due to the generation of internal waves at the interface between two layers of different densities, thereby creating additional resistance to the vessel's motion [1]. The aim is to model and analyze these waves by combining theoretical and numerical approaches. We develop a linear model of ship motion in a two-layer stratified fluid, in which the ship velocity is variable. A spectral version of the model, including a Rayleigh damping term, is studied. We prove that the associated Cauchy problem admits a unique solution when the velocity and the initial conditions are sufficiently regular [2]. The case of constant velocity is analyzed, highlighting the existence of a critical speed that separates two dynamical regimes and plays a central role in wave propagation at the interface between the two fluids [3]. For the numerical method, we use a scheme based on the discrete Fourier transform in space and an exponential integrator in time [4], reducing numerical dissipation and dispersion. One- and two-dimensional simulations illustrate the theoretical results. If time permits, we will also introduce optimal control results. In this context, the aim is to minimize internal waves caused by the passage of the ship, while ensuring that the ship reaches its destination.

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SHOCK-INDUCED TRANSITION FROM UNIFORM TO JETTING BUBBLE COLLAPSE IN LIQUIDS

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ABSTRACT

We examine the conditions under which a gas bubble embedded in a shocked liquid collapses quasi-uniformly or develops a re-entrant jet. The central hypothesis is that collapse morphology is governed by the ratio of the shock–bubble interaction time, τ_i , to the inertial collapse time, τ_c . When $\tau_i/\tau_c \ll 1$, the bubble experiences an effectively uniform pressure loading and collapses nearly spherically; when $\tau_i/\tau_c = O(1)$ or larger, finite shock-transit effects generate strong asymmetry and jet formation. Using a Rayleigh-type estimate for τ_c and the Rankine–Hugoniot jump conditions for the shocked liquid, we show that for bubbles larger than a minimum radius set by surface tension, the timescale ratio depends primarily on the shock jump conditions and becomes small only for weak shocks. Two-dimensional inviscid simulations will be used to map this transition from acoustic/weak-shock loading to strong-shock jetting, and to quantify the work required for collapse. An analytical model for uniform adiabatic collapse is developed as a baseline and compared with non-uniform simulations, showing that jetting introduces an excess energetic cost associated with asymmetric deformation and jet formation.

INTRODUCTION

Shock-driven collapse of gas cavities in liquids exhibits a transition from nearly spherical compression to strongly asymmetric collapse with a high-speed re-entrant jet. This problem is relevant to cavitation damage, shock focusing, and the response of heterogeneous liquids and fluid-filled porous materials subjected to impulsive loading [1, 3, 4]. In addition to controlling local deformation and hot-spot formation, bubble dynamics influence the effective compressibility and wave structure of bubbly media, making collapse morphology important for both mesoscale mechanics and continuum-scale shock response [2].

The present work focuses on identifying when a shocked bubble behaves as though it were subjected to an approximately uniform pressure rise and when finite shock-transit effects instead drive jetting. Our central idea is that the relevant regime boundary can be organized using the ratio of the shock–bubble interaction time to the inertial collapse time. Surface tension introduces a lower size limit below which the collapse becomes size dependent, while for sufficiently large bubbles the transition is governed mainly by the shocked-liquid jump conditions. This framework motivates a set of two-dimensional inviscid simulations spanning weak to strong shocks and provides a physically transparent way to connect shock strength, bubble size, collapse symmetry, and collapse energetics.

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COLLAPSE CRITERION AND ENERGETIC ANALYSIS

Let R_0 denote the initial bubble radius, U_s the shock speed in the liquid, and $\Delta p = p_1 - p_0$ the pressure jump across the incident shock. We define the shock–bubble interaction time as

$$\tau_i \sim \frac{2R_0}{U_s}, \quad (1)$$

and estimate the inertial collapse time using a Rayleigh-type scaling,

$$\tau_c \sim 0.915 R_0 \sqrt{\frac{\rho_\ell}{\Delta p + 2\sigma/R_0}}, \quad (2)$$

where ρ_ℓ is the liquid density and σ is the surface tension. Uniform collapse is expected when

$$\Pi \equiv \frac{\tau_i}{\tau_c} \ll 1, \quad \text{while jetting is expected when } \Pi = O(1) \text{ or larger.} \quad (3)$$

Using the liquid Rankine–Hugoniot relation

$$U_s^2 = \frac{\Delta p}{\rho_0(1 - \rho_0/\rho_1)}, \quad (4)$$

we obtain

$$\Pi \sim \frac{2}{0.915} \left[\left(1 - \frac{\rho_0}{\rho_1}\right) \left(1 - \frac{2\sigma}{R_0 \Delta p}\right) \right]^{1/2}. \quad (5)$$

Equation (5) shows that surface tension matters only when $2\sigma/R_0$ is comparable to Δp , giving a minimum size scale

$$R_{\min} \sim \frac{2\sigma}{\Delta p}. \quad (6)$$

For $R_0 \gg R_{\min}$, the collapse criterion depends primarily on the shock jump conditions. Since $1 - \rho_0/\rho_1$ is small only for weak liquid shocks, Eq. (5) predicts that uniform collapse is restricted to weak shocks or acoustic-wave loading, whereas stronger shocks favor jetting.

An energetic analysis will be presented in terms of the work required to drive the bubble from its initial state to its minimum volume. A uniform-collapse model provides the baseline estimate for the reversible compression work, while the simulated non-uniform collapses are used to determine the additional work associated with asymmetric interface deformation, lateral momentum redistribution, and jet formation. In this way, the analysis separates the work needed for idealized spherical compression from the excess energetic cost of jetting.

PLANNED SIMULATIONS AND EXPECTED OUTCOMES

Two-dimensional inviscid simulations will be performed over a range of shock strengths chosen to span $\Pi \ll 1$ to $\Pi = O(1)$. The calculations will test the proposed regime boundary, quantify the onset of non-uniform collapse, and measure how the additional work needed to form a jet grows with increasing shock strength. We expect the results to show that bubbles collapse nearly uniformly only for weak shocks or acoustic-wave loading, whereas stronger shocks produce increasingly asymmetric collapse and a larger excess energetic cost.

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TOWARDS THE DEVELOPMENT OF ROBUST MESH MOTION STRATEGIES FOR A FIRST ORDER ARBITRARY-LAGRANGIAN EULERIAN CONSERVATION LAW FRAMEWORK

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ABSTRACT

The Arbitrary Lagrangian–Eulerian (ALE) formulation in solid dynamics was originally developed to mitigate excessive mesh distortion in highly deformable hypo- and hyper-elasto-plastic processes [1]. In addition to the standard material (initial) and spatial (current) configurations, ALE introduces an intermediate referential (intrinsic) configuration, enabling the decoupling of material and mesh motion. This additional flexibility makes ALE methods particularly well suited for problems involving large deformations, where maintaining mesh quality is critical. This poster builds on ongoing work within the group, with a particular focus on the development of robust and adaptive mesh motion strategies within a novel ALE-based first-order conservation law framework for multi-material shock hydrodynamics. Under isothermal, non-dissipative conditions, the governing mass and linear momentum conservation laws are formulated and solved in the reference configuration, while more complex irreversible processes are treated through the coupled evolution of internal state variables. Central to the proposed approach is the formulation of mesh motion as a momentum-type conservation law, driven by an energy potential defined as a convex combination of material and spatial deformation measures. This enables a dynamic and adaptive redistribution of the mesh, significantly improving element quality in the presence of large, and potentially irreversible, deformations. In parallel, the deformation gradient tensor is obtained via a multiplicative decomposition into two auxiliary fields, each governed by additional first-order conservation laws, ensuring consistent convergence of kinematic and kinetic variables. A variationally consistent, vertex-centred finite volume discretisation is employed [2], ensuring conservation and compatibility with the underlying continuum formulation. The resulting scheme satisfies a global discrete entropy inequality, maintaining consistency with the second law of thermodynamics [4]. The effectiveness of the proposed mesh motion strategy is demonstrated through a range of benchmark problems, highlighting improved robustness and accuracy for both reversible and irreversible processes (e.g. thermal, viscoelastic, and viscoplastic behaviour).

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ALE FORMULATION

Building on References [3, 4], the formulation is based on a system of first-order conservation laws posed in the referential domain as

$$\left. \frac{\partial \mathcal{U}_\chi}{\partial t} \right|_\chi + \text{DIV}_\chi \mathcal{F}_\chi = \mathcal{S}_\chi,$$

where the column vectors of unknowns $\mathcal{U}_\chi$, fluxes $\mathcal{F}_\chi$, and source terms $\mathcal{S}_\chi$ are given by

$$\mathcal{U}_\chi = \begin{bmatrix} p_\chi \\ \mathbf{F}_\Phi \\ \mathbf{F}_\Psi \\ J_\Psi \end{bmatrix}, \quad \mathcal{F}_\chi = - \begin{bmatrix} (P + J_\Psi^{-1} p_\chi \otimes \mathbf{W}) \mathbf{H}_\Psi \\ \hat{\mathbf{v}} \otimes \mathbf{I} \\ \mathbf{W} \otimes \mathbf{I} \\ \mathbf{H}_\Psi^T \mathbf{W} \end{bmatrix}, \quad \mathcal{S}_\chi = \begin{bmatrix} \mathbf{f}_\chi \\ \mathbf{0} \\ \mathbf{0} \\ 0 \end{bmatrix},$$

where $p_\chi = \rho_X J_\Psi v$ is the linear momentum per unit of reference volume; ρ_X is the material density; $\mathbf{F}_\Phi$ and $\mathbf{F}_\Psi$ are deformation gradients defined from the referential to the initial and current domains, respectively, with $\mathbf{H}_\Psi$ and J_Ψ being the co-factor and Jacobian of the latter; $\hat{\mathbf{v}}$ and $\mathbf{W}$ are the corresponding spatial and material velocities related to the physical velocity $\mathbf{v}$ via $\hat{\mathbf{v}} = \mathbf{v} + \mathbf{F}\mathbf{W}$ with $\mathbf{F} = \mathbf{F}_\Phi \mathbf{F}_\Psi^{-1}$; $\mathbf{f}_\chi$ denotes a body force per unit referential volume, and $\mathbf{P}$ is the first-Piola Kirchhoff stress tensor. Additional first order evolution equations along with suitable constitutive closure models can be added to describe reversible and non-reversible processes (i.e. thermal, viscoelastic, viscoplastic), and appropriate Rankine-Hugoniot jump conditions can be added when dealing with different materials across a moving interface [5].

ADAPTIVE MATERIAL MESH MOTION

An adaptive material mesh motion $\mathbf{W}$ is introduced through the definition of a material momentum $\mathbf{p}_w = \rho_X \mathbf{W}$, which is governed by a momentum-type of conservation equation of the form

$$\left. \frac{\partial \mathbf{p}_w}{\partial t} \right|_\chi - \text{DIV}_\chi \mathbf{P}_w = \mathbf{0}; \quad \mathbf{P}_w = (1 - \alpha) \frac{\partial \Psi_w(\mathbf{F}_\Psi)}{\partial \mathbf{F}_\Psi} + \alpha \mathbf{F}^T \frac{\partial \Psi_w(\mathbf{F}_\Phi)}{\partial \mathbf{F}_\Phi},$$

where the material stress tensor $\mathbf{P}_w$ is derived consistently from an energy potential $\Psi_w(\mathbf{F}_\Phi, \mathbf{F}_\Psi)$ defined as an α -convex combination of material and spatial deformation measures. This formulation enables a flexible and adaptive control of mesh motion through the choice of the underlying energy functional. Particular emphasis is placed on the selection of alternative energy potentials (e.g. higher-order Mooney–Rivlin and ARAP formulations) to assess their influence on mesh deformation and quality. For irreversible, plasticity-dominated processes, an alternative mesh motion strategy is proposed, whereby the material mesh motion is driven to approximate the inverse of the plastic deformation within the context of a multiplicative decomposition. The proposed approach highlights the enhanced capabilities of ALE formulations compared to Total Lagrangian methods, particularly in maintaining mesh quality under large deformations.

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TOWARDS DIFFERENTIABLE MULTIPHYSICS ALE SIMULATIONS FOR AUTOMATED INVERSE DESIGN AND OPTIMIZATION

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ABSTRACT

Keywords: gradient-based optimization; adjoint methods; shock hydrodynamics; multi-material hydrodynamics; Lagrangian methods; ALE methods; multiphysics simulation.

INTRODUCTION

Gradient-based optimization has transformed modern machine learning by enabling efficient training of models with extremely high-dimensional parameter spaces. A similar revolution is now within reach for scientific computing, where multiphysics simulation codes could be used not only for forward prediction, but for automated inverse design, sensitivity analysis, and in-situ uncertainty quantification (UQ). However, obtaining accurate and scalable gradients from multiphysics ALE simulation codes remains challenging due to their complex computational graphs, tightly coupled physics modules, nonlinear material models, and the use of adaptive/moving meshes. Current gradient-free approaches for inverse design and calibration in multiphysics settings typically require ensembles of up to $O(100K)$ simulations and scale poorly with parameter dimension, effectively limiting practical design spaces to $O(10)$ parameters. We will present a new research initiative at LLNL to develop and demonstrate differentiable multiphysics codes that enable adjoint-based “back-propagation in time” for large-scale optimization problems with up to $O(1M)$ design parameters.

Our approach leverages structure inherent in high-order finite element discretizations to make automatic differentiation (AD) practical for high-performance computing (HPC). Rather than differentiating an entire MPI-parallel simulation as a monolithic black box, we use the Finite Element Operator Decomposition (FEOD), which expresses nonlinear operators in a form that separates topology-dependent transformations from pointwise nonlinear physics evaluations at quadrature points [1]. This decomposition enables pushing differentiation to the innermost, local operator component, dramatically reducing memory overhead and improving GPU performance. We build on the emerging ∂ FEM interface in MFEM, pairing partial assembly



(PA) techniques with compiler-level AD via Enzyme [2], which operates on the LLVM compiler’s intermediate representation and can generate efficient forward- and reverse-mode derivatives without invasive code rewrites. The resulting framework aims to expose key derivative operations needed for optimization and adjoint workflows, including Jacobian-vector products (JVPs), vector-Jacobian products (VJPs), and derivatives of quantities of interest (QoIs), with performance portability across CPU and GPU architectures (CUDA/HIP).

We are developing adjoint methods for multiphysics on moving ALE meshes for multimaterial, compressible shock hydrodynamics [3] and thermal radiative transfer with matter-energy coupling. Key challenges and research directions for ALE multiphysics include developing robust approaches for nonsmooth physics, such as min/max operations and absolute values, using regularization, smoothing, or subgradient methods. This includes extending gradient computations for multimaterial closure models and enabling shock capturing with differentiable artificial viscosity. Another priority is developing gradient enabled ALE remap methods, including differentiable re-meshing and bounds-preserving ALE remap, and assessing whether it’s possible to remap gradients directly rather than computing gradients of remap operators. Finally, we consider the case of dynamic checkpointing to reduce reverse-mode adjoint memory costs for time-dependent simulations. We are making progress on all these fronts, and we highlight the current state in this work.

ACKNOWLEDGMENT

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344 and was supported by the LLNL-LDRD Program under Project No. 26-SI-002. LLNL-ABS-2017440.

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OPENRADIOSS : POWERFUL, INDUSTRY-PROVEN SOLVER FOR DYNAMIC EVENT ANALYSIS NOW AVAILABLE TO ALL

Thierry Schwoertig^{a*}

^a SIEMENS

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ABSTRACT

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- MULTIMATERIAL - ALE
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EXTENSION TO PLASTICITY OF A FINITE-VOLUME UPDATED-LAGRANGIAN METHOD FOR FLUID-STRUCTURE INTERACTION

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ABSTRACT

We extend an updated-Lagrangian solver for the hyperelasticity system to plastic flows. To this end, we adopt a multiplicative decomposition of the deformation gradient and derive a plastic flow equation from thermodynamic constraints. Two models are proposed to enforce the von Mises yield criterion, both relying on a splitting between the purely elastic evolution and the enforcement of the plastic constraint. The first method, referred to as the relaxation approach, is based on a relaxation algorithm (see, e.g., [6, 11]). The second method, referred to as the projection approach, consists in a projection of the stress state onto the von Mises yield surface. In the relaxation method, the stiffness induced by the relaxation is handled using an exponential integration technique. In the projection method, the constitutive law is inverted using a fixed-point algorithm, and the deformation gradient is updated through a polar decomposition.

These methods are embedded into a second-order accurate partitioned numerical framework for the simulation of fluid–structure interaction problems [3, 4]. Under standard definiteness assumptions inherited from both the fluid [5, 9] and solid [2, 8] discretizations, the resulting coupled system is well-posed and admits a unique solution.

The relaxation and projection approaches are first compared on a one-dimensional test case. Then, a series of numerical experiments in two and three space dimensions, focusing on the projection method, demonstrates the robustness of the approach for various constitutive laws, including cases with strain hardening. Comparisons with well-established reference codes (ABAQUS [10], EUROPLEXUS [1], and HERA [7]) are provided to assess the accuracy and overall performance of the method.

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A STRUCTURE-PRESERVING HIGH-ORDER MATRIX-FREE FINITE ELEMENT METHOD FOR HYPERBOLIC PROBLEMS

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ABSTRACT

Many multiphysics applications require high-order, physically consistent and computationally efficient discretizations of hyperbolic PDEs. In this talk, we will present a new mass-matrix-free finite element (MF-FEM) scheme, which provides an explicit and arbitrary high order approximation of the smooth solutions of the hyperbolic PDEs both in space and time. The design of the scheme allows for an efficient diagonalization of the mass matrix without any loss of accuracy. This is achieved by coupling the FEM formulation with a Deferred Correction (DeC) type method for the discretization in time. The advantage of such a matrix-free approach consists in preserving a compact approximation stencil even at high orders, which reduces the computational cost compared to classical finite element techniques and provides potential benefit for exascale computing on future computer architectures. We have assessed our method on several challenging benchmark problems for one- and two- dimensional Euler equations and the scheme has proven to be robust and to achieve the theoretically predicted high order of accuracy on smooth solutions. We will discuss how structure-preserving properties of the proposed MF-FEM method can be enforced using convex limiting for blending the high-order and low-order element residuals, and showcase the method using benchmark problems for compressible Euler, shallow water, and Navier-Stokes equations.

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ADVANCES IN DAMAGE MODELING WITH SMOOTHED PARTICLE HYDRODYNAMICS

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ABSTRACT

The simulation of material fracture and fragmentation for ductile metals is a complex process that is highly sensitive to the numerical method or scheme, mesh resolution, material models, and spatial perturbation of damage or strength parameters introduced for stochastic behavior. The choice made in each of these areas can significantly impact the qualitative nature of the solution, which could lead to fundamentally different results. With respect to material models, a particular area of interest is the lode angle dependence on material failure, something that is often observed in the high strain-rate fragmentation experiments of different geometries such as rings, cylinders, and hemispherical shells. The usage of a non-convex yield surface can also be important in capturing the anisotropic nature of the material, something that is not observable with the traditional J2 yield surface. The development of analytic perturbation models to emulate the stochastic behavior of fragmentation can be adapted from fields such as turbulence, where seeding initial conditions are key to avoiding mesh imprinting and resolution dependence. Finally, the choice of modeling parameters in the smoothed particle hydrodynamics (SPH) scheme and finite element erosion criteria can greatly affect the overall fragment statistics. This work surveys some advances in damage modeling made in ALE3D, an Arbitrary Lagrangian-Eulerian hydrodynamics code with the SPH capabilities of Spheral developed at Lawrence Livermore National Laboratory (LLNL).

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STUDY AND DEVELOPMENT OF A FINITE VOLUME METHOD ON MOVING MESHES FOR THE NUMERICAL SIMULATION OF HYPERSONIC FLOWS AROUND DEFORMABLE BODIES

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ABSTRACT

This work addresses the development of robust and accurate numerical methods for the simulation of multidimensional hypersonic flows, with a particular focus on applications involving deformable bodies such as atmospheric re-entry vehicles. In such contexts, the strong coupling between flow dynamics and evolving geometries poses significant challenges for standard computational approaches. The present study aims to contribute to this field by combining advanced Finite Volume techniques with moving mesh strategies within the Arbitrary Lagrangian-Eulerian (ALE) framework.

1 INTRODUCTION

The present work is part of the study and development of numerical methods dedicated to the simulation of multidimensional hypersonic flows. Such flows are typically encountered during the atmospheric re-entry of space vehicles. They are characterized by the presence of strong shock and expansion waves, as well as extremely high levels of pressure, temperature, and heat flux [1]. For these applications, the robustness and accuracy of the underlying numerical methods are of paramount importance.

A particularly robust Finite Volume method has been developed for unstructured meshes [3], which greatly facilitates its application to complex geometries. This method relies on the construction of numerical fluxes at interfaces derived from approximate Riemann solvers that preserve positivity and ensure entropy stability. More recently, this approach has been extended to a multipoint scheme [5], in which conservation is enforced at mesh nodes rather than across cell interfaces. This strategy is inspired by methods originally designed for equations in a Lagrangian framework [6].

2 ALE FRAMEWORK

2.1 Context

During atmospheric re-entry, the geometry of a space vehicle may evolve for at least two reasons: thermal protection system ablation and the presence of moving components such as control surfaces. In all cases, accounting for time-dependent geometric deformation requires the use of a moving mesh in order to track these

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changes. This leads naturally to the implementation of a Finite Volume method on moving meshes, commonly referred to as the Arbitrary Lagrangian–Eulerian (ALE) method in the literature [4]

2.2 Governing equation

. This approach is based on a formulation of the conservation laws of fluid mechanics that lies between the Lagrangian and Eulerian descriptions, whose conservative form reads

$$\left. \frac{\partial JU}{\partial t} \right|_{\chi} + \nabla_{\chi} \cdot (J[\mathbb{F} - U \otimes w] \mathbf{M}^{-T}) = 0 \quad (1)$$

where U denotes the vector of conservative variables, $\mathbb{F}$ the flux tensor, $\mathbf{M}$ the spatial transformation Jacobian, and J its determinant.

This equation is derived by introducing a mapping between the reference domain (with coordinates χ) and the spatial domain (with coordinates x), as illustrated in Figure 1.

Within the ALE framework, the mesh velocity w is a free parameter. This flexibility makes it possible to benefit from the advantages of the Lagrangian description, in particular the exact representation of mass convection without numerical diffusion, i.e., the ability to track material interfaces without resorting to subcell reconstruction techniques. At the same time, it allows one to mitigate its drawbacks, such as severe mesh distortions that may lead to loss of convexity or even mesh tangling.

The objective of this work is to develop a multipoint scheme within the ALE framework and to define relevant mesh motion criteria for applications to atmospheric re-entry vehicles.

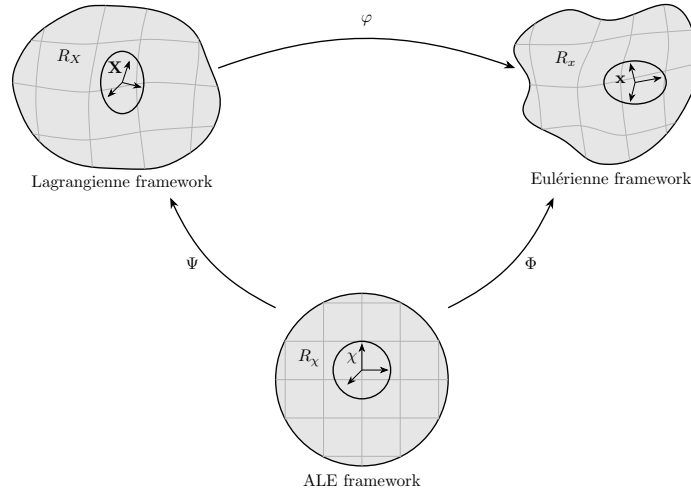


FIGURE 1: Description of the transition between the Eulerian, Lagrangian, and ALE domains.

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A STABILIZED SCHEME FOR THE SIMULATION OF TWO IMMISCIBLE AND COMPRESSIBLE FLUIDS.

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ABSTRACT

In this work we develop a stabilized scheme for the simulation of a mixture of two fluids, supposed immiscible and compressible. The interface between these two fluids is tracked using a level-set function and a cut-cell scheme defines the balance in split cells. During the presentation, we will show how we define this numerical stabilized scheme and some numerical results.

INTRODUCTION

The simulation of the interaction of two fluids is the subject of numerous studies, and several methods were developed for this purpose. A first approach consists in schemes developed to capture to a given degree of accuracy the contact discontinuities found in the underlying hyperbolic model [2]. The drawback of these approaches are the numerical diffusivity induced on contact discontinuities. To overcome this drawback, the sharp interface methods were developed. We cite for instance the ALE approach, where the mesh is deformed to follow the discontinuities [6] ; the tracer methods, where the interface is followed in a Lagrangian framework [3] ; and the reconstruction methods, where the interface is reconstructed using an implicit description [4]. Our method stands in this latest family. The interface is tracked implicitly using a level-set function which acts as a signed distance to the interface ; each phase is either on the positive or the negative side of the 0-level. Using this distance function, one can rebuild the interface in each cell (albeit being possibly discontinuous between two cells), and apply a cut-cell scheme to update the state of each fluid. This method has been used several times, often with great success [5]. However, this method also has a drawback: oscillations will necessarily appear if the scheme is kept conservative, according to [1].

Thus, we propose here to analyze a scheme where the conservation is sacrificed (to a certain margin) but ensures the preservation of galilean invariance for an enhanced stability.

MODEL, SCHEME, GALILEAN INVARIANCE

The two fluids are governed by the compressible Euler equations, written in conservative form:

$$\frac{\partial}{\partial t} \rho + \nabla \cdot (\rho \mathbf{u}) = 0, \quad \frac{\partial}{\partial t} (\rho u) + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u} + p \mathbf{I}) = 0, \quad \frac{\partial}{\partial t} (\rho E) + \nabla \cdot ((\rho E + p) \mathbf{u}) = 0, \quad (1)$$

where ρ is the density, $\mathbf{u}$ the velocity and $E = e + \frac{1}{2}|\mathbf{u}|^2$ the total energy. The previous system is equipped with a thermodynamics closure (equation of state EOS) $p = p(\rho, e)$ where e is the specific internal energy given by the perfect gas law with constant $\gamma > 1$ such that $p = (\gamma - 1)\rho e$.

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We will denote $\mathbf{U} = (\rho, \rho \mathbf{u}, \rho E)$ and $F(\mathbf{U}) = (\rho \mathbf{u}, \rho \mathbf{u} \otimes \mathbf{u} + p \mathbf{I}, (\rho E + p) \mathbf{u})$ such that the previous system is simply written $\partial_t \mathbf{U} + \nabla \cdot F(\mathbf{U}) = 0$. Integrating this system over a cell ω with faces f cut by moving interface γ gives the relation

$$\frac{d}{dt} \int_{\omega} \mathbf{U} dx = - \int_f F(\mathbf{U}) \cdot \mathbf{n} ds - \int_{\gamma} (F(\mathbf{U}) - \mathbf{U} V_t) \cdot \mathbf{n} ds,$$

where V_t is the interface velocity.

In our presentation, we will focus on the interface flux term $\phi_t = (F(\mathbf{U}) - \mathbf{U} V_t)$. We will show why this term is a source of problem for galilean invariance and how we decide to use it to ensure an enhanced stability using a scheme designed in a space-time cell.

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A STAGGERED GRID VIRTUAL ELEMENT METHOD FOR LAGRANGIAN HYDRODYNAMICS

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ABSTRACT

The virtual element method (VEM) [1] is a mesh agnostic generalization of the finite element method (FEM) that can also be seen as an extension of the mimetic finite difference (MFD) method [3]. In this work, we develop a staggered-grid Lagrangian virtual element method for compressible flow. The scheme utilizes a conforming global VEM discretization for the kinematic variables and an L^2 discontinuous finite element approximation with scaled monomial basis functions for the thermodynamic variables. The method allows for curvilinear deformations of polyhedral meshes and high-order convergence on smooth problems. The method is validated against standard compressible flow problems and elastic-plastic deformation test problems [2].

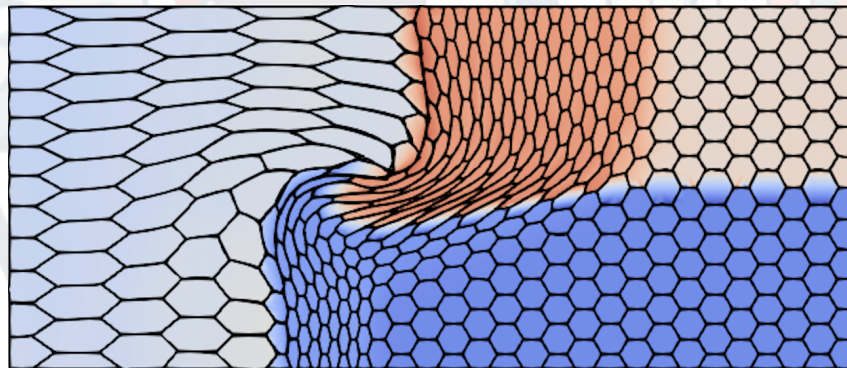


FIGURE 1: VEM simulation of the triple point problem with quadratic hexagonal elements.

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LA-UR-26-22824



AIR WATER SIMULATIONS WITH CAVITATION AND EVAPORATION

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ABSTRACT

In this work we develop a thermal equilibrium approach to multi-material simulations involving phase change. In particular we focus on the scenario when a material which can undergo liquid-vapor phase transitions (water) interacts with another gas described by an ideal gas (air). Upon mixing with air, the low partial pressure of water in the gas allows the water to evaporate. The evaporation is associated with the absorption of heat. We present simulations of air water mixing and evaluate the importance of these effects.

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INTRODUCTION

In this paper we will present a numerical investigation of turbulent mixing of air and water. We carry out implicit large eddy simulation (ILES) calculations by numerical solution of the inviscid Euler equations [1]. The equations are discretized using a finite volume conservative scheme. The algorithm has been implemented for three dimensional Cartesian structured meshes within the AMReX framework [3] for modern computer architectures.

AIR WATER MODELING

Water is well known for undergoing phase transitions between liquid and gas phases. The phase diagram (1) illustrates the stark changes in density between liquid and vapor phases. The large change in density corresponds to a large enthalpy of vaporization. Fluid flows involving this phase change are therefore also associated with large amounts of energy release or absorption which consequently affects the flow.

This is particularly apparent in the realm of meteorological forecasting, where the presence or absence of humidity plays a huge role. In particular the development of storms is linked to the heat release and subsequent buoyancy driven updrafts associated with the condensation of water vapor into liquid droplets within the atmosphere.

Previous work [2] has focused on modeling cavitation of liquid water due to a reduction in pressure. A single thermal-equilibrium equation of state was developed for the liquid-vapor mixture. Using the assumption that the liquid and vapor components of the mixture are well mixed (which is contingent on the computational cell size being larger than the length scale associated with surface tension) it can be assumed that the liquid and vapor components of the mixture are always in thermal equilibrium. Such an approach to cavitation modeling has proved to be robust and easy to implement in practice.

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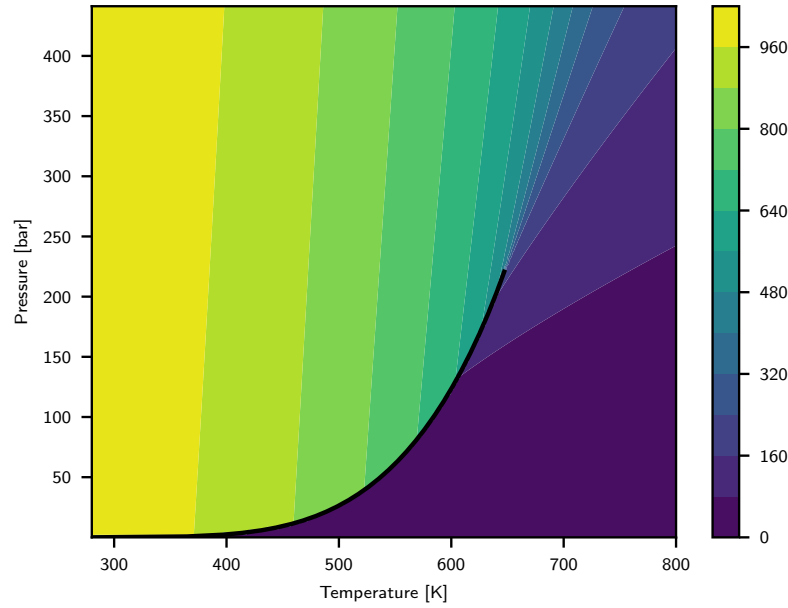


FIGURE 1: The phase diagram of water is illustrated by the density (in kgm^{-3}) as a function of pressure and temperature. The discontinuity in the density field corresponds to the phase transition between liquid and vapor phases.

The model as presented in [2] cannot be applied directly to air-water mixtures. This is because liquid water will evaporate on mixing with a sufficient quantity of dry air. While the partial pressure of water vapor remains below the saturation pressure then evaporation will continue. Water will thus exist in the vapor phase when mixed with air even at temperatures and pressures at which pure water will only exist in the liquid phase.

It is therefore reasonable to expect that turbulent mixing of water and air will lead to significant quantities of water evaporating into the vapor phase, and a corresponding amount of heat will be absorbed.

In this work we present numerical calculations evaluating the effect of evaporation on the dynamics of the turbulent mixing of air and water.

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