NUMERICAL METHODS FOR MULTI-MATERIAL FLUID FLOW (MULTIMAT 2015)

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BOOK OF ABSTRACTS

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General Information

The seventh International Conference on Numerical Methods for Multi-Material Fluid Flow (MULTIMAT 2015) will focus on mathematical and numerical aspects of Lagrangian, Eulerian, and Arbitrary Lagrangian Eulerian (ALE) methods for multiphase and multicomponent flow problems.

The topics of particular interest are:

- modeling of complex multi-material flows
- free and moving boundary problems
- radiation hydrodynamics
- advanced discretization techniques
- interface reconstruction methods
- mesh adaptation and remapping
- discrete maximum principles
- constrained optimization

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SCHEDULE

	2015/09/07 Monday	2015/09/08 Tuesday	2015/09/09 Wednesday	2015/09/10 Thursday	2015/09/11 Friday
09:00 - 10:15	Barlow Dumas Francois	Brauenig Clair Waltz	Shashkov Owen Del Pino	Barlow Burton Maire	Owen Raskin Ma
10:15 - 10:45	Coffee Break				
10:45-12:25	Sidilkover Rider Miller Popov	Loubère Boscheri Dumbser Blanchard	Luttwak Menshov Serezhkin Zakharov	Morgan Chiravalle Charest Vazquez-Gonzalez	Cook Williams Zhang Doebling
12:25 - 14:00	Lunch				
14:00-15:40	Bochev Kramer Hill De Vuyst	Dobrev Liska Váchal Kuchařík	Peterson Costes Pouderoux Kenamond	Posters	Qi Hahn Sváček
15:40 - 16:10	Coffee Break				
16:10 - 17:50	Hoch Claisse Breil Bukač	Siefert Kolev Masser Georges	Robinson Dai Ferguson Ragusa	Posters (until 17:00)	

POSTERS

Baolin	Basting C.	Basting S.	Bayraktar	Bement	Chen
Coffing	Costes	Dawes	Fung	Gasc	Gibson
Holec	Klíma	Kosík	Lohmann	Mabuza	Marboeuf
Morel	Ragusa	Rieben	Rousculp	Smith	

Contents

TALKS

Further developments of an interface-aware subscale dynamics closure model for multimaterial cells

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Keywords: shock hydrodynamics; multi-material hydrodynamics; ALE methods; closure models.

ABSTRACT

Multimaterial cells are often used in Arbitrary Lagrangian Eulerian (ALE) codes to represent material interfaces that undergo high deformation and cannot be modelled robustly with a Lagrangian treatment. A separate set of material properties is normally maintained for all the materials in each multimaterial cell along with the volume fractions that define the proportion of the cells volume occupied by each material. A closure model is then required to close the governing equations, which are otherwise underdetermined, that is, to define how the volume fractions and states of the individual material components evolve during the Lagrangian step. The challenge in developing closure models is how to accurately update the thermodynamic states of the individual material components in the multimaterial cell, and determine the nodal forces that such a zone generates - despite the lack of information about the velocity distribution within multimaterial cells.

The interface-aware sub-scale-dynamics (IA-SSD) closure model [1] consists of two stages. During the first, bulk stage, the well known equal compressibility model is used. During the second stage, sub-scale interactions of the materials inside the multimaterial cell are taken into account. Each material interacts in a pair-wise fashion with the materials with which it has a common boundary. The interactions are based on the solution of the acoustic Riemann problem between each pair of materials and is limited using physically justifiable constraints: positivity of volume, positivity of internal energy and controlled rate of pressure relaxation.

A number of further improvements and simplifications for the IA-SSD algorithm are presented including; a simpler procedure for extending the method to n materials, a modified Riemann solver that avoids the need to interpolate velocities for the material components, multiphase artificial viscosities and subzonal pressures are also developed to improve the bulk phase. The extension of the method to include additional interface physics such as void closure and opening is also considered and results are presented for test problems and a more realistic projectile impact problem to demonstrate the performance of the algorithm and allow comparisons to be made with results presented in [1] for the original IASSD method and results obtained with other closure models.

References

[1] A. Barlow R. Hill and M. Shashkov, "Constrained optimization framework for Interface-aware sub-scale dynamics closure model for multimaterial cells in Lagrangian and arbitrary Lagrangian-Eulerian hydrodynamics", *Journal of Computational Physics*, 276, pp. 92–135, 2014.

Towards effective (very) high accurate remapping method on polyhedrons using a posteriori limiting

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Keywords: ALE methods; projection methods; high accuracy; a posteriori limiting; MOOD.

ABSTRACT

In this presentation, we will focus on the development of high accurate 3D conservative projection method on polyhedral meshes following the first attempts in [1]. Our technique is based on intersection polyhedra calculation between the initial mesh onto which the cell-centered data are defined and the target mesh onto which the data are remapped.

With this method, if the intersection and the integration are exact and highly accurate respectively, the main error of the projection method is due to the representation of the underlying data. To obtain a formal higher accurate method, it is sufficient to increase the accuracy of the representation of the underlying data (i.e. reconstructing N-th accurate polynomials implies a $(N+1)$-th nominal order of accuracy).

Unfortunately, in practice, some limiting must be apply to the polynomial reconstruction to avoid over-undershoots or Gibbs phenomenon. Classical limiters have been designed for piece-wise linear reconstruction, conversely the MOOD paradigm (multi-dimensional optimal order detection [2, 3]) can manage higher polynomial reconstruction ($\mathbb{P}_N$ with $N > 1$) thanks to an 'a posteriori' detection that identifies problematic cells. Those "bad" cells are successively re-updated after some local order decrementing of the polynomial reconstruction. This iterative process eventually stops when the problematic cell is updated with a $\mathbb{P}_0$ reconstruction. In this case, the local effective order of accuracy is bounded by 1 (as it must be close to any discontinuous solutions).

In this work we have implemented an exact polyhedral intersection coupled with a high accurate numerical integration. Polynomial reconstructions of maximal degree up to 5 are considered with MOOD limiting. We will emulate an ALE code by remapping density, momentum and total energy profiles showing how density, specific internal energy and pressure could be maintained in bounds. Cyclic remapping test cases on general polyhedral meshes will be considered and we will show that effective high accuracy can be reached on smooth problems.

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A variational flux recovery approach for elastodynamics problems with interfaces

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ABSTRACT

We present a new explicit algorithm for linear elastodynamic problems with material interfaces. The method discretizes the governing equations independently on each material subdomain and then connects them by exchanging forces and masses across the material interface. The exchanged quantities approximate the surface traction force between the material subdomains, which provides a Neumann boundary condition for the subdomain problems. Variational flux recovery techniques motivate the formulation of the mass and force exchanges.

The new algorithm has attractive computational properties. It allows different discretizations on each material subdomain and enables partitioned solution of the discretized equations. This makes it possible to also use the algorithm as a coupling tool for different codes operating in different material subdomains. The method passes a linear patch test and recovers the solution of a monolithic discretization of the governing equations when interface grids match. Numerical examples illustrate these properties and show that the method is second-order accurate.

[1] Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Direct Arbitrary-Lagrangian-Eulerian ADER-MOOD Finite Volume Schemes for Multidimensional Hyperbolic Conservation Laws

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Keywords: Arbitrary-Lagrangian-Eulerian; a posteriori limiter; MOOD paradigm; ADER schemes; moving unstructured triangular and tetrahedral meshes; high order of accuracy in space and time; high performance computing (HPC); hyperbolic conservation laws.

ABSTRACT

We present a new family of efficient high order accurate direct Arbitrary-Lagrangian-Eulerian (ALE) one-step ADER-MOOD finite volume schemes for the solution of nonlinear hyperbolic systems of conservation laws for moving unstructured triangular and tetrahedral meshes. This family is the next generation of the ALE ADER-WENO schemes presented in [1, 2]. Here, we use again an element-local space-time Galerkin finite element predictor method to achieve a high order accurate one-step time discretization, while the somewhat expensive WENO approach on moving meshes, used to obtain high order of accuracy in space, is replaced by an *a posteriori* MOOD loop which is shown to be less expensive but still as accurate. This *a posteriori* MOOD loop ensures the numerical solution in each cell at any discrete time level to fulfill a set of user-defined detection criteria. If a cell average does not satisfy the detection criteria, then the solution is locally re-computed by progressively decrementing the order of the polynomial reconstruction, following a so-called *cascade* of predefined schemes with decreasing approximation order. A so-called parachute scheme, typically a very robust first order Godunov-type finite volume method, is employed as a last resort for highly problematic cells. The cascade of schemes defines how the decrementing process is carried out, i.e. how many schemes are tried and which orders are adopted for the polynomial reconstructions. The cascade and the parachute scheme are choices of the user or the code developer. Consequently the iterative MOOD loop allows the numerical solution to maintain some interesting properties such as positivity, mesh validity, *etc*, which are otherwise difficult to ensure. We have applied our new high order unstructured direct ALE ADER-MOOD schemes to the multi-dimensional Euler equations of compressible gas dynamics. A large set of test problems has been simulated and analyzed to assess the validity of our approach in terms of both accuracy and efficiency (CPU time and memory consumption).

References

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Adaptation of multimaterial Lagrange-Remap schemes for efficient parallel computation.

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Keywords: shock hydrodynamics; multi-material hydrodynamics; Eulerian methods.

ABSTRACT

The framework of the study is the design of eulerian Lagrange-Remap schemes for compressible multimaterial fluid flows simulation adapted to HPC constraints. This type of scheme belongs to the Finite Volume family and is added with a sharp interface capturing VOF like.
First, the use of fine grids implies that the scheme is convergent, thus conservation of mass, momentum and total energy is necessary. The most natural way to achieve this is to use a conservative formalism and here following [1] Maire et al, i.e. a collocated lagrangian scheme and a collocated remap. The interface capturing method is adapted with classical techniques, but with explicit pressure relaxation. Moreover, the data structure organization has to be as vectorized as possible for parallelization efficiency. A collocated scheme is thus well adapted compare to staggered schemes since all quantities are positioned at cell centres, so they can be remapped generically and independently.
Second, the parallelization efficiency and scalability of a computational code is related to the number of communication phases in the algorithm. In this context and especially in three dimensions of space, the use of directional splitting for the remap phase should be avoided because communications occur at each step of the splitting. A one step multidimensional remap requires only one point of synchronization while a directional splitting requires three points in three dimensions, and fluxes in all directions can be computed independently. However the issue with multidimensional Finite Volume remap is that corner fluxes are needed to be accurate, especially when using sharp interface capturing. A simple proposition will be described for multimaterial corner fluxes computation on structured orthogonal meshes.
Results will be presented, showing that the multidimensional Lagrange-Remap scheme provides good results compare to classical staggered schemes, so is an interesting option to build an efficient eulerian parallel code.

References

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A 3D Anisotropic Diffusion Scheme on ALE-AMR Meshes

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Keywords: 3D Anisotropic Diffusion; ALE-AMR Meshes

ABSTRACT

In the context of High Energy Density Physics (HEDP) and more precisely in the field of laser plasma interaction, Lagrangian schemes are commonly used. The lack of robustness due to strong grid deformations requires the regularization of the mesh through the use of Arbitrary Lagrangian Eulerian (ALE) methods. Theses methods usually add some diffusion and a loss of precision is observed. In this talk we propose to use Adaptative Mesh Refinement (AMR) techniques to recover this loss of accuracy. We will focus our presentation on the resolution of the anisotropic diffusion operator on ALE-AMR grids (cf Figure 1). The scheme obtained is an extension of the CCLADNS [1] scheme in 3D [2] which is able to handle this kind of meshes.

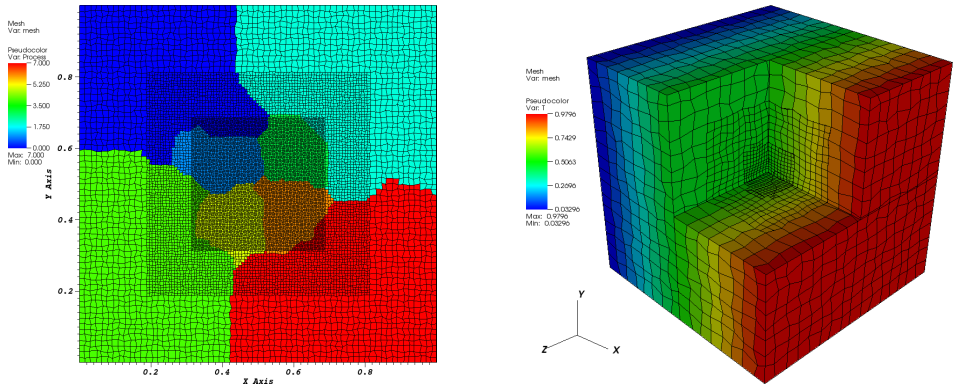

Figure 1: 2D and 3D ALE-AMR grids

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A partitioned numerical scheme for the interaction between fluid, an elastic structure and a poroelastic material

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Keywords: fluid-structure interaction; poroelastic materials; fluid-porous media interaction; partitioned numerical scheme.

ABSTRACT

The interaction between a fluid, elastic structure, and poroelastic structure plays a fundamental role in many biomedical applications. Examples of such applications are the interaction between the blood, blood vessel, and blood clot, as well as the blood flow through dissected artery, where the partially thrombosed false lumen can be modeled as a poroelastic material. This multi-physics problem features three different types of coupling: fluid-elastic structure coupling, fluid-poroelastic medium coupling, and elastic structure-poroelastic medium coupling, resulting in a fully coupled, non-linear, moving boundary problem. As a consequence, numerical algorithms that split the fluid dynamics, structure mechanics, and poroelastic structure dynamics are a natural choice. In this work, we propose a partitioned method to solve the coupled problem. We use this method to model the interaction between the blood, vessel wall, and thrombus under physiological conditions.

Corner gradient reconstruction (CGR) and the reduction of dissipation in Lagrange cell-centered hydrodynamics (CCH)

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Keywords: Lagrangian methods, shock hydrodynamics, cell-centered hydrodynamics (CCH) higher-order reconstruction, corner gradient reconstruction (CGR), dissipation

ABSTRACT

This work presents an extension of a second order cell-centered hydrodynamics scheme (CCH2) on unstructured polyhedral cells [1]. The goal is to reduce dissipation, especially on shockless flows. This is accomplished by multiple piecewise linear reconstructions of conserved quantities within the cell. The reconstruction is based upon gradients that are calculated at the nodes, a procedure that avoids the least-square solution of a large equation set for polynomial coefficients. Conservation and monotonicity are guaranteed by adjusting the gradients within each cell corner. Results are presented for a wide variety of test problems involving smooth and shock-dominated flows, fluids and solids, 2D and 3D configurations, as well as Lagrange, Eulerian, and ALE methods.

Figure 2 shows the interaction of shock wave with a cylindrical helium bubble surrounded by air at 788 μs. Schlieren images from the experiment [2] are on the left, ALE results using CGR are in the center, and second order CCH2 are on the right. The CGR results are in excellent agreement with the experiment while the CCH2 are clearly more dissipative.

Figure 2: Comparison of Schlieren images from experiment [2], CGR, and CCH2.

References

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[2] J.F. Haas and B. Sturtevant, “Interaction of weak-shockwaves”, *J. Fluid Mech.*, 181:4176, 1987.

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A High-Order Central ENO Method for ALE Simulation of Three-Dimensional Compressible Flows

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Keywords: shock hydrodynamics; ALE methods; high-order finite-volume methods.

ABSTRACT

Arbitrary Lagrangian-Eulerian (ALE) methods incorporate dynamic mesh motion in an attempt to combine the advantages of both Eulerian and Lagrangian kinematic descriptions. They are especially attractive for modelling compressible flows since their moving meshes are able to capture large distortions of the continuum without excessively smearing free surfaces or material/fluid interfaces. It is desirable to combine these ALE descriptions with high-order spatial and temporal discretizations because, for a given accuracy, high-order methods offer the potential to greatly reduce computational costs. However, the application of high-order methods to ALE is complicated by changing mesh geometry and certain stability requirements such as geometric conservation. In addition to these challenges, it is also difficult to obtain accurate high-order discretizations of conservation laws without any unphysical oscillations across discontinuities, especially on multi-dimensional unstructured meshes. One high-order method that was proved to be efficient and robust for static meshes is the central essentially non-oscillatory (CENO) finite-volume method. Here, the CENO approach was extended to an ALE formulation on tetrahedral meshes. The proposed unstructured method is vertex-based and uses a direct ALE approach that avoids the temporal splitting errors that are sometimes introduced by traditional Lagrange-plus-remap ALE methods [1]. The new approach was applied to the conservation equations governing compressible flows and assessed in terms of accuracy and computational cost. For all problems considered, which included various idealized flows, CENO demonstrated excellent reliability and robustness. High-order accuracy was achieved in smooth regions and essentially non-oscillatory solutions were obtained near discontinuities. The high-order schemes were also more computationally efficient for high-accuracy solutions, i.e., they took less wall time to achieve a desired level of error than the lower-order schemes.

References

[1] J. Waltz. Operator splitting and time accuracy in lagrange plus remap solution methods. J. Comput. Phys., 253:247–258, 2013.

A 3D Finite Element ALE Method using an Approximate Riemann Solution

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Keywords: shock hydrodynamics; multi-material hydrodynamics; ALE methods.

ABSTRACT

Finite element methods have been widely used to study the hydrodynamics of compressible flows involving strong shocks in the arbitrary Lagrangian Eulerian (ALE) framework [1]. Recently Lagrangian methods have been proposed that solve a multidimensional Riemann-like problem at the cell center in a staggered grid hydrodynamic (SGH) arrangement [2, 3]. Our work builds upon and improves an earlier Lagrangian code called Cercion-3D [4] by implementing a multidimensional Riemann-like solution for finite element SGH. In addition we extend to three dimensions a mesh relaxation and remapping technique developed in 2012 [5]. Our ALE scheme uses a compatible discretization that ensures conservation of total energy.

A test suite of three dimensional problems is explored to evaluate the fidelity of the numerical techniques in our improved Cercion-3D, including the Sedov, Noh, Verney collapsing shell, and spherically converging Sod problems. We compare the analytic solutions for these problems to our calculated results using both pure Lagrangian and ALE approaches.

To further evaluate our remapping technique we consider the steady state 3D Taylor-Green vortex problem and show that our method using an approximate Riemann-like solution does not generate excessive dissipation and is able to preserve the initial velocity magnitude on an Eulerian mesh. Finally we explore the three dimensional triple point problem involving an annular contact discontinuity and a strong shock, conditions that generate a large amount of shear-driven vorticity. We compare the amount of roll-up at the triple point with our finite element SGH method to that produced by the higher order multi-material advection technique employed in the Eulerian code, PAGOSA.

References

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A multidimensional finite-volume direct ALE cell-centered scheme for hydrodynamics simulations

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Keywords: multi-material hydrodynamics; Direct ALE methods; Artificial viscosity;

ABSTRACT

We describe in this paper a finite-volume multidimensional cell-centered solver belonging to the class of the direct ALE methods. The Euler equations for masses, momentum and total energy are solved in an arbitrarily moving coordinate frame, which leads to the appearance of advective terms depending on the grid velocity in the governing equations. It results in a continuous rezoning capability, with no extra time cost, which offers the possibility to handle greater distortion than allowed by a purely Lagrangian method, with more resolution than that provided by a purely Eulerian approach.

The stabilization of the proposed scheme results in the combination of two ingredients: on the one hand, the advection fluxes are upwinded regarding to the direction of the relative velocity $\overrightarrow{\mu} = \overrightarrow{v} - \overrightarrow{w}$, where $\overrightarrow{v}$ is the flow velocity and $\overrightarrow{w}$ the grid velocity, and on the other hand, a viscous tensor, working in any system of coordinates, is added to both conservation equations for momentum and total energy.

The multimaterial formulation of the solver is based on several ideas inherited from the diffuse-interface method proposed by Allaire *et al.* [1]. A VOF strategy is used to characterize the multimaterial cells by using the volume fraction α. Interfaces are never explicitely reconstructed within these cells. On the contrary, we do not use explicitely the topological relation to get the evolution of the interface, but we propose instead a specific procedure which predicts at each timestep the number of pure cells that may potentially become multimaterial. The main feature of this procedure is to use the upwind volume fraction as switches between monomaterial and multimaterial cells, which results in a strict control of the mass diffusion.

Numerical Results for both monomaterial and multimaterial hydrodynamics problems will be proposed to prove the robustness of our methods.

References

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2D Axisymmetric extention of the Lagrangian CSTS (Conservative Space- and Time-Staggered) hydrodynamic scheme

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Keywords: Lagrangian methods; staggered scheme; leap-frog; VNR; compatible scheme; conservative scheme.

ABSTRACT

In the context of Lagrangian computation of compressible fluid dynamics, space- and time-staggered (STS) schemes have been widely used since the pioneering work of von Neumann and Richtmyer [1]. These schemes are known to be non conservative in total energy and present some distorsions for accurately capturing Hugoniot relationships at shock discontinuities (on shock level and on propagation velocity). We proposed in [2, 3] a modification, in the spirit of [4], of the basic STS scheme, denoted by CSTS scheme, which is conservative, entropic, compatible, positive definite in kinetic energy, explicit in momemtum equation and second order accurate (even for variable time steps). Corrections have thus been brought to the simplest STS scheme in order to recover energy conservation.
Variable node masses are recommended for axisymmetric geometry in order to avoid strong axial singularities, but they create spurious momemtum fluxes unaccounted in usual (C)STS (as noticed by [4]). We proposed herein a new modification of CSTS scheme with variable node masses to handle such axisymmetric geometries. As in [5], this modification conserves mass, momemtum and total energy and keeps the same algorithm structure than CSTS. We will study different definitions of node masses (planar and 3D descriptions). Various numerical examples will be shown, and we will discuss the preservation of 1D symmetry for cylindrical spherical flows.

References

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High-order Eulerian Simulations of Multi-material Flows

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Keywords: shock hydrodynamics; multi-material hydrodynamics; Eulerian methods

ABSTRACT

Rayleigh-Taylor (RT), Richtmyer-Meshkov (RM) and Kelvin-Helmholtz (KH) instabilities serve as efficient mixing mechanisms in a wide variety of flows, from supernovae to jet engines. In computing these instabilities, the primary challenges are to: (1) capture all relevant physics, (2) conserve mass, momentum and energy, (3) resolve an adequate range of scales, (4) minimize numerical errors and (5) bring the results into agreement with experiments. Carefully crafted numerical simulations, like experiments, can sometimes lead to the discovery of previously unknown flow phenomena. Over the past decade, we have used the Miranda code to temporally integrate the multi-component Navier-Stokes equations at spatial resolutions up to 29 billion grid points. The code employs 10th-order compact schemes for spatial derivatives, combined with 4th-order Runge-Kutta time advancement. Some of our major findings are as follows: The rate of growth of a mixing layer is equivalent to the net mass flux through the equi-molar plane. RT growth rates can be significantly reduced by adding shear. RT instability can produce shock waves. The growth rate of RM instability can be predicted from known interfacial perturbations. Thermal fluctuations in molecular dynamics simulations can seed instabilities along the braids in KH instability. And finally, enthalpy diffusion is essential in preserving the second law of thermodynamics.

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Mesh regularization for an ALE code based on the limitation of the fluid vorticity

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Keywords: multi-material hydrodynamics; ALE methods; mesh regularization; L.E.L method

ABSTRACT

For the simulation of flow with strong shock the Lagrangian approach is usually used. Moreover, in the case of multi-material flows the Lagrangian approach is particulary well suited to treat the material interface. Unfortunately, this formulation can lead to very large deformations of the mesh [1]. To overcome this drawback the Arbitrary Lagrangian Eulerian (ALE) method uses a mesh regularization usually based on an analysis of the cells' geometry, *e.g.* [2]. The regularization step may be considered as a method used to correct the tangled and potential non-convex cells constituting the mesh.

In this talk we present a new approach for the mesh regularization. Instead of using a pure geometric criterion we propose to compute the mesh evolution based on the flow vorticity. This approach called L.E.L method (Large Eddy Limitation) is aimed at being introduced into a direct ALE method.

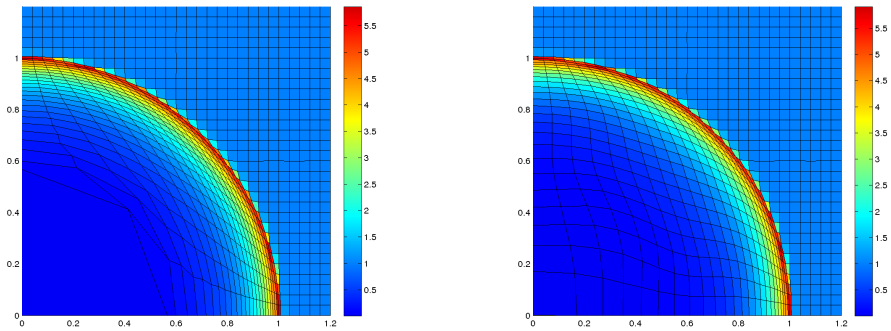

Figure 3: Sedov test case, pressure field at $t = 1\ s$: Lagrangian method (left) and L.E.L. method (right).

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On Operator-splitting Technique for Plasma 3-T Radiation Diffusion in Two and Three Dimensions

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Keywords: 3-T; radiation.

ABSTRACT

Solving plasma 3-T radiation diffusion equation is a critical step in multi-physics simulations, Often these simulations involve mixed cells, and within a mixed cell there are more than one material. Treatment of mixed cells is important for many applications.

Two typical implicit methods are the backward Euler method and Crank-Nicolson method. The backward Euler method is only first order accurate in time, and the size of time step in Crank-Nicolson method is limited. The formulation for large time steps is very important for problems involving dramatically different materials even for time-dependent problems. A given time step may be considered so large for some material that the formulation for steady state is more appropriate for the material than the formulation with the second order of accuracy, but the time step is so small for other materials that accuracy in time is more important. The scheme we will present is second order accurate in both space and time and works for any size of time steps.

For systems of multi-materials with dramatically different material properties, the correct treatment for the discontinuity of material properties is important. A typical approach for this is to use mathematical approximations, which could introduce numerical errors when thermal properties of two materials are very different. We use the governing physics principle to give formula for effective diffusion coefficient across a material interface for flux calculations on polyhedral meshes.

In addition to the aspects mentioned above, we will focus on another issue in numerical simulations for plasma 3-T radiation equations, i.e., numerical treatment for interaction between radiation and material that involves nonlinearity. The 3-T radiation diffusion equations are often solved through some operator-splitting technique. Several approaches that are typically used in numerical simulations have serious drawbacks for some problems even for very small time steps.

The numerical scheme to be presented is an extension of previous work to include mixed cells, unstructured meshes, fully coupling, full nonlinearity, and operator-splitting. For mixed cells, we consider the interface reconstruction with any number of materials in both two- and three-dimensional meshes with adaptive mesh refinement (AMR).

In this talk, we will first describe the procedure for interface reconstruction for both two- and three-dimensions for AMR meshes with any number of materials, and then we will present the scheme for the set of equations for 3-T radiation diffusion in both two- and three-dimensions. Comparing with the results obtained from a fully nonlinear scheme in which material and radiation are fully coupled, we will demonstrate serious errors of typical operator-splitting approaches for some problems. We will finally present our operator-splitting technique that generates reasonable solutions for the problems previous operator-splitting techniques failed to give reasonable solutions.

Stable and accurate compressive interface capturing advection schemes

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ABSTRACT

Anti-dissipative transport schemes have known an increasing interest for interface capturing problems and multi-component compressible flows [1, 2, 3, 4] during the past years. Their simplicity of implementation and natural extension to 3D computations make them attractive alternative methods compared to interface tracking methods like VOF. They also present advantages for High Performance Computing on multicore/manycore architectures [5]. However, they still know accuracy issues and interfaces instabilities in some cases. This work is aimed at improving both stability and accuracy issues of compressive interface capturing methods. We have developed a "shape-preserving" local extremum diminishing explicit conservative advection scheme that takes into account some local geometrical properties of the interface. The example below shows the case of the classical Rider-Kothe advection problem on the unit square with forward and reverse flow ($T = 5$):

$$u(x, y, t) = -\left(-\sin^2(\pi x)\sin(2\pi xy), \sin(2\pi x)\sin^2(\pi y)\right)\cos\left(\pi\frac{t}{T}\right) \tag{1}$$

One can observe that the process is able to restore the initial disk with a quite good accuracy.

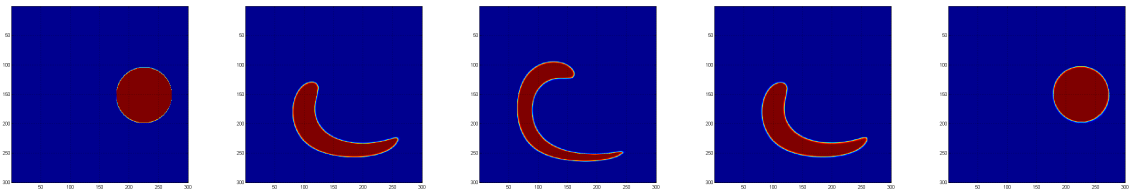

Figure 4: Kothe-Rider advection test case, with reverse velocity. The grid size is 300x300. Interface representations at times $t = 0$, $t = 1.25$, $t = 2.5$, $t = 3.75$ and $t = 5$ respectively. http://youtu.be/dz5mCgg5g3E.

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An asymptotic preserving multidimensional ALE method for the Scannapieco-Cheng model

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Keywords: multi-fluid, friction, Lagrangian, ALE, asymptotic-preserving.

ABSTRACT

Multi-fluid models allow the description of multiple fluids mixture. There exists many kind of multi-fluid models. In particular, one can consider muti-velocity models where each fluid is described by its own mass density, velocity, total energy density and equation of state.

In this presentation, we consider the discretization of the Scannapieco-Cheng[1] model. This multi-velocity model describes the interpenetration of plasma. If one neglects electromagnetic interactions, this model reduces to a collection of Euler equations that are coupled by friction terms.

We propose and study an asymptotic preserving discretization for this model. The considered asymptotic being achieved when friction tends to infinity. This kind of scheme has already been studied in [2] in Eulerian coordinates using directional splitting. We present a multidimensional approach based on cell-centered Lagrangian schemes [3, 4].

Each fluid being characterized by its own velocity field, we provide a grid to each of them. The proposed Lagrangian scheme requires these grids to coincide at the beginning of the timestep, and since these grids evolve differently during the Lagrangian step, an ALE procedure is mandatory to relocate them for next timestep.

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Multi-material Remap Algorithms for High-order Finite Element Arbitrary Lagrangian-Eulerian (ALE) Simulations

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Keywords: high-order discretizations, multi-material shock hydrodynamics; ALE methods; remap methods.

ABSTRACT

Arbitrary Lagrangian-Eulerian (ALE) methods are the basis of many multi-physics simulation codes. Our group develops ALE algorithms based on high-order finite element discretizations using the so-called "Lagrange plus remap" approach. During the Lagrange phase of ALE, the computational mesh follows the physical motion which in the presence of large deformations (e.g. vortical flow) leads to unacceptable mesh quality degradation. In order to correct this issue, a remesh step is introduced followed by an interpolation (remap) step to transfer the physical fields from the old mesh to the new. In multi-material problems, this algorithm naturally leads to the introduction of mesh elements (zones) which contain multiple materials —- mixed zones, which require careful treatment during the Lagrangian and remap steps of the algorithm.

In this talk we describe our approach to mixed zone representation based on high-order discontinuous material indicator functions and focus on the multi-material remap algorithms we developed. Our approach to the remap problem is based on an advection formulation where the transition from the old Lagrangian mesh to the new mesh is given as a deformation field evolving in pseudo-time between the two states. We discretize this problem using a high-order discontinuous Galerkin (DG) scheme which is applied to the material indicator functions (or indicators) as well as the other physical fields. An important property of the indicators, that we want to preserve during remap, is that they are non-negative and sum to one. To ensure this, we consider synchronized monotonicity treatment based on flux corrected transport/remap (FCT/FCR) algorithm. Such corrections represent modifications to the volume transferred from one zone to another, and have to be taken into account when other fields, e.g. density, are remapped. In addition, special care must be used when all material-specific fields are transported to a zone, where that material was not previously present, in order to avoid creating new extrema. We will present our approach to resolving these conservation and monotonicity requirements, based on synchronized FCT treatment, and illustrate it with various multi-material examples.

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The LANL Code Verification Test Suite

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Keywords: code verification; hydrodynamics; high explosives; test problems

ABSTRACT

The LANL Code Verification Test Suite (VTS) is a repository of tools and test problems to enable standardized code verification testing. Such testing provides an objective evaluation of code accuracy and spatial convergence, as well as an objective basis for comparing test problem results across codes. The standardization and configuration management of the suite ensures consistency and repeatability in the verification analysis. The tools and test problems are formulated such that they are usable, maintainable, customizable, and extendable by the code end-user community at LANL. This ease of use and maintenance ensures that verification test results are kept "fresh" and that new test problems as well as instances of test problems in new codes and with new code options can continually be added. The VTS has five fundamental components: (1) Standardized test problem definitions, representing the same test problem across different computational physics codes; (2) Test problem exact solutions via the software package *ExactPack*, ensuring that the same test problem solution is used for all code verification analyses; (3) Tools and standards for generating and managing code input decks and executing simulations; (4) Code verification analysis tools (also part of *ExactPack*) to perform tasks such as loading data, computing error norms, performing convergence analyses, and creating plots; and (5) Automated documentation capabilities, for consistent, customizable, and archive-quality reporting. The presentation will also cover a description of the suite of tests currently in the VTS, as well as some sample results and demonstrations of the customizable analysis capabilities.

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A new volume-preserving and continuous interface reconstruction method for multimaterial flow

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Keywords: multi-material hydrodynamics; interface reconstruction; dynamic programming.

ABSTRACT

A new interface reconstruction method which ensures continuity of the interface and perserves volumic fractions is presented here. It is made of two steps, first the minimization of a cost functional based on volumic fractions least square errors by using dynamic programming, a fast and efficient scheme well known in imagery [1], and then a local correction phase. In each cell, the interface is then made of two line segments joining two edges. This new interface reconstruction method, called DPIR (*Dynamic Programming Interface Reconstruction*) has been coupled with various advection schemes, among them the Lagrange + remap scheme. Figure 5 gives a reconstruction detail of a square type shape immersed in a rotating field, and compares the reconstruction with DPIR and the reconstruction with the Youngs method ([2]) after few iterations in time. With an almost negligible additional cost, it has been observed that the DPIR reconstruction method is more accurate and less diffusive, in various test cases that will be presented at the conference (single vortex flow field, Rayleigh Taylor instabilities, etc...).

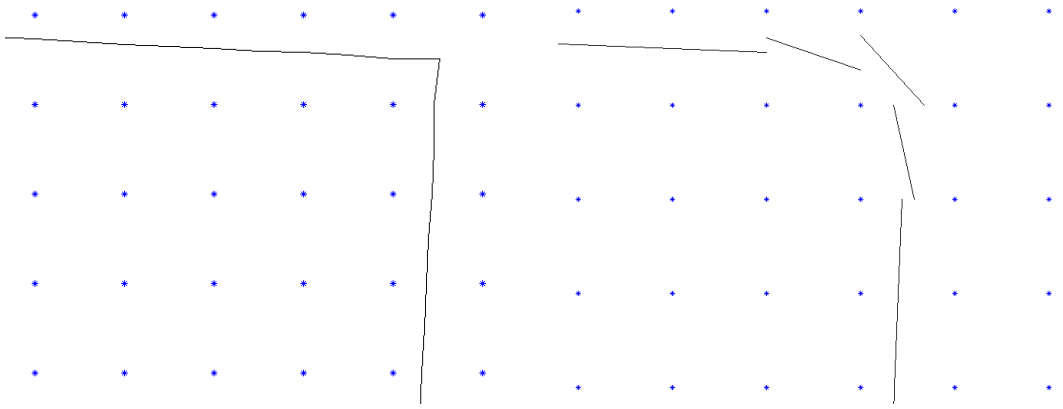

Figure 5: Interface reconstruction with DPIR (left) and Youngs (right).

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A novel a posteriori subcell finite volume limiter for the discontinuous Galerkin method on space-time adaptive grids

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Keywords: Arbitrary high-order ADER discontinuous Galerkin schemes; a posteriori ADER-WENO sub-cell finite volume limiter; MOOD paradigm; high order space-time adaptive mesh refinement (AMR); ADER-DG and ADER-WENO finite volume schemes; hyperbolic conservation laws.

ABSTRACT

In our talk we will present a novel *a posteriori* finite volume subcell limiter technique for the Discontinuous Galerkin finite element method for nonlinear systems of hyperbolic conservation laws in multiple space dimensions that works well for *arbitrary* high order of accuracy in space *and time* and that does *not* destroy the natural *subcell resolution* properties of the DG method. High order time discretization is achieved via a one-step ADER approach that uses a local space-time discontinuous Galerkin predictor method to evolve the data locally in time within each cell.

Our new limiting strategy is based on the so-called MOOD paradigm, which *a posteriori* verifies the validity of a discrete candidate solution against physical and numerical detection criteria after each time step. Here, we employ a relaxed discrete maximum principle in the sense of piecewise polynomials and the positivity of the numerical solution as detection criteria. Within the DG scheme on the main grid, the discrete solution is represented by piecewise polynomials of degree N. For those troubled cells that need limiting, our new limiter approach recomputes the discrete solution by scattering the DG polynomials at the previous time step onto a set of $N_s = 2N + 1$ finite volume subcells per space dimension. A robust but accurate ADER-WENO finite volume scheme then updates the subcell averages of the conservative variables within the detected troubled cells. The recomputed subcell averages are subsequently gathered back into high order cell-centered DG polynomials on the main grid via a subgrid reconstruction operator. The choice of $N_s = 2N + 1$ subcells is optimal since it allows to match the maximum admissible time step of the finite volume scheme on the subgrid with the maximum admissible time step of the DG scheme on the main grid, minimizing at the same time the local truncation error of the subcell finite volume scheme. It furthermore provides an excellent subcell resolution of discontinuities.

Our new approach is therefore *radically different* from classical DG limiters, where the limiter is using TVB or (H)WENO *reconstruction*, based on the discrete solution of the DG scheme on the *main grid* at the new time level. In our case, the discrete solution is instead *recomputed* within the troubled cells using a *different and more robust* numerical scheme on a *subgrid level*.

We illustrate the performance of the new *a posteriori* subcell ADER-WENO finite volume limiter approach for very high order DG methods via the simulation of numerous test cases run on Cartesian grids in two and three space dimensions, using DG schemes of up to *tenth* order of accuracy in space and time ($N = 9$). The method is also able to run on massively parallel large scale supercomputing infrastructure, which is shown via one 3D test problem that uses a tenth order scheme and **10 billion** space-time degrees of freedom per time step.

At the end of our talk, we will also present the extension of this novel *a posteriori* subcell limiter approach to space-time adaptive Cartesian grids (AMR) in two and three space dimensions, together with time-accurate local time stepping (LTS). The combination of the high order DG scheme and the sub-cell resolution of the new limiter with the advantages of AMR allows for an unprecedented ability in resolving even the finest flow details. The spectacular resolution properties of the new scheme have been shown through a wide number of test cases performed in two and in three space dimensions, both for the Euler equations of compressible gas dynamics and for the magnetohydrodynamics (MHD) equations.

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Radiative-shock solutions from grey Sn-transport with temperature- and density-dependent cross-sections

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Keywords: radiation hydrodynamics; radiative shocks; code-verification;

ABSTRACT

Radiative shocks are known to exist in extreme astrophysical environments, and have been replicated in high-energy-density-laboratory astrophysical experiments in the last decade. Accurate computational simulations of radiative shocks in both of these environments are important to understanding the underlying cause of the shock formation, and the effect of the shock on both the pre-shocked ambient material and the post-shocked highly-stressed material. The standard literature discussing radiation hydrodynamics assumes a nonequilibrium-diffusion radiation model, which assumes that the Eddington factor is a constant value of 1/3 everywhere. We have previously presented semi-analytic time-independent radiative-shock solutions which used grey Sn-transport to model the radiation and constant cross-sections. This radiation model allows the spatially-dependent variable-Eddington factor (VEF) to be determined, which qualitatively changes the structure of the radiative shock solution, even for simple constant cross-section solutions. Since that presentation, these solutions have been used in the astrophysics communnity as a code-verification tool. We present new radiative-shock solutions which incorporate temperature- and density-dependent cross-sections, as found in Bremstrahlung scattering. This temperature- and density-dependent model for the cross-section allows for a sharp variation of the VEF in the upstream region, which separates a hot translucent region from a cold opaque region. We will present these new results and discuss important modifications to our code which made the results possible. We will also discuss our future directions of code development, such as frequency-dependent solutions, which may also produce qualitatively different radiative-shock profiles.

Interface reconstruction algorithms in 2D and 3D for many-core and multi-core computer architectures

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ABSTRACT

With the increasing heterogeneity of high-performance computing hardware and the multitude of vendor-specific hardware, a major challenge to computational physicists is to work in close collaboration with computer scientists to develop portable and efficient algorithms and software on these novel computer architectures. In this work, we have written a single portable and efficient code, named PINION, using NVIDIA's Thrust library to perform interface reconstruction in two-dimensions and three-dimensions on structured Cartesian meshes. Interface reconstruction is a technique commonly used in volume tracking methods for simulations of multi-material flows. The Thrust library provides a high-level interface to program on GPUs as well as multi-core CPUs because it supports CUDA, OpenMP, and Intel Threading Building Blocks. However, the Thrust library has a simplistic data model and only employs one-dimensional vectors, making it challenging to perform multi-dimensional physics-based simulations. Therefore, we have designed two-dimensional and three-dimensional mesh data structures that are mapped to the one-dimensional vectors used by Thrust. Since our mesh data structures present an interface using familiar terminology (such as cells, vertices, and edges), they are simple to use in physics algorithms. With these new data structures in place, we have implemented a recursive volume-of-fluid initialization algorithm and standard piecewise interface reconstruction algorithms in two-dimensions and in three-dimensions, and have tested them on multiple architectures. Our work provides a single implementation of these algorithms that can be compiled to multiple backends (including multi-core CPUs, NVIDIA GPUs, and Intel Xeon Phi coprocessors), making efficient use of the available parallelism on each. Performance results will be shown to illustrate the utility of this approach.

A cell-centered Finite Volume method for solving multi-dimensional hyper-elasticity equations written under total Lagrangian form

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Keywords: finite volume method; cell-centered; unstructured meshes; hyper-elasticity equations; multi-dimensional flows; Lagrangian methods.

ABSTRACT

Finite Volume discretization of non-linear elasticity equations seems to be a promising alternative to the traditional Finite Element discretizations currently employed [1]. In this work, we intend to derive a Finite Volume discretization to compute the large deformations of elastic isotropic isothermal materials including shock waves. The materials under consideration are characterized by an hyper-elastic constitutive law for which the second Piola Kirchhoff stress tensor is the derivative of a strain energy function with respect to the right Cauchy Green tensor. In this manner, the material model satisfies the principle of material frame indifference and is thermodynamically consistent. The set of governing equations consists of the linear momentum equation, which is written under total Lagrangian form, and the geometric conservation law (GCL), which is nothing but the time rate of change of the deformation gradient. Extending the methodology described in [2] for Lagrangian gas dynamics, we present a nominally second-order cell-centered discretization for solving the equations of non-linear elasticity on tetrahedral grids. This work can also be viewed as an extension of the two-dimensional first-order scheme introduced in [3]. We provide a spatial discretization of the deformation gradient for which the Piola compatibility condition is satisfied. Further, the numerical fluxes at cell interfaces are approximated to ensure a thermodynamic-like dissipation inequality. The robustness and the accuracy of this Finite Volume method for non-linear elasticity are assessed by means of numerous representative test cases.

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ALE-FEM for Two-Phase Flows with Surfactants

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Keywords: multi-material hydrodynamics; ALE methods; Surfactants

ABSTRACT

The influence of surfactants (surface active agents) on the deformation of droplets and the structure of the surrounding flow field is an active research area with numerous applications. The convective transport induced by the flow field generates a local accumulation of surfactants and the resulting Marangoni forces may lead to a destabilization of the interface with essential consequences on the flow structure. This is a complex process whose tailored use in applications requires a fundamental understanding of the mutual interplay.

We present a finite element method for the flow of two immiscible, incompressible fluids in two and three dimensions. Thereby the presence of soluble and insoluble surfactants is considered.

We consider a bounded domain $\Omega \subset \mathbb{R}^d$, $d = 2, 3$, filled with two incompressible, immiscible fluids, which occupy at time t the domains $\Omega^i(t)$, $i = 1, 2$. Let $\partial\Omega^i(t)$ denote the boundary of $\Omega^i(t)$, $i = 1, 2$, and $\Gamma(t) = \partial\Omega^1(t) \cap \partial\Omega^2(t)$ the interface of $\Omega^1(t)$ and $\Omega^2(t)$. Further, let $n(t, \cdot)$ be the outer unit normal on $\Gamma(t)$ with respect to $\Omega^1(t)$ and $V(t, \cdot)$ the normal velocity of the interface with respect to n. The velocity and pressure fields of the two fluids at time t are denoted by $u^i(t, \cdot)$ and $p^i(t, \cdot)$, respectively. The surfactant concentration in the bulk phases are denoted with c^i and the surface surfactant concentration with c_Γ. Together with the Navier-Stokes equation, the convection diffusion equations for bulk and surface, and boundary conditions on the interface the mathematical model read

$$\partial_t u^i + (u^i \cdot \nabla)u^i - \nabla \cdot \mathbb{S}(u^i, p^i) = f, \quad \nabla \cdot u^i = 0 \quad \text{in } \Omega^i(t), \tag{2}$$

$$[-\mathbb{S}]n = \sigma(c_\Gamma)\kappa n + \nabla_\Gamma \sigma(c_\Gamma), \quad [u] = 0, \quad V = u \cdot n \quad \text{on } \Gamma(t), \tag{3}$$

$$\partial_t c^i - D^i \Delta c^i + (u^i \cdot \nabla)c^i = 0 \quad \text{in } \Omega^i(t), \tag{4}$$

$$[D\partial_n c] = -S(c^1, c^2, c_\Gamma) \quad \text{on } \Gamma(t), \tag{5}$$

$$\partial_t c_\Gamma - D_\Gamma \Delta_\Gamma c_\Gamma + \nabla_\Gamma \cdot (c_\Gamma u|_\Gamma) = S(c^1, c^2, c_\Gamma) \quad \text{on } \Gamma(t). \tag{6}$$

for $i = 1, 2$. Where, $\mathbb{S}$ is the usual stress tensor for Newtonian fluids, f describes gravitational forces, $[h] := h^1 - h^2$ denotes a jump of quantity h across the interface, $\sigma(c_\Gamma)$ is the surface tension coefficient, κ denotes the mean curvature of the interface, D^i is the diffusion coefficient for the bulk $\Omega^i(t)$, D_Γ is the surface diffusion coefficient, ∇_Γ and Δ_Γ are the surface version of the corresponding differential operators, S describes ad- and absorption of surfactant at the interface and while ∂_t denotes the time derivative, ∂_n denotes the spatial derivative in normal direction.

Our finite element method uses the Arbitrary Lagrangian Eulerian (ALE) technique, which tracks the interface by moving grids. We use second order finite elements and a second order interface approximation, which allows precise incorporation of surface tension forces and Marangoni forces.

We study the influence of surfactants on the dynamics of two-phase flows. In several numerical tests we compare cases of soluble and insoluble surfactants and surfactant free settings.

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Local slide line merging capability

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Keywords: multi-material hydrodynamics; Lagrangian methods; Eulerian methods; ALE methods; Slide line merging.

ABSTRACT

Slide lines [1, 2] allow material interfaces to be accurately represented where frictional forces are applied, different shock speeds in materials create thin shear layers, or mesh tangling is likely to occur. Allowing the interfaces to move, or slide, relative to each other with pure Lagrangian or minimal ALE motion avoids the internal elements of the mesh becoming distorted in each material, and also allows for additional physics to control the extent of the slide movement. Where the slide interface becomes distorted, for example due to high local curvature on the slide line, robustness issues may be introduced in ensuring correct node movement along the slide line. In this case, to allow the slide line node movement to be compatible with the local mesh movement, it may be beneficial to merge or partially zip the slide line and ALE the interface instead.

Development of a capability to merge slide lines on spatially decomposed meshes is presented. This process involves allowing slipped slide line nodes to move along the slide line to the co-ordinates of their corresponding master slide line nodes via an iterated local remap once the merge condition has been triggered. Once merged, mesh connectivity is updated, with ghost data created if the merged node lies on a processor boundary. The merged interface may then evolve due to multimaterial ALE mesh motion. The method allows slide lines to be merged completely, or for slide nodes to be gradually zipped once the local merge condition has been met for each node. Examples are shown demonstrating the performance of the method.

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Local stability for third-order schemes on conical unstructured meshes

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Keywords: Conical meshes, finite volume method, third-order reconstruction, remapping, advection, a posteriori iterative limitation, flux corrected transport.

ABSTRACT

We focus on local stability for third-order method dedicated to transport equation in two space dimension. The finite volume method is third-order accurate, both on conservative quantities (using Least-Squares reconstruction [1, 7, 4]) and geometry (using conical meshes) [6] see Figure 6. The stability for transport schemes is obtained by combination and extension of works [3, 4, 2, 5].

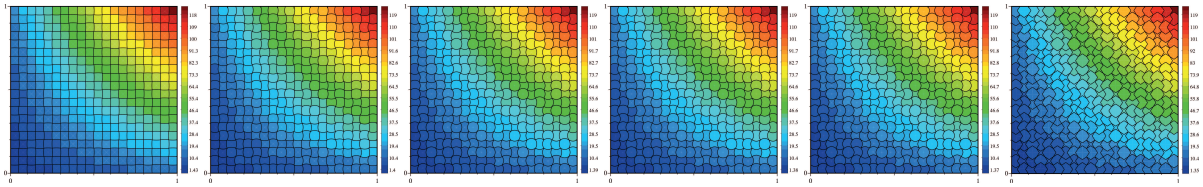

Figure 6: Reconstruction of quadratic polynoms is exact on arbitrary conical cells: a first step for fully third-order schemes (geometry **and** conservative unknowns).

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Advances in Dendritic Mesh Generation, LA-UR 15-21449

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Keywords: shock hydrodynamics; multi-material hydrodynamics; Lagrangian methods; ALE methods; mesh generation; dendritic meshing; mesh paving.

ABSTRACT

The Lagrangian Application Project (LAP) at Los Alamos National Laboratory develops the FLAG ALE code as part of the Advanced Simulation and Computing (ASC) program. FLAG operates on dendritic unstructured polyhedral meshes. Figure 7 shows two examples.

Dendritic mesh generators enable users to construct meshes of complex geometry that conform to material interfaces, are regular and have specified anisotropic cell sizes and distributions. These mesh qualities are desirable for accurate Lagrangian and ALE shock hydrodynamics simulations. The current dendritic mesh generation capability used by FLAG [1] is based on a block-structured approach with edge removal in only one logical direction. The unidirectional feathering constraint restricts anisotropic cell size control and often requires more careful block decomposition. We present two advances in dendritic mesh generation: dendritic paving and multi-directional feathering.

The dendritic paving concept adapts the all-quad paving or advancing front techniques such as wedge, tuck, seam, repair, etc. to leverage dendrites. As with traditional paving, mesh blocks can be unstructured and mesh block geometry can be more general, thus simplifying the mesh generation process. However it also produces meshes that are regular and satisfy anisotropic cell size and distribution specifications. In addition, quad paving constraints such as even number of boundary nodes no longer apply.

Multi-directional feathering of structured dendritic blocks, which is being developed under contract with Kitware, enables anisotropic cell size control. This provides added flexibility to users when considering how to decompose the computational domain into mesh blocks. It also extends to three dimensional structured dendritic mesh blocks, where tri-directional feathering can be used to maintain anisotropic cell sizes in all three logical directions.

We present the methodology, current status, results, issues and future direction for these dendritic mesh generation research efforts.

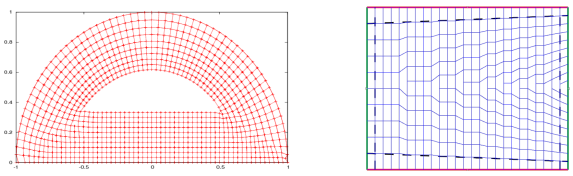

Figure 7: Dendritic paving (left) and feathering (right) examples.

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Closure Models for High-Order Finite Element Hydrodynamics

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Keywords: high-order discretizations, multi-material shock hydrodynamics; ALE methods; closure models.

ABSTRACT

In this talk we present our approach in developing a multi-material extension of the high-order finite element Lagrangian method described in [1]. Lagrangian codes solve the hydrodynamics equations on a moving mesh. In order to compute correct pressure, such algorithms must be able to handle the so-called mixed cells where a single computational element contains multiple materials. Mixed cells appear when aligning the mesh to the material interfaces is not desirable, or the Lagrangian algorithm is combined with a remesh procedure. The goal of a closure model is to define evolution of material volumes, during a Lagrangian simulation, in a physically reasonable way.

We reformulate some of the existing methods (e.g. [2]) for the low-order, cell-centered case, as multi-material mathematical models on a continuous level, thus extracting and separating the model from the discrete algorithm. Then we apply a high-order finite element discretization to this continuous model. This combination results in a pressure equilibration procedure that defines terms which control the evolution of material volume and the transfer of internal energy between distinct materials. These terms are computed at each integration point of a mixed cell, complying with the high-order finite element concept of sub-cell resolution without the need of reconstructing an explicit material interface.

Using the single-material discretization in [1] as a base, we duplicate the material density and energy for every material present in a zone, but use a single velocity, motivated by the fact that the conforming computational mesh has a single motion during a Lagrangian computation. In addition, a set of new variables, i.e. volume fractions, is added to the zonal data that describes the distribution of the materials within the zone. These volume fractions can be represented as pointwise values at a chosen set of integration points on a reference cell, or arbitrarily high-order finite element functions. This spatial discretization is combined with high-order explicit time stepping methods.

We will show the details of the above discretization and illustrate the numerical performance of the resulting algorithms on a set of model multi-material test problems.

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A Conformal Decomposition Finite Element Method with Guaranteed Quality Dynamic Discretization*

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Keywords: Enriched finite element methods; Moving interface methods; Mesh quality.

ABSTRACT

Enriched finite element methods such as the Generalized Finite Element Method (GFEM), the eXtended Finite Element Method (XFEM), and the Conformal Decomposition Finite Element Method (CDFEM), are powerful tools for multiphase and multimaterial problems. These methods provide discretizations that dynamically adapt to moving material and phase boundaries such that interfacial physics and discontinuities are accurately captured. In the CDFEM, new degrees of freedom are assigned to nodes that are added at the intersection of a level set surface with the edges of the background mesh.

Time integration in enriched finite element methods is challenging because the degrees of the freedom change in a discontinuous manner as nodes or elements change material or phase. The degrees of freedom at a node depend on the phases or materials that intersect the elements supported by the node. As materials move through the domain, unknowns are created and destroyed in order to accommodate the dynamic discretization. We present a novel method for handling the dynamic discretization produced by the CDFEM [1], based on moving mesh methods for fixed discretizations and using ideas from Arbitrary Lagrangian-Eulerian methods. First or second order accuracy in time is demonstrated, for both strong and weak discontinuities that vary in time and space.

Because an interface can come arbitrarily close to background mesh nodes, the linear system of equations generated by a CDFEM problem can become poorly conditioned due to the presence of small elements. This is often mitigated by snapping the interface to the nearest background mesh node when a minimum separation is reached, so the small element is not generated, but this snapping introduces an error in the location of the interface. An alternative approach is presented here that removes the poor conditioning without introducing an error in the interface location. When an edge is crossed by the interface near one of its ends, the nearest node of the edge is moved to the crossing instead of moving the crossing to the node. This method is similar to that used in Isosurface Stuffing [2], and improves the quality of the resulting decomposed mesh to produce discrete systems of equations with dramatically better conditioning. Because no error is introduced in this process, larger snapping tolerances can be used to produce high accuracy and robustness.

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Multi-Scale Pressure-Residual-Based Anti-Hourglass Scheme in Compatible Staggered Lagrangian Method

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Keywords: multi-material hydrodynamics; Lagrangian methods; compatible staggered discretization; hourglass treatment.

ABSTRACT

Hourglassing is a well-known pathological numerical artifact produced by the Lagrangian methods, decreasing robustness of the simulation and resulting in its early breakdown. There exist a large number of methods dealing with hourglass-control, many of them are summarized in the seminal work [1]. In the community of the staggered compatible Lagrangian methods, the approach of subzonal pressure forces [2] is widely used. However, in case of multi-material simulations, one needs to deal with the material pressure or density in each subzone to construct such forces, which requires to perform material reconstruction on the subzonal level. To avoid this problem, we have adapted the multi-scale residual-based stabilization [3] for the staggered compatible discretization. Here, we describe two discretizations of the new approach and demonstrate its properties on selected numerical problems.

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Divergence preserving reconstruction of nodal components of the vector field from its normal components to the faces

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Keywords: vector reconstruction; divergence preservation; Lagrangian hydrodynamics based on Godunov method.

ABSTRACT

We deal with the problem of how to compute the vector field components at mesh nodes from their normal components to the edges of computational mesh. This problem appears naturally e.g. in Lagrangian gas dynamics discretizations based on Godunov's method, where the normal component of a vector on an edge between two cells is computed from the solution of a 1D Riemann problem, but the Cartesian components are needed at nodes in order to compute the nodal motion,

This problem has been treated in [1] by two methods based on least squares approximation of the vector field using piece-wise constant or piece-wise linear reconstruction. Using these two methods the two discrete approximation of the divergence (one from the normal components to the edges and another one from Cartesian components at nodes) are different. They even do not converge for the zeroth order method using piece-wise constant reconstruction. They converge to each other for the first order method using piece-wise linear reconstruction. We require that these two discrete divergences give the same result in all computational cells. We treat this problem by constrained optimization employing Lagrangian multipliers, which leads to the solution of a global system similar to a system obtained when solving elliptic problem with cell centered scalar function and nodal discretization of vector function. The new divergence preserving method has been developed on 2D logically rectangular mesh. Numerical examples demonstrating the properties of the method include reconstruction of smooth and non-smooth vector fields on smooth and non-smooth, randomly perturbed, meshes.

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A direct high accurate ALE numerical scheme with a posteriori stabilization technique

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Keywords: shock hydrodynamics; hydrodynamics; Lagrangian methods; Eulerian methods; ALE methods; a posteriori stabilization.

ABSTRACT

We will present a new family of efficient high order accurate direct Arbitrary-Lagrangian-Eulerian (ALE) one-step ADER-MOOD finite volume schemes for the solution of nonlinear hyperbolic systems of conservation laws for moving unstructured triangular and tetrahedral meshes. This family is the next generation of the ALE ADER-WENO schemes presented in [3]. Here, we use again an element-local space-time Galerkin finite element predictor method to achieve a high order accurate one-step time discretization, while the somewhat expensive WENO approach on moving meshes, used to obtain high order of accuracy in space, is replaced by an *a posteriori* MOOD loop which is shown to be less expensive but still as accurate.

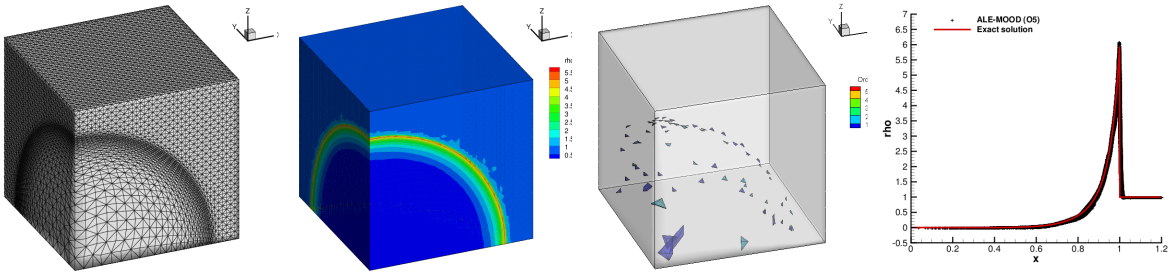

Figure 8: Sedov problem in 3D on 32×10^4 thetrahedra at $t = 1$. Left→right: mesh, density, density as a function of cell radius, polynomial degree of reconstructions in cells.

This *a posteriori* MOOD loop [2] ensures the numerical solution in each cell at any discrete time level to fulfill a set of user-defined detection criteria. If a cell average does not satisfy the detection criteria, then the solution is locally re-computed by progressively decrementing the order of the polynomial reconstruction, following a so-called *cascade* of predefined schemes with decreasing approximation order. A so-called parachute scheme, typically a very robust first order Godunov-type finite volume method, is employed as a last resort for highly problematic cells. The cascade of schemes defines how the decrementing process is carried out, i.e. how many schemes are tried and which orders are adopted for the polynomial reconstructions. The cascade and the parachute scheme are choices of the user or the code developer. Consequently the iterative MOOD loop allows the numerical solution to maintain some interesting properties such as positivity, mesh validity, *etc*, which are otherwise difficult to ensure. We have applied our new high order unstructured direct ALE ADER-MOOD schemes to the multi-dimensional Euler equations of compressible gas dynamics [1]. A large set of test problems has been

simulated and analyzed to assess the validity of our approach in terms of both accuracy and efficiency (CPU time and memory consumption), see the Sedov problem for our ALE-ADER-MOOD-$\mathbb{P}_0\mathbb{P}_4$ code in Figure 8.

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On Extension of Monotonicity to Multi-Dimensional Flows

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Keywords: shock hydrodynamics; multi-material hydrodynamics; Lagrangian; Eulerian; ALE; slope limiters; flux limiters;

ABSTRACT

In a high order scheme, the distribution of the variables in a zone depends (e.g. through a Taylor expansion) on the gradients of these variables. Near discontinuities these gradients may become unbounded. To prevent non-physical fluctuations in the solution, either the *slopes* or the resulting *fluxes* must be *limited* . The *slope-limiter* or *flux-limiter* algorithms are designed to prevent such *monotonicity violations*. Only the advent of such limiters made possible the use of high order schemes for compressible flows. The concept of monotonicity in one dimensional space is well established. A density profile is monotonic if its value anywhere in the zone lies in between the corresponding values in the left and right neighbors. However the extension of monotonicity to multi-dimensional space is not trivial. It was customary to apply the limiters separately to each (e.g. Cartesian) component of a vector or tensor. However, as it was shown [1, 2], such a procedure is not *frame invariant* and it can break the symmetries present in the problem. For a vector variable (e.g. velocity) the *convex hull* based *VIP* (vector image polyhedron) [1,2] is the natural extension of an one-dimensional range to vectors in multiple dimensions. The symmetry breaking could be also avoided by applying the limiting in flow related directions [3]. For tensors, the natural extension of VIP would be again a convex hull based *TIP* (tensor image polyhedron) [1]. Alternative approaches were also considered [4]. The importance of using frame-invariant limiters for vectors and tensor is more and more recognized [5]. The definition of monotonic behaviour of a scalar field in multiple dimensions also raises some questions. Requiring, the value of the density in a zone to stay in between the smallest and largest value of the densities in all neighbour zones, would lead to a frame invariant, but too dissipative scheme. Alternatively the VIP approach could be applied to the density gradients [6]. In the current work, we discuss the monotonicity conditions to be used in multiple dimensions and their effect on some test cases. In particular we will consider more in detail the *TIP* limiter to be used for the stress tensor in elastic plastic flow simulations.

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The *VIP* limiter and related ideas emerged through many discussions with prof. Joseph Falcovitz.

Comparison of Material Point Method (MPM) and Volume of Fluid (VOF) Method in simulation of HE material fragment impact

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Keywords: shock hydrodynamics; multi-material hydrodynamics; Lagrangian methods; Eulerian methods; ALE methods; fluid-structure interaction.

ABSTRACT

The Material Point Method (MPM) and Volume of Fluid Method (VOF) are two major methods in simulations of multi-material interaction. MPM utilizes a Lagrangian approach used in the LANL code CartaBlanca, while the VOF approach is Eulerian and is used in the LANL code Pagosa. The two approaches offer many similarities in capability. For example, both methods can efficiently track material interfaces, and can handle incompressible and compressible flow with strong shocks. Both can handle changes in the global topology of the interface, such as fronts that either break up into droplets or collide and merge. Additionally, both provide advantages over other interface tracking methods, such as the Level-Set method, as they naturally conserve the mass of each material (or fluid). However, a detailed quantitative comparison of the two methods to identify distinguishing characteristics has yet to appear in the literature. To investigate these approaches, we perform simulations of a high-velocity fragment impact on canned high explosives using both approaches, and the results are presented and compared. Results suggest that MPM outperforms VOF in cases of large deformation, but that VOF outperforms MPM in the accuracy of the interface topology.

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A Cell-centered Finite Volume method on Lagrangian grid for solving elastic-plastic flows in two-dimensional axisymmetric geometry

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Keywords: shock hydrodynamics; Lagrangian methods; elastic-plastic flows; cell-centered Finite Volume method.

ABSTRACT

The numerical simulation of the response of solid materials undergoing large strains is of particular interest in many industrial applications such as high-velocity impacts [3]. In this presentation, we shall describe a cell-centered Lagrangian scheme devoted to the numerical simulation of solid dynamics on two-dimensional unstructured grids. This method is the extension to axisymmetric geometry of the work initially presented in [2]. The underlying physical modeling relies on the classical elastic-plastic material model initially proposed by Wilkins [4]. This hypoelastic model is characterized by the decomposition of the Cauchy stress tensor into the sum of its deviatoric part and the thermodynamic pressure which is defined by means of an equation of state. Regarding the deviatoric stress, its time evolution is governed by a classical constitutive law for isotropic material. The plasticity model employs the von Mises yield criterion and is implemented by means of the radial return algorithm. The numerical scheme relies on a finite volume cell-centered method wherein numerical fluxes are expressed in terms of sub-cell force. The generic form of the sub-cell force is obtained by requiring the scheme to satisfy a semi-discrete dissipation inequality. Sub-cell force and nodal velocity to move the grid are computed consistently with cell volume variation by means of a node-centered solver, which ensures total energy conservation. The nominally second-order extension is achieved by developing a two-dimensional extension in the Lagrangian framework of the Generalized Riemann Problem methodology, introduced by Ben-Artzi and Falcovitz [1]. We also address and solve the issue of developing a piecewise linear monotonic reconstruction of the stress tensor which maintains the Galilean invariance of the second-order spatial discretization. Finally, the robustness and the accuracy of the numerical scheme are assessed through the computation of several test cases.

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A Comparative Study of Thermodynamic Closures for Multimaterial Cells in Lagrange–Plus–Remap Algorithms

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Keywords: shock hydrodynamics; multi-material hydrodynamics; Eulerian methods; ALE methods.

ABSTRACT

Several hydrocodes successfully employ a homogenized picture of multimaterial cells to perform updates of momentum and energy equations. Frequently, these schemes require a closure model to distribute the changes in volume and internal energy of a mixed cell to its material components. A Lagrange–plus–Remap version of Los Alamos National Laboratory's adaptive mesh refinement code, xRage, implements four closure models, including two variants of the uniform strain approximation, the Tipton pressure relaxation method and pressure–temperature equilibrium. Despite well–known flaws with the approximations of these schemes, each of these closure models prove to be robust and applicable to diverse combinations of mixed cell constituents. In this presentation, we provide a detailed description of these four closure models, along with descriptions of historical alternatives to provide context. We describe the implementation of the closure models in xRage, with additional details regarding tabular equation–of–state constraints. We compare these closure models on a set of test problems ranging from one–dimensional, two–material shock tube problems to two–dimensional solid impact problems.

An Eulerian Method for Computing Gas-Solid Two-Phase Flows

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Keywords: dispersed two-phase flows; non-conservative Euler equations; moving grids; Eulerian methods; Rusanov scheme.

ABSTRACT

In our presentation we address the development of a numerical method that solves the system of governing equations for dispersed solid-gas two-phase flows in non-equilibrium regimes when the phase velocities and temperatures are different enough. The mathematical model is described by conservation laws of mass, momentum, and energy for the solid and gas phases. The intergranular pressure is introduced in the solid phase, which depends on the solid volume fraction and vanishes as the volume fraction becomes less than a critical value of the close-packed structure. The solid phase equations degenerate in this case and are no longer strictly hyperbolic. Due to so-called nozzling terms in the right-hand side, the gas phase equations are not conservative. In the present paper, we discuss how to correctly take into account these two singularities of the governing equations at the discrete level.

We split the equations into two sub-systems – one for the solid phase and another for the gas phase. The first sub-system (solid) is integrated with the Godunov method. With this aim, we state the appropriate Riemann problem that describes elementary solid-solid interactions. Under minor assumptions this problem can be solved analytically in the non-linear formulation; the solution provides the flux approximation that correctly works in the whole range of volume fraction. The linear approximation of the solution is shown to be insufficient and leads to incorrect numerical results.

The sub-system of the gas phase is referred to the class of non-conservative Euler equations (shallow water, quasi-1D gas dynamics, two-phase flow). These equations have intensively investigated during the last decade. Most results obtained concern a fixed in space function of volume fraction [1]. In our case this function varies both in space and in time. We develop the Rusanov method [2] to solve numerically the gas dynamics constrained by moving solid porous material. First, the Rusanov flux approximation is recast so that it could be applied to moving Eulerian grids. Then, we extend the Rusanov-type method for the non-conservative Euler equations with fixed in space volume fraction [1] to account for moving grids with maintaining the property of well-balancing. Finally, the Rusanov-type method is proposed to calculate gas dynamics in the moving skeleton of the solid phase. The method is proved to guarantee the well-balancing property.

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An Edge-Centered Tensor Artificial Viscosity

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Keywords: artifical vscosity; shock hydrodynamics; Lagrangian methods;

ABSTRACT

Artificial viscosity is frequently used to allow numerical solution of shock problems. There have been many variations [5], [3], [2], [1], [4], and research into improved forms is ongoing. We present an alternative artificial viscosity, or "Q". We were guided by the need for Galilean invariance, reduced mesh sensitivity to mesh topology, robustness in high aspect ratio zoning, and reduced velocity diffusion in non-compressing directions.

We employ a tensor formulation to obtain an edge-centered Q. The Q force opposes only the compressing direction of the local velocity field. We examine sensitivity to several methods of obtaining a velocity gradient. We use a tensor length scale to capture the effects of local mesh geometry. We show that careful treatment of the length scale is a critical part of forming a physically reasonable Q in the limit of high aspect ratio zoning. We find that because the force direction will be parallel to one of the eigenvectors of the Q tensor, it is advantageous to formulate Q as a symmetric tensor to force its eigenvectors to be perpendicular. We present several standard 2D test problem results (Noh, Sedov, Saltzman) and some high aspect ratio variations.

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A 3D Arbitrary Lagrangian Eulerian hydrodynamic approach for tetrahedral meshes

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Keywords: Shock hydrodynamics; Riemann solver; Lagrangian; Eulerian; ALE; Tetrahedral meshes.

ABSTRACT

We present a three dimensional (3D) arbitrary Lagrangian Eulerian (ALE) hydrodynamic scheme suitable for modeling complex compressible flows on tetrahedral meshes. The new approach stores the conserved variables (mass, momentum, and total energy) at the nodes of the mesh and solves the conservation equations on a control volume surrounding the point. This type of an approach is termed a point-centered hydrodynamic (PCH) method. The conservation equations are discretized using an edge-based finite element (FE) approach with linear basis functions. All fluxes in the new approach are calculated at the center of each tetrahedron. A multidirectional Riemann-like problem is solved at the center of the tetrahedron. The advective fluxes are calculated by solving a 1D Riemann problem on each face of the nodal control volume. Second-order spatial accuracy is achieved on smooth flows by reconstructing the solution over the nodal control volume with a linear Taylor series expansion. The gradient of the reconstruction is limited around discontinuities for monotone solutions. A 2-stage Runge-Kutta method is used to evolve the solution forward in time, where the advective fluxes are part of the temporal integration. For ALE motion, the mesh velocity is smoothed by solving a Laplacian equation. The details of the new ALE hydrodynamic scheme are discussed. Results from a range of numerical test problems including shock driven flows and smooth flows are presented. Results are presented for Lagrangian [1], Eulerian and ALE motion [2].

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Conservative Reproducing Kernel Smoothed Particle Hydrodynamics for Solids

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Keywords: shock hydrodynamics; multi-material hydrodynamics; solid mechanics; Lagrangian methods; meshfree methods.

ABSTRACT

Conservative Reproducing Kernel Smoothed Particle Hydrodynamics (CRKSPH [1]) is a new meshfree method related to Smoothed Particle Hydrodynamics (SPH [4]). The reproducing kernel (RK) extension of SPH has been known since the mid-90's [3, 2], but has primarily been utilized for incompressible flows in engineering applications. The interpolation theory of reproducing kernels represents a significant improvement in accuracy compared with standard SPH interpolation, but breaks the underlying symmetries that allow the SPH discretization equations to be written such that momentum and energy are rigorously conserved. For this reason RK methods have found limited use, particularly for problems involving strong shocks or large deformations. In [1] we derive a fully conservative method based on reproducing kernels (CRKSPH) appropriate for use in compressible flows, including shock physics and/or fluid instabilities. This talk will discuss extensions of CRKSPH for modeling solids including material strength effects, and consider a variety of tests of our new formalism for problems requiring material strength.

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Conservative, Multimaterial ReALE Hydro on a Staggered Grid

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Keywords: ALE methods; Multimaterial hydro; Mesh reconnection; Voronoi mesh generation.

ABSTRACT

Reconnection-ALE (ReALE) is a generalization of the “Lagrange + Remap" update that characterizes most ALE hydrodynamics codes [1]. The ALE update is augmented by a mesh rezoning phase in which the Lagrangian mesh is replaced by an automatically-generated Voronoi tessellation. The physical state from the deformed Lagrangian mesh is mapped to the new Voronoi mesh by means of an intersection-based overlay. The simulation proceeds as before under a new mesh topology and geometry.

ReALE development has primarily focused on cell-centered discretizations for Lagrangian hydro. This greatly simplifies the conservative remapping of fluid variables. Our approach utilizes a spatially-staggered hydro discretization that is compatibly differenced to achieve conservation of mass, momentum, and energy [2]. As a result of this discretization, subzonal fluid information must be treated during the ReALE update to maintain conservation of momentum.

This talk will focus on a new algorithm for conservatively treating subzonal information that avoids a direct subzone-to-subzone overlay [3]. Subzonal information is reconstructed using coarsened representations of the data on the primary (zone) and dual (node) mesh elements. Reconstructing the data is equivalent to solving a linear least-squares problem that is global yet sparse. I will outline the algorithm, discuss its extension to multimaterial data, and demonstrate its effectiveness on a variety of multimaterial hydro tests using ReALE.

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Optimization-based mesh correction with volume and convexity constraints

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Keywords: Lagrangian motion; incremental remap; semi-Lagrangian transport; departure volume correction; volume fraction; passive tracer.

ABSTRACT

We consider the problem of finding a mesh such that 1) it is the closest, with respect to a suitable metric, to a given source mesh having the same connectivity, and 2) the volumes of its cells match a set of prescribed positive values that are not necessarily equal to cell volumes in the source mesh. This volume correction problem arises in important simulation contexts, such as satisfying a discrete geometric conservation law [3] and solving transport equations by semi-Lagrangian [2] or characteristic schemes [1].

In this talk we formulate volume correction as a constrained optimization problem. Specifically, the distance to the source mesh defines an optimization objective, while the prescribed cell volumes, mesh validity and/or cell convexity specify the constraints. We solve the optimization problem numerically using a sequential quadratic programming (SQP) method whose performance scales with the mesh size. To achieve scalable performance we develop a specialized multigrid-based preconditioner for optimality systems that arise in the application of the SQP method to the volume correction problem. Numerical examples illustrate the importance of volume correction, and demonstrate the accuracy, robustness and scalability of our approach.

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Maximum principle preserving finite element method for nonlinear conservation laws

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Keywords: shock hydrodynamics; high-order methods; limiters; Eulerian methods; invariant domains.

ABSTRACT

Maximum principle, entropy stability, convergence of viscosity approximations, and design of high-order methods based on limiting is a very well developed area in nonlinear scalar conservation laws. However, in the case of nonlinear systems many of the above problems are still open. We will present a new viscosity approximation for nonlinear hyperbolic systems based on a graph Laplacian viscosity [3]. In the case of the one-dimensional p-system we will show that this new method has a local invariant domain property which is the analog of a local maximum principle in the case of systems. We will derive sharp bounds for the viscosity coefficients for the invariant domain property to hold and show that this approximation is consistent with all entropy inequalities. Based on this first order viscous method, we will construct a second order limited method. The limiting is done in the spirit of Boris-Book and Zalezak [1, 2] where similar to the scalar case (see [4]) we use an entropy viscosity scheme for the high-order method in the limiting process. We will show that the limited method also preserves the local invariant domain property.

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ShaPo: A Framework for Generating 2D Voronoi Meshes

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Keywords: Voronoi; Tessellation; Remeshing; Parallelisation; Remeshing.

ABSTRACT

Voronoi meshes are involved in numerous applications from astrophysics to biology or computer graphics. Their properties are especially widely used in geophysical flows and computational fluid dynamics. Our main interest in Voronoi meshes related to Reconnection-Based ALE family of methods introduced in [1].

In this talk we present ShaPo, a cross platform C++ software library accessible from different programming languages (C, Fortran and Python) that integrates algorithms to generate, in serial or in parallel, 2D Voronoi meshes from a set of generators into a domain defined by non-convex multi-connected boundary polygons. ShaPo allows to generate either *Constrained Voronoi* or *Clipped Voronoi* tessellations respectively inspired from [2, 3] and [4], and provides the full cells, points and edges connectivity.

We describe the two different robust Voronoi construction algorithms implemented in ShaPo both based on the dual Delaunay triangulation computation. Proposed optimizations in regard to the original algorithms are also described. As ShaPo can also be used in a data-parallelism context where generators and boundaries are distributed across processors, a quick overview of the parallel algorithm based on an MPI communication layer is presented. Finally we describe the *remeshing* functionality of ShaPo which enables the generation of a Voronoi mesh in the sub-domain of an existing unstructured mesh - see Figure 9.

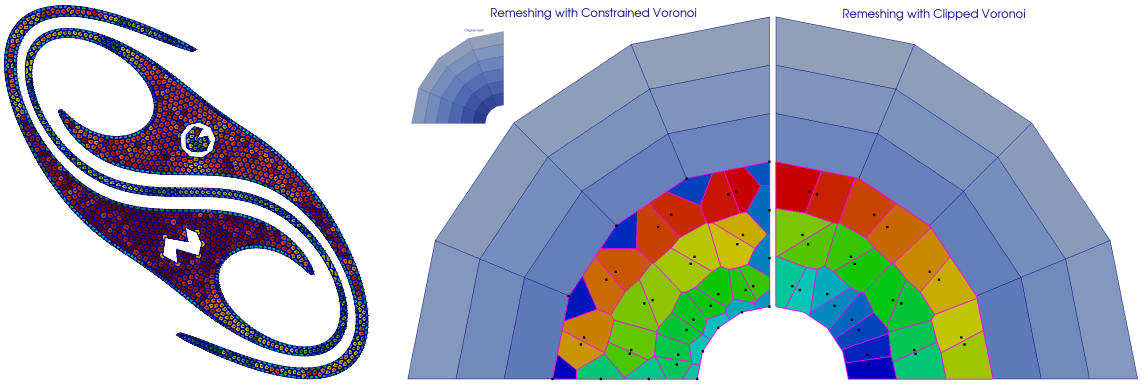

Figure 9: Left: Constrained Voronoi tessellation of a complex domain. Right: Comparison of Constrained vs. Clipped Voronoi tessellations for remeshing a subdomain of a radial mesh.

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A remapping-free high-order ALE method based on undistorted temporal-spatial control volumes

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Keywords: ALE method; irrotationality; temporal-spatial control volume; generalized Riemann problem.

ABSTRACT

Arbitrary Eulerian Lagrangian (ALE) methods [1] play a dominant role in the simulation of hydrodynamics problems with large deformation. ALE methods often consist of three steps: a Lagrangian step, a rezone step and a remap step, among which the remap step is a static process. However, that fluid flows between two meshes is a dynamic process, which leads to remapping-free ALE methods in [2][3][4] that directly couple mesh movement into physical variables' update to reflect the temporal evolution during the two meshes.

From the viewpoint of the temporal-spatial control volume, this work develops a remapping-free high-order ALE method based on undistorted temporal-spatial control volumes. According to the Hodge decomposition theorem [5], a vector field can always be decomposed into a divergence-free component and an irrotational component. This work generates mesh moving velocities by the irrotational component of fluid' s velocity, so the ALE mesh avoids Lagrangian mesh's rotation and keeps control volumes of no twist. Then based on the finite volume framework, 2-D Euler equations in integral form are discretized in such undistorted hexahedral temporal-spatial control volumes. Besides numerical fluxes are computed by generalized Riemann problem solver [6] to get a high-precision approximation. Typical numerical examples test and verify the new method.

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Entropy-based artificial viscosity stabilization for non-equilibrium Grey Radiation-Hydrodynamics

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Keywords: shock radiation-hydrodynamics; artificial viscosity method; entropy viscosity method.

ABSTRACT

The entropy viscosity method is extended to the non-equilibrium Grey Radiation-Hydrodynamic equations. The method employs a viscous regularization to stabilize the numerical solution with an artificial viscosity coefficient modulated by the entropy production which exhibits peaks in shock regions. The added dissipative terms are consistent with the entropy minimum principle. A new functional form of the entropy residual, suitable for the Radiation-Hydrodynamic equations, is derived. We demonstrate that the viscous regularization preserves the equilibrium diffusion limit. The equations are discretized with a standard Continuous Galerkin Finite Element Method and a fully implicit temporal integrator within the MOOSE multiphysics framework. The method of manufactured solutions is employed to demonstrate second-order accuracy in both the equilibrium diffusion and streaming limits. Several typical 1-D radiation hydrodynamic test cases with shocks (from Mach 1.05 to Mach 50) are computed to establish the ability of the technique to capture and resolve shocks.

CRKSPH - A Conservative Reproducing Kernel Smoothed Particle Hydrodynamics Scheme

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Keywords: shock hydrodynamics; Lagrangian methods; reproducing kernels; artificial viscosity.

ABSTRACT

Suitable modifications to the SPH interpolation scheme first suggested by [1] allow for the exact reproduction of constant, linear, or higher order fields, and these modifications are commonly referred to as reproducing kernel methods (RPKM). However, efforts in this realm have run into difficulties maintaining conservation of momentum when the kernel functions are no longer symmetric. We demonstrate a version of smoothed particle hydrodynamics that employs a first-order consistent smoothing function that exactly reproduces linear fields, building on RPKMs, while also maintaining momentum conservation. This scheme confers all of the benefits of traditional particle methods, such as Galilean invariance and natural conservation of momentum, while also eliminating some of their shortcomings, such as overly aggressive artificial viscosity and their inability to reproduce linear fields. We employ a simple fix to the momentum equation first derived for moving least-squares SPH methods [2] to our reproducing kernels that restores conservation. We also show how the reproducing kernel method's more accurate approximation of the velocity gradient allows for a much more conservative form of artificial viscosity, which hitherto fore has been a barrier to particle codes being employed for problems featuring fluid instabilities such as the Kelvin-Helmholtz instability.

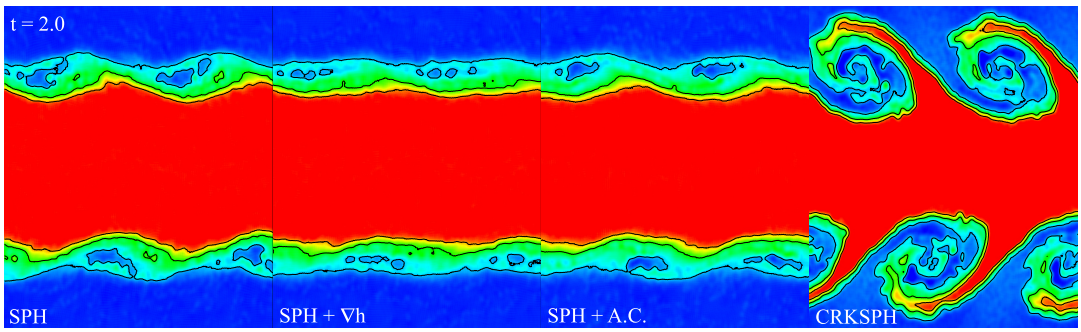

Figure 10: Snapshots at $t = 2.0 \approx 5\tau_{\mathrm{KH}}$ of the growth of a Kelvin-Helmholtz instability in density for (from left-to-right) traditional SPH, SPH with "grad-h" corrections, SPH with artificial conduction, and CRKSPH.

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Evolution Equations for Developing Improved High-Resolution Schemes

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Keywords: shock hydrodynamics; numerical analysys, variation, dissipation

ABSTRACT

The development of high-resolution numerical methods has been a tremendous achievement in computational physics. These methods have provided an essential balance of accuracy (fidelity or resolution) with physical admissibility combined with computational tractability. While these methods were a tremendous achievement, their recent progress has stalled in several respects. Here, I will provide some concepts that may spur further development through the utilization of evolution equations and the analysis of numerical methods using modified equation analysis. These concepts were essential in ideas that were key in the formulation of the original generation of methods[2] and was utilized to show that monotone methods produced vanishing viscosity entropy solutions. High resolution methods allowed the barrier theorem of Godunov[1] to be overcome and paved the way for further developments. Harten's work provided the work to tie these streams of work together by introducing the total variation concepts to formalize the mathematics[3]. Subsequently there have been several attempts to move beyond the first generation of high resolution methods, but each has met with limited success. I am proposing revisiting the foundational aspects of high-resolution methods by returning to modified equation analysis of numerical methods and providing connections to providing proof of physically admissible solutions. To conduct such analysis I am suggesting the study of the energy evolution of equations, and/or the continuous variation evolution. Each equation will admit a vanishing viscosity solution, and the modified equation analysis can provide a connection of the numerical method to admissibility. For a simple hyperbolic PDE, $u_t + f(u)_x = 0$, the basic physical admissibility condition can be given $u_t + f(u)_x = \nu u_{xx}, \nu \rightarrow 0$. Similarly, the variation evolution may be derived and used to similar effect, $|V|_t + f'(u)$, $|V|_x + f''(u)V^2 = 0$ where $V = u_x$, and its vanishing viscosity solution can be similarly stated $|V|_t + f'(u)|V|_x + f''(u)V^2 = \nu |V|_{xx}$. Finally, we will utilize modified equation analysis to produce analysis of existing and new clases of methods that offer the promise of greater resolution and more provable connections to physical admissibility. One basic concept is to uses TVD methods to tie high-order discretizations and admissibility conditions.

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A UQ Enabled Aluminum Tabular Multiphase Equation-of-State Model

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Keywords: shock hydrodynamics; equation-of-state; EOS; uncertainty quantification; UQ.

ABSTRACT

To begin to truly understand the boundaries of predictivity in computational simulation, we need to require uncertainty quantification (UQ) in the material models used in the numerical solution of continuum equations. A conceptual framework for the representation and propagation of the uncertainty in the equation-of-state (EOS) for hydrodynamic modeling has been proposed by the authors [1]. The framework includes the use of Bayesian inference to determine the probability density function for the parameters in the EOS models through the use of Markov Chain Monte Carlo (MCMC) methods and the tabular representation of this EOS using principal component analysis (PCA). We have also stressed the importance of an integrated software approach to employing UQ sampling methodologies directly in a continuum modeling code. This work has now been extended to include multiphase models with tens of parameters and multiple phases. We require an advanced adaptive MCMC approach, careful control over acceptable phase boundary shapes in the EOS model, an unstructured EOS tabular format using triangular linear basis functions, smooth mapping of the phase boundaries and interior grids between sample tables to minimize noise in the PCA analysis, and an efficient tabular mesh generation system. Every aspect of the Bayesian modeling coupled with the phase boundary and meshing system must be robust and fast enough to be usable. These requirements are difficult to achieve. We describe the requirements and the solutions found to effectively build a wide range aluminum model using this approach. We also show how the uncorrelated random variables arising from the PCA analysis can be evaluated and understood in terms of probability density shape and independence. For a UQ modeling approach to be effective all material closure properties with significant potential variability should be included in the analysis. The UQ framework described above is thus being extended to include electrical conductivity transport properties and we describe current efforts along these lines.

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A Simple, Accurate Lagrangian Hydrocode

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Keywords: shock hydrodynamics; Lagrangian methods; mesh imprinting; temporal limiting.

ABSTRACT

Lagrangian hydrocodes play an important role in the computation of transient, compressible, multi-material flows. Here a simple cell-centered Lagrangian method for the Euler equations is presented that respects multidimensional physics while achieving second order accuracy. Algorithms that acknowledge the multidimensional physics associated with vorticity transport and acoustic wave propagation are needed in order to increase accuracy and prevent spurious mesh distortions. As such, one-dimensional Riemann solvers and spatial gradient limiters, which are common to traditional Godunov-type schemes, have been abandoned. Instead, we employ multidimensional vertex fluxes that automatically define the mesh motion and temporal, physics-based flux limiting. The first- and second-order accurate Lagrangian methods presented here are an extension of the vorticity preserving Lax-Wendroff-type methods detailed in [1]. In addition to the base schemes, a nonlinear, limited method has also been developed by taking inspiration from the Flux-corrected transport (FCT) framework. Here a simple temporal-based flux limiter reduces the antidiffusive flux in order to reduce overshoots. The Lagrangian schemes developed here suffer from minimal mesh imprinting and are able to preserve radial symmetry, even when solving the Noh problem on a Cartesian mesh as shown in Figure 11. Additional numerical results will be presented to illustrate current successes and ongoing challenges.

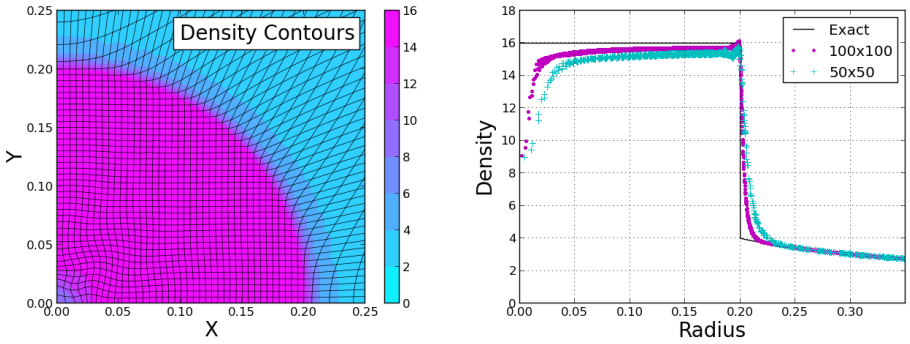

Figure 11: Limited second order density solutions for the Noh problem ($\gamma = 5/3$, $t = 0.6$): Left - Density contours with mesh, 50×50 cells, Right - Radial plots for 50×50 mesh and 100×100 mesh

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Numerical Simulation of Detonation in Condensed Porous Explosives

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Keywords: two-phase non-equilibrium gas-solid flow, porous explosives, numerical modeling

ABSTRACT

The present paper addresses a method for numerical modeling of deflagration and detonation processes in condensed porous reactive materials. The physical model is developed that takes into account such important factors as velocity and temperature nonequilibrium between non-reacted explosives (the solid phase) and products of reactions (the gas phase) and elasto-plastic properties of the solid phase. The solid volume fraction is assumed to change due to combustion and interphase deformation processes that force the pore linear size to change. The mathematical model is derived on the base of the Bayer-Nunziato description of two-phase heterogeneous medium. We modify this model to account for elasto-plastic properties of the condensed phase by implementing a modification of the Prandtl-Reus approach. Nonequilibrium processes include the velocity relaxation by the interface drag (Ergun correlations), the interphase mass exchange (the model of Lee-Tarver), the temperature relaxation by the convective and radiative heat transfer, and the interphase deformation (the model of Kiselev).

The system of governing equations of the model is hyperbolical, but has nonconservative form because of "nozzle effects" terms and source terms of the interphase interaction. To solve these equations numerically we develop a Godunov-type discretization on a moving eulerian grid. First, we split the system into two subsystems. One describes pure hydrodynamics of the nonequilibrium two-phase flow with no interphase interaction. Only gas dynamics in porous solid medium and deformation of the solid skeleton are treated at this stage. We extend the Rusanov flux approximation considered in [1] for the non-conservative Euler equations with fixed porosity to the case of variable in time porosity. The well-balancing property is formulated and proved for the numerical flux proposed. The solid phase equations are solved with a Godunov-type method proposed in [2]. At the second stage, the obtained numerical solutions are corrected by the stress model and the interphase interaction terms.

Finally, we show numerical results that verify the proposed method. We demonstrate that the method exactly reproduces steady-state solutions and warranties the well-balancing property on any arbitrary moving Eulerian grids. Comparisons are done for the Sod tests of [1] reformulated for moving porosity. Interphase models are tested on a plane shock/detonation wave propagation in elasto-plastic porous reacted material. Applications concern 2D simulation of detonation in a porous condensed medium.

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Adaptive Reconnection-based Arbitrary Lagrangian Eulerian Methods

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Keywords: shock hydrodynamics; multi-material hydrodynamics; ALE methods, Reconnection, Voronoi;

ABSTRACT

We present a new adaptive reconnection-based Arbitrary Lagrangian Eulerian methods - ReALE methods. The main elements in a standard ReALE method, [1], are: An explicit Lagrangian phase on arbitrary polygonal mesh in which the solution and positions of grid nodes are updated; a rezoning phase in which a new grid is defined - number of mesh cells in rezoned mesh is *not changing*, but the connectivity of the mesh is allowed to change (it is based on using Voronoi tessellation; and a remapping phase in which the Lagrangian solution is transferred onto the new grid. In standard ReALE method rezoned mesh is smoothed by using one or several steps toward centroidal Voronoi tessellation, but it is not adapted to the solution in any way. In current paper we present two adaptive ReALE methods. Both methods are based on following design principles. First,it is using monitor (error indicator) function based on gradient or Hessian of some flow parameter(s), which is measure of interpolation error. Second, using equidistribution principle for monitor function as criterion for creating of adaptive mesh. Third, using weighted centroidal Voronoi tessellation as a tool for creating adaptive mesh. Fourth, we modify raw monitor function - we scale it to avoid very small and very big cells and smooth it to create smooth mesh and allow to use theoretical results related to weighted centroidal Voronoi tessellation. In first method - R-ReALE (R stands for Relocation) - number of mesh cells is chosen at the beginning of the calculation and does not change with time, but mesh is adapted to modified monitor function at rezone stage at each time step. In second method - A-ReALE (A stands for Adaptive) - both number of cells and their locations allowed to change at rezone stage on each time step. The number of generators is chosen to guarantee required spatial resolution where the modified monitor reaches its maximum value. We present all details required for implementation of new adaptive ReALE methods and demonstrate their performance in comparison with standard ReALE method. on series of numerical examples.

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Factorizable methods for compressible flow computations: Recent developments

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Keywords: shock hydrodynamics; Eulerian methods.

ABSTRACT

The term "factorizable schemes" was coined in the late 90's (see [1]). It describes a discretization scheme for the compressible flow equations such that does not introduce any non-physical coupling between the acoustics and the advection of vorticity factors. Such a method can be regarded as a representative of a general class of the so-called mimetic methods. A scheme that was constructed that strictly obey this requirement on uniform quadrilateral meshes (independently of the cells' aspect ratio and skewness . The assumption (verified by numerical experiments) was that the coupling appearing in the case of non-uniform, though smooth, meshes was negligible from a practical perspective. A version of the scheme for (regular) triangular meshes was also proposed. The benefits of this approach comparing to the standard dimension-by-dimension methods are as follows:

- accuracy and efficiency for the low Mach number flows;
- facilitation for construction of "optimally" efficient fast solvers;
- improved resolution of vortical flow.

In this presentation we shall summarize some developments which took place during the recent years. We shall present a new more general formulation (two- and three-dimensional) based upon more complete theoretical grounds. The new scheme is less sensitive to the grid non-uniformity. Some numerical examples illustrating the performance of the scheme will be presented.

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Implicit Solvers for Higher-Order Discretizations

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ABSTRACT

Higher order discretizations are of increasing interest in the hydro community as they allow for increased accuracy away from shocks as well as potentially allowing for improved performance on advanced architectures. In operator-split magnetohydrodynamics or thermal applications, these additional problems require implicit solution. We present multilevel preconditioning techniques for several canonical problems in this (and other related) arenas, focusing on the issue of coarsening in polynomial degree to allow us to use more traditional multigrid methods while coarsening in space. Application areas will include electrostatics and fully-implicit flow models.

Numerical simulation of flow induced vibrations of a vocal fold model with consideration of different boundary conditions

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Keywords: Arbitrary Lagrangian-Eulerian method; fluid-structure interaction; finite element method.

ABSTRACT

This paper is focus on the numerical simulation of fluid-structure interaction(FSI) problems within biomechanics. Particularly, the attention is paid to the the mutual interaction of fluid flow and vibrating vocal fold, where the voice creation process is addressed. One approach in speech modelling is to model the interaction of the vocal folds using a simplified model, cf. [3], based on a simplified description of both fluid and structure dynamics. For these approaches a simplification of flow problem was used, e.g. potential flow or Bernoulli equation. The application of simplified mathematical models can provide valuable information as well as better understanding of the phenomena. However, the reality is much more complex: the air flow coming from lungs accelerates in the narrowest glottal part causing the vibrations of the vocal folds compiant tissue. The glottis is almost (or completely) closing during vibrations and the vocal folds collide generating the sound. The modelling of such a complex phenomena encounters many difficulties as it is a result of coupling between complex fluid dynamics and complex structural behaviour including contact and acoustic problems.

In this paper we consider the coupled FSI problem of air flow through vibrating glottal region, where the choice of the inlet/outlet boundary conditions is discussed, cf. [2]. The flow is described by the incompressible Navier-Stokes equations (flow velocities in the human glottal region are lower than 100 m/s and the influence of compressibility on the flow induced instability can be neglected). The motion of the computational domain is treated using the arbitrary Lagrangian-Eulerian method (ALE), cf. [4]. The flow problem is the numerically approximated by the fully stabilized finite element (FE) method, cf. [1]. The system of ordinary differential equations describing the structure motion is time discretized and coupled to the flow problem. The numerical results are shown.

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Symmetry and Volume Compatibility in an r-z Staggered Scheme

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Keywords: Axi-symmetric; Spherical symmetry; Geometric conservation law; Subcell pressure forces; Staggered grid Lagrangian.

ABSTRACT

This presentation is focused on the issue of symmetry preservation, energy and volume conservation and other important properties of staggered Lagrangian hydrodynamic schemes in cylindrical geometry. Typical advantages and drawbacks of existing area-weighted (AW) and genuinely r-z schemes will be pointed out. With quadrilateral cells it is known that, in r-z, spherical symmetry preservation, perfect satisfaction of the Geometric Conservation Law (GCL), and total energy conservation are incompatible [4], even if the grid conforms to the solution.

Recently [3] we were able to symmetrize an artificial viscosity that had very desirable properties but did not conserve sphericity, that is, we modified the viscosity to retain all of those properties yet also conserve sphericity on a conforming grid. In this work we use a similar symmetrization technique to modify the energy-conserving geometry-conserving scheme of [2], thereby creating a new symmetric (symmetry-conserving on a conforming grid) scheme that conserves energy and reduces the geometric conservation error. As indicated above, this is the most we can hope for. To make this method useful and robust also for non-symmetric grids and/or problems, we incorporate the mechanism of subcell pressures similarly as it has been suggested in [1] for the Cartesian case, but keeping in mind the objective to reduce the geometric conservation error. Symmetrization of various types of subcells will be shown, and their properties compared, such as the anti-hourglassing effect and overall performance on grids with initially perturbed symmetry.

The issue of wall heating in the Noh problem and other tests is also addressed.

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A mimetic approach to enforce geometric and energetic consistency on a simple and robust fluid-dynamics ALE scheme

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Keywords: ALE methods; shock hydrodynamics; energetic and geometric consistency.

ABSTRACT

A novel numerical scheme is developped for compressible fluid dynamics in the presence of shocks, large deformations and advection. This scheme fulfills various constraints such as: exact conservation of mass, momentum and total energy, thermodynamic and geometric consistency of pressure work, arbitrary evolution of the computational domain and grid, robustness and stability in the presence of (strong) shocks, etc.

Several important ingredients are used for the derivation of the new scheme:

- The fluid velocities are located at half integer time steps. This discretization provides second order accuracy, geometric consistency between the variables, and continuity with existing space- and time-staggered schemes such as [1]. This choice may seem to be inconsistent with total energy conservation but recent studies have shown that total energy can be conserved using time-staggered Lagrangian approaches Llor et al. [2].
- Advection relative to grid is defined by a simple first order upwind scheme so as to preserve the linearity of the continuous generalized momenta. This may appear contradictory with the second order features but it is acceptable as the motion relative to the grid is presumed to be a correction over the global motion captured by the mesh.
- A discrete space-and-time least-action variational principle is used to derive the numerical scheme. This variational approach is appealing because it produces a thermodynamically consistent discretization of the pressure gradient (a critical ingredient in many cases). Such variational approach have seldom been used in the context of hydrodynamics but appear to be special cases of numerical mimetism [3].

The usual test cases of Sod, Sedov, Noh and the Triple point shock tube are performed using several strenuous grid conditions in 1D and 2D so as to verify the robustness, the stability, and the indifference and versatility of the scheme relative to grid motion strategies.

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A Direct ALE Approach for Multimaterial Flows on 3D Unstructured Grids

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Keywords: shock hydrodynamics; multi-material hydrodynamics; Lagrangian methods; Eulerian methods; ALE methods.

ABSTRACT

The standard technique within the shock hydrodynamics community for the solution of the arbitrary Lagrangian-Eulerian (ALE) hydrodynamic equations[1] is the Lagrange-plus-remap method: following a Lagrange step, the mesh is smoothed or relaxed to minimize grid distortion, and the solution is then "remapped" to the new mesh. An alternative approach is the so-called direct ALE method. In this approach, the advection terms are solved directly with the force and stress terms, analogous to direct Eulerian methods, with no explicit Lagrange step [2]. Direct ALE methods used in conjunction with approximate Riemann solvers and node-centered unknowns have been recently applied to shock hydrodynamics [3, 4] and shown to give excellent results on a wide range of problems.

In this work we describe the extension of the direct ALE method to multi-material flows. The hydrodynamic equations are extended from the single material case to the multiple material case, but still written in a flux-conservative form for an arbitrary reference frame. These equations are supplemented with a volume fraction equation for each material, that also must be solved in direct sequence with the hydrodynamic equations, *i.e.* without operator splitting. We describe the overall solution algorithm, including time integration, interface treatment, and modifications to the approximate Riemann solvers. Results are presented for a variety of standard test problems on 3D unstructured grids composed of tetrahedral cells.

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Simulating ejecta production

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Keywords: ejecta; material interface modelling; shock hydrodynamics; multi-material hydrodynamics; surface tension.

ABSTRACT

The interaction of strong shocks with material surfaces is known to generate significant amounts of particulate ejecta, generated by defects on the surfaces. We are developing a capability for simulating ejecta based on standard material models. This talk will discuss aspects of the development of this model, specifically the determination of the sizes of particles produced. This requires a model for the surface tension of fluid droplets which is capable of capturing the particle development without introducing numerical biases, and the ability to accurately track the motion of the material surface within an otherwise Eulerian code to minimize the effects of finite mesh resolution.

A Composite Riemann Solver for Improving Interface Capturing in Multimaterial Calculations

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Keywords: multi-material hydrodynamics; Eulerian methods; Godunov methods; interface capturing.

ABSTRACT

We consider an Eulerian finite-volume method for numerical calculations of multimaterial fluid flows. The medium to be considered consists of several components with different EOS governed by the Euler equations. The mathematical model of a heterogeneous multiphase fluid with the equilibrium in velocity, pressure, and temperature is used to describe multimaterial dynamics.

Our method belongs to the class of interface capturing methods. Once we use the conventional Godunov method for the flux approximation based on the exact or approximate Riemann solver the method looks as a diffuse interface one. It means that the interface between different materials is represented by a set of mixed cells occupied by the heterogeneous mixture of the components. A drawback of the method is that the interface is numerically smeared within from ten to hundreds computational cells, and its exact position in space is lost.

Another drawback is revealed in calculations of the flow of condensed and gaseous materials with rarefaction waves. The problem is that the EOSs in this case are quite different and admit different regions of thermodynamic parameters. Solids admit negative pressure while the gaseous phase not. Because of the equilibrium, the pressure in mixed cells should be always positive. This leads to an artificial numerical effect that we name as pseudo-fracture. It develops as a small region of mixed cells near the pure solid region where the solid volume fraction drastically decreases.

In order to fix these drawbacks one can sharpen smeared interfaces by implementing some techniques commonly referred to as anti-diffusive. We suggest an alternative way that is based on a numerical flux approximation that takes into account the position of the interface in mixed cells or in other words the material sub-cell structure. In doing so, we come to an extended formulation of the Riemann problem that accounts along with the initial discontinuity also the contact one located apart[1]. We name this formulation as Composite Riemann Problem (CRP). The solution of the CRP provides more accurate approximation of the numerical flux in mixed cells. We demonstrate numerical results that show that the CRP technique allows us to reduce the mixed zone to only one computational cell in 1D calculations and a few cells for multidimensional problems.

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Modeling Continuum to Disperse State Transitions

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Keywords: dual domain material point method, fragmentation

ABSTRACT

Transition from a continuum state to a disperse state happens when a material pulverizes under a significant impact. There have been many conceptual and numerical issues related to the modeling of these transitions. The conceptual issues include descriptions of the transition and the applicability of the continuum description.

From the point of view of numerical calculations, different numerical methods are typically employed for different material states. For instance, the finite element method is often used for solids, finite difference and finite volume methods are often used for fluids, and the discrete element method is often used for granular materials. To model the transition from a continuum to a disperse state, should we use different numerical methods in each stage of the material deformation? If so, how and when should the numerical method be switched?

In this talk, I will present a unified framework and an associated numerical method for these types of material motions. The theoretical framework is based on ensemble phase averaging theory. Under this theory, the continuum approach and the associated equations are applicable if the related variables are regarded as averages, however, the average material strain rate cannot be directly calculated from the gradient of the average velocity because of the change in material connectivity during process of the material disintegration. Models between the material strain rate and the gradient of the average velocity are needed. I will also show that under a wide variety of such models, the averaged equations can be solved efficiently using the dual domain material point method, an improved version of the material point method.

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POSTERS

High-order numerical simulations of compressible two-phase flows with the complex equation of states

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Keywords: compressible two-phase flows; complex equation of states; monotonicity-preserving limiter; Rusanov approximate Riemann solver.

ABSTRACT

In this paper, we investigate the applicability of high-order numerical resolution of compressible homogeneous two-phase flows governed by a quasi-conservative five-equation model of Allaire et al. [1], in which the flow regime of interests is assumed to be homogeneous with no jumps in the pressure and velocity (the normal component of it) across the interfaces that separate two regions of different fluid components. In contrast to many algorithms where in different regions different algorithms are used (for example: in regions away from the interfaces where the flow is a single phase, a standard reconstruction scheme such as MUSCL is used while a special method is used in regions near the interfaces where two different fluid components are present within a cell), our practical algorithm is the same in all regions. To be more specific, the Rusanov approximate Riemann solver is used to obtain the flux at cell edges/faces and the fifth-order upwind scheme with the modified monotonicity-preserving limiter [2] in the standard reconstruction process. Furthermore, based on Surel [3] and Johnsen [4]'s work, for the consistency with the Rusanov approximate Riemann solver, the algorithm is also used to solve the advection equation of the volume fraction and the primitive variables are used in the reconstruction process. Temporal integration of the algorithm is done by employing a third-order strong stability-preserving Runge-Kutta method.

Several one- and two-dimensional problems with different equations of states (such as the ideal-gas EOS, stiffened gas EOS, van der Waals EOS and Mie-Grüneisen EOS for characterizing the materials) are used to demonstrate the feasibility of the proposed method.

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Optimal control and parabolic reinitialization for level set methods

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Keywords: Level Set Methods; Reinitialization; Optimal Control; Variational Formulation; Finite element methods.

ABSTRACT

In the context of numerical simulation for evolving interfaces, we consider the problem of preserving the signed distance function (SDF) property of level set functions. A well-designed reinitialization method produces a signed distance function that has the same zero contour as the original level set function. Many methods tackling this problem exist and can roughly be separated into geometric and PDE-based approaches. Sussman et al. [2] suggest a PDE-based approach that recovers the signed distance function by solving a hyperbolic PDE to steady state. In our recent publication [1], a suitable potential function is minimized yielding an elliptic PDE. The displacement of the zero contour is prevented by adding an appropriate penalty term. On this poster, we will present two related PDE-based approaches.

In the first method we formulate an optimal control problem that incorporates the residual of the Eikonal equation into its objective. The state equation is based on the level set transport equation but extended by an additional source term, correcting the solution so as to minimize the objective functional. By definition, the interface can not be displaced. The system of first order optimality conditions is derived, linearized, and solved numerically. The control will also prevent numerical instabilities, so that no additional stabilization techniques are necessary. This approach offers the flexibility to include other desired design criteria into the objective functional.

The second approach utilizes the elliptic regularization term introduced in [1] in the context of a minimization problem for the residual of the Eikonal equation. In contrast to [1], the elliptic regularization term is embedded into a parabolic correction step.

Both approaches are evaluated numerically and compared to other PDE-based reinitialization methods such as the convected level set method [3].

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An interface fitted Arbitrary Lagrangian-Eulerian finite element approach for free and moving boundary problems

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Keywords: ALE methods; two-phase flows; fluid-structure interaction; front tracking; mesh optimization

ABSTRACT

Classical moving mesh methods for free and moving boundary problems usually suffer from mesh distortion if large displacements of the problem domain or interfaces are considered.

On this poster, we present a finite element framework based on moving meshes which aims at resolving these problems. The approach is based on the classical arbitrary Lagrangian-Eulerian (ALE) formulation of the fluid equations, but allows for temporal discontinuities of the ALE parametrization. In contrast to traditional ALE based mesh moving/front tracking methods, the deformation of the computational mesh is not directly derived from an extension of the interface displacement. Instead, the mesh is obtained from a variational mesh optimization technique which yields meshes that are aligned with the interface, retain connectivity and can be shown to be of optimal quality.

The presented approach allows for large deformations of the interface while preserving attractive features of front tracking methods: an accurate description of the interface, and (consequently) the design of problem-tailored finite element spaces. The framework is introduced and evaluated in the context of problems from two-phase flows with surface tension, particulate flows and fluid-structure interaction.

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Numerical Solutions of a Coupled CFD-Enthalpy Model for Partly Molten Polymer Processes in Complex Geometries

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Keywords: multiphase; screw extruder; CFD; numerical simulation; mathematical modelling; enthalpy model; phase change.

ABSTRACT

Many processes in the field of chemical process engineering involve multi-phase and/or even multimaterial problems. In the recent past there is a significant progress in the field of computational treatment of such processes. Our work is motivated by a particular polymer compounding process in twin screw extruders. The CFD based simulation of fully filled parts in such extruders is already possible even though the large aspect ratios (sub millimeter gaps and diameters or screw length in the range of several centimeter), rotating domains (for twin screws there is no possibility of coordinate transformation) and complex rheology (nonlinear shear dependent and temperature dependent viscosities) lead to a rather challenging setup. Our ingredients in the code Extrud3d are higher order finite elements (Q2P1), parallelization with domain decomposition, dynamic mesh deformation based on monitor functions and Newton-multigrid solvers. Extrud3D is an adaption of FeatFlow, further developments on Extrud3D are necessary when the simulation also include a secondary disperse polymer phase fed to the process. Polymer engineers make use of an intrinsic cooling behavior by these secondary feed strategies. From an engineering point of view there are several questions which should be answered by using numerical simulations. How do particles interact and distribute downstream? What are the local and integral thermodynamic impacts on the flow due to the phase change in the melting process? How does the morphology of particles change in the combined melting/compounding process? In our approach, we have used an adapted version of the so called enthalpy model. Whenever possible, we compare our results with experiments which are conducted at our partner institute KTP (Kunststofftechnik Paderborn).

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Implementation of the SURF high explosive burn model in FLAG

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Keywords: high explosives; reactive burn; shock hydrodynamics; multi-material hydrodynamics; Lagrangian methods; Eulerian methods.

ABSTRACT

SURF is a high explosive (HE) burn model based on the ignition and growth concept of hot-spot reaction and is described in [1] and [2]. In contrast to other models, the reaction rate for SURF is a function of the lead shock pressure rather than the local pressure. The model includes an algorithm for detecting the lead shock based on the Hugoniot energy function. In this poster, we present an assessment of the SURF reactive HE model implementation in the Los Alamos National Laboratory developed multiphysics ALE code FLAG. Specific attention is paid to the assessment of the lead shock detection method and its performance in conjunction with the standard staggered grid hydrodynamics in FLAG. Comparisons of this algorithm in other codes and hydrodynamics methods are also presented. Finally, results for standard HE test problems employing PBX 9502, such as run-to-detonation, are presented for both the FLAG implementation as well as SURF implementations in other codes.

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A GKS-ALE Method For Multi-material Flows With General Equation Of State

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ABSTRACT

Based on a gas kinetic scheme (GKS) and the finite volume method, we propose a new Arbitrary Lagrangian–Eulerian (ALE) method for compressible multi-material flow problems with general equation of state (EOS) on arbitrary computational grids. In the current ALE scheme, after a coordination transformation, the Riemann problems on moving grids can be transferred to fix grids, thus we can make use of a non-oscillatory gas kinetic scheme (the NOK scheme proposed in [1]), which can deal with general EOS, to evaluate the numerical flux, and this avoids constructing a Riemann solver for general EOS. Furthermore, material interfaces are tracked by requiring them to move with fluid (Lagrangian) velocity, while the internal nodes are rezoned to improve the geometrical quality. In the rezoning step, an optimization-based rezoning method on structured grids [2] is extended to arbitrary grids, the new method can preserve three good geometrical requirements: (1) convex, (2) smooth, (3) uniform. Figure 1 shows the numerical results of an underwater explosion problem, a typical multi-material problem with general EOS, computed by our new ALE scheme. It is clearly that the material interfaces can be sharply resolved, while the computational grid can be kept in good quality for a wide range of problems.

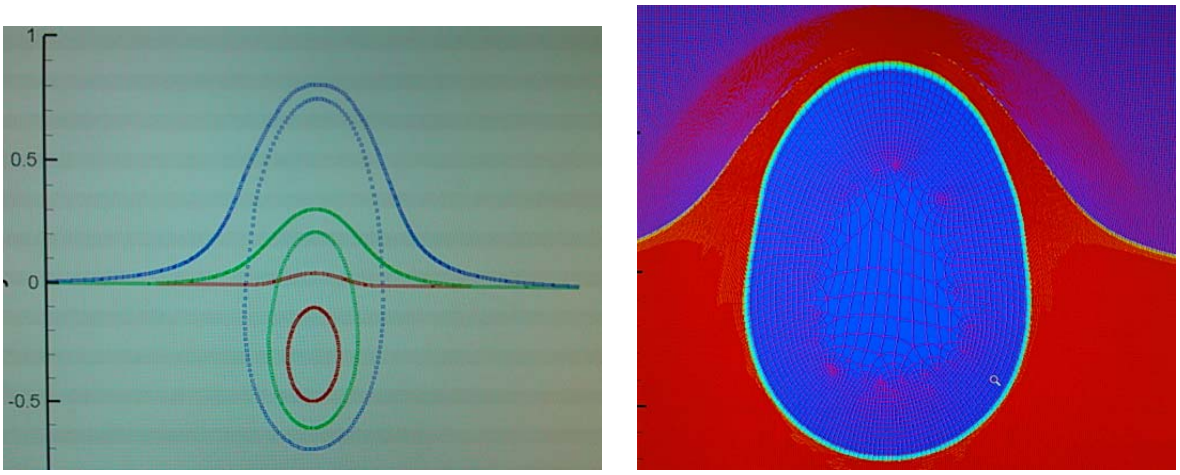

Figure 12: Numerical results of underwater explosive problem computed by new ALE method. Left: Evolution of material interface, right, the computational grid near the material interface.

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Gradient Operator Optimization for 3D Unstructured Meshes (LA-UR-15-21404)

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Keywords: unstructured mesh; arbitrary Lagrange-Eulerian; multi-core architecture; parallelization.

ABSTRACT

FLAG is a code that solves the arbitrary Lagrangian-Eulerian (ALE) form of the conservation equations to model multi-material and multi-physics problems [1]. The particular ALE algorithm implemented in FLAG can be split into three main steps: performing a Lagrangian solution update, generating a new computational mesh with improved characteristics, and remapping the Lagrangian solution onto the new mesh. A particularly costly and repeated operation in a remapping step is the calculation of discrete gradients of various solution quantities, such as density or pressure. The gradient operator reconstructs field quantities at the nodes of a mesh by using the averaged fields and geometries of the surrounding zones.

FLAG's gradient operator is only implemented serially, is not optimized, and cannot be parallelized due to data race conditions. Furthermore, FLAG employs MPI primarily to achieve parallelization by using single-core computation spread to a number of number of processors – utilizing the many-core and multi-core processing power of the next generation architecture is a current challenge of similar 3D unstructured mesh simulation codes [2]. The gradient algorithm used in FLAG is similar to the algorithms used in many unstructured fluid dynamics codes and comparable to commonly used spatial operators. As such, FLAG's gradient operator serves as an excellent case for testing parallelization of spatial operators on a 3D unstructured mesh.

Starting with a mini-application designed to simulate the basic features of FLAG, a variety of gradient operator alternatives and optimizations were tested. The most successful of those algorithms were then implemented directly into FLAG to demonstrate their computational performance compared to the currently used methods. They include different renumbering schemes, data restructuring, and connectivity inversion. This research also investigates the feasibility of a hybrid OpenMP and MPI parallelization solution for FLAG and similar hydrocodes. Preliminary research suggests over 20 times the performance increase of the current methods and the initial tests suggest that the new alternative gradients will translate well to multi-core, multi-processor environments.

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Computing flows with sharp interfaces between pure and mixed cells

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Keywords: multi-material hydrodynamics; interface capturing; Eulerian method; two-fluid model

ABSTRACT

Numerical modeling of flows in two-fluid Euler-Euler formulation can be done either via an averaged physical model [1] or via a numerical model with interfaces [3]. The first vision has the advantage of simplifying interface tracking at the cost of spurious numerical diffusion in mixing zones. The method with interface capturing has a higher numerical cost but prevents numerical diffusion between materials. In this work, a numerical method is proposed for managing both approaches. In addition to the theoretical study and implementation of the model, this poster will focus on the case of three materials cells which contain both a mixture of fluids and an interface with a pure cell.

The proposed numerical model aims at extending the two-fluid FVCF scheme without interface [2] to the interface capturing case and the multimaterial FVCF [3] to two-fluid models. A minimal four equations and one dimension model is considered. Dissipative or corrective terms are neglected and an algebraic differential pressure between fluids is considered. The equations of state considered are polytropic and close to those used for air-water flows modeling.

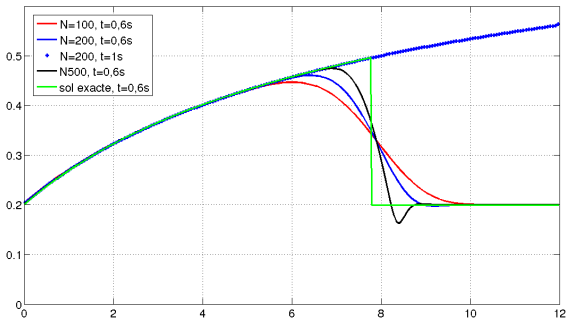

Figure 13: Ransom faucet test case: comparison of the numerical results of void fraction to the exact solution.

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3D multi-material polyhedral methods for diffusion

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Keywords: multi-material; Eulerian methods; ALE methods; diffusion; implicit; explicit.

ABSTRACT

The process of energy diffusion is an important physical mechanism for the exchange within materials and across material interfaces. For the Arbitrary Lagrangian Eulerian or pure Eulerian frameworks, material boundaries will be miss-aligned with the computational mesh creating multi-component or mixed cells. To capture the dynamics of energy diffusion in mixed cells we will describe an implicit 3D multi-material polyhedral based scheme. In this paper we will also outline an alternative scheme based upon explicit super-time stepping. We will present results, and compare and contrast the different approaches.

Geodesic and prismatic mesh generation

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Keywords: three-dimensional mesh generation; unstructured grids; dendritic meshes; Lagrange hydrodynamics.

ABSTRACT

In ALE simulations with moving meshes, mesh topology has a direct influence on feature representation and code robustness. In three-dimensional simulations, modeling spherical volumes and features is particularly challenging for a hydrodynamics code. Calculations on traditional spherical meshes (such as spin meshes) often lead to errors and symmetry breaking. Although the underlying differencing scheme may be modified to rectify this, the differencing scheme may not be accessible. This work documents the use of spherical geodesic meshes to mitigate solution-mesh coupling. These meshes are generated notionally by connecting geodesic surface meshes to produce triangular-prismatic volume meshes. This mesh topology is fundamentally different from traditional mesh topologies and displays superior qualities such as topological symmetry. This work describes the geodesic mesh topology, including motivating demonstrations with the FLAG hydrocode, and extensions of related prismatic meshes into cylindrical and other meshes.

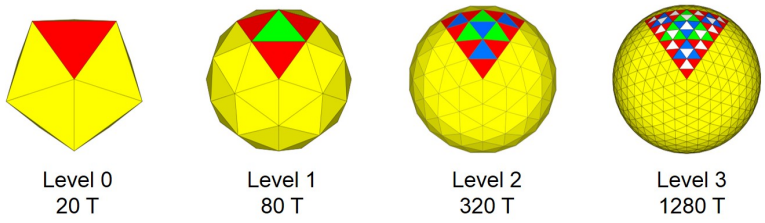

Figure 14: Triangular discretizations of the sphere admit to straightforward refinement techniques.

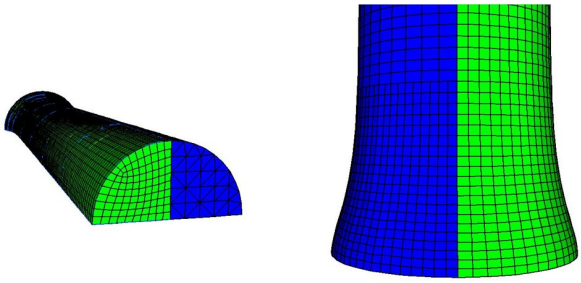

Figure 15: Taylor impact comparison between simulations on a hexahedral mesh (green) and a triangular prismatic mesh (blue).

Performance modeling and optimization of a Lagrange-Remap algorithm on multicore processors

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Keywords: performance modeling; Roofline model; ECM model; Lagrange-Remap methods.

ABSTRACT

Performance modeling aims at building simple analytical models which allow to predict the performance of an algorithm on a target computing architecture from the knowledge of the main features of both the algorithm and the processor.

Such models provide a deep understanding of the performance of an algorithm and help to identify suitable optimization strategies. Performance models are robust and stable tools, since they are derived from algorithm study and are not based on one of its specific implementation. They can also be seen as decision-making tools.

We will present recent results of the performance study of a reference staggered Lagrange-Remap algorithm for compressible gas dynamics obtained using *Roofline* and *ECM* models. As a result, we are able to predict the whole performance on modern processors with errors of order 5%, which is very accurate.

Moreover, as a consequence, the analysis also gave us highlights for designing a new Lagrange-Remap-like solver with expected better performance. In particular, using low diffusive interface capturing methods rather than interface tracking strategies appears to be promising because of their SIMD features. This will be address in the companion talk by De Vuyst et al. in this workshop.

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Improvements to multi-material modelling in a 3D ALE code

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Keywords: multi-material hydrodynamics; ALE methods; interface reconstruction.

ABSTRACT

AWE's three-dimensional Arbitrary Lagrangian Eulerian (ALE) code, Pegasus, has been enhanced to make use of Youngs' interface reconstruction method [1, 2] in the advection and pin crossings algorithms.

The new advection scheme, replacing the Cale algorithm [3, 4], first determines the order in which the materials in a multi-material cell should be advected, as described by Bell and Hertel [5], based on the abundance of each material in the donor and acceptor cells. The normal to the interface between each material is calculated in isoparametric coordinates so that distorted elements can be treated as unit cubes, allowing Youngs' interface reconstruction method to then be used to determine the overlap of each material with the advection volume. The new algorithm is of comparable speed and the results of test problems are presented which show that numerical errors such as beading are reduced.

Youngs' method has also been used in the new pin crossings algorithm. The original algorithm established when pins crossed a Lagrangian surface while the new algorithm is based on multi-material cell representation of the surface, which is useful when the material surface is no longer in line with the Lagrangian surface as a result of an ALE calculation. Knowledge of the location of each pin is maintained, so when a pin is seen to enter a pure (single-material) cell of the material of interest it is immediately recorded as having crossed the material. If the pin enters a mixed (multi-material) cell, first the isoparametric coordinates of the pin within the cell are calculated and compared with the location of the interface as calculated using Youngs' algorithm. Thus it can be determined if the pin has crossed the material interface within the multi-material cell. The results of test problems demonstrating the accuracy of the new algorithm are presented.

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On Nonlocal Transport Based Closure Relations for Radiation Hydrodynamics

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Keywords: radiation hydrodynamics; closure relations; nonlocal transport; Bhatnagar-Gross-Krook collision operator; higher order methods; diffusion asymptotic; discontinuous Galerkin.

ABSTRACT

The nonlocal theory of the energy transport in radiative plasmas of arbitrary ratio of the characteristic spatial scale length to the photon and electron mean free paths is applied to define the closure relations of hydrodynamic system. The corresponding transport phenomena cannot be described accurately with the usual fluid approach dealing only with local values and derivatives. Thus, the parabolic terms like viscous force and energy flux are calculated directly by solving a simplified transport equation allowing one to take into account the effect of long-range particle transport. The key feature of the proposed method is the application of the Bhatnagar-Gross-Krook collision operator delivering a calculation efficiency and an inherent coupling to the fluid plasma parameters in an implicit way. In combination with a higher order discontinuous Galerkin scheme of the transport equation, the solution obeys both limiting cases, i.e. the collisional diffusion asymptotic usually present in radiation hydrodynamics models and the collisionless transport of free-streaming particles. As a result we present a robust method to model the energy transport exhibiting a correct physical behavior controlled by the particles mean free path.

Remapping by combined intersection- and swept-based methods in 2D ALE simulations of single-material flows

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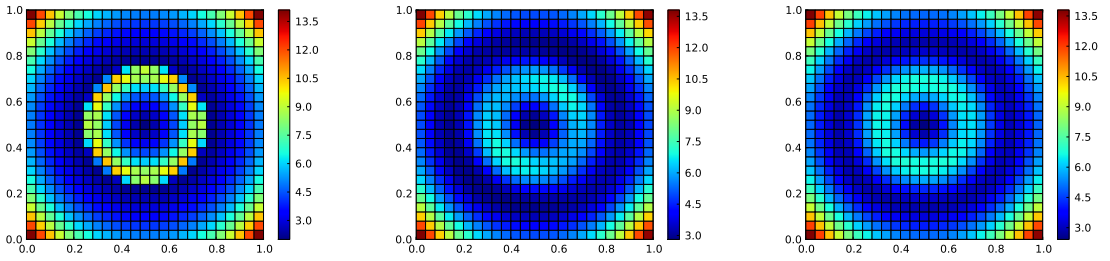
Keywords: ALE methods; Remap; Symmetry preservation.

ABSTRACT

A typical Arbitrary Lagrangian-Eulerian (ALE) algorithm consists of a Lagrangian step, where the computational mesh moves with the fluid flow, a rezoning step, where the computational mesh is smoothed and repaired in case it gets too distorted, and a remapping step, where all fluid quantities are conservatively interpolated on this new mesh. In single-material simulations, the remapping process is often represented with fluxes constructed by integrating a reconstructed function over regions swept by edges of the computational cells. This method is robust and fast because the swept regions are formed from the old and new positions of cell vertices and therefore no polygon intersection calculation is needed. However, this method can produce inaccuracies if the mesh is moved in the direction of the cell corners during rezoning, distorting the symmetry of the quantities distribution (see Figure 16). An error with similar cause is also produced when the cell edge is rotated during rezoning ("hourglass" motion).

An alternative to the swept-based method is to integrate over the intersections of the computational cells. This approach requires a robust intersection algorithm, which is often more complex and expensive in terms of computational resources. Inspired by the hybrid algorithms combining both methods in multi-material simulations we propose a similar "pseudo-hybrid" algorithm for single-material flows. Based on an error analysis, it employs exact intersections only in certain parts of the computational mesh, and the swept-based method is used elsewhere. This way our algorithm can retain the beneficial symmetry preserving capabilities of intersection remapping while keeping the overall computational cost moderate.



(a) Initial state (b) Swept-based method (c) Intersection-based method

Figure 16: Effect of a periodic diagonal mesh rezoning on a radially symmetrical density distribution.

Anisotropic slope limiting in discontinuous Galerkin methods for transport equations

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Keywords: hyperbolic conservation laws; discontinuous Galerkin methods; anisotropic slope limiting; inequality-constrained optimization.

ABSTRACT

In this paper, we present an anisotropic version of a vertex-based slope limiter for discontinuous Galerkin (DG) methods. The limiting procedure is carried out locally on each mesh element utilizing the bounds defined at each vertex by the largest and smallest mean value from all elements containing the vertex. The application of this slope limiter guarantees the preservation of monotonicity. Unnecessary limiting of smooth directional derivatives is prevented by constraining the x- and y-components of the gradient separately. In contrast to optimization-based methods based on solving small linear programming (LP) problems, we derive a closed-form formula for calculating the correction factors for the x- and y-derivatives. We also provide the necessary generalizations for using the anisotropic limiting strategy in an arbitrary rotated frame of reference. The performance of the new anisotropic slope limiter is illustrated by two-dimensional numerical examples.

Physics-compatible numerical approximations to the Fokker-Planck model of fiber orientation

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Keywords: fiber suspension flows, Fokker-Planck equation, orientation tensors, Galerkin approximation, Fourier analysis, spherical harmonics.

ABSTRACT

The rheological behavior of fiber suspension flows depends on orientation tensors [1] which represent even-order moments of an orientation probability density function ψ. The evolution of this function is governed by the Fokker-Planck equation which describes the transport and rotation of fibers in a flow field satisfying the generalized Navier-Stokes equations. When it comes to the design of numerical approximations to the Fokker-Planck equation, it is essential to use algorithms that preserve nonnegativity of ψ or at least positive semi-definiteness of the orientation tensors. Otherwise, nonphysical orientation states may arise rendering the results of a computationally expensive simulation worthless.

In this work, we use operator splitting to decompose the Fokker-Planck equation into subproblems associated with spatial convection and orientation changes. The space derivatives are discretized using linear finite elements, whereas the orientation angles are discretized using a Fourier series expansion (in 2D) or spherical harmonics (in 3D). The so-defined tensor product approximation to the probability density function may attain nonphysical negative values, and the orientation tensors determined by the first coefficients of this approximation may fail to satisfy the condition of positive semi-definiteness. In order to rectify this deficiency of the standard Galerkin discretization, we consider two correction techniques. The first one modifies the coefficients of the Fourier expansion/spherical harmonics or adds numerical diffusion to keep the orientation tensors positive semi-definite [2]. The second approach is based on maximum entropy reconstruction of nonnegative probability density functions from their first coefficients (cf. [3]). It leads to a nonlinear least squares problem which we solve using the Levenberg-Marquardt algorithm. As a useful byproduct, the reconstruction-based approach makes it possible to use higher-order coefficients of reconstructed nonnegative functions instead of heuristic closure approximations in the evolution equations for the low-order coefficients. The results of a numerical study for 2D and 3D test problems illustrate the potential of reconstruction-based closures.

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Positivity preserving schemes for the reactive flow of solutes from a viscous fluid to a poroelastic medium

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Keywords: reactive transport; ALE methods; flux corrected transport; positivity preservation.

ABSTRACT

In this study, we consider a mathematical model for the reactive transport of chemical solutes from a viscous fluid to a poroelastic medium. The solutes are dissolved in an incompressible fluid and they are transported to the poroelastic medium through a moving interface due to fluid-structure interaction. In the poroelastic medium the solutes undergo chemical reactions where they are deposited to the solid material. The character of the fluid and the structure are not affected by the chemistry. We derive some positivity preserving numerical schemes for the flow with moving meshes using the ALE-FCT type of design. The schemes ensure mass conservation. We simulate the phenomena starting with flow in a fixed channel with a thick porous wall where the fluid flow via steady and time-dependent velocity profiles. We then consider flow in a moving domain where the fluid flow is defined by the Navier-Stokes equations and the structure is modeled by a Biot law. Consequences of these result are significant in the numerical simulation of nano-particle cancer drug delivery. Our results are an exploration of ways to enhance targeted adsorption of cancer drugs carried by nano-particles via the human vasculature.

Numerical study of dissipative terms in the Lagrangian CSTS (Conservative Space- and Time-Staggered) hydrodynamic scheme

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Keywords: Lagrangian methods; staggered scheme; leap-frog; artificial viscosity; hourglassing

ABSTRACT

In the context of Lagrangian computation of compressible fluid dynamics, we proposed in [1, 2] a modification, in the spirit of [3], of the basic STS scheme [4], denoted by CSTS scheme, which is conservative, entropic, compatible, positive definite in kinetic energy, explicit in momemtum equation and second order accurate (even for variable time steps). Corrections have thus been brought to the simplest STS scheme in order to recover energy conservation.
In this work, we propose a numerical study on the dissipative terms of such CSTS scheme. In particular, we will focus on artificial viscosity and hourglassing. The connection between these two processes will be highlighted and higher order formulation will be considered. Several relevant numerical tests will be shown.

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Second-Order Discretization in Space and Time for Grey S_2 Radiation-Hydrodynamics

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Keywords: radiation-hydrodynamics; MUSCL-Hancock; S_2 radiation.

ABSTRACT

We combine the MUSCL-Hancock method for hydrodynamics with the linear-discontinuous finite-element and trapezoidal/BDF-2 time integration methods for S_2 radiation transport. There are several important properties of our approach. First, the scheme is directly applicable to Sn radiation transport. Second, we deal with the fact that there are two different definitions for the material internal energy slopes - one arising from the MUSCL-Hancock method and another arising from the linear-discontinuous discretization associated with the exchange of radiation energy with the internal energy field. In particular, we are able to obtain second-order accuracy and preserve the equilibrium-diffusion limit by using different slopes in different parts of the calculation. Third, we conserve total momentum in this approximation, which is in contrast to a similar method previously developed using grey radiation diffusion in P_1 form [1]. Fourth, we expect this approach to easily generalize to multidimensions.

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An Explicit, Positivity-Preserving Flux-Corrected Transport Scheme For The Radiation Transport Equation

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Keywords: radiation transport equation; entropy viscosity method; flux-corrected transport.

ABSTRACT

High-order numerical solutions of the radiation transport equation

$$\vec{\Omega} \cdot \vec{\nabla}\psi + \sigma\psi = q$$

are known to exhibit negativities, or undershoots, as a well as overshoots. These numerical artefacts can lead to numerical difficulties, notably in simulations where radiation transport is coupled to hydrodynamics equations. Here, we solve the time-dependent transport equation using a P_1 continuous finite element (CFEM) discretization, stabilized using the entropy viscosity method (an artificial viscosity technique). A flux-corrected transport (FCT) technique is applied to this higher-order solution in order to produce a positivity preserving scheme that satisfies a local discrete maximum principle (DMP). Explicit time discretizations are employed, including explicit Euler and strong-stability-preserving Runge-Kutta (SSPRK) schemes such as the 3-stage, 3rd-order-accurate Shu-Osher scheme (SSPRK33). Results are presented for 1-D test problems, demonstrating that the entropy viscosity method stabilizes the pure Galerkin discretization but does not satisfy a DMP (undershoots and overshoots are still present). On the other hand, the "entropy viscosity + FCT" solution is both stable and discrete-maximum-principle satisfying.

Scalable High-order ALE Simulations

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ABSTRACT

The Arbitrary Lagrangian-Eulerian (ALE) framework forms the basis of many large-scale multi-physics codes, and in particular those centered around radiation diffusion and shock hydrodynamics. Current ALE discretization approaches consist of a Lagrange phase, where the hydrodynamics equations are solved on a moving mesh, followed by a three-part "advection phase" involving mesh optimization, field remap and multi-material zone treatment. While traditional low-order ALE methods have been successful at extending the capability of pure Lagrangian methods, they also introduce numerical problems of their own including breaking of symmetry, and lack of energy conservation.

In this talk, we present a general high-order finite element discretization framework that aims to improve the quality of current ALE simulations of radiation-hydrodynamics, while also improving their performance on modern data-centric computing architectures. We use the de Rham complex to guide the discretization of different physics components. In particular, kinematic quantities (e.g. velocity, position) are discretized with continuous (H1) finite elements, thermodynamic quantities (e.g. internal energy) use continuous (L2) elements, while H(div)-conforming finite elements are used for the fluxes in radiation diffusion.

Our Lagrangian hydrodynamics algorithm is based on Galerkin variational formulation of momentum and energy conservation using the high-order de Rham finite elements. The use of high-order position description enables curvilinear zone geometries allowing for better approximation of the mesh curvature, which develops naturally with the flow. The remap phase of ALE is posed as an advection problem in artificial pseudo-time, describing the evolution of the post-Lagrangian mesh into the improved new mesh. This is discretized using a finite element Discontinuous Galerkin (DG) approach on high-order curvilinear meshes. The semi-discrete DG method results in high-order accuracy for sufficiently smooth fields, but can produce non-monotonic results for discontinuous fields. We consider several non-linear approaches to enforce monotonicity, including high-order algebraic Locally Scaled Diffusion (LSD), Flux Corrected Transport (FCT) and Optimization Based Remap (OBR). The ALE evolution of different materials in our framework uses high-order "material indicator" functions, and we have developed high-order closure models to model the sub-zonal material behavior during the Lagrangian phase.

We have started exploring approaches for discretizing high-order multi-group radiation diffusion on general curvilinear grids and will report some initial results on the coupling with the high-order hydrodynamics. We will also present numerical tests illustrating the robustness and scalability of our discretization algorithms and discuss recent work to further improving their performance on modern architectures.

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Modeling of the Damaged Surface Hydrodynamics Experiments

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Keywords: shock hydrodynamics; multi-material hydrodynamics; ALE methods; fluid-particle methods; magnetohydrodynamics.

ABSTRACT

das Three cylindrical, pulsed-power driven, damaged surface hydrodynamics (DSH) experiments have been conducted at the Los Alamos Neutron Science Center's (LANSCE) proton radiography facility. There the Precision High Energy-density Liner Implosion eXperiment (PHELIX) capacitor bank delivered 3.6 MAmp, 6 μs pulses in order to magnetically accelerate a thin aluminum liner (Diam. $= 5.4$ cm, thickness $= 0.5$ or 0.8 mm) to 1 km/s. The liner impacted an aluminum target cylinder (Diam. $= 3.0$ cm, thick $= 0.1$ mm) that was coated with a thin (100 μm) layer of micron size tungsten powder. The powder was shock launched into vacuum and 120 psia of Nobel gases (Ar or Xe). A 21-frame proton radiograph data set was collected for each experiment. Shocks in the gas, particle-cloud structure, and the target cylinder are clearly visible in the radiographs. See Figure 17.

This well-controlled, well-diagnosed set of experiments has produced a data set that challenges Lagrangian and ALE methods for modeling multi-material converging flows. While single-fluid, resistive magnetohydrodynamics (MHD) is adequate for modeling the condensed-state, converging liner, the main question is how best to describe the thin tungsten powder layer and its transport into both gas and vacuum. Three methods of increasing complexity are investigated. First, a fully fluid description where ALE is necessary to evolve the azimuthal structure and radial flow. Second, hybrid fluid-particle methods where Lagrangian material cells are shock converted into particles and transported through a background fluid, without particle-particle interactions. Finally, granular material models where full particle-particle interactions are taken into account.

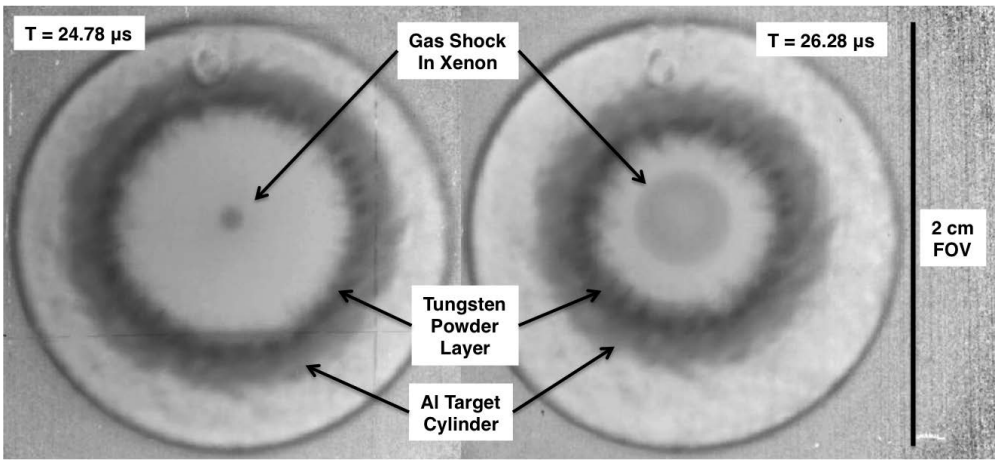

Figure 17: Axial proton radiographs of the DSH-2 experiment at two different times showing the shock in the Xe gas, the tungsten power layer, and the Al target cylinder.

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Remapping and Advection Considerations in FLAG

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Keywords: advection; ALE; remapping; subcycling.

ABSTRACT

Events such as the activation of a physics package or a change in mesh strategy may benefit from massive mesh relaxation. Two methods to massively relax mesh exist in the FLAG hydrocode—advection subcycling and mesh remapping. In an advection subcycle, the proposed relaxation of each point is scaled uniformly based on an advection volume limit. Advection subcycling may require hundreds or thousands of subcycles to massively relax the mesh. Variables are advected with second-order accuracy, causing each subcycle to incur advection error if fields are nonlinear. In contrast, mesh remapping calculates exact intersections between the original and massively relaxed mesh, then performs a single second-order conservative remap. Both methods use identical relaxers and preserve the topology of the original mesh. An identical set of variables is updated in both methods.

This work compares the accuracy of advection subcycling and mesh remapping. Simple test problems including 1) linear fields, 2) nonlinear fields, and 3) slip surfaces are used to investigate each method.

The first test examines linear fields on unit square meshes that are initially distorted. Initial meshes are biased in the x, and both x and y directions. A third initial mesh is biased in both the x and y directions, with a random perturbation. The final mesh is uniformly relaxed. Several linear fields are remapped using both methods. In all tests, density (mass) is the field of interest, although both methods are generalized for any conserved quantity. Both advection subcycling and mesh remapping were found to be exact for linear fields.

The second test investigates nonlinear fields. The mesh is initially biased in both x and y directions, and randomly perturbed for various resolutions. Again, the final mesh is uniformly relaxed. Both methods converge with approximate second-order accuracy. For all simulations, mesh remapping has lower L1 relative error. The difference in L1 error between advection subcycling and mesh remapping is $\sim$10x for a hyperbolic tangent field, which approximates a discontinuity.

The third test simulates the alignment of a slip surface. Adjacent slip surfaces can be cleanly stitched together if both surfaces are aligned before their removal. However, both advection subcycling and mesh remapping incur faceting error as the discretized boundary is relaxed. Faceting error causes unphysical field defects along curved boundaries which can disrupt simulations and preclude the clean removal of slip surfaces. This test consists of a unit density field on a mesh with a non-uniform curved boundary. The final mesh is uniformly relaxed along the curved boundary. Both methods demonstrated field perturbations due to faceting error, although the severity is less with mesh remapping. As implemented in FLAG, mesh remapping can by followed by a process that repairs faceting error along slip surfaces. This is accomplished by scaling conserved quantities on a per-zone basis by the post-remap_zone_volume/intersection_volume. Conservation is enforced by applying a uniform factor to conserved quantities in zones adjacent to the slip surface. In testing, this correction is able to faithfully represent the original conserved field.

Tests of nonlinear fields indicate mesh remapping is more accurate, and with a correction, may reduce the effect of faceting error along slip surfaces. Motivated by the differences found in these simple tests, advection subcycling and mesh remapping will be compared in integrated simulations. The results will inform best practices for user simulations.