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Title: High-order hydrodynamic algorithms for exascale computing

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High-order hydrodynamic algorithms for exascale computing

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Introduction

Hydrodynamic algorithms are at the core of many programs of national importance ranging from simulating inertial confinement fusion (ICF) implosions to the design of high-explosive experiments to climate modeling to circulation of blood in cardiovascular systems. The hydrodynamic algorithms commonly employed at the laboratory and in industry (1) typically *lack requisite accuracy* for complex multi-material vortical flows and (2) are not well suited for exascale computing due to *poor data locality* and *poor compute intensity*. Exascale computing requires transformational advances in both computer science and numerical algorithms. We propose to research the second requirement and create a revolutionary new high-order arbitrary Lagrangian Eulerian hydrodynamic algorithm that has both excellent data locality and compute intensity, and is suitable for accurately simulating multi-material vortical flows involving metals, gasses and viscous fluids on fully unstructured polytopal meshes.

Project Goals

The history of hydrodynamic research at Los Alamos is rich and full of many revolutionary discoveries. Approximately 66 years ago von Neumann and Richtmyer [36] developed the Lagrangian (mesh moves with the flow) staggered grid hydrodynamic (SGH) method. In this framework, the velocity and thermodynamic variables are spatially staggered. The SGH method is the basis of many LANL and LNLL hydrodynamic codes and is the world standard. Ruppel and Harlow [1] proposed the Lagrangian cell-centered hydrodynamic (CCH) method in the early 80's. Recently, the CCH method has seen renewed interest and researchers around the world are building on these foundational ideas [15, 27, 28, 8]. Burton et. al. [8, 9] extended the Lagrangian CCH method to support multi-material cells on arbitrary polytopal cells and account for complex nonlinear material models such as those associated with metals. From von Neumann to Burton, Los Alamos has been a world leader in hydrodynamic research. The objective of this research is to build on this heritage and substantially advance numerical algorithms of relevance to Laboratory and national missions and lead the world in multi-material hydrodynamics research.

While hydrodynamic algorithms have advanced, challenges still exist with accurately simulating vortical flows such as those seen in imploding ICF capsules, shaped charge munitions, hydrodynamic experiments, atmospheric flows, and a beating heart. The need for additional research was recently acknowledged by the predictive science panel (PSP) that listed as a top priority the need to investigate the predictive capabilities of hydrodynamic codes at simulating complex vortical multi-material flows. Many hydrodynamic methods are prone to generating spurious vorticity, while other methods can artificially suppress physical vorticity. New hydrodynamic methods must be derived with careful attention on accurately generating, evolving and dissipating vorticity.

Computational physics is facing addition, new challenges that are arising with emerging computer architectures. Heterogeneous processors (GPUs and MICs) are forcing the simulation community to reconsider long held paradigms such as relying on mesh refinement with lower order

methods. Emerging architectures are forcing algorithmic development to move towards higher compute intensity methods with excellent data locality and internal parallelism. The goal is to maximize the compute intensity per memory footprint (FLOP/memory ratio) and to eliminate the communication between distance cells (e.g., good data locality). Lower order methods typically have excellent data locality, but they have poor compute intensity and because of high numerical diffusion, struggle to accurately simulate vortical flows at reasonable mesh resolutions. Higher-order methods boost significantly the accuracy and FLOP/memory ratio, reduce numerical diffusion and dispersion, and often, have excellent data locality. The challenge, however, is that prior research on high-order methods has focused on single-phase, single-material flows. A DR-level investment is needed to develop high-order Arbitrary Lagrangian Eulerian hydrodynamic methods suitable for simulating multiphase multi-material complex flows in a strongly deformable medium that arise in many applications.

This research proposal seeks to develop a revolutionary new high-order multi-material hydrodynamic method with excellent data locality and compute intensity that has superior accuracy to existing methods on multi-material vortical flows with gasses, metals, and viscous fluids. This research will impact a broad range of areas including numerical theory, discrete mathematics, vorticity evolution, solid dynamics, gas dynamics, interface instability evolution, turbulent flows, fluid dynamics, and shock driven flows. If successful, the proposed research has the potential to radically transform hydrodynamic simulation capabilities, place the laboratory as a leading research institution in the world on high-order hydrodynamics and help position the laboratory for computing at the exascale and competing for external funding from other agencies.

Why not programmatic funding? Numerous research challenges exist so this proposed project lies outside the scope of ASC that is heavily focused on (1) enabling the current codes to run on the Trinity machine, (2) researching and developing computer science capabilities for exploiting task-based parallelism essential for the next generation code (NGC), and (3) implementing known algorithms into NGC to meet an aggressive development scheduled. NGC must perform 3D multi-physics calculations by 2020 (~4 years away) and such a task historically has taken more than 4 years to accomplish. The short timeframe forces the adoption of established numerical methods that do not have risk and concentrating programmatic funds on implementation and not research. The proposed research fits very well with the LDRD program that supports the pursuit of higher-risk, high-reward technologies.

Background and Statement of Problem

Conventional hydrodynamic algorithms are lower-order, cannot accurately simulate vortical multiphase multi-material flows at manageable mesh resolutions and lose efficacy on emerging computer architectures. For example, in AMR Eulerian codes such as xRAGE [21], spurious vorticity is created by numerical errors [20] so that mesh resolutions on the order of a micron are typically required in ICF simulations to reduce the magnitude of the vorticity errors [31]. Micron mesh resolutions are currently impractical for 3D ICF simulations and create challenges for exascale computing due to poor FLOP/memory ratios. The staggered grid Arbitrary Lagrangian Eulerian (ALE) finite volume method, that are used in many LANL and LLNL codes [29, 6, 7], comprise the current world standard. For these schemes, artificial viscosity and mesh stability models combined with a lack of kinematic degrees of freedom artificially suppress vorticity and lead to unphysical symmetric flows. Refining the mesh resolution with these methods can, in some instances, improve the accuracy, but lack of compute intensity makes this strategy ineffi-

cient for future computing architectures. Modern high-order collocated finite volume methods [10] are very accurate, but these schemes have poor data locality and require communication with distant elements. An alternative strategy is to develop new high-order 2D/3D ALE hydrodynamic algorithms that correctly capture vorticity and other complexities at reasonable mesh resolutions and yet have excellent FLOP/memory ratios and data locality. Such algorithms are suitable for emerging architectures such as GPUs and MICs and exascale computing.

High-order solutions of complex multidimensional flows, such as vorticity, require more kinematic degrees of freedom in the element than present in current hydrodynamic methods [11, 12]. The current methods use elements with linear surfaces, whereas, high-order elements have edges described by high-order polynomials or splines or NURBS. To capture vorticity, the edges must bend and flex in the Lagrangian limit in which the mesh moves with the flow (Fig. 1). The necessity of high-order elements is illustrated by calculating a 2D vortex (Fig. 2) proposed in [34]. This test problem is calculated using cubic quadrilateral elements in the Lagrangian limit. Analytic mesh deformation results are provided to facilitate comparisons (Fig. 2b). As illustrated, the linear elements struggle to follow the rotating flow (Fig. 2c), whereas, the cubic elements readily deform with the flow (Fig. 2d).

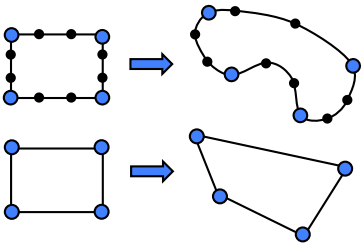
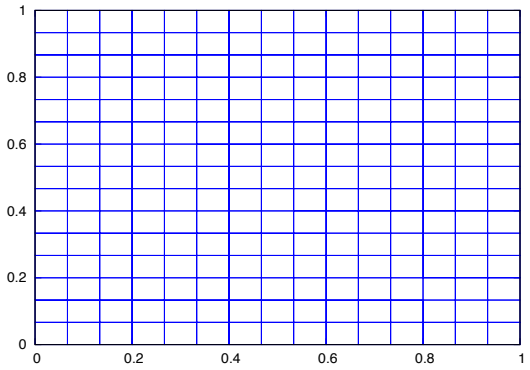
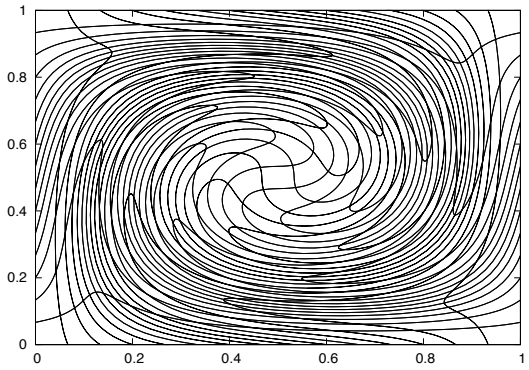


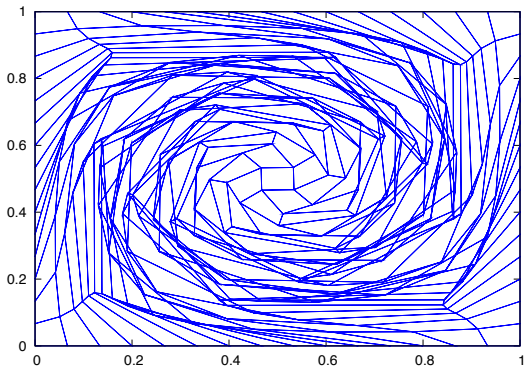
Fig. 1: High order elements (top) can bend, whereas, linear elements (bottom) are stiffer



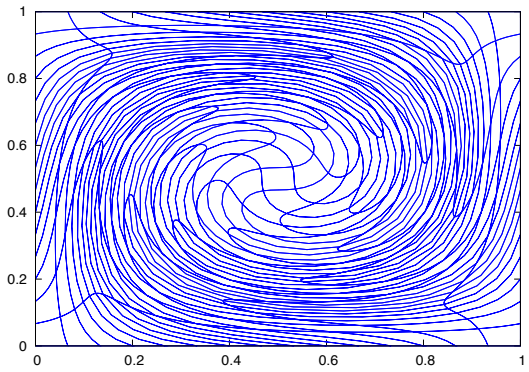
(a) Initial mesh



(b) Analytic mesh deformation



(c) Standard linear elements tangle



(d) Cubic elements can bend

Fig. 2: The high-order elements better capture the details of the flow (2d) compared to linear elements (2c). The results shown correspond to the center element rotating 360°.

High-order elements have merits in the Eulerian limit, in which the mesh is stationary, and with ALE, in which the mesh moves arbitrarily between the Eulerian and Lagrangian limits. Most multi-material multi-physics ALE codes use a three-step solution procedure. The first step is a Lagrange calculation that deforms the mesh, the second step creates an improved mesh (e.g., a smoother mesh), and the third step is to remap the physical quantities to the improved mesh. This type of approach is termed "Lagrange+remap." The high-order elements are able to more accurately capture the non-linear variation of the flow along the faces of the elements; this translates into a more accurate estimate of the remap volume and a more accurate reconstruction of the fields (density, velocity, energy, etc.) over the element. Current methods typically use linear elements and assume a linear variation of the fields over the element. Neglecting complex variations in the flow is inadequate for simulations at manageable mesh resolutions. Fig. 3 graphically illustrates the need for high-order elements in the Eulerian limit.

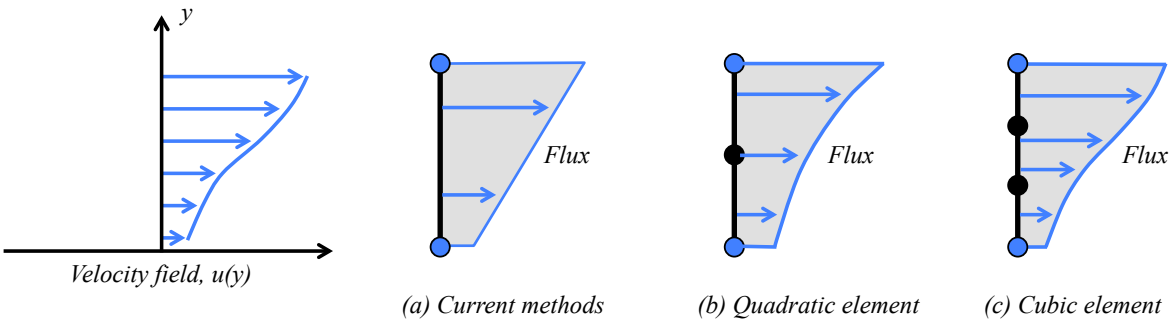


Fig. 3: A velocity field is prescribed on an element face and the corresponding remap volumes (grey region) are calculated for the Eulerian limit (remap back to the original mesh) using the current method (3a), a quadratic element (3b), and a cubic element (3c).

Proposed Innovation and Significance

The proposed innovation is to develop the *first* Lagrange+remap ALE cell centered discontinuous Galerkin [33] hydrodynamic (DGH) method on high-order elements suitable for realistic simulations of complex multi-material 2D and 3D flows involving metals, gases, and viscous fluids. The method will have an excellent FLOP/memory ratio and data locality, which is necessary for emerging architectures such as MICs, GPUs and exascale computing. The Lagrangian DGH research to date is very limited in focus with only a few papers published on the topic [22, 24, 25, 35]. The sparse literature only addresses single material gas dynamics with a simple analytic equation of state, so the few published Lagrangian DGH methods are incapable of simulating applications of relevance to laboratory missions. *This research proposal will close many gaps in the theory and numerical algorithms essential for simulating hydrodynamic experiments including the support of multi-material cells, tensor quantities (e.g., stress, strain) [8], tabular equations of state (EOS), explosives, constitutive models, tensile failure, material damage evolution, 2D/3D unstructured polytopal meshes [26], curved surfaces and material interfaces in both 2D axisymmetric R-Z coordinates and 3D Cartesian coordinates, contact surfaces and high-order remaps.* This list reflects the complexity of real-life simulations and highlights the vast range of topics that *have not been studied* for Lagrangian or ALE DGH. Many past research efforts [38] have failed to create robust low-order ALE methods suitable for complex multi-material flows so the proposed research will be navigating uncharted waters that have technolog-

ical risk. To help mitigate this risk, a multidisciplinary team of experts will perform the research that has experience covering DG theory, finite element methods, and ALE multi-material CCH.

The motivation for researching the DGH method is that it has advantages over other methods such as the high-order finite volume hydrodynamic (FVH) method [11, 12, 10] and the high-order finite element hydrodynamic (FEH) method [16]. The FEH method requires artificial viscosity, whereas, the DGH method solves a Riemann problem that can improve the accuracy on shock problems. The DGH method also requires solving only a local mass matrix, so it has excellent data locality when compared to high-order FEH and FVH methods [10].

The research in [23] demonstrates order-of-magnitude performance gains on GPUs with a high-order DGH method for solving Maxwell's electromagnetic equations in 3D for linear, isotropic, and time-invariant materials. Additional reductions in computing time can be realized with high-order methods because fewer elements are required for a given level of accuracy. The numerical error in a 4th-order accurate method is proportional to the edge length (dx) to the 4th power ($error \propto dx^4$), whereas, the numerical error in current, 2nd-order accurate methods is $error \propto dx^2$. The 3D calculation time typically scales as $1/dx^4$ so using 2 to 4 times larger elements can significantly reduce the computing time. Fig. 4 shows the wall clock time required to reach a given level of accuracy on a 3D vortex problem using 4th-order and 2nd-order accurate Eulerian FVH methods on an unstructured mesh [10]. As shown, a 4th-order accurate method can reach the same level of accuracy approximately 20X faster than current, 2nd-order accurate methods with sufficient mesh resolution (red arrow in Fig. 4). Alternatively, for the same wall clock time, the errors can be reduced by approximately 100x using the 4th-order accurate method with sufficient mesh resolution (blue arrow in Fig. 4). For reasons such as these, the European Union exascale program is researching the single material gas dynamics moving mesh DGH method in [3, 4].

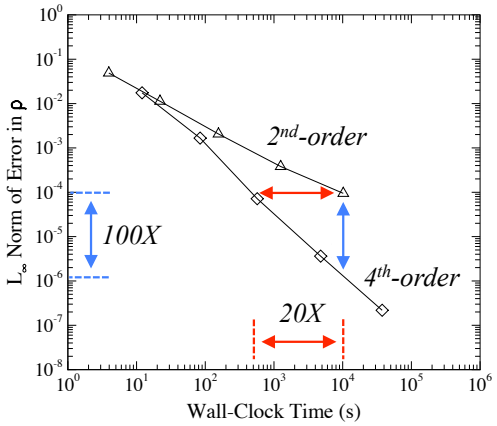


Fig. 4: The plot shows the max density error in a calculation of a 3D vortex as a function of wall-clock time. Significant speed-ups and improvements in accuracy can be achieved with high-order hydrodynamic methods.

Technical impact

A range of important mathematical topics neglected in the existing research will be investigated including numerical stability of high-order Lagrangian methods, compatible discrete equations, entropic discrete equations, and mimetic formulations. Extending the mimetic approach to high-order methods is of great importance to topics beyond hydrodynamics including radiation transport, diffusion, and electromagnetics. The research can positively impact simulations of both viscous and inviscid flows that arise in diverse applications ranging from blood flowing through a heart to vortical flows in ICF capsules to ocean currents to molten metal flows in additive manufacturing and casting processes.

Mission impact

Improvements to hydrodynamics algorithms are of great importance to science-based prediction in programmatic applications. Simulations at LANL are regularly used to (1) design hydrody-

namic experiments where many exceed a million dollars to execute, (2) aid understanding of experiments, (3), interpolate between different experiments, (4) estimate margins and uncertainties, (5) investigate high strain-rate deformation of metals, and (6) extrapolate experiments into regimes and scales that are not readily accessible. This research proposal will likely impact many key Laboratory programs such as the ASC and joint munitions programs. Developing high-order algorithms is also beneficial to fluid dynamic codes so the impact could be very broad, ranging from simulating molten metal flows to atmospheric vortical flows. While this research has risk, the results could radically transform the simulation capabilities at LANL and beyond. Furthermore, the research can reaffirm that the laboratory is a world leader in multiphase multi-material hydrodynamics, which is essential for attracting new staff at all career levels.

R&D Methods and Anticipated Results

The proposed cell centered DGH Lagrange+remap method is a significant departure from the algorithms in the existing LANL codes and those published in scientific journals. Some key differences include: high-order expansions for each material primitive variable in a cell (e.g., support multi-material cells), high-order expansions of tensor quantities (e.g., stress and strain), high-order contact surfaces and boundary surfaces and material interfaces, diverse types of material models, multi-material remaps (e.g. ALE), and curved surfaces with unstructured polytopal meshes in both 2D and 3D Cartesian and curvilinear coordinates.

Multi-material DGH formulation

The governing equations for evolving the specific strain rate tensor ($\boldsymbol{\gamma}$), velocity ($\mathbf{u}$), total energy (τ), and position ($\mathbf{x}$) in the Lagrangian limit are:

$$\rho\frac{\partial\boldsymbol{\gamma}}{\partial t}-\nabla\otimes\mathbf{u}=0\,,\qquad \rho\frac{\partial\mathbf{u}}{\partial t}-\nabla\cdot\boldsymbol{\sigma}=0\,,\qquad \rho\frac{\partial\tau}{\partial t}-\nabla\cdot\left(\boldsymbol{\sigma}\cdot\mathbf{u}\right)=0\,,\qquad \frac{\partial\mathbf{x}}{\partial t}=\mathbf{u}\,, \tag{1}$$

where the density is ρ, the stress tensor is $\boldsymbol{\sigma}$, and $\otimes$ is the tensor product. The proposed method assigns each material in an element a high-order polynomial expansion (e.g. Taylor-Series) for all primitive variables in the element "z" (Fig. 5). The expansions for a material "m" of some quantity are given by

$$U_z^m=\sum_k\psi^k\left(\mathbf{x}\right)U^{k,m}\qquad U^{k,m}=\left(\ \boldsymbol{\gamma}^{k,m},\ \ \mathbf{u}^{k,m},\ \ \tau^{k,m},\ \ \boldsymbol{\sigma}^{k,m},\ \ (\boldsymbol{\sigma}\cdot\mathbf{u})^{k,m},\ \right) \tag{2}$$

where $\psi^k\left(\mathbf{x}\right)$ are basis functions that spatially vary over the element, $U^{k,m}$ are temporally varying coefficients on the expansions for a material present in the element. The high-order expansions (Eq. 2) are substituted into the governing equations (Eq. 1). The governing equations are then multiplied by test functions, $\psi^j\left(\mathbf{x}\right)$, and integrated over the domain of each element. Using the divergence theorem, the resulting multi-material equations of an arbitrary order for a material undergoing Lagrangian motion are:

$$\left(\int_V\rho^m\psi^j\psi^k\phi^m\,dV\right)\frac{\partial\boldsymbol{\gamma}^{k,m}}{\partial t}=\int_{\partial V}\mathbf{n}\otimes\mathbf{u}^*\psi^j\phi^m\,dA-\int_V\mathbf{u}_k^m\otimes(\nabla\psi^j)\phi^m\,dV+\int_I\mathbf{n}\otimes\mathbf{u}^*\psi^j\,dA_I \tag{3}$$

$$\left(\int_V\rho^m\psi^j\psi^k\phi^m\,dV\right)\frac{\partial\mathbf{u}^{k,m}}{\partial t}=\int_{\partial V}\mathbf{n}\cdot\boldsymbol{\sigma}^{*m}\psi^j\phi^m\,dA-\int_V\boldsymbol{\sigma}^{k,m}\cdot(\nabla\psi^j)\phi^m\,dV+\int_I\mathbf{n}\cdot\boldsymbol{\sigma}^{*m}\psi^j\,dA_I \tag{4}$$

$$\left(\int_V \rho^m \psi^j \psi^k \phi^m \, dV\right) \frac{\partial \tau^{k,m}}{\partial t} = \int_{\partial V} \mathbf{n} \cdot \boldsymbol{\sigma}^{*m} \cdot \mathbf{u}^* \psi^j \phi^m \, dA - \int_V (\boldsymbol{\sigma} \cdot \mathbf{u})^{k,m} \cdot (\nabla \psi^j) \phi^m \, dV + \int_I \mathbf{n} \cdot \boldsymbol{\sigma}^{*m} \cdot \mathbf{u}_I^* \psi^j \, dA_I \qquad (5)$$

where ϕ^m is the material volume fraction, the superscript * denotes a Riemann solution on the element boundary, ∂V, or an internal material-material interface, I (Fig. 5). Repeated superscript indices j and k imply summation. The surface integral along material interfaces accounts for the sub-cell exchange of compression, momentum, and total energy between the materials, which obviates the need for classical closure models. Eqs. (3)-(5) form a local system of equations for each material that must be solved each time integration step. A high-order, explicit, and conservative multistage Runge-Kutta temporal integration method is used. *The proposed multi-material discrete equations presented here have never been investigated.*

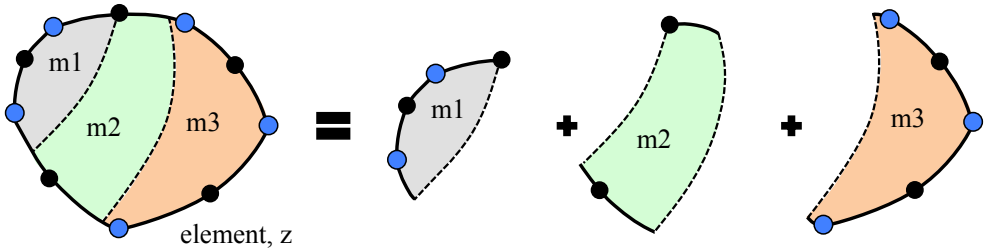


Fig. 5: A high-order element is shown with 3 distinctly different materials. The dashed lines denote material interfaces inside the element.

Multi-Material multidirectional Riemann problem

The spatial variation in velocity and stress tensor fields is given by polynomial expansions over the element (Eq. 2). Discontinuities in the velocity and stress fields can arise at the element surfaces so an approximate Riemann problem is solved to address the discontinuities. The Riemann force contributions from all materials on a segment of the element surface, ∂V_i, is $\mathbf{F}_i^* = \sum_m \phi^m \int \mathbf{n} \cdot \boldsymbol{\sigma}^{*m} \psi^j \, dA$. The Riemann stress [8] contribution per unit area from a material is $\mathbf{n} \cdot \boldsymbol{\sigma}^{*m} = \mathbf{n} \cdot \boldsymbol{\sigma}^m + \mu^m \left|\hat{\mathbf{e}} \cdot \mathbf{n}\right| \left(\mathbf{u}_p^* - \mathbf{u}^m\right)$, where $\hat{\mathbf{e}}$ is an estimate of the shock direction, μ^m is the shock impedance of a material, and $\mathbf{u}_p^*$ is the Riemann velocity at an element node. The Riemann velocity is found by enforcing conservation of momentum over all surfaces, ∂V_i, connected to the element node ($i \in p$),

$$\mathbf{u}_p^* = \frac{\sum_{i \in p} \sum_m \phi_i^m \int_{\partial V_i} \left(\mu^m \left|\hat{\mathbf{e}} \cdot \mathbf{n}\right| \mathbf{u}^m - \mathbf{n} \cdot \boldsymbol{\sigma}^m\right) \psi^j \, dA}{\sum_{i \in p} \sum_m \phi_i^m \int_{\partial V_i} \left(\mu^m \left|\hat{\mathbf{e}} \cdot \mathbf{n}\right| \mathbf{u}^m\right) \psi^j \, dA} \qquad (6)$$

The Riemann velocity is used to move an element node and to calculate the Riemann force for each material. *Multi-material multidirectional approximate Riemann solutions for arbitrary order polynomial expansions are new and have not been studied.*

Curved surfaces with fully unstructured polytopal meshes

Unstructured polytopal meshes are required for representing complex, arbitrary geometries and are essential for improved accuracy on large deformation flows [26, 13]. A polytopal element can be decomposed into sub-regions termed “sides” that are triangles (2D) or tetrahedral (3D);

this is illustrated in Fig 6. The side decomposition enables implementation and extension of complex numerical algorithms to any element type. For instance, the DGH approach requires integration of high-order polynomial expansions over the element volume and along the surface. This can be performed by using (1) established isosparametric transformations on each element side and (2) summing over the known Gauss integration points. *This side decomposition can enable adaptive mesh refinement (AMR) with curved surfaces, solutions on high-order Voronoi elements, and enable construction of curved material interfaces inside an element.*

EOS and strength models

The side decomposition (Fig. 6) enables the application of tabular EOSs and complex strength models to high-order polytopal elements. A stress tensor, $\boldsymbol{\sigma} = -p\mathbf{I} + \boldsymbol{\sigma}'$, can be defined at the Gauss integration points in each element side in a manner similar to classical finite element methods [14]. Hypo [37] or hyper [2] elastic-plastic models can be used to calculate the stress deviators, $\boldsymbol{\sigma}'$. The pressure, p, is calculated from a table or analytic function. Artificial element locking should not be an issue due to the many degrees of freedom in the side compared to linear triangles and tetrahedra (e.g. TTS [5]). For the quadratic element shown in Fig. (6), there would be 3 stress tensors per side. *Extending strength models and tabular equations of state to Lagrangian DGH has not been researched for linear or high-order polytopal elements.*

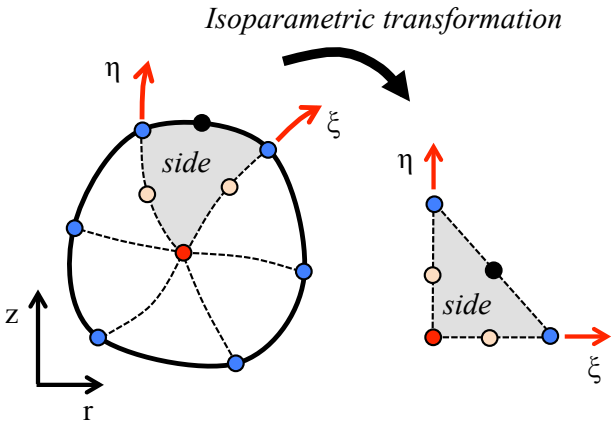


Fig 6: This research effort seeks to extend curved surfaces to arbitrary polytopal elements in 2D RZ coordinates and 3D Cartesian coordinates. To accomplish this goal, isoparametric transformations will be applied to each element side (grey region), which are either high-order triangles (2D) or tetrahedra (3D).

Contact surfaces

Contact surface algorithms enable Lagrangian meshes to impact, slide and separate. Morgan et. al. [30] proposed the first contact surface method for Lagrangian cell-centered FVH. The method solves a multidirectional approximate Riemann problem at each penetrating or touching node along the contact surface. A challenge with the method in [30] is calculating high-order polynomial reconstructions of the velocity and stress in elements along the contact surface due to an insufficient number of element neighbors. The merit of the DGH method is that the polynomial expansions are evolved forward in time so high-order solutions are feasible at mesh discontinuities such as contact surfaces. Furthermore, DGH could enable the use of curved boundary surfaces that more accurately captures bending. *The DGH method is potentially a game-changer by enabling high-order solutions along curved contact surfaces.*

Remap

While high-order elements enable significantly more mesh deformation, the need to relax or adjust the mesh positions is still required on many large deformation flows to keep spatial resolution in key regions, to increase temporal step size, and to improve accuracy. The concept in ALE is to find a more optimal mesh and then remap the mass, momentum, energy, porosity, plasticity, etc. to the new, improved mesh (Fig. 3). A merit of DGH is that the high-order polynomial ex-

pansions can be used to calculate remap fluxes, which obviates the potentially costly reconstruction step in current methods. For multi-material cells, the proposed method calculates high-order remap fluxes for each material. *Improvements to multi-material remaps are of great importance to simulating interface evolution of disparate materials (e.g., a metal-gas interface)*.

Risk mitigation

The DGH method has intrinsic risk mitigation because it can reduce to the cell-centered FVH method. Furthermore, Dumbser et. al. [17, 18, 19] proposed a generalized framework called P_nP_m that combines both FVH and DGH methods. The FVH methods evolve a cell average, P_0, and reconstruct the fields (e.g., velocity) using neighboring elements with a polynomial of order P_m. All FVH methods are P_0P_m. The DGH method evolves a polynomial expansion over the element of order P_n, and the reconstruction is equal to the polynomial expansion, P_m=P_n. DGH methods are P_nP_n, where a linear DGH method is P_1P_1. The P_nP_m framework uses the element neighbors to increase the accuracy of the reconstruction typically by one order, P_m=P_{n+1}. For instance, the DGH method can evolve a linear polynomial P_1, and build a quadratic reconstruction P_2 using neighboring elements. The P_nP_m framework enables immense flexibility in the type of solution – everything from DGH to FVH and beyond. Robust multi-material methods exist for linear Lagrangian FVH methods, P_0P_1, so the P_nP_m framework provides a research path with intrinsic risk mitigation that facilitates significant improvements over current methods.

Curved elements generate a range of technological challenges. One risk migration strategy is to approximate the curved surface as multiple, piecewise-linear segments instead of high-order polynomials or splines or NURBS. With this strategy, the convergence rate is likely to remain similar to current methods, but the numerical errors are expected to drop significantly. The element will have more degrees of freedom, which allows the mesh to deform more readily on vortical flows, and the P_nP_m framework can be used to evolve and or construct high-order polynomial expansions of each variable over the element.

Expected results

The objective is to realize 10x to 100x improvements in accuracy over current lower-order methods. The research will be performed in both research codes and the FLAG ASC code [7]. The motivation for using FLAG is that it is an excellent platform for developing and refining the new method, because it currently supports a range of algorithms for handling multi-material cells and diverse material models including strength. The project goals would not be achievable if a new computer infrastructure must be built from scratch. Leveraging the existing infrastructure in the FLAG code reduces the research and development time, and if successful, the capabilities will be immediately available to the simulation community.

Project plan

The proposed project plan is provided in Fig. 8. The project will start with a focus on developing both a linear and curved surface DGH method for 2D and 3D coordinates. The work on linear surfaces will aid research and develop of a DGH method for high-order elements. The goal is to enable single material gas dynamics on 2D and 3D arbitrary higher-order polytopal meshes by mid FY18. Research on multi-material elements, strength, contact surfaces, and remaps (*i.e.,* ALE) will start with linear elements by the end of the first year and start with high-order elements by the end of the second year. The goal at the end of this project is to simulate Rayleigh-Taylor instability growth in metals undergoing extremely high strain rates [32] using the new high-order ALE method.

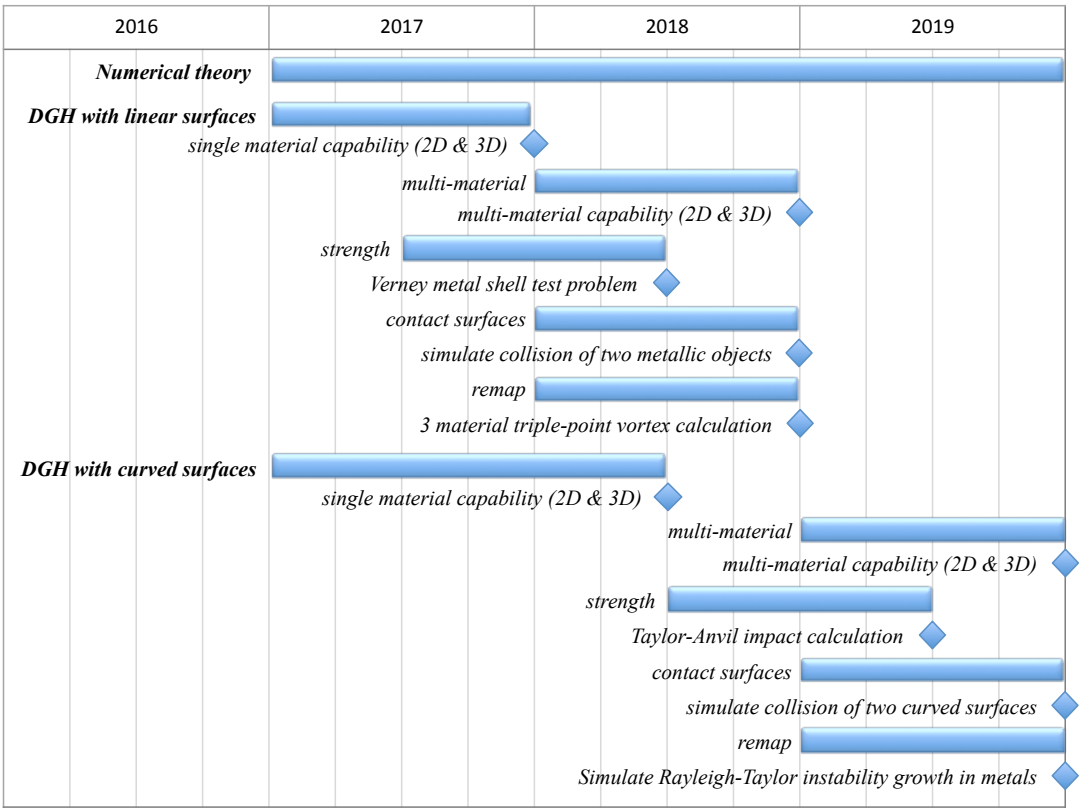


Fig. 8. The research timeline with milestone deliverables

Data management plan

The coding and simulation results will be stored on LANL HPC networks including hpss.

Transition plan

The proposed research could transition to funds under the ASC program that oversees the FLAG code and the next generation code (NGC). A merit of using the FLAG ASC code for research and development is that, if the research is successful, it is more likely to have follow-on financial support. Likewise, the NGC project will be sufficiently mature by the end of 2019 that a multi-material high-order algorithm could be adopted and follow-on computer science research could be performed. ASC funds could support work to (1) implement a successful new hydrodynamic method into NGC, (2) develop strategies to take advantage of the superior FLOP/memory ratio, and (3) investigate techniques for moving towards exascale.

The Joint Munitions program (JMP) seeks to advance conventional munitions collaboratively with the DoD. Computer simulations are integral to the design, execution, and interpretation of experimental results. The principle code used by JMP at LANL is the CTH code from SNL. The proposed high-order hydrodynamic method would be a monumental advance over the lower-order method in CTH. The JMP could adopt a LANL ASC code for hydrodynamic simulations.

Budget Request

Many difficult research tasks will be undertaken so multiple, experienced staff members are required to work at more than half time and some closer to full time. $1.6M/year is necessary to cover the associated staffing costs.

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Computing Resource Needs

All persons listed on the research proposal have access to LANL high performance computers such as Moonlight. Sufficient computing resources currently exist for the proposed research and sufficient storage is available to store software and all simulation results.

Appendix

Donald E. Burton (118576, XCP-4) has a Ph.D. in Theoretical Physics. He has over 45 years of code development experience, leading TENSOR, GROK, and FLAG code projects as well as weapons effects projects at LLNL. He created two of the surviving ASC code projects, one at LLNL and the Shavano Project at LANL and led the latter for nearly 10 years. He held numerous group and section leader positions at both laboratories. He has many journal publications on Lagrangian and ALE hydrodynamics. His role in the project will involve developing the theory and numerical algorithms, design and implementation in FLAG, and documentation. (0.70 FTE)

Some journal publications of relevance to the project are provided.

- D. Burton, N. Morgan, T. Carney, M. Kenamond: *Reduction of dissipation in Lagrange cell-centered hydrodynamics (CCH) through corner gradient reconstruction (CGR)*. J. Comp. Phys. 2015; 299:229-280.
- D. Burton, T. Carney, N. Morgan, S. Sambasivan, M. Shashkov: *A cell-centered Lagrangian Godunov-like method for solid dynamics*. Comp. & Fluids 2013; 83:33-47.
- S. Sambasivan, M. Shashkov, D. Burton: *A finite volume cell-centered Lagrangian hydrodynamics approach for solids in general unstructured grids*. Int. J. Num. Meth. Fluids. 2013;72:770-810.
- N. Morgan, M. Kenamond, D. Burton, T. Carney, D. Ingraham: *An Approach for Treating Contact Surfaces in Lagrangian Cell-Centered Hydrodynamics*. J. Comp. Phys. 2013; 250:527-554.
- S.K. Sambasivan, M.J. Shashkov, and D.E. Burton. *Exploration of new limiter schemes for stress tensors in Lagrangian and ALE hydrocodes*. Comput. Fluids, 86:98–114, 2013.
- S.K. Sambasivan, M.J. Shashkov, and D.E. Burton. *A cell-centered Lagrangian finite volume approach for computing elasto-plastic response of solids in cylindrical axisymmetric geometries*. J. Comput. Phys., i237:251-288, 2012.
- A. Barlow, D. Burton, M. Shashkov: *Compatible, energy and symmetry preserving 2D Lagrangian hydrodynamics in rz – cylindrical coordinates*. Proc. Comp. Sci. 2010;1:1887-1895.
- E. Caramana, C. Rousculp, D. Burton: *A compatible, energy and symmetry preserving Lagrangian hydrodynamics algorithms in three-dimensional Cartesian geometry*. J. Comp. Phys. 2000;157:89-119.
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- D.E Burton. *Multidimensional discretization of conservation laws for unstructured polyhedral grids*. SAMGOP-94: 2nd International Workshop on Analytical Methods and Process Optimization in Fluid and Gas Mechanics, VNIIEF, Holiday Base, Arzamas-16, Russia, September 10-16, 1994.

Marc Charest (276524, XCP-1) received a Ph.D. in Aerospace Engineering from the University of Toronto in Ontario, Canada. He came to the lab as a Nicholas C. Metropolis Postdoctoral Fellow in Computational and Computer Sciences working in XCP-8. His current research involves developing high-order methods for Eulerian and ALE hydrodynamics that can be used in conjunction with adaptive mesh refinement and unstructured grids. He is also currently developing/implementing advanced remapping strategies for arbitrary polygonal meshes in FLAG. All of this work focuses on designing highly-scalable algorithms specifically for next-generation computer architectures. Prior to joining LANL in 2013, he was the MITACS Postdoctoral Fellow at the University of Toronto's Institute for Aerospace Studies. In Toronto, he researched high-order solution methods for large eddy simulation of practical turbulent flames. This research was funded by Rolls-Royce Canada to help improve their ability to predict harmful emissions from gas turbine combustion engines. Throughout his career, his research has focused on improving the accuracy and performance of finite-volume methods. This included implementing various discontinuous Galerkin and finite element solvers for comparison purposes. (0.35 FTE)

Some recent publications related to the project are provided.

- M.R.J. Charest, C.P.T. Groth, P.Q. Gauthier: *A high-order central ENO finite-volume scheme for three-dimensional low-speed viscous flows on unstructured mesh*. Communications in Computational Physics, 17(3):615–656, 2015.
- M.R.J. Charest, T.R. Canfield, N.R. Morgan, J. Waltz, J.G. Wohlbier: *A high-order vertex-based central ENO finite-volume scheme for three-dimensional compressible flows*. Computers & Fluids, 114:172–192, 2015.
- N.R. Morgan, J.Waltz, D.E. Burton, M.R.J. Charest, T.R. Canfield, J.G.Wohlbier: *A point-centered arbitrary Lagrangian Eulerian hydrodynamic approach for tetrahedral meshes*. Journal of Computational Physics, 290:239–273, 2015.
- J.Waltz, J.G.Wohlbier, L.D. Risinger, T.R. Canfield, M.R.J. Charest, A.R. Long, N.R. Morgan: *Performance analysis of a 3D unstructured mesh hydrodynamics code on multi- and many-core architectures*. International Journal for Numerical Methods in Fluids, 77(6):319–333, 2015.
- N.R. Morgan, J. Waltz, D.E. Burton, M.R.J. Charest, T.R. Canfield, J.G. Wohlbier: *A Godunov-like point-centered essentially Lagrangian hydrodynamic approach*. Journal of Computational Physics, 281:614–652, 2014.

Konstantin Lipnikov (179388, T-5) has Ph.D. in applied mathematics. He has over 18 years of experience in scientific computing including the development, implementation and theoretical analysis of compatible discretization methods on unstructured polytopal meshes with non-planar faces. Currently, he is a team leader of Numerical Analysis Team at T-5, and the Discretization Task lead for the Advanced Simulation Capability for Environmental Management (ASCEM) multi-Labs DOE project. For the last 10 years, he was implementing mimetic discretization schemes in the ASC code FLAG for multi-material diffusion problems, artificial viscosity, and, this year, resistive MHD. He has co-authored 2 books and more than 80 peer reviewed papers on (a) the theory of discretization methods including the DG methods, (b) the theory of a priori error estimates on adaptive anisotropic meshes, and (c) the theory of iterative solvers. In 2015, he participated in the Legion bootcamp training on writing high-performance applications for distributed heterogeneous architectures. His role in the project will involve theory, derivation of algorithms on unstructured meshes, implementation in FLAG and C++ test codes, and documentation. (0.5 FTE)

Seven publications related to the project are provided.

- K.Lipnikov, I.Yotov, D.Vassilev: *Discontinuous Galerkin and mimetic finite difference methods for coupled Stokes-Darcy flows on polygonal and polyhedral grids*. Numer. Mathematik, 2014;126:321-360.
- F.Brezzi, K.Lipnikov, M.Shashkov: *Convergence of mimetic finite difference method for diffusion problems on polyhedral meshes with curved faces*. M3AS: Math. Models and Meth. in App. Sciences, 2006;16:275-297.
- V.Gyrya, K.Lipnikov, G.Manzini: *The arbitrary order mixed mimetic finite difference method for the diffusion equation*. M2AN: Math. Model. Numer. Anal. (2016), accepted.
- N. Morgan, K. Lipnikov, D. Burton, M. Kenamond: *A Lagrangian staggered grid Godunov-like approach for hydrodynamics*. J. Comp. Phys. 2014; 259:568-597.
- K.Lipnikov, D.Svyatskiy, and Y.Vassilevski: *A monotone finite volume scheme for advection-diffusion equations on unstructured polygonal meshes*. J. Comp. Phys., 2010; 229:4017-4032.
- R.Garimella and K.Lipnikov, *Solution of the diffusion equation in multi-material domains by subdivision of elements along reconstructed interfaces*. Int. J. Numer. Meth. Fluids, 2011; 65:1423-1437.
- K.Lipnikov and M.Shashkov. *A mimetic tensor artificial viscosity method for arbitrary polyhedral meshes*. Procedia Computer Science, 2010; 1:1915-1923.

Robert B. Lowrie (119261, CCS-2) has a Ph.D. in Aerospace Engineering. Lowrie is currently the project leader for three very successful radiation transport codes in the ASC Program at Los Alamos: Implicit Monte Carlo (IMC), PARTISN (S_N neutron), and Capsaicin (S_N thermal). The S_N method for radiation transport is the origin of the discontinuous Galerkin method, and Lowrie's original dissertation research was on discontinuous Galerkin for shock hydrodynamics using space-time elements. His current research focus is on radiation transport and coupled radiation-hydrodynamics. He has also published in a range of numerical methods topics and physics application areas, including shock hydrodynamics, advection schemes, asymptotic-preserving methods for kinetic equations, numerical methods and theory for hyperbolic conservation laws, and numerical methods for multi-physics time integration. Lowrie will investigate multi-physics coupling issues with the new hydro methods, time-integration, and treatment of multi-material mesh cells (0.2 FTE).

Some recent journal publications of relevance to the project are provided.

- T. S. Haut, C. Ahrens, A. Jonko, R. B. Lowrie, and A. Till. *A New Multigroup Method for Cross-sections that Vary Rapidly in Energy*. Submitted to J. Quantitative Spectroscopy and Radiative Transfer, April 2016.
- D. Lee, R. Lowrie, M. Petersen, T. Ringler, M. Hecht, *A High Order Characteristic Discontinuous Galerkin Scheme for Advection on Unstructured Meshes*. Submitted to J. Computational Physics, April 2016.
- A. B. Wollaber, H. Park, R. B. Lowrie, R. M. Rauenzahn, and M. A. Cleveland. *Radiation Hydrodynamics with a High-Order, Low-Order Method*. Proceedings of the ANS M&C Nashville, TN, April 2015.
- T. S. Haut, R. B. Lowrie, H. Park, R. M. Rauenzahn, and A. B. Wollaber. *A Linear Stability Analysis of the Multigroup High-Order Low-Order (HOLO) Method*. Proceedings of the ANS M&C Nashville, TN, April 2015.
- R. B. Lowrie and T. S. Haut. *Reconstructing opacities for multigroup thermal radiative transport*. Technical Report LA-UR-14-24608 and Proceedings of the Nuclear Explosives Code Developers Conference, 2014
- R. B. Lowrie and A. B. Wollaber. *Simple material-motion corrections for thermal radiative transport*. Transport Theory and Statistical Physics, vol. 43, 2014.

Darby J. Luscher (173969, T-3) has a Ph.D. in Mechanical Engineering. Luscher is an expert in multiscale and nonlocal computational mechanics and has been a staff member at LANL for 15 years. Luscher has served as team leader for seven staff members and two-post docs on a computational modeling team. Throughout his career, Luscher has mentored two staff members, seven GRAs, and three UGSs on research comprising constitutive theory, computational mechanics, crystal plasticity, and multi-physics modeling. Luscher is currently PI on an LDRD-ER focused on continuum modeling of coupled dislocation transport with crystal plasticity been involved as a co-investigator on two LDRD-ER and two LDRD-DR projects addressing various areas of computational mechanics of materials. Most recently, Luscher's research has centered on developing and implementing physics-based models for the response of FCC, BCC, orthorhombic, and triclinic single crystals under shock loading conditions and developing theoretical models reflecting the role of anisotropic thermal expansion, intragranular slip, and distributions of crystal orientation on the thermal ratchet growth of TATB-based explosive composites. (0.5 FTE)

Some recent journal publications of relevance to the project are provided.

- Luscher, D., F. Addessio, Cawkwell, M., and K. Ramos. *A dislocation density based continuum model of the anisotropic shock response of single-crystal alpha-RDX*. in review
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- Luscher, D., J. Mayeur, H. Mourad, A. Hunter, and M. Kenamond, M. *Coupling continuum dislocation transport with crystal plasticity for application to shock loading conditions*. Int. J. Plasticity 76, 111–129, 2016
- Mayeur, J., H. Mourad, Luscher, D., A. Hunter, and M. Kenamond, M., *Numerical implementation of a crystal plasticity model with dislocation transport for high strain rate applications*. Mod. Sim. Mat. Sci. & Eng., 24(4), 2016
- Alleman, C., D. Luscher, C. Bronkhorst, and S. Ghosh. *Distribution-enhanced homogenization framework and model for heterogeneous elasto-plastic problems*. J. Mech. Phys. Solids, 85, 176-202, 2015
- Buechler, M. and D. Luscher. *A semi-implicit integration scheme for a combined viscoelastic-damage model of plastic bonded explosives*. Int. J. Num. Meth. in Eng. 99(1), 54–78, 2014
- Luscher, D., C. Bronkhorst, C. Alleman, and F. Addessio. *A model for finite-deformation nonlinear thermomechanical response of single crystal copper under shock conditions*, J. Mech. Phys. Solids, 61, 2013.
- Luscher, D., C. Bronkhorst, and D. McDowell. *Effects of local and nonlocal substructure spin on localization in tantalum top-hat specimen*, Technische Mechanik, vol. 2–5, pp. 393–407, 2012.
- Luscher, D., D. McDowell, and C. Bronkhorst. *A second gradient theoretical framework for hierarchical multiscale modeling of materials*, Int. J. Plasticity, vol. 26, 2010.

Nathaniel R. Morgan (178925, XCP-8) has a Ph.D. in Mechanical Engineering. He has over 11 years of experience at LANL in multi-material, multi-physics Lagrangian and ALE hydrodynamics. He also has 2 additional years of experience at LANL as an experimentalist in multi-phase fluid dynamics. He is the current ALE hydrodynamics project leader for the next generation code (NGC) in the ASC program. He has many journal publications on Lagrangian and ALE hydrodynamic algorithms including being an author on 5 journal papers on finite element hydrodynamic methods on unstructured 3D meshes. He was selected in 2012 by the Laboratory Director to serve on his small peer-review committee to independently review various scientific activities and assessments at LANL in accordance with US law. He continues to work on the peer-review committee at the request of the Director. Besides leading the research effort, his role in the project will involve theory, algorithm derivation, implementation in FLAG, and documentation. (0.60 FTE)

Some recent journal publications of relevance to the project are provided.

- D. Burton, N. Morgan, T. Carney, M. Kenamond: *Reduction of dissipation in Lagrange cell-centered hydrodynamics (CCH) through corner gradient reconstruction (CGR)*. J. Comp. Phys. 2015; 299:229-280.
- M. Charest, T. Canfield, N. Morgan, J. Waltz, J. Wohlbier: *A high-order vertex-based central ENO finite-volume scheme for three-dimensional compressible flows*. Comp. & Fluids 2015; 114:172-192
- N. Morgan, J. Waltz, D. Burton, M. Charest, T. Canfield, J. Wohlbier: *A point-centered arbitrary Lagrangian Eulerian hydrodynamic approach for tetrahedral meshes*. J. Comp. Phys. 2015; 290:239-273.
- N. Morgan, J. Waltz, D. Burton, M. Charest, T. Canfield, J. Wohlbier: *A Godunov-like point-centered essentially Lagrangian hydrodynamic approach*. J. Comp. Phys. 2015; 281:614-652.
- N. Morgan, K. Lipnikov, D. Burton, M. Kenamond: *A Lagrangian staggered grid Godunov-like approach for hydrodynamics*. J. Comp. Phys. 2014; 259:568-597.
- D. Burton, T. Carney, N. Morgan, S. Sambasivan, M. Shashkov: *A cell-centered Lagrangian Godunov-like method for solid dynamics*. Comp. & Fluids 2013; 83:33-47.
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- J. Waltz, T. Canfield, N. Morgan, L. Risinger, J. Wohlbier: *Verification of a three-dimensional unstructured finite element method using analytic and manufactured solutions*. Comp. & Fluids 2013; 81:57-67.
- J. Waltz, N. Morgan, T. Canfield, M. Charest, L. Risinger, J. Wohlbier: *A three-dimensional finite element arbitrary Lagrangian-Eulerian method for shock hydrodynamics on unstructured grids*. Comp. & Fluids 2013; 92:172-187.

Postdoc TBD A post doc with experience in high-order hydrodynamic methods will be hired to work on this project full time. (1 FTE)