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Title: An Invariant-Preserving ALE Method for Solids under Extreme Conditions

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Sambasivan, Shiv Kumar and Christon, Mark

Abstract

We are proposing a fundamentally new approach to ALE methods for solids undergoing large deformation due to extreme loading conditions. Our approach is based on a physically-motivated and mathematically rigorous construction of the underlying Lagrangian method, vector/tensor reconstruction, remapping, and interface reconstruction. It is transformational because it deviates dramatically from traditionally accepted ALE methods and provides the following set of unique attributes: (1) a three-dimensional, finite volume, cell-centered ALE framework with advanced hypo-/hyper-elasto-plastic constitutive theories for solids; (2) a new physically and mathematically consistent reconstruction method for vector/tensor fields; (3) advanced invariant-preserving remapping algorithm for vector/tensor quantities; (4) moment-of-fluid (MoF) interface reconstruction technique for multi-material problems with solids undergoing large deformations. This work brings together many new concepts, that in combination with emergent cell-centered Lagrangian hydrodynamics methods will produce a cutting-edge ALE capability and define a new state-of-the-art. Many ideas in this work are new, completely unexplored, and hence high risk. The proposed research and the resulting algorithms will be of immediate use in Eulerian, Lagrangian and ALE codes under the ASC program at the lab. In addition, the research on invariant preserving reconstruction/remap of tensor quantities is of direct interest to ongoing CASL and climate modeling efforts at LANL. The application space impacted by this work includes Inertial Confinement Fusion (ICF), Z-pinch, munition-target interactions, geological impact dynamics, shock processing of powders and shaped charges. The ALE framework will also provide a suitable test-bed for rapid development and assessment of hypo-/hyper-elasto-plastic constitutive theories. Today, there are no invariant-preserving ALE algorithms for treating solids with large deformations. Therefore, this is a high-impact effort that will significantly advance the state of ALE methods and position LANL as world leaders in advanced ALE methods.

Research Goals

The primary goal for this research is to establish the numerical algorithms for accurately treating solid materials subjected to high-rate loading conditions and severe deformation in an Arbitrary Lagrangian-Eulerian (ALE) framework. The correct representation of the material behavior is intimately tied to conservation principles, kinematics, and ultimately the accurate evolution of stress/strain fields. ***Currently, there are no accepted algorithms for reconstructing, limiting and remapping vector/tensor quantities that are guaranteed to preserve fundamental and critical properties of the stress/strain fields while faithfully representing the material behavior.***

We are proposing a fundamentally new approach to ALE methods for large deformation problems that is based on a physically-motivated and mathematically rigorous construction of the underlying Lagrangian method, vector/tensor reconstruction and limiting, remapping, and interface reconstruction. The framework is physics-inspired because the governing conservation laws and Galilean invariance are intrinsically satisfied. Additionally, it is also mathematically consistent as the properties of vector/tensor quantities and the identities of vector/tensor calculus are preserved at the most conceptual level. Specifically, we are proposing an ALE framework that incorporates the following attributes:

- Physically and mathematically consistent, monotonicity-preserving, high-order reconstruction techniques for vector/tensor fields in the presence of discontinuities
- Physically and mathematically consistent remapping techniques for vector/tensor quantities that preserve conservation laws and invariant properties of all physical variables
- A unified framework for accurately treating advanced hyper-/hypo-elastic-plastic constitutive theories for a broad spectrum of strain rates and materials
- Invariant-preserving properties that reduce the coupling errors between kinematics and material evolution in the presence of severe loading conditions and large deformations
- An efficient interface reconstruction treatment that can accurately represent multi-material interfaces and accommodates important interface mechanics
- A robust framework that can be used for hybrid mesh topologies that include tetrahedral, hexahedral, pyramid, wedge and polyhedral elements.

This work brings together many new ideas, which in combination with emergent cell-centered Lagrangian methods [1, 2, 3, 4, 5, 6, 7] will produce a cutting-edge ALE capability and define a new state-of-the-art. This research will yield a robust capability for handling a broad class of lab-centric problems that include applications such as Inertial Confinement Fusion (ICF), Z-pinch, munitions-target interactions, and geological impact dynamics. This framework will also provide a convenient platform for rapid development, evaluation and deployment of advanced constitutive theories.

Background & Significance

Modeling the response of finite-strength real materials subjected to high-rate loading conditions is of broad interest to the DOE defense program laboratories and industry. Applications, where high-rate loading and material strength play a key role, vary from weapons design to automotive crashworthiness and impact design for cell phones. Large deformations due to high-rate loading conditions are characterized by initial elastic deformation followed by plastic flow of the material. Arbitrary-Lagrangian-Eulerian methods are typically used for solving such large deformation problems because they provide an optimal choice between purely Lagrangian methods, ideal for modeling material response, and Eulerian methods that do not suffer the deleterious effects of large mesh deformation. Despite continuous development and widespread acceptance, there are multiple outstanding issues that limit the robustness and accuracy of these methods.

Limitations of Existing Methods: Over the past 20 years, there have been a number of significant hydrocode efforts based on Eulerian [8, 9, 10, 11, 12, 13, 14], Lagrangian [15, 16, 17, 18, 19, 20], and ALE [21, 22, 23, 24, 25] methods. In spite of their number, existing hydrocodes are known to exhibit multiple numerical, physical and mathematical inconsistencies. In the Lagrangian component of ALE methods, the pathologies stem from the use of inherently low-order staggered-grid discretizations, ad-hoc artificial viscosities, unconstrained mesh instabilities (hourglass modes), and poor pressure-gradient approximations on distorted grids [26]. Furthermore, the current remapping algorithms, designed to move vector and tensor data from the Lagrangian to the final ALE reference frame, are fundamentally flawed. It is typical for remapping algorithms to fail to preserve invariants of vector/tensor quantities leading to mathematically inconsistent results, such as, non-symmetric stress tensors, and inaccurate representation of material behavior. In addition, high-order monotonicity preserving reconstruction techniques for vector/tensor quantities remains an open question for both the Lagrangian and ALE communities.

In the context of multi-material hydrocodes, Eulerian methods [9, 10] suffer from a lack of local conservation, particularly when level-sets are used. A more typical approach is to use volume-of-fluid or volume-tracking techniques for the ALE remapping step. Here, the errors, associated with component-by-component reconstruction, dimensionally split remapping, and a failure to preserve vector/tensor invariants, constitute significant limitations. Repeated application of the remapping and reconstruction methods are known to introduce cumulative errors that lead to abrupt termination of the solution procedure [27]. These errors emanate from remapping and reconstruction algorithms that do not preserve Galilean invariance and vector/tensor invariants.

Scientific Impact: There is a clear gap in the knowledge base for ALE methods that spans the interconnected areas of high-order reconstruction and remapping of vector/tensor quantities, treatment of hypo-/hyper-elasto-plastic material behavior, and multi-material interface reconstruction. Building on emergent cell-centered Lagrangian methods, that avoid many of the pathologies associated with current techniques, the proposed research is aimed at developing physically and mathematically consistent algorithms for reconstructing and remapping vector/tensor quantities. ***As there are no such invariant-preserving algorithms today, this high-impact effort will significantly advance the state of ALE methods.***

R&D Approach

Our proposed approach is transformational as it deviates dramatically from the traditionally accepted ALE methods by building on the following algorithmic components:

1. A three-dimensional, finite volume, cell-centered ALE framework with advanced constitutive theories for solids
2. A new physically and mathematically consistent reconstruction method for tensor fields
3. A new invariant-preserving remapping algorithm for vector/tensor quantities
4. Advanced moment-of-fluid (MoF) interface reconstruction for multi-material problems with solids undergoing large deformations

1. A Cell-centered ALE framework with advanced constitutive theories:

Advanced hypo- and hyper-elasto-plastic constitutive theories: Two main approaches are used to describe material behavior in large deformation problems: hypo-elasto-plastic and hyper-elasto-plastic models. In the hypo-elasto-plastic model, an evolution equation is solved to determine the elastic contribution to the strain, and the associated plastic flow is modeled via an appropriate yield model. An objective derivative is required to ensure frame invariance, which yields a non-conservative formulation for the stress evolution equation. However, in light of their comprehensive and simplistic nature, hypo-elastic models are preferred for engineering applications. In the hyper-elastic model, the stress field is computed from the direct evaluation of the potential energy functional constructed using the invariants of the deformation gradient, thereby circumventing the need for an objective derivative [17, 22, 28]. The plastic response, however, is still described in rate form using a Lie derivative [22]. With respect to conservative formulations, hyper-elasto-plastic models with intrinsic frame invariance offer important advantages. Nevertheless, modeling the plastic response for a broad range of materials remains an open question for hyper-elasto-plastic models. ***We are proposing an ALE framework that is material model invariant and permits the use of both existing and new hypo-/hyper-elasto-plastic constitutive theories.***

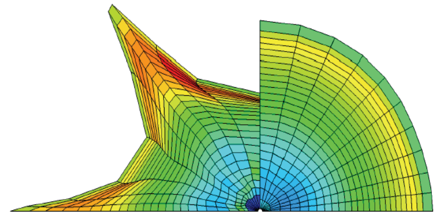

Figure 1: Pressurized ball test. Staggered-grid failure (left) vs. cell-centered success (right).

<u>*What is currently done:*</u> Today, state-of-the-art lab and commercial, Lagrangian and ALE hydrocodes are based on staggered methods. In staggered methods, the momentum equation is solved at the vertices of the mesh, and the thermodynamic variables are evolved at element centroids. The staggering decouples the kinematic and thermodynamic quantities, leading to multiple numerical pathologies. An instance in which staggered schemes fail miserably is shown in Figure 1. In spite of such prominent failure modes, staggered schemes are prevalent in large-scale finite-element and finite-volume codes throughout the world (e.g., LS-DYNA [23], Abaqus/Explicit [24], ALEGRA [29]).

<u>*What is new:*</u> In contrast to staggered schemes, we propose to use a cell-centered formulation for the underlying Lagrangian method. Cell-centered methods [1, 2, 3, 4, 30], wherein all quantities are stored and evolved at element centroids, are devoid of mesh imprinting and spatial instabilities. Also, they do not require ad-hoc artificial stabilizing parameters, and are free of spurious vorticity generation, and inherently preserve symmetry. ***Using a cell-centered formulation for solving large deformation problems is a radical departure from traditional methods.*** Current studies with cell-centered schemes have focused on simple two-dimensional gas dynamics (with the exception of our preliminary studies discussed below). Extension to three-dimensional applications will be a contribution that is both significant and unique. However, the proposed work aims at pushing the envelope further. In this work, we will formulate our cell-centered framework to seamlessly integrate advanced hypo-/hyper-elasto-plastic constitutive theories.

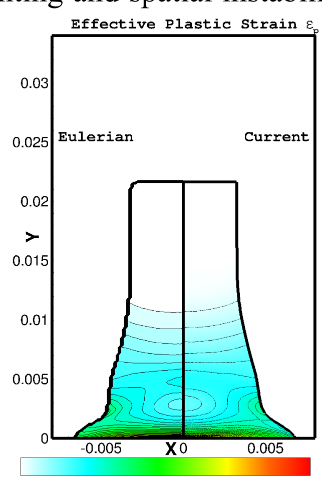

Figure 2: Impact of a copper rod at 227 m/s - Eulerian (left) and cell-centered Lagrangian (right) calculations.

<u>*Preliminary studies, key challenges and risk factors:*</u> Our preliminary studies for complex two-dimensional large deformation problems have shown impressive results for hypo-elasto-plastic models. We note that past efforts for modeling large deformation problems

using cell-centered schemes have had limited success. ***Our two-dimensional formulation is the first of its kind for solving large deformation problems with material strength, and provides the path forward to advance cell-centered Lagrangian schemes***. Extensive comparisons with existing Eulerian and Lagrangian hydrocodes indicate that our two-dimensional formulation is both robust and accurate, and performs well on arbitrary polygonal mesh topologies (Figure 2). This is particularly crucial as we propose to build our framework for arbitrary mesh topology. A key risk factor, in extending this methodology to three-dimensions, involves the deduction of an efficient and generic quadrature rule that holds true for polyhedral grids. To circumvent this issue, a quadrature rule based on splitting polyhedron into multiple tetrahedral elements can be used. This can be automated, but comes at the expense of the overall efficiency of the method – a trade off we will evaluate.

2. A Physically and mathematically consistent high-order reconstruction technique:

Reconstruction: High-order reconstruction of vector and tensor quantities is essential for achieving a high-fidelity hydrocode. Achieving high-order accuracy requires reconstruction of solution variables, which can violate monotonicity criteria, i.e., the reconstruction procedure may introduce new minima/maxima into the field variable. The two prevalent techniques for reconstruction, namely polynomial reconstruction [31] and Taylor series expansion [32], employ slope limiters (gradient limiters) to ensure monotonicity of the reconstructed field.

Limitations of Slope Limiters: Slope limiters have always been designed for scalar variables. Traditionally, limiters for vectors and tensors have been formulated by applying the scalar limiter to individual components of the vector/tensor variables. This approach treats individual components of the tensor field as unrelated scalars, and therefore do not preserve fundamental tensor properties. Furthermore, such component-wise limiters are frame dependent and do not preserve features such as rotational or planar symmetry. Existing limiters have been devised to enforce rudimentary monotonicity constraints without respecting the physics. ***Currently, there are no limiters that are both frame invariant and preserve fundamental tensor properties for second or higher-rank tensor fields.*** This motivated us to examine a consistent formulation for limiter schemes in the context of hypo-elasto-plastic models for two-dimensional applications.

Physical and Mathematical Constraints: Our preliminary studies [33] indicate that a limiter constructed from the second and third stress invariants may hold the key to properly limit tensor quantities. ***The limiter design is driven by mathematical and physical requirements that include: (a) the reconstructed stress tensor should remain symmetric and retain its invariants, (b) the reconstructed stress tensor should be consistent with conserved elastic and plastic energy, (c) the reconstructed stress tensor should lie on the proper yield surface, and (d) no new extrema should be introduced in the reconstructed tensor.*** Similar constraints apply for vector quantities.

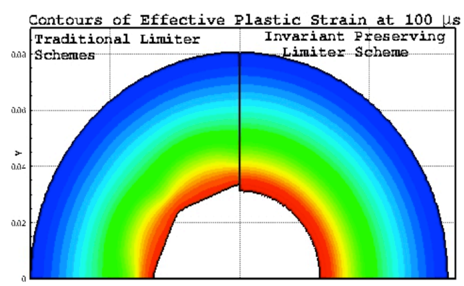

Figure 3: Contours of effective plastic strain for the collapse of a spherical Beryllium shell – traditional limiter (left) and invariant-preserving limiter (right)

Preliminary studies, key challenges and risk factors: Limiters that respect the second invariant of the stress tensor, satisfy the requirements stated above [33]. A representative result of this work is shown in Figure 3. ***The limiter formulation from our preliminary studies is being used in the cell-centered Lagrangian hydro implementation in FLAG [4, 25], a well-established hydrocode developed and maintained in X-CP.*** In contrast to our previous work, the proposed approach aims at constraining the first, second and third invariants of the total stress tensor. This is particularly crucial for hyper-elasto-plastic constitutive theories, which were not considered in our preliminary studies. Since our preliminary investigations were restricted to two-dimensions, the proposed work examines the possibility of extending such an approach to three-dimensional and hypo-/hyper-elasto-plastic applications. The challenge here is to ensure that the reconstructed stress tensor remains symmetric. Moreover, extracting a linearity and bound preserving slope limiter from invariants of the tensor is not a trivial task. ***This area is of high interest, need, and priority for multiple projects at LANL including ASC, climate modeling, CASL. However, this research is considered too high risk for programmatic funding.***

3. A Physically and mathematically consistent remapping technique:

Remapping: This is the process of transferring the solution field from the source (old un-optimized) to the target (new optimized) grid. Remapping vector and tensor quantities is both an essential component and an outstanding issue for ALE methods [27]. Conventional techniques for remapping tensor quantities include advection or interpolation of individual components of the tensor field [22]. These procedures are ad-hoc, fundamentally flawed and suffer from similar issues outlined in the preceding sections. In addition, errors accrued over time due to repeated remapping lead to abrupt termination of the solution. Accurate and invariant-preserving remapping is vitally important for accurate and reliable simulation of large deformation problems.

What we don't want to do - dispelling the inadequacies: The advection and interpolation approaches, that have been popularized, are mathematically and physically inconsistent. This is clearly demonstrated when the stress evolution equation for hypo-elasto-plastic theory is examined. The stress evolution equation for the Eulerian, Lagrangian and ALE reference frames are

$$\text{Eulerian:}\quad \underbrace{\frac{\partial \mathrm{S}_{ij}}{\partial t} + \mathrm{u}_k \frac{\partial \mathrm{S}_{ij}}{\partial \mathrm{x}_k}}_{\text{Advection}} + \underbrace{\mathrm{S}_{ij}\Omega_{jk} - \mathrm{S}_{kj}\Omega_{ji}}_{\text{Objective}} = \mathrm{G}\underbrace{\left(\frac{\partial \mathrm{u}_i}{\partial \mathrm{x}_j} + \frac{\partial \mathrm{u}_j}{\partial \mathrm{x}_i} - \frac{2}{3}\frac{\partial \mathrm{u}_i}{\partial \mathrm{x}_k}\delta_{ki}\right)}_{\text{Strain-rate}}$$

$$\text{Lagrangian:}\quad \underbrace{\frac{DS_{ij}}{Dt}}_{Material-Derivative} + \underbrace{S_{ij}\Omega_{jk} - S_{kj}\Omega_{ji}}_{Objective} = G\underbrace{\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3}\frac{\partial u_i}{\partial x_k}\delta_{ki}\right)}_{Strain-rate}$$

$$\text{Remap/Advection:}\quad \frac{\partial S_{ij}}{\partial t} + u_k \frac{\partial S_{ij}}{\partial x_k} = 0$$

It is important to recognize the presence of the objective term in both reference frames. This term ensures rotational invariance of the stress tensor. ***In contrast, the remap/advection equation typically used in ALE methods omits the objective term and therefore the remapped stress tensor is guaranteed not to remain rotationally invariant.*** Repeated application of the remap algorithm leads to non-symmetric stress tensors, which violate angular momentum conservation, and ultimately results in complete failure of the solution. Ultimately, the issue with remapping stress stems from the fact that stress is not a conserved quantity.

Proposed approach and risk factors: We propose to construct a unified remapping algorithm for hypo-/hyper-elasto-plastic constitutive theories that satisfies the following design criteria: (a) the stress tensor remains symmetric before and after remap, (b) constitutive theories are satisfied before and after remap, and (c) the strain energy or the total deformation remains conserved. We propose two fundamentally new approaches. In our first approach, the deformation tensor is remapped ensuring that the strain energy and the total deformation realized before and after remap are conserved. Since the total deformation is a conserved quantity, simple advection or intersection-based techniques can be applied. An intersection-based technique, in which the source and the target grids are overlaid to determine the regions of intersection, can be employed to interpolate the deformation and stress tensors to the new target grid. The interpolated stress tensor is then corrected for rotational and stretch effects based on the new remapped deformation tensor. For the hyper-elasto-plastic model, the stress state can be determined from the potential energy functional based on the remapped deformation tensor. ***The proposed approach is completely unexplored, and hence relatively high risk.*** In our second approach, we plan to remap invariants and eigenvectors. Using the remapped invariants and eigenvectors, the stress state can be reconstructed on the target grid.

4. Interface reconstruction technique for solids undergoing large deformations:

Interface Reconstruction: Multi-material problems involve sharp interfaces and demand specialized treatment in ALE methods. Volume-tracking methods are frequently used in multi-material ALE codes. They are conservative and rely on a reconstruction procedure to represent sharp interfaces. Volume-tracking methods, also known as, volume-of-fluid methods have been used for approximately 30 years and may be found in laboratory and commercial hydrocodes. In many of these codes (e.g., LS-DYNA [23], Abaqus/Explicit [24], ALEGRA [29]), the state-of-the-art is represented by Young's method [34]. Young's method is first-order accurate and is often used with a spatially split (operator-split) remapping procedure. This can result in grid-scale artifacts, "flotsam and jetsom", being created at material interfaces (Figure 4). In addition to the low-order accuracy and grid-scale break-up, the reconstructed interface is material-order dependent and can result in completely incorrect representations of the interfaces.

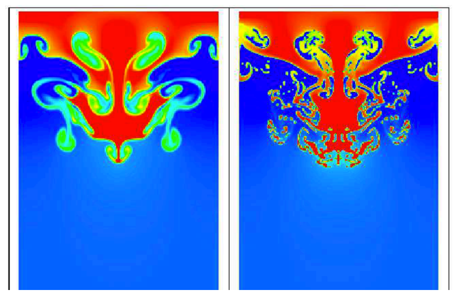

Figure 4: Rayleigh-Taylor calculation. Diffuse interface treatment (left) vs. Young's interface reconstruction with flotsam and jetsom (right).

What we want to do: The moment-of-fluid (MoF) method (developed at LANL [35, 36, 37, 38]) is dimension and topology independent, delivers second-order accuracy, unique and order independent multi-material reconstruction. MoF is emerging as a new standard for interface reconstruction because of its ability to treat complex interfaces on arbitrary grids as shown in Figure 5. ***The MoF method for multi-material ALE computations with material strength is new, and constitutes a significant technological step forward. We plan to use MoF with intersection-based remapping.***

Proposed approach and risk factors: Our primary focus is on intersection-based remapping with MoF reconstruction. Although MoF has been extended to 3-D, it has not been extended to 3-D on unstructured hybrid meshes comprised of arbitrary polyhedral elements. Our approach will rely on a tetrahedral decomposition of the elements and subsequent intersection for remapping. We will adopt existing algorithms for material-order independent reconstruction. If the tetrahedron decomposition proves too computationally expensive, we will revert to a more traditional flux-based remap but retain MoF reconstruction.

Exascale Implementation and Scalability: The Hydra multi-physics toolkit [39] will be used for code development. The Hydra toolkit provides a rich suite of components that permits rapid application development, supports multiple discretization techniques, provides I/O interfaces to permit reading/writing multiple file formats for meshes, plot data, time-history, surface-based and restart output. The toolkit also provides run-time parallel domain decomposition with datamigration for both static and dynamic load balancing. The toolkit has been demonstrated to scale up to 8000 cores. The Hydra toolkit already supports single and multi-material Lagrangian hydro algorithms, and a second-order cell-centered Lagrangian hydro method is already implemented and being tested. Worksets suitable for mapping to GPU centric architectures are currently being explored for the multiple Lagrangian hydro algorithms in Hydra. Hydra will provide a convenient vehicle for mapping our new ALE algorithms to exascale architectures.

Expected results

This work will set a new standard for 3-D ALE methods for treating solid materials subjected to high strain-rate loading conditions. In addition, our current work suggests that we will achieve significant algorithmic advances in the treatment of hypo-/hyper-elastic materials, reconstruction and remapping of tensors, and enhanced interface treatment in multi-material problems. This will set a new standard for ALE methods and position LANL as a world-leader in advanced ALE methods. The theoretical and algorithmic results will be presented to the broader scientific community through workshops and open publications.

Schedule and Milestones

Year 1:	• Establish 3D parallel framework for hypo-/hyper-elasto-plastic constitutive theories applicable on arbitrary mesh topology • Formulate high-order monotonicity preserving reconstruction for vectors and tensor fields in in the context of hypo-/hyper-elasto-plastic constitutive theories • Verify on canonical benchmark problems using hypo-/hyper-elasto-plastic materials
Year 2:	• Develop a remap framework that preserves monotonicity, fundamental conservation laws and invariant properties of the vector and tensor fields for single material • Develop robust multi-material interface reconstruction technique for capturing large deformations and interpenetrations of the deforming solid materials • Implement and verify for single material three-dimensional applications
Year 3:	• Extend single material remap framework to multi-material • Verification and validation for representative problems for Inertial Confinement Fusion (ICF) and Z-pinch, munitions-target interactions, and geological impact

Mission Relevance & Program Development Plan

The accurate treatment of materials with strength in the context of emerging cell-centered hydro methods is an important research issue that will impact multiple programs and codes at LANL. This project will provide the necessary research on algorithms for treating hypo-/hyper-elastic-plastic materials, reconstruction and remapping of tensor quantities, and accurate interface reconstruction required to advance new and existing hydro capabilities. Specifically, the research and resulting algorithms will be of immediate use in Eulerian, Lagrangian and ALE codes at the lab under the ASC program. Multiple aspects of this research are of direct interest to CASL and climate modeling efforts at LANL. The ALE framework will also provide a suitable test-bed for rapid development and assessment of hypo-/hyper-elasto-plastic models. The application space impacted by this work includes Inertial Confinement Fusion (ICF), Z-pinch, munition-target interactions, geological impact dynamics, shock processing of powders and shaped charges. The following managers are aware of the proposed work: Jerry Brock (XCP-1), Ed Dendy (CCS-2), Mark Schraad (T-3). We will work closely with these individuals to guide the research effort and develop future funding sources for this work.

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