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A cell-centered Lagrangian Godunov-like method for solid dynamics

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ABSTRACT

This work presents a spatially and temporally second-order cell-centered Lagrangian formulation (CCH) suitable for elasto-plastic materials on unstructured polyhedral cells in multiple dimensions. In the development of our scheme, we follow a mimetic approach, based upon the finite volume method, as a guide to the derivation of the difference equations. In doing so, we consider not only the governing equations, but a number of ancillary relationships. The finite volume equations for solids are cast in Lagrangian form with particular attention to the discrete form of the Second Law of Thermodynamics. We expand upon previous work and propose a new entropy production expression. A new tensor dissipation model is presented that guarantees the viscous stress tensor is symmetric. The new tensor dissipation model shows increased mesh robustness. In the second-order formulation, a limiter for the stress gradient is presented, as well as a vorticity limiter for the velocity gradient. Numerical results are demonstrated for common test problems involving both gas and solid constitutive models.

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1. Introduction

Cell-centered hydrodynamics schemes in which all conservation equations are solved on a common control volume (called a cell) are commonly applied to Eulerian methods, but not Lagrange. A cell-centered Lagrange method was first suggested by Godunov [24,25] and later by Ruppel and Harlow leading to the CAVEAT code [1,20]. In CAVEAT, the surface fluxes were obtained by solving an approximate Riemann problem at cell faces. Nodal velocity was then inferred from the adjacent face velocities. This resulted in a geometric volume change that was inconsistent with that obtained from the finite volume (FV) evolution equation, thereby violating the so-called Geometric Conservation Law (GCL) discussed in Section 4.1.

After a hiatus of several years, interest in cell-centered methods has increased, especially in the area of gas dynamics [2,14,17,36,15,39]. These schemes have been enabled by the seminal work of Després and Mazeran [17] in a scheme named GLACE. In finite volume formulations, conservation is commonly enforced by assuming continuity of fluxes at the cell surface. In GLACE, however, continuity of velocity was assumed at nodes, but continuity of stress and total energy was replaced by a weaker statement of momentum and energy conservation. This crucial idea led to the

* Corresponding author. E-mail address: burton@lanl.gov (D.E. Burton). construction of a node-centered approximate Riemann solver and consequently a volume evolution equation that satisfied the GCL.

Subsequent work by Maire et al. [36] and Maire [39] revealed a strong sensitivity in GLACE to cell aspect ratio, leading to numerical instabilities. To overcome this flaw, Maire and his co-authors proposed an alternative scheme named EUCCLHYD that addressed the aforementioned difficulty and resulted in a second form for the nodal solver.

In a series of ground-breaking papers, both the GLACE [14,18,33] and EUCCLHYD [38,37,39,40,22,23,41] schemes for gases have been extended in areas such as second order, unstructured grids, axial symmetry, multi-dimensionality, and arbitrary Lagrange–Euler (ALE).

We built upon the methodology of previous investigators to extend the formalism to solids, yielding a second-order scheme for unstructured meshes in 1D, 2D, and 3D planar and curvilinear geometry [9,10]. In the following we provide additional information on this cell-centered hydrodynamics scheme, named CCH. We note that Kluth and Després [33] proposed a first-order extension of the GLACE scheme to solid dynamics using an hyper-elastic model and that other investigators [42,48] have since extended EUCCLHYD to include solids. In our formulation, we cast the Lagrangian evolution equations for solids in FV form with particular attention to the discrete form of the Second Law of Thermodynamics for solids. This led to a new tensor dissipation relation that differs from that previously assumed by other investigators,





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applies to both solids and gases, and guarantees a symmetric viscous stress tensor. This dissipation relation led to a third form for the nodal solution.

In the course of this investigation, we observed additional instabilities in the EUCCLHYD methodology that we attribute to a non-symmetric viscous stress, thereby violating a condition for rotational equilibrium. We found the non-symmetric stress tensor to be a consequence of the dissipation relation assumed in both GLACE and EUCCLHYD. Our new nodal solver was observed to remove the instabilities, substantially improving mesh robustness.

The formulation applies to arbitrarily connected meshes in all dimensions. As part of the second-order formulation we also propose a simple extension to the velocity gradient limiter that reduces spurious vorticity [21], as well as a second-order limiter on the stress tensor.

1.1. Implementation

As the following is intended to address the theoretical underpinnings of the method and not its implementation, we briefly summarize the latter here. The Lagrange cycle is divided into a predictor step that uses a forward Euler scheme to advance the solution from time *n* to n + 1/2 and a corrector step that uses a central difference scheme to advance from n to n + 1. The steps are identical aside from the time increments. Within each step conserved quantities within cells are redistributed linearly using monotonicity preserving linear gradients. This isolates stress and velocity discontinuities, and consequently entropy production, to the interfaces between cells. Next, a Riemann-like problem is solved to obtain fluxes at the cell mesh points. These fluxes are then integrated using the finite volume method to yield the rates of change of conserved quantities that are then integrated in time. The rate of change of internal energy is inferred from the total and kinetic energy rates. Finally, an equilibrium constitutive model is invoked to determine stress in the cell.

1.2. Organization

The paper is constructed as follows. In Section 2, we discuss the mimetic foundations of cell-centered discritization, mesh topology and notational conventions, and present a brief overview of the FV method as applied here. We present in Section 3 the FV equations for conserved quantities in Lagrangian form, a general hypoelastic closure model, and a decomposition of the energy equation that leads to a numerical definition of the Second Law of Thermodynamics. Section 4 presents a number of ancillary relations that need to also be satisfied. Section 5 extends the formulation to second order, presents details of the velocity and stress redistribution, and offers a new shock-based vorticity limiter. Section 6 reviews the foundations of dissipation models and presents the new tensor dissipation model. Section 7 couples the dissipation models to the conservation of momentum, yielding a Riemann-like solution for the nodal velocities as well as the surface stresses. Section 8 presents numerical results for a number of common test problems involving both gas and solid constitutive models as described in Appendix A. Conclusions appear in Section 9.

2. Mimetic foundations

There are many ways to difference the governing equations of hydrodynamics. In the development of our scheme, a mimetic approach, based upon the finite volume method, was followed as a guide to the derivation of the difference equations. The term *mimetic* was apparently coined by Hyman [30] and conveyed the idea that a discrete scheme should mirror the mathematical properties

of the physical system. Initially, mimetic methods focused on discrete approximations to differential operators. In our methodology, we consider not only the governing equations (Section 3), but also discrete forms of ancillary equations (Section 4) such as geometric conservation, angular momentum conservation, equilibrium and rotational equilibrium, as well as differential curl and divergence operators. Although these ancillary equations may be satisfied analytically, they are not necessarily satisfied in a numerical scheme. Once decisions about mesh topology and conservation are made, the mimetic approach greatly constrains the formulation of the difference equations and reduces the introduction of inadvertent inconsistencies. As shown in Section 4, the key to satisfying the ancillary equations is twofold: locating the surface fluxes at the mesh points and constructing a symmetric viscous stress tensor.

2.1. Multi-dimensional mesh topology and notation

A discretization stencil describes how information defined on grids is spatially connected. It is important that the mathematical formulation be consistent with the stencil. This gives rise to the relatively unconventional notation described below. For regular grids, stencils can be quite simple. For polygonal grids, the potential complexity is overcome by finding a simpler but universal stencil. Our stencil is a minor extension of the multi-dimensional unstructured stencil of Ref. [7] and is formed by decomposing polygonal cells into triangular (2D) or tetrahedral (3D) substructures. We assume a tessellation of space that gives rise to a number of geometrical entities. The various control positions *p*, *z*, *f*, and *e* denote respectively points, zones or cells, faces, and edges. In 2D, depicted in Fig. 1, the face and edge control positions are degenerate.

The *iota* is the smallest letter in the Greek alphabet, and will be used to denote the smallest simplex definable with this set of control points. Depending upon the dimensionality, the iota is bounded by one of each of the types of control points. The stencil also includes connectivity to adjacent iotas. The cell *corner* c consists of those iotas sharing a common z and p.

In the discrete equations, it will be necessary to refer to physical quantities in relation to the iota connectivity structure. The iota will be indicated by a superscript. The logical location of the variable relative to a particular iota is identified with a subscript. For example, \mathbf{u}_{z}^{i} and \mathbf{u}_{p}^{i} denotes velocity at cell center and point respectively relative to iota *i*, while σ_{z}^{i} and σ_{p}^{i} denote the stress at the same respective locations. A geometrical quantity associated with an iota is the outward directed surface normal $\mathbf{N}^{i} = N^{i} \hat{\mathbf{n}}^{i}$ with area N^{i} and direction $\hat{\mathbf{n}}^{i}$.

2.1.1. Sums

It will be necessary to perform sums over iotas or other quantities. Conventional mathematical expressions for this are more



Fig. 1. 2D and 3D discretization stencil showing relation of the iota to a computational cell and control points. The f and e positions are degenerate in 2D, and also the p position in 1D. The shell between o and p is used to model discontinuities.

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