Review of "Numerical methods for Lagrangian and ALE hydrodynamic simulations" by Pavel Váchal

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November 10, 2021

1 Overview

The ten articles authored or co-authored by Pavel Váchal included in his habilitation are an impressive record of scientific contribution to Arbitrary-Lagrangian-Eulerian Hydrodynamic (ALE) methods. The selected papers have impact across the breadth of the numerical algorithms required for ALE simulation codes.

In ALE (Lagrange+remap) methods, there are three phases of the calculation:

1. A Lagrangian phase where forces are calculated and the mesh moved with the local velocity
2. A Mesh relaxation or rezoning phase where a new mesh is calculated based on the Lagrangian mesh
3. A Remap or conservative interpolation of field values from the Lagrangian mesh to the relaxed mesh.

P. Váchal has made important contributions to all of these phases.

In papers A.1, A.2, A.3, A.4, and A.5 improvements to staggered grid Lagrangian schemes are reported. This includes key insights on the connection of artificial viscosity, a key technique for shock-capturing in the Lagrangian phase, to Riemann solvers used in cell-centered schemes. It also includes other developments in artificial viscosity and insights in symmetry preservation. In A.6, improvements to interpolation used for tabular equation-of-states are illustrated. This is an important detail for Lagrangian calculations of practical interest.

In paper A.7, a novel extension of condition number mesh relaxation has been proposed and demonstrated. This paper has led to extensive international effort further extending the ideas presented in this work.

In A.8 and A.9, improvements to the widely used flux-corrected transport algorithms employed in many ALE remap steps are presented. The simultaneous preservation of solution monotonicity, accuracy, and symmetry in the remap process continues to be a subject of great practical interest for ALE code development, and the papers show significant progress in that area.

In A.10 demonstration of the utility of ALE schemes for laser and plasma simulation to provide insight into physical experiments is shown.

This body of work has had a clear impact on the community and is a credit to Pavel Váchal. It is also noteworthy that Pavel Váchal has collaborated broadly across countries and institutions with many of the leading researchers in ALE methods.

Specific comments are detailed below.

2 A.1 "Staggered Lagrangian Discretization Based on Cell-Centered Riemann Solver and Associated Hydrodynamics Scheme", P.-H. Maire, R. Loubère, and P. Váchal

This work derives a staggered-grid compatible Lagrangian hydrodynamics scheme in 1d and 2d using a cell centered Riemann solver and artificial viscosity. The connection is made with familiar compatible schemes in the use of subcell pressure forces for hourglass control. The paper made significant contributions to the community:

- Further the understanding of connections between cell-centered Lagrangian schemes and classical staggered-grid schemes,
- The use of a cell-centered velocity, determined using Galilean invariance, thermodynamic, and symmetry properties.
- The formulation of artificial viscosity in terms of the jump between nodal and cell-centered velocities
- Extension of Barth-Jespersen limiter to vector fields in a manner which preserves rotational symmetry.

This is an important paper in the development of modern, total energy conserving Lagrangian hydrodynamic schemes.

3 A.2 “3D staggered Lagrangian hydrodynamics scheme with cell-centered Riemann solver-based artifical viscosity”, R. Loubère, P.-H. Maire, and P. Váchal

This extends the previous work in A.1 to 3D. While the extension to 3D is generally straightforward, the implementation details can be challenging. In particular, the extension of the rotationally invariant Barth-Jespersen limiter to 3D is noteworthy. It is noted the implementation and extension of the limiter were specific contributions of P. Váchal.

4 A.3 “A symmetry preserving dissipative artificial viscosity in an r-z staggered Lagrangian discretization” P. Váchal and B. Wendroff

This work presents a systematic derivation of the treatment of the acceleration of nodes on the axis of symmetry. Historically these nodes are considered to have zero mass, so the acceleration is treated in another (often ad-hoc) way. Through symmetry conditions, a straightforward formula for the acceleration of such nodes is derived and is a significant improvement to current practice.

5 A.4 “Volume change and energy exchange: How they affect symmetry in the Noh problem”

The Noh problem is a well-known Lagrangian hydrodynamics test problem for which many common schemes show exceedingly poor results including wall heating, loss of symmetry, and mesh tangling. This short note illuminates how inconsistent application of edge based artificial viscosity where some edges may have viscosity applied even with the bulk cell is not under compression leads to poor performance. In addition, a proposed energy exchange between adjacent cells which can mitigate wall-heating while improving symmetry.

6 A.5 “On preservation of symmetry in r-z staggered Lagrangian schemes” P. Váchal and B. Wendroff

This paper presents a novel geometric correction that can be applied to a total energy conserving axisymmetric scheme to preserve radial symmetry while only introducing a small error to the satisfaction of the geometric conservation law.

The method is of significant practical application. However, it also furthers the understanding of the construction of symmetry preserving schemes.

7 A. 6 "HerEOS: A framework for consistent treatment of the equation of state in ALE hydrodynamics" M. Zeman, M. Holec, and P. Váchal

This paper describes the consistent interpolation and evaluation of tabular and analytic equations of state based on Hermite interpolation of the Helmholtz free energy. The use of Hermite interpolation for tabular EOS data is well-established and has been extensively developed by the Livermore Equation-of-State (LEOS) effort at Lawrence Livermore National Laboratory. (see *Fritsch, F.N. LIP: The Livermore Interpolation Package, Technical Report LLNL-TR-406719-REV-1, Lawrence Livermore National Laboratory, 2009* and subsequent reports)

That said, this paper makes an important contribution to the field. The automatic identification and correction of problematic section of tabular EOS has been of been of long-standing interest (P. Stern, Lawrence Livermore National Laboratory, Private Communication.) However, little work has been published on the issues involved and attempts to address them. This paper provides clear examples of the known issues and viable approaches for solution. It is the hope this will stimulate further work in the area.

8 A. 7. "Discretization for weighted condition number smoothing on general unstructured grids", P. Váchal and P.-H. Maire

This paper demonstrates a novel extension of the condition number smoothing method of P. Knupp to use a spatially varying weight function to concentrate zoning in regions of interest. The paper provides a clear description of the method and demonstration of its utility. The work here used an analytic expression of the weight function as the gradient and Hessian of that weight function are generally required for implementation. Possible approaches for extension to discretely defined weights were mentioned but not explored in this work.

The condition number mesh relaxation method has become very popular in ALE codes at LANL and LLNL due to its robustness and local character. However, the lack of the ability to adapt the mesh to local features as is available in well-known equipotential mesh smoothing techniques ("Winslow smoothing") has limited its use with users. Attempts have been made to mix equipotential and condition number smoothing to obtain the robustness of CN smoothing with the user-controlled weighting of equipotential smoothing. This work provides a means to directly extend CN smoothing to accommodate weights. Subsequent work has focused on the extension to discrete weights and material interfaces *P.T. Greene, S. P. Schofield, R. Nourgaliev Dynamic mesh adaptation for front evolution using discontinuous Galerkin based weighted condition number relaxation, J. of Comp. Physics, 335:664-687. 2017* . The novel ideas in A.7 have led to significant progress in solution sensitive mesh relaxation in ALE codes.

9 A. 8. "Synchronized flux corrected remapping for ALE methods", R. Liska, M. Shashkov, P. Váchal, and B. Wendroff

This paper describes an extension of flux corrected transport to consistent monotonicity enforcement for mass, momentum, and energy. In ALE remap methods, there are broadly two categories of monotonicity enforcement (1) slope limiting (van Leer, Barth-Jespersen, etc) and (2) flux corrected transport. In some codes, both are applied as slope limiting by itself absent corner fluxes may not be sufficient guarantee monotonicity.

FCT splits a high-order flux into a first order monotonic flux plus an anti-diffusive flux which should be higher order accurate. It then scales back the anti-diffusive flux to maintain local bounds under worst-case scenarios. Traditionally, it is applied field by field, which can introduce pathologies where inconsistencies between the limited mass, momentum vector components, and internal energy lead to spurious values and rotations of vector fields. This paper develops a synchronized method which computes FCT like limiters simultaneously for all fields avoiding those issues. The constrained optimization solve is only applied at faces where constraints are violated, so this method may be practical for production use.

10 A.9 "Symmetry - and essentially bound preserving - flux corrected remapping of momentum in staggered ALE hydrodynamics" J. Velochovsky, M. Kucharik, R. Liska, M. Shashkov, and P. Váchal

This paper describes a symmetry preserving FCT method for symmetry preservation in ALE calculations on polar grids. In many ways, this paper complements the extension of the Barth-Jespersen limited for vector fields developed in A.1. It provides proofs of the symmetry preservation for the linear reconstruction used in the remap as well as for the flux corrected remap. This paper is important for many of reasons discussed above in A.8 due to the prevalence of FCT like methods used in ALE codes.

There is an in-depth discussion of DeBar consistency (the consistency of the remap of the cell-centered mass and nodal momentum control volumes in a staggered grid hydrocode).

11 A.10 "Modeling of annular-laser-beam-driven plasma jets" V. Kmetík, J. Limpouch, R. Liska, and P. Váchal

This paper provides a useful application of the ALE techniques developed by P. Váchal and co-workers to problems of interest in lasers and plasmas.