Preprint
UCRL-JC-140555

A Staggered Grid Lagrangian Method With Local Structured Adaptive Mesh Refinement For Modeling Shock Hydrodynamics

R. W. Anderson, R. B. Pember, N. S. Elliot

This article was submitted to
15th American Institute of Aeronautics and Astronautics
Computational Fluid Dynamics Conference
Anaheim, CA
June 11-14, 20001

U.S. Department of Energy
Lawrence Livermore National Laboratory

September 26, 2000

A Staggered Grid Lagrangian Method with Local Structured Adaptive Mesh Refinement for Modeling Shock Hydrodynamics

R. W. Anderson*, R. B. Pember†, N.S. Elliot‡

Center for Applied Scientific Computing
Lawrence Livermore National Laboratory
P.O.Box 808
Livermore, CA, 94551

Abstract

A new method for the solution of the unsteady Euler equations has been developed. The method combines staggered grid Lagrangian techniques with structured local adaptive mesh refinement (AMR). This method is a precursor to a more general adaptive arbitrary Lagrangian Eulerian (ALE-AMR) algorithm under development, which will facilitate the solution of problems currently at and beyond the boundary of soluble problems by traditional ALE methods by focusing computational resources where they are required. Many of the core issues involved in the development of the ALE-AMR method hinge upon the integration of AMR with a Lagrange step, which is the focus of the work described here. The novel components of the method are mainly driven by the need to reconcile traditional AMR techniques, which are typically employed on stationary meshes with cell-centered quantities, with the staggered grids and grid motion employed by Lagrangian methods. These new algorithmic components are first developed in one dimension and are then generalized to two dimensions. Solutions of several model problems involving shock hydrodynamics are presented and discussed.

*Mail Stop: L-551. Phone: (925) 424-2858. E-mail: anderson110@llnl.gov
†Mail stop: L-560. Phone: (925) 422-4549. E-mail: pember@mercury.llnl.gov
‡Mail stop: L-560. Phone: (925) 422-4004. E-mail: elliott22@llnl.gov

1 Introduction

The numerical simulation of compressible flows with shocks and discontinuities is a computational challenge in many important application areas including inertial confinement fusion (ICF), astrophysics, fluid-solid interactions, and plasma physics. Resolution of small scale flowfield features such as shocks, material interfaces, and regions of inviscid instability requires a large number of computational cells in these regions. Lagrangian and ALE techniques have often been favored in the above application areas [1], in part due to the self-adapting nature of Lagrangian grid motion, e.g., contact discontinuities are tracked automatically, and cells are clustered into high density regions behind shocks. However, this inherent form of adaption present in Lagrangian and ALE methods, while an advantage over pure Eulerian codes in some applications, is not ideal. One particular drawback relative to a more general adaption method is that the number of cells in any such calculation, which may be thought of as a "resolution capacity," is constant, while the resolution requirements for many applications may change substantially throughout the simulation. A relatively simple initial condition may evolve into a highly complex system with many regions of complex interactions requiring high resolution. It becomes necessary in such situations to match the resolution capacity of the initial grid with the greatest resolution requirement present throughout the simulation. This is not optimal since it requires a priori knowledge of the dynamics of the system and the eventual resolution requirements, and secondly, it is wasteful of computational resources during the portions of the simulation time for which resolution requirements are submaximal.

An approach which has proven effective in addressing these problems is structured grid local adaptive mesh refinement (AMR) [2, 3, 4, 5]. AMR involves the addition and removal of mesh cells as required to maintain a specified level of accuracy, as opposed to maintaining a fixed cost, which is the case for a traditional Lagrangian calculation. As illustrated in Figure 1, this technique involves the successive refinement of regions of a structured mesh where additional resolution is required. Extension of the AMR idea to Lagrangian and in turn ALE solution techniques is nontrivial due to several factors. The first is that AMR was originally developed in the context of algorithms that employ cell-centered variables. Lagrangian methods, by contrast, are often developed by utilizing a staggered grid, where thermodynamic

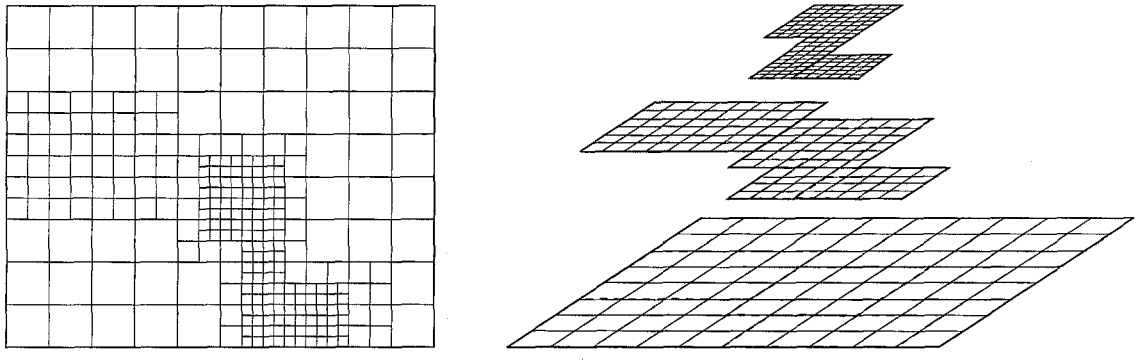

Figure 1: *An example of adaptive mesh refinement showing a properly nested hierarchy of grids. There are three levels, a base level and two levels of refinement, each generated from the next coarser level using a refinement ratio of two. There are three grids at each of the fine levels. Note that one of the grids at the finest level spans two grids at the intermediate level.*

quantities such as density and energy are located at cell centers, while the kinematic quantities of position and velocity are located at the mesh intersections, or nodes. This change manifests itself in the AMR algorithms in several ways. New or modified operators which transfer quantities between the coarse and fine meshes in a conservative manner must be developed. Furthermore, the methods responsible for synchronization of fine grid and coarse grid solutions via "refluxing" must be modified to suit a Lagrangian context on a staggered grid. Finally, the grid motion itself is a new component with respect to AMR methods, and the coupling between fine and coarse grid nodes in the AMR hierarchy must be established. Although some work has been done with moving structured grids in an Eulerian context [6], the methodology presented here is a departure from this previous work.

It is important to note that Lagrangian methods suffer from mesh tangling difficulties for many relevant applications. This is the impetus for the ALE-AMR effort which will extend this initial investigation of a purely Lagrangian AMR algorithm.

2 Methodology Overview

The governing equations to be solved are the Euler equations in Lagrangian form:

$$\frac{D\rho}{Dt} + \rho\vec{\nabla}\cdot\vec{V} = 0 \tag{1}$$

$$\rho\frac{D\vec{V}}{Dt} + \vec{\nabla}p = 0 \tag{2}$$

$$\rho\frac{De}{Dt} + p\vec{\nabla}\cdot\vec{V} = 0. \tag{3}$$

where ρ, e, p, and $\vec{V}$ are the fluid density, internal energy, pressure, and velocity respectively, and t is time.

The solution of the system (1),(2),(3) proceeds through a succession of Lagrange steps on a hierarchy of structured meshes. The form of the Lagrange step employed is independent of the mesh configuration, except with respect to boundary conditions as will be discussed in section 2.2. First, we will outline the established methodology upon which the method is based.

2.1 Established Methods

The Lagrange step methodology employed on the grid interior follows the general approach taken by Tipton [7]. It employs a predictor-corrector discretization in time, and the HEMP spatial discretization [8],[9]. The scheme employs a monotonic artificial viscosity due to Christensen [10], and a simple kinematic hourglass filter [11].

The model AMR methodology which is being adapted for the Lagrangian method is that of Berger, Oliger, and Colella [3, 12]. In this approach, a hierarchical grid structure is employed which changes dynamically in time, and is composed of logically rectangular, uniform grids of varying resolution. The grid hierarchy is constructed so that a coarse grid cell is covered precisely by l^n fine grid cells, where l is a user specified integer called the refinement ratio, and n is the spatial dimension of the simulation. The solution is defined on all cells, including coarse cells which underlay cells of finer resolution. The collection of grids at a given resolution is referred to as a level. The hierarchy can have an arbitrary number of levels and any number of grids at a given level. The time step is a recursive procedure which we describe here for a two level calculation.

The first step is to regrid the current solution by refining regions of the flow requiring greater resolution. Cells requiring refinement are tagged and then grouped with untagged cells to create relatively

large blocks of the coarse grid that will be refined. These blocks are then subdivided to create the new fine grids. When new fine grid cells are generated in the process, the solution is defined by a conservative interpolation of the coarse grid data. The modified interpolation operator employed in the Lagrangian context is discussed in the following section.

The next step is a coarse grid advance, in which the coarse grid data is integrated to some new time, $t + \Delta t$. The fine grid is then advanced through multiple time steps to the same time as the coarse grid. The principal consideration in the fine grid advance is the boundary conditions employed on the fine mesh, in particular at coarse-fine mesh boundaries. Typically this is achieved through time and space interpolation of coarse grid data to provide Dirichlet boundary conditions. Required modifications to this procedure are discussed in the following section.

The final step in a traditional hierarchy advance is synchronization of the coarse grid and fine grid data. This is accomplished in two steps. First, a conservative coarsening or "averaging down" takes place that replaces any coarse grid data for which fine grid data is available. Second, the coarse cells which are adjacent to a fine grid boundary are updated to reflect the fluxes which were provided by the fine grid at those boundaries over the succession of fine grid advances. This is necessary to ensure conservation, since the coarse grid and fine grid fluxes will not in general be the same. For a Lagrange scheme, the synchronization step requires a modified approach.

2.2 Novel Extensions

The integration of AMR with a Lagrangian method on a staggered grid requires in essence four modifications of standard AMR methodology. The four modified elements are the refinement operators, the coarsening operators, the treatment of boundary conditions on finer grids, and the synchronization of coarse grid and fine grid data after a hierarchy advance.

Refinement operators for shock hydrodynamics applications of AMR ought to obey at a minimum four essential properties. They ought to maintain the order of accuracy of the underlying integration (typically 2nd order accuracy), they should be conservative, they should not generate new extrema in the solution, and they should obey a reciprocity relation with their corresponding coarsening operators. Refinement

operators which obey these properties on a staggered mesh configuration are developed first in one dimension, and then generalized to two dimensions. The coarsening operators are also modified to conform to the staggered grid configuration, first in one dimension, and then in two dimensions. Conservation and reciprocity with the refinement operators are established.

The treatment of boundary conditions on finer grids requires additional algorithmic developments over traditional AMR, since in the Lagrange step, the node locations and hence the mesh are determined as part of the integration. This has no counterpart in an Eulerian AMR solution method, and care must be taken at coarse-fine boundaries to ensure conservation. Solutions for this problem are presented in one dimension and then in the more challenging case of two dimensions. The formerly distinct concepts of fine grid boundary conditions and coarse-fine synchronization become coupled in a Lagrangian context. No additional synchronization step to ensure mass conservation is required as a result of the fine grid boundary condition treatment, but synchronizing adjustments for momentum and energy must be made in an appropriate way to ensure conservation. The modified synchronization step is developed in one dimension and generalized to two dimensions, and conservation is established.

2.3 Implementation and Preliminary Results

The implementation of these algorithms is accomplished using SAMRAI [13], an object-oriented framework for the development of structured grid adaptive mesh refinement applications. The AMR specific portions of the code development that benefit from higher level abstractions are implement using C++, and the lower level portions of the algorithm where performance is the dominant factor are implemented in FORTRAN 77. All inner loop computations are performed at the FORTRAN level of implementation.

Preliminary results using a one-dimensional Lagrangian AMR (LAMR) algorithm are displayed in Figure 2 for the Sod shock tube problem [14]. This is a two level calculation with a refinement ratio of $n = 4$. Both the coarse and fine mesh solutions are shown on the same axes at the time $t = .245$, corresponding to the Sod initial conditions of $\rho_L = 1.0$, $p_L = 1.0$, $\rho_R = .125$, $p_R = 0.1$, and $u_L = u_R = 0$, where L and R subscripts denote states in the left and right halves of a shock tube extending between $-1 < x < 1$. This is a simple demonstration

of a functional LAMR algorithm in one dimension. Performance on more challenging problems in both one and two dimensions will be presented.

3 Acknowledgment

This work was performed under the auspices of the U.S. Department of Energy by University of California Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.

References

[1] Benson, B. J., "An Efficient, Accurate, Simple ALE Method for Nonlinear Finite Element Programs," *Comp. Meth. Appl. Mech. Eng.*, Vol. 72, 1989, pp. 205–350.

[2] Bell, J., Berger, M., Saltzman, J., and Welcome, M., "Three Dimensional Adaptive Mesh Refinement for Hyperbolic Conservation Laws," *SIAM J. Sci. Comp.*, Vol. 15, 1994, pp. 127–138.

[3] Berger, M. and Oliger, J., "Adaptive Mesh Refinement for Hyperbolic Partial Differential Equations," *J. Comput. Phys.*, Vol. 53, 1984, pp. 484–512.

[4] Berger, M. and Colella, P., "Local Adaptive Mesh Refinement for Shock Hydrodynamics," *J. Comput. Phys.*, Vol. 82, 1989, pp. 64–84.

[5] Pember, R., Bell, J., Colella, P., Crutchfield, W., and Welcome, M. L., "An Adaptive Cartesian Grid Method for Unsteady Compressible Flow in Complex Geometries," *J. Comput. Phys.*, Vol. 120, 1995, pp. 278–304.

[6] Bell, J., Colella, P., Trangenstein, J., and Welcome, M., "Adaptive Mesh Refinement on Moving Quadrilateral Grids," *Proceedings, AIAA 9th Computational Fluid Dynamics Conference*, Buffalo, New York, June 14-16, 1989, p.471-579.

[7] Tipton, R., Unpublished report, Lawrence Livermore National Laboratory, 1990.

[8] Wilkins, M. L., "Calculation of Elastic-Plastic Flow," *Meth. Comp. Phys.*, Vol. 3, 1964, pp. 211–263.

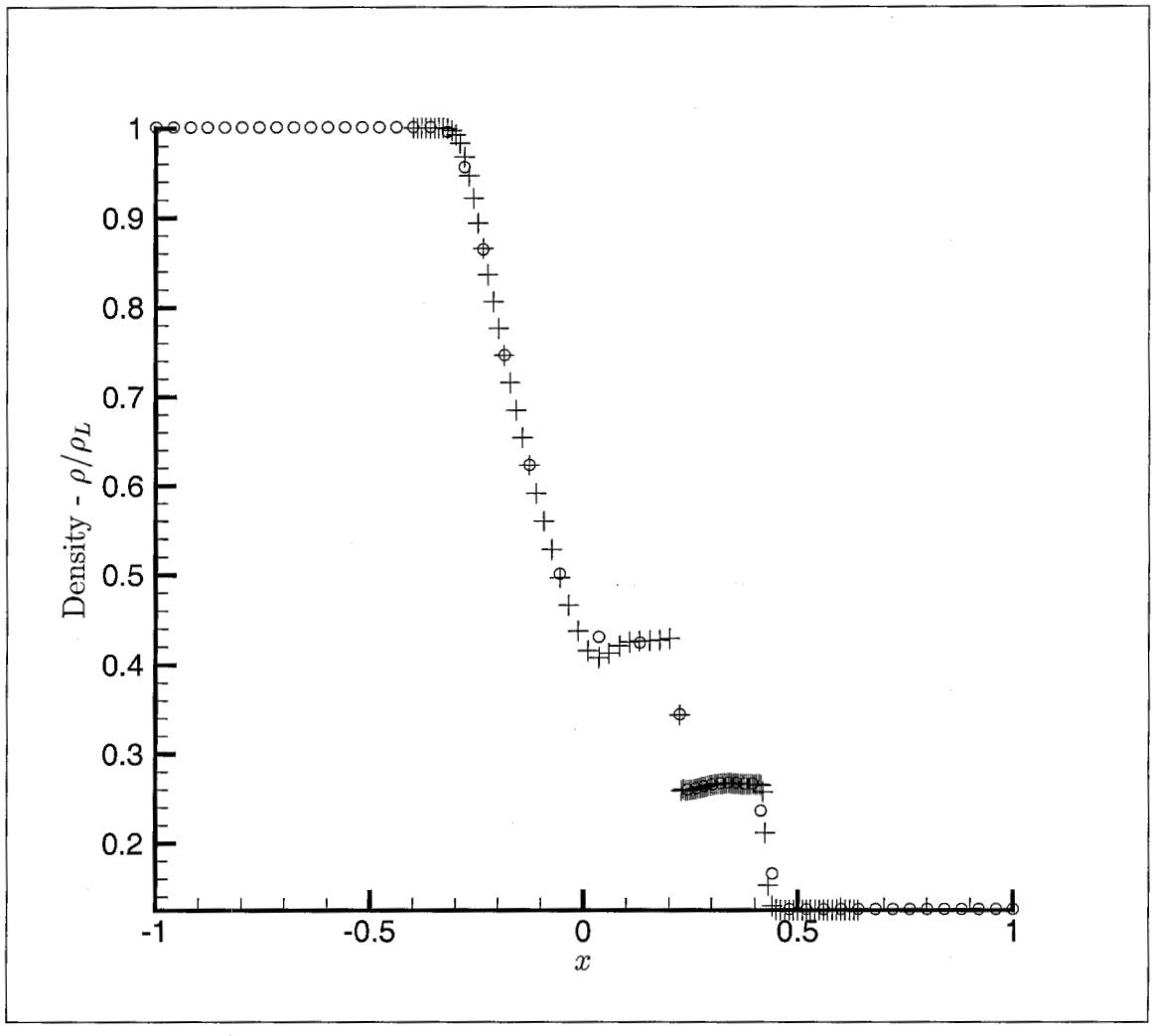

Figure 2: Sod problem density profile at t=.245. ∘ - Coarse mesh solution. + - Refined mesh solution with refinement ratio $n = 4$.

[9] Sharp, R., "HEMP Advection Model," Tech. Rep. UCID-17809, Lawrence Livermore National Laboratory, 1978.

[10] Christensen, R., "Godunov Methods on a Staggered Mesh — An Improved Artificial Viscosity," Tech. Rep. UCRL-JC-105269, Lawrence Livermore National Laboratory, 1990.

[11] Margolin, L. and Pyun, J., "A Method for Treating Hourglass Patterns," Tech. Rep. LA-UR-87-439, Los Alamos National Laboratory, 1987.

[12] Berger, M. and Colella, P., "Local Adaptive Mesh Refinement for Shock Hydrodynamics," *J. Comput. Phys.*, Vol. 82, 1989, pp. 64–84.

[13] Hornung, R. and Kohn, S., "Future Directions for Adaptive Mesh Refinement in ASCI and other LLNL Simulation Projects," Tech. Rep. UCRL-ID-12833, Lawrence Livermore National Laboratory, September, 1997.

[14] Sod, G., "A survey of several finite difference methods for systems of nonlinear hyperbolic conservation laws." *J. Comput. Phys.*, Vol. 27, No. 1, 1978.