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A Hybrid Adaptive Multiresolution Approach for the Efficient Simulation of Reactive Flows

Brandon Gusto, Tomasz Plewa

Department of Scientific Computing
Florida State University

Contact Information:
Brandon Gusto
blg13@my.fsu.edu

Introduction

Many physical systems are characterized by the presence of multiple spatial scales. Numerical simulation of such types of systems poses a significant challenge. One of the most widely-adopted approaches to address this issue involves the use of a non-uniformly spaced mesh with a hierarchy of grid resolutions. Such approaches can be broadly classified as adaptive mesh refinement (AMR) methods.

Rather than refine one computational cell individually, AMR methods typically create a hierarchy of grid levels by refining large collections of cells (blocks) around non-smooth solution features. Block-based refinement is typically preferred over cell-based refinement for reasons of computational efficiency. Shown in Figure (1) is a quadtree structure used to organize the block hierarchy.

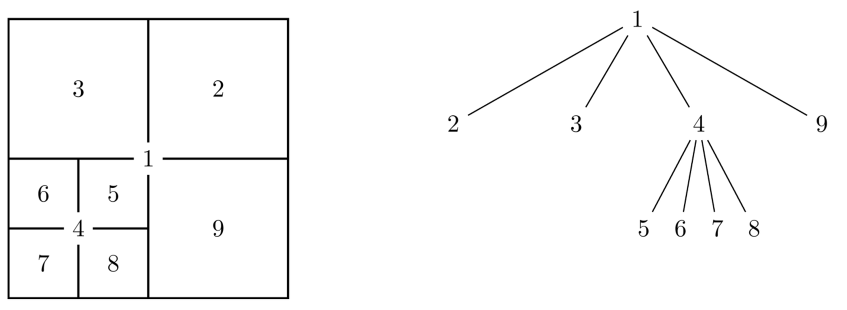

Figure 1: An example of a quadtree structure with three mesh levels. Blocks 2, 3, 5, 6, 7, 8, and 9 are leaf blocks on which the numerical solution is advanced.

One major drawback of block-structured AMR is the 'over-resolution' of many cells in the mesh which occupy a smooth part of the solution and are only required to satisfy the block structure format. A sub-optimal mesh can also be the result of the following rules governing mesh refinement:

i. There can be a difference in refinement level between adjacent blocks no greater than one.
ii. A complete set of child blocks must be produced for any block that is refined.

A method for dealing with multi-scale problems on *uniform* grids was introduced by Harten [1], which uses a multiresolution (MR) representation of the data in order to decrease excessive computations in smooth regions. The idea was to reduce the number of costly flux evaluations while maintaining a prescribed level of accuracy. In the present work, this scheme is generalized to block-structured AMR discretizations. We denote the new scheme as the hybrid adaptive multiresolution (HAMR) scheme. Furthermore, we expand the procedure to adaptively calculate the equation of state (EoS) and reactive source terms, as these are often the most computationally demanding aspects of complex, multiphysics flow simulations.

Hybrid adaptive multiresolution scheme

The MR approach considers a set of nested grids

$$\mathcal{G}^l = \{x_i^l\}_{i=0}^{N_l}, \quad x_i^l = i \cdot h_l, \quad h_l = 2^{L-l} \cdot h_L, \quad N_l = N_L / 2^{L-l}, \tag{1}$$

on the given domain where $l = 1$ represents the coarsest level of resolution and $l = L$ represents the finest. The width of a computational cell on level l is h_l. **The MR procedure encodes solution data on the finest grid as coarse-grid values plus a series of differences obtained on finer levels.** These differences are the smoothness indicators, known as detail coefficients. They are computed as the difference between the data on level $l+1$ and values interpolated from data on level l,

$$d_i^l = u_{2i}^{l+1} - \tilde{u}_{2i}^{l+1}, \tag{2}$$

where $\tilde{u}_{2i}^{l+1}$ is the interpolated data. Then an adaptive mesh may be defined by truncating coefficients whose absolute values are smaller than a given tolerance ε.
Once the significant detail coefficients are identified, a block-structured mesh is constructed. The coefficients are then used to identify regions of the mesh where costly evaluation of the numerical flux, reactive source term, or EoS may be avoided and replaced with interpolation of values already obtained nearby. This workflow is shown for an example AMR mesh in Figure (2).

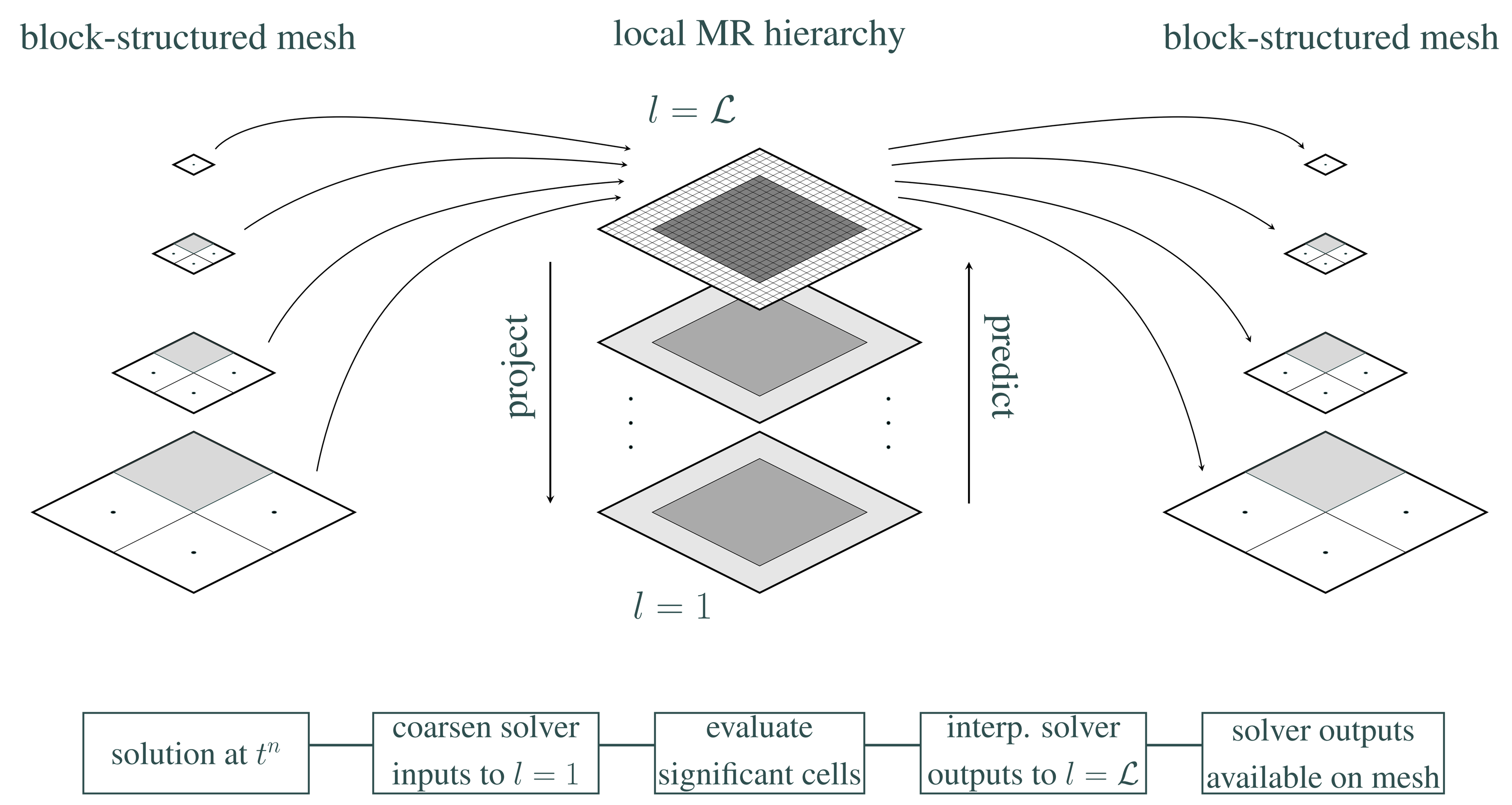

Figure 2: General flow of procedures for the solver-adaptive component of the HAMR scheme. On the local MR hierarchy, lighter regions indicate the ghost cell region of the block.

Results

In the Hawley-Zabusky problem [3], a planar shock passes through an oblique density-stratified interface. The density contrast creates a rolling tendency along the interface as the wave is allowed to travel faster in the less dense medium than in the denser medium. The top left panel of Figure (3)

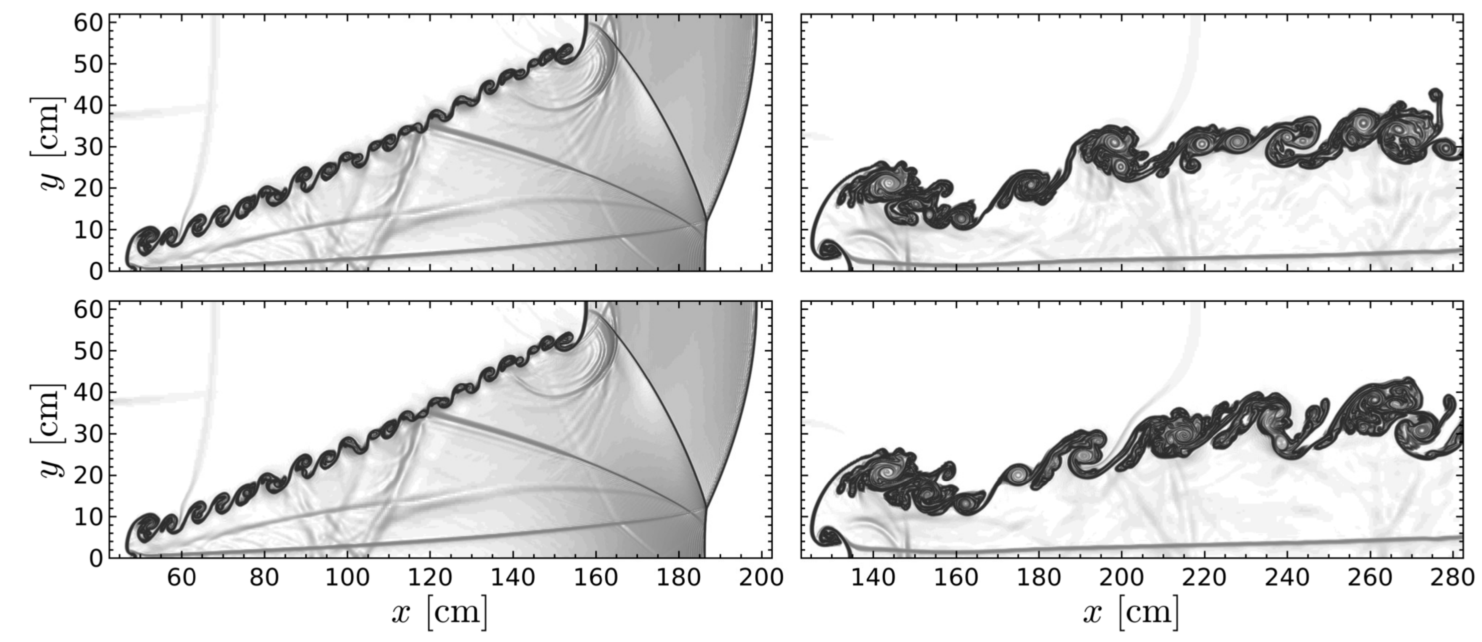

Figure 3: The morphology of the flow in the Hawley-Zabusky problem is shown with numerical schlieren density images for the baseline AMR solution (top row) and HAMR solution with $\kappa = 1 \times 10^{-2}$ (bottom row). The panels in the left column show the morphology shortly after the shock passed through the interface ($t \approx 180$ s), while the structure of the interface at the final simulation time is shown in the right column. Note that the structure of the HAMR solution closely matches that of the baseline solution at early times. There are however discernable differences in the small scale structure of the mixed region at the final time.

shows the initial roll-up along the interface for the baseline AMR solution, while the top right panel shows the mixed region at late time. The bottom panels show the HAMR solution at the corresponding times. While there are some differences in the flow structures, the overall behavior is much the same.

We test the effect of interpolating fluxes on the adaptive mesh according to the significant detail coefficients and find that the error remains well controlled, even at late times. The given simulation uses a tolerance of $\varepsilon = 10^{-2}$ for mesh refinement and multiplicative safety factors ranging from of 10^{-4} to 10^{-1} for flux interpolation. The left panel of Figure (4) shows the evolution of the integrated vorticity at late time for the uniform mesh, baseline AMR, and HAMR simulations. In the right panel is the corresponding error. We see that the effect of interpolating fluxes does not introduce significantly more error than the AMR itself.

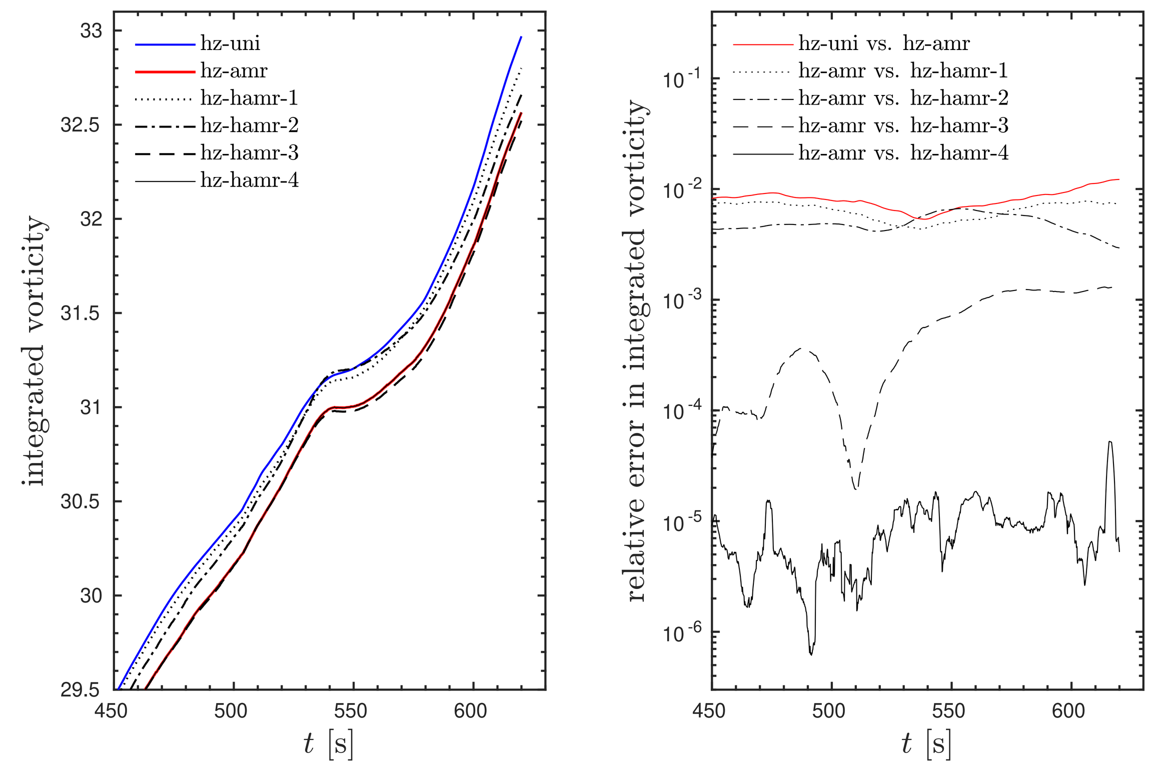

Figure 4: The integrated vorticity evolution for the Hawley Zabusky problem is shown in the left panel for the reference uniform mesh solution (solid blue line), AMR solution (solid red line), and a set of HAMR models (black lines). The time evolution of the relative error in integrated vorticity is shown in the right panel during the same time window for each HAMR solution.

Future work

Adaptive models with robust error estimation

The main disadvantage of using MR indicators for time-dependent problems is that the indicators alone cannot reliably be used detect time-dependent features. Some intuition as to where features may develop must be supplied by the user.
In order to estimate the local truncation error (LTE) for time-dependent problems, the technique known as Richardson extrapolation may be employed. This requires the solution to be advanced on grids of differing spatial resolution. Then the error on the coarser grid can be estimated according to

$$E_{h/2} \approx \frac{u_{h/2} - u_h}{2^p - 1}, \tag{3}$$

where p is the nominal order of the method. **This can be used to guide the AMR, or to provide additional error estimates for MR methods.**

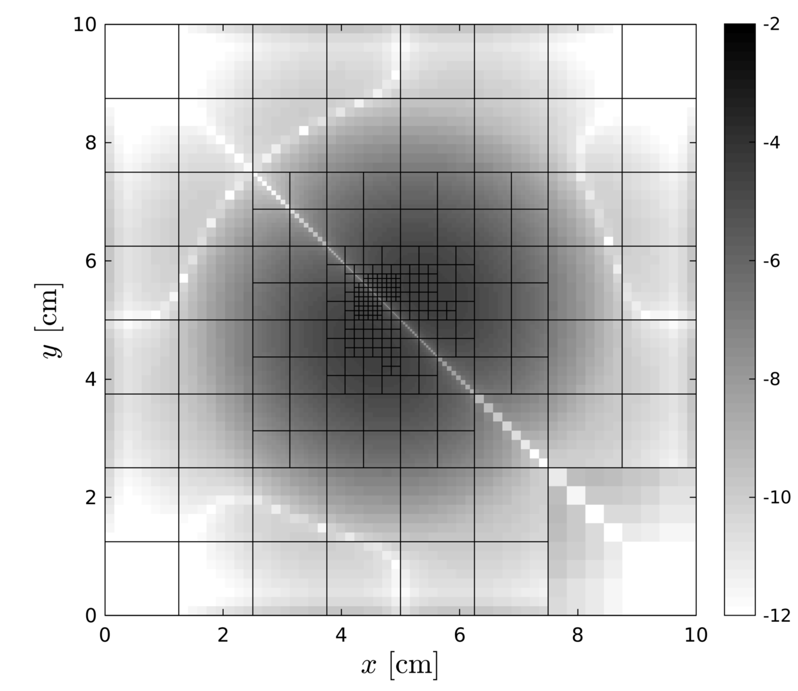

Figure 5: LTE estimates and resultant block-structured adaptive mesh for the Isentropic vortex problem.

Estimates of the LTE for the Isentropic vortex problem [2] are shown in Figure (5). These estimates will be compared with the actual error obtained using the analytic solution.

References

[1] A. Harten. Adaptive multiresolution schemes for shock computations. *Journal of Computational Physics*, 115(2):319–338, 1994.

[2] H.C Yee, N.D Sandham, and M.J Djomehri. Low-dissipative high-order shock-capturing methods using characteristic-based filters. *Journal of Computational Physics*, 150(1):199–238, 1999.

[3] N. Zabusky and J. Hawley. Vortex paradigm for shock-accelerated density-stratified interfaces. *Physical Review Letters*, 63:1241–1244, 1989.