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A Multiresolution Hybrid Adaptive Approach for Turbulent Reactive Flows

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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.

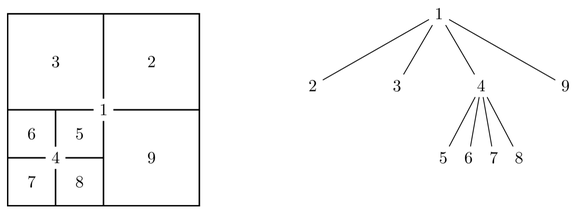

Figure 1: An example of a quadtree structure with three mesh levels. Blocks 2, 3, 5, 6, 7, 8, and 9 are leaf blocks on which the numerical solution is advanced.

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. Furthermore, we expand the original Harten's method 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.

Methods

Preliminaries

In the present work we are interested in numerically solving conservation laws of the form

$$\begin{cases} \boldsymbol{u}_t + \boldsymbol{f}(\boldsymbol{u})_x + \boldsymbol{g}(\boldsymbol{u})_y = \boldsymbol{s}(\boldsymbol{u}), \quad \boldsymbol{x} \in \mathbb{R}^2 \\ \boldsymbol{u}(\boldsymbol{x}, 0) = \boldsymbol{u}_0(\boldsymbol{x}), \end{cases} \tag{1}$$

where $\boldsymbol{u}$ represents the vector of conserved quantities, $\boldsymbol{f}(\boldsymbol{u})$ and $\boldsymbol{g}(\boldsymbol{u})$ are the flux functions, and $\boldsymbol{s}(\boldsymbol{u})$ is a source term. In the finite volume formulation, the solution quantities are approximated by a volume average defined over a target cell $I_{i,j} = \left[x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}\right] \times \left[y_{j-\frac{1}{2}}, y_{j+\frac{1}{2}}\right]$ as

$$v_{i,j}(t) \approx \frac{1}{h^2} \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \int_{y_{j-\frac{1}{2}}}^{y_{j+\frac{1}{2}}} u(\hat{x}, \hat{y}, t) d\hat{y} d\hat{x}, \tag{2}$$

where h is the cell width. We introduce a set of nested grids

$$\boldsymbol{\mathcal{G}}^l = \left\{ (x_i^l, y_j^l) \right\}_{i,j=0}^{N_l}, \quad x_i^l = i \cdot h_l, \;\; y_j^l = j \cdot h_l, \;\; h_l = 2^{L-l} \cdot h_L, \;\; N_l = N_L / 2^{L-l}, \tag{3}$$

on the given domain where $l = 1$ represents the coarsest level of resolution and $l = L$ represents the finest. A multiresolution decomposition is performed on the solution field at each timestep, given by

$$\boldsymbol{M}\boldsymbol{v}^L = \left(\boldsymbol{d}^L, \boldsymbol{d}^{L-1}, \ldots, \boldsymbol{d}^1, \boldsymbol{v}^1\right), \tag{4}$$

where $\boldsymbol{M}$ is the linear transform operator and $\boldsymbol{d}^l$ are the detail coefficient vectors. The detail coefficients are a measure of the local smoothness of the solution. They are then used to guide the block-structured mesh adaptation by creating a mask $\boldsymbol{\mathcal{M}}$ as

$$\mathcal{M}_{i,j}^l = \begin{cases} 1, & \text{if } |d_{i,j}^l| > \varepsilon_l \\ 0, & \text{else,} \end{cases} \tag{5}$$

where ε_l is a level-dependent threshold, determined by the user.

Multiresolution scheme

Once the mesh is fixed, the multiresolution basis is used to interpolate quantities that are otherwise expensive to calculate in the over-resolved regions of the mesh. We consider a general function of the solution,

$$\boldsymbol{\phi}(\boldsymbol{v}) = \int_\Omega \boldsymbol{q}(\boldsymbol{v}(\boldsymbol{x})) \tag{6}$$

that must be obtained at the locally finest level of the mesh. The function $\boldsymbol{q}$ is assumed to depend smoothly on $\boldsymbol{v}$, meaning that the regularity analysis on $\boldsymbol{v}$ is a good estimate for the regularity analysis on $\boldsymbol{q}$ itself or $\boldsymbol{\phi}$. Specifically we use the function $\boldsymbol{\phi}$ as a placeholder for the *divergence of the flux*, *reactive source term*, and *EOS*. The compressed multiresolution basis is used to obtain an approximate representation $\tilde{\boldsymbol{\phi}}^L$ such that the error between it and the true function is bounded by

$$||\boldsymbol{\phi}^L - \tilde{\boldsymbol{\phi}}^L|| < \varepsilon. \tag{7}$$

The process of obtaining $\tilde{\boldsymbol{\phi}}^L$ proceeds by first calculating directly the values at the coarsest level of resolution $\boldsymbol{\phi}^1$. Then the values at finer levels are either computed directly or interpolated from the adjacent coarse level depending on the mask $\boldsymbol{\mathcal{M}}$.

Results

Hawley-Zabusky problem

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 in figure (2) shows the initial roll-up along the interface, while the lower panel shows the MR detail coefficients which clearly have larger values in region occupied by non-smooth flow features such as shocks, acoustic waves and material interfaces.

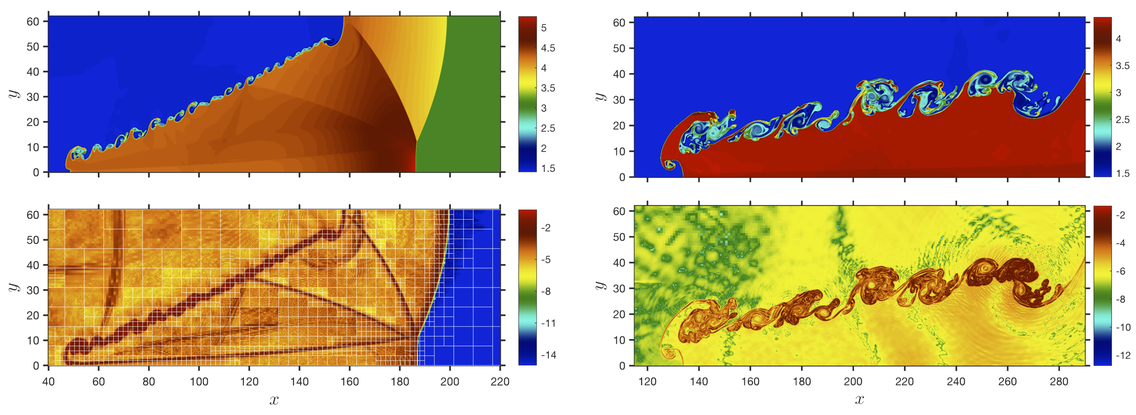

Figure 2: Left: Multiresolution coefficients are used to identify the shock waves, vortices, and weak acoustic signals, and guide the mesh refinement accordingly (bottom). Block outlines are shown in white. Right: The vortical structures along the interface at final time (top). Solution error between the reference and MR solution at the same time (bottom).

We test the effect of interpolating fluxes on the adaptive mesh according to the mask. Due to the complex and frequent interaction of acoustic signals, this problem does not offer much savings for the MR scheme, however it is useful for error analysis. We find that the error remains well controlled, even at late times. The given simulation uses a tolerance of $\varepsilon = 10^{-3}$ for mesh refinement and 10^{-4} for flux interpolation. The bottom right panel of figure (2) shows the difference between the reference and MR solutions on the adaptive mesh. The error is within the expected ranges.

Cellular detonation

The cellular detonation problem [2] involves two-dimensional detonation of carbon under degenerate conditions and is designed to study the complex interaction of transverse shocks behind a perturbed detonation front. The detonation front instability is triggered by small density perturbations introduced in the upstream region. This instability ultimately manifests itself into triple points which oscillate along the detonation front over time. Emanating from these triple points are transverse waves which create the conditions for turbulence behind the front. We use this problem as a test bed for the EOS and reactive source term interpolation. The computationally expensive Helmholtz EOS is required due to the extreme conditions necessary for burning to occur. This combined with the integration of the reaction network itself dominate the total cost of the simulation. Figure (3) shows the detonation front in quasi-steady state. Most of the savings from the MR scheme in this problem come from the region ahead of the detonation front, where the mesh is highly refined but the solution is constant. The error is assessed by computing the difference in the lateral average of several species (carbon and silicon) and the nuclear energy generation rate, $\dot{e}$. We find that the error is within the expected tolerance. Figure (4) shows the difference in the lateral averages around the detonation front.

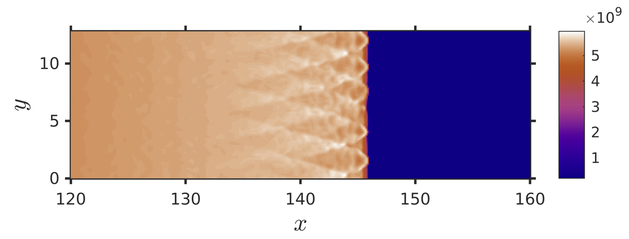

Figure 3: Detonation front in quasi-steady state. The triple point hotspots (regions of high pressure and temperature) are clearly visible along the detonation front, as are the transverse waves in the wake.

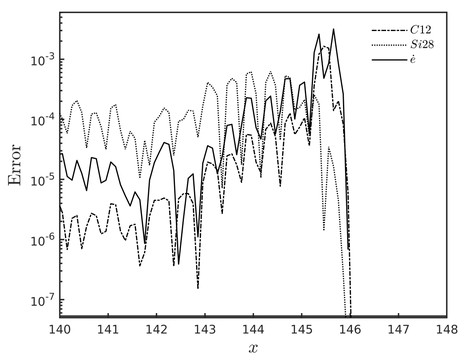

Figure 4: Error in lateral (spanwise) averages of species and nuclear energy generation rate.

Conclusions

The multiresolution scheme is used to reduce the number of flux, EOS, and source term calculations on block-structured AMR grids. It is found that the scheme significantly reduces computational effort without adversely affecting the numerical solution.

References

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

[2] F. Timmes et al. On the cellular structure of carbon detonations,. *The Astrophysical Journal*, 543:938–954, 2000.

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