

Case Study

1. Title of Case Study: HAMISH: a dynamic adaptive mesh refinement solver for turbulent reacting flows

2. Grant Reference Number: EP/P022286/1, EP/R029369/1

3. One sentence summary: A dynamic adaptive mesh refinement solver, which allows to capture small-scale flow structures in reacting flows at a reasonable computational cost, is being developed through the collaboration between STFC Daresbury Laboratory, Cambridge University and Newcastle University.

4. One paragraph summary: In order to carry out high-fidelity turbulent reacting flow simulations of physical processes with a large range of length scales (e.g. flame/wall interaction, localised ignition, deflagration to detonation transition) at a reasonable computational cost, a dynamic adaptive mesh refinement (AMR) CFD solver, HAMISH, is being developed, through the collaboration between STFC Daresbury Laboratory, Cambridge University and Newcastle University. The numerical framework of HAMISH relies on a finite-volume approach for spatial discretisation together with a high-order Runge-Kutta algorithm for time stepping. An unstructured AMR Cartesian mesh allows for adaptive local refinement and de-refinement operations based on the fidelity requirements prescribed by the numerical solution. The data structure is built by representing the unstructured mesh as a bitree/quadtree/octree and spanning the tree leaves with the help of the Morton space filling curve, allowing efficient cell addressing and parallel domain decomposition. The code, which is still under development, has already shown advantages compared to the fixed mesh solvers in some benchmark tests.

- 5. Key outputs in bullet points:**
- The application of Morton code and octree structure in an adaptive mesh refinement CFD solver with detailed chemical description.
 - MPI-based parallel octree structure for high-order numerical scheme with dynamic load balance.
 - High-order flux reconstruction method for numerical simulation of turbulent reacting flows.

6. Main body text

In combustion simulations, it is necessary to resolve the thin reaction layer where the high magnitudes of temperature and species gradients exist. Typically, 10-20 grid points are kept within the flame thickness in order to resolve key thermo-chemical processes within the flame. The grid resolution requirements become increasingly stringent with increasing complexity of the chemical mechanism. In order to carry out high-fidelity simulations of turbulent reacting flow simulations of physical processes with a large range of length scales (e.g. flame/wall interaction, localised ignition, deflagration to detonation transition) at a reasonable computational cost, a dynamic adaptive mesh refinement (AMR) solver, HAMISH, is being developed.

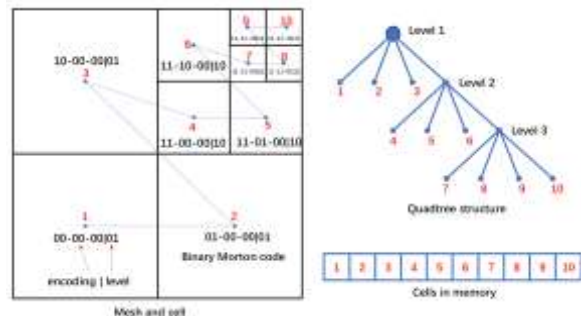


Figure 1. Sketch of a Morton code of a 2-D AMR mesh and its quadtree structures.

The Navier-Stokes equations for multi-component variable property mixtures are discretised using the finite-volume method in HAMISH. The spatial discretisation follows a distributed octree structure (see Fig.1 for a 2-D example). In a 3D case, the individual cells are cubic and a cell of side $2h$ is divided into 8 identical cubic cells with a side of h for the purpose of adaptive refinement. The cell-averaged conserved variables are stored in each individual cell. The cells are indexed with the help of Morton coding (see Fig. 1 for a 2-D example), which enables mapping of three-dimensional physical space into one-dimensional computational space. Morton codes are saved globally and individual code is assigned to each individual cell. An octree data structure is utilised to identify each individual cell in the mesh and this octree is distributed for parallel architecture so that load balancing is achieved through distributing octree and Morton code across the processors.

The HAMISH code has been tested in a series of benchmarks. The Rayleigh–Taylor instability problem and mixing-layer problem have demonstrated the advantage of the AMR technique in capturing the interface between two fluids, as shown in Fig. 2. The test in the 3-D Taylor-Green vortex case has shown its ability in resolving vortical simulations. Figure 3 shows that the AMR solver can ensure higher resolution near the region with strong turbulent fluctuations. Further tests in 2D and 3D channel flows have further demonstrated the ability of the HAMISH in simulating wall bounded flow, as shown in Fig. 4. The mesh is automatically refined in the near-wall region, where small-scale flow structures appear. Currently, HAMISH is still under development in terms of optimisation of the parallel performance. Figure 5 shows the results from the unstrained laminar premixed 1D planar flame, the mesh refinement algorithm is able to track the flame and the total number of cells decrease from 2048 to 157 without any loss of accuracy in this case.

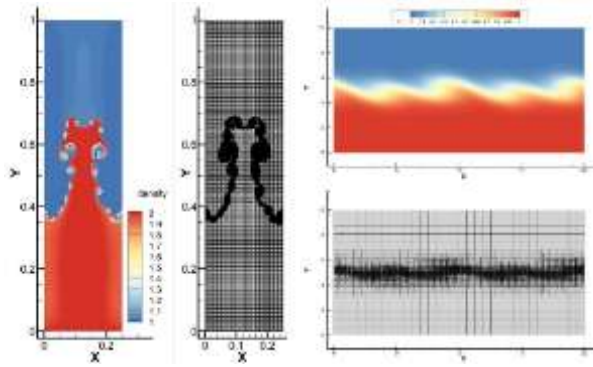


Figure 2. Instantaneous density field in a Rayleigh–Taylor instability problem (a), and mass fraction field in a mixing-layer case (b).

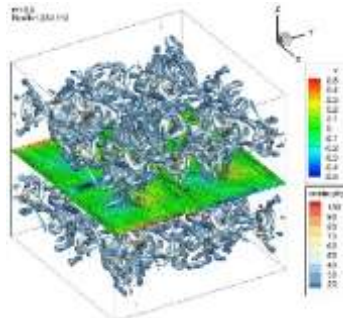


Figure 3. Instantaneous coherent structures in the 3D Taylor-Green vortex case

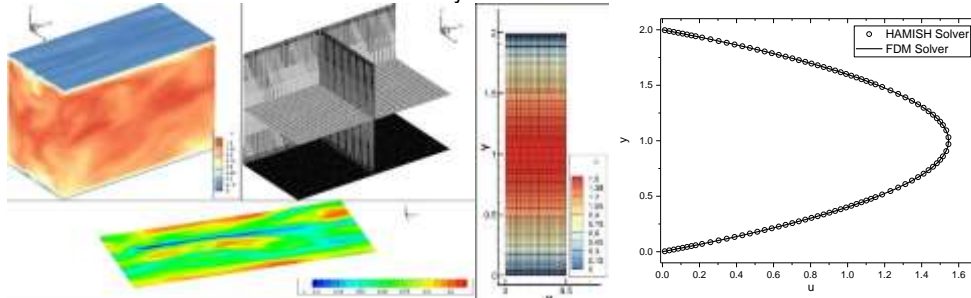


Figure 4. Application of HAMISH to the 2D/3D channel flows (left). Validation of the velocity profile against a high-order finite-difference solver (right)

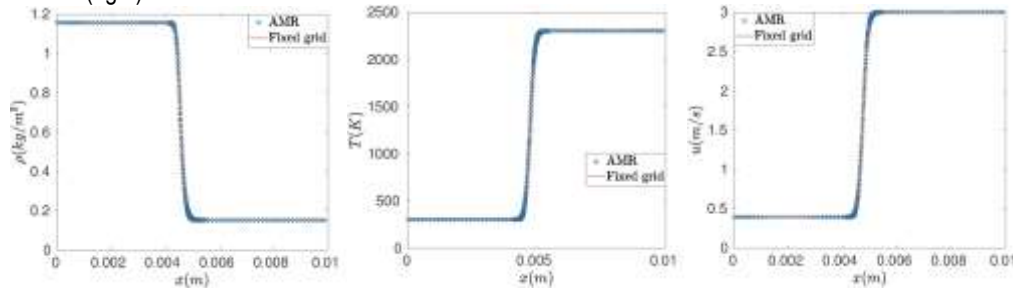


Figure 5. Application of HAMISH to the unstrained laminar 1D flame. Profiles of density (left), temperature (middle) and velocity (right) are shown for both AMR and non-AMR calculations.

7. Names of key academics and any collaborators:

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8. Sources of significant sponsorship (if applicable):

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10. Please indicate if you would like this case study to be included on the Consortium's ARCHER web-page. Yes