Numerical simulation of reacting flows using an unstructured adaptive mesh refinement based code HAMISH

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Outlines

- Background
- Introduction to the HAMISH Code
- Code Tests
  - 1-D thermal diffusion
  - 1-D planar flame
  - 1-D HOQ
  - 2-D thermal diffusion
  - 3-D TGV
  - 3-D isotropic decaying turbulence
- Scalability and Code Profiling
- Summary and Perspectives

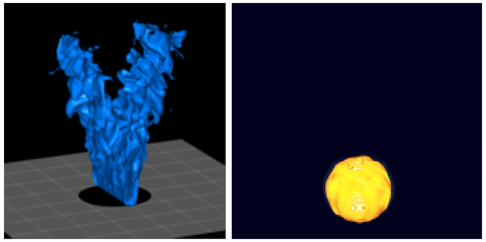
Background

- **Adaptive Mesh Refinement (AMR)**
  - AMR is a method of dynamically adapting the accuracy of a solution within certain regions of a simulation, i.e. during the time the solution is being calculated.
  - The main idea of AMR is to enable higher accuracy at lower cost, through an automatically optimal distribution of mesh cells in the concerned computational region.

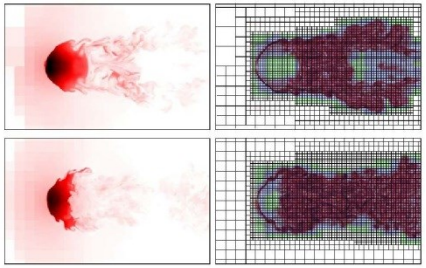
Background

- **Advantages of AMR**
  - Computational savings over a static mesh approach.
  - Storage savings over a static mesh approach.
  - Full control of the mesh resolution.
  - More detailed physics for the same number of cells as for a static mesh.
- **Main Applications**
  - To solve hyperbolic systems of conservation laws.
  - Problems with large dynamic range of scales.
  - Local enhancement of resolution is sufficient.

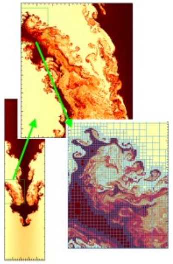
Background



Flames (Boxlib)

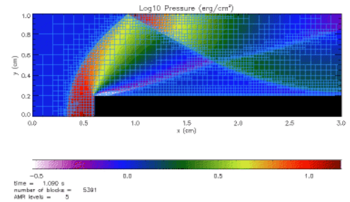


R-T instability (ENZO Code)

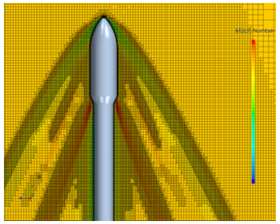


(FLASHCode)

Problems with interfaces

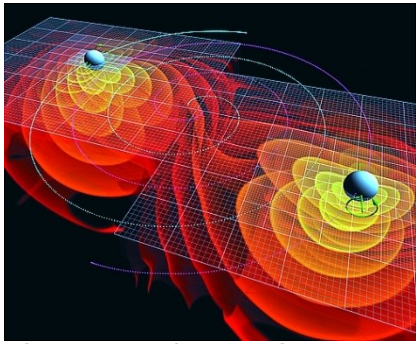


Moving Shock-Wave (PARAMESH)

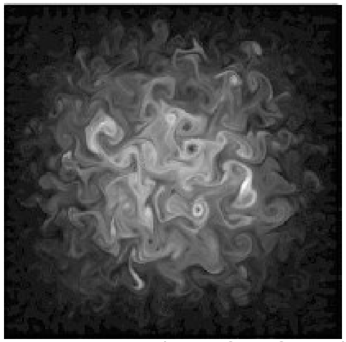


Supersonic Vehicle

Problems with discontinuities

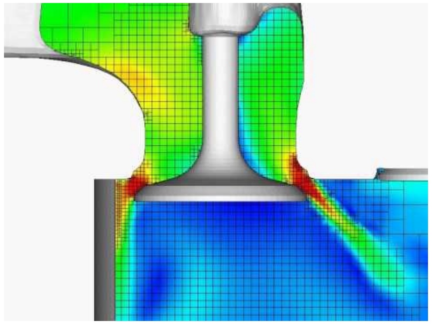


Computing Cosmic Cataclysms

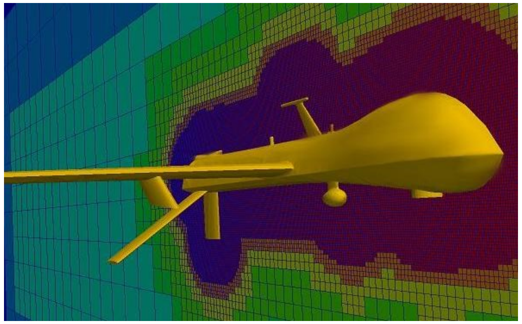


Turbulence (FLASH Code)

Problems with great variety of scales



Engine Combustion



Drone

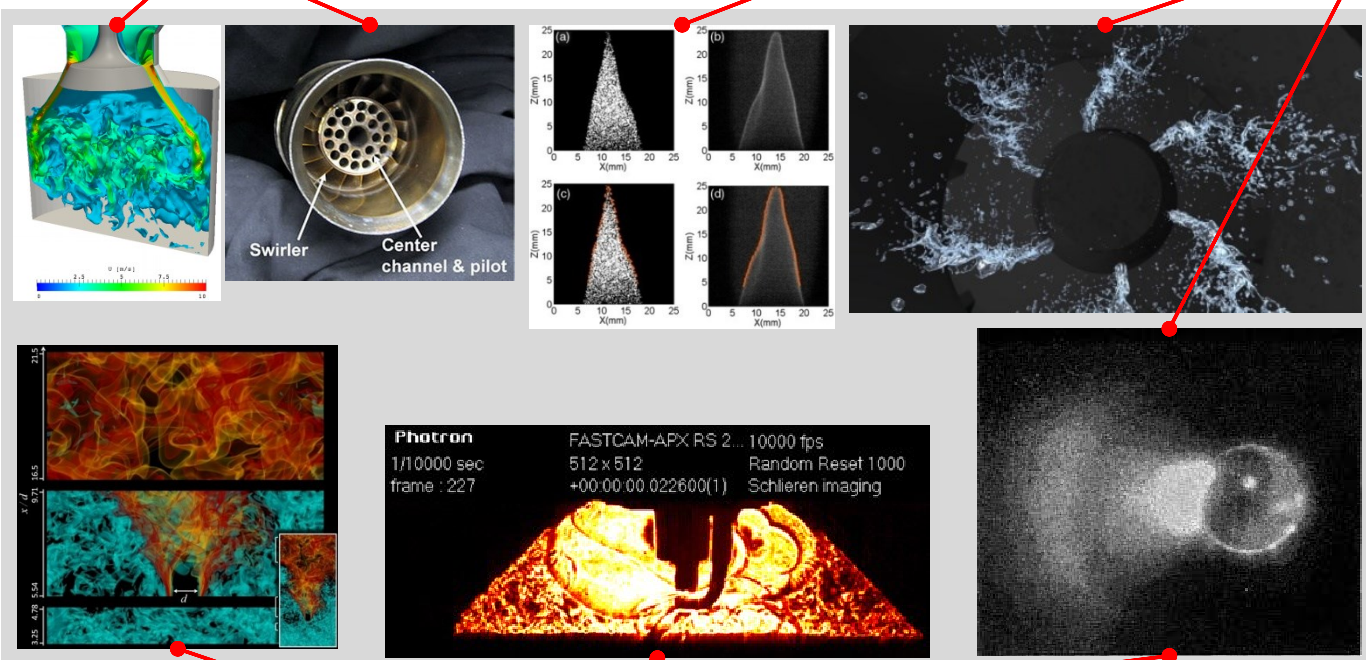
Problems with complex geometries

Background

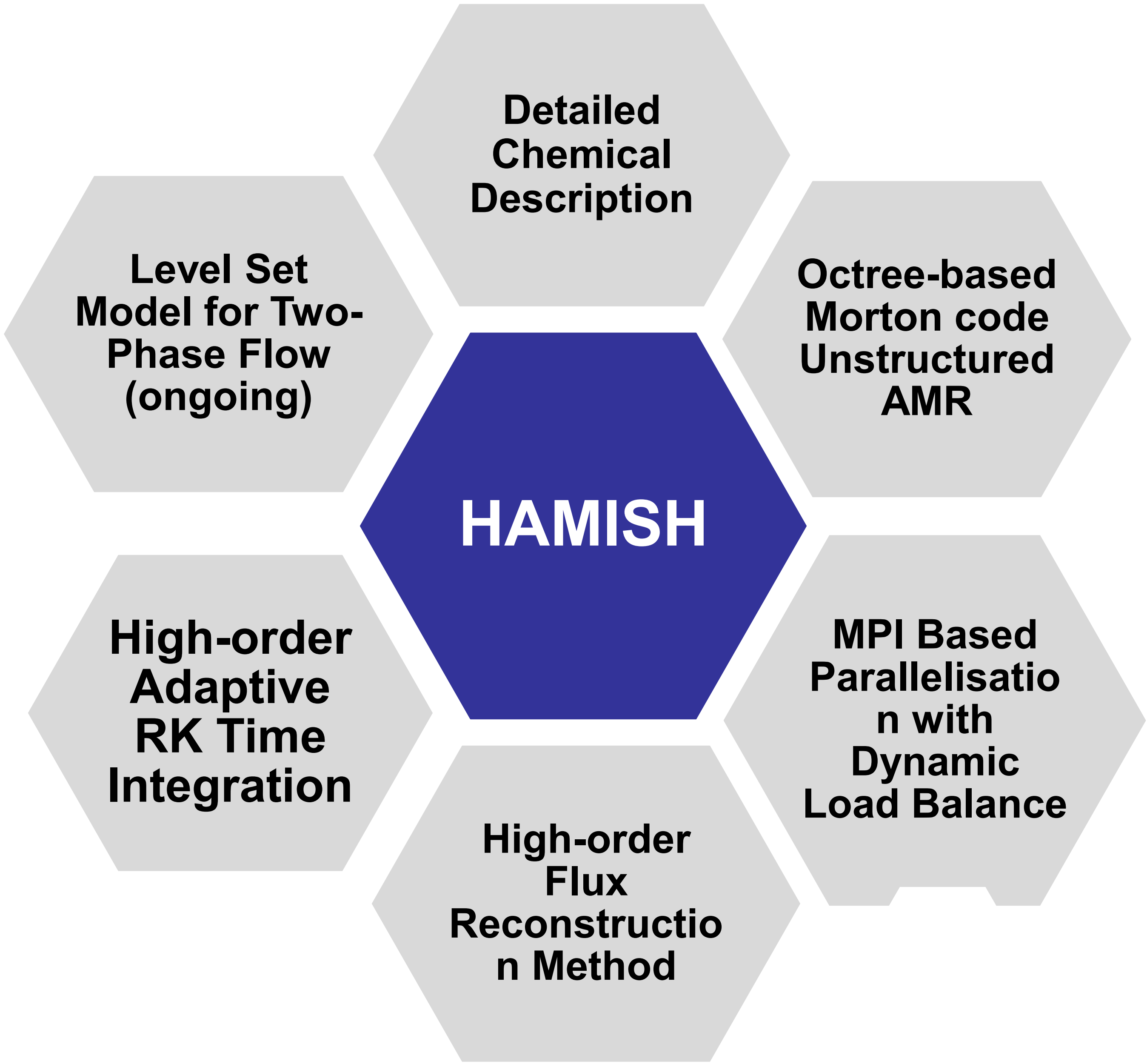
- **Flow dynamics in combustion**

Geometry Complexity
- •Swirler
- •Piston
- •Igniter
- •Spray

Interface
- •Flame front
- •Gas/Liquid interface
- •Droplets surface

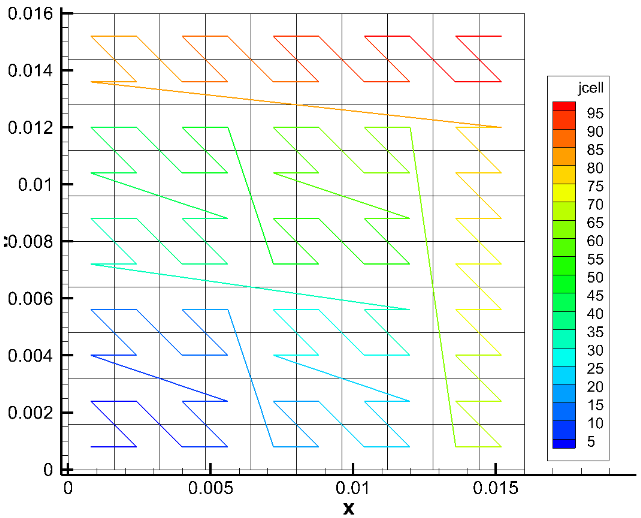


Scale-variety
- •Turbulence
- •Flame
- •Shock-wave
- •Droplets

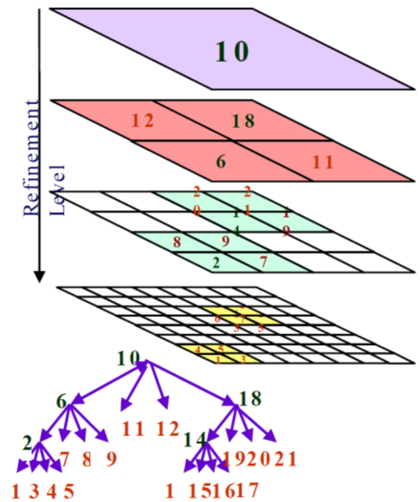

Detailed Chemical Description
Level Set Model for Two-Phase Flow (ongoing)
Octree-based Morton code Unstructured AMR
HAMISH
High-order Adaptive RK Time Integration
MPI Based Parallelisation with Dynamic Load Balance
High-order Flux Reconstruction Method

Introduction to the HAMISH Code

- **AMR in HAMISH (h-refinement)**

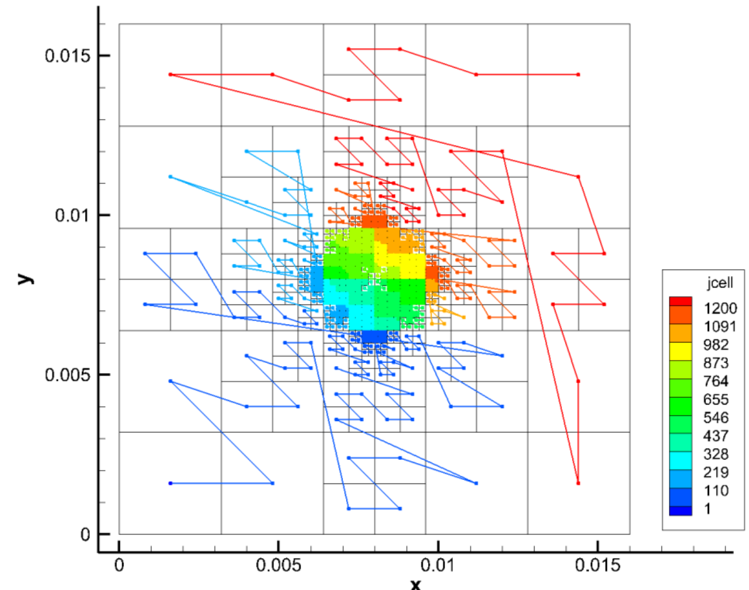


M-Code



Tree data structure

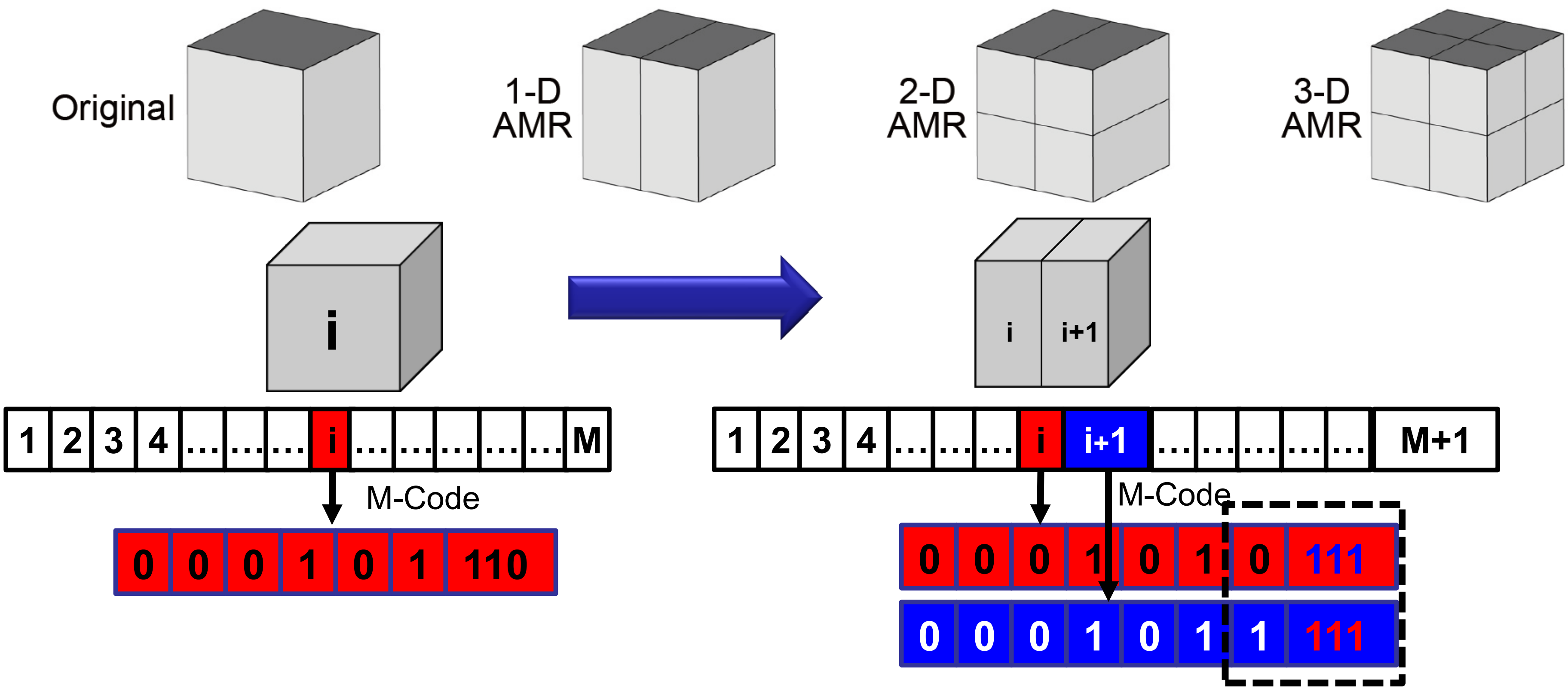
Binary tree/Quadtree/Octree



AMR cell structure

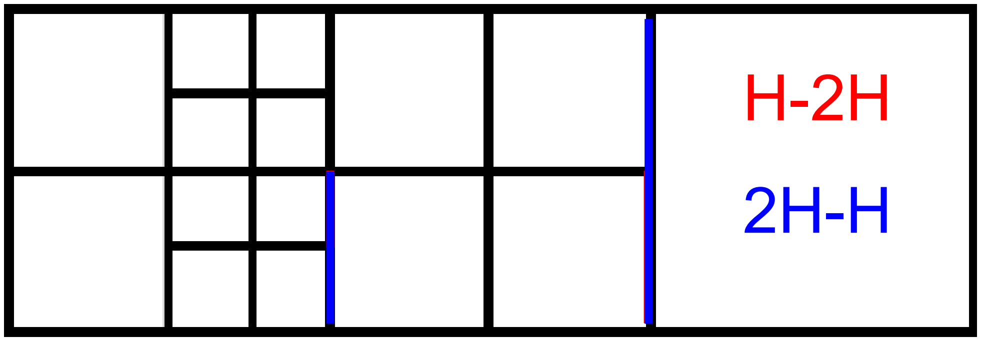
Introduction to the HAMISH Code

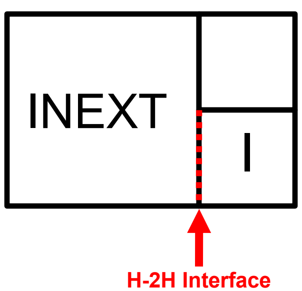
- **Data Structure**



Introduction to the HAMISH Code

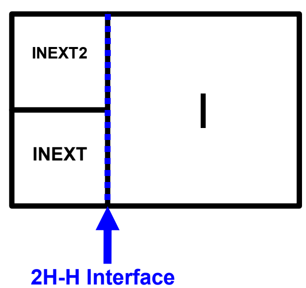
- **Flux Calculation (linear scheme)**





$$f_{Interface} = \frac{1}{2}(f_I + f_{INEXT})$$

$$\left.\frac{\partial f}{\partial x}\right|_{Interface} = \frac{(f_I - f_{INEXT})}{0.5(L_I + L_{INEXT})}$$



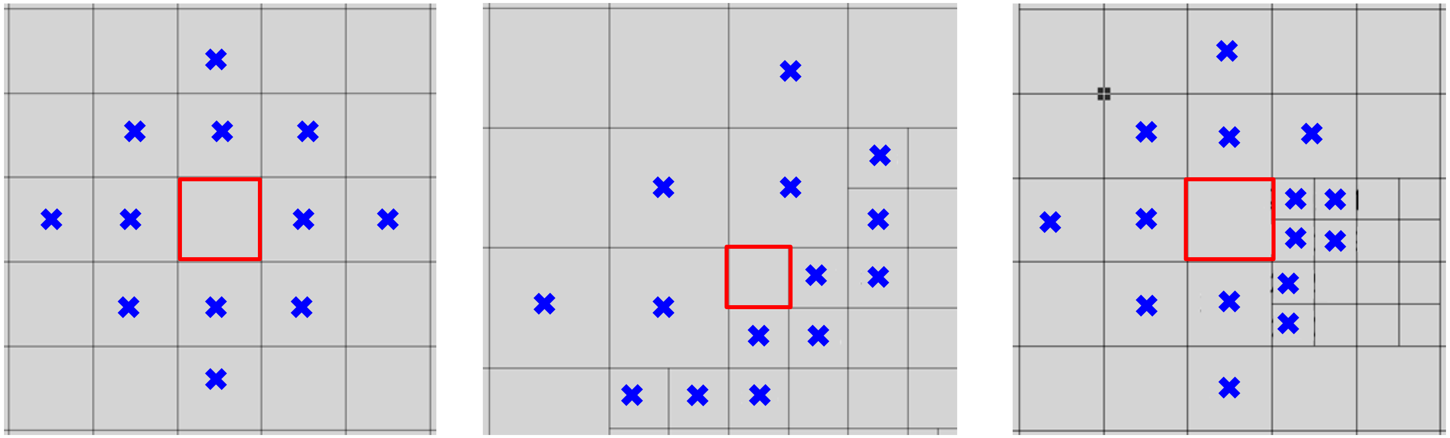
$$f_{Interface} = \frac{1}{2}(f_I + 0.5(f_{INEXT} + f_{INEXT2}))$$

$$\left.\frac{\partial f}{\partial x}\right|_{Interface} = \frac{(f_I - 0.5(f_{INEXT} + f_{INEXT2}))}{0.5(L_I + L_{INEXT})}$$

Conservation is preserved

Introduction to the HAMISH Code

- **Flux Calculation (CENO Flux Reconstruction)**



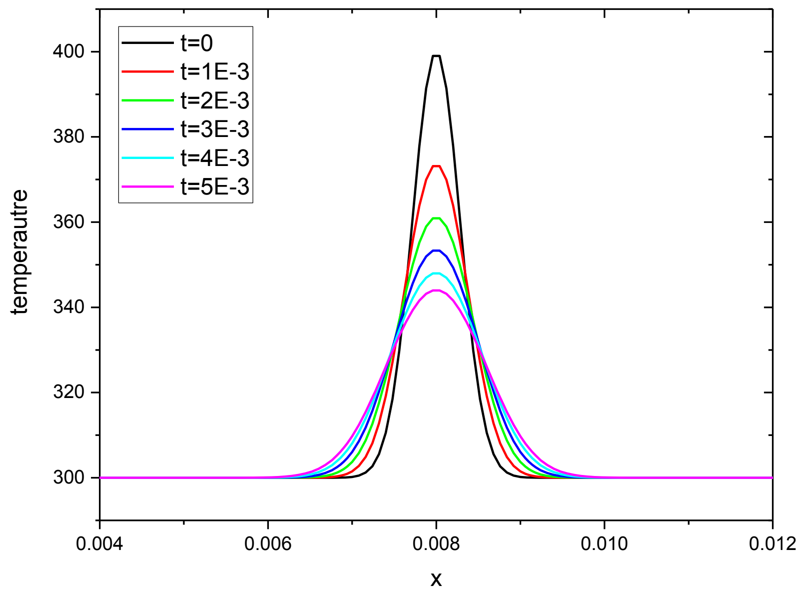
Stencil in 2D case

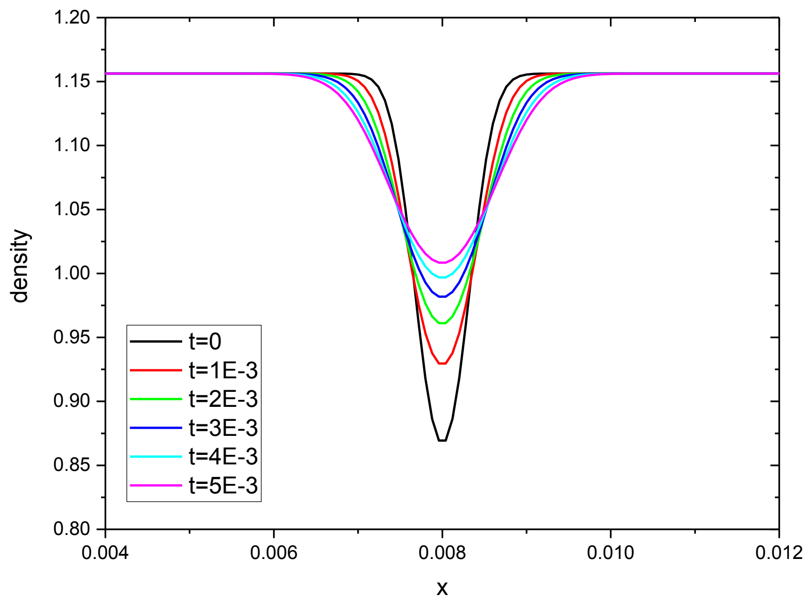
Code Tests

- **1-D thermal diffusion problem**

•Pure Diffusion Case
•Periodic Condition for All Boundaries
•No Chemical Reaction
•Initial condition

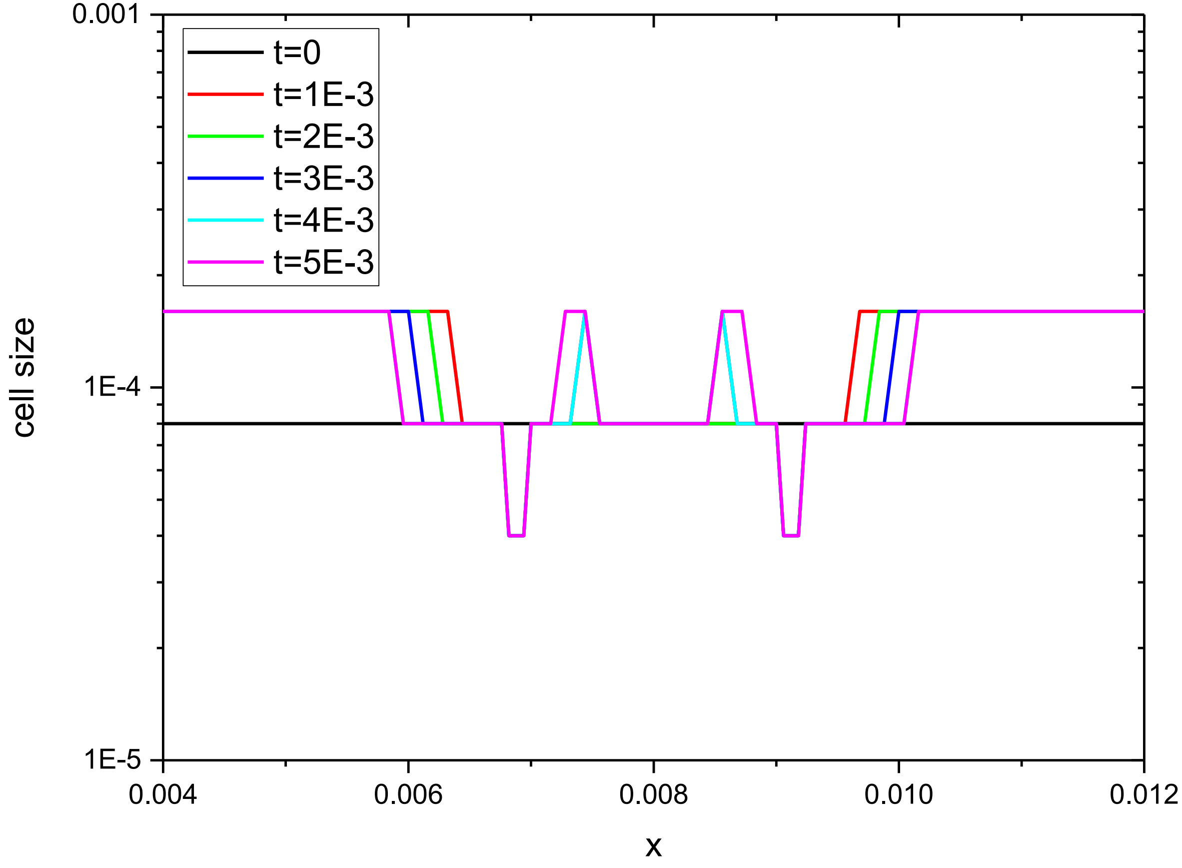
$$T = 300 + 100exp\left(-\frac{(x - x_0^2)}{4\delta}\right)$$





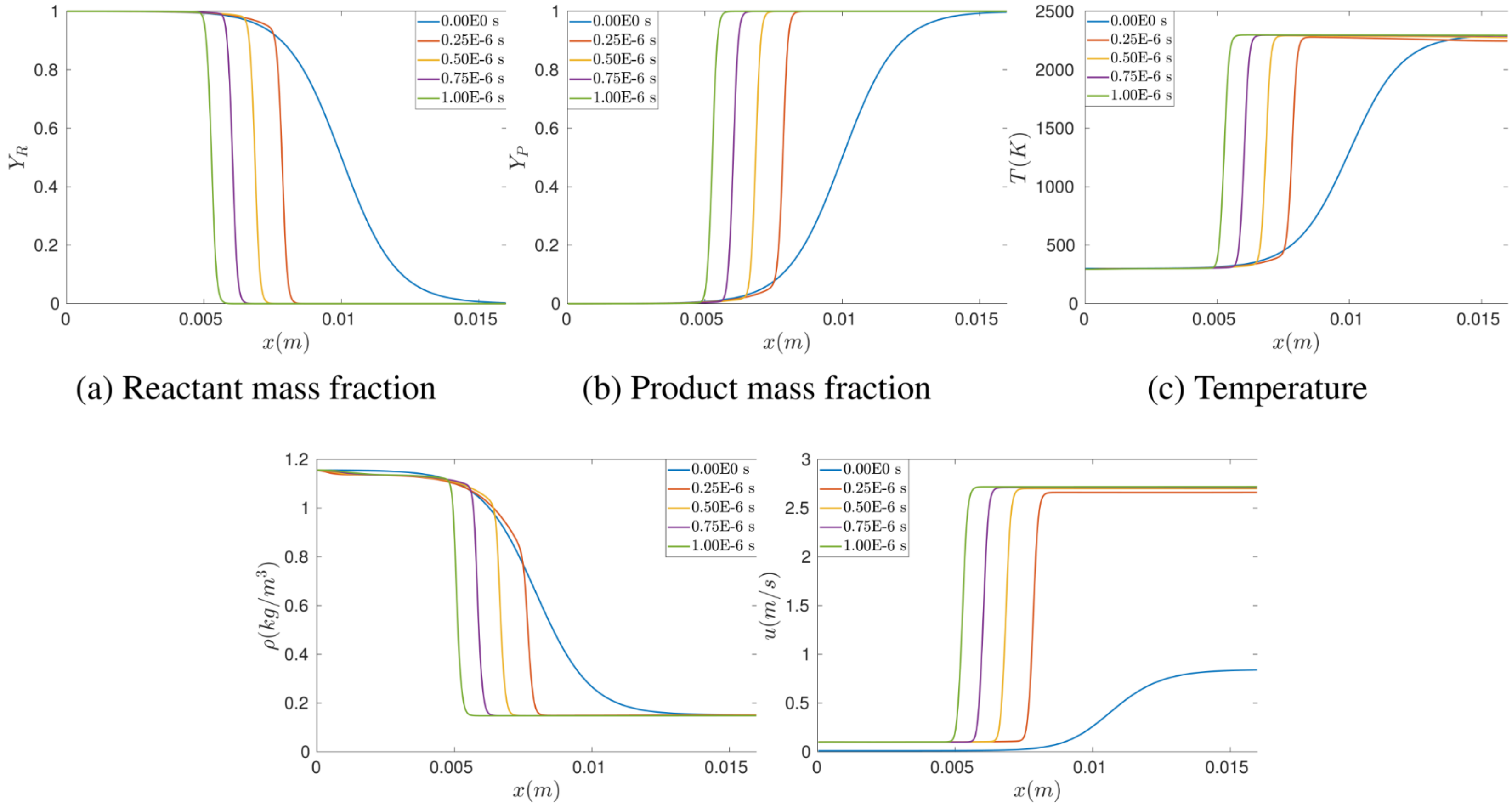
Code Tests

- **1-D thermal diffusion problem**



Code Tests

- **1-D planar flame results**



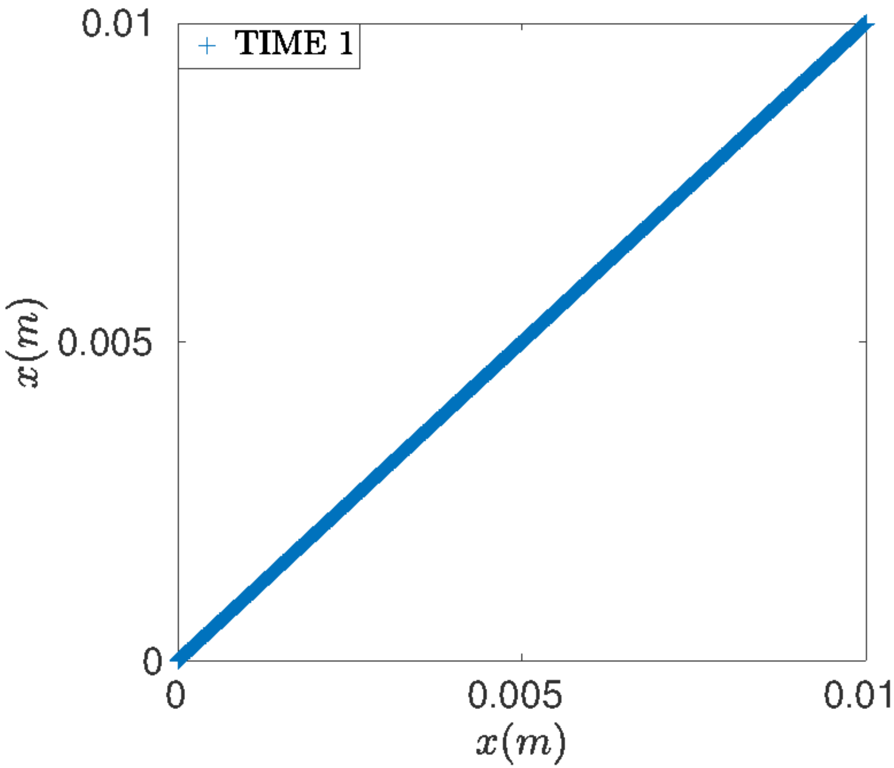
(a) Reactant mass fraction (b) Product mass fraction (c) Temperature

(d) Density (e) Velocity

Code Tests

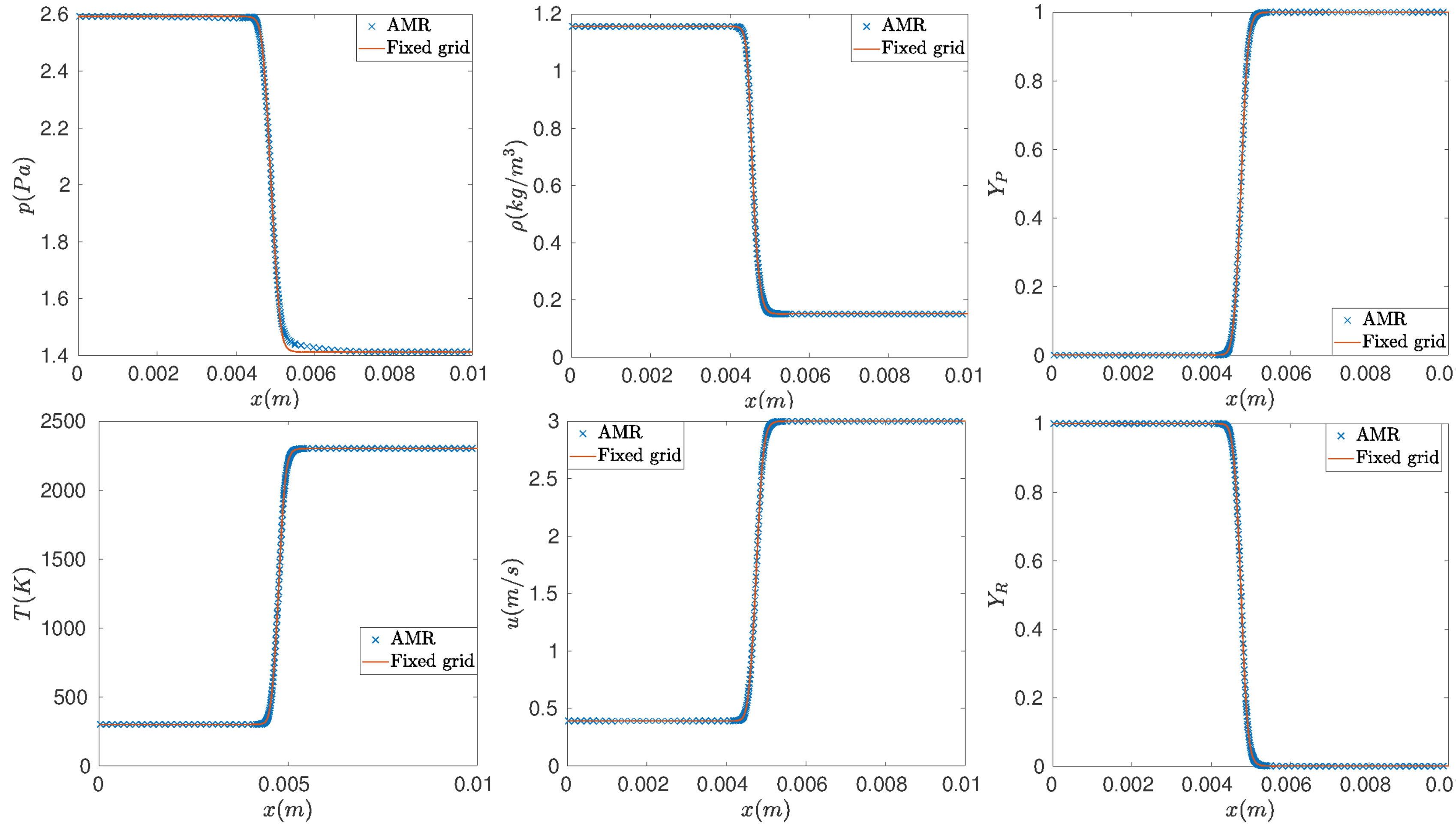
- **1-D planar flame results with AMR**

[redacted]



Code Tests

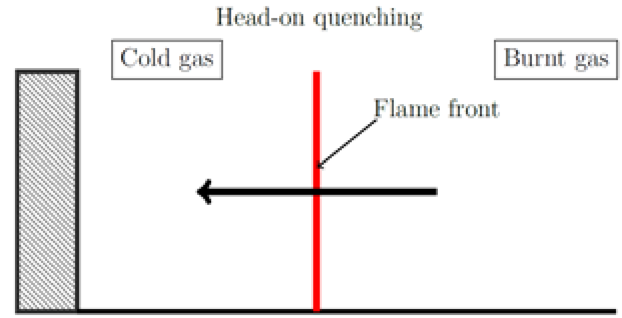
- **1-D planar flame results with AMR**

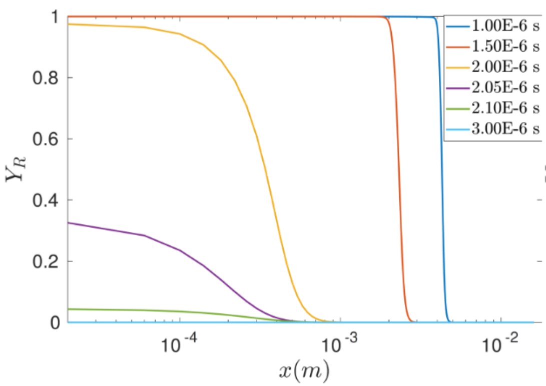


- Fixed grid simulation with 2048 cells.
- AMR simulation finished with 157 cells.

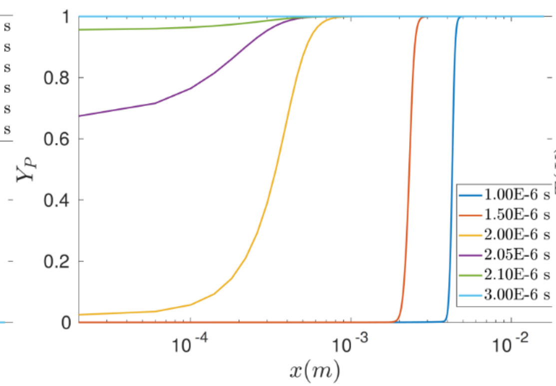
Code Tests

- **1-D HOQ flame results**

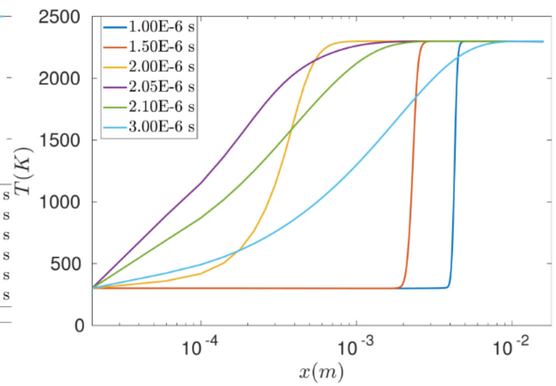




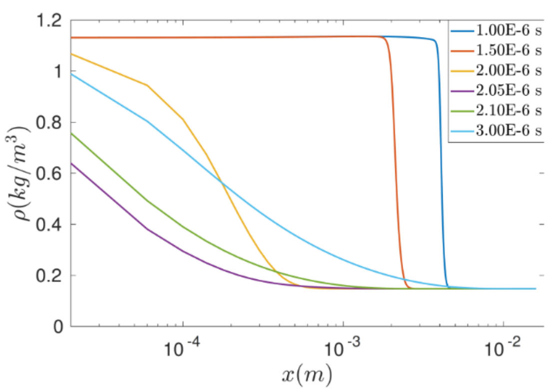
(a) Reactant mass fraction



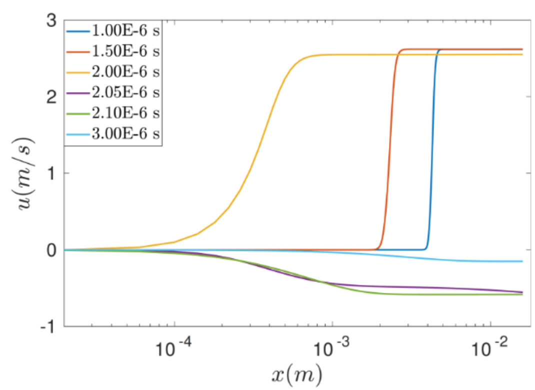
(b) Product mass fraction



(c) Temperature



(d) Density



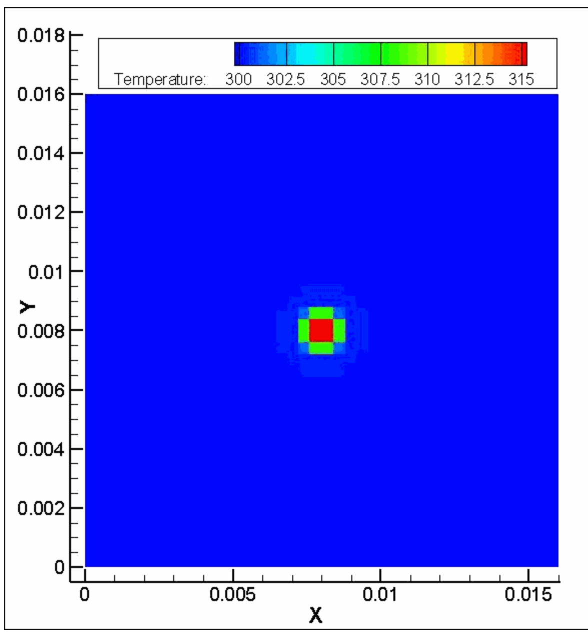
(e) Velocity

Code Tests

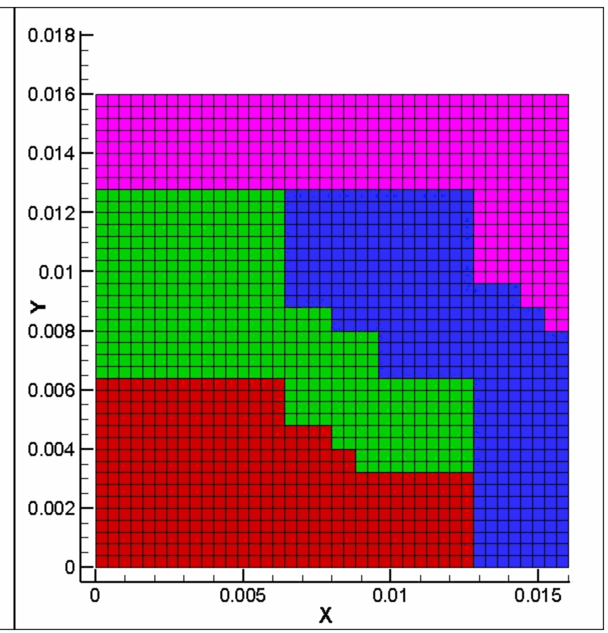
- **2-D thermal diffusion problem**

•Pure Diffusion Case
•Periodic Condition for All Boundaries
•No Chemical Reaction
•Initial condition

$$T = 300 + 100exp\left(-\frac{(x - x_0^2) + (y - y_0^2)}{4\delta}\right)$$



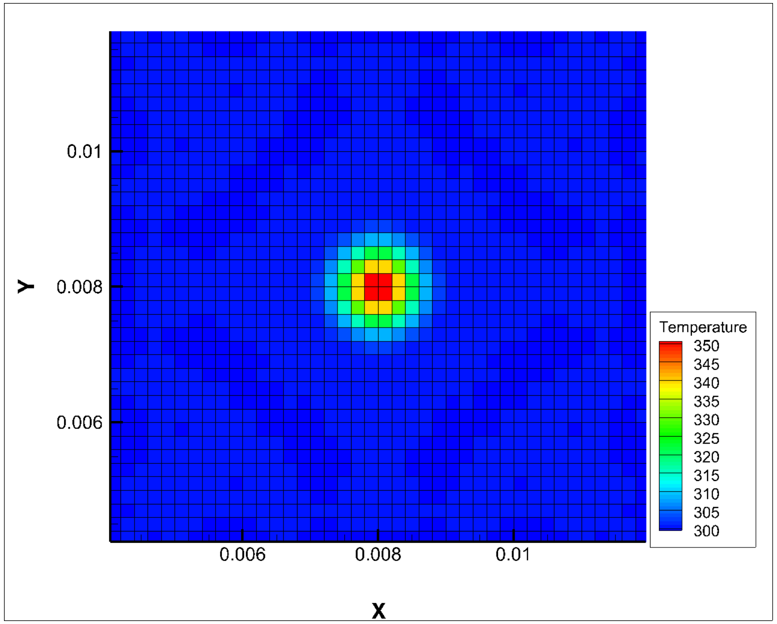
Temperature



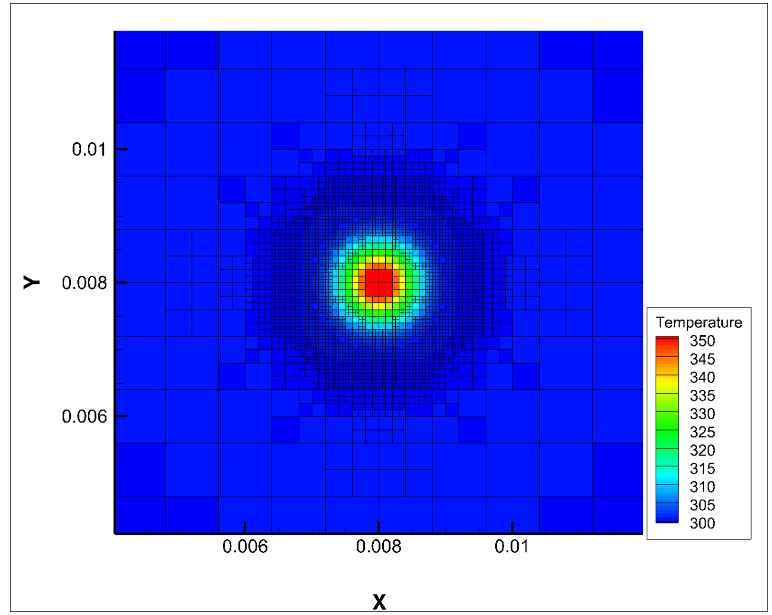
Dynamic load balance

Code Tests

- **2-D thermal diffusion problem**



HAMISH with Fixed Mesh of **6400** cells

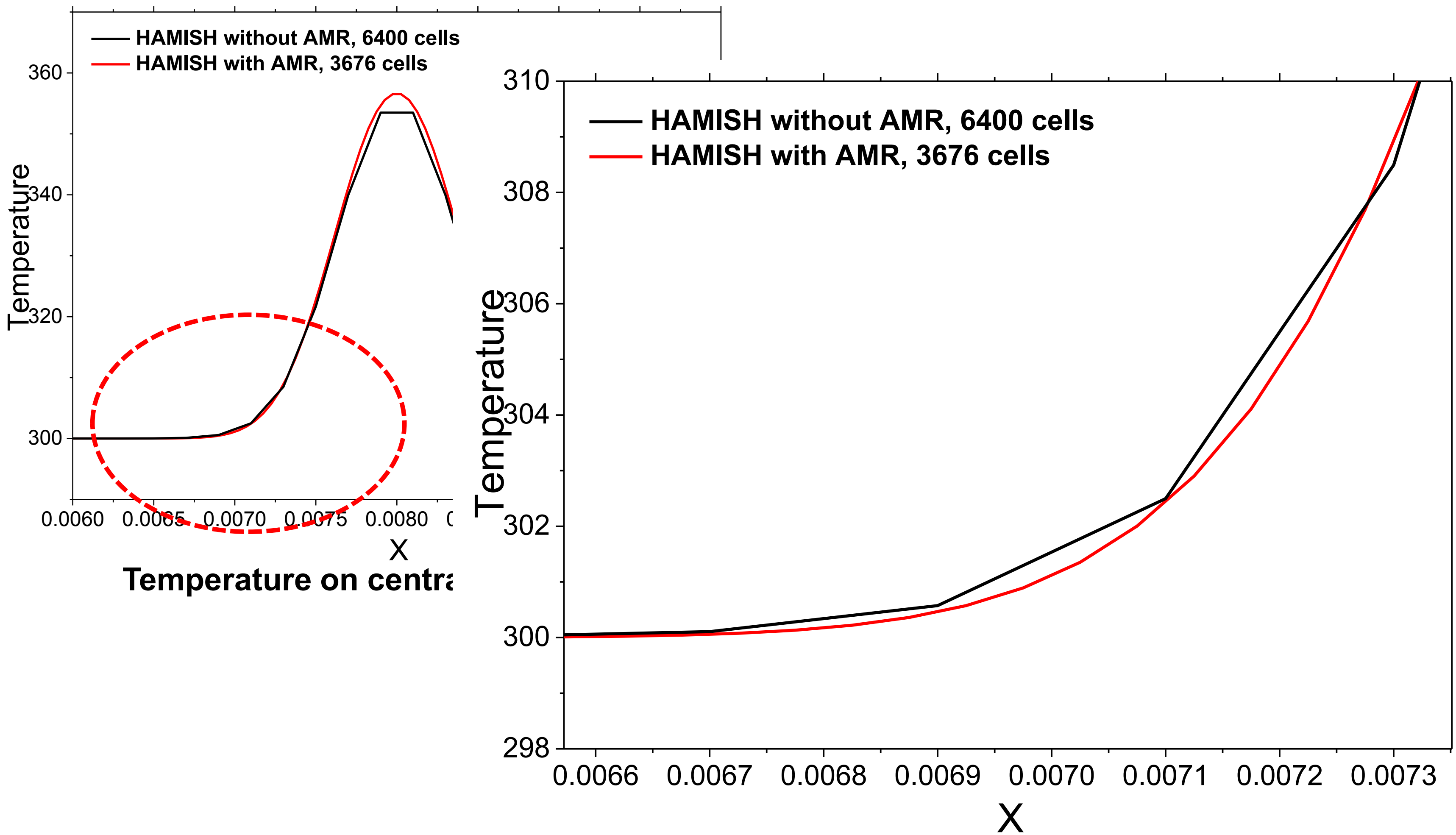


HAMISH with Adaptive Mesh of **3676** cells

Temperature at t=0.001

Code Tests

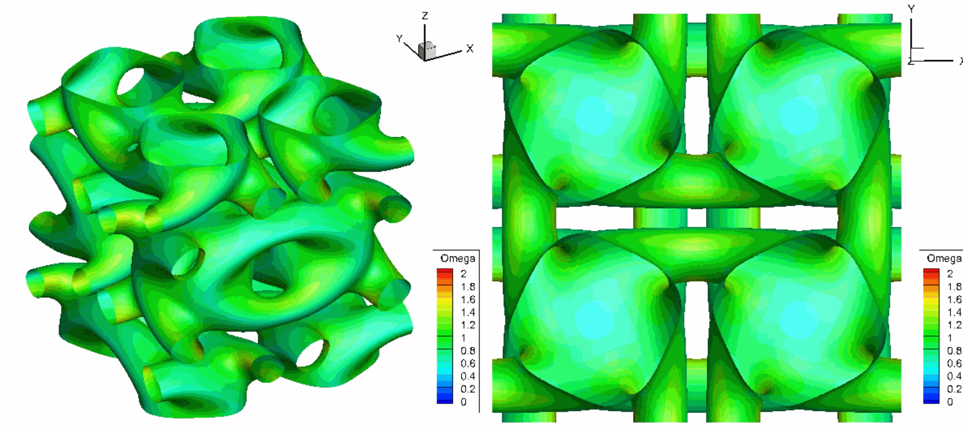
- **2-D thermal diffusion problem**



Code Tests

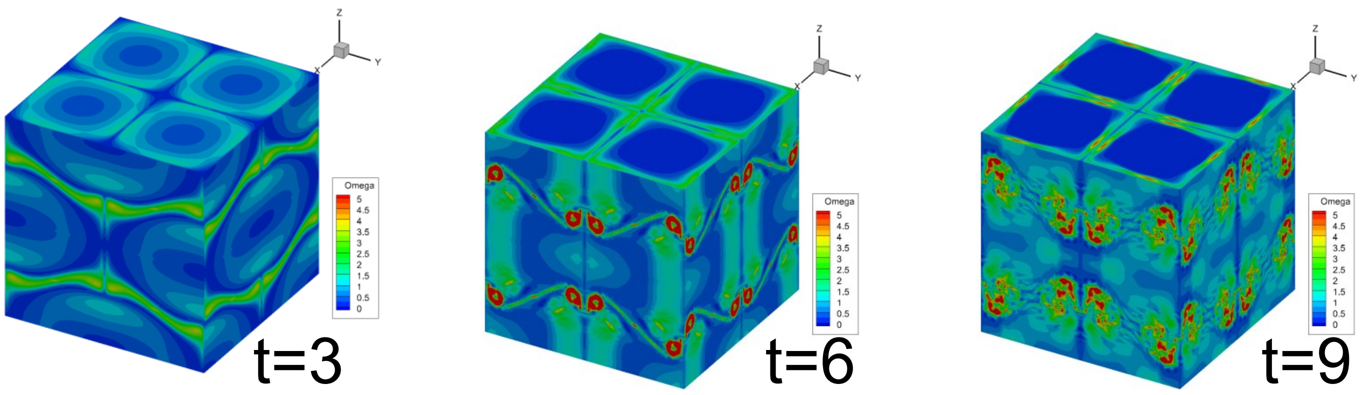
- **3-D Taylor-Green Vortex**

$$u = U_0 \sin(x/L)\cos(y\,/\,L)\cos(z\,/\,L)$$
$$v = -U_0 \cos(x/L)\sin(y\,/\,L)\cos(z\,/\,L)$$
$$w = 0$$
$$p = p_0 + \frac{\rho_0 U_0^2}{16}[\cos(2x/L) + \cos(2y/L)][\cos(2z\,/\,L) + 2]$$
$$\rho = \rho_0$$
$$T = \frac{p}{\rho R}$$



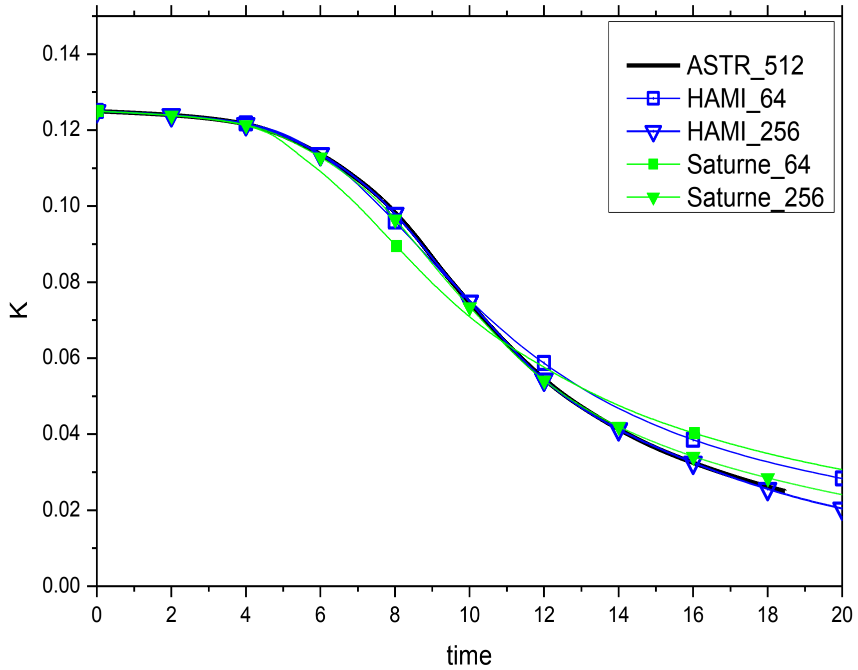
$2\pi \times 2\pi \times 2\pi$, Re=1600, Ma=0.1

J. R. Bull and A. Jameson. "Simulation of the Taylor–Green Vortex Using High-Order Flux Reconstruction Schemes", AIAA Journal, Vol. 53, No. 9 (2015), pp. 2750-2761.

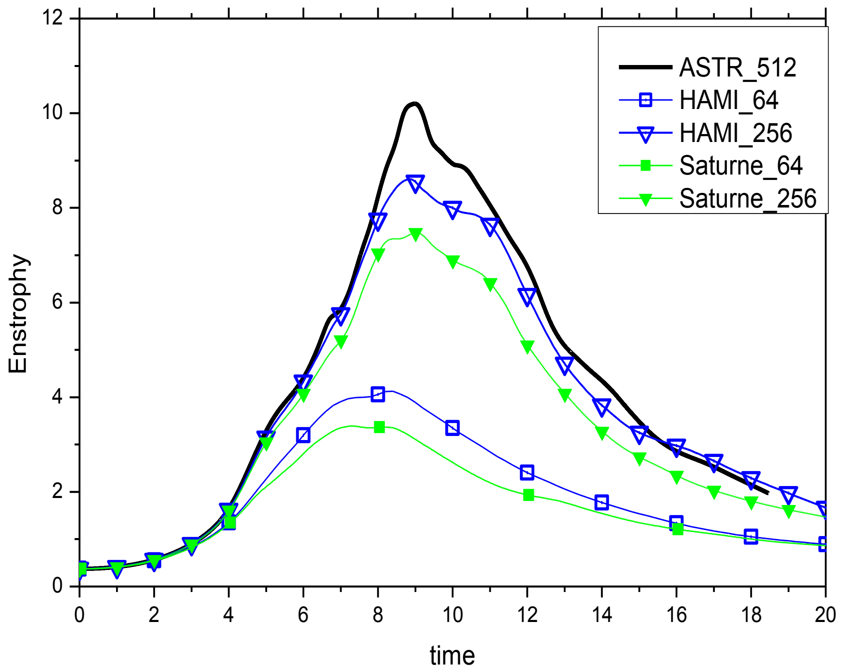


Code Tests

- **3-D Taylor-Green Vortex**



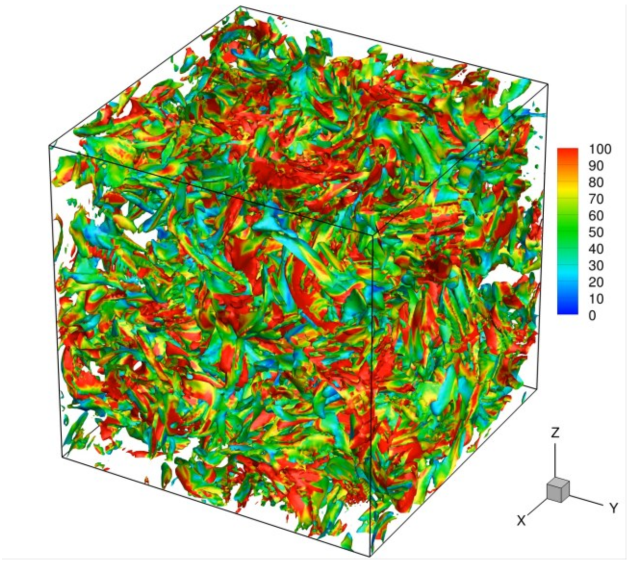
KE temporal evolution



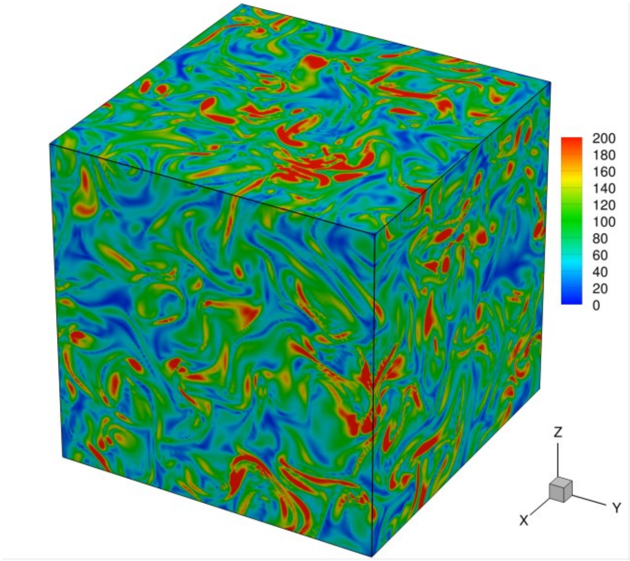
Enstrophy temporal evolution

Code Tests

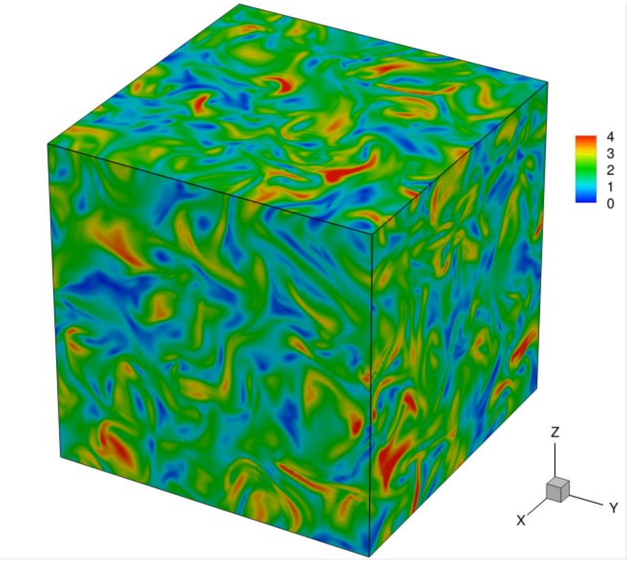
- **3-D Isotropic decaying grid turbulence**



Q-Criterion



Vorticity magnitude



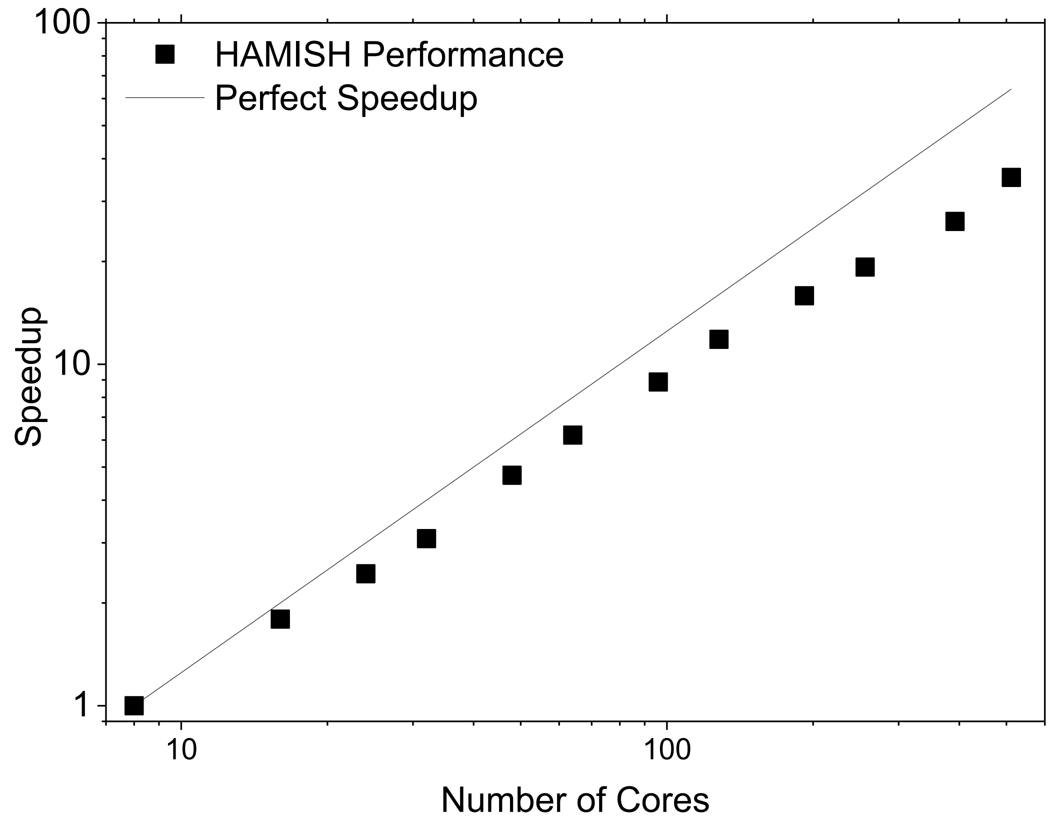
Velocity magnitude

- Fixed grid 128x128x128
- The choice of AMR criterion needs to be adjusted.
- Currently enstrophy based AMR criterion is being tested.

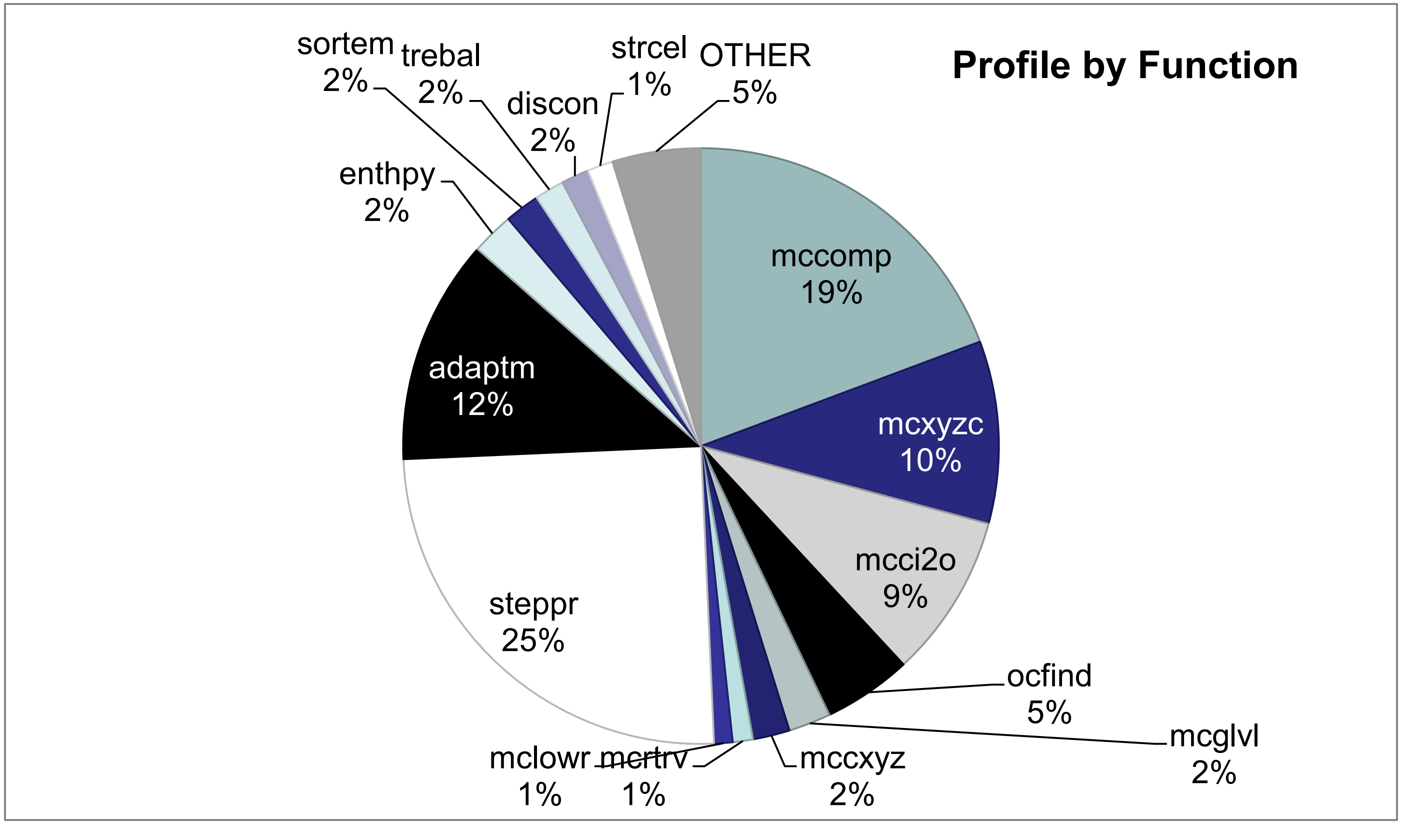
Scalability and Code Profiling

- Scalability of HAMISH with AMR off (128^3 cells)

Cores	Runtime / s	Speedup
8	1632.8	1.00
16	910.6	1.79
24	670.5	2.44
32	529.1	3.09
48	345.1	4.73
64	263.2	6.20
96	184.0	8.87
128	138.0	11.83
192	102.9	15.87
256	84.82	19.26
392	62.3	26.20
512	46.3	35.26



Scalability and Code Profiling



More than 60% of the computations of one step is cost for M-Code, Octree, AMR related subroutines.

MCCOMP	Compares two Morton codes in their entirety
MCXYZC	Converts xyz coordinates into a Morton code at the specified level
MCCI2O	Converts an encoded integer array to an octal string
OCFIND	Searches the local Octree using a given Morton code
STEPPR	Time stepping of the solution, including calculating RHS
ADAPTM	Adapts the spatial mesh

Summary and Perspectives

- The HAMISH code was tested and its accuracy was assessed.
- Good performance and scalability were observed.
- Adaptive mesh refinement presents a better capability in resolving flame front, using fewer computational cells, compared to a simulation using the fixed mesh-based solver.
- More than 60% of the CPU resource is spent in the mesh adaptation-related computations when AMR is activated at every time-step.
- The current HAMISH code shows its capability in capturing small-scale structures and interfaces in turbulent reacting flows.

- Code optimisation.
- Level set model for two-phase flow.
- Post-processing module for turbulence simulation.
- OpenMP support.

Acknowledgements

The project is supported by the UKCTRF (EP/K024574/1) and EPSRC Software Flagship Project ((EP/P022286/1).)