Test of the HAMISH code

for the 1-D/2-D Thermal Diffusion Case

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1. Introduction of the HAMISH Code

HAMISH is a CFD solver for turbulent reacting flows using the adaptive mesh refinement (AMR) technology. The Navier-Stokes (N-S) equations with mass fraction transport equations and chemical reactions are solved within the framework of cell-centred finite volume method. The cells are labelled following a Morton code [1] pattern (shown in Figure 1), and the cell-connection is dynamically build via a bintree(1-D)/quadtree(2-D)/octree(3-D).

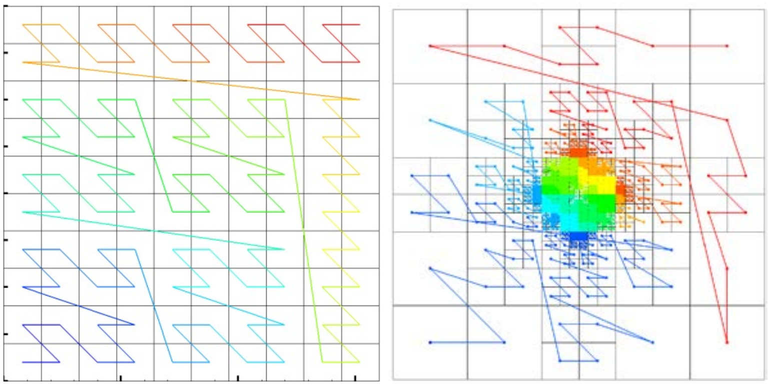


Figure 1. Example of data structure for an uniform mesh (left) and for a dynamically refined mesh using AMR (right). Both follows a Morton code pattern.

When the mesh is dynamically refined/de-refined, the maximum ratio of the size between 2 neighbouring cells is limited to 2, i.e. only h-h and 2h-h/h-2h connections are allowed (see Figure 2).

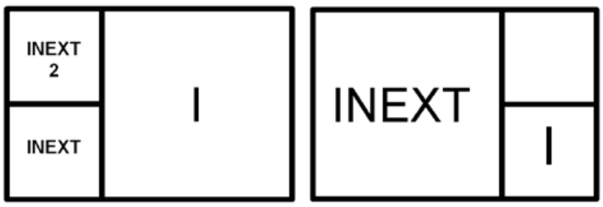


Figure 2. sketches of 2h-h (left) and h-2h (right) cell connection.

A 2nd-order central scheme is used to calculate the flux at the cell's interface, although high-order scheme with a large stencil are also possible when using a Morton code based on unstructured data.

For the 2h-h and h-2h interface, the flux is calculated as,

$$f_{1/2}^{2h-h} = \frac{f_I}{2} + \frac{f_{INEXT} + f_{INEXT2}}{4} \tag{1}$$

$$f_{1/2}^{h-2h} = \frac{f_I + f_{INEXT}}{2} \tag{2}$$

to ensure flux consistency calculated from each side for the interface.

The parallelisation of the HAMISH code is based on domain decomposition and MPI. (CM: YOU MIGHT WANT TO DEVELOP A BIT HERE, EXPLAINING HOW YOU PARTITION THE CODE AT THE MOMENT).

2. Case Description and Setup

A simple thermal diffusion problem is used as the baseline test case of the HAMISH code, in which the diffusion of an initial hot spot in the centre of the computational domain is simulated. No chemical reaction is activated and periodic conditions are applied to all boundaries.

The initial temperature field is set up in the SUBROUTINE FLAMIN, giving the formula of the 1-D case (x-direction) as,

$$T = T_0 + \Delta TC \cdot e^{-\left(\frac{x-x_c}{2\theta}\right)} \tag{3}$$

where $T_0 = 300K$, $\Delta T = 2000K$, $C = 0.05$, $x_c = 0.008$ (based on the size of domain which is[0.016]), and $\theta = 2 \times 10^{-4}$.

The code reads an input file, namely *cont.dat* where all the parameters to setup a case are available. The *cont.dat* file for the 1-D and 2-D cases are shown as follows,

```
****************************************************
**                                                **
**       HAMISH: Run control data file            **
**                                                **
****************************************************

Global domain size (x,y,z) in metres
1.6d-2  0.d0  0.d0

Global cells (nx) initial, base/max levels, step switch (0=fixed, 1=adaptive)
160      4          10          1

Time step; start step, no of steps, step switch (0=fixed, 1=adaptive)
1.0D-7    1   1000000  0

Intervals between dumps, reports, stats, results, dump o/p flag, results flag
10000    10000    10000    10000  0    0

Cold start switch (0=cold start, 1=restart), dump i/p flag (0/1=un/formatted)
0     0

Initial turbulence generator
switch (0=off, 1=new, 2=inlet); random seed; turbulence parameters Rij, L
 1      -1      1.0D0  1.0D0  1.0D0  0.0D0  0.0D0  0.0D0  5.0D-4

Flame generator switch (0=off, 1=on)
1

Default initial conditions
pressure, temperature, velocity components u,v,w, level set
 1.0D5   3.0D2   0.0D0  0.0D0  0.0D0  0.0D0
mass fractions
 2
 1    1.0D0
 2    0.0D0

Global outer boundary condition types
one per line: x-left; x-right; y-left; y-right; z-left; z-right
(1=periodic; 1a=inlet; 2b=outlet; 3c=wall; a,b,c denotes BC subtype)
(four integer and four real parameters allowed for each)
1      0    0    0   0   1.0D5     2.87D-1  1.0D-3    0.0D0
1      0    0    0   0   1.0D5     2.87D-1  1.0D-3    0.0D0
1      0    0    0   0   0.0D0     0.0D0    0.0D0     0.0D0
1      0    0    0   0   0.0D0     0.0D0    0.0D0     0.0D0
1      0    0    0   0   0.0D0     0.0D0    0.0D0     0.0D0
1      0    0    0   0   0.0D0     0.0D0    0.0D0     0.0D0

End of file
```

Initial number of cells

AMR is activated

highest level of cells

Lowest level of cells

Periodic B.C.

A 2-D case is defined

```
*************************************************
**                                             **
**        HAMISH: Run control data file        **
**                                             **
*************************************************

Global domain size (x,y,z) in metres
1.6D-2  1.6D-2    0.D0

Global cells (nx) initial, base/max levels, step switch (0=fixed, 1=adaptive)
 80      4         9        1

Time step; start step, no of steps, step switch (0=fixed, 1=adaptive)
1.0D-7   1   10000000  0

Intervals between dumps, reports, stats, results, dump o/p flag, results flag
1000   1000    1000   1000  0    0

Cold start switch (0=cold start, 1=restart), dump i/p flag (0/1=un/formatted)
0     0

Initial turbulence generator
switch (0=off, 1=new, 2=inlet); random seed; turbulence parameters Rij, L
 0      -1      1.0D0  1.0D0  1.0D0  0.0D0  0.0D0  0.0D0  5.0D-4

Flame generator switch (0=off, 1=on)
1

Default initial conditions
pressure, temperature, velocity components u,v,w, level set
 1.0D5   3.0D2   0.0D0  0.0D0  0.0D0  0.0D0
mass fractions
 2
 1    1.0D0
 2    0.0D0

Global outer boundary condition types
one per line: x-left; x-right; y-left; y-right; z-left; z-right
(1=periodic; 1a=inlet; 2b=outlet; 3c=wall; a,b,c denotes BC subtype)
(four integer and four real parameters allowed for each)
1      0    0    0   0   0.0D0     0.0D0    0.0D0     0.0D0
1      0    0    0   0   0.0D0     0.0D0    0.0D0     0.0D0
1      0    0    0   0   0.0D0     0.0D0    0.0D0     0.0D0
1      0    0    0   0   0.0D0     0.0D0    0.0D0     0.0D0
1      0    0    0   0   0.0D0     0.0D0    0.0D0     0.0D0
1      0    0    0   0   0.0D0     0.0D0    0.0D0     0.0D0

End of file
```

3. Results

Both 1-D and 2-D cases are simulated using 4 MPI tasks.

3.1. 1-D case

The temperature profiles at t=0 s to t=10^{-2} s are shown in Figure 3 (left), from which we can see the reduction of the peak of temperature and the widening of the heat source, which is typical to a thermal diffusion process. The profile of the cells' size is also shown in Figure 3 (right). The mesh is refined at the edge of the heat source, where the gradients are the steepest and de-refined elsewhere. The history of the total number of cells is presented in Figure 4 which shows the dynamic change of the mesh. The total number of cells is largely reduced from the initial value during the first 4 time-steps.

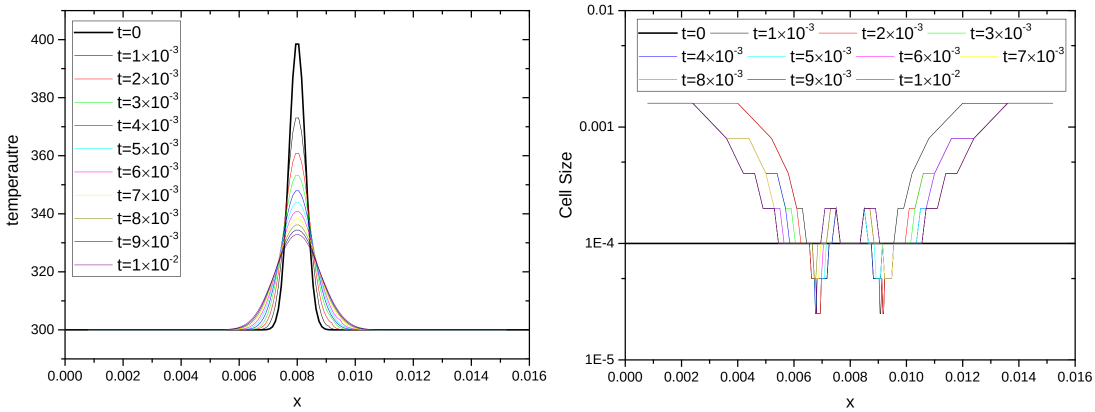


Figure 3. Profiles of temperature (left) and cell size (right) from t=0 s to t=10^{-2} s.

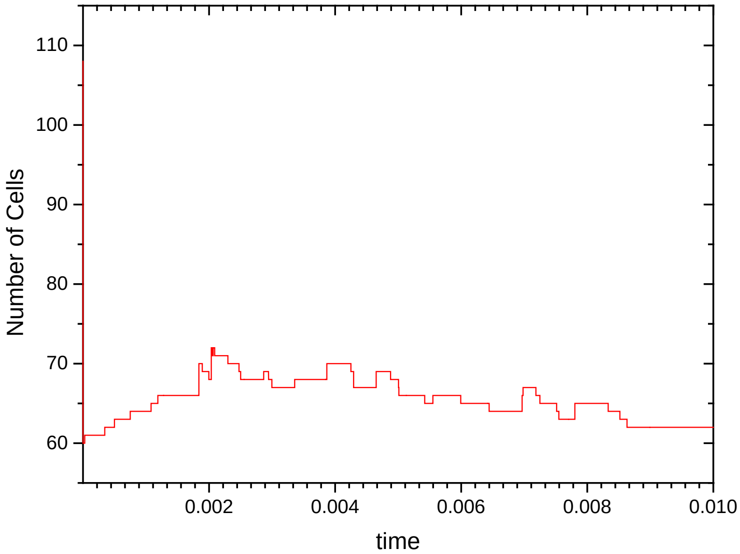


Figure 4. Temporal evolution of the total number of cells.

3.1. 2-D case

The temperature field at t=0 s, 5×10^{-4} s, 1×10^{-3} s, 1.5×10^{-3} s is shown in Figure 5 and a movie is provided from t=0 s to t=5×10^{-3} s (see Animation 1). The diffusion of the central heat source can be seen with the mesh being refined around the edge of the heat source and de-refined in the rest of the field. The temperature profile across the centre line is shown in Figure 6, and a faster reduction of the peak temperature than for the 1-D case is observed, as presented in Figure 6 (right).

The history of the total number of cells is shown in Figure 7, and we can see that the mesh being refined during the simulation.

The distribution of the cells in the four MPI processors is shown in Figure 8, presenting the migration of cells among processors by the following two subroutines, SUBROUTINE PARBALM and SUBROUTINE PAROCTINT for the purpose of load balance.

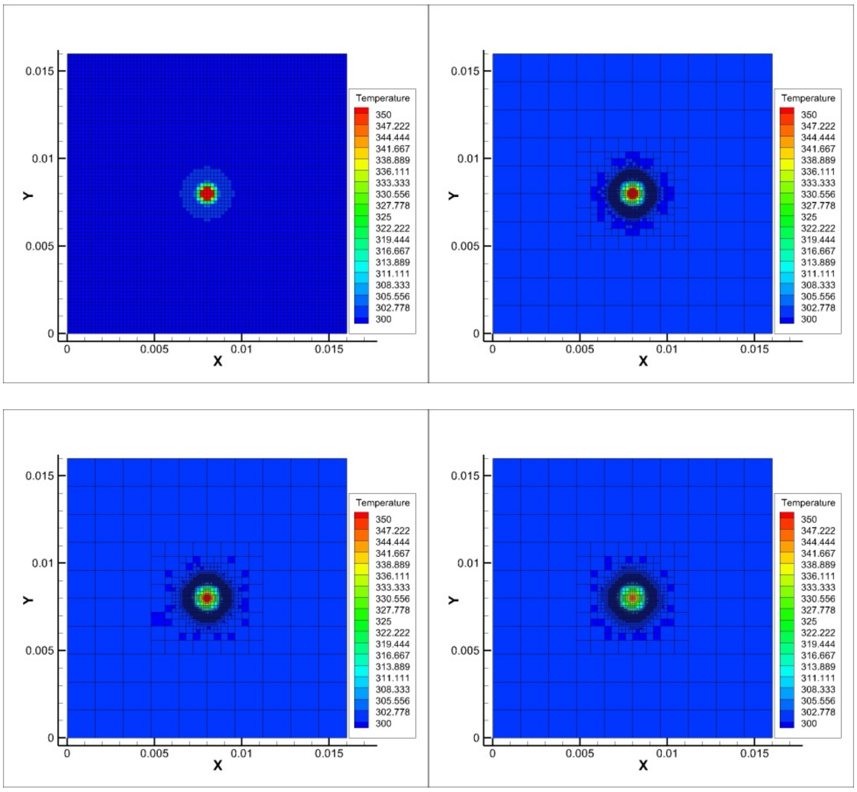
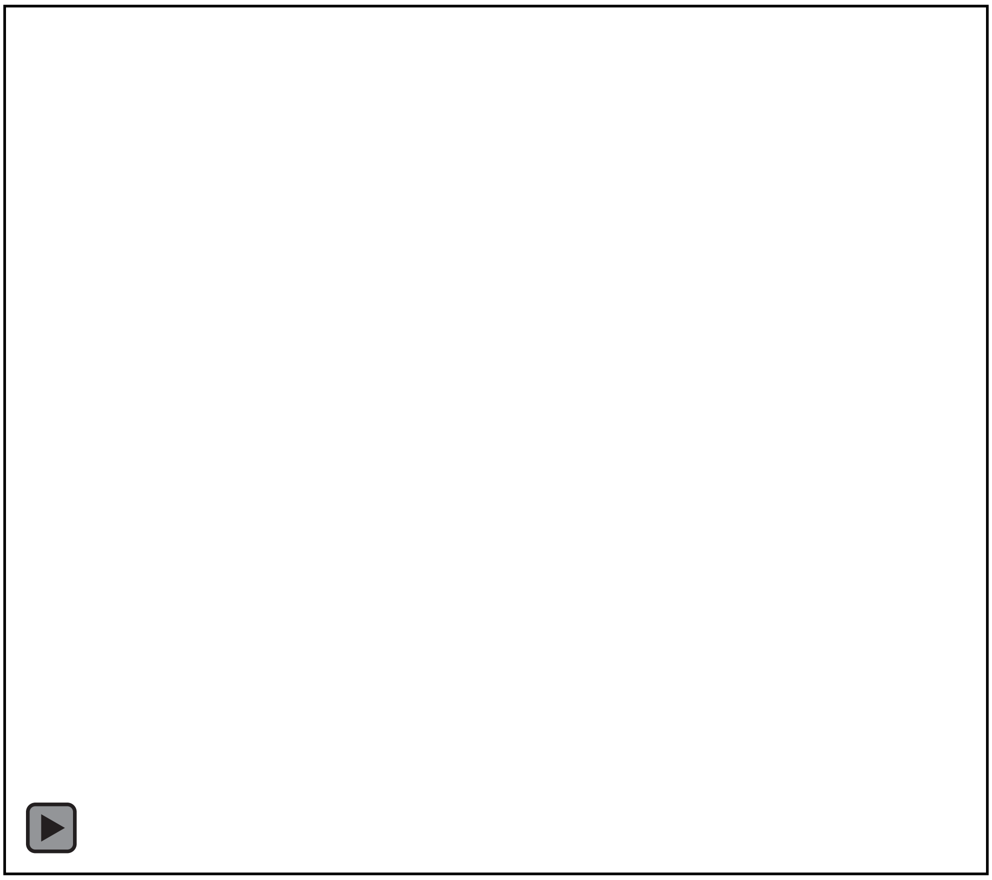


Figure 5. Temperature field at t=0 s, 5×10^{-4} s, 1×10^{-3} s, 1.5×10^{-3} s.



Animation 1. Temperature field from t=0 s to t=5×10^{-3}s.

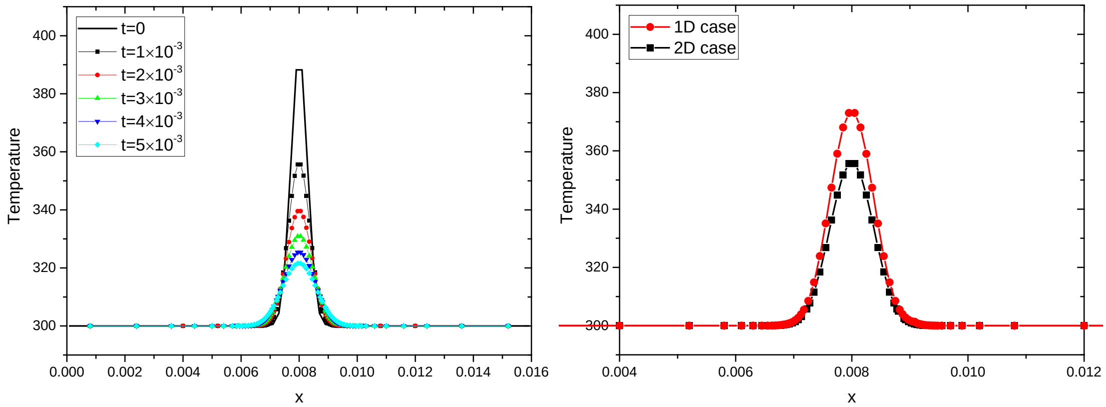


Figure 6. Temperature profiles across the centre line (y=0.008 m) from t=0 s to t=5×10^{-3} s (left) and comparison between 1-D and 2-D profiles at t=1×10^{-3} s (right).

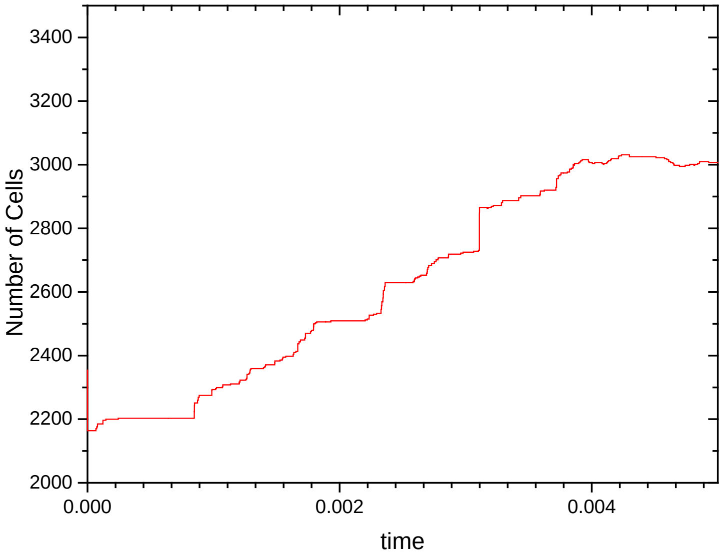


Figure 7. Temporal evolution of the total number of cells.

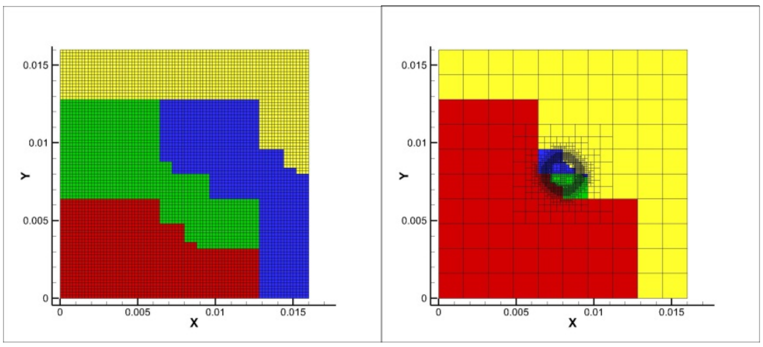


Figure 8. Cell distributions per MPI processor at t=0 s (left) and t=1.5×10^{-3} s (right). Red corresponds to processor 0, Green to processor 1, Blue to processor 2 and Yellow to processor 3.

3. Summary

The HAMISH code has been validated, focusing on dynamic mesh refinement for a simple thermal diffusion case. Both 1-D and 2-D cases are studied. The mesh is properly refined around the edge of the heat source and de-refined in the rest of the domain. The flow field is smooth and free of wiggles, which indicates that the flux construction and flow interpolation functionalities work well.

Reference

[1] Morton, G. M. (1966), A computer Oriented Geodetic Data Base; and a New Technique in File Sequencing, Technical Report, Ottawa, Canada: IBM Ltd