Physical Models, Post Processing

Michael A. Gallis

Engineering Sciences Center
Sandia National Laboratories
Albuquerque, New Mexico, USA

magalli@sandia.gov

DSMC15 Short Course

Sept. 2015 – Kapaa, Hawaii

U.S. DEPARTMENT OF ENERGY

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

NNSA National Nuclear Security Administration

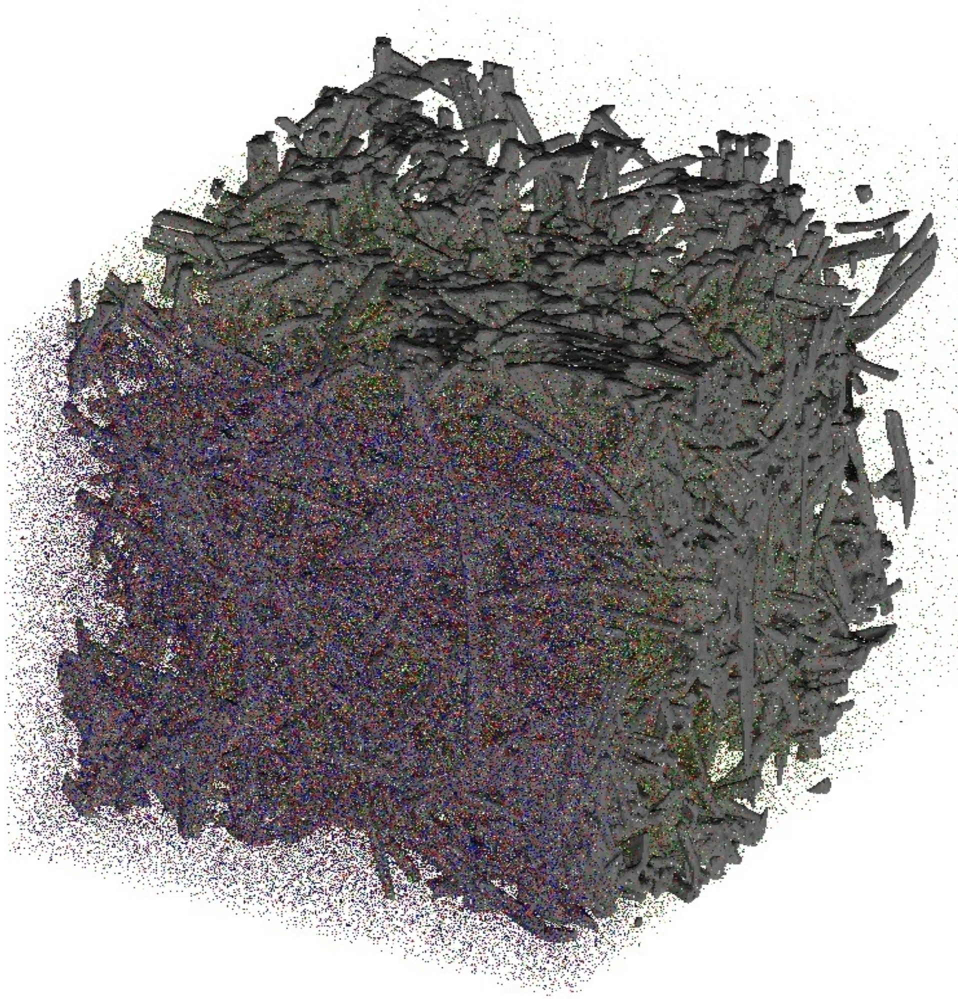
Physical Models in Sparta

- **Molecular models**
  - VSS, VHS
- **Energy Exchange**
  - Continuous Borgnakke Larsen with variable relaxation rates.
  - Quantized vibrational mode (diatomics only)
- **Chemical Reactions**
  - TCE
  - QK (diatomics only) Currently using the same data files.
- **Ionized flows**
  - Ambipolar diffusion
  - No electrostatic fields

Boundary conditions

- **Inflow**
  - Hypersonic free stream
- **Outflow**
  - Outflow (vacuum)
  - Specular and diffuse walls
  - Axis of symmetry
  - Chemically reacting walls (absorption, dissociation, exchange)

Surface Recession on Ablative Thermal Protection System



- Marching Cube algorithm used to generate surface
- Surface moves in time
- Formation of CO and CO_2 molecules during surface oxidation
- Extension of surface chemistry model to new reactions
- Addition of new gas chemical reactions
- Study of multiple porous media used to to manufacture TPS: FiberForm, felts, woven TPS…

A. Borner, F. Panerai, N. N. Mansour
NASA Ames Research Center:
Session 5 - Tuesday 12:40pm

Inflow boundary conditions

- Currently the open-loop hypersonic inflow boundary condition has been implemented
  - Bird 1994 eq. 4.65
- Uniform conditions or variable from file
- The inflow boundary condition can be applied to:
  - Bounding box
  - Surfaces

Grid adaptation

- User specified
  - Multiple levels (up to 16 in 64 bit architecture)

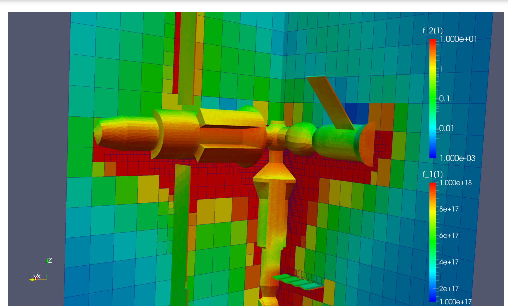
```
create_grid 100 100 100 level 2 25*75 25*75 25*75 2 2 2
create_grid 5 5 1 level 2 * * * 5 5 1 level 3 * * * 2 2 1
```

- Automated grid adaptation
  - Static

```
adapt_grid refine coarsen surf 0.15 iterate 1 dir 1 0 0
```

  - Dynamic

```
fix 10 adapt 10 refine coarsen value c_1[1] 4500 5500 &
fix 10 adapt 100 refine coarsen value c_1b[2] 1.00 2.00 &
      combine min thresh less more  maxlevel 5 cells 2 2 1
```



Steady State in Sparta

- Traditional DSMC codes define "steady state" at some time during the run.

- Sparta defines a series of "runs"
- Steady state is defined as a run where the maximum collision probability is not re-set.
- Moment accumulators are reset between runs
- Moments are accumulated as instantaneous or running averages during runs

Output in Sparta

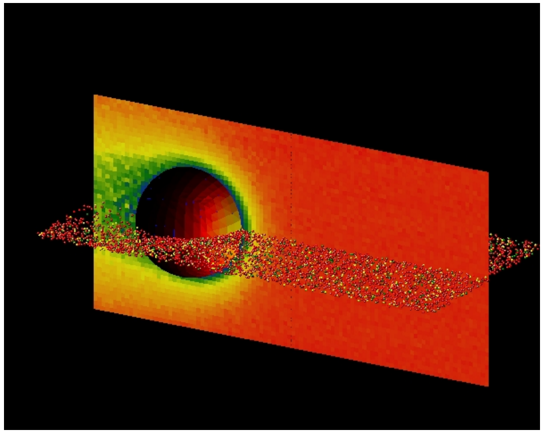
- Grid output

```
compute             2 grid all nrho temp trot
fix                 2 ave/grid 1 1000 1000 c_2 ave one
compute             4 tvib/grid species
fix                 4 ave/grid 1 1000 1000 c_4 ave one
compute             5 sonine/grid all thermal
fix                 5 ave/grid 1 1000 1000 c_5 ave running
dump                1 grid all 1000 tmp_flow.%.* id f_2 f_4 f_5
```

- surface output

```
compute             3 surf all all press ke
fix                 3 ave/surf all 1 1000 1000 c_3 ave running
dump                3 surf all 1000 tmp_surf.* id f_3
```

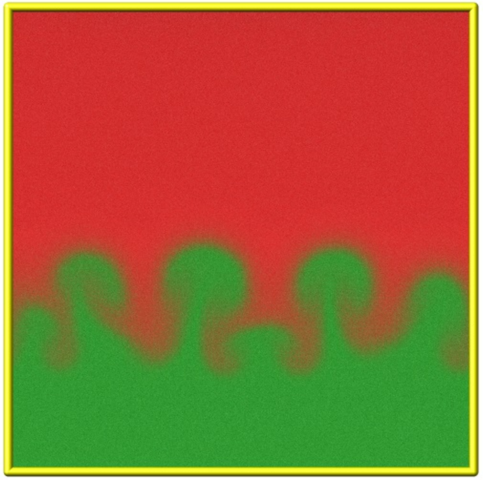
In-Situ Visualization



Not a replacement for interactive viz, but ...
Quite useful for debugging & quick analysis
At end of simulation (or during), instant movie

Render a JPG snapshot every N time steps:

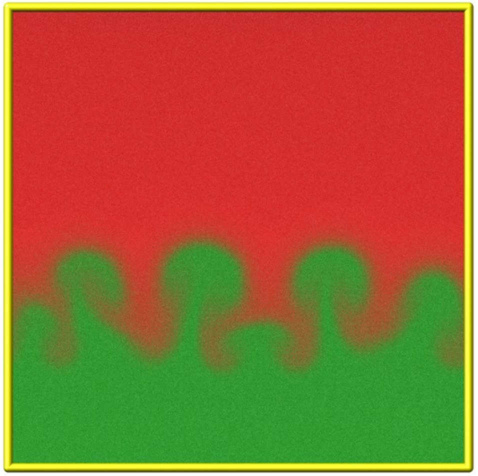
- Each processor starts with blank image (1024x1024)
- Processor draws its cells/surfaces/molecules with depth-per-pixel
- Merge pairs of images, keep the pixel in front, recurse
- Draw is parallel, merge is logarithmic (like MPI Allreduce)

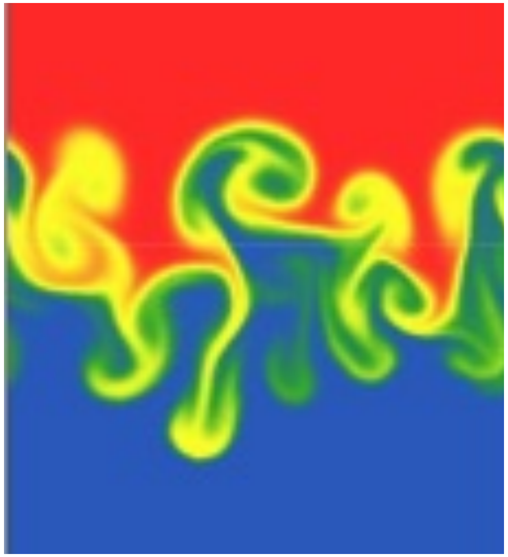


Images are ray-traced quality

In-Situ Visualization in Sparta

- Options
  - Color molecules in cells





  - Color cell according to some variable (density)
- Extract **quantitative** data using image processing software
  - Full output is a computationally **very** expensive operation
  - There is a memory overhead for this operation

Examples of in-situ Visualization Richtmyer-Meshkov Instability (RMI)

At pre-defined time steps, JPEG images were created in which each cell of the domain was colored to represent the gas with the most molecules in it.

Through image analysis, the time-stamped series of images was post-processed to provide quantitative values for the instability growth.

Field Post Processing for Paraview

- Python scripts operate on surface and field data
  - grid2paraview.py
  - The script will launch as many threads as needed (maximum the number of cores on the machine)

```
pvpython grid2paraview.py shuttle_slice.txt flow -r tmp_flow.*.1000 –xc
100 –yc 100 –zc 100
```

- Example of *.txt file

```
dimension           3
create_box          -4.0 6.0 -5.0 5.0 -5.0 5.0
read_grid           grid.5000
create_grid         10 10 10
```

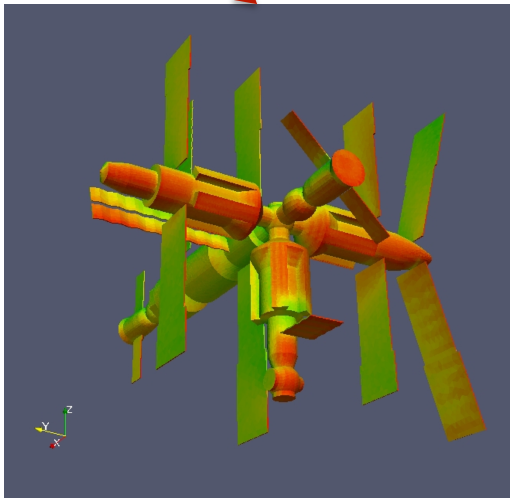
- Slicer for 3D flow fields
  - For 3D flow fields grid2paraview can process pre-specified slices of the 3D domain
  - ```
    slice               1 0 0 0.0 0.0 0.0
    slice               0 1 0 0.0 0.0 0.0
    slice               0 0 1 0.0 0.0 0.0
    ```
    ```

Surface post-processing

- Surface python script
  - surf2paraview.py

```
pvpython surf2paraview.py sdata.shuttle surf -r tmp_surf.*.1000
```

Surface description



In situ-Paraview

- Paraview (http://www.paraview.org) can also be used in-situ.
- Fix command in input script

```
fix me catalyst 100 script.txt
```

- Paraview command file

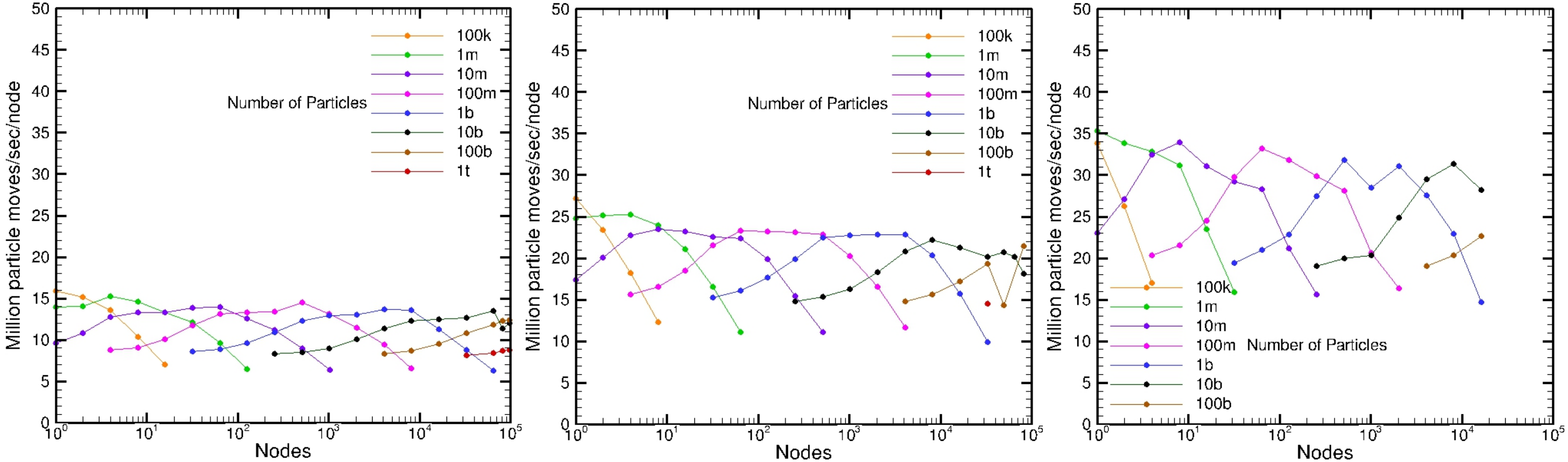
```
begin catalyst
  color by scalar = f_1[2]
  show axes = true
  show orientation axes = true
  show edges = true
  clip = point 0.0 0.0 0.0 normal 0 1 0
end
```

SPARTA Benchmarking

- Flow in a closed box
  - Stress test for communication
    - No preferred communication direction
  - 3D regular grid, 10^4-10^{11} (0.1 trillion) grid cells
  - 10 molecules/cell, 10^5-10^{12} (1 trillion) molecules
- Effect of threading
  - 2 threads/core = 1.5 speed
  - 4 threads/core = 2x speed

SPARTA Benchmarking

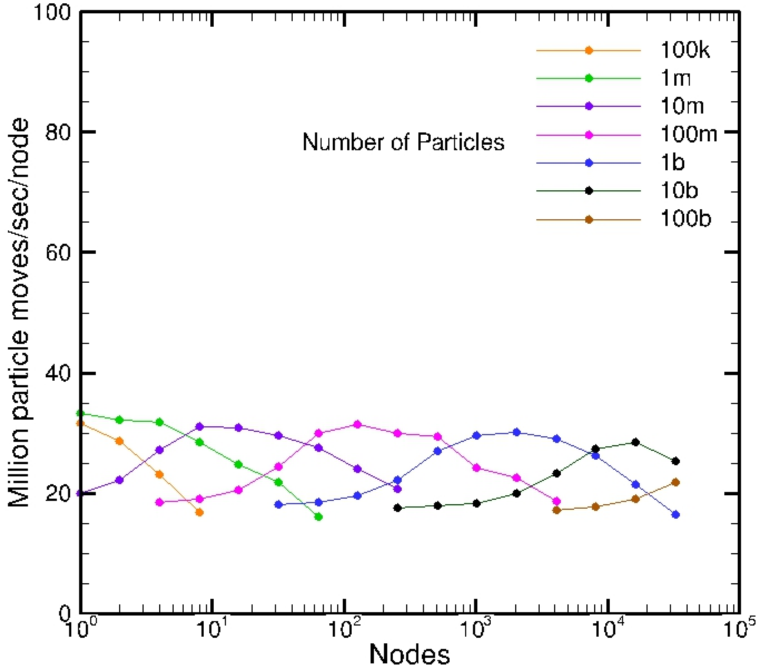
16 cores/node 1 task/core	16 cores/node 2 tasks/core	16 cores/node 4 tasks/core



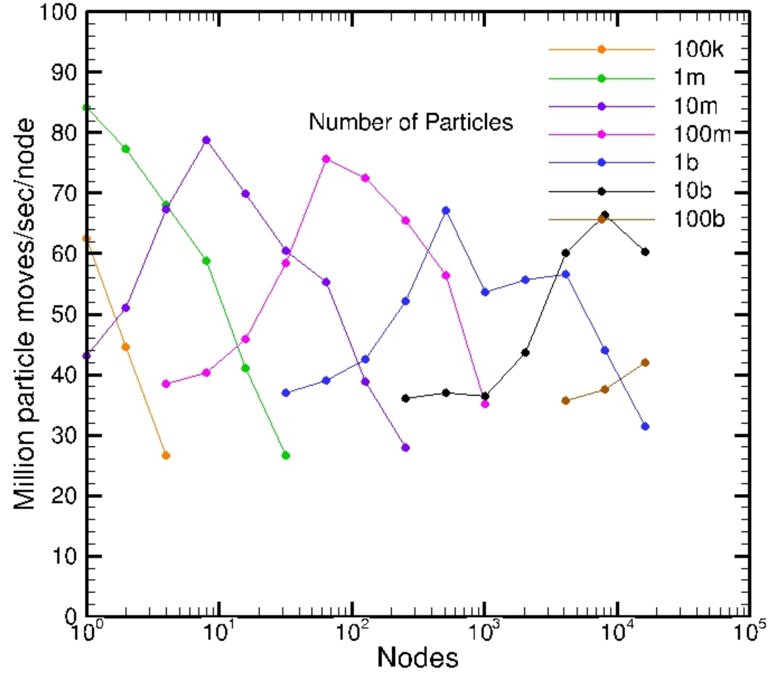
- Weak scaling indicates, 10% peak performance reduction from 1 to 10^6 cores
- 2 tasks/core gives 1.5x speedup, 4 tasks/core gives 2x speedup
- A total of 1 trillion molecules can be simulated on one third of the BG/Q
- Maximum number of tasks is 2.6 million

SPARTA Benchmarking (FM)

16 cores/node, 1 task/core



16 cores/node, 4 tasks/core



- Free-molecular (FM) calculations stress-test for communications
- 2x speedup compared to collisional