"I have had my results for a long time, but I do not yet know how I am to arrive at them."

–Carl Friedrich Gauss, 1777-1855

DIY Parallel Data Analysis

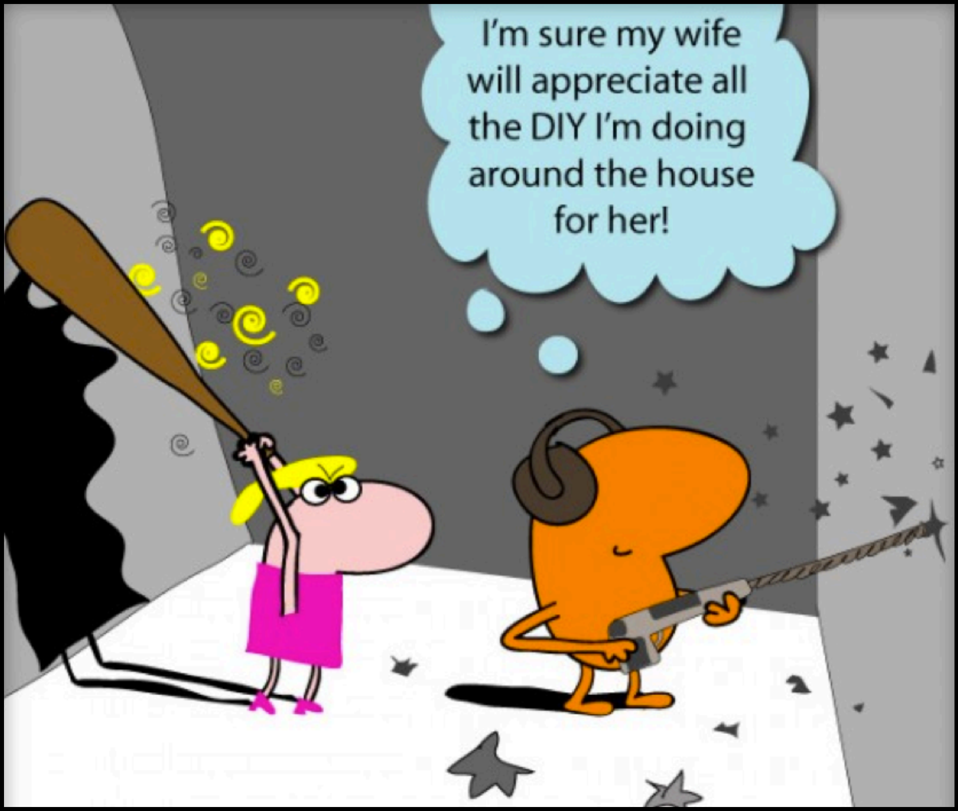

Image courtesy pigtimes.com

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APTESC Talk 8/6/13

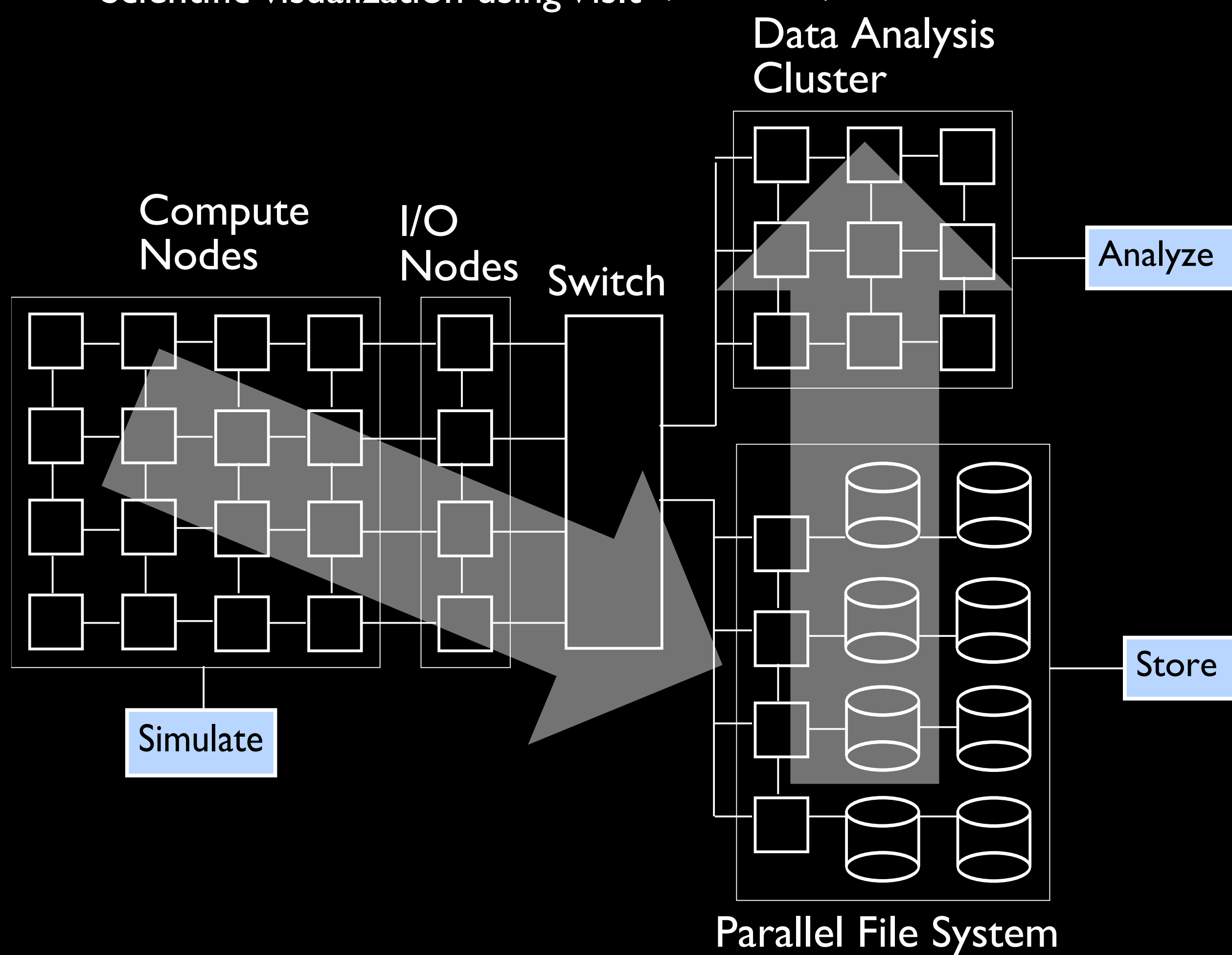
Postprocessing Scientific Data Analysis in HPC Environments

Examples:

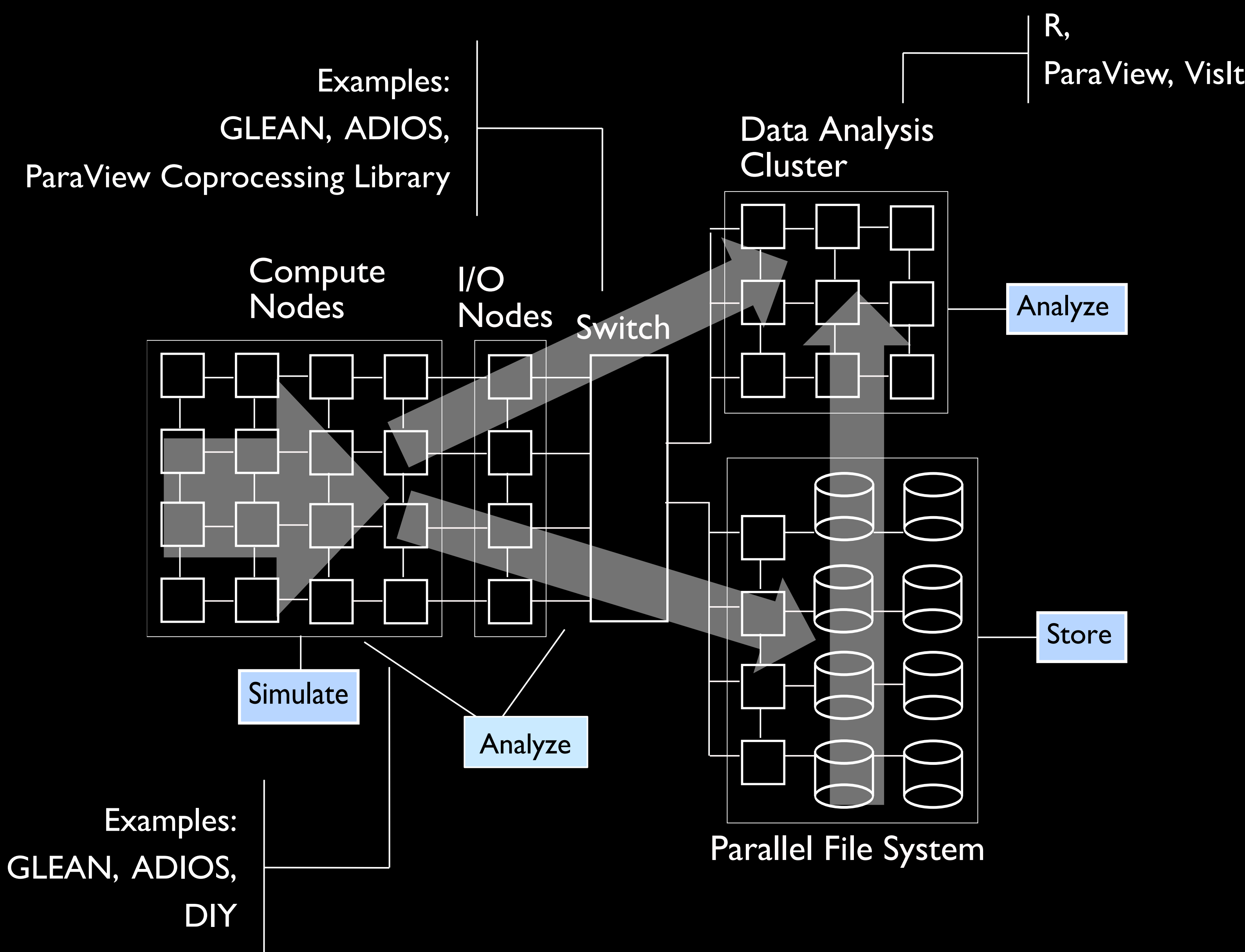
2D statistical graphics using R

3D scientific visualization using ParaView

Scientific visualization using VisIt



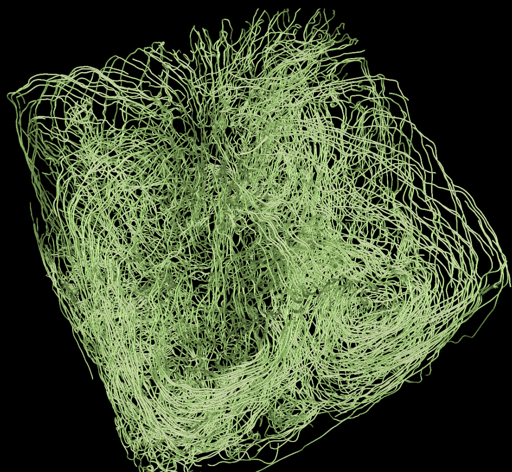
Run-time Scientific Data Analysis in HPC Environments



Scientific Data Analysis Today

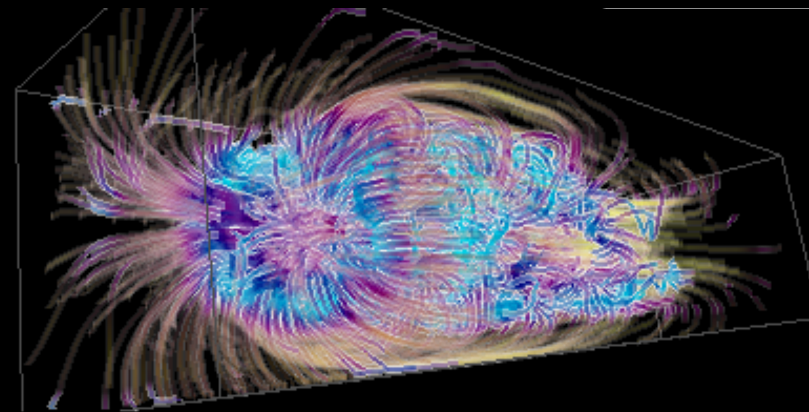
- Big science = big data, and
  - Big data analysis => big science resources
- Data analysis is data intensive.
  - Data intensity = data movement.
- Parallel = data parallel (for us)
  - Big data => data decomposition
  - Task parallelism, thread parallelism, while important, are not part of this work
- Most analysis algorithms are not up to the challenge
  - Either serial, or
  - Communication and I/O are scalability killers

Data Analysis Comes in Many Flavors



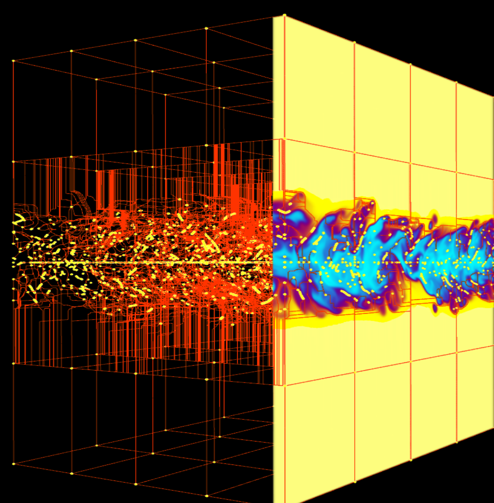
Visual

Particle tracing of thermal hydraulics flow



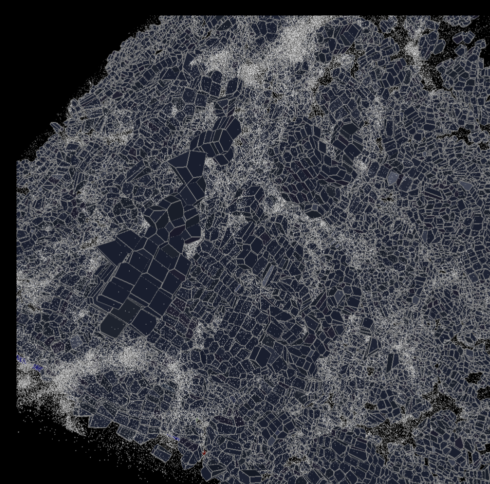
Statistical

Information entropy analysis of astrophysics



Topological

Morse-Smale Complex of combustion

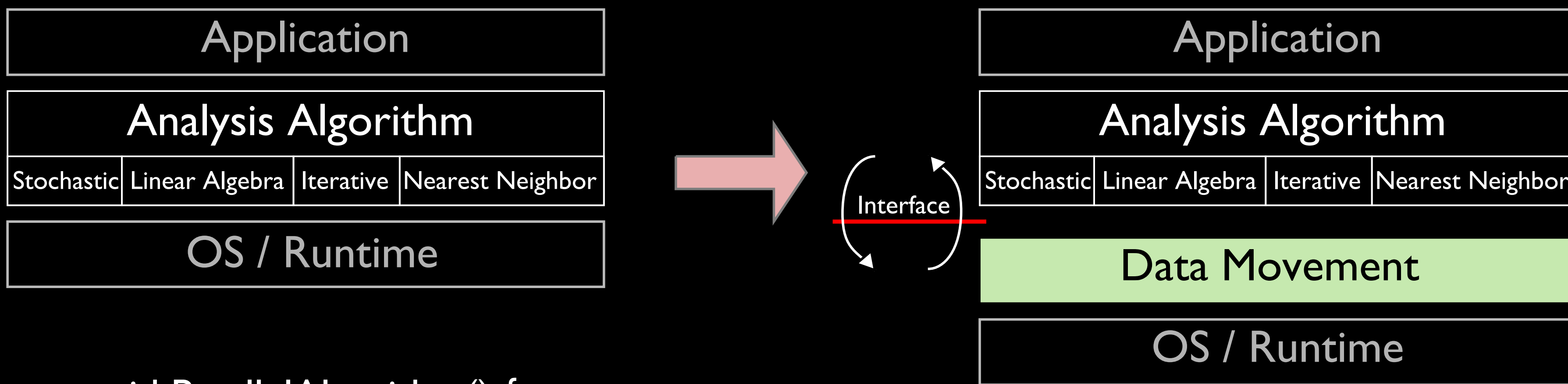


Geometric

Voronoi tessellation of cosmology

You Have Two Choices to Parallelize Data Analysis

By hand — or — With tools




```
void ParallelAlgorithm() {
  …
  MPI_Send();
  …
  MPI_Recv();
  …
  MPI_Barrier();
  …
  MPI_File_write();
}
```

```
void ParallelAlgorithm() {
  …
  LocalAlgorithm();
  …
  DIY_Merge_blocks();
  …
  DIY_File_write()
}
```

DIY

helps the user write data-parallel analysis algorithms by decomposing a problem into blocks and communicating items between blocks.

Features

Parallel I/O to/from storage

Domain decomposition

Network communication

Utilities

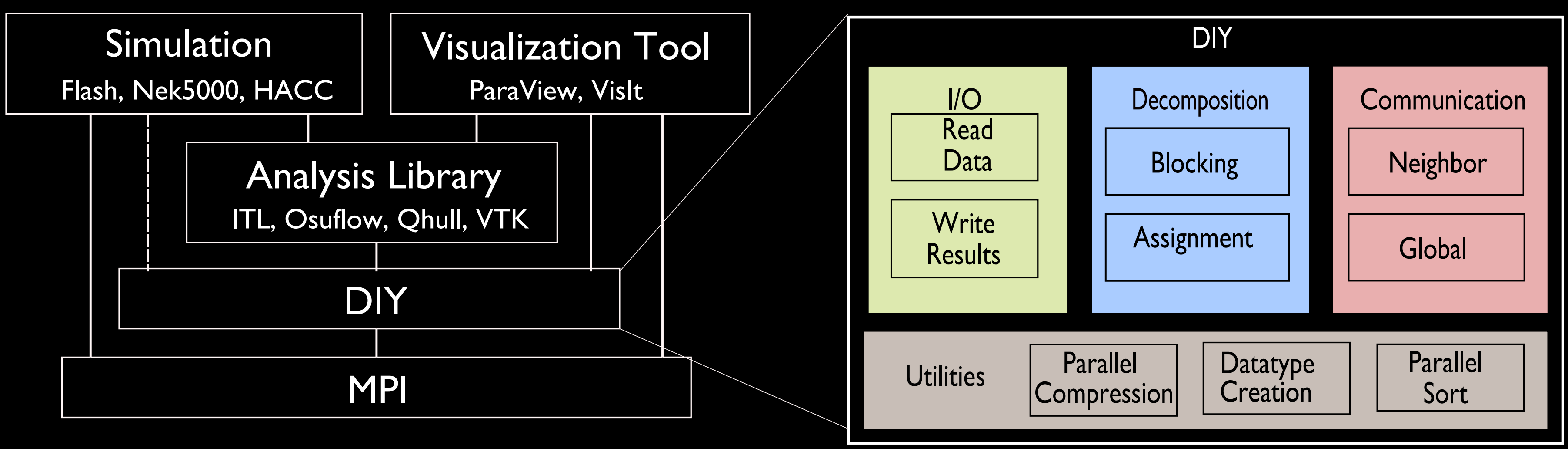
Library

Written in C++ with C bindings

Autoconf build system (configure, make, make install)

Lightweight: libdiy.a 800KB

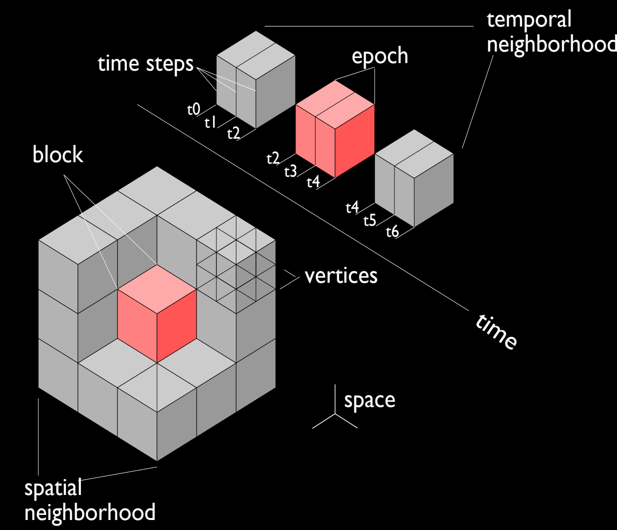
Maintainable: ~15K lines of code, including examples

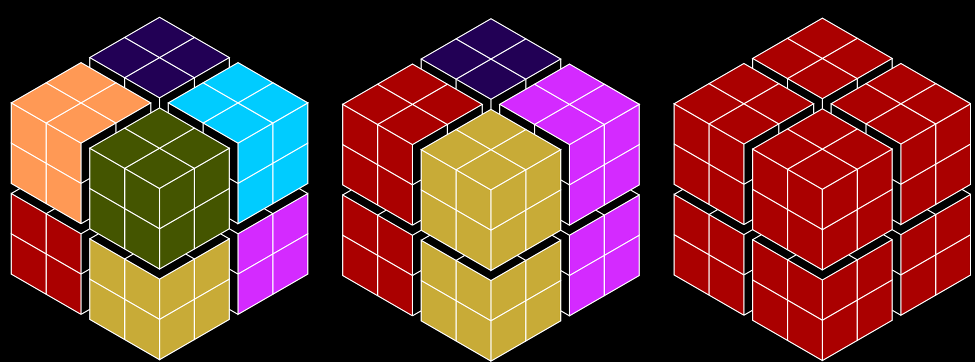


DIY usage and library organization

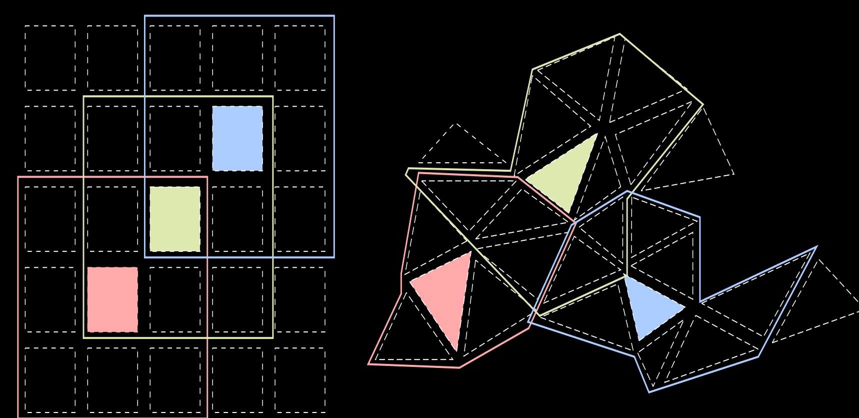
Nine Things That DIY Does

1. Separate analysis ops from data ops
2. Group data items into blocks
3. Assign blocks to processes
4. Group blocks into neighborhoods
5. Support multiple multiple instances of 2, 3, and 4
6. Handle time
7. Communicate between blocks in various ways
8. Read data and write results
9. Integrate with other libraries and tools





8 processes 4 processes 1 process



Two examples of 3 out of a total of 25 neighborhoods

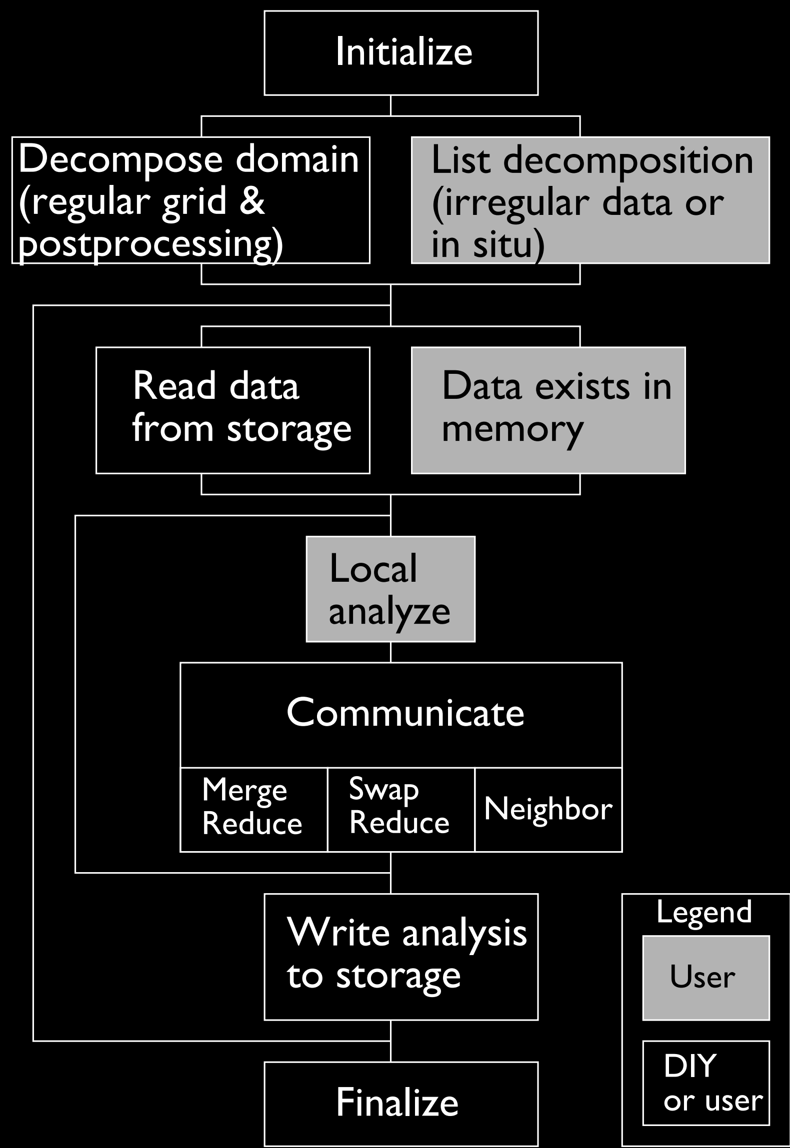
Writing a DIY Program

Documentation

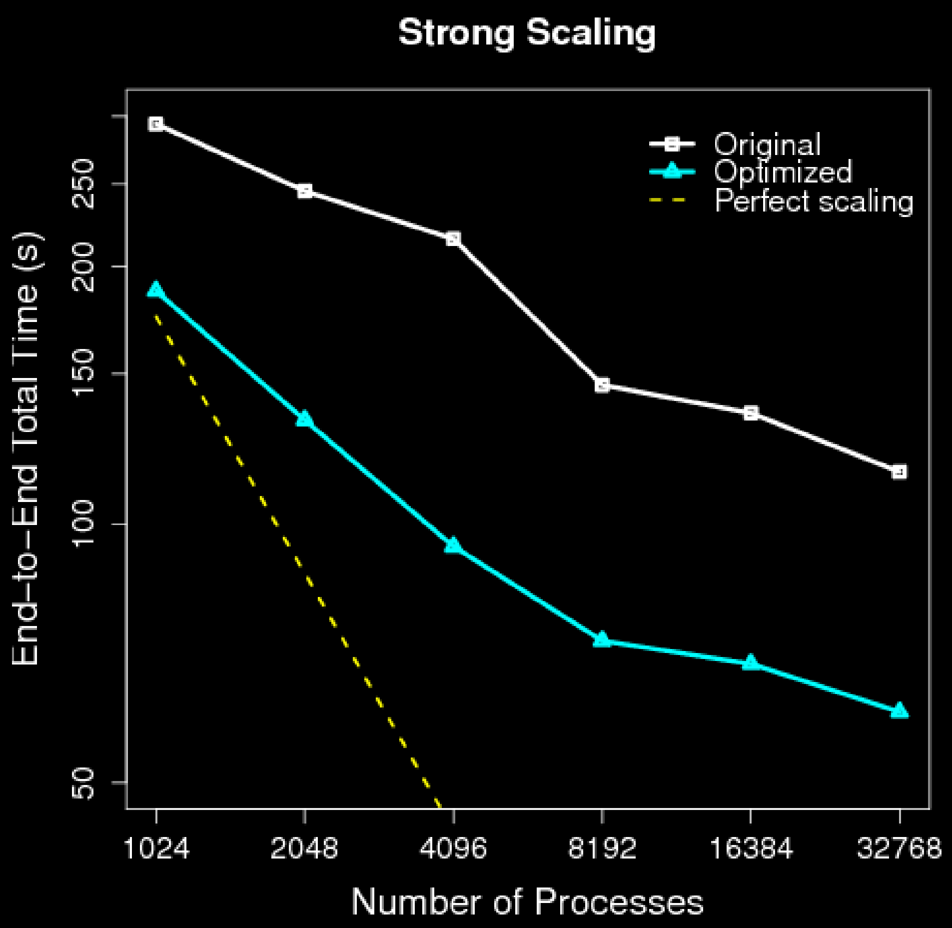
- README for installation
- User's manual with description, examples of custom datatypes, complete API reference

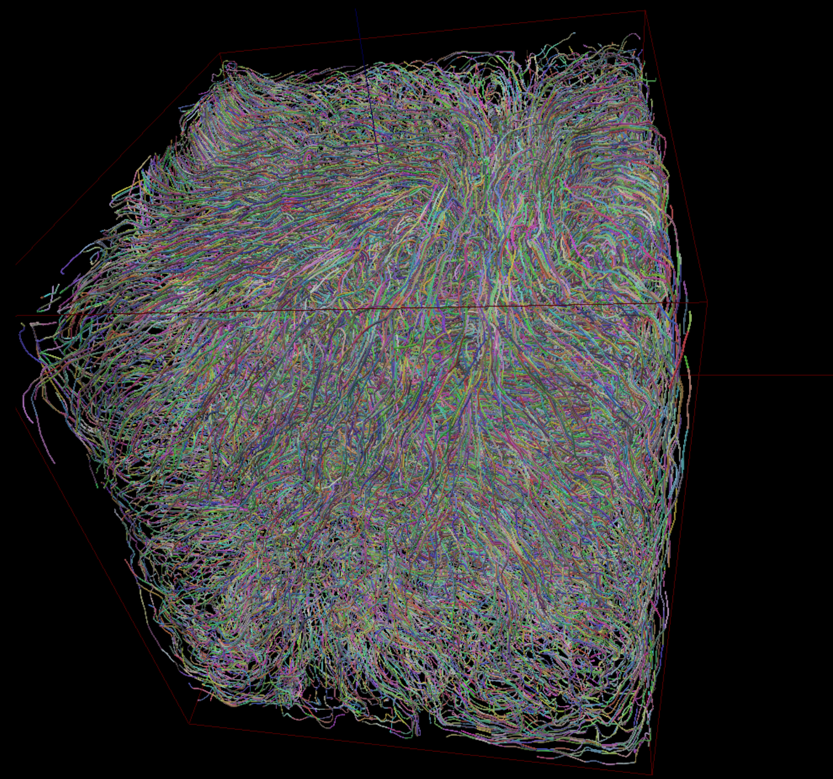
Tutorial Examples

- Block I/O: Reading data, writing analysis results
- Static: Merge-based, Swap-based reduction, Neighborhood exchange
- Time-varying: Neighborhood exchange
- Spare thread: Simulation and analysis overlap
- MOAB: Unstructured mesh data model
- VTK: Integrating DIY communication with VTK filters
- R: Integrating DIY communication with R stats algorithms
- Multimodel: multiple domains and communicating between them



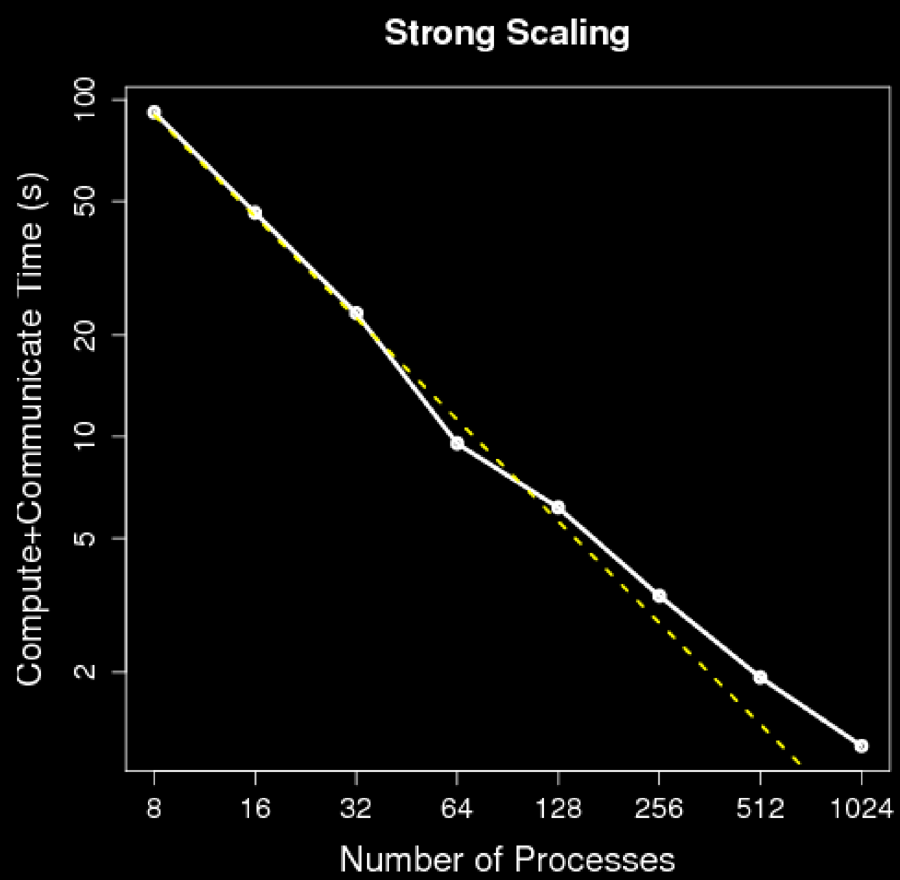
Particle Tracing

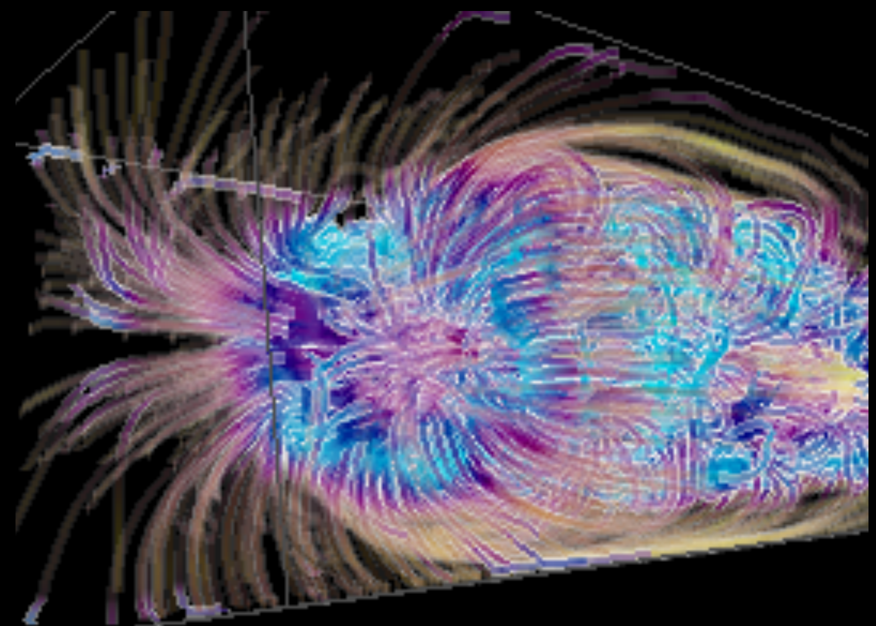




Particle tracing of ¼ million particles in a 2048^3 thermal hydraulics dataset results in strong scaling to 32K processes and an overall improvement of 2X over earlier algorithms

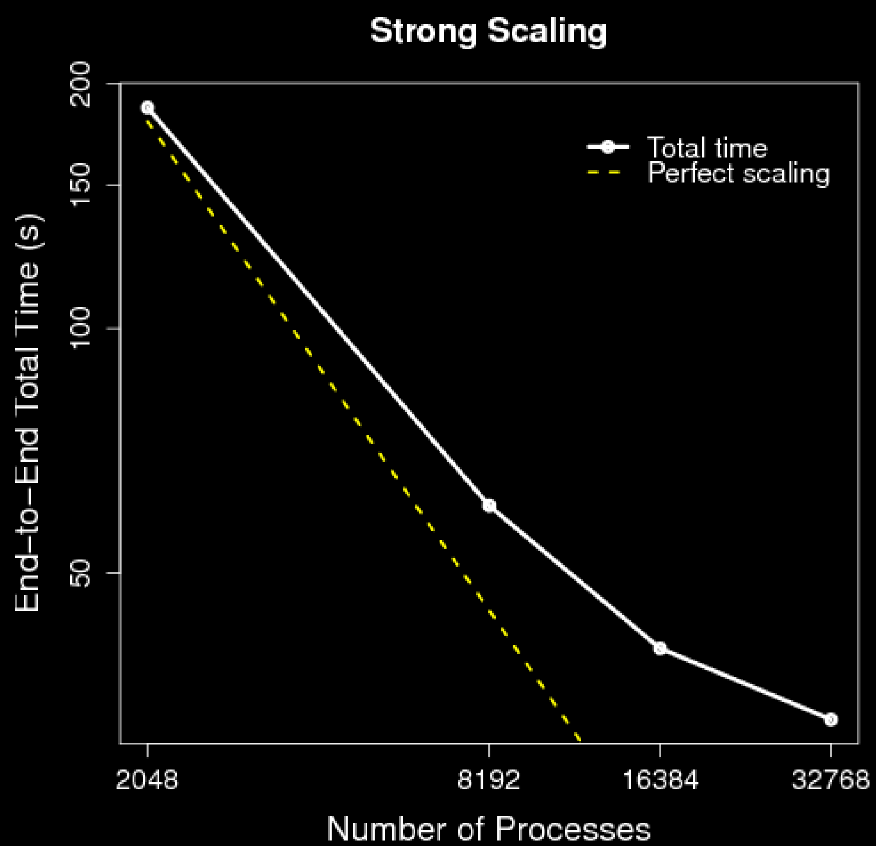
Information Entropy

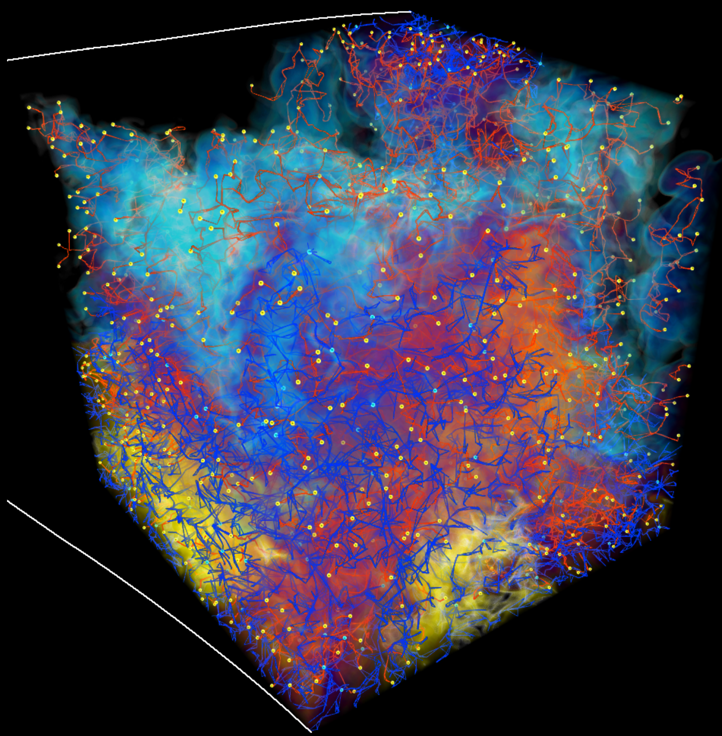




Computation of information entropy in 126x126x512 solar plume dataset shows 59% strong scaling efficiency.

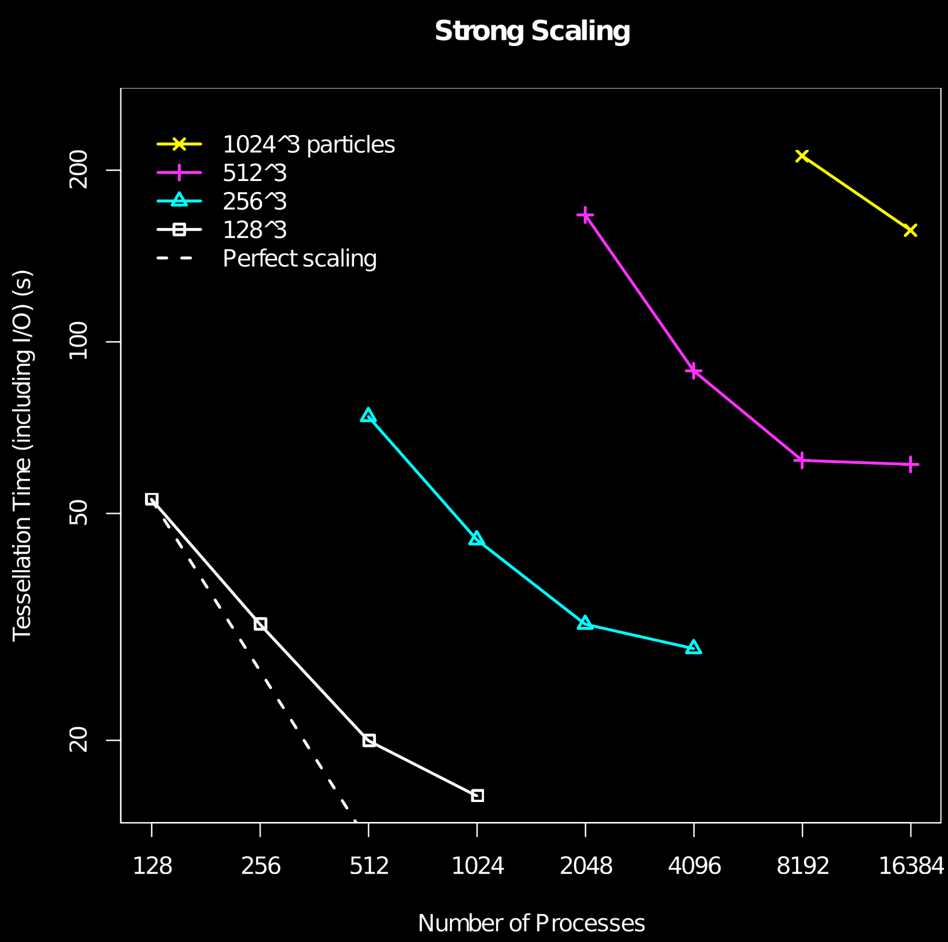
Morse-Smale Complex

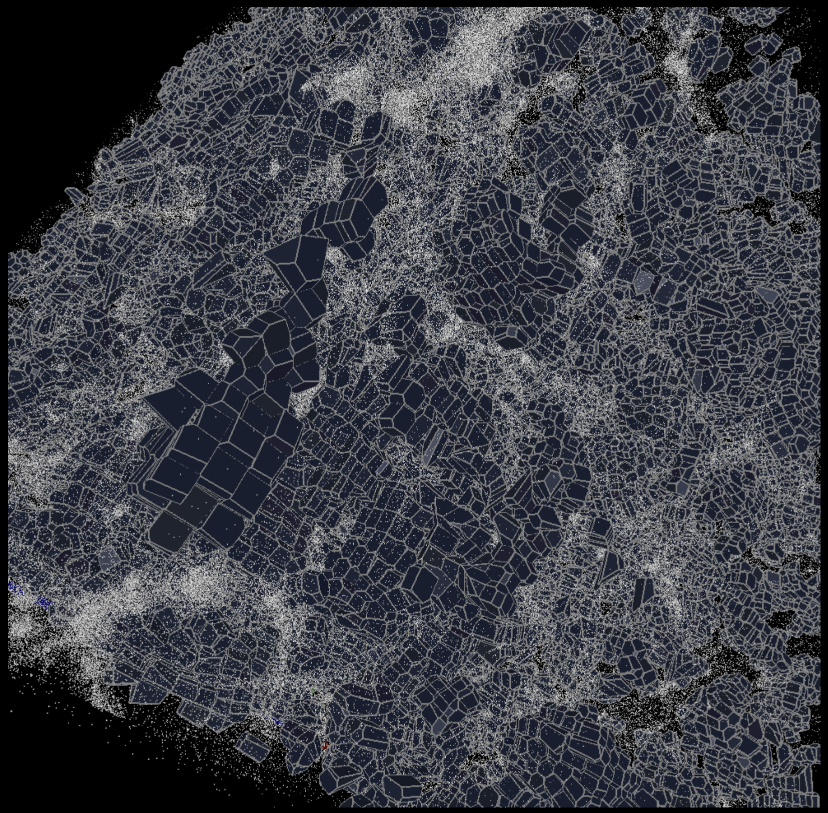




Computation of Morse-Smale complex in 1152^3 Rayleigh-Taylor instability data set results in 35% end-to-end strong scaling efficiency, including I/O.

In Situ Voronoi Tessellation





For 128^3 particles, 41 % strong scaling for total tessellation time, including I/O; comparable to simulation strong scaling.

Further Reading

DIY

- Peterka, T., Ross, R., Kendall, W., Gyulassy, A., Pascucci, V., Shen, H.-W., Lee, T.-Y., Chaudhuri, A.: Scalable Parallel Building Blocks for Custom Data Analysis. Proceedings of Large Data Analysis and Visualization Symposium (LDAV'11), IEEE Visualization Conference, Providence RI, 2011.
- Peterka, T., Ross, R.: Versatile Communication Algorithms for Data Analysis. 2012 EuroMPI Special Session on Improving MPI User and Developer Interaction IMUDI'12, Vienna, AT.

DIY applications

- Peterka, T., Ross, R., Nouanesengsey, B., Lee, T.-Y., Shen, H.-W., Kendall, W., Huang, J.: A Study of Parallel Particle Tracing for Steady-State and Time-Varying Flow Fields. Proceedings IPDPS'11, Anchorage AK, May 2011.
- Gyulassy, A., Peterka, T., Pascucci, V., Ross, R.: The Parallel Computation of Morse-Smale Complexes. Proceedings of IPDPS'12, Shanghai, China, 2012.
- Nouanesengsy, B., Lee, T.-Y., Lu, K., Shen, H.-W., Peterka, T.: Parallel Particle Advection and FTLE Computation for Time-Varying Flow Fields. Proeedings of SC12, Salt Lake, UT.
- Peterka, T., Kwan, J., Pope, A., Finkel, H., Heitmann, K., Habib, S., Wang, J., Zagaris, G.: Meshing the Universe: Integrating Analysis in Cosmological Simulations. Proceedings of the SC12 Ultrascale Visualization Workshop, Salt Lake City, UT.
- Chaudhuri, A., Lee-T.-Y., Zhou, B., Wang, C., Xu, T., Shen, H.-W., Peterka, T., Chiang, Y.-J.: Scalable Computation of Distributions from Large Scale Data Sets. Proceedings of 2012 Symposium on Large Data Analysis and Visualization, LDAV'12, Seattle, WA.

"The purpose of computing is insight, not numbers."
–Richard Hamming, 1962

Acknowledgments:

Facilities
Argonne Leadership Computing Facility (ALCF)
Oak Ridge National Center for Computational Sciences (NCCS)

Funding
DOE SDMAV Exascale Initiative
DOE Exascale Codesign Center
DOE SciDAC SDAV Institute

http://www.mcs.anl.gov/~tpeterka/software.html
https://svn.mcs.anl.gov/repos/diy/trunk

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