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Title: The PISTON Software Framework for Visualization and Analysis on Next-Generation Multi-core Architectures

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The PISTON Software Framework for Visualization and Analysis on Next-Generation Multi-core Architectures

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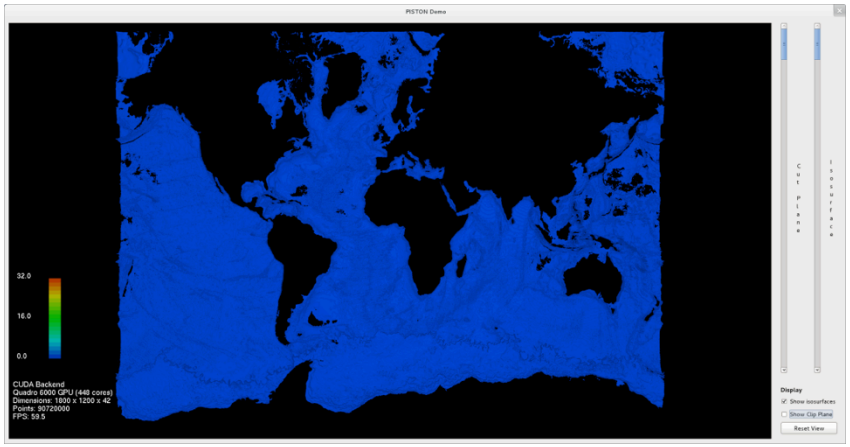

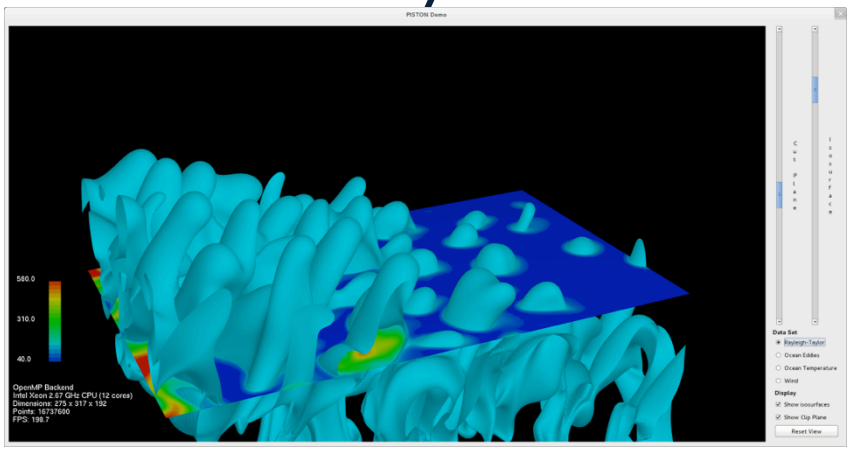

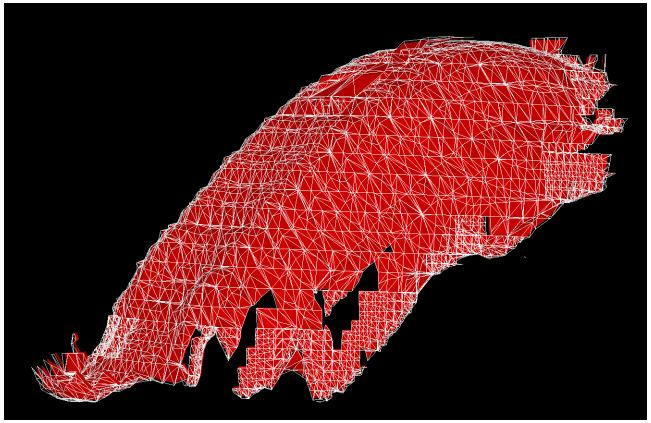

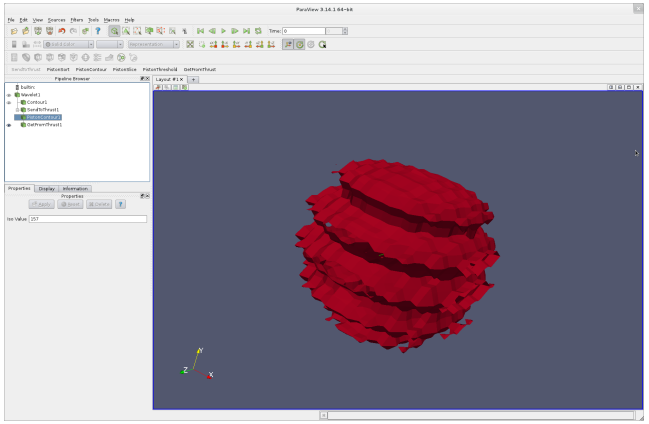

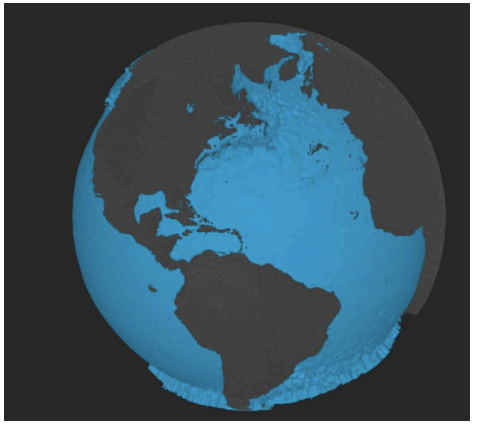

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Overview

- Goal: Portability and performance for visualization and analysis operators on current and next-generation supercomputers
- Main idea: Write operators using only data-parallel primitives (scan, reduce, etc.)
- Requires architecture-specific optimizations for only for the small set of primitives
- PISTON is built on top of NVIDIA's Thrust Library

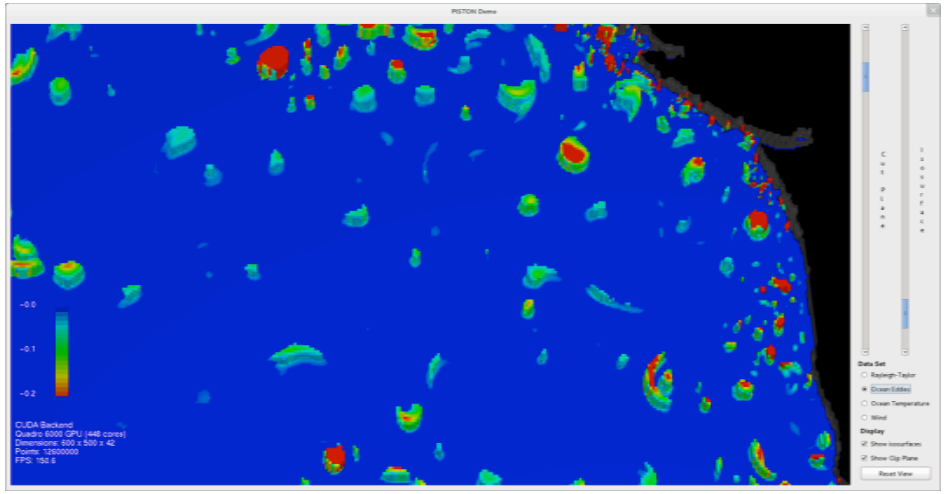
Motivation and Background

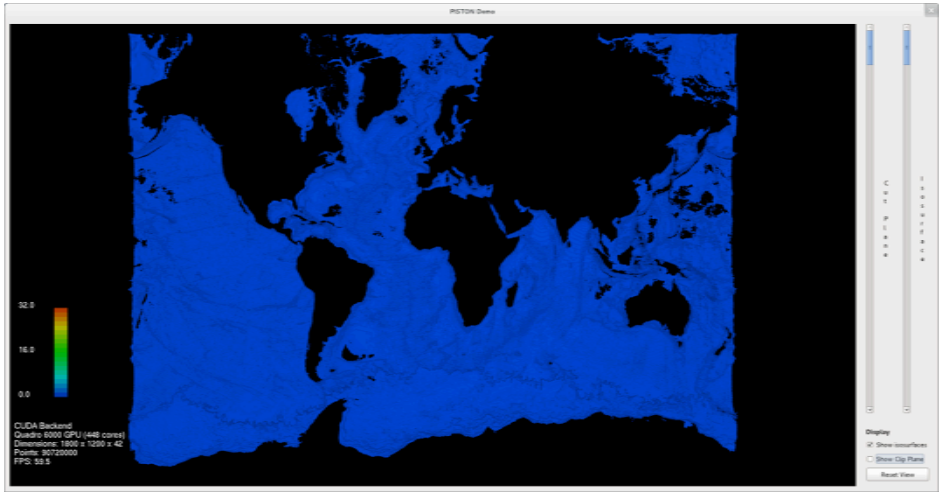
- Current production visualization software does not take full advantage of acceleration hardware and/or multi-core architecture
- Research on accelerating visualization operations are mostly hardware-specific; few were integrated in visualization software
- Standards such as OpenCL may allow program to run cross-platform, but usually still requires many architecture specific optimizations to run well
- Data parallelism: independent processors performs the same task on different pieces of data (see Blelloch, "Vector Models for Data Parallel Computing")
- Due to the massive data sizes we expect to be simulating we expect data parallelism to be a good way to exploit parallelism on current and next generation architectures
- Thrust is a NVidia C++ template library for CUDA. It can also target other backends such as OpenMP, and allows you to program using an interface similar the C++ Standard Template Library (STL)

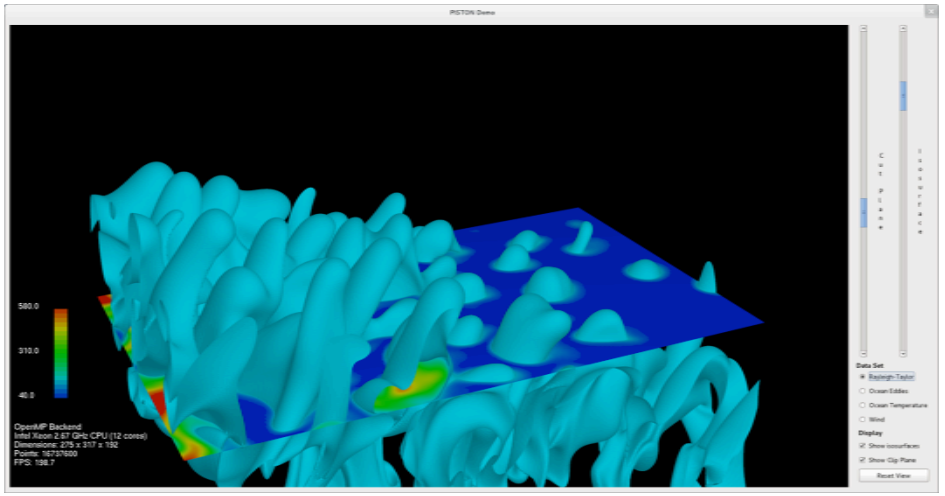
Questions for the Panel

- What fundamental problem are you trying to solve?
  - Portable performance for visualization and analysis operators
- What are your plans to deal with exascale-specific issues (massive concurrency, distributed memory, memory overhead, fault tolerance)?
  - Data-parallel programming model; requires architecture-specific optimizations for a limited set of "embarrassingly parallel" primitive operators
- What is your philosophy for dealing with ambiguity of the exascale architecture (multiple swim lanes, heterogeneous architectures)?
  - Data-parallel programming model; requires architecture-specific optimizations for a limited set of "embarrassingly parallel" primitive operators
- How is your technology implemented?
  - Extension of NVIDIA's Thrust library
- What is the long-term result for this effort? (Production software? Research prototype?)
  - Open-source repository (available on-line now); integrated into VTK/ParaView (available on-line now)

Videos of PISTON in Action







Brief Introduction to Data-Parallel Programming and Thrust

What algorithms does Thrust provide?

- Sorts
- Transforms
- Reductions
- Scans
- Binary searches
- Stream compactions
- Scatters / gathers

Challenge: Write operators in terms of these primitives only

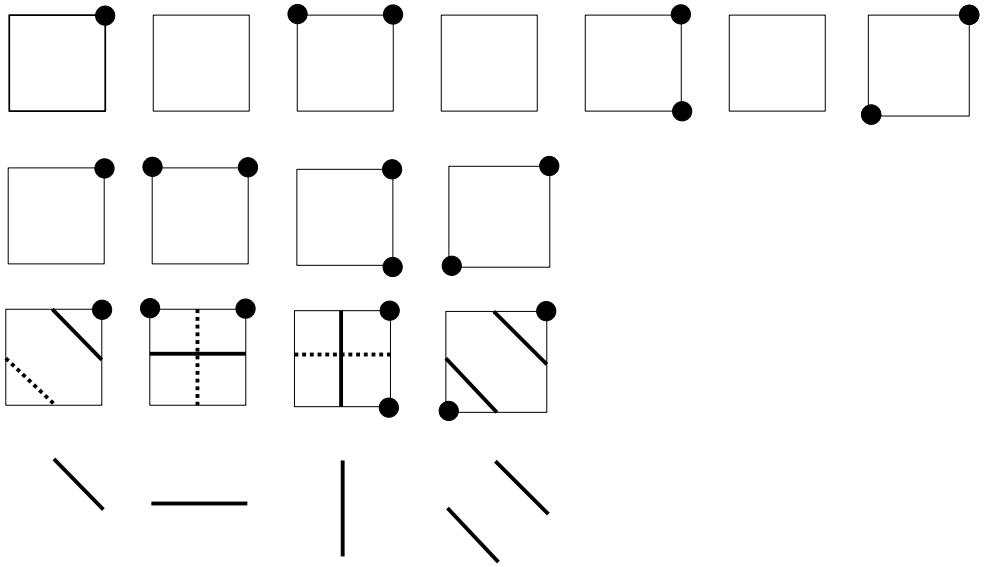
Reward: Efficient, portable code

```
input                      4  5  2  1  3
-------------------------------------------
transform(+1)              5  6  3  2  4
inclusive_scan(+)          4  9 11 12 15
exclusive_scan(+)          0  4  9 11 12
exclusive_scan(max)        0  4  5  5  5
transform_inscan(*2,+)     8 18 22 24 30
for_each(-1)               3  4  1  0  2
sort                       1  2  3  4  5
copy_if(n % 2 == 1)        5  1  3
reduce(+)                                15

input1                     0  0  2  4  8
input2                     3  4  1  0  2
-------------------------------------------
upper_bound                3  4  2  2  3
permutation_iterator       4  8  0  0  2
```

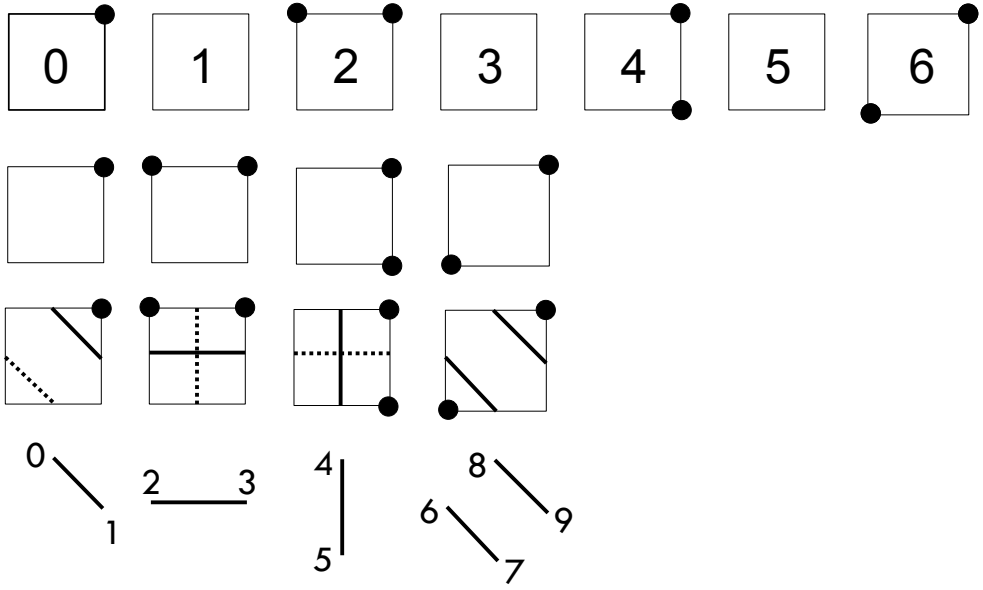
Isosurface with Marching Cube – the Naive Way

- Classify all cells by *transform*
- Use *copy_if* to compact valid cells.
- For each valid cell, generate same number of geometries with flags.
- Use *copy_if* to do stream compaction on vertices.
- This approach is too slow, more than 50% of time was spent moving huge amount of data in global memory.
- Can we avoid calling *copy_if* and eliminate global memory movement?



Isosurface with Marching Cube – Optimization

- Inspired by HistoPyramid
- The filter is essentially a mapping from input cell id to output vertex id
- Is there a "reverse" mapping?
- If there is a reverse mapping, the filter can be very "lazy"
- Given an output vertex id, we *only* apply operations on the cell that would generate the vertex
- Actually for a range of output vertex ids



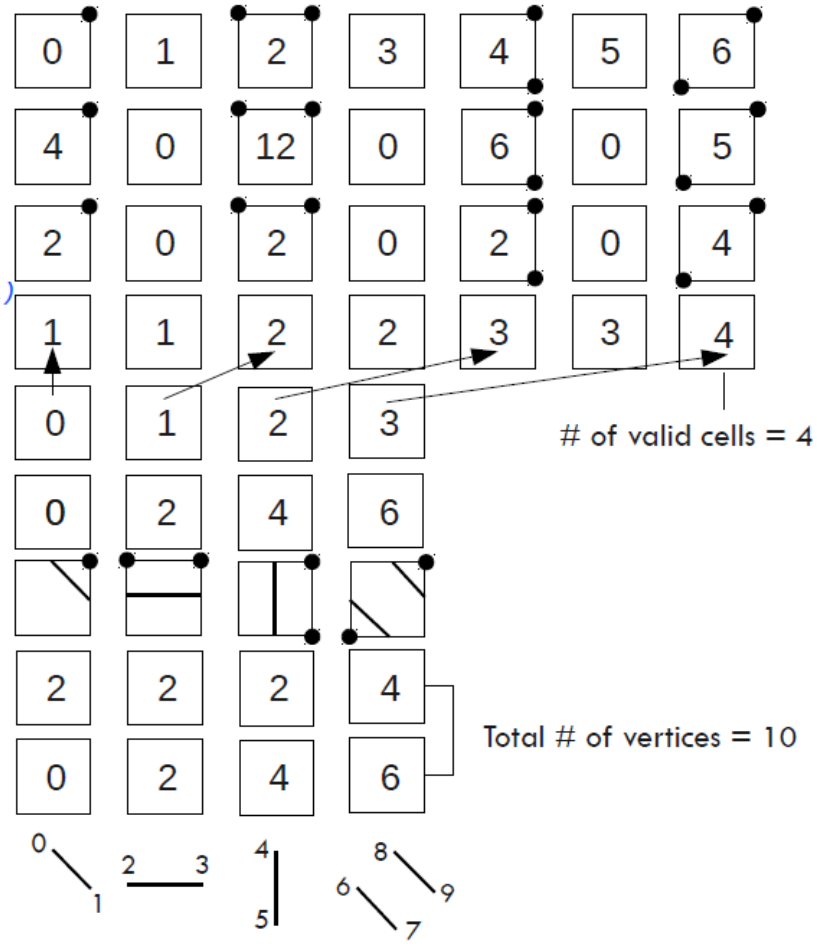
Isosurface with Marching Cubes Algorithm

1. input
   transform(classify_cell)
2. caseNums

3. numVertices
   transform_inclusive_scan(is_valid_cell)
4. validCellEnum

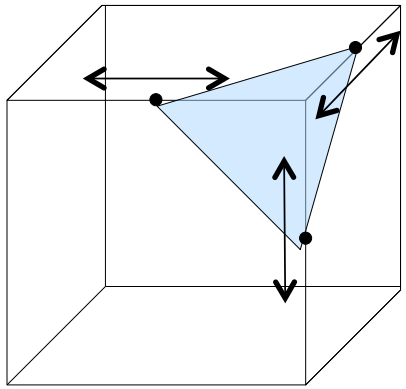
5. CountingIterator
   upper_bound
6. validCellIndices

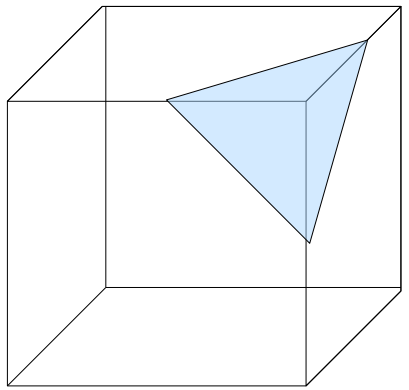
   make_permutation_iterator
7. numVerticesCompacted
   exclusive_scan
8. numVerticesEnum
   for_each(isosurface_functor)
9. outputVertices

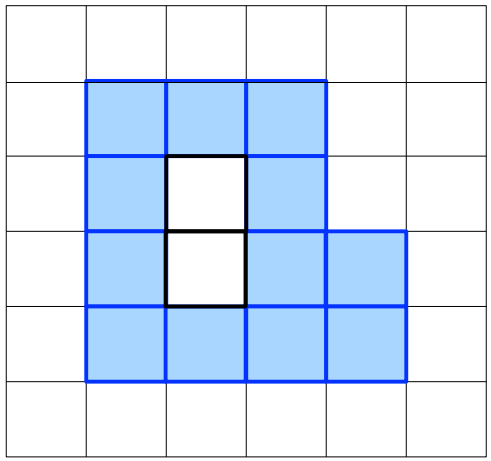


Variations on Isosurface: Cut Surfaces and Threshold

- Cut surface
  - Two scalar fields, one for generating geometry (cut surface) the other for scalar interpolation
  - Less than 10 LOC change, negligible performance impact to isosurface
  - One 1D interpolation per triangle vertex
- Threshold
  - Classify cells, this time based on whether value at each vertex falls within threshold range, then stream compact valid cells and generate geometry for valid cells
  - Additional pass of cell classification and stream compaction to remove interior cells







Additional Operators

Blelloch's "Vector Models for Data-Parallel Computing"

Data Structures
- Graphs: Neighbor reducing, distributing excess across edges
- Trees: Leaffix and rootfix operations, tree manipulations
- Multidimensional arrays

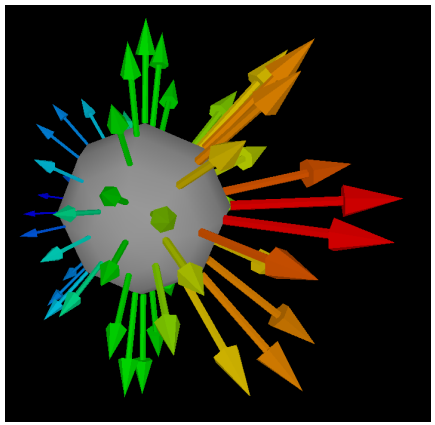
Computational Geometry
- Generalized binary search
- k-D tree
- Closest pair
- Quickhull
- Merge Hull

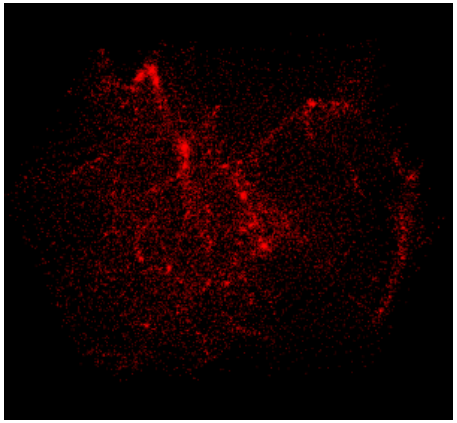
Graph Algorithms
- Minimum spanning tree
- Maximum flow
- Maximal independent set

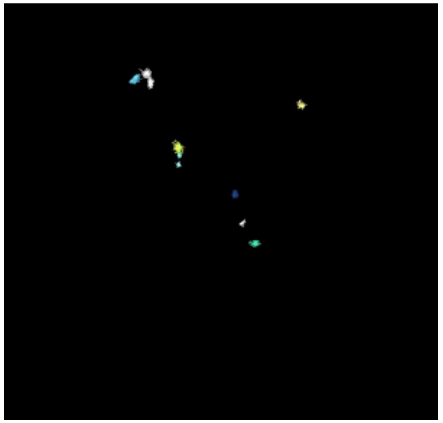
Numerical Algorithms
- Matrix-vector multiplication
- Linear-systems solver
- Simplex
- Outer product
- Sparse-matrix multiplication

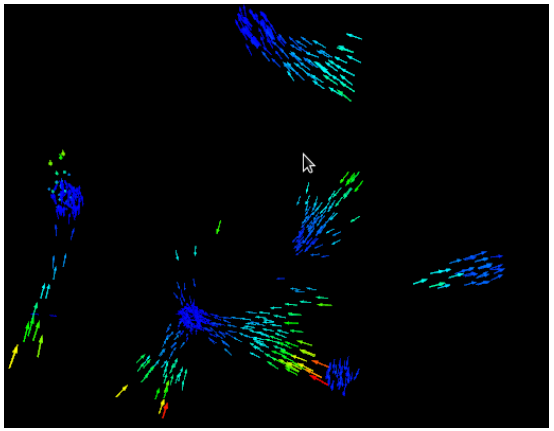
Current prototypes

- Glyphs
- Halo finder for cosmology simulations
- "Boid" simulation (flocking birds)

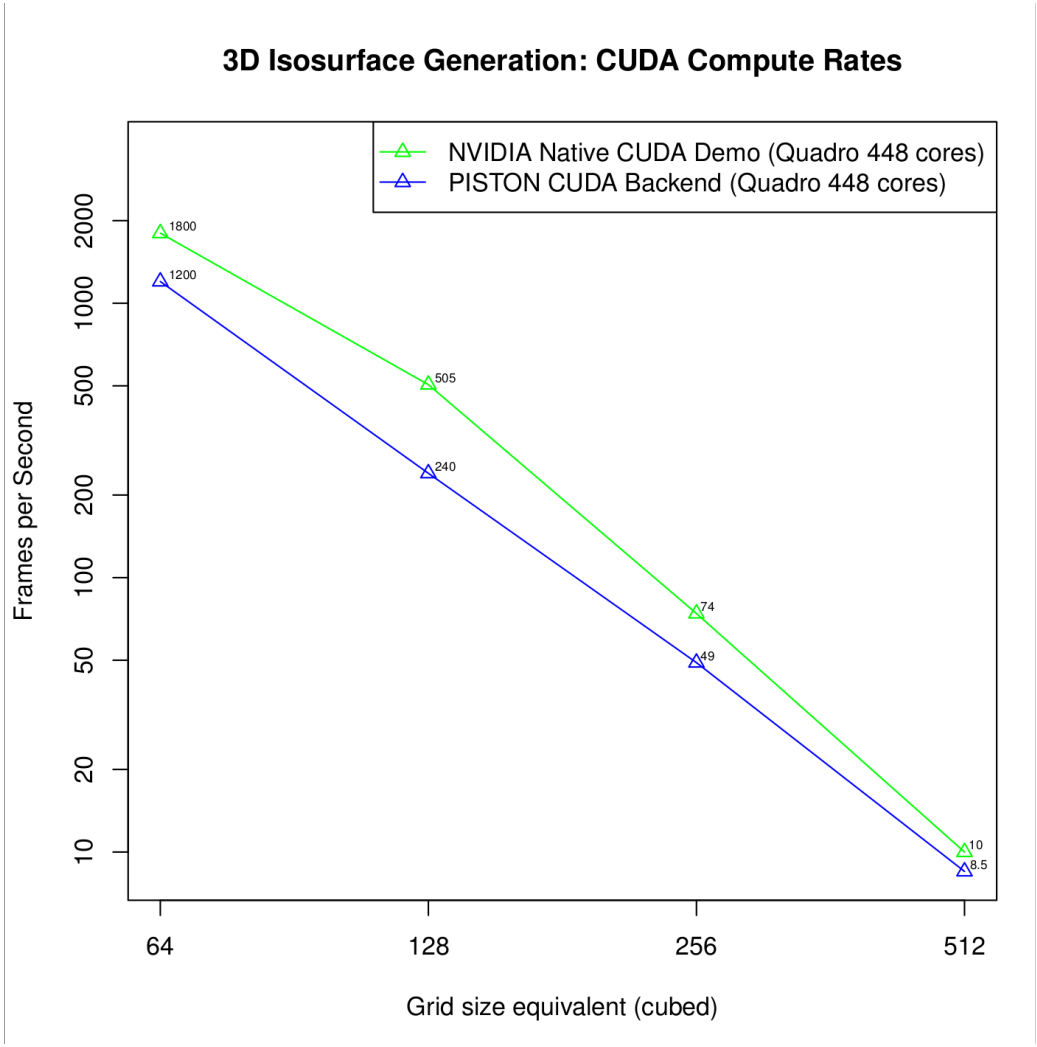


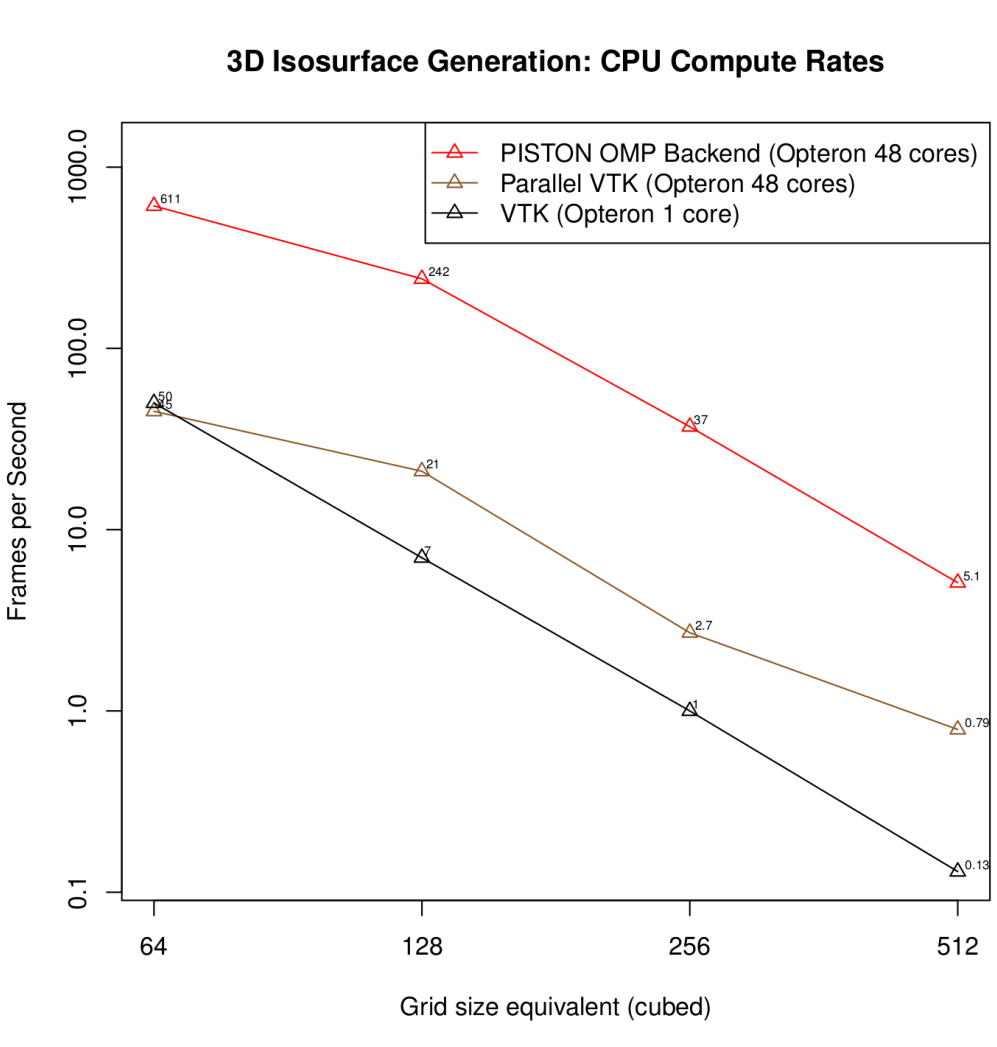






PISTON Performance





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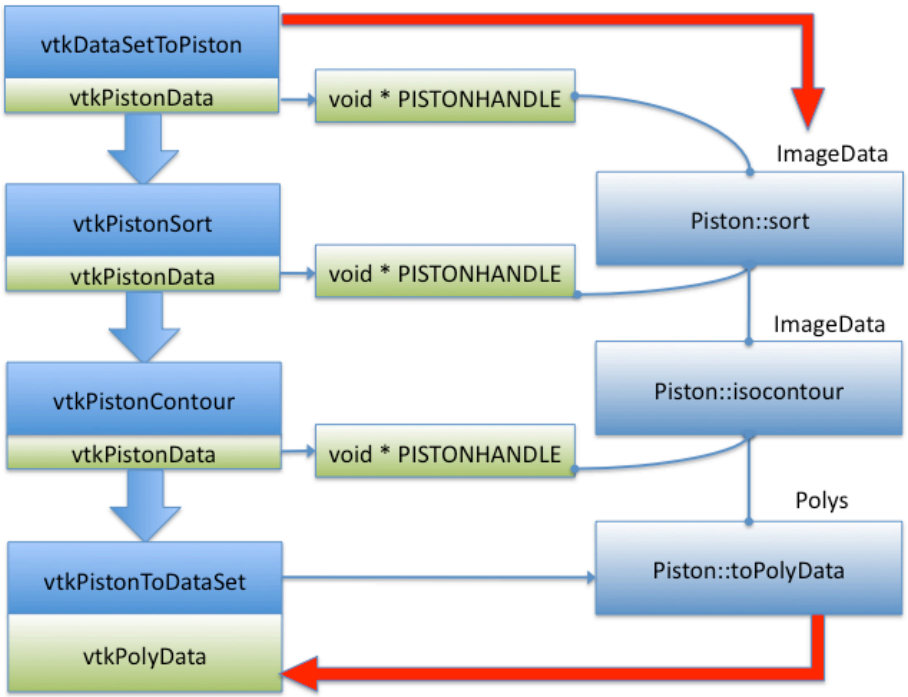
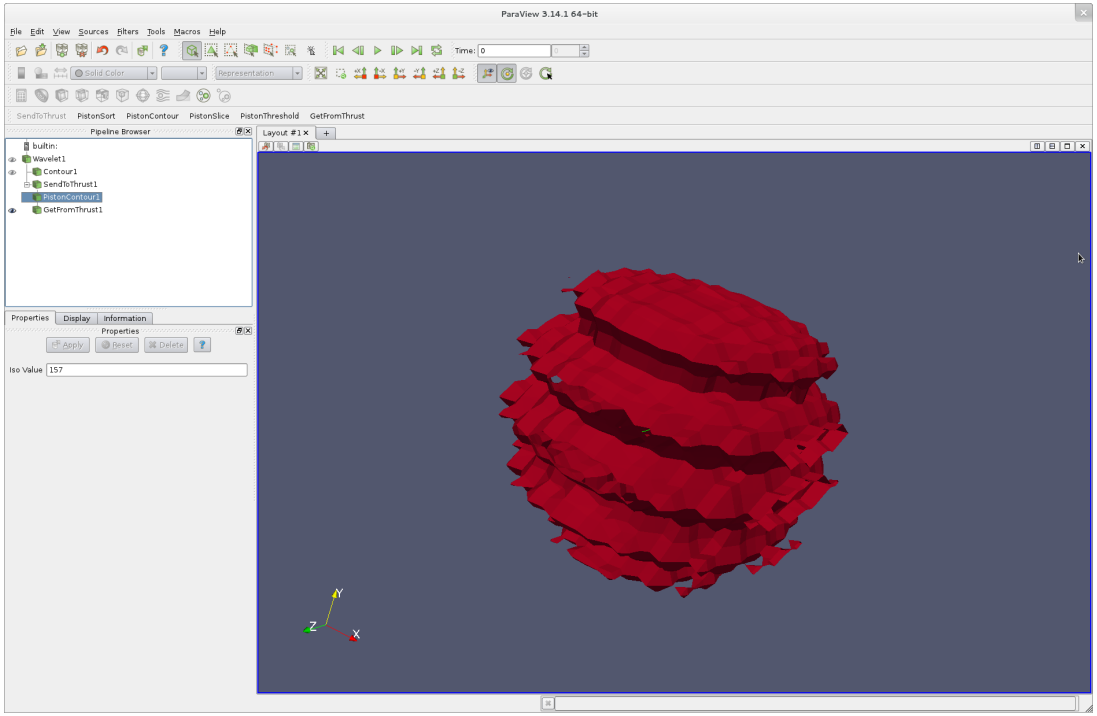
Integration with VTK and ParaView

- Filters that use PISTON data types and algorithms integrated into VTK and ParaView
- Utility filters interconvert between standard VTK data format and PISTON data format (thrust device vectors)
- Supports interop for on-card rendering

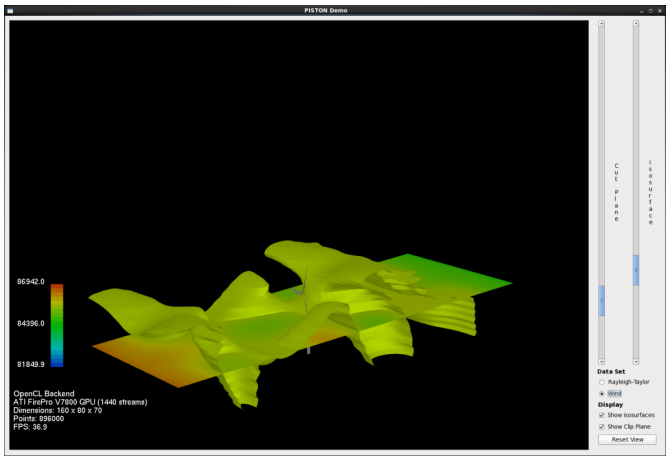


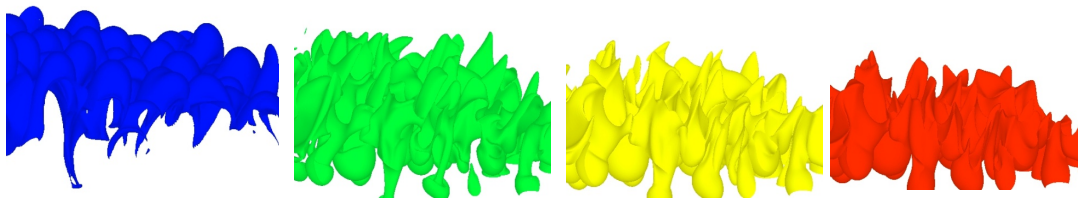


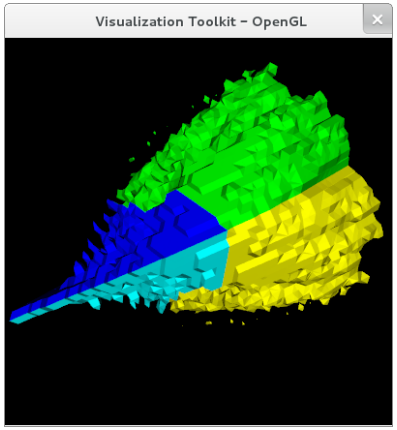
Developed with Dave DeMarle and Utkarsh Ayachit at Kitware

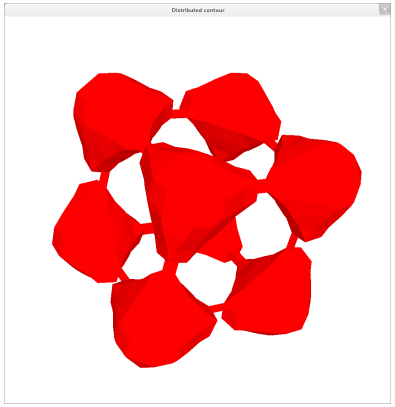
Extending PISTON's Portability: Architectures

- Prototype OpenCL backend
  - Successfully implemented isosurface and cut plane operators in OpenCL with code almost identical to that used for the Thrust-based CUDA and OpenMP backends
  - With interop on AMD FirePro V7800, we can run at about 6 fps for 256^3 data set (2 fps without interop)
- Renderer
  - Allows generation of images on systems without OpenGL
  - Rasterizing and ray-casting versions (using K-D Tree)
- Inter-node parallelism
  - VTK Integration
    - Domain partitioned by VTK's MPI libraries
    - Each node uses PISTON filters to compute results for its portion of domain
    - Results combined by VTK's compositors
  - Distributed implementations of Thrust primitives using MPI (in progress)



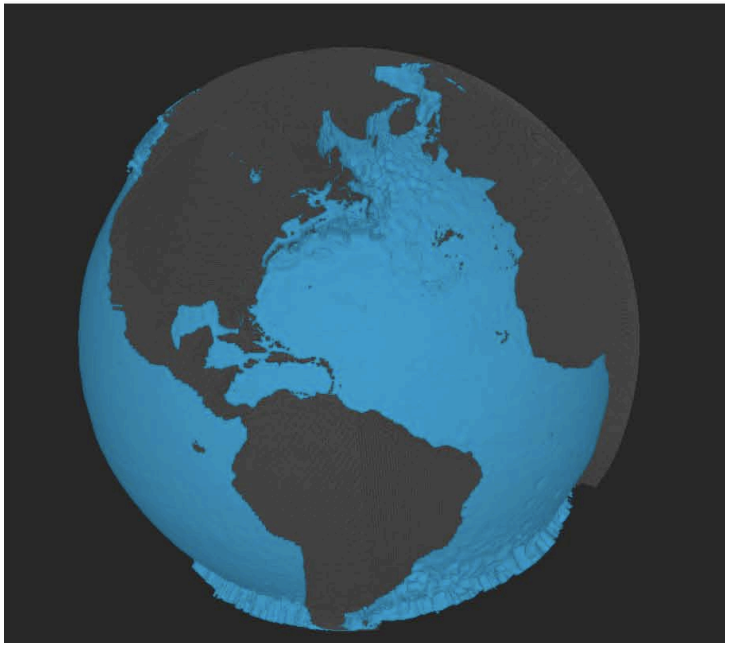


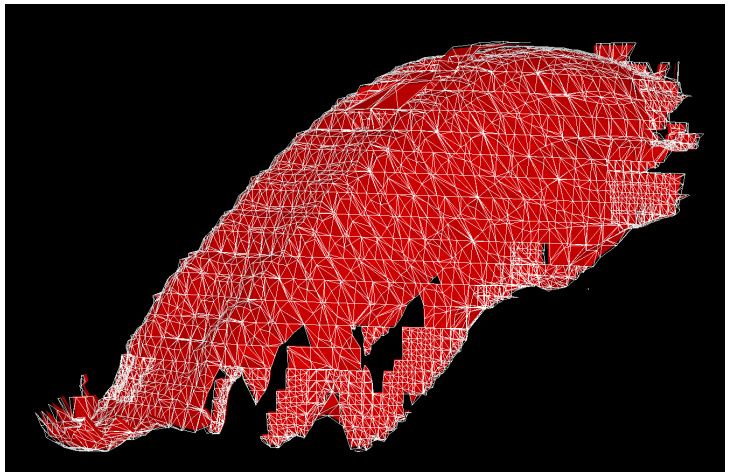




Extending PISTON's Portability: Data Types

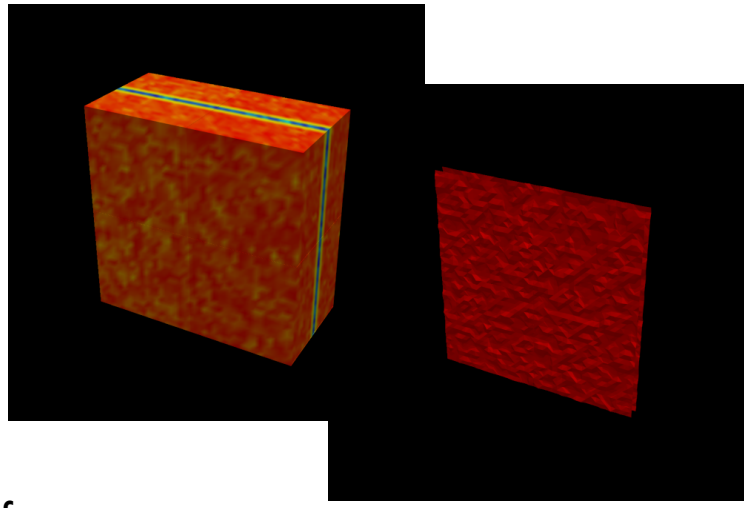
- Curvilinear coordinates
  - Multiple layers of coordinate transformations
  - Due to kernel fusion, very little performance impact
- Unstructured / AMR data
  - Tetrahedralize uniform grid or unstructured grid (e.g., AMR mesh)
  - Generate isosurface geometry based on look-up table for tetrahedral cells
  - Next step: Develop PISTON operator to tetrahedralize grids, and/or to compute isosurface directly on AMR grid



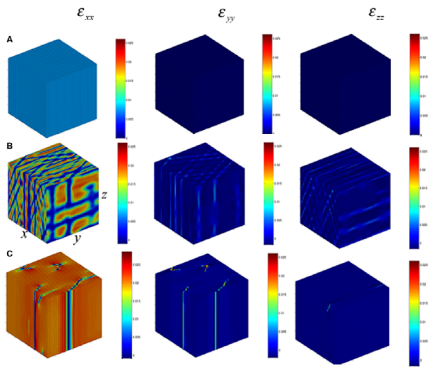


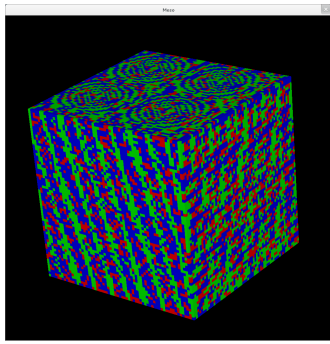
PISTON In-Situ

- VPIC (Vector Particle in Cell) Kinetic Plasma Simulation Code
  - Implemented first version of an in-situ adapter based on Paraview CoProcessing Library (Catalyst)
  - Three pipelines: vtkDataSetMapper, vtkContourFilter, vtkPistonContour
- CoGL
  - Stand-alone meso-scale simulation code developed as part of the Exascale Co-Design Center for Materials in Extreme Environments
  - Studies pattern formation in ferroelastic materials using the Ginzburg–Landau approach
  - Models cubic-to-tetragonal transitions under dynamic strain loading
  - Simulation code and in-situ viz implemented using PISTON



Output of vtkDataSetMapper and vtkPistonContour filters on Hhydro charge density at one timestep of VPIC simulation

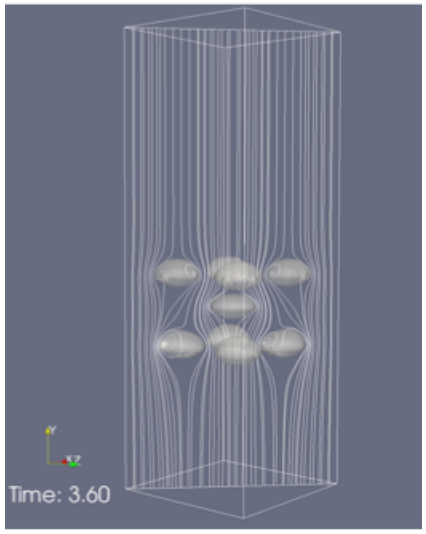


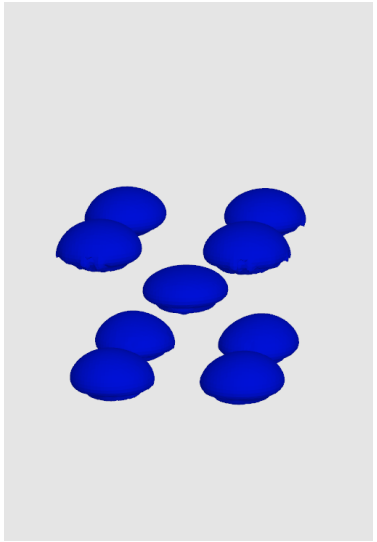


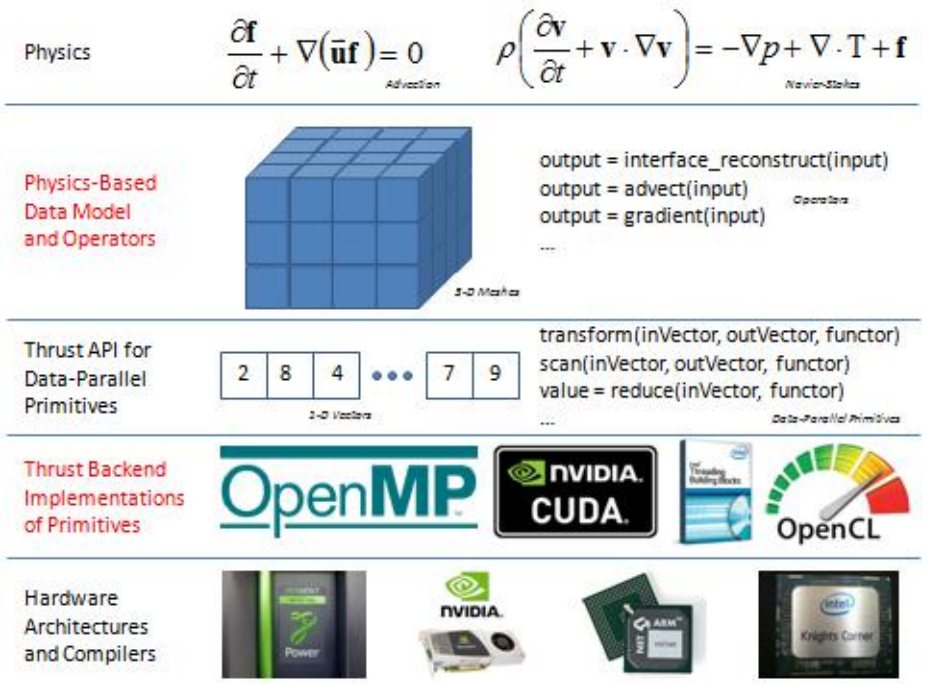
Strains in x,y,z (above); PISTON in-situ visualization (right)

PISTON's New Companion Project: PINION

- A portable, data-parallel software framework for physics simulations
  - Data structures that allow scientists to program in a way that maps easily to the problem domain rather than dealing directly with 1D host/device vectors
  - Operators that provide data-parallel implementations of analysis and computational functions often used in physics simulations
  - Backends that optimize implementations of data parallel primitives for one or two emerging supercomputer hardware architectures







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PISTON Open-Source Release

- Open-source release
  - Stable tarball: http://viz.lanl.gov/projects/PISTON.html
  - Current repository: https://github.com/losalamos/PISTON

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- Los Alamos Laboratory Directed Research and Development Program