The SDAV Software Frameworks for Visualization and Analysis on Next-Generation Multi-core Architectures

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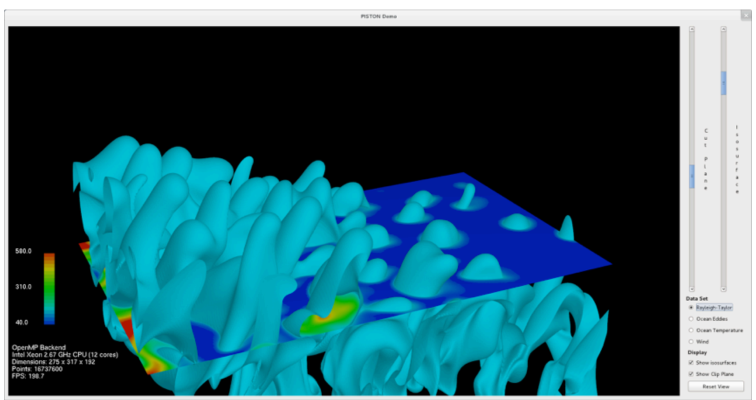
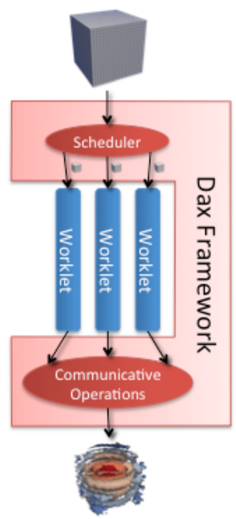
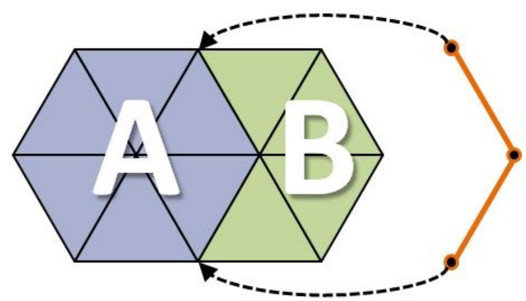
DAX — Ken Moreland (Sandia National Laboratories)

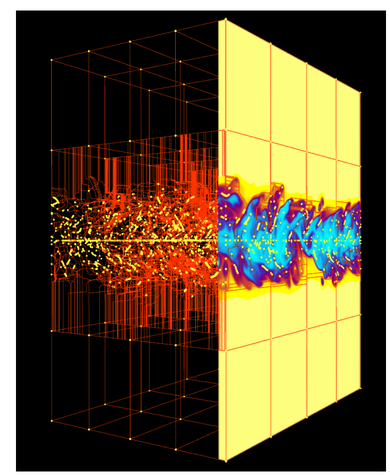
EAVL — Jeremy Meredith (Oak Ridge National Laboratory)

DIY — Tom Peterka (Argonne National Laboratory)









Productization support provided by Kitware

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SDAV VTK-m Frameworks

- Objective: Enhance existing multi/many-core technologies in anticipation of in situ analysis use cases with LCF codes
- Benefit to scientists: These frameworks will make it easier for domain scientists' simulation codes to take advantage of the parallelism available on a wide range of current and next-generation hardware architectures, especially with regards to visualization and analysis tasks
- Projects
  - EAVL, Oak Ridge National Laboratory
  - DAX, Sandia National Laboratory
  - DIY, Argonne National Laboratory
  - PISTON, Los Alamos National Laboratory
- Work on integrating these projects with VTK is on-going, in collaboration with Kitware

EAVL: Extreme-scale Analysis and Visualization Library

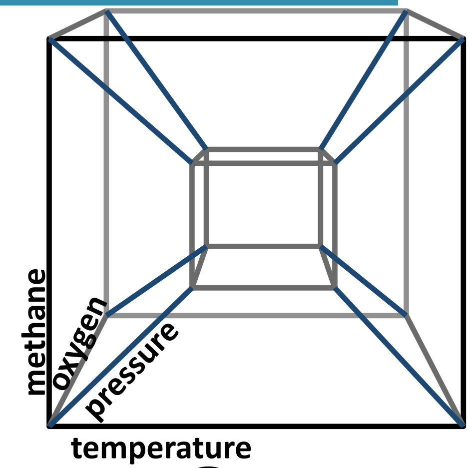
- Targets approaching hardware/software ecosystem:
  - Update traditional data model to handle modern simulation codes and a wider range of data.
  - Investigate how an updated data and execution model can achieve the necessary computational, I/O, and memory efficiency.
  - Explore methods for visualization algorithm *developers* to achieve these efficiency gains and better support exascale architectures.

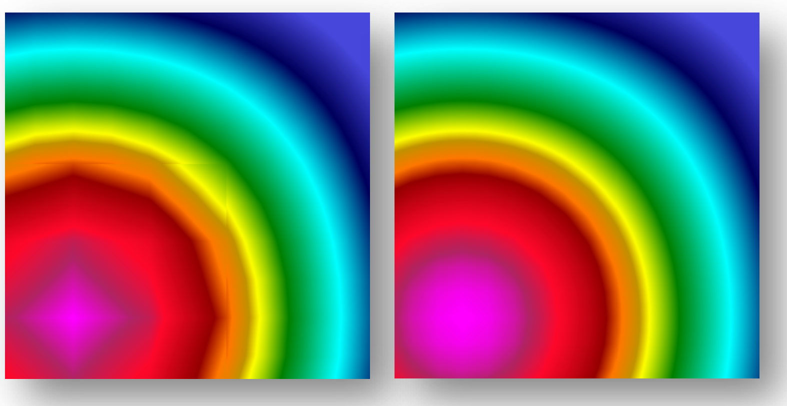
http://ft.ornl.gov/eavl

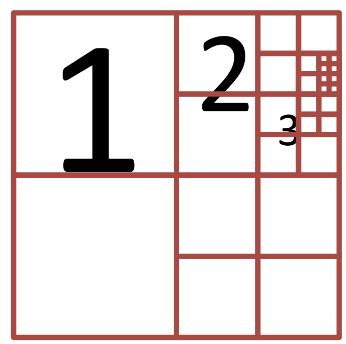
https://github.com/jsmeredith/EAVL

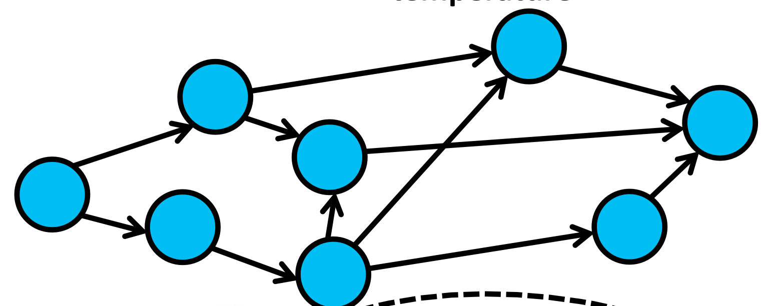
An Efficient Data Model in EAVL

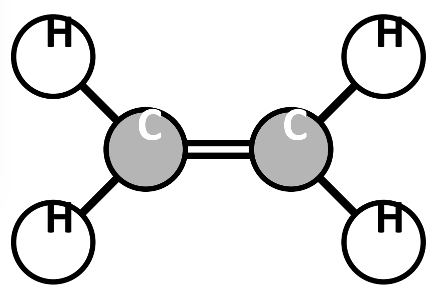
- More efficiently support existing data types with more flexible mesh structures
- Better support non-physical and new types of data (high-order, high-dim)
- Algorithms execute faster due to fewer data transformations.

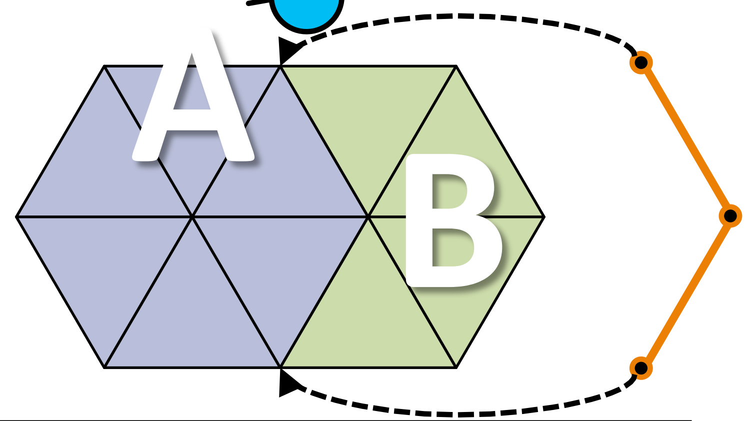




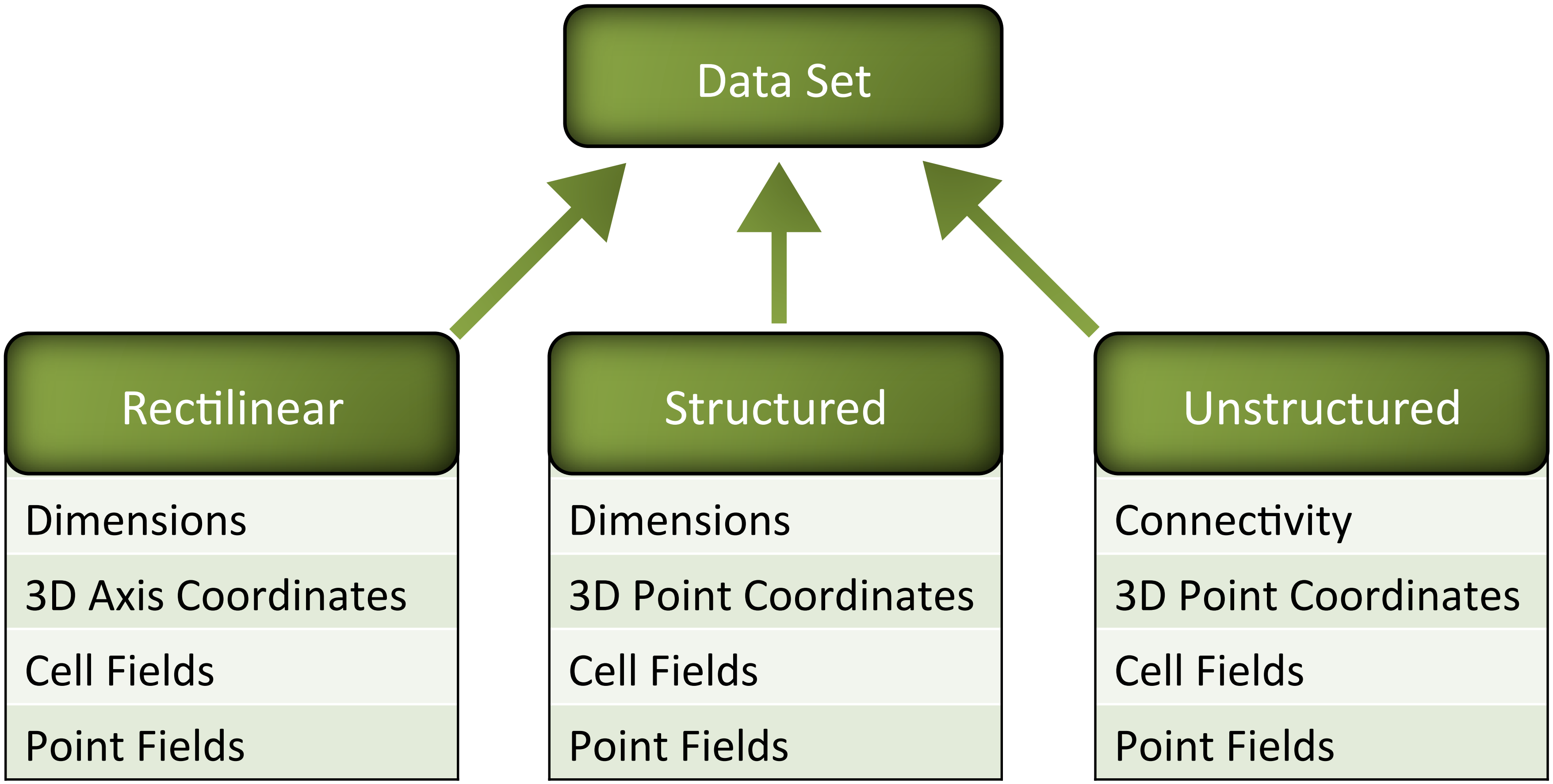




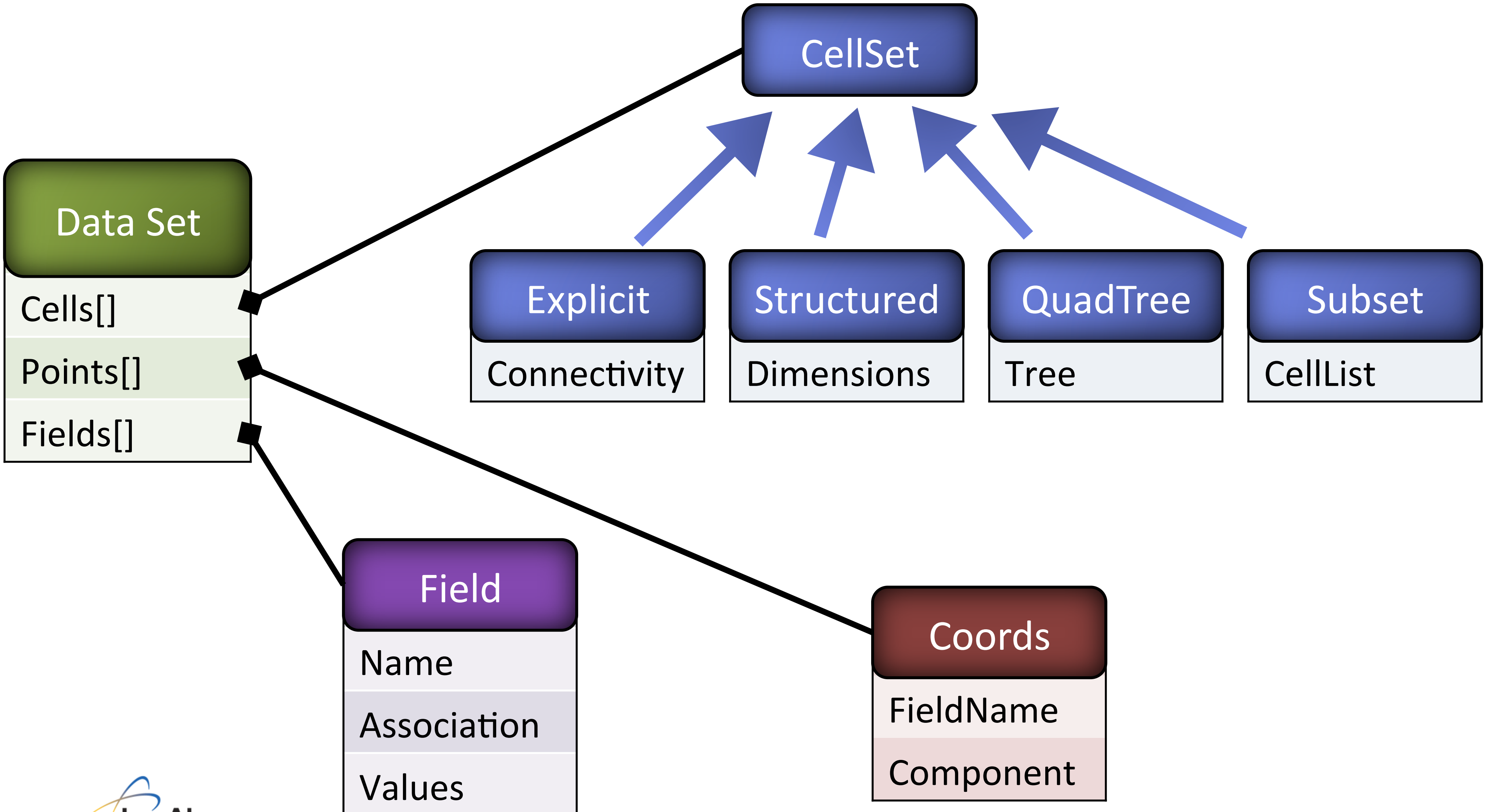




A Traditional Data Set Model

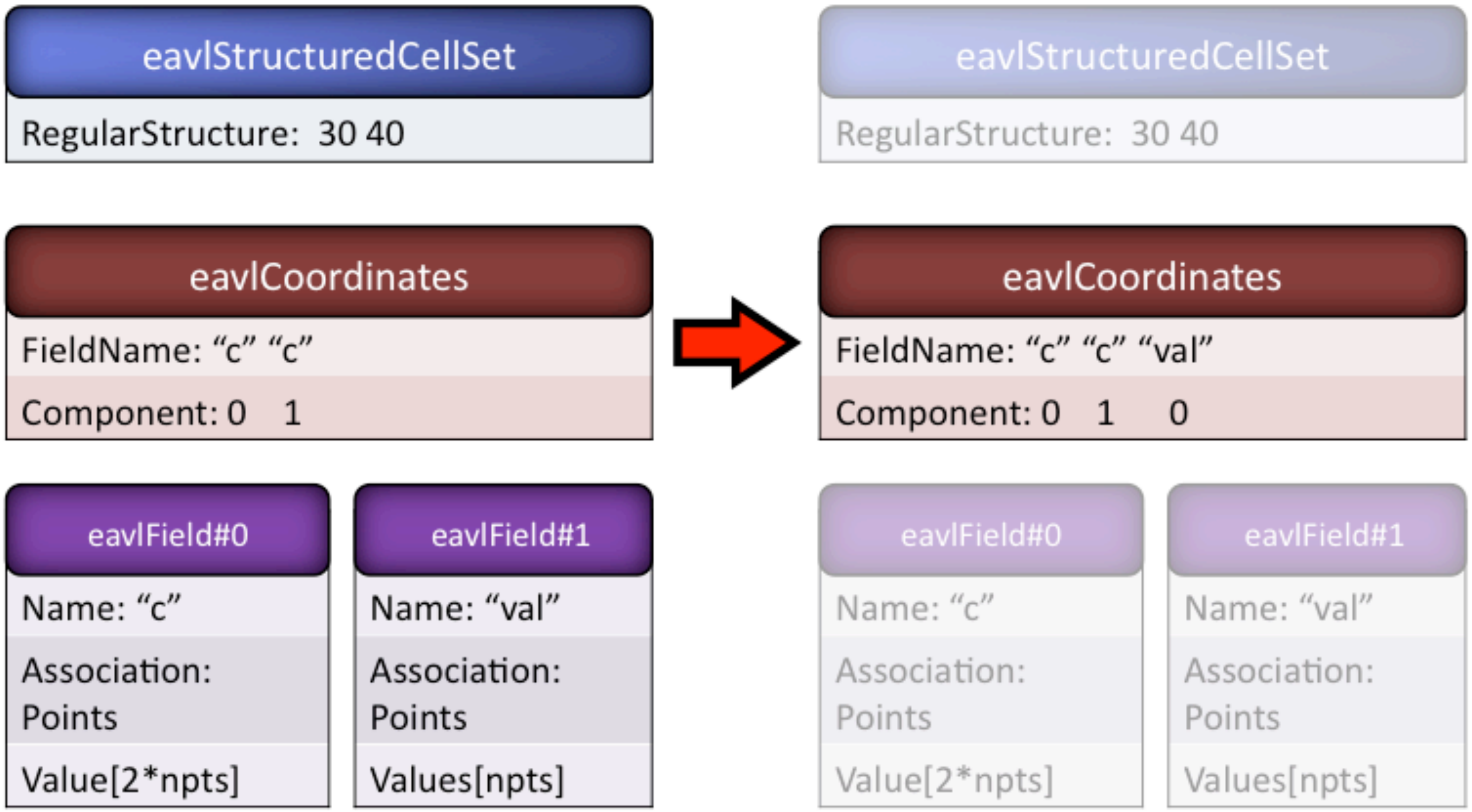


The EAVL Data Set Model



EAVL Example: Elevating a Structured Grid

- No problem-sized data modifications.
  - Interleaved and separated coordinates can be used simultaneously.



Productive Algorithm Development in EAVL

- Topological iterators encapsulate data-parallel patterns
- Functors provide optimized execution on CPU and GPU
- Transparent heterogeneous memory space support

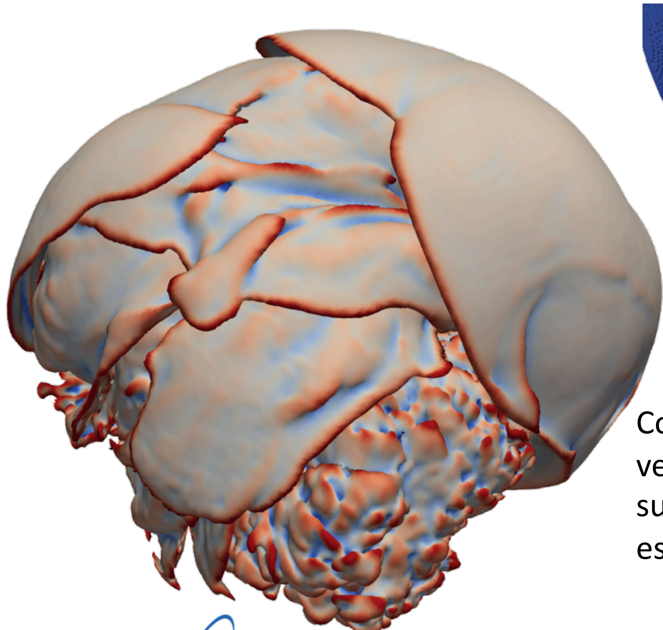
```
struct PolyNormalFunctor
{
  void operator()(float *x, float *y, float *z, float *n)
  {
    // get two adjacent edge vectors
    float ax = x[1]-x[0],  ay = y[1]-y[0],  az = z[1]-z[0];
    float bx = x[2]-x[1],  ay = y[2]-y[1],  az = z[2]-z[1];
    // calculate their cross product
    n[0] = ay*bz - az*by;  n[1] = az*bx - ax*bz;   n[2] = ax*by - ay*bx;
  }
};

void FaceNormalFilter::Execute(...)
{
  executor->AddOperation(new NodeToCellOp3(xcoord, ycoord, zcoord, outputnormals,
                                           inputcells, PolyNormalFunctor()));
}
```

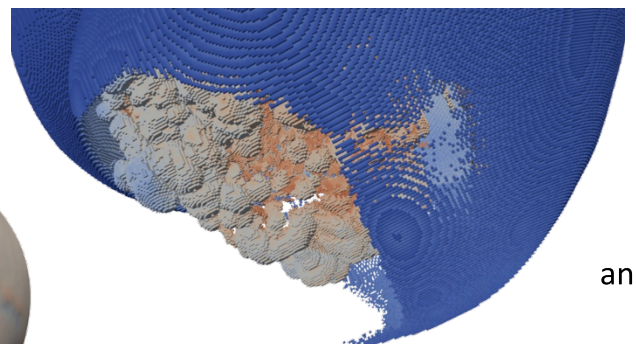
Dax: A Toolkit for Analysis and Visualization at Extreme Scale

The primitives necessary to design finely-threaded algorithms

http://daxtoolkit.org

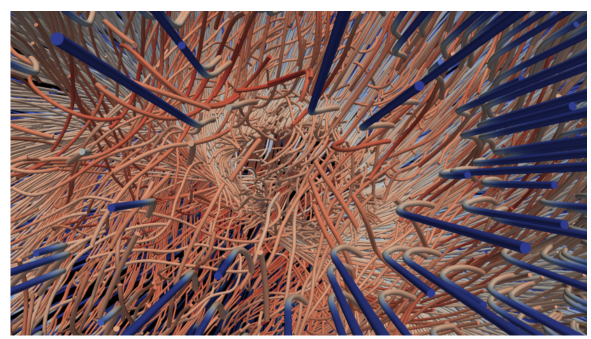
- “Worklets” ease design in serial, scheduled in parallel
- Basic visualization design objects (think VTK for many-core)
- Communicative operations provide neighborhood-wide operations without exposing read/write hazards



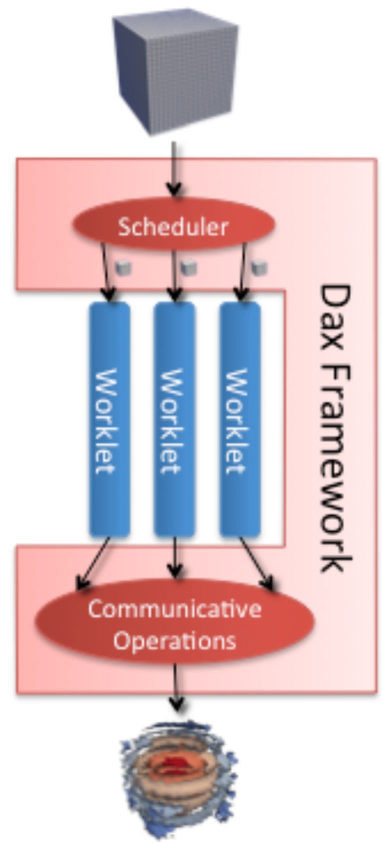


Extracted cells of large gradient and compacted points

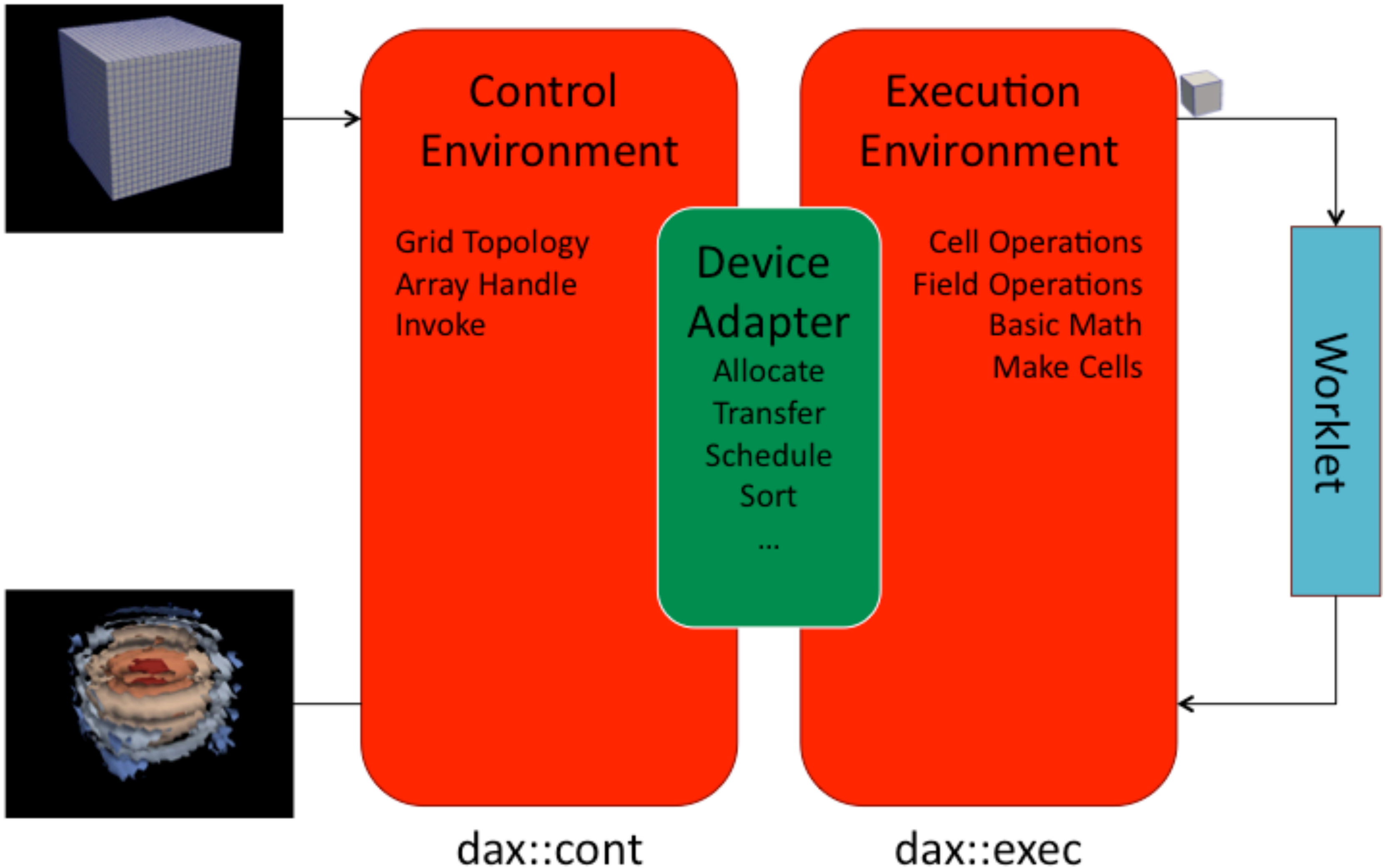
Contour with subsequent vertex welding, coarsening, subdivision, and curvature estimation



Streamlines (preliminary work)



Dax Framework



Example Dax Worklet

```
struct Normal: dax::exec::WorkletMapField
{
        typedef void ControlSignature(Field(In),Field(Out));
        typedef _2 ExecutionSignature(_1);

        template<typename T>
        T operator()(const T& coord) const
        {
        dax::Scalar dot = dax::dot(coord,coord);
        return coord * dax::math::RSqrt(dot);
        }
};
```

Example Dax Control Code

```
int main()
{
using namespace dax::cont;
 std::vector<dax::Vector3> coords(10);
 for(int i=0; i < 10; i++)
    {
    const dax::Scalar x(1.0f + i);
    coords[i] = dax::Vector3(dax::math::Sin(x)/i+1,
                             1/(x*x),
                             0);
    }
 //make a dax array handle to the coordinates
 ArrayHandle<dax::Vector3> coordHandle =
          make_ArrayHandle(coords);

 //make a dax array handle to store the results
 ArrayHandle<dax::Vector3> normals;


 Schedule< > scheduler;
//note two parameters passed to scheduler like the control
// signature requests
 scheduler(Normal(), coordHandle, normals);


  std::vector<dax::Vector3> results(normals.GetNumberOfValues());
 normals.CopyInto (results.begin());
}
```

DIY (Do-It-Yourself): Overview

Main Ideas and Objectives

-Large-scale parallel analysis (visual and numerical) on HPC machines

-For scientists, visualization researchers, tool builders

-In situ, coprocessing, postprocessing

-Data-parallel problem decomposition

-MPI + threads hybrid parallelism

-Scalable data movement algorithms

-Runs on Unix-like platforms, from laptop to supercomputer (including all IBM and Cray HPC leadership machines)

Features

-Parallel I/O to/from storage

-Domain decomposition

-Network communication

-Written in C++

-C bindings, can be called from Fortran, C, C++

-Autoconf build system

-Lightweight: libdiv.a 800KB

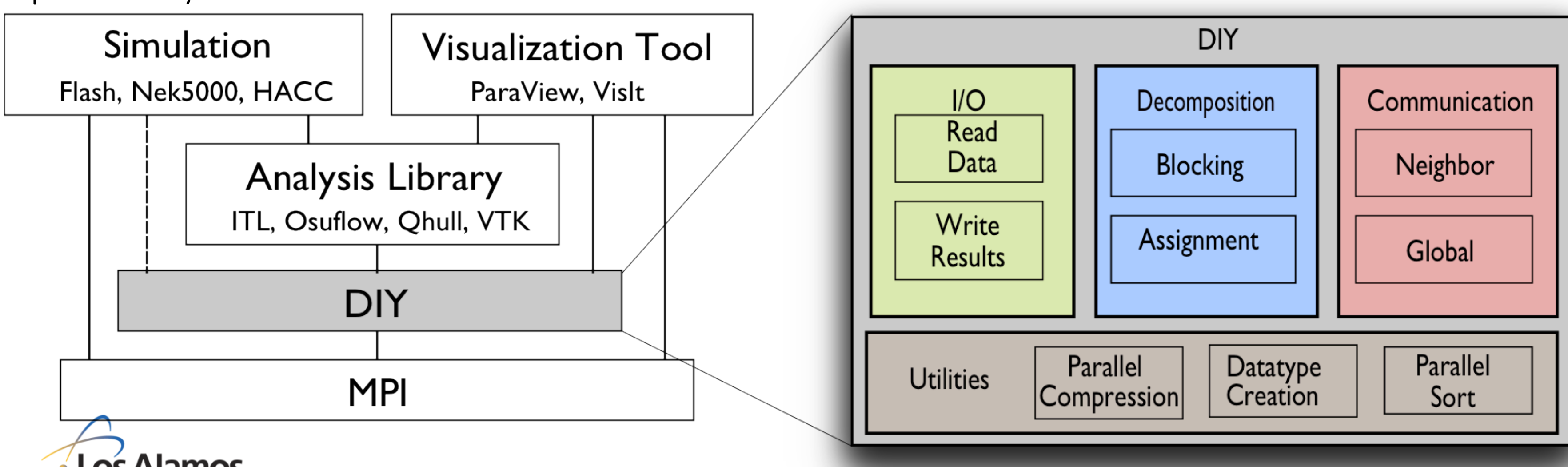
-Maintainable: ~15K lines of code

Benefits

-Researchers can focus on their own work, not on parallel infrastructure

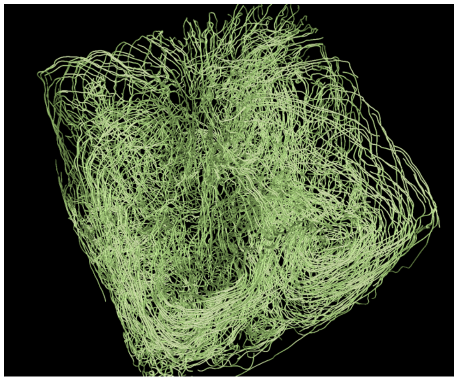
-Analysis applications can be custom

-Reuse core components and algorithms for performance and productivity

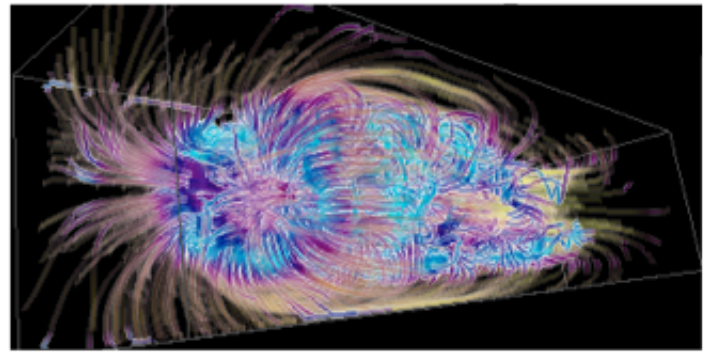


DIY usage and library organization

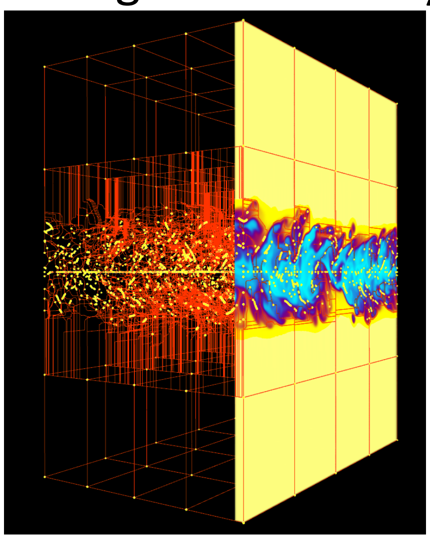
DIY: Applications



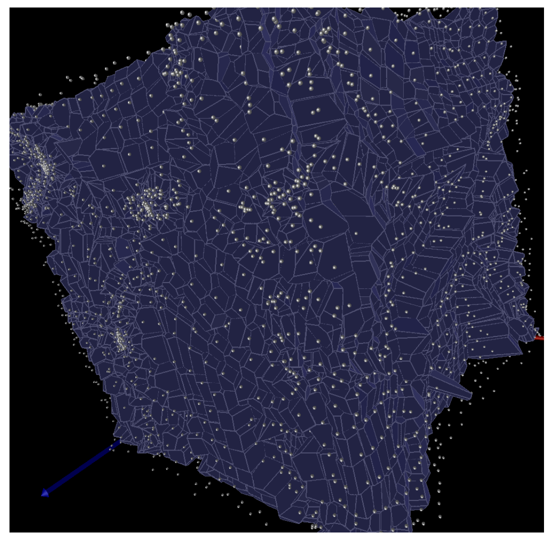
Particle tracing of thermal hydraulics flow



Information entropy analysis of astrophysics



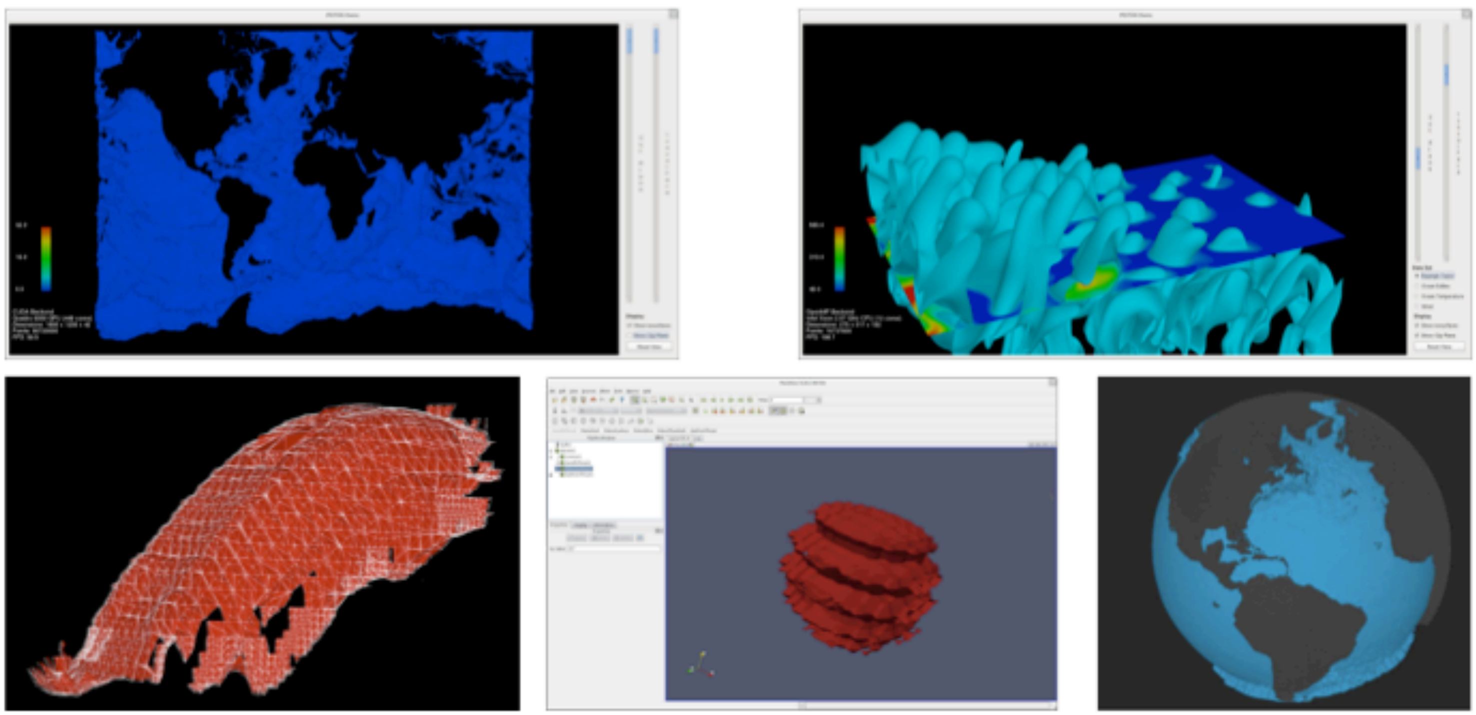
Morse-Smale complex of combustion



Voronoi tessellation of cosmology

PISTON: A Portable Data-Parallel Visualization and Analysis Framework

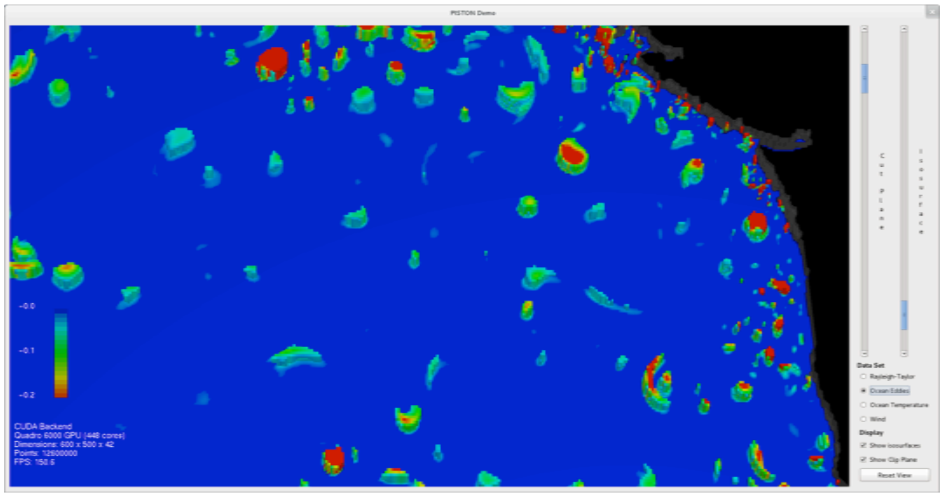
- Goal: Portability and performance for visualization and analysis operators on current and next-generation supercomputers
- Main idea: Write operators using only data-parallel primitives (scan, reduce, etc.)
- Requires architecture-specific optimizations for only for the small set of primitives
- PISTON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

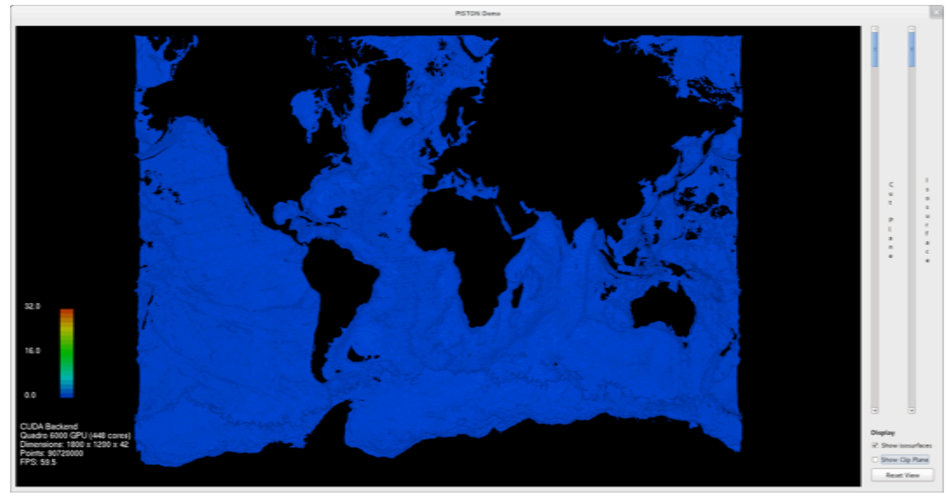


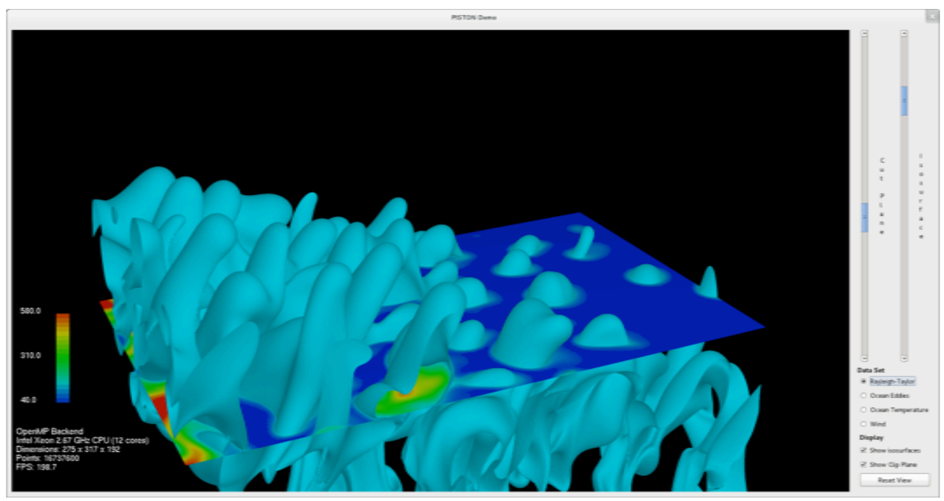
Motivation and Background

- 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)

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

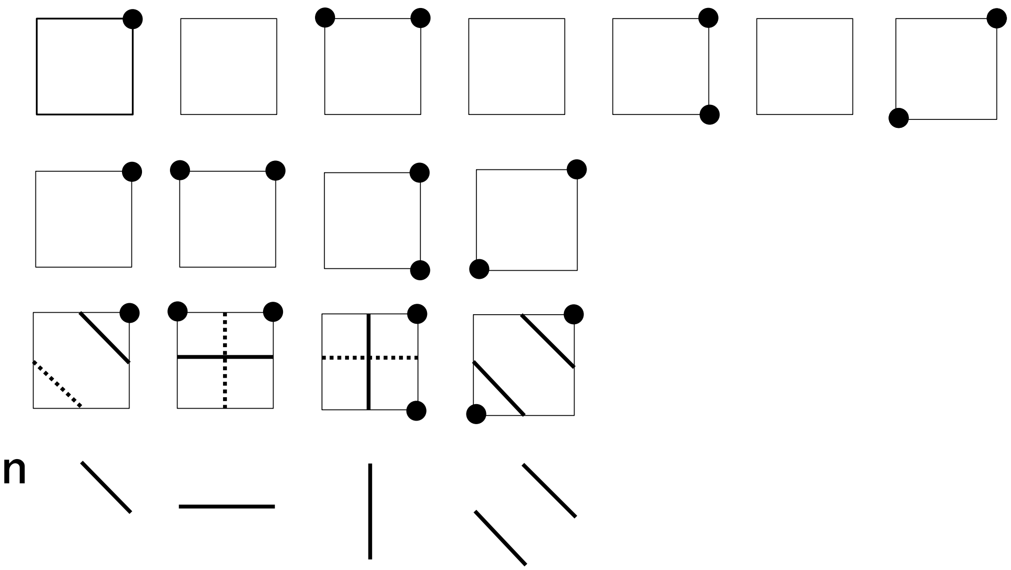
```
input                    4  5  2  1  3
--------------------------------------
transform(+1)            5  6  3  2  4
inclusive_scan(+)        4  9 11 12 15
exclusive_scan(+)        0  4  9 11 12
exclusive_scan(max)      0  4  5  5  5
transform_inscan(*2,+)   8 18 22 24 30
for_each(-1)           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

Challenge: Write operators in terms of these primitives only

Reward: Efficient, portable code

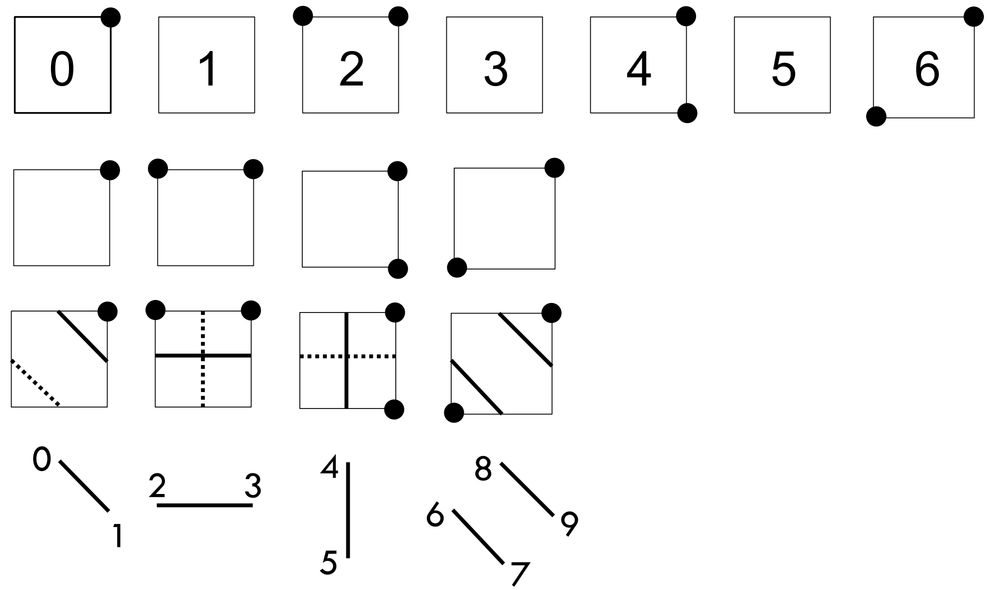
Isosurface with Marching Cube – the Naive Way

- 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?



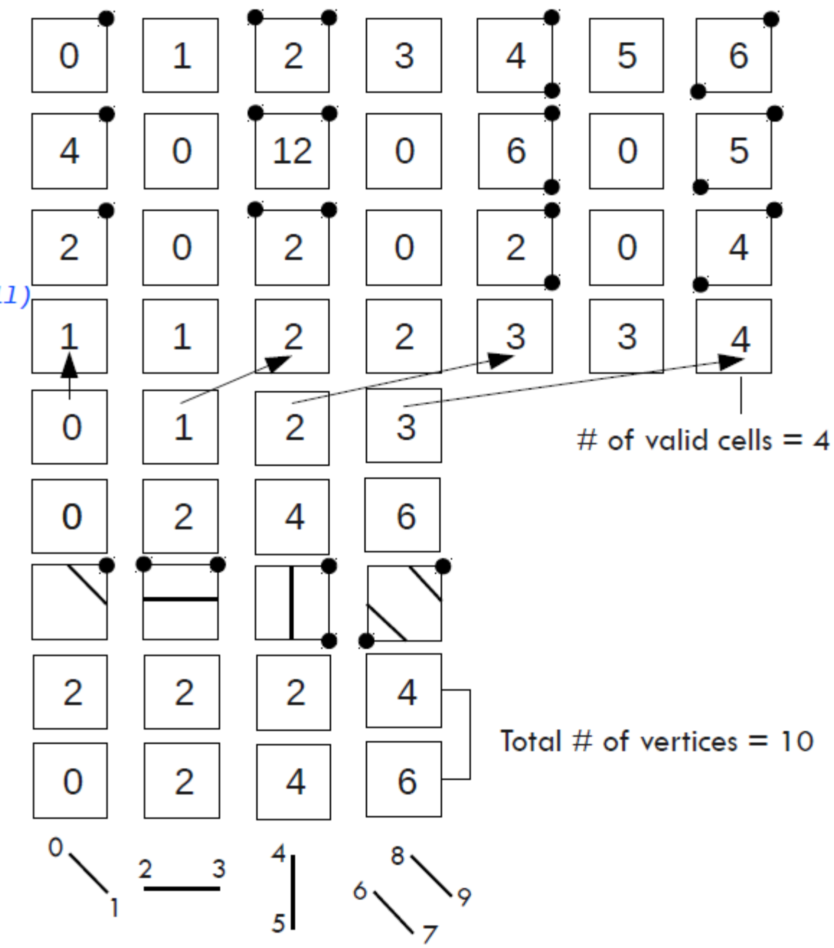
Isosurface with Marching Cube – Optimization

- 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



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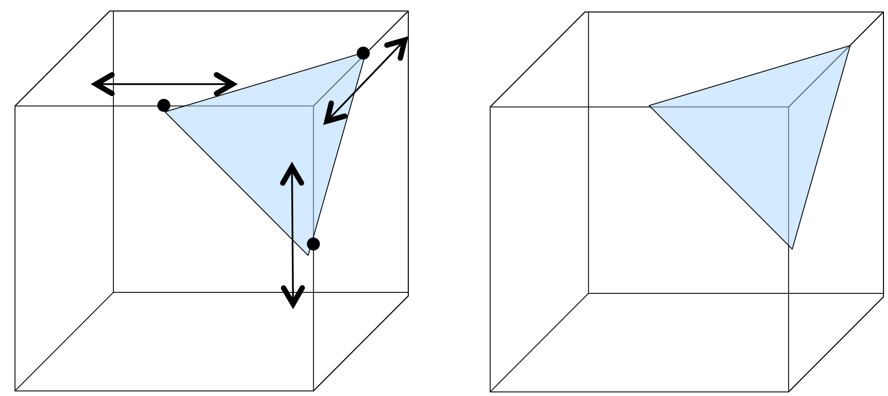
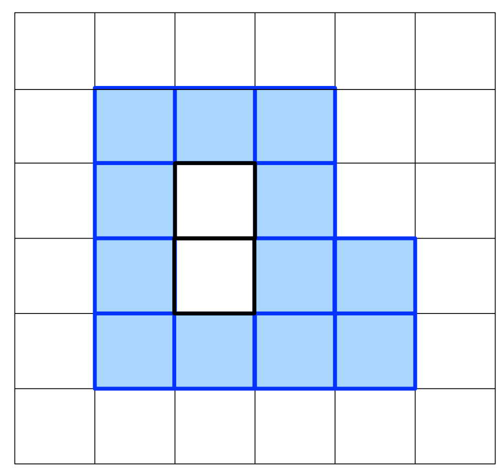
Variations on Isosurface: Cut Surfaces and Threshold

- 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



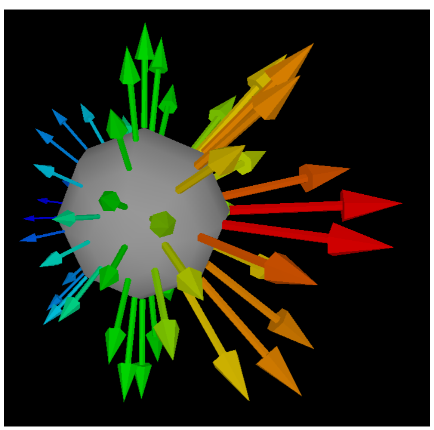
Additional Operators

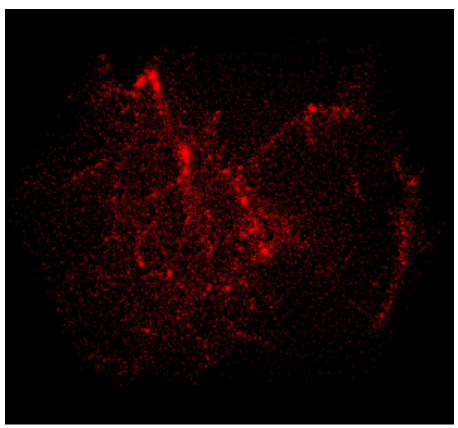
Blelloch's "Vector Models for Data-Parallel Computing"

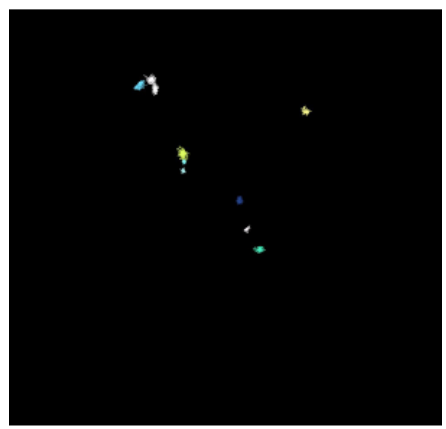
- Data Structures
  - Graphs: Neighbor reducing, distributing excess across edges
  - Trees: Leaffix and rootfix operations, tree manipulations
  - Multidimensional arrays
- Computational Geometry
  - Generalized binary search
  - k-D tree
  - Closest pair
  - Quickhull
  - Merge Hull
- Graph Algorithms
  - Minimum spanning tree
  - Maximum flow
  - Maximal independent set
- Numerical Algorithms
  - Matrix-vector multiplication
  - Linear-systems solver
  - Simplex
  - Outer product
  - Sparse-matrix multiplication

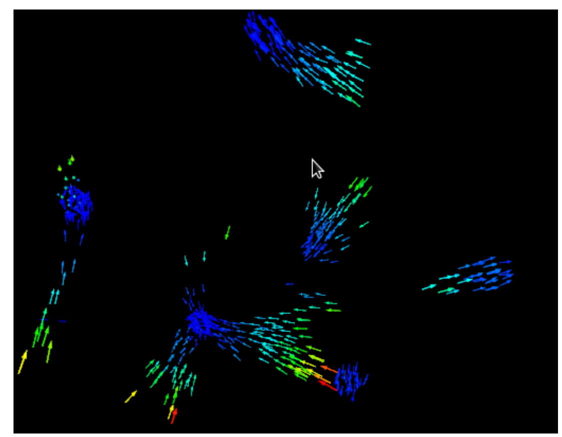
Current prototypes

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

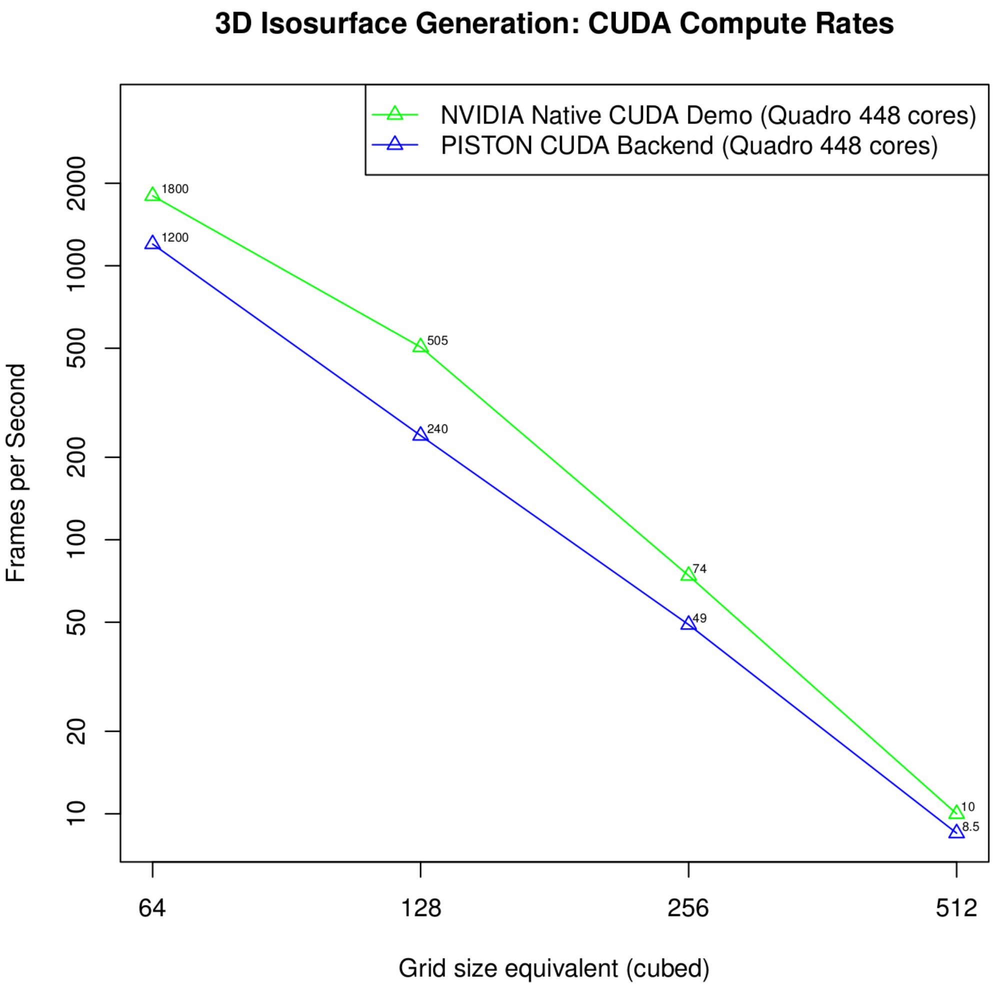


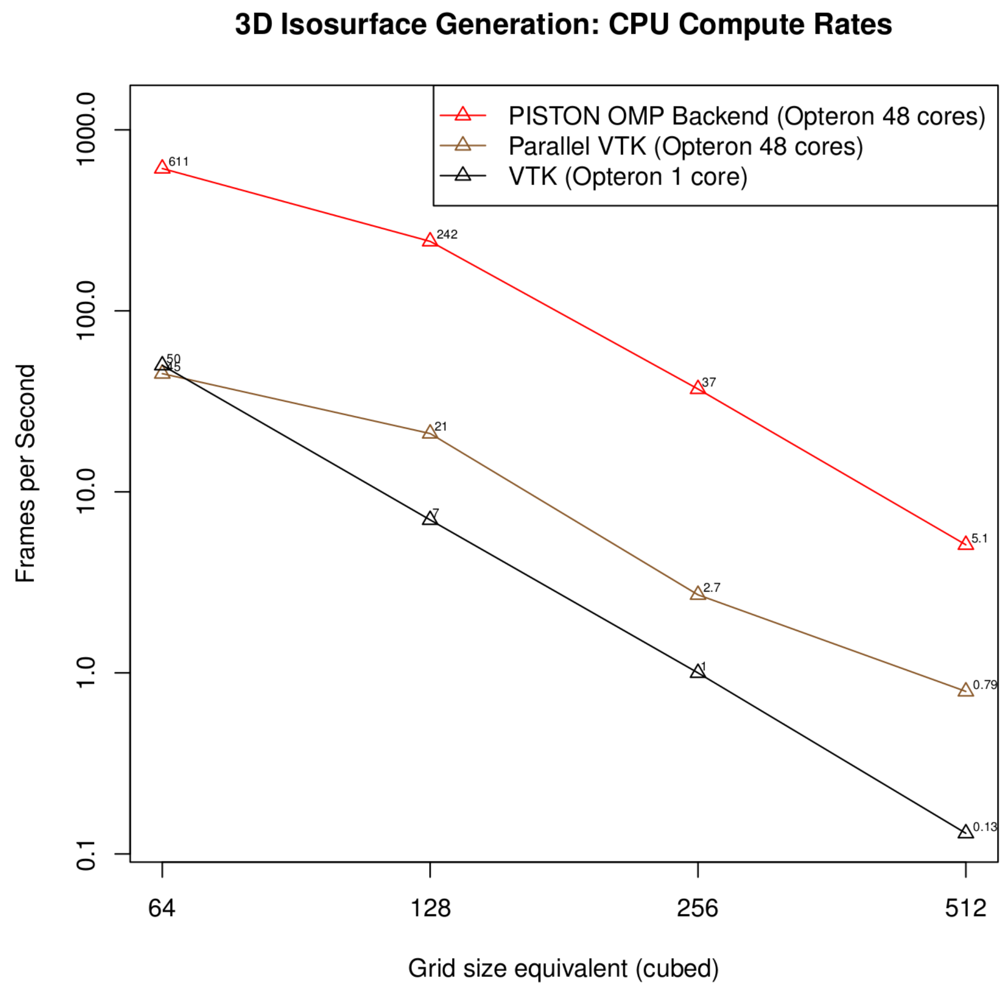






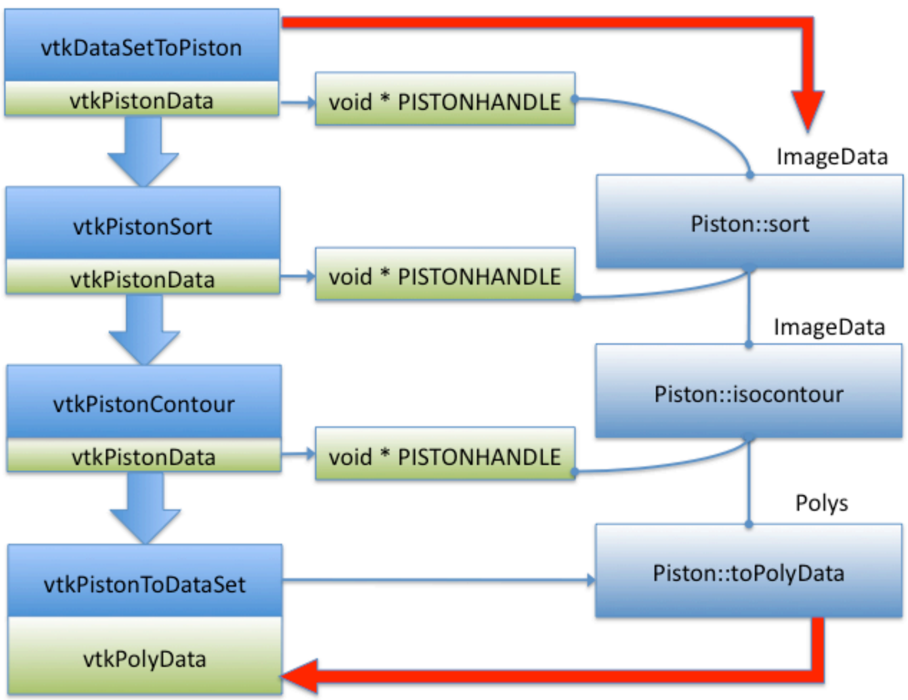
PISTON Performance

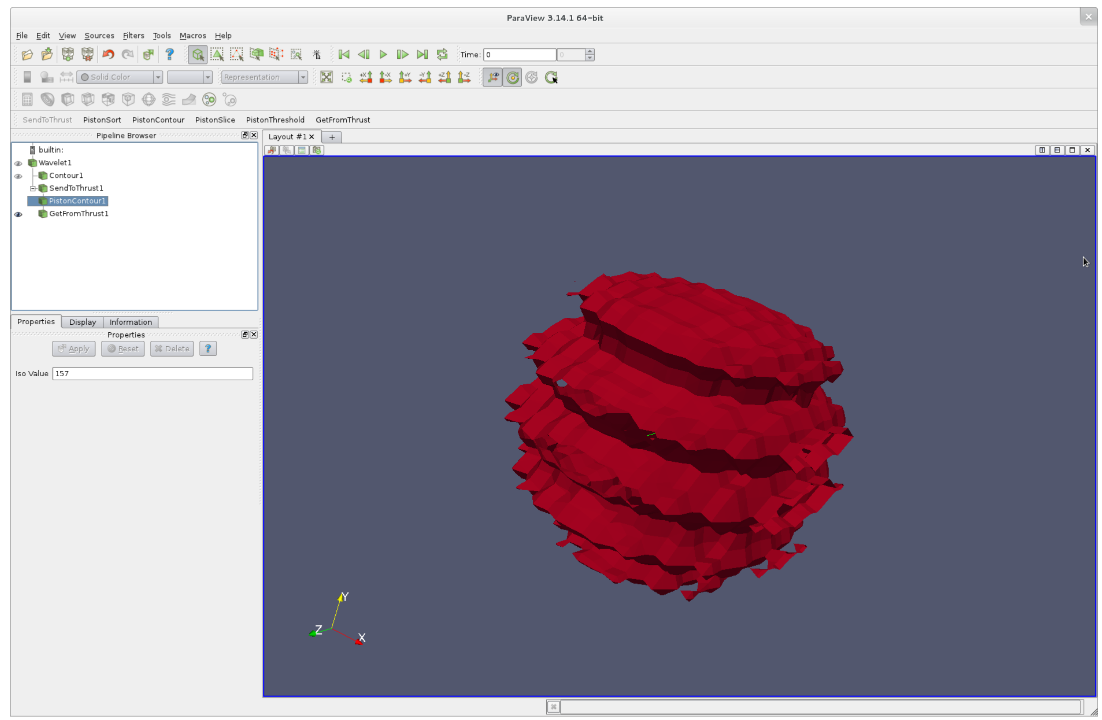




Integration with VTK and ParaView

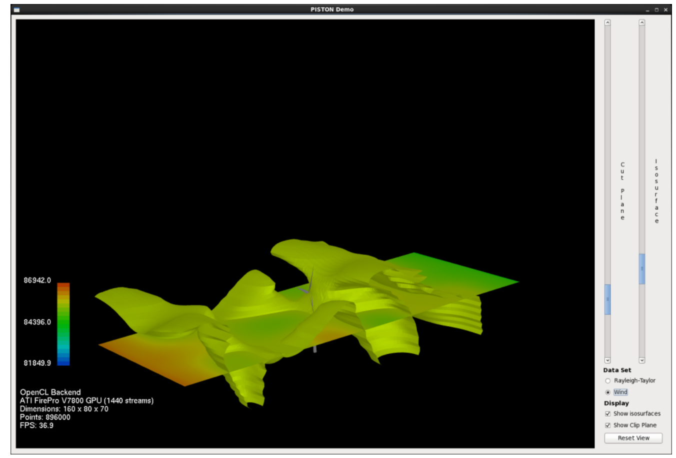
- Filters that use PISTON data types and algorithms integrated into VTK and ParaView
- Utility filters interconvert between standard VTK data format and PISTON data format (thrust device vectors)
- Supports interop for on-card rendering



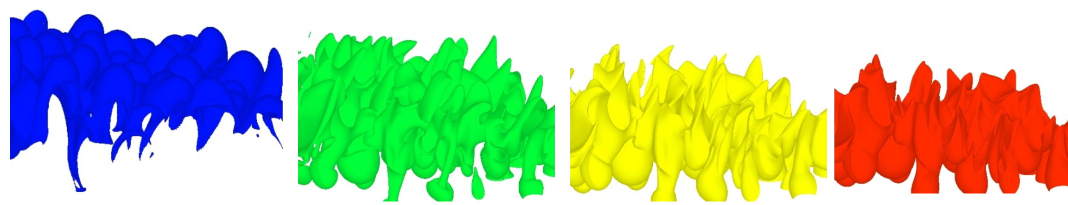


Extending PISTON's Portability: Architectures

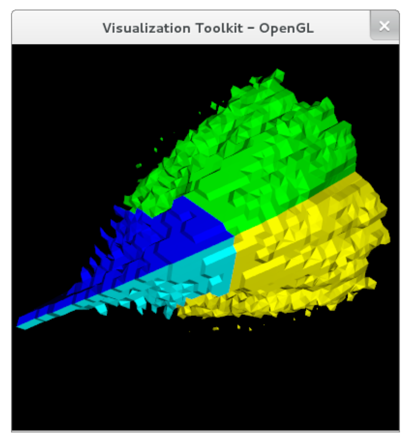
- Prototype OpenCL backend
  - Successfully implemented isosurface and cut plane operators in OpenCL with code almost identical to that used for the Thrust-based CUDA and OpenMP backends
  - With interop on AMD FirePro V7800, we can run at about 6 fps for 256^3 data set (2 fps without interop)

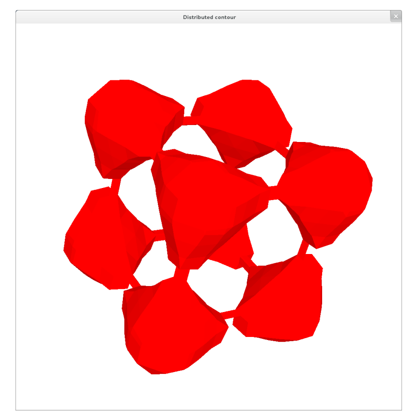


- Renderer
  - Allows generation of images on systems without OpenGL
  - Rasterizing and ray-casting versions (using K-D Tree)



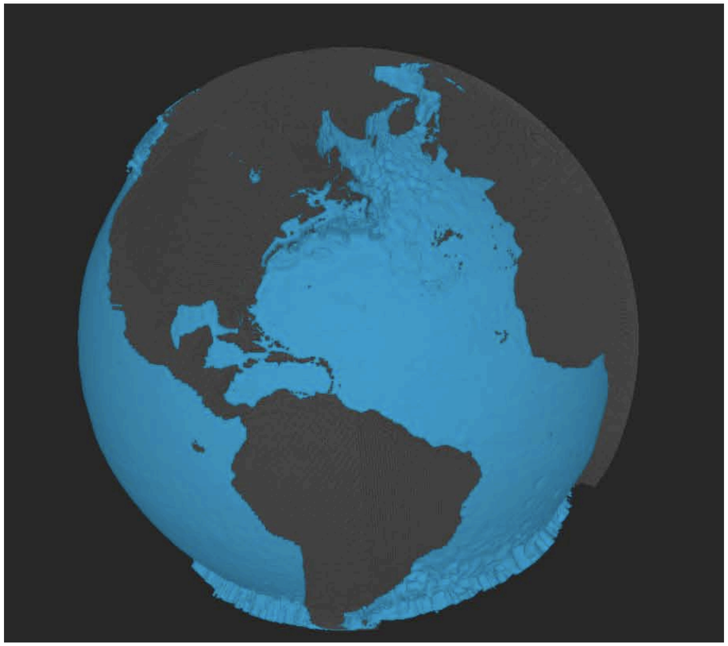
- Inter-node parallelism
  - VTK Integration
    - Domain partitioned by VTK's MPI libraries
    - Each node uses PISTON filters to compute results for its portion of domain
    - Results combined by VTK's compositors
  - Distributed implementations of Thrust primitives using MPI (in progress)

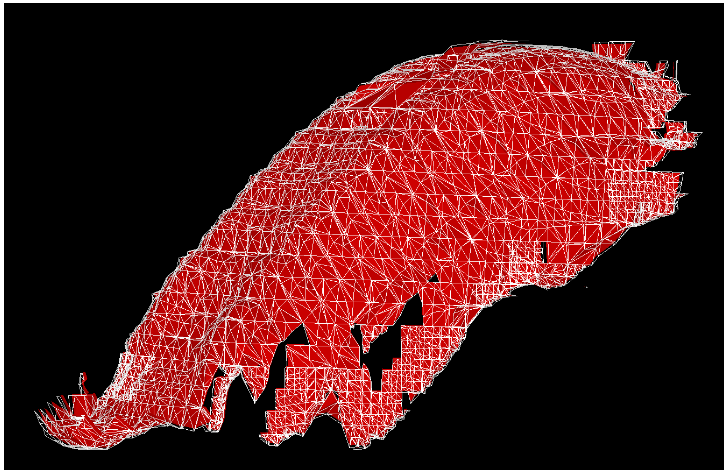




Extending PISTON's Portability: Data Types

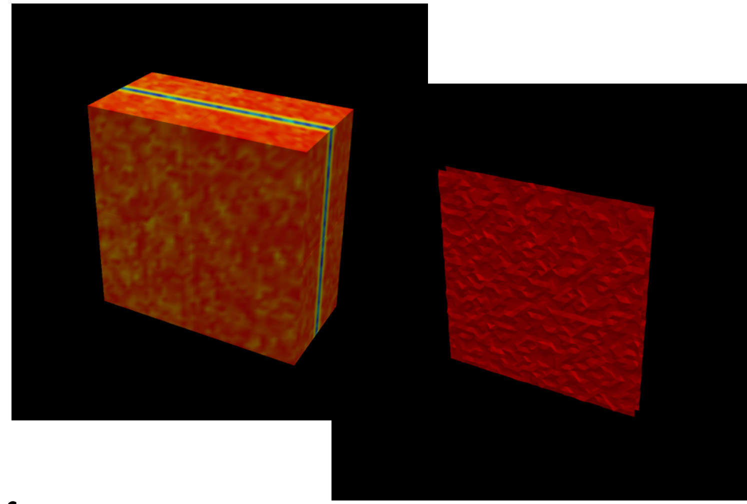
- Curvilinear coordinates
  - Multiple layers of coordinate transformations
  - Due to kernel fusion, very little performance impact
- Unstructured / AMR data
  - Tetrahedralize uniform grid or unstructured grid (e.g., AMR mesh)
  - Generate isosurface geometry based on look-up table for tetrahedral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





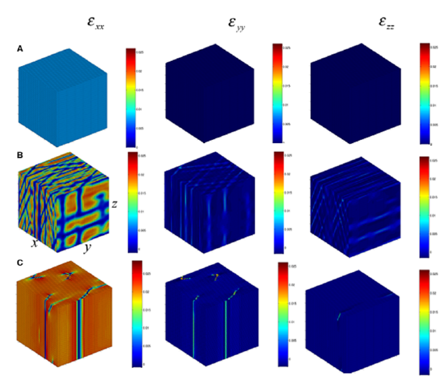
PISTON In-Situ

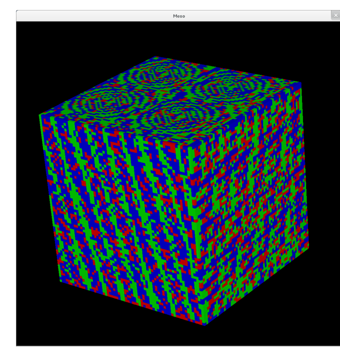
- VPIC (Vector Particle in Cell) Kinetic Plasma Simulation Code
  - Implemented first version of an in-situ adapter based on Paraview CoProcessing Library (Catalyst)
  - Three pipelines: vtkDataSetMapper, vtkContourFilter, vtkPistonContour



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

- 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

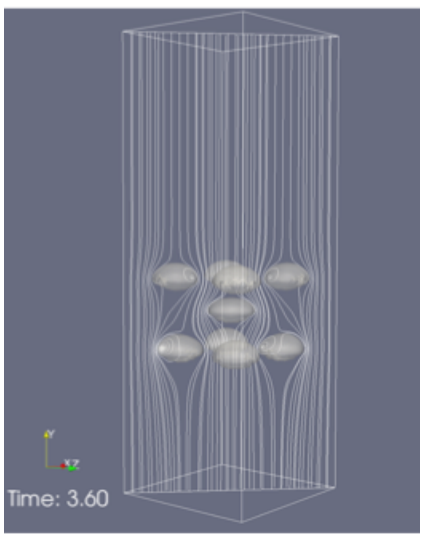


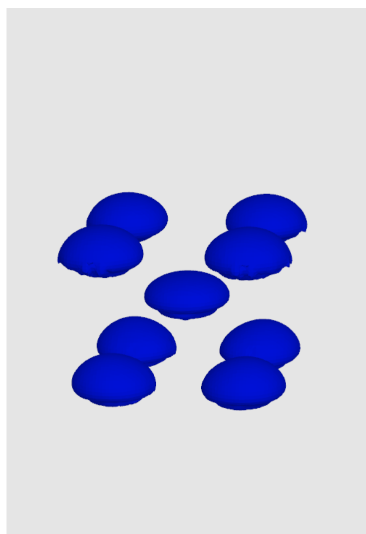


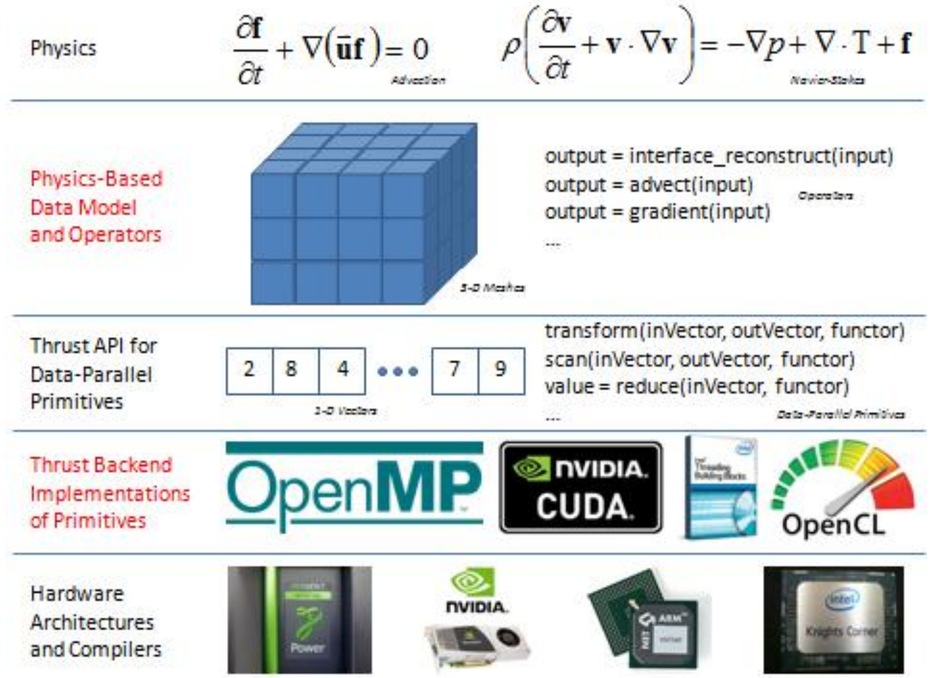
Strains in x,y,z (above); PISTON in-situ visualization (right)

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







PISTON Open-Source Release

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

Acknowledgments and Resources

- http://sdav-scidac.org/
- Panel at SC12: "Visualization Frameworks for Multi-Core and Many-Core Architectures" Hank Childs, Jeremy Meredith, Patrick McCormick, Christopher Sewell, Kenneth Moreland
  - Wednesday, November 14, 3:30 – 5:00, 355-BC
- The SciDAC Institute of Scalable Data Management, Analysis and Visualization (SDAV) is funded by the DOE Office of Science through the Office of Advanced Scientific Computing Research.
  - SciDAC Institute Director: Arie Shoshani
  - Visualization Project Chairs: James Ahrens, Wes Bethel
- Related PISTON projects also funded by ASC Program, ASCR, LANL LDRD