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

Christopher Sewell
Ken Moreland
Jeremy Meredith
Tom Peterka
Li-ta Lo
James Ahrens

The Seventh Workshop on Ultrascale Visualization, The International Conference for High Performance Computing, Networking, Storage, and Analysis, November 12, 2012
The SDAV Software Frameworks for Visualization and Analysis on Next-Generation Multi-core Architectures

Presentation by Chris Sewell, Los Alamos National Laboratory

PISTON
Chris Sewell, Li-ta Lo, James Ahrens

DAX
Ken Moreland

EAVL
Jeremy Meredith

DIY
Tom Peterka

Productization support provided by Kitware
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

- **Rectilinear**
  - Dimensions
  - 3D Axis Coordinates
  - Cell Fields
  - Point Fields

- **Structured**
  - Dimensions
  - 3D Point Coordinates
  - Cell Fields
  - Point Fields

- **Unstructured**
  - Connectivity
  - 3D Point Coordinates
  - Cell Fields
  - Point Fields
The EAVL Data Set Model

Data Set
- Cells[]
- Points[]
- Fields[]

Field
- Name
- Association
- Values

Cell Set
- Explicit Connectivity
- Structured Dimensions
- QuadTree Tree
- Subset CellList

Coords
- FieldName
- Component
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

```cpp
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];
        // calculate their cross product
        n[0] = ay*bx - 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

- “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

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

Streamlines (preliminary work)

Extracted cells of large gradient and compacted points

http://daxtoolkit.org
Dax Framework

Control Environment
- Grid Topology
- Array Handle
- Invoke

Execution Environment
- Cell Operations
- Field Operations
- Basic Math
- Make Cells

Device Adapter
- Allocate
- Transfer
- Schedule
- Sort
- ...

dax::cont

dax::exec

Worklet
Example Dax Worklet

```cpp
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

```cpp
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);

    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.CopyTo (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

Simulation
Flash, Nek5000, HACC

Visualization Tool
ParaView, VisIt

Analysis Library
ITL, Osuflow, Qhull, VTK

DIY

MPI

I/O
Read Data
Write Results

DIY

Decomposition
Blocking
Assignment

Communication
Neighbor
Global

Utilities
Parallel Compression
Datatype Creation
Parallel Sort
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

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
   \texttt{transform(classify\_cell)}
2. caseNums
3. numVertices
   \texttt{transform\_inclusive\_scan(is\_valid\_cell)}
4. validCellEnum
5. CountingIterator
   \texttt{upper\_bound}
6. validCellIndices
   \texttt{make\_permutation\_iterator}
7. numVerticesCompacted
   \texttt{exclusive\_scan}
8. numVerticesEnum
   \texttt{for\_each(isosurface\_functor)}
9. outputVertices

\begin{tikzpicture}
\fill[blue!10] (0,0) rectangle (5,5);
\fill[red!10] (0,5) rectangle (5,10);
\fill[green!10] (5,0) rectangle (10,5);
\fill[orange!10] (5,5) rectangle (10,10);
\end{tikzpicture}

\textbf{Total # of vertices} = 10
\textbf{# of valid cells} = 4
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

3D Isosurface Generation: CUDA Compute Rates

- NVIDIA Native CUDA Demo (Quadro 448 cores)
- PISTON CUDA Backend (Quadro 448 cores)

3D Isosurface Generation: CPU Compute Rates

- PISTON OMP Backend (Opteron 48 cores)
- Parallel VTK (Opteron 48 cores)
- VTK (Opteron 1 core)
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

- 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 Hydro 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
PISTON Open-Source Release

- Open-source release
  - Current repository: [https://github.com/losalamos/PISTON](https://github.com/losalamos/PISTON)
Acknowledgments and Resources

- [http://sdav-scidac.org/](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