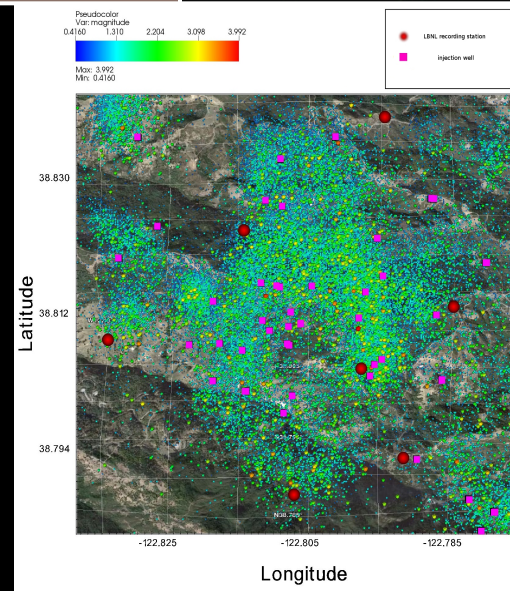
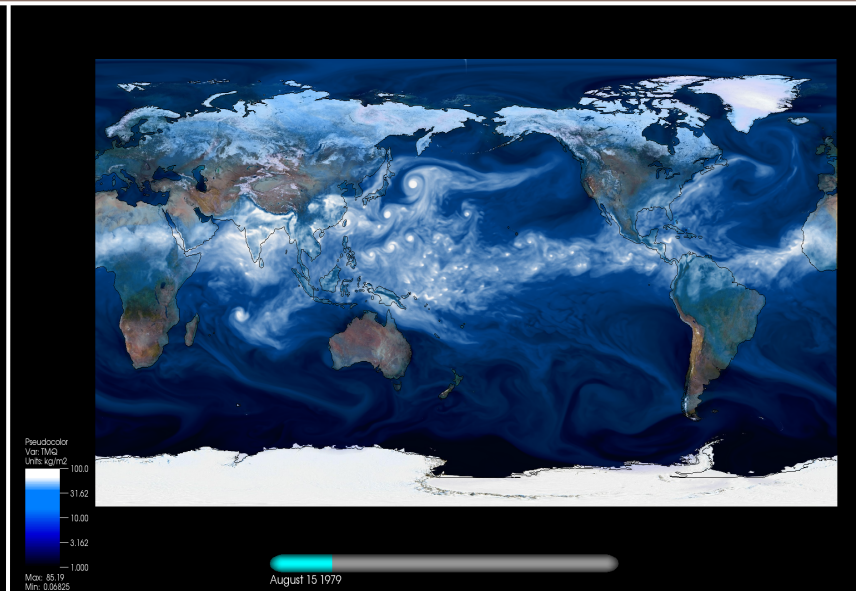
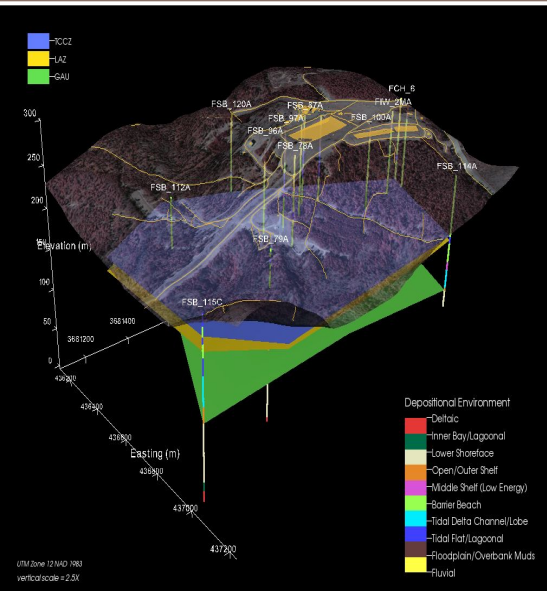


Challenges and Solutions for Visual Data Analysis on Current and Emerging HPC Platforms

SEG WORKSHOP

High Performance Computing in the Geosciences

BERKELEY, CALIFORNIA USA
18-21 JULY 2011



July 20, 2011

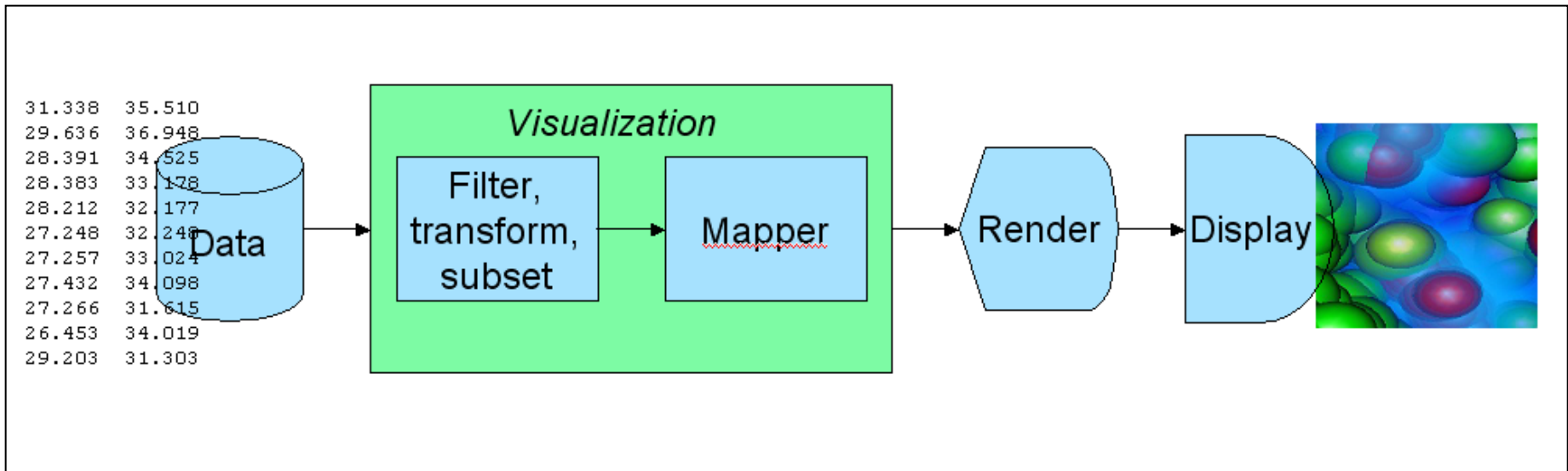
Wes Bethel & Hank Childs, Lawrence Berkeley Lab

Outline

- Petascale & Exascale issues (Childs)
- Tools: how the community comes together to collectively solve large data visual data analysis problems (Childs)
- Achieving extreme performance in visual data analysis (Bethel)
- Recent examples/case studies (Bethel)

Visualization 101

- Transformation of numbers (data) into readily comprehensible images.
- Plays an integral part in the scientific and analytic processes.
- Data intensive.

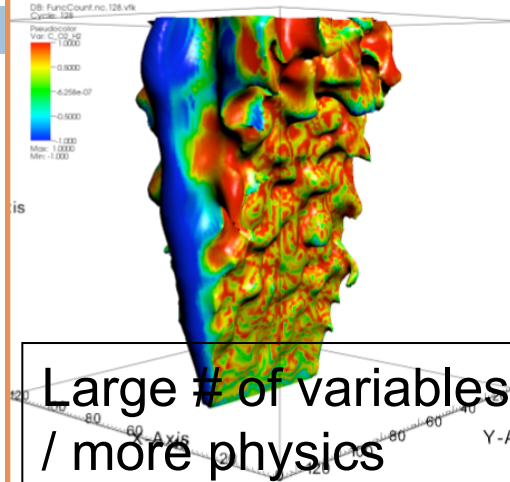
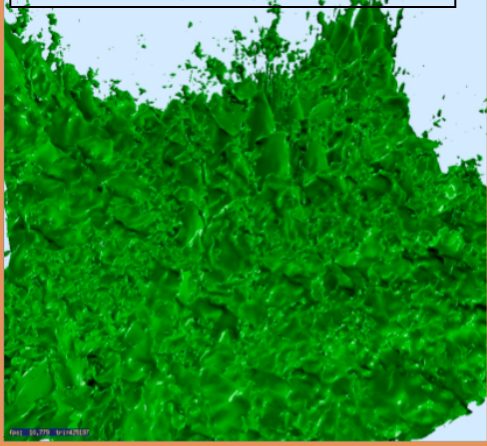


Why are supercomputing trends going to change the rules for visualization and analysis?

- Michael Strayer (U.S. DoE Office of Science) in 2006:
“petascale is not business as usual”
 - ▣ Especially true for visualization and analysis!
- Large scale data creates two incredible challenges:
scale and **complexity**
- **Scale** is not “business as usual”
 - ▣ Will discuss this assertion throughout this talk
 - ▣ Solution: we will need “smart” techniques in production environments
- More resolution leads to more and more **complexity**
 - ▣ Will the “business as usual” techniques still suffice?

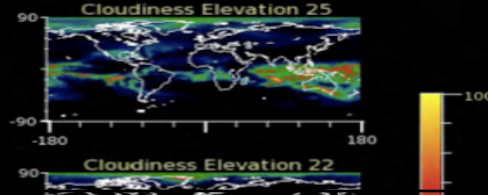
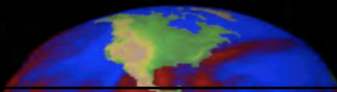
How does increased computing power affect the data to be visualized?

High-res meshes

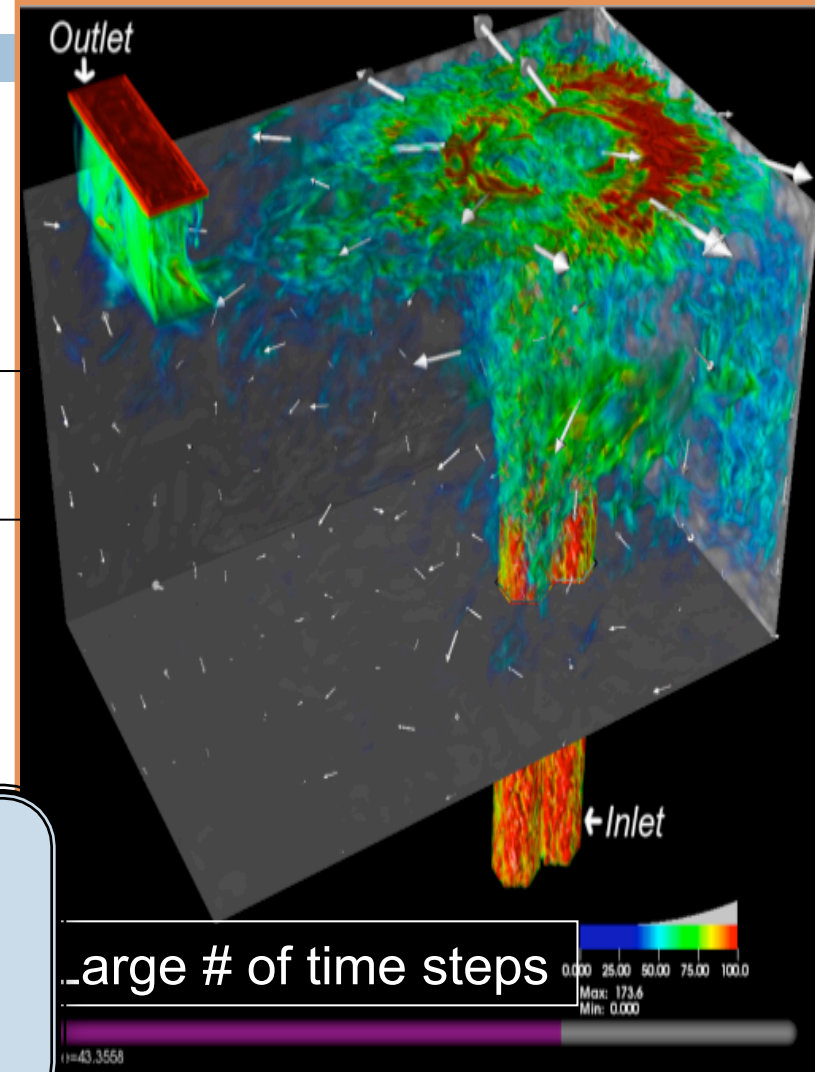


Large ensembles

Variable: cloud area fraction in atmosphere layer



Your mileage may vary; some simulations produce a lot of data and some don't.



Slide credit: Sean Ahern (ORNL) & Ken Joy (UCD)

Today's production visualization tools use "pure parallelism" to process data.

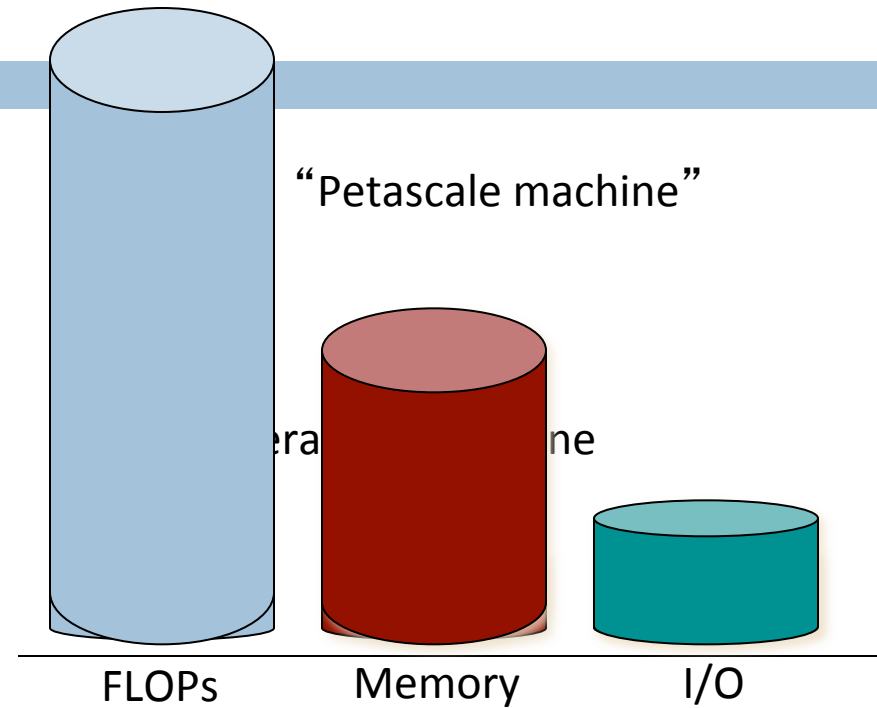


Pure parallelism

- Pure parallelism: “brute force” ... processing full resolution data using data-level parallelism
- Pros:
 - ▣ Easy to implement
- Cons:
 - ▣ Requires large I/O capabilities
 - ▣ Requires large amount of primary memory

I/O and visualization

- Pure parallelism is almost always $>50\%$ I/O and sometimes 98% I/O
- Amount of data to visualize is typically $O(\text{total mem})$
- Two big factors:
 - ① how much data you have to read
 - ② how fast you can read it
- \rightarrow Relative I/O (ratio of total memory and I/O) is key



Why is relative I/O getting slower?

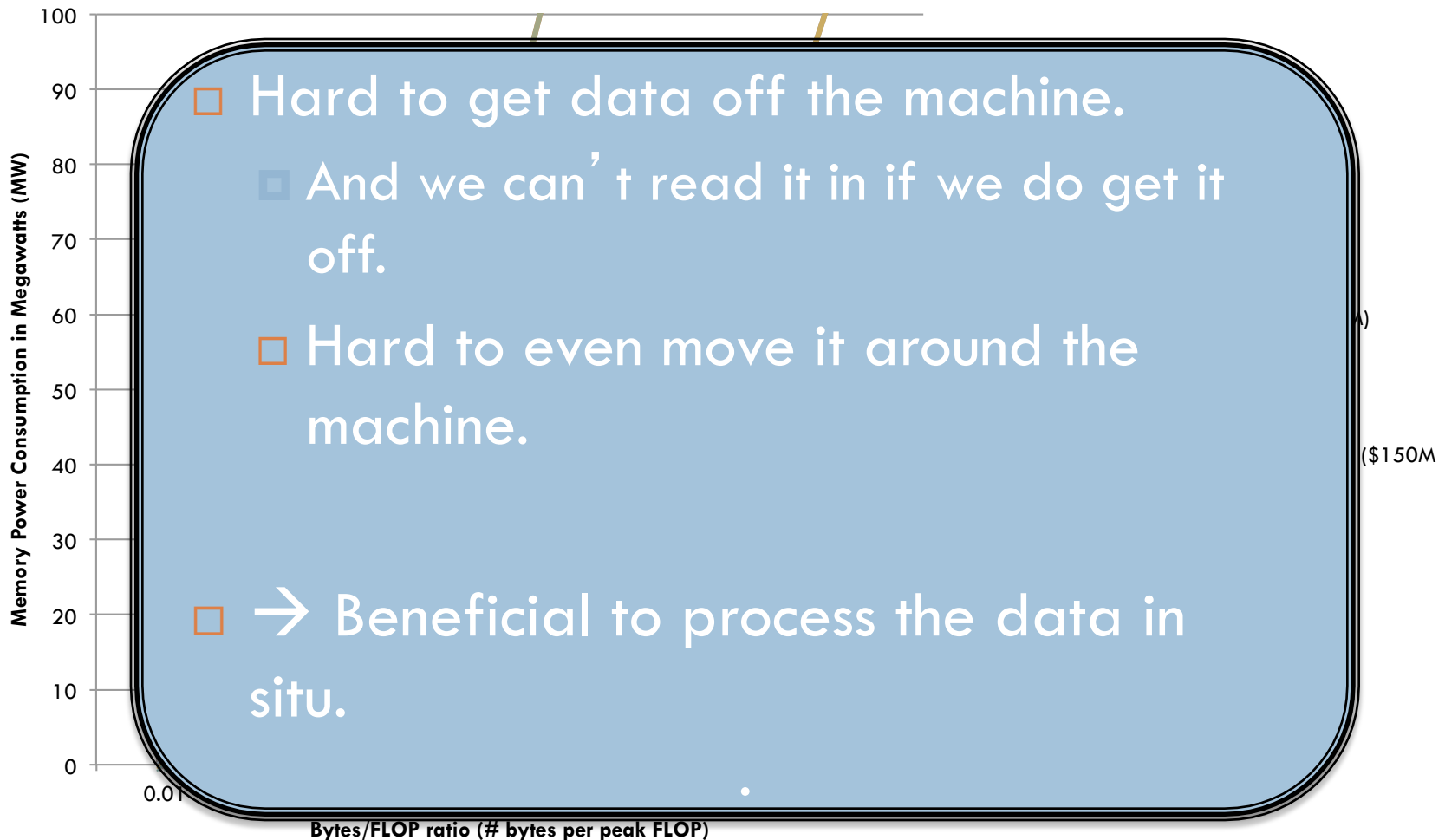
- I/O is quickly becoming a dominant cost in the overall supercomputer procurement.
 - ▣ And I/O doesn't pay the bills.
- Simulation codes aren't as exposed.

We need to de-emphasize I/O in our visualization and analysis techniques.

There are “smart techniques” that de-emphasize memory and I/O.

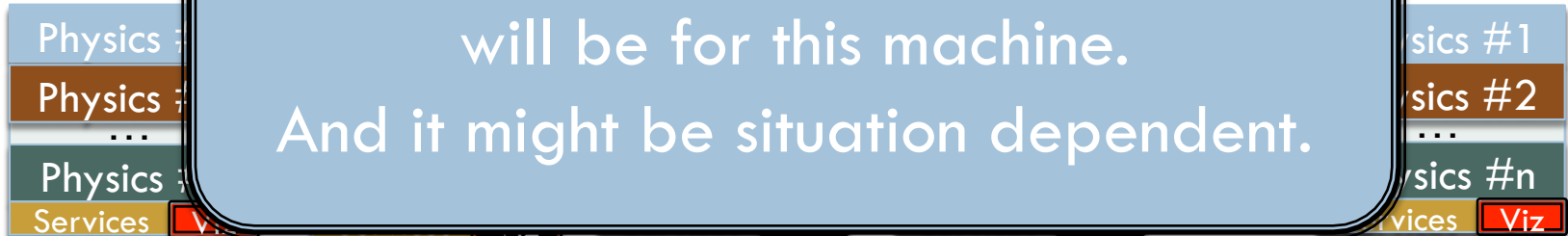
- Out of core
 - Data subsetting
 - Multi-resolution
 - In situ
-
- ... the community is currently getting these techniques deployed in production tools.
-
- This will be the primary challenge of the <100PFLOP era.

Exascale hurdle: memory bandwidth eats up the entire power budget



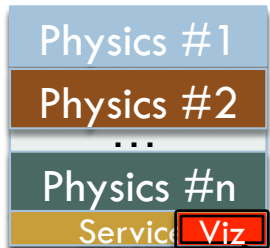
Possible in situ visualization scenarios

Visualization



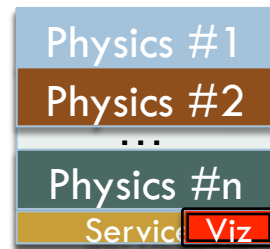
We don't know what the best technique will be for this machine. And it might be situation dependent.

... or visualization could be done on a separate node located nearby dedicated to visualization/analysis/IO/etc. (loosely coupled)



We will possibly need to run on:

- The accelerator in a lightweight way
- The accelerator in a heavyweight way
- A vis cluster (?)



to high memory of
exascale machine
(e.g. GPU)

the data is reduced and sent to dedicated resources off machine!

Additional exascale challenges

- Programming language:
 - ▣ OpenCL? Domain-specific language?
 - ▣ We have a substantial investment in CPU code; we can't even get started on migrating until language is resolved.
- Memory efficiency
- How do we explore data?
 - ▣ In situ reductions that are post-processed afterwards?
- Resiliency
- New types of data – massive ensembles, multi-physics, etc – will require new techniques
- Reducing complexity

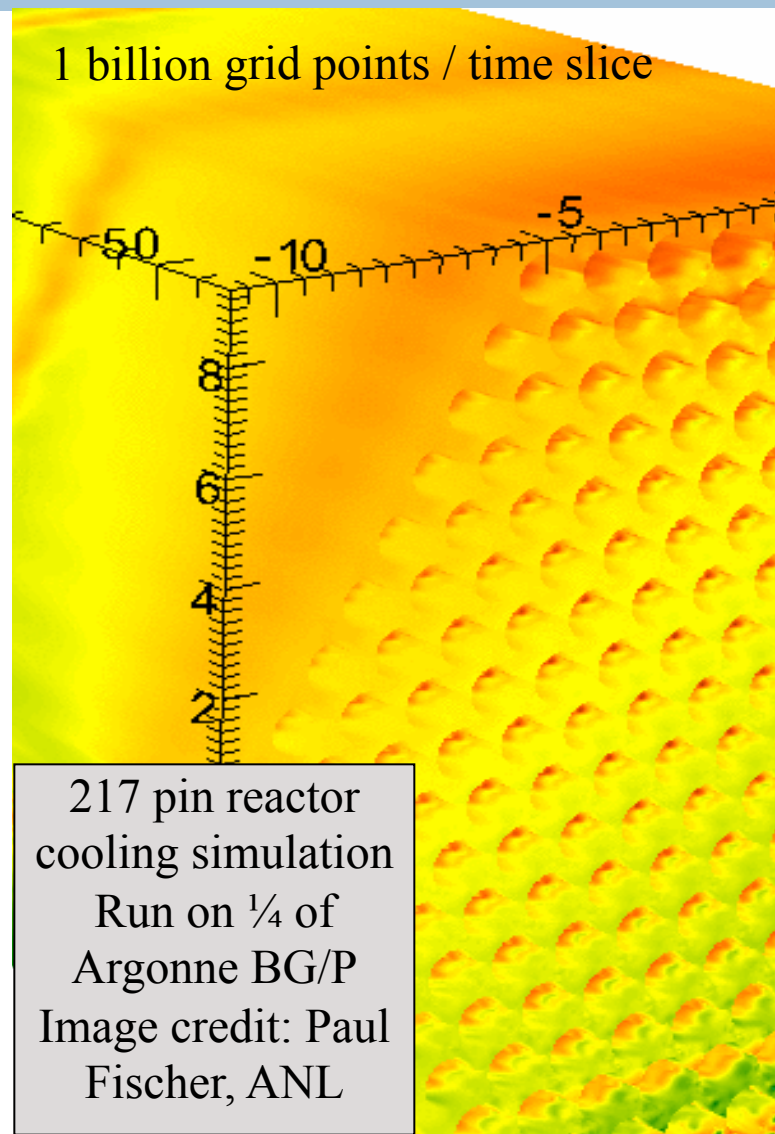
Tools: the VDA community achieves an economy of scale by collectively developing a shared infrastructure that is used by many application areas.



Food co-op, Ralston, Iowa

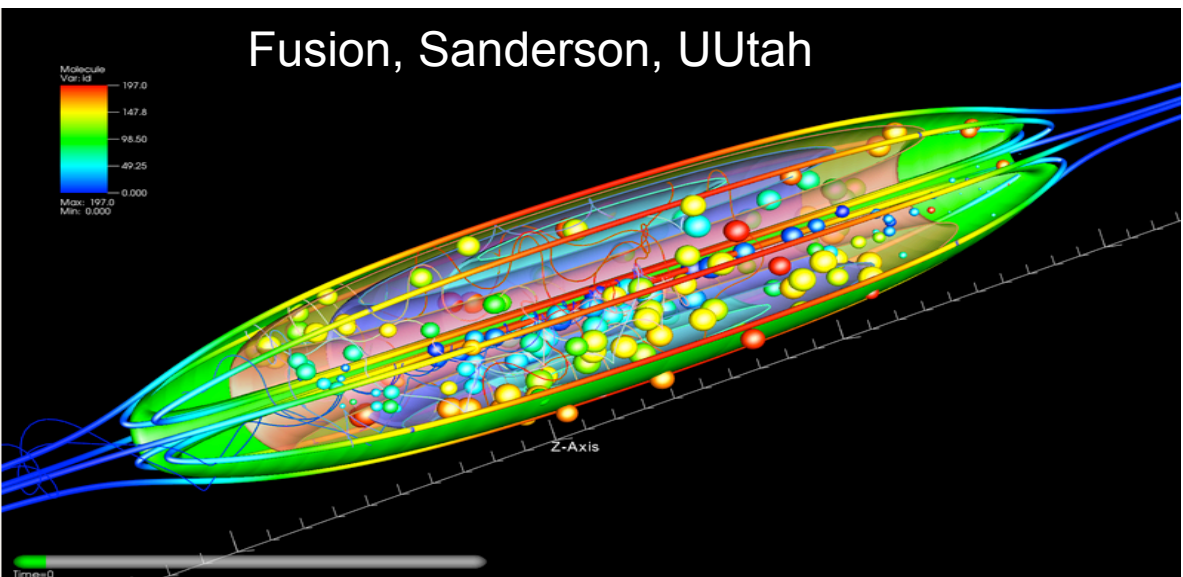
VisIt is an open source, richly featured, turn-key application for large data.

- Terribly named!!!:
 - ▣ Visual debugging
 - ▣ Quantitative & comparative analysis
 - ▣ Data exploration
 - ▣ Presentations
- Popular
 - ▣ R&D 100 award in 2005
 - ▣ Used on many of the Top500
 - ▣ >>>100K downloads

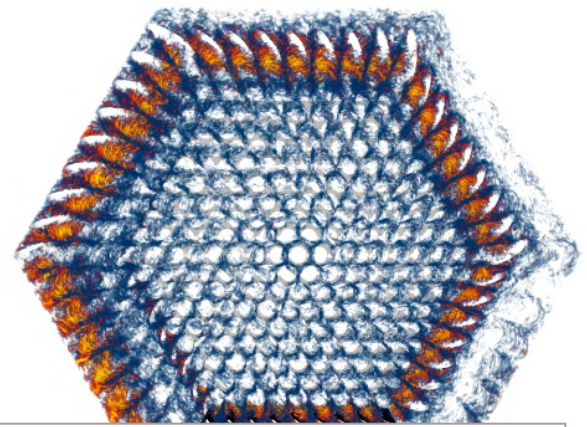
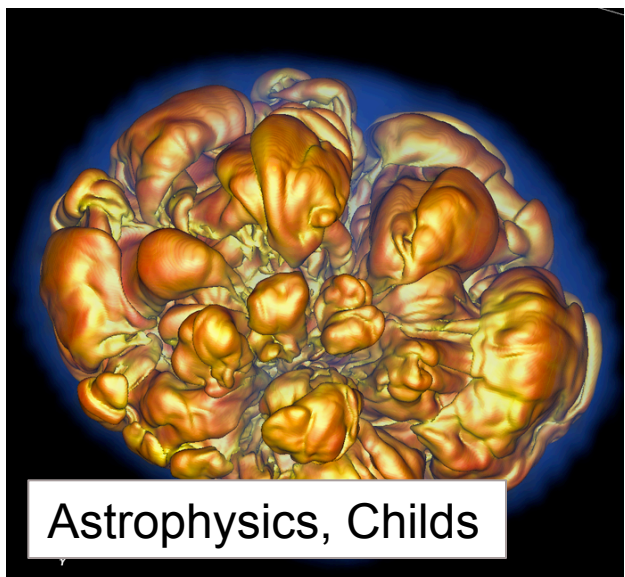


VisIt is used to look at lots of types of simulated and experimental data.

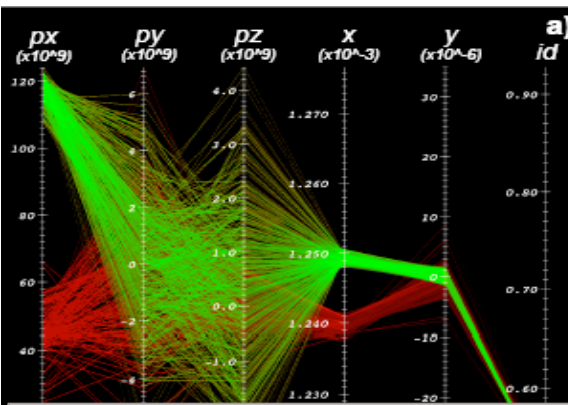
Fusion, Sanderson, UUtah



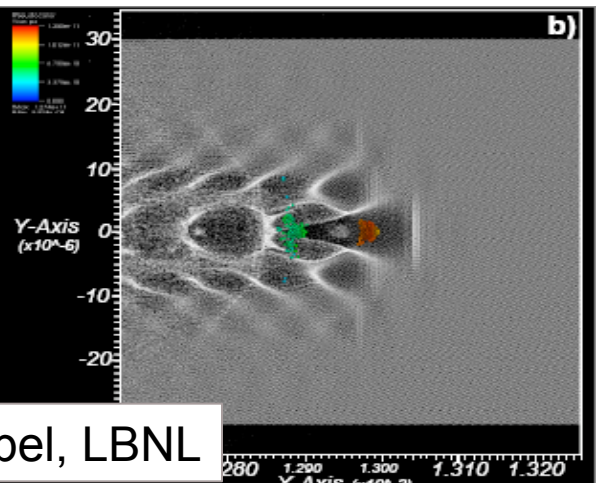
Astrophysics, Childs



Nuclear Reactors, Childs



Particle accelerators, Ruebel, LBNL



It has taken a lot of research to make VisIt work

A Contract Based System for Large Data Visualization
Eric Brugler, Anthony Bonito, Jeremy Hoesly, Steve Kary, and Bob Whitlock

Abstract: Large-scale visualization of the kind of unstructured data sets that are produced by modern scientific and engineering applications is a significant challenge. The visualization of such data sets is often limited by the amount of data that can be processed by the visualization system. This paper describes a contract-based system for large data visualization that is designed to overcome these limitations. The system is based on a contract-based architecture that allows the visualization system to be scaled to the size of the data set. The system is designed to be flexible and extensible, allowing the visualization system to be adapted to a wide range of data sets and visualization techniques. The system is designed to be easy to use and to integrate with existing visualization systems. The system is designed to be scalable and to support a wide range of visualization techniques. The system is designed to be easy to use and to integrate with existing visualization systems.

Systems research:
Adaptively applying algorithms in a production env.

Extreme Scaling of Production Visualization Software on Diverse Architectures
Mark Hesterman, Paulsen, Heather H. Wilson, and A. Tito Beldar - Lawrence Berkeley National Laboratory

Abstract: The visualization of large-scale scientific and engineering data sets is a significant challenge. The visualization of such data sets is often limited by the amount of data that can be processed by the visualization system. This paper describes a contract-based system for large data visualization that is designed to overcome these limitations. The system is based on a contract-based architecture that allows the visualization system to be scaled to the size of the data set. The system is designed to be flexible and extensible, allowing the visualization system to be adapted to a wide range of data sets and visualization techniques. The system is designed to be easy to use and to integrate with existing visualization systems. The system is designed to be scalable and to support a wide range of visualization techniques. The system is designed to be easy to use and to integrate with existing visualization systems.

Scaling research:
Scaling to 10Ks of cores and trillions of cells.

Fast, Memory-Efficient Cell Location in Unstructured Grids for Visualization
Chengxin Guo and Robert L. Gray - AMMBAC, LLC

Abstract: The visualization of large-scale scientific and engineering data sets is a significant challenge. The visualization of such data sets is often limited by the amount of data that can be processed by the visualization system. This paper describes a contract-based system for large data visualization that is designed to overcome these limitations. The system is based on a contract-based architecture that allows the visualization system to be scaled to the size of the data set. The system is designed to be flexible and extensible, allowing the visualization system to be adapted to a wide range of data sets and visualization techniques. The system is designed to be easy to use and to integrate with existing visualization systems. The system is designed to be scalable and to support a wide range of visualization techniques. The system is designed to be easy to use and to integrate with existing visualization systems.

Algorithms research:
Accelerating field evaluation of huge unstructured grids

A Scalable, Hybrid Scheme for Volume Rendering Massive Data Sets
Heath Thurman, Erik DeWitt, and Kenzie Lu - Los Alamos National Laboratory

Abstract: The visualization of large-scale scientific and engineering data sets is a significant challenge. The visualization of such data sets is often limited by the amount of data that can be processed by the visualization system. This paper describes a contract-based system for large data visualization that is designed to overcome these limitations. The system is based on a contract-based architecture that allows the visualization system to be scaled to the size of the data set. The system is designed to be flexible and extensible, allowing the visualization system to be adapted to a wide range of data sets and visualization techniques. The system is designed to be easy to use and to integrate with existing visualization systems. The system is designed to be scalable and to support a wide range of visualization techniques. The system is designed to be easy to use and to integrate with existing visualization systems.

Algorithms research:
How to volume render efficiently in parallel.

Scalable Computation of Streamlines on Very Large Datasets
Chengxin Guo, Robert L. Gray, and Erik DeWitt - AMMBAC, LLC

Abstract: The visualization of large-scale scientific and engineering data sets is a significant challenge. The visualization of such data sets is often limited by the amount of data that can be processed by the visualization system. This paper describes a contract-based system for large data visualization that is designed to overcome these limitations. The system is based on a contract-based architecture that allows the visualization system to be scaled to the size of the data set. The system is designed to be flexible and extensible, allowing the visualization system to be adapted to a wide range of data sets and visualization techniques. The system is designed to be easy to use and to integrate with existing visualization systems. The system is designed to be scalable and to support a wide range of visualization techniques. The system is designed to be easy to use and to integrate with existing visualization systems.

Algorithms research:
How to efficiently calculate particle paths in parallel.

High Performance Multivariate Visual Data Exploration for Extremely Large Data
Ulises Ribes, Tommaso, Rodrigo W. Hank, Chris, Jeremy Hoesly, Connor G. Caputo, Emily Carson-McNeil, Tom Hanks, Jonathan R. Meyer, Roger Hesterman, and Bob Whitlock

Abstract: The visualization of large-scale scientific and engineering data sets is a significant challenge. The visualization of such data sets is often limited by the amount of data that can be processed by the visualization system. This paper describes a contract-based system for large data visualization that is designed to overcome these limitations. The system is based on a contract-based architecture that allows the visualization system to be scaled to the size of the data set. The system is designed to be flexible and extensible, allowing the visualization system to be adapted to a wide range of data sets and visualization techniques. The system is designed to be easy to use and to integrate with existing visualization systems. The system is designed to be scalable and to support a wide range of visualization techniques. The system is designed to be easy to use and to integrate with existing visualization systems.

Systems research:
Using smart DB technology to accelerate processing

Streamline Integration using MPI-Hybrid Parallelism on a Large Multi-Core Architecture
David Carpi, Stuart Moore, Eric Chengxin Guo, Robert L. Gray, Chengxin Guo, and Robert L. Gray - AMMBAC, LLC

Abstract: The visualization of large-scale scientific and engineering data sets is a significant challenge. The visualization of such data sets is often limited by the amount of data that can be processed by the visualization system. This paper describes a contract-based system for large data visualization that is designed to overcome these limitations. The system is based on a contract-based architecture that allows the visualization system to be scaled to the size of the data set. The system is designed to be flexible and extensible, allowing the visualization system to be adapted to a wide range of data sets and visualization techniques. The system is designed to be easy to use and to integrate with existing visualization systems. The system is designed to be scalable and to support a wide range of visualization techniques. The system is designed to be easy to use and to integrate with existing visualization systems.

Architectural research:
Hybrid parallelism + particle advection

Large Data Visualization on Distributed Memory Multi-CPU Clusters
Heath Thurman, Erik DeWitt, and Kenzie Lu - Los Alamos National Laboratory

Abstract: The visualization of large-scale scientific and engineering data sets is a significant challenge. The visualization of such data sets is often limited by the amount of data that can be processed by the visualization system. This paper describes a contract-based system for large data visualization that is designed to overcome these limitations. The system is based on a contract-based architecture that allows the visualization system to be scaled to the size of the data set. The system is designed to be flexible and extensible, allowing the visualization system to be adapted to a wide range of data sets and visualization techniques. The system is designed to be easy to use and to integrate with existing visualization systems. The system is designed to be scalable and to support a wide range of visualization techniques. The system is designed to be easy to use and to integrate with existing visualization systems.

Architectural research:
Parallel GPU volume rendering

Visualization and Analysis-Oriented Reconstruction of Material Interfaces
Jeremy S. Hesterman and David Carpi - Los Alamos National Laboratory

Abstract: The visualization of large-scale scientific and engineering data sets is a significant challenge. The visualization of such data sets is often limited by the amount of data that can be processed by the visualization system. This paper describes a contract-based system for large data visualization that is designed to overcome these limitations. The system is based on a contract-based architecture that allows the visualization system to be scaled to the size of the data set. The system is designed to be flexible and extensible, allowing the visualization system to be adapted to a wide range of data sets and visualization techniques. The system is designed to be easy to use and to integrate with existing visualization systems. The system is designed to be scalable and to support a wide range of visualization techniques. The system is designed to be easy to use and to integrate with existing visualization systems.

Algorithms research:
Reconstructing material interfaces for visualization

Frameworks for Visualization at the Extreme Scale
Kenneth L. Liu, Mark Weber, Frank Omer, A. Tito Beldar, John Chao, and Robert L. Gray - Los Alamos National Laboratory

Abstract: The visualization of large-scale scientific and engineering data sets is a significant challenge. The visualization of such data sets is often limited by the amount of data that can be processed by the visualization system. This paper describes a contract-based system for large data visualization that is designed to overcome these limitations. The system is based on a contract-based architecture that allows the visualization system to be scaled to the size of the data set. The system is designed to be flexible and extensible, allowing the visualization system to be adapted to a wide range of data sets and visualization techniques. The system is designed to be easy to use and to integrate with existing visualization systems. The system is designed to be scalable and to support a wide range of visualization techniques. The system is designed to be easy to use and to integrate with existing visualization systems.

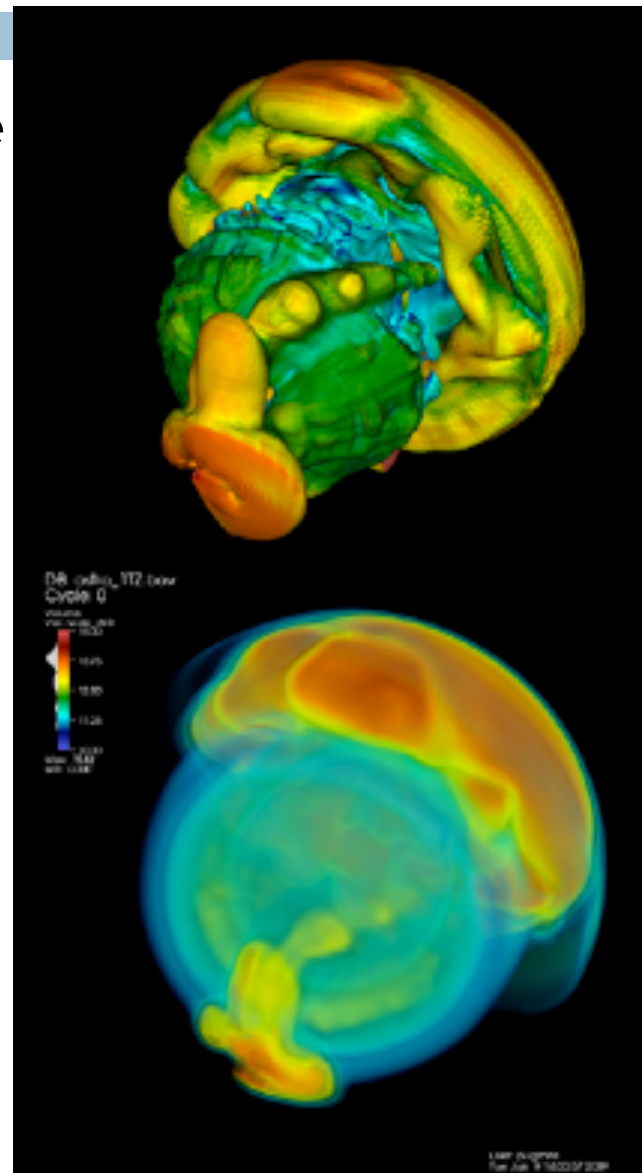
Methods research:
How to incorporate statistics into visualization.

VisIt recently demonstrated good performance at unprecedented scale.

- Weak scaling study: $\sim 62.5\text{M}$ cells/core

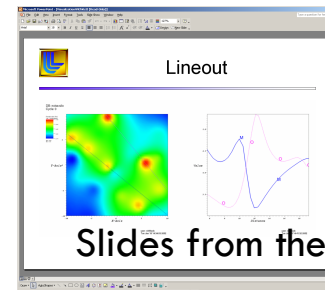
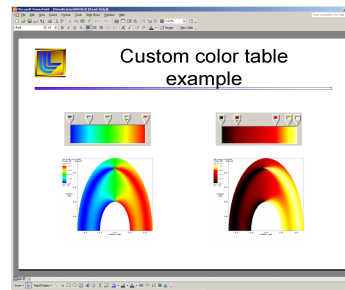
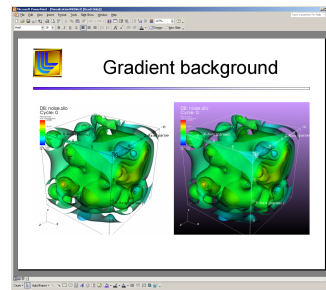
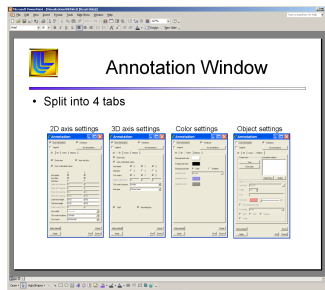
Machine	Model	Problem Size	#cores
Franklin	Cray XT4	1T, 2T	16K, 32K
Dawn	BG/P	4T	64K
JaguarPF	Cray XT5	2T	32K
Juno	X86_64	1T	16K
Purple	IBM P5	0.5T	8K
Ranger	Sun	1T	16K

Two trillion cell data set,
rendered in VisIt by
David Pugmire on ORNL
Jaguar machine



The VisIt team focuses on making a robust, usable product for end users.

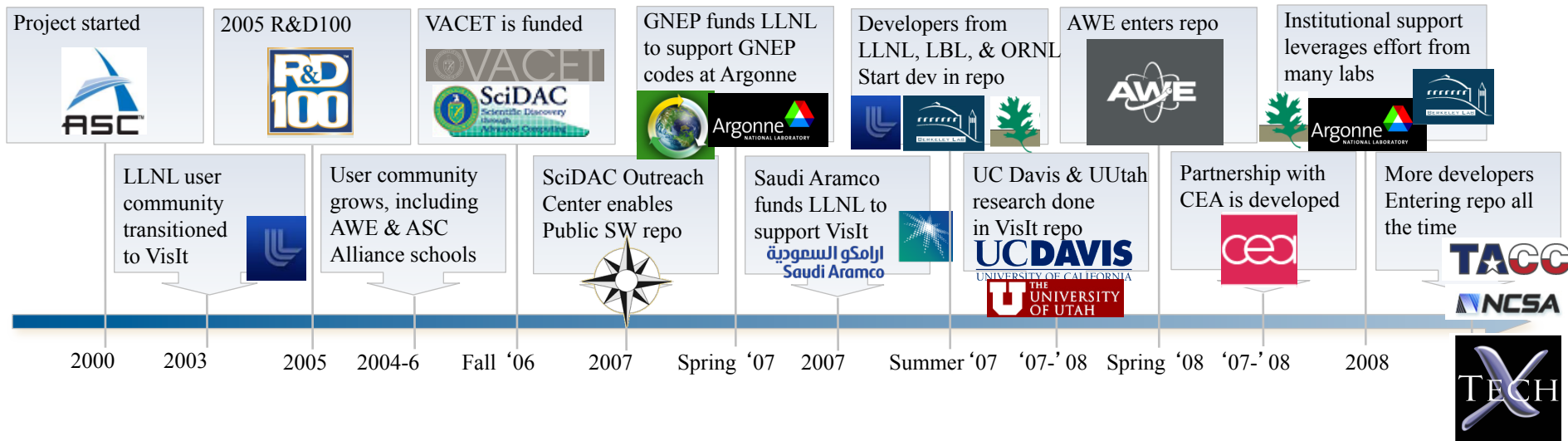
- Manuals
 - 300 page user manual
 - 200 page command line interface manual
 - “Getting your data into VisIt” manual
- Wiki for users (and developers)
- Revision control, nightly regression testing, etc
- Executables for all major platforms
- Day long class, complete with exercises



Slides from the VisIt class

VisIt is a vibrant project with many participants.

- Over 75 person-years of effort
- Over 1.5 million lines of code
- Partnership between: Department of Energy's Office of Science, National Nuclear Security Agency, and Office of Nuclear Energy, the National Science Foundation XD centers (Longhorn XD and RDAV), and more....



Achieving Extreme Performance

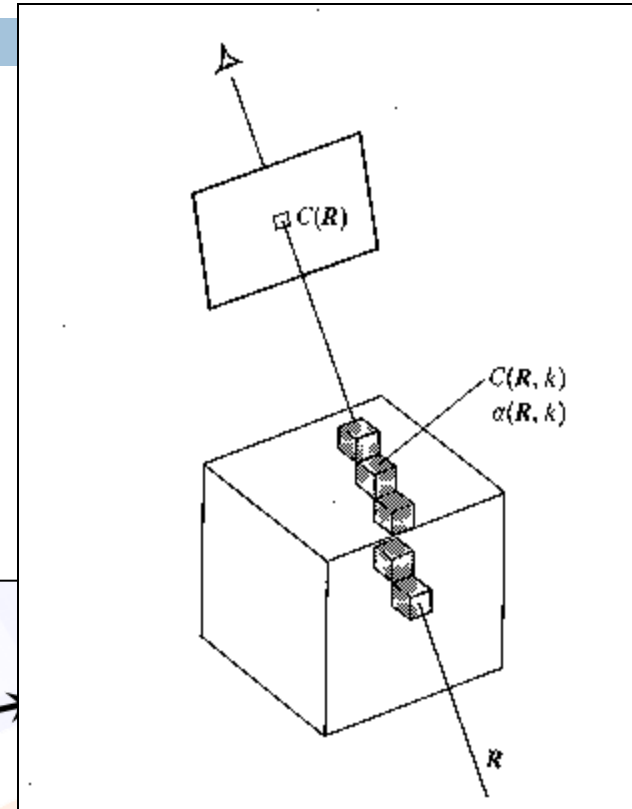
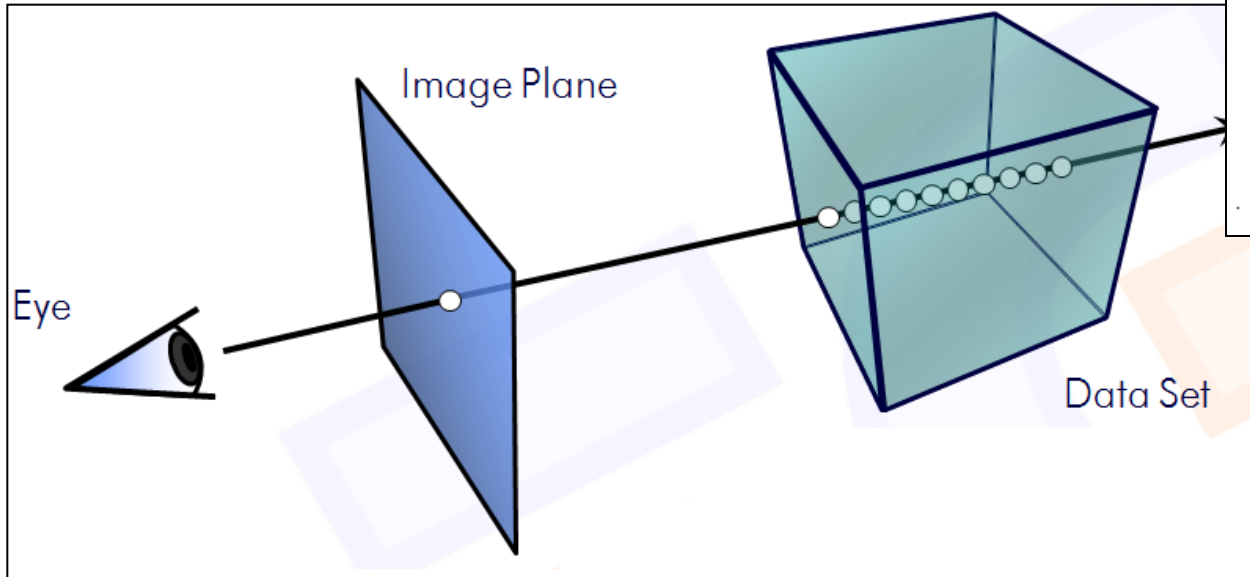


Achieving Extreme Performance

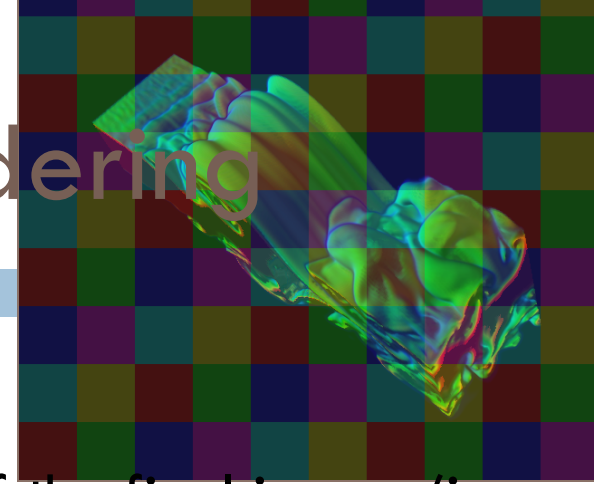
- The lessons of auto-tuning and multi-/many-core architectures:
 - ▣ Performance can vary by as much as 5x depending upon how tunable algorithmic parameters.
- Hybrid-parallelism:
 - ▣ MPI-only approaches not sustainable to extreme levels of concurrency.
 - ▣ Our results show hybrid parallelism runs faster, consumes less memory, requires less data movement.

Algorithm Studied: Raycasting VR

- Overview of Levoy's method
 - ▣ For each pixel in image plane:
 - Find intersection of ray and volume
 - Sample data (RGBA) along ray, integrate samples to compute final image pixel color



Parallelizing Volume Rendering

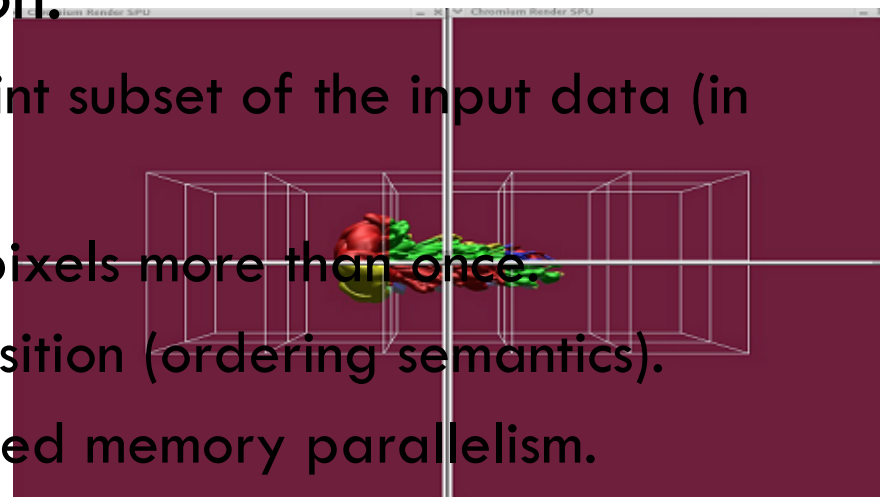


□ Image-space decomposition.

- ▣ Each process works on a disjoint subset of the final image (in parallel)
- ▣ Processes may access source voxels more than once, will access a given output pixel only once.
- ▣ Great for shared memory parallelism.

□ Object-space decomposition.

- ▣ Each process works on a disjoint subset of the input data (in parallel).
- ▣ Processes may access output pixels more than once.
- ▣ Output requires image composition (ordering semantics).
- ▣ Typical approach for distributed memory parallelism.



Autotuning and Performance Optimization

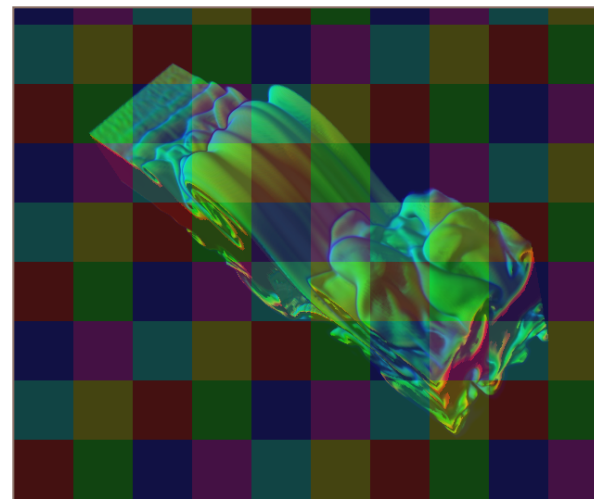
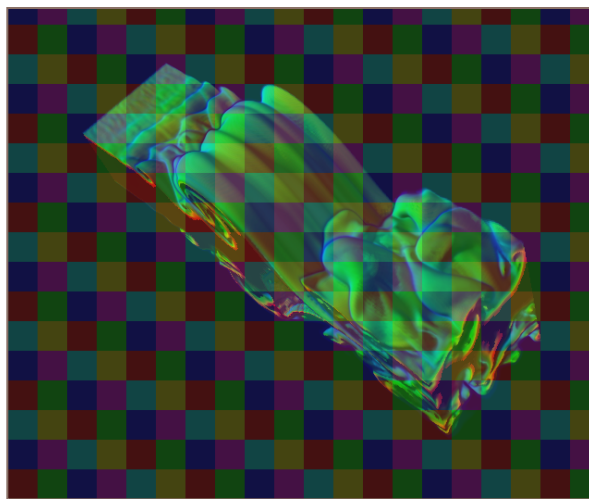
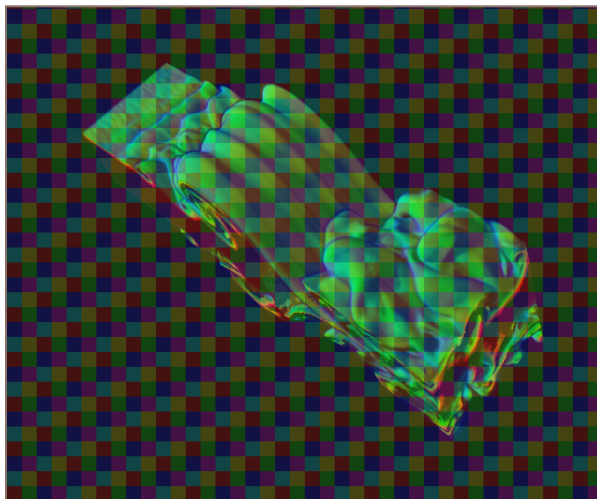


Motivation

- Many algorithms have “tunable” parameters
 - CUDA: size/shape of thread block.
 - Image-parallel volume rendering: size of image tile.
- Choice of tunable parameters can have a huge impact on algorithm performance.
 - May vary by specific problem, architecture.
 - Examples that follow:
 - Shared-memory volume rendering: 2.5x difference between best and worst depending upon image tile size (unpublished work)
 - CUDA: 10x performance difference on stencil-based code (unpublished work, led to half of work for SC09 paper submission).
 - Other examples:
 - Multi-core CPU and GPU: 49x performance gain for a clinical medical imaging application. (Submitted to SC09)
 - Autotuning framework and multi-core CPUs and GPUs applied to stencil-based code. (CUG 2009, Best Paper Award)

Work Decomposition: Image Tile Size

- Final image divided into spatially disjoint regions, or work blocks.
- User specifiable block size/shape:
 - ▣ E.g., 8x8, 64x64, 512x1, 1x512
- Do some block sizes and shapes result in better performance than others?



Does Block Size/Shape Impact Performance?

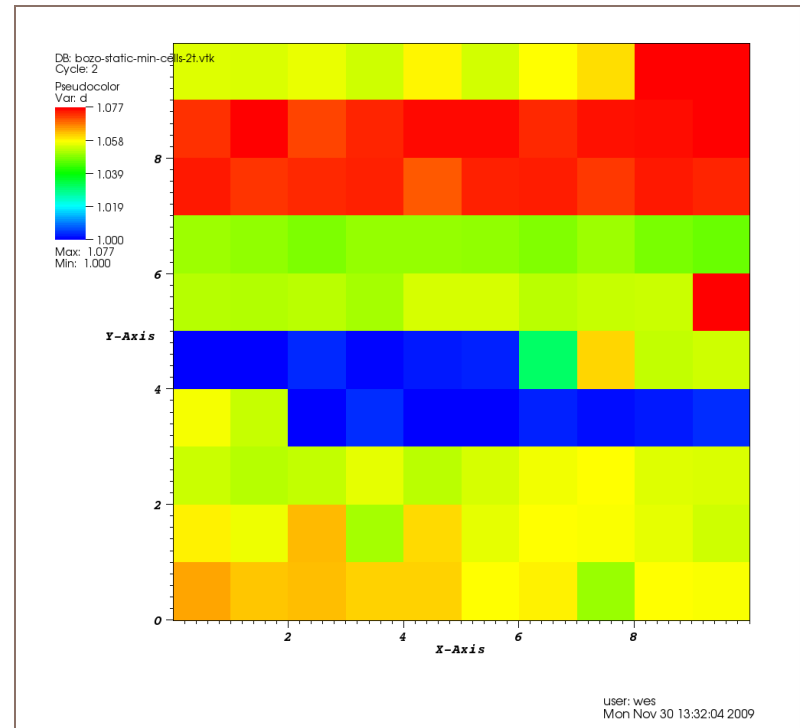
Platform	Concurrency	Nearest-neighbor	Trilinear	Phong, NN	Phong, Trilinear
AMD/Italy	1	2.62	1.35	5.74	4.33
Intel/Nehalem	1	0.76	0.66	1.22	0.66
AMD/Italy	2	7.74	5.29	11.21	8.93
Intel/Nehalem	2	4.85	5.40	5.20	5.40
AMD/Italy	4	68.39	74.78	79.49	76.03
Intel/Nehalem	4	65.25	73.34	72.85	73.34
AMD/Italy	8	63.23	67.71	70.60	77.60
Intel/Nehalem	8	226.85	246.61	244.44	246.61

Percent variation in runtime across entire test battery.

- Yes! Huge impact!
 - ▣ Greater variation at increasing concurrency.
 - ▣ Greater variation for more memory intensive algorithmic configurations.

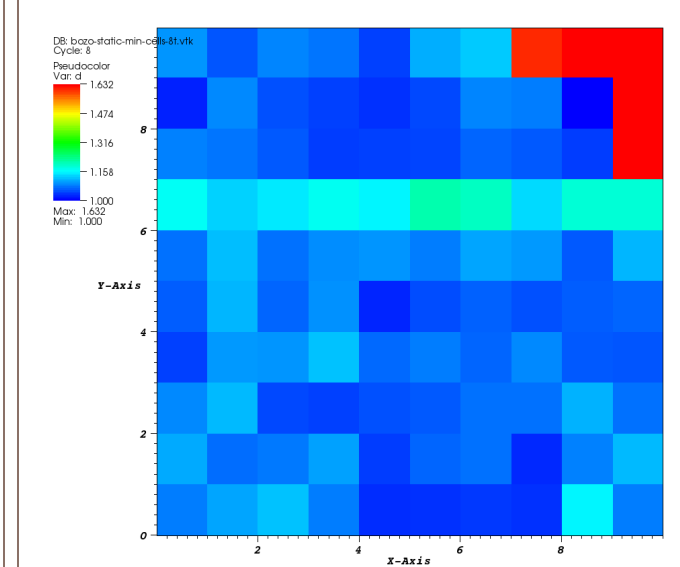
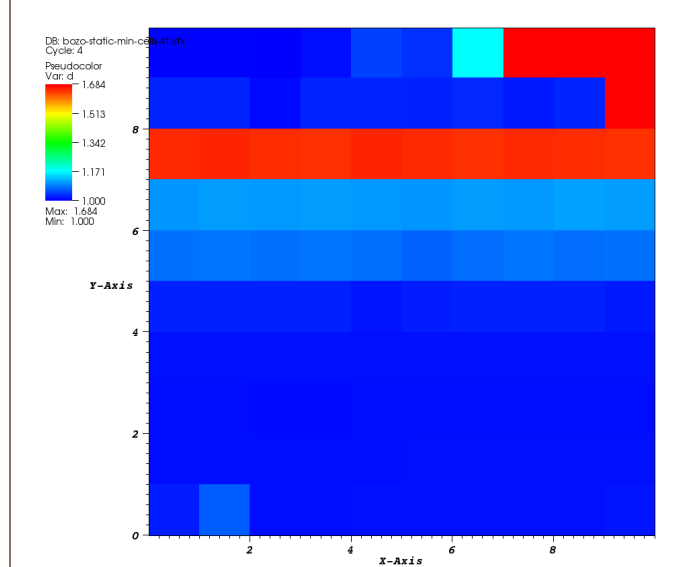
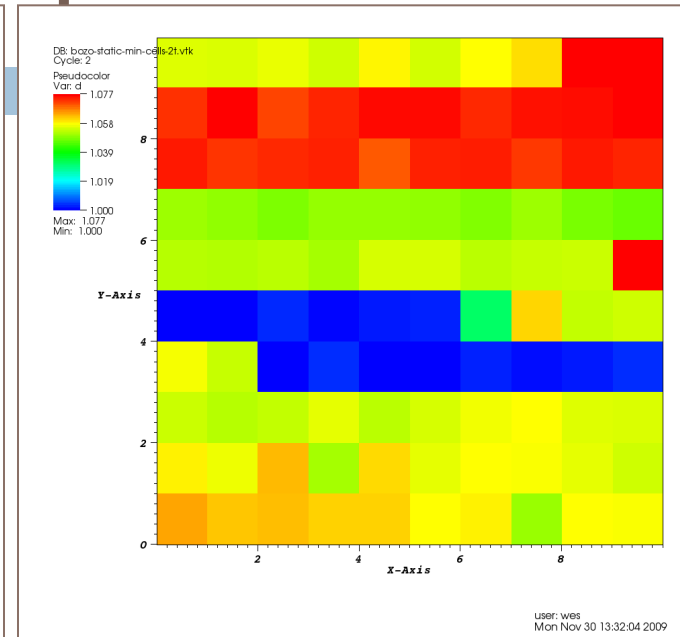
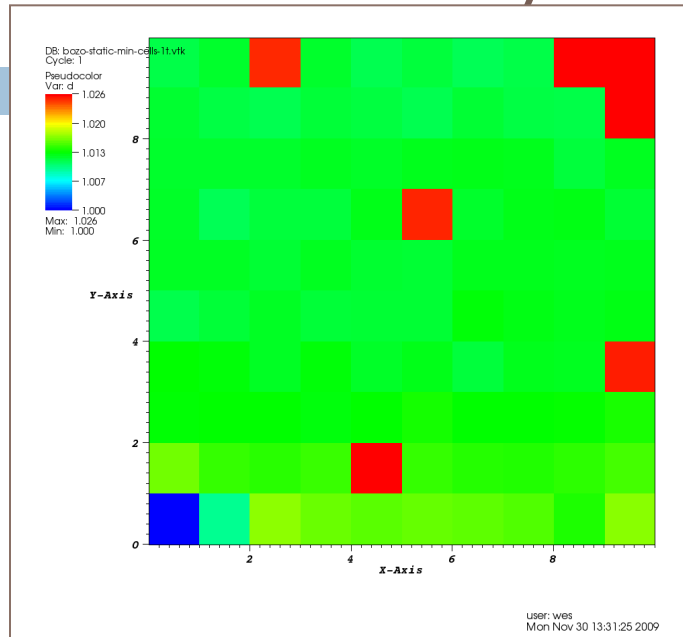
Optimal Block Size/Shape?

- Raw render time normalized by minimum render time value (shows sweet spots)
- This example:
 - 2 threads, AMD/Italy
 - X-axis/Y-axis: block sizes
 - Blue: sweet spot
 - Red: sour spot



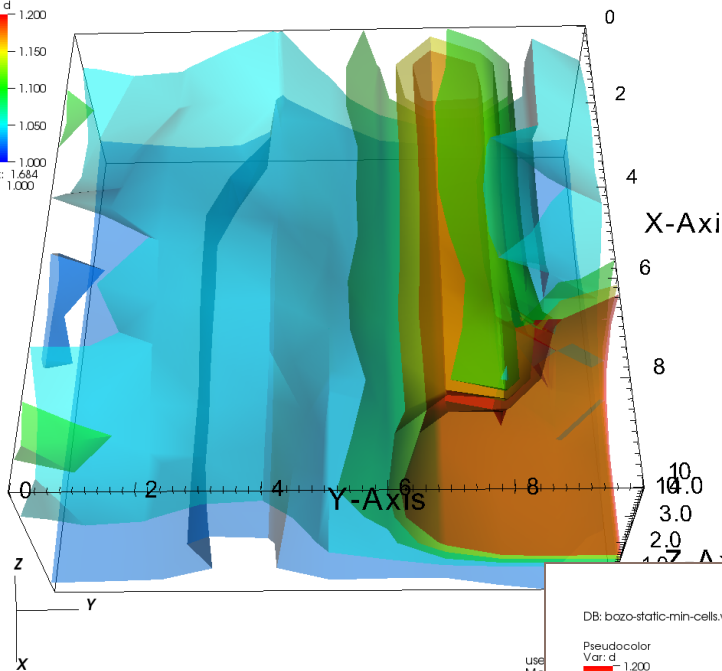
Optimal Block Size/Shape?

- Avg render time.
- 1, 2, 4, 8 threads.
- NN, NL.
- Bw=128 is really bad at t=2, 4, and bad at t-8.
- Dual socket, dual core machine.



DB: bozo-static-min-cells.vtk

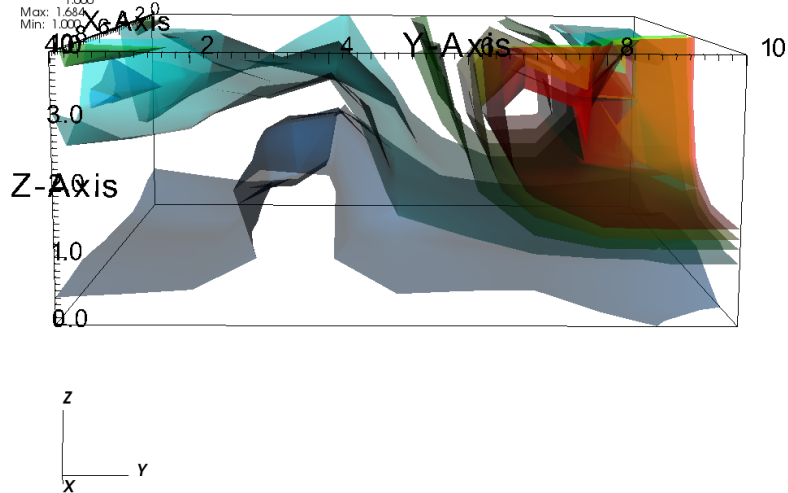
Pseudocolor
Var: d
Max: 1.684
Min: 1.000



Size /

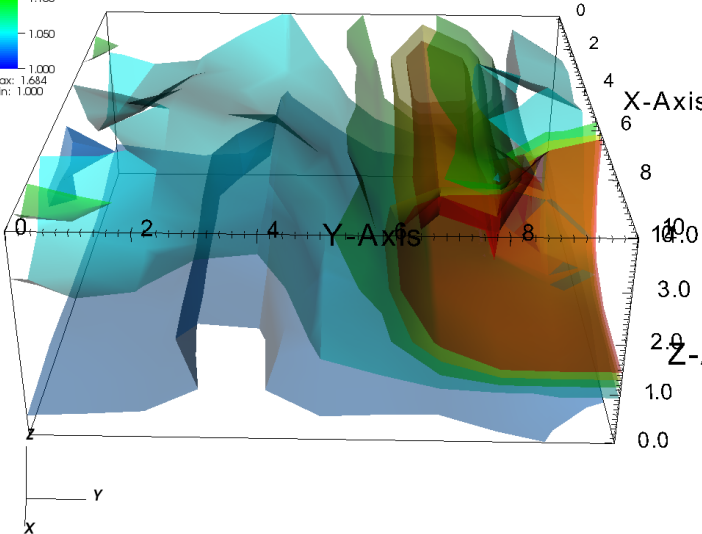
DB: bozo-static-min-cells.vtk

Pseudocolor
Var: d
Max: 1.684
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DB: bozo-static-min-cells.vtk

Pseudocolor
Var: d
Max: 1.684
Min: 1.000

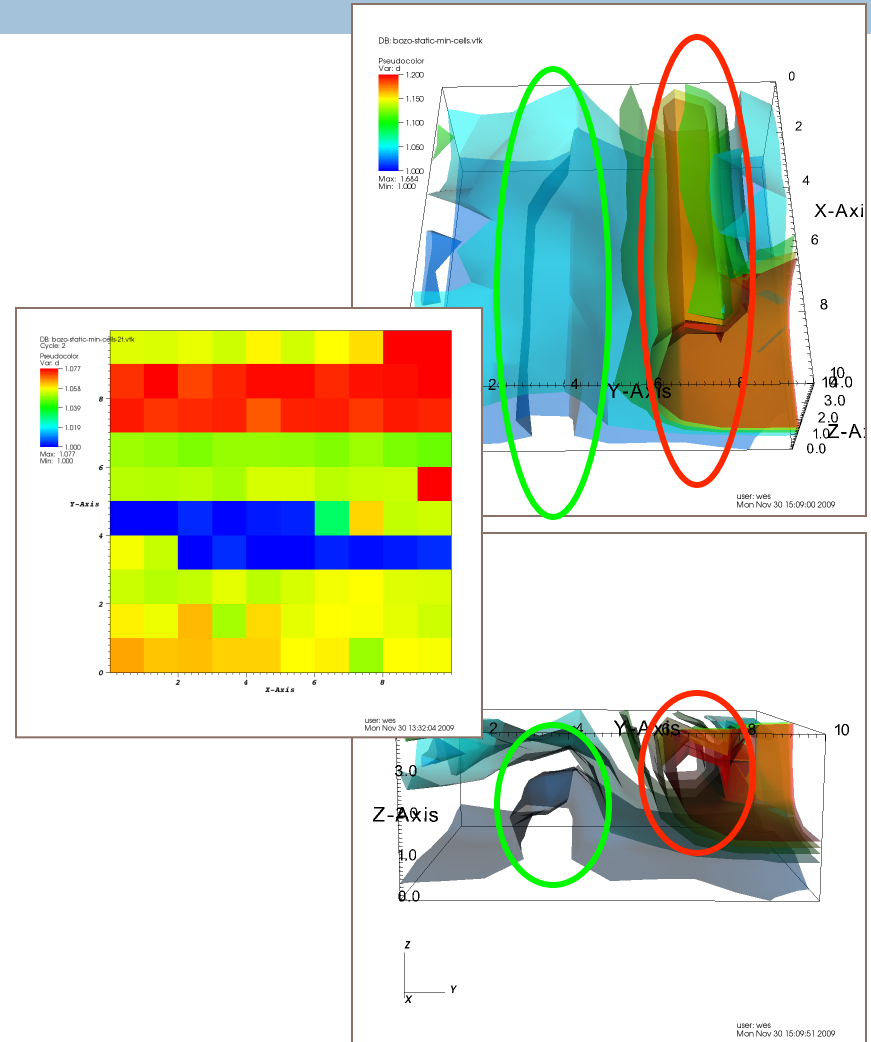


user: wes
Mon Nov 30 15:09:51 2009

user: wes
Mon Nov 30 15:09:26 2009

Optimal Block Size/Shape?

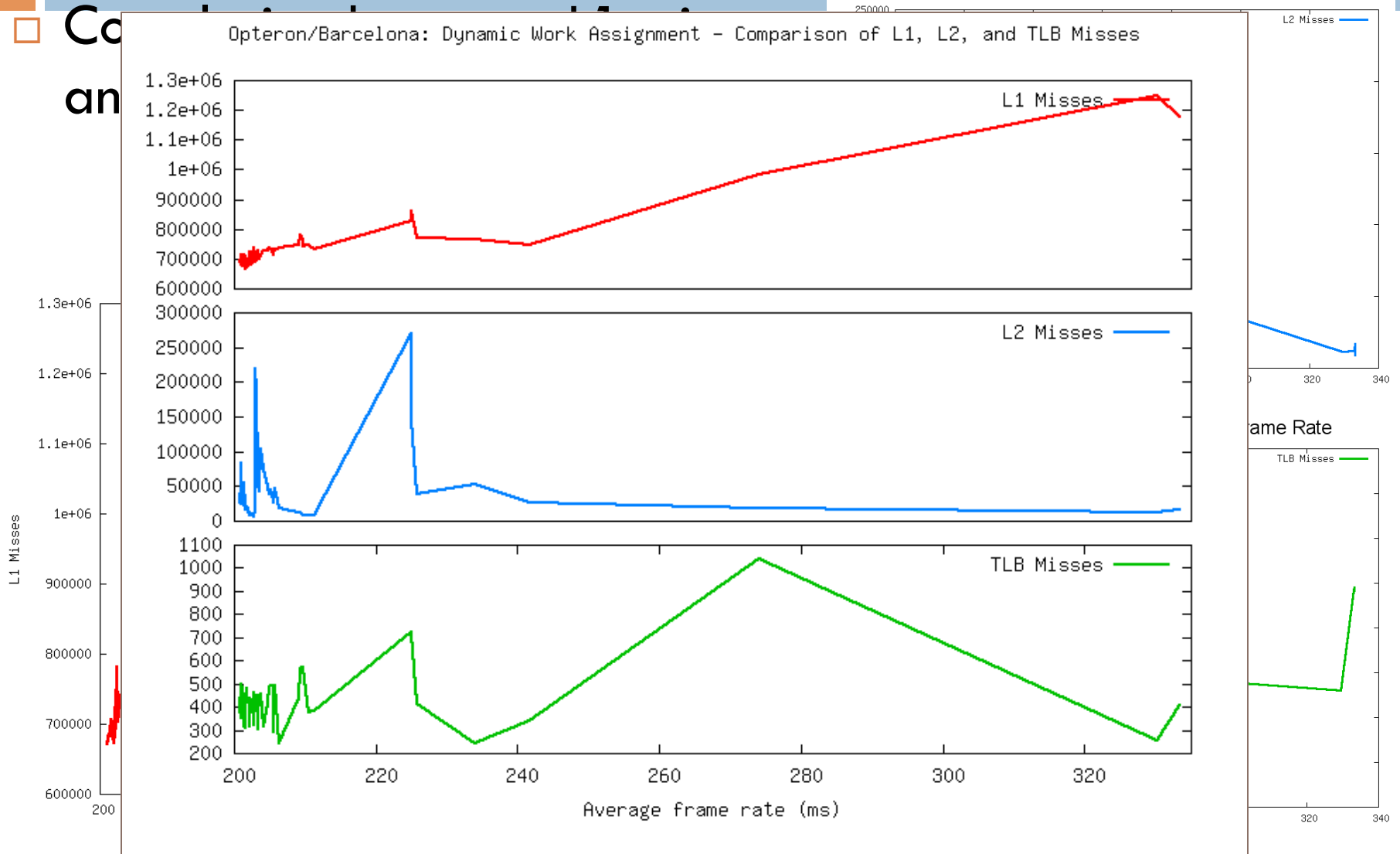
- AMD/Opteron-Italy
- Sweet spot/region: ○
 - Block width: 2^3 - 2^4
 - Block height: 2^2 - 2^6
- Sour spot/region: ○
 - Block width: 2^7 - 2^8
 - Block height: all



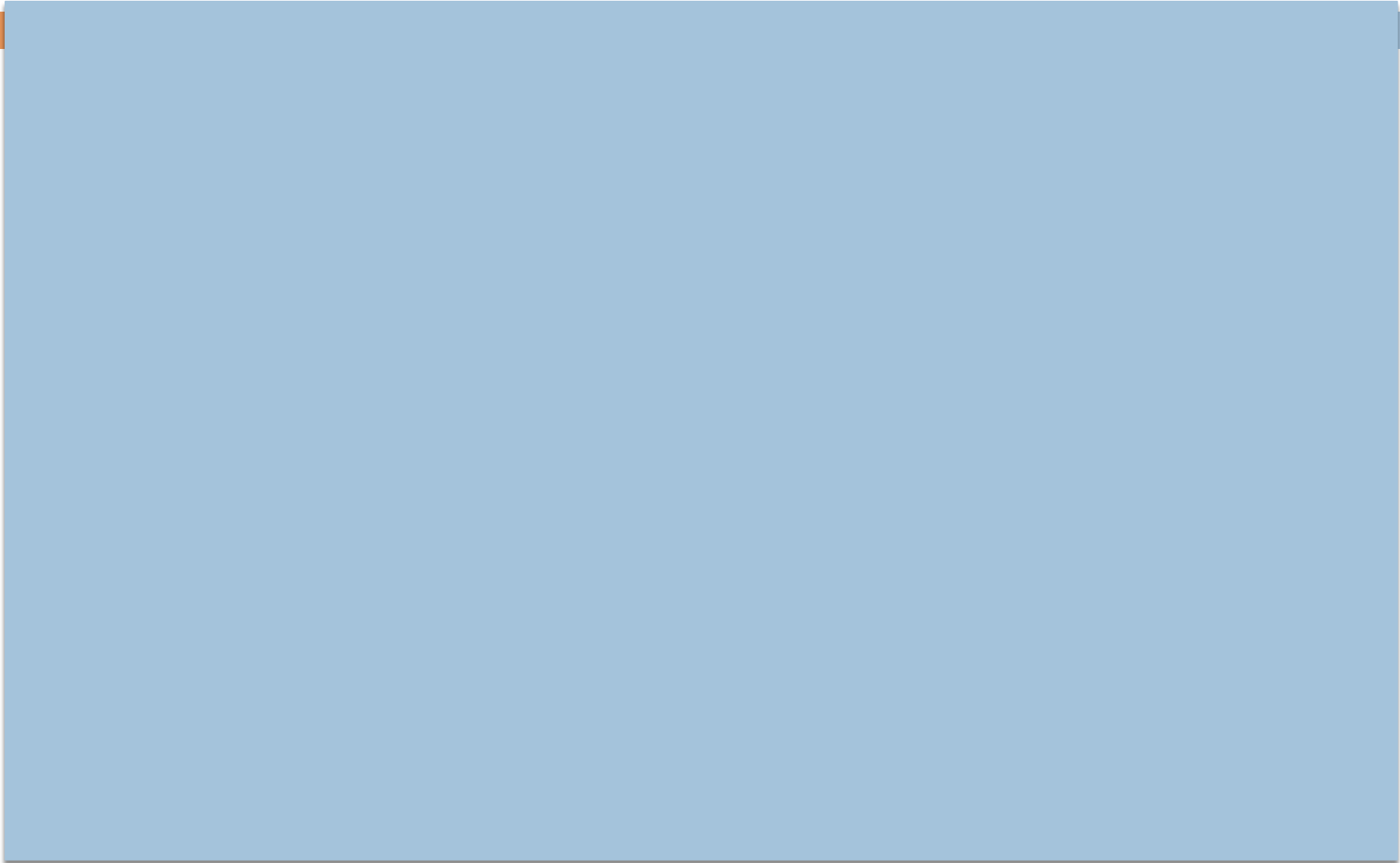
Cache Utilization and Block Size

□ Co
an

Opteron/Barcelona: L2 Misses and Frame Rate



Many-core Platform: GPU



Performance Optimization and Auto-tuning: Summary

- Different settings for tunable algorithmic parameters can have a huge impact on performance on m-core platforms.
- Our results show roughly 2.5x variation on 6-core CPUs, up to 4.5x variation on GPUs.
- Code: unstructured memory access, largely memory bound rather than compute bound.
- Optimal settings from this study feed into the next study...

Hybrid Parallelism



State of Parallelism in Scientific Computing

- Most production codes written using MPI, vendor MPI implementations optimized for their architecture.
- HPC community wondering how well MPI will scale to high concurrency, particularly on 100-core CPUs.
- What to do?
 - ▣ Some alternatives: data parallel languages (CUDA), PGAS languages (UPC), global shared memory (CAF).
 - ▣ Various research projects explore different aspects of this space: Chombo in Titanium, autotuning, hybrid parallelism.

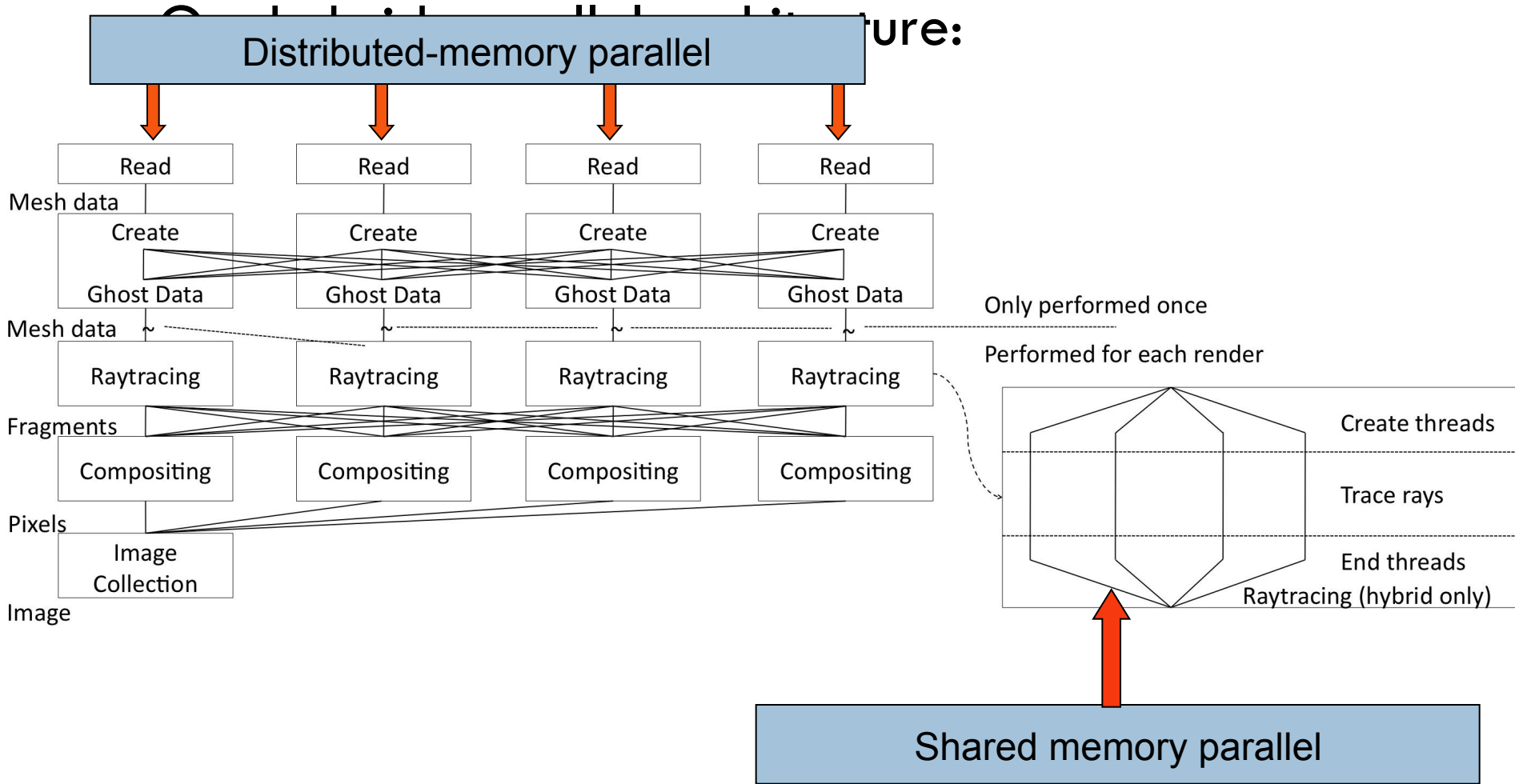
This Study

- First-ever study of hybrid parallelism on visualization: raycasting volume rendering.
 - ▣ Parallels similar work done for scientific computing.
- Hybrid-parallel implementation/architecture.
- Performance study.
 - ▣ Runs at 216K-way parallel: 6x larger than any published results (circa May 2010).
 - ▣ Look at:
 - Costs of initialization, Memory use comparison, Scalability, Absolute runtime.

Hybrid Parallel Volume Rendering

- Hybrid-parallelism a blend of shared- and distributed-memory parallelism.
- Distributed-memory parallelism:
 - ▣ Each socket assigned a spatially disjoint subset of source data, produces an image of its chunk.
 - ▣ All subimages composited together into final image.
 - ▣ MPI implementation.
- Shared-memory parallelism:
 - ▣ Inside a socket, threads use image-space partitioning, each thread responsible for a subset of the final image.
 - What is the best image tile size? (Autotuning presentation)
 - ▣ Implementations (2): pthreads, OpenMP.

Hybrid Parallel Volume Rendering

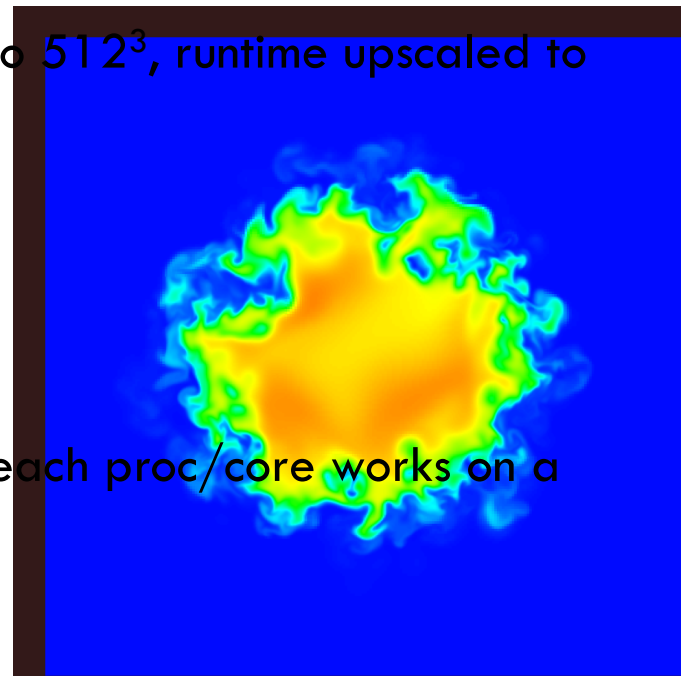


Our Experiment

- Thesis: hybrid-parallel will exhibit favorable performance, resource utilization characteristics compared to traditional approach.
- How/what to measure?
 - ▣ Memory footprint, communication traffic load, scalability characteristics, absolute runtime.
 - ▣ Across a wide range of concurrencies.
 - ▣ Algorithm performance somewhat dependent upon viewpoint, data:
 - Vary viewpoints over a set that cut through data in different directions: will induce different memory access patterns.
- Strong scaling study: hold problem size constant, vary amount of resources.

Experiment: Platform and Source Data

- Platform: JaguarPF, a Cray XT5 system at ORNL
 - 18,688 nodes, dual-socket, six-core AMD Opteron (224K cores)
- Source data:
 - Combustion simulation results, hydrogen flame (data courtesy J. Bell, CCSE, LBNL)
 - Effective AMR resolution: 1024^3 , flattened to 512^3 , runtime upscaled to 4608^3 (to avoid I/O costs).
- Target image size: 4608^2 image.
 - Want approx 1:1 voxels to pixels.
- Strong scaling study:
 - As we increase the number of procs/cores, each proc/core works on a smaller-sized problem.
 - Time-to-solution should drop.



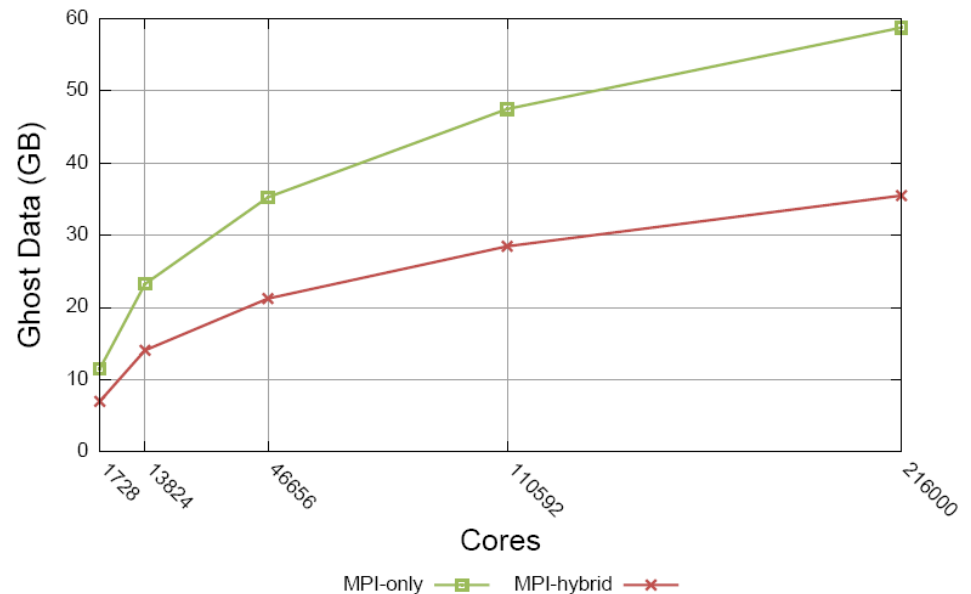
Memory Use – MPI_Init()

- Per PE memory:
 - ▣ About the same at 1728, over 2x at 216000.
- Aggregate memory use:
 - ▣ About 6x at 1728, about 12x at 216000.

Cores	Mode	MPI PEs	MPI Runtime Memory Usage		
			Per PE (MB)	Per Node (MB)	Aggregate (GB)
1728	MPI-hybrid	288	67	133	19
1728	MPI-only	1728	67	807	113
13824	MPI-hybrid	2304	67	134	151
13824	MPI-only	13824	71	857	965
46656	MPI-hybrid	7776	68	136	518
46656	MPI-only	46656	88	1055	4007
110592	MPI-hybrid	18432	73	146	1318
110592	MPI-only	110592	121	1453	13078
216000	MPI-hybrid	36000	82	165	2892
216000	MPI-only	216000	176	2106	37023

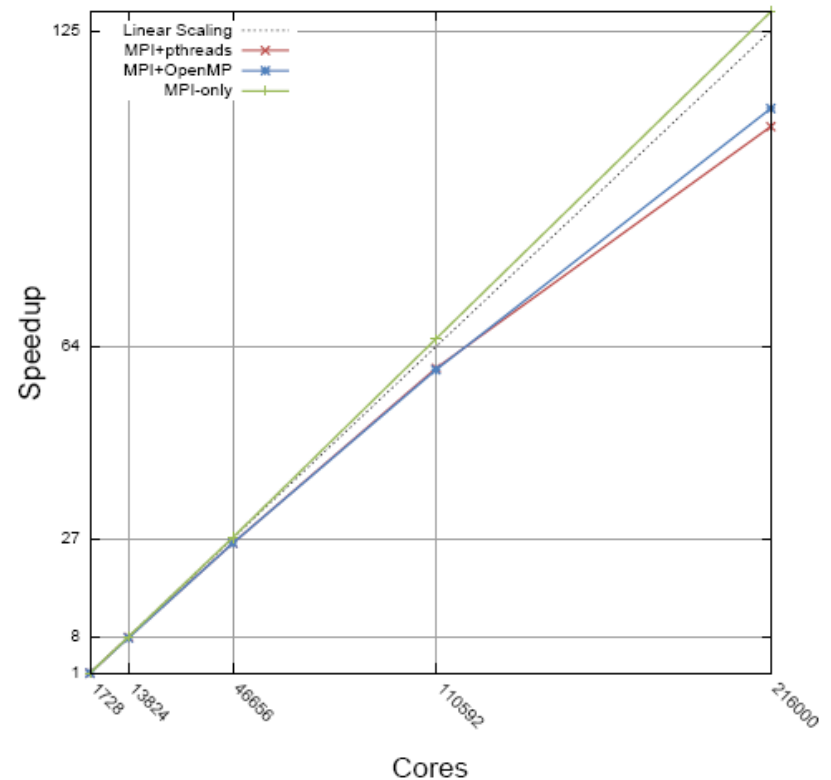
Memory Use – Ghost Zones

- Two layers of ghost cells required for this problem:
 - ▣ One for trilinear interpolation during ray integration loop.
 - ▣ Another for computing a gradient field (central differences) for shading.
- Hybrid approach uses fewer, but larger data blocks.
 - ▣ ~40% less memory required for ghost zones (smaller surface area)
 - ▣ Reduced communication costs



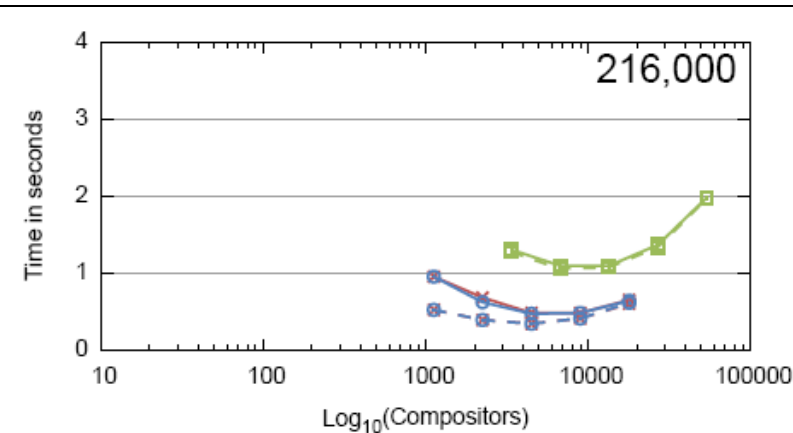
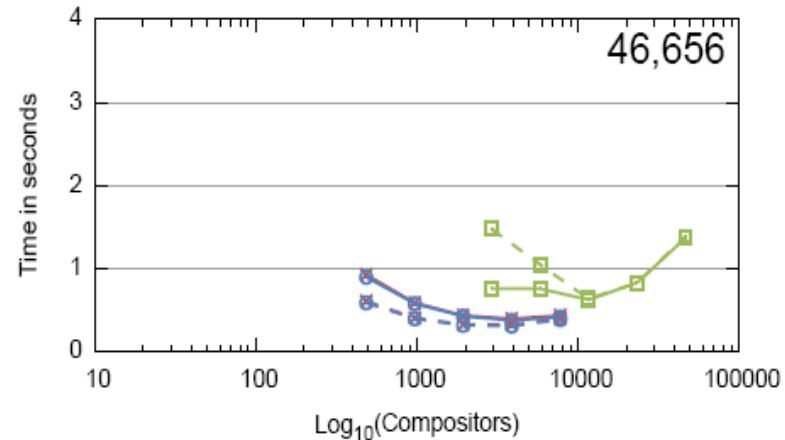
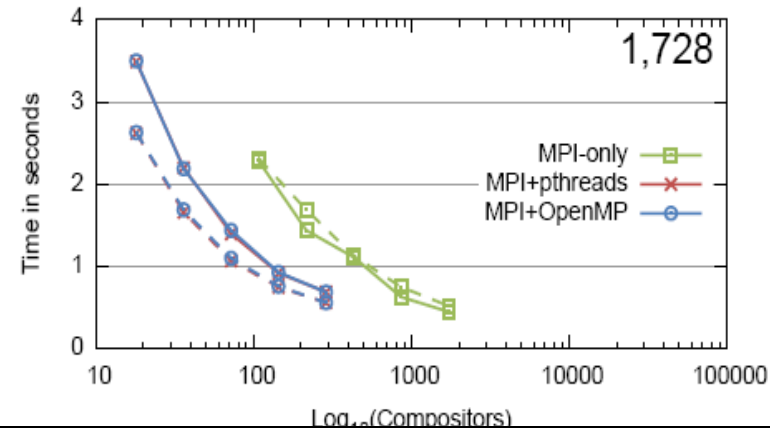
Scalability – Raycasting Phase

- Near linear scaling since no interprocess communication.
- -hybrid shows sublinear scaling due to oblong block shape.
- -only shows slightly better than linear due to reduced work caused by perspective foreshortening.



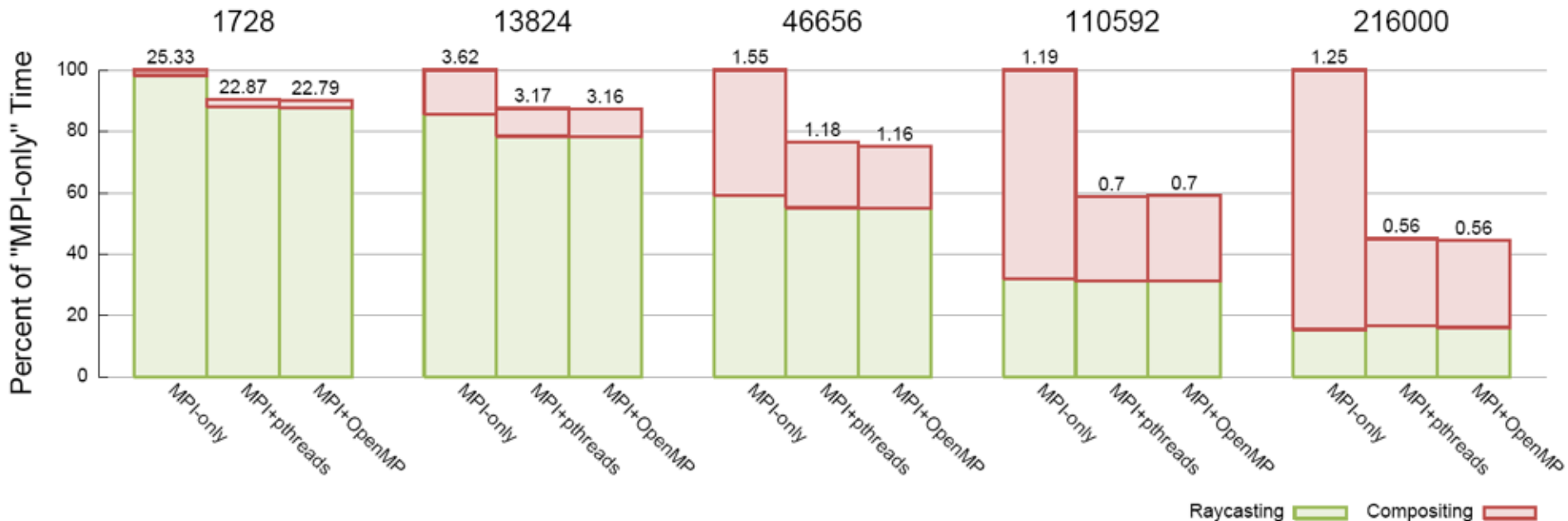
Scalability – Compos

- How many composers to use?
 - ▣ Previous work: 1K to 2K for 32K renderers (Peterka, 2009).
 - ▣ Our work: above $\sim 46K$ renderers, 4K to 8K works better.
 - ▣ -hybrid cases always performs better: fewer messages.
 - ▣ Open question: why the critical point?



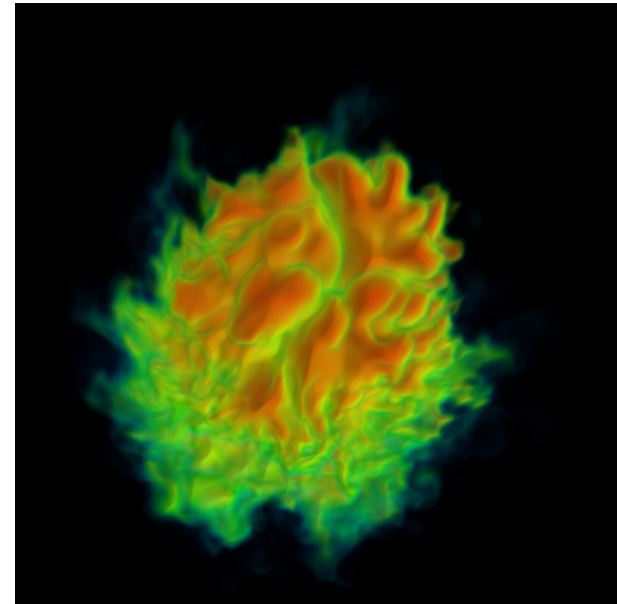
Absolute Runtime

- -hybrid outperforms -only at every concurrency level.
- ▣ At 216K-way parallel, -hybrid is more than twice as fast as -only.



Summary of Results

- Absolute runtime: -hybrid twice as fast as -only at 216K-way parallel.
- Memory footprint: -only requires 12x more memory for MPI initialization than -hybrid
 - ▣ Factor of 6x due to 6x more MPI PEs.
 - ▣ Additional factor of 2x at high concurrency, likely a vendor MPI implementation (an N^2 effect).
- Communication traffic:
 - ▣ -hybrid performs 40% less communication than -only for ghost zone setup.
 - ▣ -only requires 6x the number of messages for compositing.
- Image: 4608^2 image of a $\sim 4500^3$ dataset generated using 216,000 cores on JaguarPF in ~ 0.5 s (not counting I/O time).



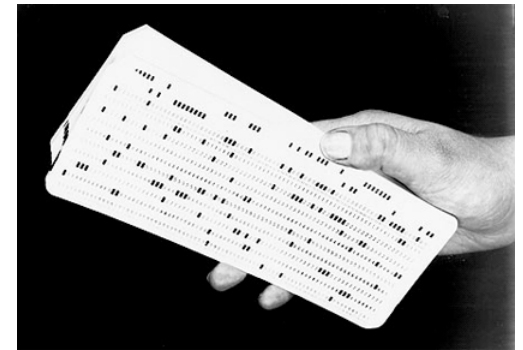
Examples/Case Studies

- 1995: Concurrent (in situ) visualization: UTCHEM simulation code and AVS.
- 2011: Advanced Simulation Capability for Environmental Management (ASCEM).

Reservoir modeling and VDA

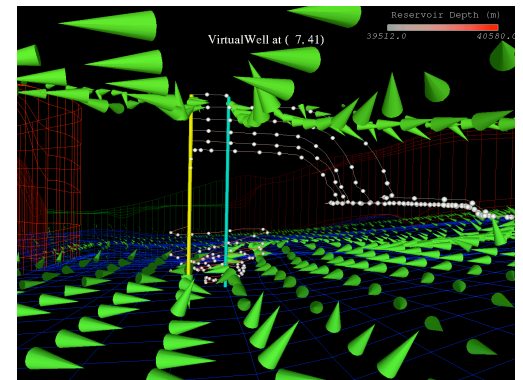
□ Problem(s):

- Setting up inputs (well locations) to optimize production (secondary, tertiary recovery, or EM applications) is tricky; input “card deck.”
- Simulations generate tabular output, difficult to quickly gain insight.



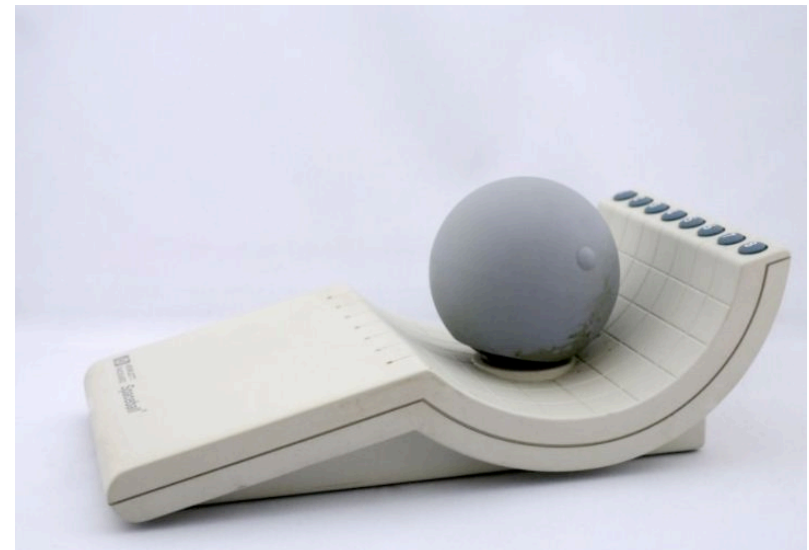
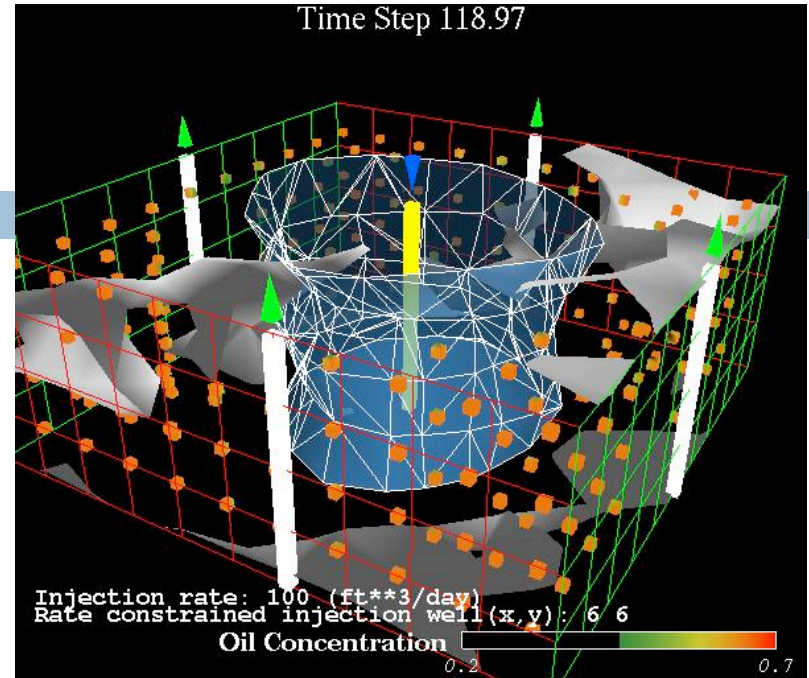
□ Approach:

- Couple model setup with intuitive input devices.
- Couple simulation directly with VDA software.
- Closed-loop system easy to use, quickly converge on optimal setup.

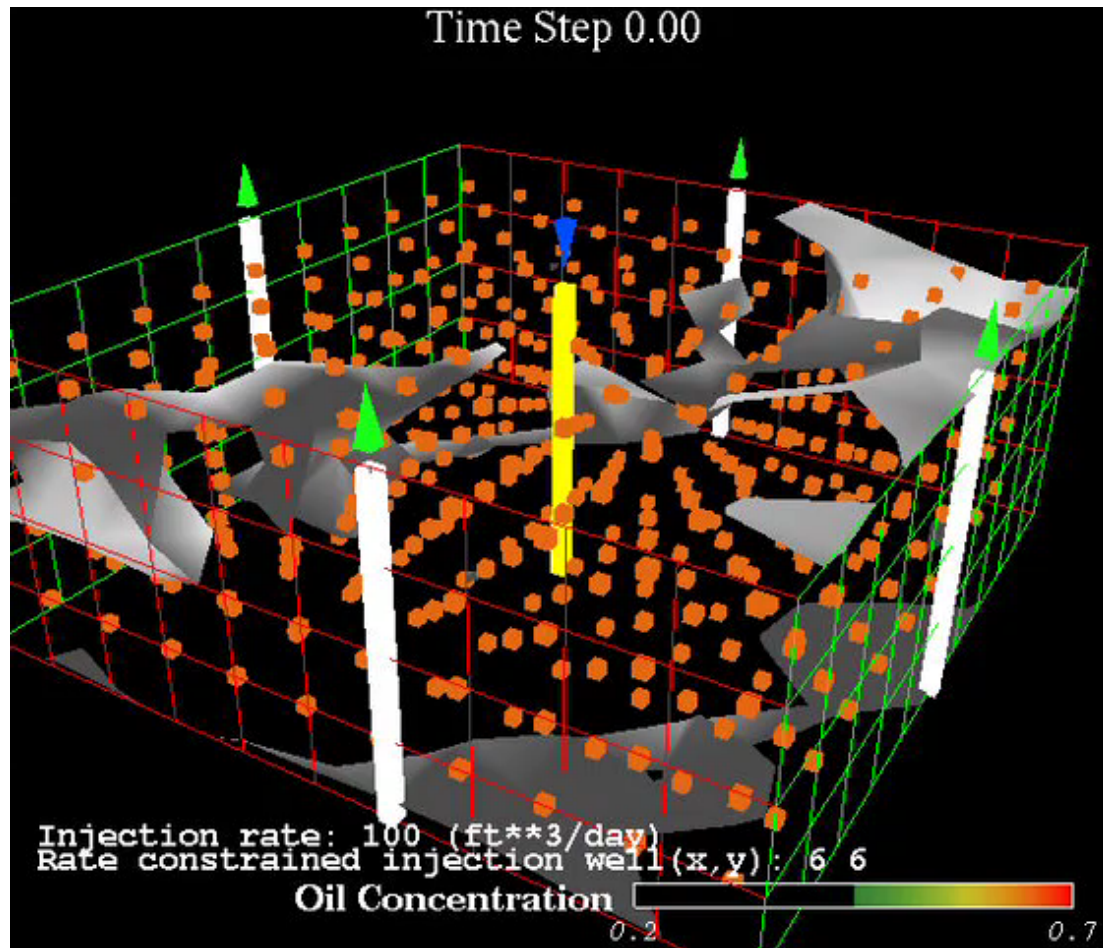


Problem Setup

- Placement of production and injection wells to optimize recovery/mobilization.
- Supplant manual editing of card deck with 3D input device for easy well placement.
- (movie, next slide)



UTCHEM+AVS



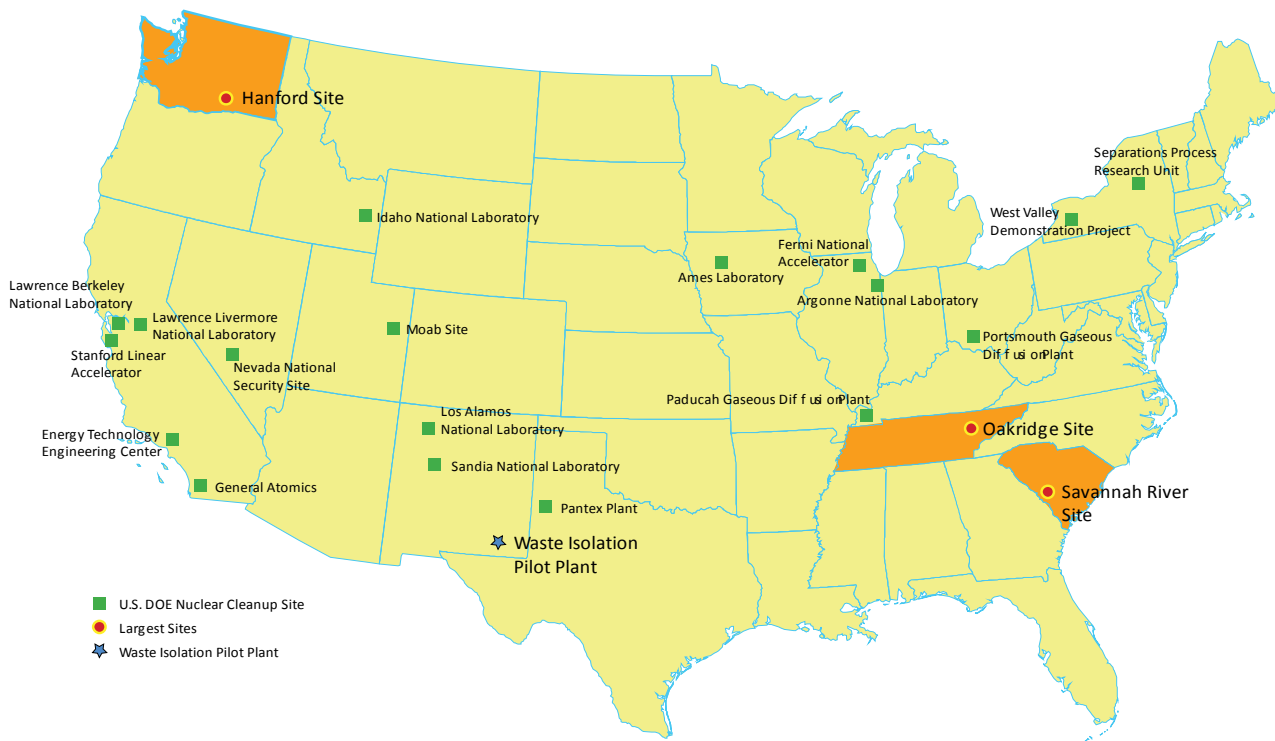
Movie file located here: <http://vis.lbl.gov/Research/utchem-1993/images/utchem.mov>

Environmental Management



Environmental Management - Mission

“Complete the safe cleanup of the environmental legacy brought about from five decades of nuclear weapons development, production, and Government-sponsored nuclear energy research.”



- 6.4 trillion liters & 40 million cubic meters of contaminated groundwater and soil respectively
- Distributed across 30 states and 10,000 individual sites

Solving highly complex technical problems with transformational technologies can lead to billions of dollars of savings and improved clean up

The Challenge

- ❑ Current practices work for some sites and lead to closure
- ❑ Many of the subsurface contamination problems at DOE sites have no practical remedy



❖ Some successes: SRS F-Area groundwater contaminated with metals and radionuclides

- Pump & treat system cost \$1M/month to operate and generated waste products
- Barrier system installed in 2006 costs <\$10K/month and generates no waste products

❖ Need more options to address costly systems and meet regulatory requirements for closure of sites

- Hanford pump & treat systems for the 200 Area cost ~ \$10M/year
- Oak Ridge mercury contamination in debris, soil, groundwater, and stream systems is estimated to cost \$1B to meet regulatory requirements

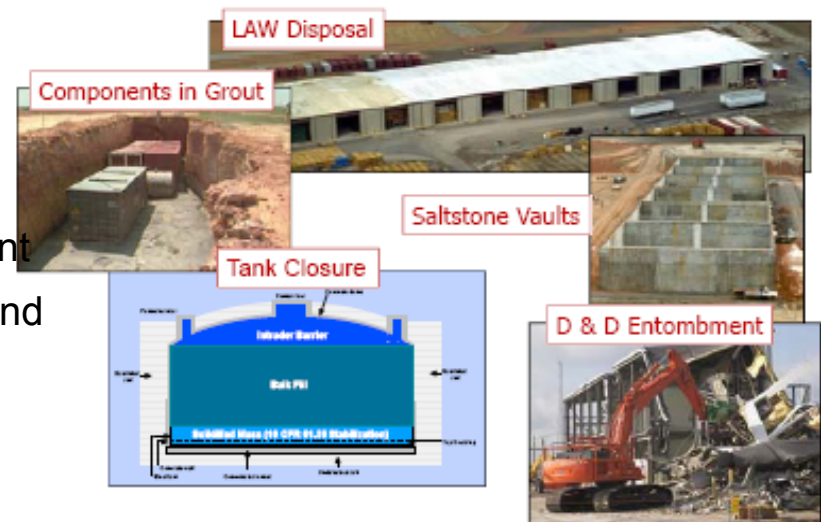
ASCEM Challenge and Impact

➤ Challenge

- Reduce time required and financial cost of remedial actions at sites within EM complex by providing scientifically defensible modeling and simulation tools that accurately address complex environmental management situations
- Develop an integrated, high-performance computer modeling capability to simulate multiphase, multi-component, multi-scale flow and contaminant transport, waste degradation and contaminant release, including
- Provide (software) tools for decision making: parameter estimation, visualization, uncertainty quantification, data management, risk analysis, and decision support
- Leverage investments made by SC, NE, RW, and FE as well as other Federal agencies to capitalize on significant investments and reduce the lifecycle development time and costs

➤ Impact

- Near-term: *technically underpin* existing site RA's and PA's
- Inform strategic data collection for model improvement
- Scientifically defensible and standardized EM RA's and PA's



ASCEM Leverages SciDAC and ASC

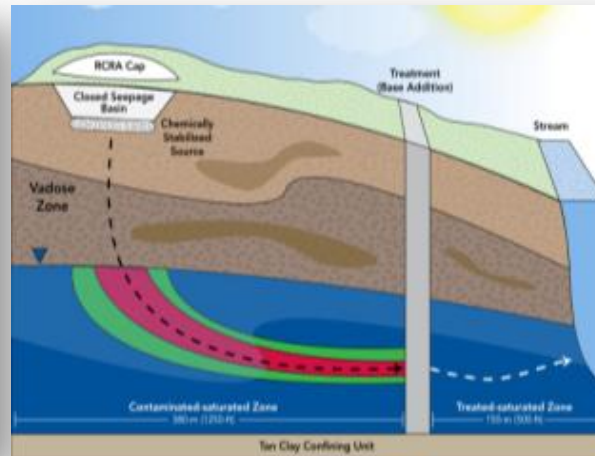
- Significant leveraging of investments by Advanced Simulation and Computing (ASC /DOE NNSA) and Advanced Scientific Computing Research (ASCR/DOE SC)
- Examples include:
 - VisIt – visualization and graphic analysis tool developed by ASC and ASCR **SciDAC** Program
 - PSUADE – uncertainty analysis tool developed by **ASC**
 - Trilinos Framework – services for parallel programming and integrated software packages developed by **ASC** and ASCR **SciDAC** program
 - PETsc – Portable, Extensible Toolkit for Scientific Computation developed by ASCR **SciDAC** Program
 - BoxLib – parallel AMR framework developed by ASCR **Base Math** and **SciDAC**
 - MFD – Mimetic Finite Difference discretization methods developed by ASCR **Base Math** Program
 - Geochemistry Toolset – developed by computational scientists funded through DOE SC **BER**

ASCEM Delivered via a National Laboratory Consortium



Savannah River Site F-Area Background

- Disposal of low-level radioactive, acid waste solutions (1955–1989) created groundwater plume (pH 3–3.5, NO_3 , U, ^{90}Sr , ^{129}I , ^{99}Tc , tritium)
- Ongoing remediation includes capping (1989), active pump and treat (1997-2003), and pH manipulation since 2004
- ***Natural attenuation is desired as a long-term remediation strategy***

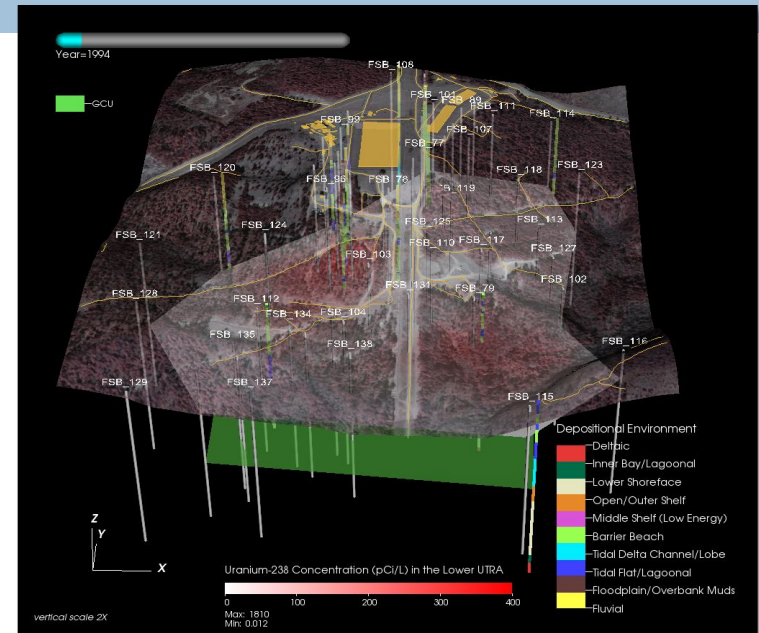
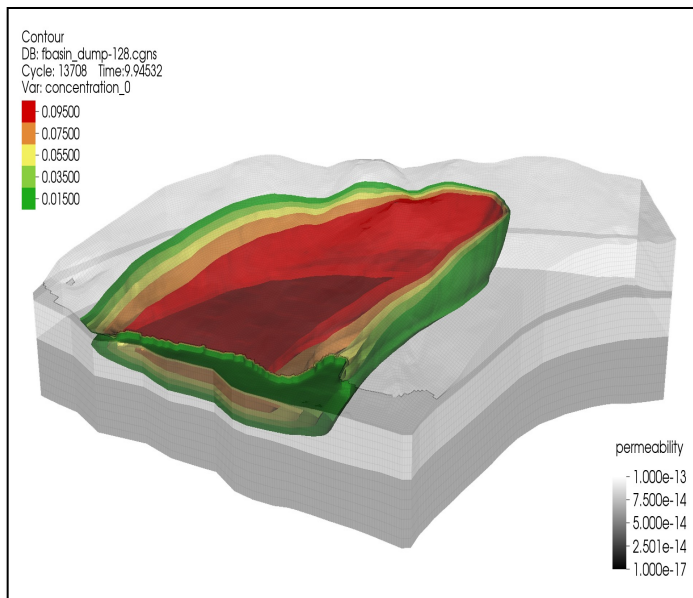


Goals: Phase/Year 1 Demonstration

Platform Data Management	Platform Visualization	Platform Uncertainty Quantification	HPC
<ul style="list-style-type: none">• Depositional data entered into databases• Contaminant concentrations entered into databases• Browsing and query interface with tabled output	<ul style="list-style-type: none">• 3D navigation of concentration data• Visualization of time lapse contaminant concentrations through subsurface domain• Selectively enable several types of data	<ul style="list-style-type: none">• Initial Monte Carlo sampling capability• Automatic creation of forward simulation runs• Visualization of relationships between key parameters and model outputs	<ul style="list-style-type: none">• 3D simulation• Richards' equation• Parallel (100 cores)• Reactive transport of uranium• Advection of non-reactive species• Aqueous speciation• Sorption• Mineral precipitation, and dissolution

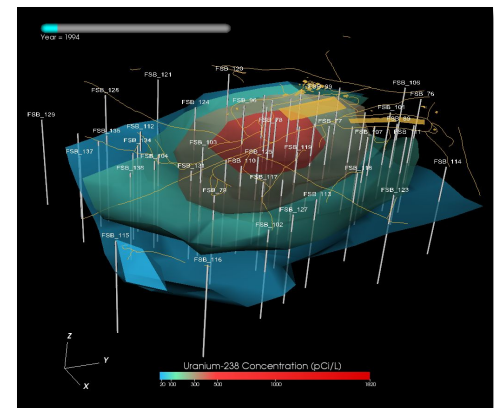
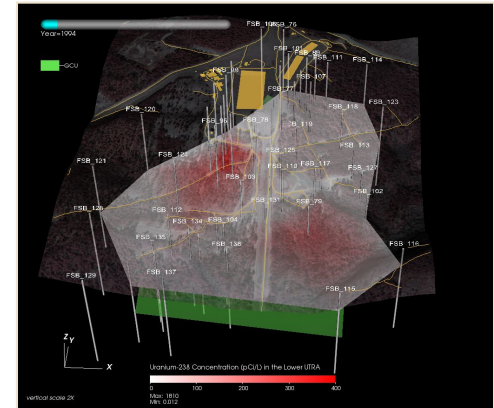
ASCEM Visualization Year 1 Objectives

- Visual data exploration of
 - Part 1: Historical field data.
 - Part 2: Simulation data.
 - Part 3: Ensemble data.

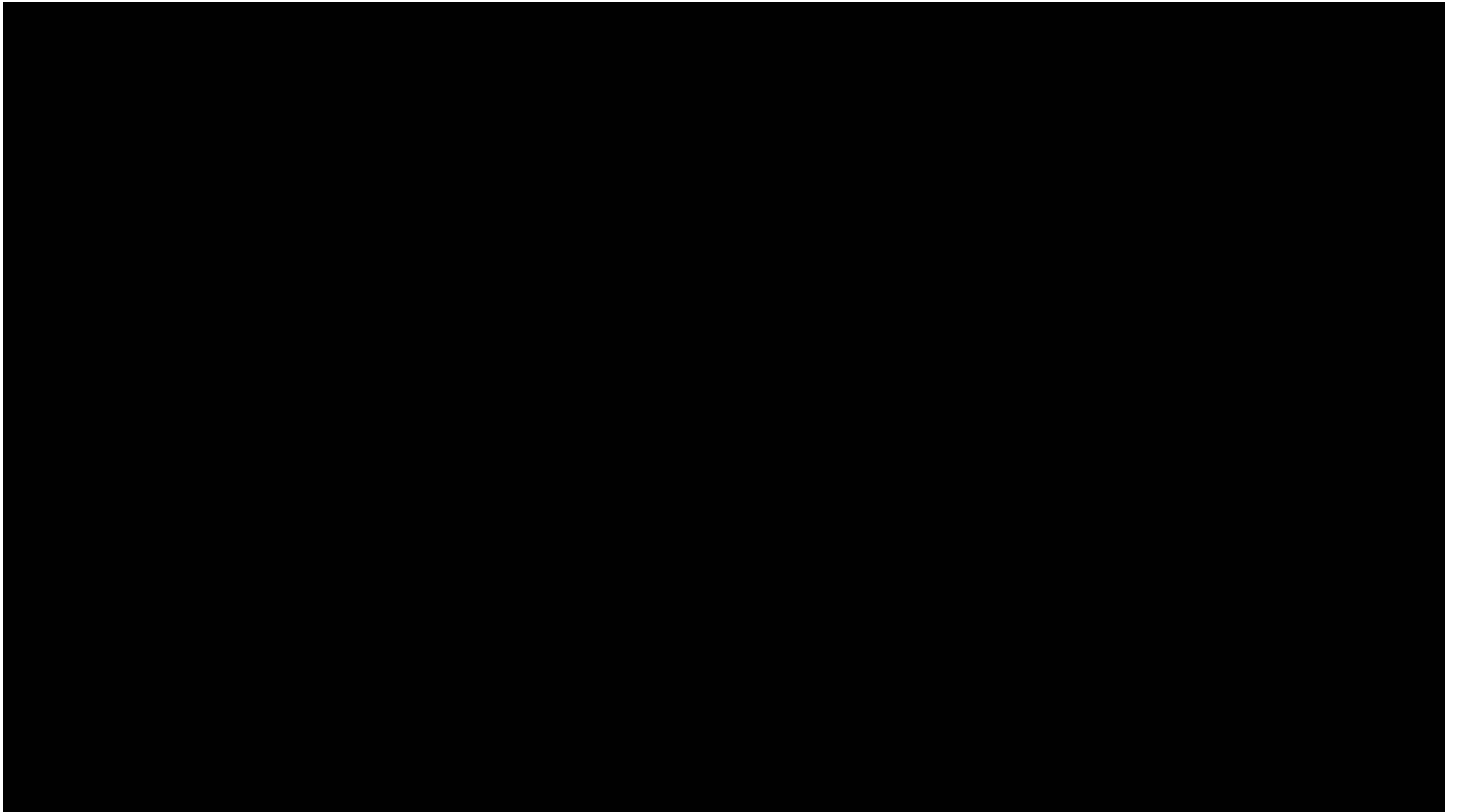


Visualization – Goals and Approach (Part 1)

- Visual data exploration of different types of geospatially registered data for the F-area seepage basin:
 - Observation wells, surface topography, depositional environment, observed concentration from many years, GIS data.
- Phase I Demonstration Objectives:
 - 3D navigation through the F-area historical concentration data.
 - Temporal browsing to show time evolving contaminant plume.
- Approach
 - Add new capabilities to well-established, production-quality, open source visual data analysis and exploration software infrastructure to meet ASCEM needs.
 - Demonstrate viability via application to ASCEM-specific problems.



ASCEM Animation



Movie file located here: <http://vis.lbl.gov/Vignettes/ASCEM/ascem.mp4>

Summary

- DOE and LBNL Visualization team studying different aspects of scalable visualization and analysis, deploying working technologies to the science research community.
- Terascale: Easy. Petascale: lots of work to do. Exascale: Hard.
 - ▣ Exascale requires us to rethink everything, and requires us to change course in terms of programming models/ languages, and in how we think about performance.

