Exploring *OptIPortals* as Petascale Simulation End Stations

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• OptiPortals
  – Scalable display walls based on commodity LCD panels
  – Developed by EVL and CalIT2

• Petascale Simulations
  – Numerical simulations carried out on petaflop/s supercomputers
  – Remote resources

• End Stations
  – DOE-speak for where the science measurements get done
  – e.g., detector at a particle accelerator
Project in a Nutshell.....

Science done here
(end station)

Simulations done here

Visualizations done here
Talk Outline

• State of cosmological research (motivation)
• Laboratory for Computational Astrophysics (who we are)
• Petascale cosmological simulations (the agony and the ecstasy)
• Building a computational end station (design, issues, progress)
Evolution of the Universe

- Afterglow Light Pattern 400,000 yrs.
- Dark Ages
- Development of Galaxies, Planets, etc.
- Inflation
- Quantum Fluctuations
- 1st Stars about 400 million yrs.
- Dark Energy Accelerated Expansion

Big Bang Expansion

13.7 billion years
A Bounty of Precision Cosmological Data

Cosmic Microwave Background Anisotropies

Initial Density Fluctuations

Expansion of the Universe

Galaxy Large Scale Structure
What the Universe is Made Of

The part of the Universe we can see

Causes matter to clump and form galaxies

Causes expansion rate to accelerate

- Atoms: 4.6%
- Dark Matter: 23%
- Dark Energy: 72%
Cosmology’s Big Mysteries

• What is the dark matter?
  – Some undetected elementary particle?

• What is the dark energy?
  – Why does it exist?
  – Does it change with time, or stay constant?

• How do galaxies form?
  – What are the first galaxies like?
  – How do they evolve into spirals and ellipticals?
• What we do
  – Develop and distribute simulation software and tools for computational astrophysics and cosmology for HPC platforms
    • ZEUS (astrophysical MHD and RHD)
    • ENZO (cosmology)
  – Apply our codes to problems requiring extreme levels of computing power (and data storage)
  – Moving into building “theory data” digital collections for others to use
Enzo Project Page

This is the development site for Enzo, an adaptive mesh refinement (AMR), grid-based hybrid code (hydro + N-Body) which is designed to do simulations of cosmological structure formation. Links to documentation and downloads for all versions of Enzo from 1.0 on are available. This is not a pretty, shiny page, it's a place where work gets done.

Enzo development is supported by grant AST-0808184 from the National Science Foundation.

Download

Releases

- Enzo1.5 (released Nov. 6, 2008)
- Enzo v1.0.1 download page.

Repository

- Public Subversion repository → http://lca.ucsd.edu/svn/Enzo/public/
- Browse public repository.
- How to check out a copy.

Compiling Help

- UserGuide/CompilationRequirements
- UserGuide/BuildingEnzo

Documentation

- Enzo v1.0.1 documentation
- Latest user guide
- Tutorials for the current version
The Fate of the Universe Depends on

DARK ENERGY

How to measure expansion accurately?
Standard candles at various distances
Standard rulers to measure dark energy
Baryon Acoustic Oscillations (BAO) in the Cosmic Microwave Background
The Cosmology Simulation We Need To Do: 
$4096^3$ cells/particles in 600 Mpc Box

- Large volume to sample BOA wavelength
- High resolution to resolve cosmic structure

$2048^3$ simulation of cosmic structure
(1/20th volume shown)

2048 core Kraken Cray XT4

**Physics:** 6-species gas dynamics, N-body dark matter, self-gravity, non-eq. ionization
The Agony and the Ecstasy of Petascale Simulations

- **Ecstasy**
  - Remarkable simulations are now possible
  - $4096^3$ simulations feasible today

- **Agony**
  - 50,000 cores
  - 200 TB of data generated intermittently over many months of execution time
    - How to monitor, harvest and store?
  - Complex data analysis task best done on other, geographically-distributed resources
  - How to look at this much data?
  - How to publish the data?
Lifecycle in Words

• Simulations are run on the largest of the NSF resources (e.g., ORNL Kraken)
• Raw output is reduced on various TeraGrid systems (e.g., TACC Ranger)
• Large-scale visualization is done on specialized machines (e.g., ANL Eureka)
• Reduced data and renderings are sent to the Triton Resource at UCSD for display and analysis on our OptIPortal
• At every step, metadata is added to a central database (SimDB, Simulation Database)
• The end result is a queryable repository of publicly available data, tied to publications
That’s Point B

• We’re still at Point A
• Here’s what we need to get there:
  – Internal processes for routinely adding metadata as data is produced
  – Robust networks between large resources
  – Analysis tools with performance comparable to the simulation code
  – Storage for persistent data collections
  – Standardized interfaces to simulation data and metadata
OptIPortal @ LCA/UCSD
80 megapixels, $65,000^2$ image
A collection of resources for data-intensive HPC applications
Publishing Simulation Data: Goals

• Provide mechanisms for discovering and accessing simulation data
• Define standards for publishing simulation data and metadata to promote interoperability
Building Blocks (0/3)
IVOA Theory Interest Group (TIG)

• The IVOA defines standards for publishing astronomical data online
• Standards describe web service interfaces and metadata formats
• TIG is focusing on 3 coupled standards for simulations:
  – Simulation Data Model
  – Simulation Database
  – Simulation Data Access Protocol
Building Blocks (1/3)

Simulation Data Model (SimDM)

- Set of related classes defining simulation metadata
- Key terms:
  - Protocols (simulation and analysis codes)
  - Experiments (simulations and post-processing)
  - Snapshots (results, datasets)
- Rich--includes parameters, purpose and characterization of simulations
- Development led by Gerard Lemson (MPE)
Building Blocks (2/3)

Simulation Database (SimDB)

• Relational database schema derived from the Simulation Data Model
• Intended to be common way for publishing simulation metadata
• Service interface defined by upcoming IVOA Table Access Protocol (TAP)
• Also led by Gerard Lemson (MPE)
Simulation Data Access Protocol (SimDAP)

- Service interface for accessing actual simulation data (e.g., downloads)
- Services may also provide subsets of raw data (particle cutouts, extracted fields)
- Results described using SimDM + metadata for files and contents
- Development led by Rick Wagner (SDSC) and Claudio Gheller (CINECA)
Implementation - SimCat

- SimCat: Simulation Catalog
- Web service extending the SimDM
- RESTful API for managing the catalog
- Foundation for building SimDB and SimDAP services
- Uses Django (Python web framework)
- [http://code.google.com/p/simcat](http://code.google.com/p/simcat)
Status

• SimCat:
  – Development service running
  – Building catalog of existing simulations
  – Needs human-friendly interface
  – SimDAP service interface in development
  – SimDB service interface when TAP standard closer to completion

• IVOA Standards
  – SimDAP Note due in March 2009
  – SimDAP Working Draft out by next InterOp (May 2009)
Next Steps

• Evaluate workflow software for automating forwarding of petascale data files over the network (from ORNL to ANL to UCSD)
• Evaluate workflow software for automating forwarding of file metadata to SimCAT
• Explore use of switched fiber optic circuits on Internet2/NLR for aiding data transfers
• Get analysis software running on Triton Resource
• Push the $4096^3$ run off the cliff
Collaboration Opportunities

- Workflow automation
- Data modeling/publishing
- Scientific visualization
- Parallel analysis algorithms
- Data mining

If you are interested, could use MURPA to engage.

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