Numerical Relativity Infrastructure Meeting

APS, St Louis
April 2008
XiRel: Next Generation Infrastructure for Numerical Relativity

- Providing an open, modern and scalable cyberinfrastructure for numerical relativity to leverage new petascale computing resources.
- Involves LSU, PSU, RIT, AEI, Arizona
  - Developing highly scalable, efficient and accurate adaptive mesh refinement layers for Cactus (initially based on Carpet driver)
  - Metadata for scientific computing, data archiving, science services
- Supported community-driven infrastructure
- [http://www.cct.lsu.edu/XiRel](http://www.cct.lsu.edu/XiRel)
  - New release of Carpet
Motivation

• Petascale computers
  – Real hydro problems will require these
  – >100,000 processors, multicore, accelerators
  – NSF already funding PetaApps, PRAC, etc
  – LOT OF CYCLES RIGHT NOW

• New era for numerical relativity
  – Interactions with gravitational wave data analysis, astrophysics

• Data !!!
  – Move data, keep data, describe data

• Science
  – Progress, training students, need more people

• Funding: NSF OCI/CISE, DOE, ...
Topics for Discussion

• What technical advances will we need in the next five years?
• What infrastructure is there already for numerical relativity?
• Frameworks: Where have initiatives such as Cactus been successful? What have been the problems, are they technical or social? What level of sharing of infrastructure does the community envisage for the future (data level, sharing code, sharing infrastructure)?
• Other tools: Data models, visualization tools, community archives?
• Social aspects: How to support common infrastructure, how to get community guidance on infrastructure, how to take advantage of funding for computational/computer science/cyberinfrastructure.
Shared Infrastructure

• Data:
  – Data description (to share initial data, output data, build common visualization, analysis tools, information extraction/data mining)
  – Metadata (common way of describing data --- this is crucial and needs physics insight)
  – Provenance
  – Technologies for handling large data, e.g. moving data from centers, setting up group (``VO'') archives, subsampling data, using optical networks
Shared Infrastructure

• Coming Architectures
  – Multicore and manycore (hybrid OpenMP/MPI, new paradigms)
  – Accelerators (GPUs, Cells, clearspeed, ....)0
  – Hundreds of thousands of processors (how to scale production AMR or complex data structures)
Shared Infrastructure

• Component Frameworks
  – “Deeply integrated” (e.g. Cactus)
  – “Loosely integrated” (e.g. SOA)
  – With right interfaces/abstractions can have interoperable components
  – Components as libraries
  – Sharing of Components
    • Core computer science stuff: Carpet, Parallel I/O, interpolators
    • Common science tools that everyone uses: analysis, initial data (Einstein Toolkit)
  – Associated tools: ALPACA: debugging/profiling, verification & validation, report generation
Shared Infrastructure

• Science Gateways (TeraGrid)
  – Paradigm shift from HPC use. Enable entire communities of users associated with a common scientific goal to use national resources through a common interface. Science gateways are enabled by a community allocation whose goal is to delegate account management, accounting, certificates management, and user support to the gateway developers.
  – Varying goals and implementations. Expose specific sets of community codes so that anonymous scientists can run them, community portal that brings a broad range of new services and applications to the community, access to data collections or the ability to create data products by analyzing data in a collection, remote visualization.
Shared Infrastructure

- Relativity Services
- Automatic Code Generation
- Visualization and Steering
What is ESMF?

The Earth System Modeling Framework (ESMF) is software for building and coupling weather, climate, and related models. Read more...

News Highlights

- **Registration is now open** for the 7th Annual ESMF Community Meeting. It will be held on May 28-30, 2008 in Fort Lauderdale, FL, coincident with the AGU Joint Assembly. The meeting will include a 3-day coding workshop focused on one-to-one interactions with framework developers. April, 2008

- **ESMF on the TeraGrid**! ESMF received funding to begin comprehensive regression testing over the TeraGrid. This will exercise the TeraGrid Build & Test Service and demonstrate ESMF use on the world’s largest, most comprehensive distributed cyberinfrastructure for scientific research. March, 2008

- **New ESMF-Based National Weather Prediction System** Navy, NOAA, and Air Force operational centers are starting a two year pilot project to initiate the construction of a new weather prediction system, with ESMF as the target framework. October, 2007

- **Coupled COAMPS and NCOM** The Naval Research Laboratory successfully completed a beta test coupling COAMPS and NCOM. The coupling uses the new sparse matrix multiply in ESMFv3.0.3. October, 2007

Quick Links

- FAQ
- Download ESMF
- Release schedule
- Browse source code

Upcoming Events

Telecons

- Thursday, 4/10/08, 1:00pm MT: loxahedral interface (Neckels)
- Tuesday, 4/15/08, 1:00pm MT: Attribute interface (DeLuca)
- Thursday, 5/1/08, 1:00pm MT: Location stream integration (Dennike)

To receive telecon emails, review materials, and release notifications, join the JST mailing list.

Meetings

ESMF Annual Community Meeting, May 28-30, 2008, Fort Lauderdale, FL. Register here.

Meetings archive
The Geosciences Network (GEON) project is a collaboration among a dozen PI institutions and a number of other partner projects, institutions, and agencies to develop cyberinfrastructure in support of an environment for integrative geoscience research.

Recent News

GeoEarthScope Northern California Airborne LiDAR Data Now Available on GEON Portal.

The first processed products from the GeoEarthScope Northern California Airborne LiDAR project are now available via the GEON portal. For further info and step-by-step access instructions, click here.
The National Ecological Observatory Network (NEON) is a continental-scale research platform for discovering and understanding the impacts of climate change, land-use change, and invasive species on ecology. NEON will gather long-term data on ecological responses of the biosphere to changes in land use and climate, and on feedbacks with the geosphere, hydrosphere, and atmosphere. NEON is a national observatory, not a collection of regional observatories. It will consist of distributed sensor networks and experiments, linked by advanced cyberinfrastructure to record and archive ecological data for at least 30 years. Using standardized protocols and an open data policy, NEON will gather essential data for developing the scientific understanding and theory required to manage the nation’s ecological challenges.
NSF CDI (07603)

Create revolutionary science and engineering research outcomes made possible by innovations and advances in computational thinking. Computational thinking is defined comprehensive to encompass computational concepts, methods, models, algorithms, and tools.

- From Data to Knowledge: enhancing human cognition and generating new knowledge from a wealth of heterogeneous digital data;
- Understanding Complexity in Natural, Built, and Social Systems: deriving fundamental insights on systems comprising multiple interacting elements;
- Building Virtual Organizations: enhancing discovery and innovation by bringing people and resources together across institutional, geographical and cultural boundaries.