Northwest Indiana Computational Grid

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OSG All-Hands Consortium Meeting

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What is NWICG?

- The Northwest Indiana Computational Grid (NWICG) is a partnership of researchers and educators at three university campuses in northwestern Indiana: Purdue University-Calumet, Notre Dame University, and Purdue University-West Lafayette.

- Under NWICG, resources at all three campuses are available to each other, and all campuses coordinate and plan future infrastructure with this partnership in mind.

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Development of NWICG

- IP-Grid (Indiana-Purdue Grid) (2004)
    - NSF funded grid built on partnership for ETF proposal
    - Developed high performance networking infrastructure
- Teragrid partnership
    - Indiana and Purdue collaborated on a successful joint Teragrid proposal
- Large grid infrastructure projects were in development or underway
    - University of Michigan Grid (M-Grid) (2002)
    - UK e-Science, European Data Grid
- Motivated development of a computational grid focused on Northwest Indiana
- Purdue University (West Lafayette, Calumet), Notre Dame University
- Garnered Federal support to create Northwest Indiana Computational Grid
- Goals of NWICG
    - Leverage mutual interests amongst the three campuses with national science and research initiatives
    - Provide cyberinfrastructure to support science and educational efforts
    - Contribute to regional economic development

NWICG History

- 2004
  - NWICG first formed as a DOE-sponsored project
- 2005
  - Initial workshops
  - Condor pools at West Lafayette and Notre Dame deployed and expanded
- 2006
  - Adoption of the OSG software stack
  - Opteron cluster and storage array at Notre Dame brought online
  - Networking between West Lafayette and Notre Dame upgraded
- 2007
  - High-memory SGI Altix in West Lafayette installed
  - Condor pool at Calumet brought online
  - Networking to Notre Dame and Calumet upgraded

Networking Upgrades

- Initially, Notre Dame and West Lafayette added a dedicated 100Mb/s MREN (Metropolitan Research & Education Network) link between the two campuses

- Later Notre Dame obtained a 1 Gb/s "I-Light" link via Indiana's state-operated fiber network. Benchmarks were done to ensure this link is performing as expected between Notre Dame and West Lafayette.

- Calumet has brought online another DS3 circuit as a stop-gap measure pending their own I-Light connection.

NWICG HPC Resources

- **Calumet**
  - Condor pool of over 200 Pentium4 Windows lab machines, accepting flocking from West Lafayette's Condor gatekeeper
  - Small parallel computing cluster deployed at Calumet for use in training users and testing locally before involving NWICG grid partners

- **Notre Dame**
  - 144-core Opteron Sun Fire X2100 system
  - 36 TB NetApp FAS3050 storage array
  - Condor pool containing more than 500 machines
    - Predominantly 32-bit and 64-bit Linux machines with some Sun machines

NWICG HPC Resources

- ## **West Lafayette**
    - 128-processor Itanium SGI Altix 4700 with 512 GB of RAM (unique high-memory system to complement Notre Dame Opteron cluster)
    - 30 TB SGI InfiniteStorage 4000 system
    - 8-core FPGA SGI 450 RASC RC100 system (4 Xilinx Virtrex FPGAs)
    - Tesla Quad-GPU system (CUDA) with dual 16-lane PCI buses
    - Condor pool with over 7,000 processors of various type

- **Also smaller dedicated systems at each campus to support other resources**

Workflow Improvements

- Added Condor job submission hosts at each campus
  - Users won't need to configure local Globus/Condor-G clients.

- Dedicated interactive compilation node for the SGI Altix
  - Allows researchers to easily and quickly develop and test codes
  - Jobs submitted through Globus/Condor-G to SGI Altix

- Dedicated Serialize-Place-and-Route node being tested now at West Lafayette for grid users of the Altix 450 FPGAs
  - Allows researchers to create their own algorithms for the FPGAs and install/run them easily.

Organization / Communication

- Calumet and Notre Dame have dedicated AccessGrid facilities
  - AG used for regular coordination meetings

- NWICG website
  - Features a wiki for documenting and explaining how users can access NWICG resources.

Education / Outreach

- Condor workshop held in 2007 at Purdue
  - Introduced potential users and systems administrators to Condor
  - Demonstrations on using and configuring Condor
- Parallel computing workshop held at Calumet
  - Train students and faculty in parallel and distributed computing concepts and methods.
- Contributed funds to help build a teaching lab for high-performance computing at Purdue

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Scientific Research using NWICG

- September 11 Word Trade Center attack simulations using LS-DYNA
  http://www.youtube.com/watch?v=cddIgb1nGJ8

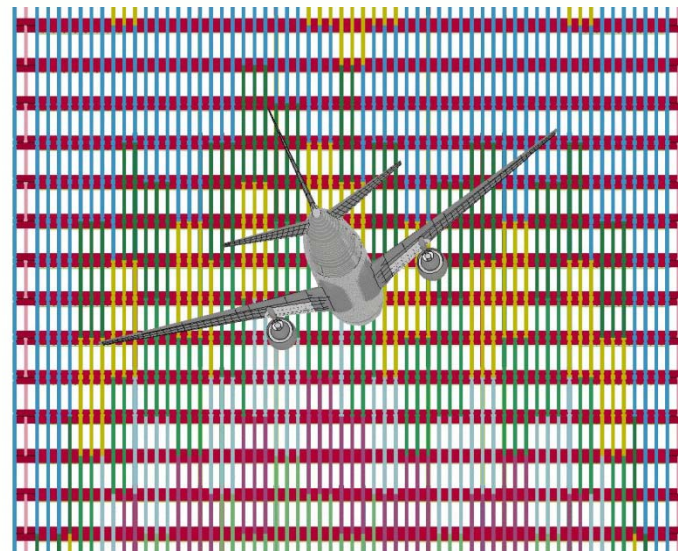- Purdue FPGAs confirmed to meet published BLAST benchmarks from SGI of 65.9x speedup over a normal CPU.
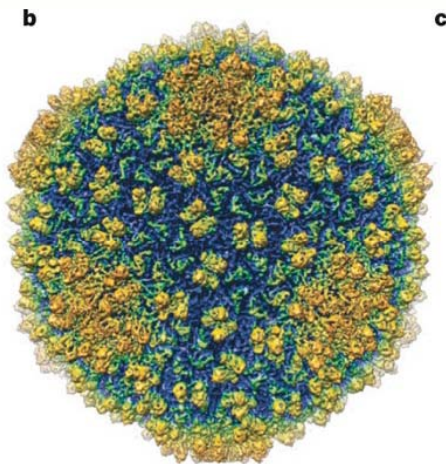

Image shows façade before impact. Reproduced courtesy of Mete A. Sozen, Ayhan Irfanoglu, Christoph M. Hoffmann.

- Ozone degradation research, including a very large 6-week job not able to be accommodated at national centers. This is the largest calculation ever completed for this problem.

Scientific Research using NWICG

Image of virus structure.
Reproduced courtesy of Wen Jiang.

- Purdue work to identify specific infectious virus structure using image reconstruction from electron cryomicroscopy. This work was published in Nature in February.

- Notre Dame research modeling of optimum automotive structures subjected to complex crash interactions using hybrid cellular automaton.

Scientific Research using NWICG

- Research on adsorption and reaction thermodynamics relevant to NO oxidation on Pt(111) at as a function of oxygen coverage (Notre Dame).

- Large prime number factorization research support (Purdue).

- Hurricane simulations from the 2000-2005 seasons as part of the Florida State University Mesoscale Superensemble Project (FMSP) (Notre Dame)
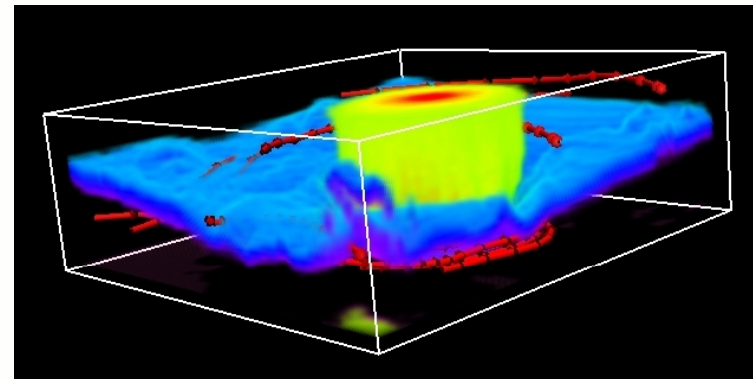

Image shows a 3-dimensional volume rendering of central pressure of Hurricane Katrina. The red vectors depict flow around and within the hurricane. Imagery produced by VAPOR (www.vapor.ucar.edu), a product of the National Center for Atmospheric Research.

NWICG Current Status

- Actively engaging users of major existing computational resources (Notre Dame cluster, West Lafayette high-memory Altix).
- In partnership with Teragrid, developing better processes for using FPGAs in a shared production setting, including issues related to bit-file generation, end executable compilation, and scheduling and execution on and of both host and FPGAs
- Setting up visualization facilities at Calumet now and actively recruiting a Calumet visualization center director.
- Awaiting major upgrade to Calumet networking via I-Light connection.
- Holding regular coordination and planning meetings for both infrastructure and steering committees, usually via AccessGrid on each campus.

Future Plans: Calumet

- Investigating curriculum development around simulation and modeling to be used in conjunction with existing programs.
- Support for much larger job/data transfer via upgraded network capacity.
- Development of visualization center and facilities for use by local users in conjunction with remote processing via NWICG partners.
- Investigating extension of Molecular Dynamics n-body techniques to Astrophysics problems using accelerator technologies.
- Exploring other research proposals as well.

Future Plans: Notre Dame

- Research into "Grid Heating"—the reuse of HPC waste heat as a heating-energy source.

- Work with FSU on satellite remote sensing techniques to improve and verify climate models.

- Deploying OSG Storage Element resource.

- Exploring other research proposals as well.

Future Plans: West Lafayette

- Open and refine access to FPGA resources already on the floor.
- Analyze power consumption of FPGA resources and determine power-time savings for certain jobs over normal CPU usage.
- Investigation of additional accelerator technologies for possible deployment, including GPUs and Cell processors.
- Development of image-processing service to use Tesla GPU (CUDA) system.
- Testing DVI over IP use as part of real-time remote visualization with NWICG partner institutions.
- Interoperate with TeraDRE to allow Condor-flocking of rendering jobs to other NWICG sites, and make TeraDRE resources available to NWICG users.
- Expanding cooperative Condor use to additional Indiana colleges via the BoilerGrid project.
- Exploring other research proposals as well.

Research Collaborators

- Ed Bensman
- Gary Bertoline
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- Paul Brenner
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- Christoph Hoffmann
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- Doug Thain
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NWICG Personnel

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  - John Alberts