Advancing Science & Engineering through Computational Science
Advancing Computational Science through Gravity

Edward Seidel
Director, Center for Computation & Technology, LSU
Cray Professor of Physics and Computer Science, LSU
IEEE 2006 Sidney Fernbach Award Lecture, SC2006

Center for Computation & Technology
AT LOUISIANA STATE UNIVERSITY
Powerful Beyond Imagination

“Computers are incredibly fast, accurate, and stupid. Human beings are incredibly slow, inaccurate, and brilliant. Together they are powerful beyond imagination.”

SC06 Tag Line
“Computers are incredibly fast, accurate, and stupid. Human beings are incredibly slow, inaccurate, and brilliant. Together they are powerful beyond imagination.”

50 years later: Computers are $\sim 2^{35}$ times faster now! Extending human intelligence (a la Kurzweil) to allow us to solve equations Einstein could not! He would be very pleased with progress!
Einstein’s Equations and Gravitational Waves

*Two major motivations/directions for numerical relativity*

- Exploring Einstein’s General Relativity
- Developing theoretical lab to probe this fundamental theory
  - Fundamental theory of Physics
  - Among most complex equations of physics
  - Dozens of coupled, nonlinear hyperbolic-elliptic eqs: 1000’s of terms
    - Barely have capability to solve after a century
    - Predict black holes, gravitational waves, etc, but want much more
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Gravity waves collapse to BH. Pure theory, no experiment, requires supercomputer!

BH forms!
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- Exciting new field about to be born: Gravitational Wave Astronomy
  - LIGO, VIRGO, GEO, LISA, … ~ $1 Billion worldwide!
  - Fundamentally new information about Universe
  - A last major test of Einstein’s theory: do they exist?
    - Eddington: “Gravitational waves propagate at the speed of thought”
    - 1993 Nobel Prize Committee: Hulse-Taylor Pulsar (indirect evidence)
    - 20xx Nobel Committee: ??? (For actual detection….)
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Christian Ott, et al. AEI & U Arizona. ~ First 3D GR SN…

Kaehler viz, ZIB, AEI
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One century later, breakthroughs happening at the same time!

HPC + grids + algorithm + theory all essential ingredients.
Grand Challenge Collaborations

Science and Eng. Go Large Scale: Needs Dwarf Capabilities

NASA Neutron Star Grand Challenge

- 5 US Institutions, 3 years, $1.4M
- Solve problem of colliding neutron stars (try...)

[Image of a simulation of two neutron stars colliding]
Grand Challenge Collaborations

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- **NSF Black Hole Grand Challenge**
  - 8 US Institutions, 5 years, $4M
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Science and Eng. Go Large Scale: Needs Dwarf Capabilities

- EU Network Astrophysics
  - 10 EU Institutions, 3 years, €1.5M
  - Continue these problems
  - *Entire Community becoming Grid enabled*

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• Examples of Future of Science & Engineering
  – Require large scale simulations, and collaborations
  – Bring together cross disciplinary teams
  – Demands on software engineering
  – Solving problems simply beyond reach until now…
Early Experiments
First 3D Black Hole Collisions, 1994
NSF Black Hole Grand Challenge Era

Event Horizon in green
Ψ₄ (gravitational waves) in blue-yellow

- Smarr thesis now a “test problem” for 3D
- Possible due to 2D studies, 512 node CM-5
Relativity Workbench (1992)

*Inspired by Mike Norman*

- Above work very tedious! Want workflow, resource selection, live viz, etc
- Choose resources, compute initial data, visualize
- Evolve, visualize
- Archive, store results
- Early grid, portal ideas!
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G. Heinz
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G. Heinz
CAVE, SC93, 94, 97

- Golden Age of numerical relativity, but takes so long!
  - Visualizing results: could not wait for physics!
- Developed 3D visualization during simulation
  - Why? Better science, better understanding, fewer errors

G, H codes for EEs. CM-5 allowed 3D!

SC97: Garching, Germany - San Jose
Wanted multiple views of all functions (50 3D arrays!), different viz targets, ease of use

Joan Massó, John Shalf, Tom DeFanti, Trina Roy, Jon Goldman, Carolina Cruz-Neira, et al
SC95 I-WAY

• Pivotal event
  – “Metacomputing” discussed for few years (Catlett, Smarr, et al)
  – EE’s could use all SCs available: how?
• Tom DeFanti, Ian Foster, et al
  – Networks, software layers
  – NCSA relativity group among apps
    • Single MPI job across NCSA, PSC, SDSC, Cornell, viz’d in CAVE
  – Projects “successful”, Heros of SC95!
• Software projects emerge
  – Globus Toolkit and Grids
  – Cactus Toolkit for applications: learn from above
Lessons Learned
Computational Science is Hard

• Requires incredible mix of technologies & expertise!
• Many scientific/engineering components
  – Physics, astrophysics, CFD, engineering,…
• Many numerical algorithm components
  – Finite difference? Finite volume? Finite elements?
  – Elliptic equations: multigrid, Krylov subspace,…
  – Mesh refinement, multipatch
• Many different computational components
  – Parallelism (HPF, MPI, PVM, ???)
  – Architecture (MPP, DSM, Vector, PC Clusters, FPGA, ???)
  – I/O (generate TBs/simulation, checkpointing…)
  – Visualization of all that comes out!
• New technologies
  – Grid computing
  – Steering, data archives
  – Symbolic code generation to do all above (possible!)
• Abstractions: enable all disciplines, areas of CS…
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More Modern Approaches
Cactus Emerges after GC, IW

- Free, modular, portable environment for collaboratively developing parallel, HPC multi-D simulations (Component-based)
- Developed for Numerical Relativity, now general framework for parallel computing
- Finite difference, AMR (Carpet, Samrai, Grace), new FE/FV, multipatch, unstructured meshes
- Interfaces to advanced I/O, elliptic solvers
- Active user and developer communities, main development now at LSU and AEI.
- Open source, documentation, etc

Paul Walker (JP Morgan), Joan Massó (Grid Systems), John Shalf (LBNL); Tom Goodale (Cardiff/LSU), Gabrielle Allen (LSU), Gerd Lanfermann (Phillips)

Microsoft, SGI, Intel, Sun, HP support...
Cactus Structure

Core “flesh” with plug-in “thorns”

Plug-In “Thorns” (modules)

Fortran/C/C++

input/output

interpolation

SOR solver

wave evolvers

multigrid

coordinates

extensible APIs

ANSI-C

parameters

scheduling

error handling

make system

grid variables

boundary conditions

black holes

equations of state

Computational Tools !!

AMR, unigrid, unstructured

remote steering

Your Physics !!
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Abstractions, interfaces:
- Users don’t want to write MPI!
- Plug in different AMR, parallel I/O, elliptic solvers

Computational Tools !!
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- remote steering

Your Physics !!

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Users and Toolkits

• Many numerical relativity groups around the world
  – Over 100 publications
  – Maya, Whisky, Lazarus, …

• Others:
  – CFD
  – Quantum Gravity
  – Chemical Engineering
  – Crack Propagation
  – Environmental modeling
  – Plasma physics
  – Computer science
  – Astrophysics
  – Cosmology
  – [Biology/Materials]

• Toolkits
  – Cactus Computational Toolkit
  – Einstein Toolkit
    – Many modules
    – Kranc generates entire Cactus codes from Mathematica: Sascha Husa, AEI, Jena
  – CFD Toolkit (CCT, KISTI booth)
  – (Biology Toolkit)

• Teaching
  – Over 30 student thesis/diploms
Notification, Remote Interactive Viz & Steering

Any Viz Client:
LCA Vision, OpenDX

Changing steerable parameters
• Parameters
• Physics, algorithms
• Performance

DFN grants at AEI, now EnLIGHTened and other
**Grids 1: Dynamic, Adaptive, Distributed Computing**

**SDSC IBM SP**
- 1024 procs
- $5 \times 12 \times 17 = 1020$

**NCSA Origin Array**
- $256 + 128 + 128$
- $5 \times 12 \times (4+2+2) = 480$

**Communications dynamically adapt to application and environment**

Any Cactus application. Scaling: 15% → 85%

*“Gordon Bell Prize” (SC01)*

**Thomas Dramlitsch**

**Matei Ripeanu**
Grids 1: Dynamic, Adaptive, Distributed Computing

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GigE: 100 MB/sec
(But only 2.5 MB/sec)

Cactus + MPICH-G2
Communications dynamically adapt to application and environment
Any Cactus application. Scaling: 15% -> 85%
Grids 2: GridLab

- EU 5th Framework (2002-2005)
  - 6 Million Euros
  - Led by Jarek Nabrzyski

- Focused on tools for applications
  - Cactus and numerical relativity apps
  - Gravitational Wave Data Analysis (Triana)
  - Dynamic scenarios: Early DDDAS combine GW + Numrel

- Dynamic grid apps, infrastructure, users all can:
  - Be aware of environment: services, allocation, bandwidth?
  - Decide: migrate, spawn, access data
  - Publish information: what is the app/user doing?

- 12 workpackages, including:
  - Grid services, apps, testbed, GAT, Portals, brokers, mobile...

Successful 5th Framework project --- came from GR, Cactus, other EU projects, early Globus work
Grid Application Toolkit & SAGA

- Abstract programming interface between apps and Grid services: “Cactus for Grid”. Adaptors! App runs everywhere with same code
- Designed for what apps need (move file, run remote task, migrate, write to remote file)
- Motivated by numerical relativity
- GAT led to OGF Working Group to develop a “Simple API for Grid Applications” or SAGA
  - Focus on scientific and engineering applications, simplicity
  - Better API based on use case studies
- SAGA is centerpiece for OGF at application level
  - 60-day comment period now for specification
- OMII calling for proposals to implement SAGA
- C++ implementation at LSU ongoing
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GridSphere

- GridSphere portal framework, developed in GridLab at AEI
  - Origins in '92 relativity workbench, NSF ASC project
- Generic JSR 168 compliant portlet container
- Architecture for “pluggable” web applications
- Core portlets, Grid Portlets, Cactus Portlets, D-Grid, LSU projects
- Over 250 subscribed to user mail list, around 500 unique web visits/month
Return to Future: Properly Engineered Software

Task Farming, Spawning & Migration combined

Main Cactus BH Simulation
starts in Berkeley
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Dozens of small jobs sent out to test parameters
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Data returned for main job.
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Huge job generates remote data to be visualized in Baltimore
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Physics code to do all this can be generated via symbolic algebra!
Louisiana Optical Network Initiative (LONI)
40 Gbits to all PhD campuses, 100Tflops for Louisiana
Optical Nets Enable Old & New Paradigms

Huge BH simulation, outputs ~TBs data, must be interactively viz’d & analyzed by international collaboration

• Many practical problems found above go away!
• New Distributed Computing, Data, and Viz Services
  – Data larger than memory, disk slow: multiple streaming data servers
  – Co-scheduling machines, data, and network for single event: MacLaren HARC
  – Lambda Provisioning: Karmous-Edwards EnLIGHTened NSF project
  – Same application must work with multiple nets, services: GAT/SAGA

• High Resolution: not science w/o details, analysis
  – Uncompressed HD stream: near latency-free remote viz at 1.5Gbit/sec
  – Video for colleagues: see details, read equations
  – Sterling HPC class: from LSU but LA, AR, Brno (Czech)
Current Major Numerical Relativity Efforts in Binary BH, NS, SN

Many groups use Cactus, all BBH use AMR
- share codes, modules
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Relativistic Astrophysics in 2010

- Full 3D GR simulations of binary systems for dozens or orbits and merger to final black hole
  - All combinations of black holes, neutron stars, and exotic objects like boson stars, quark stars, strange stars
  - Full 3D GR simulations of core collapse, supernova explosions, accretion onto NS, BH
  - Gamma-ray bursts
- All likely to be observed by LIGO, GEO, Virgo
- Resolve from 10,000 km down to 100 m on a domain of 1,000,000 km$^3$ for 100 secs of physical time
  - ~20Kflops per gridpoint, ~500 grid functions
  - 16 levels of refinement
  - Weeks on Pflops/sec sustained performance
  - 100 TB memory (size of checkpoint file needed)
  - PBytes storage for full analysis of output
NSF TeraGrid

- Distributed national computing facility
  - NCSA, SDSC, Chicago, Pittsburgh, ORNL, Indiana, TACC

- How to integrate computers, networks, data for advanced science?
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News Flash: LSU/LONI to join TeraGrid!
Recent NSF Awards

- NSF “Toward Petascale” (Track 2)
  - Oak Ridge National Lab/U of Tennessee
    - National Center/Regional Anchor
    - $30M Cray machine, available summer 2008
  - TACC, others coming in 2009 and beyond (LA?)

- NSF Leadership Class
  - UIUC/NCSA-LSU-GLC
  - 1PF ++, 2011
  - World’s most capable machine
  - $208M+: How we will access the output? Grids!
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Petascale Challenges for GR
(Scary)

• Basic numerical algorithms in place (new!)
  – Dozens of groups compute GR, share common tools for petascale

• Most AMR codes scale to ~ 64 processors, but petascale machine will have 500K processors!
  – Serious work to do on scaling, dynamic loadbalancing, fault tolerance, software environments, debugging tools

• Consider novel ways to break up jobs
  – Farming off non-parallelizable analysis tasks, viz, coupling codes, spawning, integrating with data analysis
  – Consider petascale machine as your grid!

• Handling all the data: storing, retrieving, visualizing, analyzing. Lambda provisioning for steering, migration, viz

• Parameter space! Metadata to describe $10^6+$ simulations
Ideas Apply to Coastal Modeling

- Event driven computing: GWs detected, hurricane coming, etc!
- Respond to data, observation, computational resources: DDDAS
  - Use computer simulations to model winds and water: surge and waves, farm on grid, couple models, data acquisition, ensembles, invoke new algorithms
- Need to have lots of CPUs ready to go!
- Where should we evacuate? Where should we rebuild?

W. Benger, S. Venkataraman
Lessons Learned for Future

• Be creative: “Imagination is more important than knowledge.” Albert E.

• Petascale machines
  – 500K processors is a universe unto itself
  – Consider not just scaling, but code-coupling, spawning, data integration, DDDAS ideas

• Abstractions are critical for
  – application scientists, computer scientists
  – collaborations

• Scientists, hardware, software, technology groups need to work together
Summary

• Einstein’s impact on HPC, computational science is huge!
  – Will be for years

• Numerical relativity has reached a new stage of maturity
  – Where CFD was decades ago
  – New era: Suddenly many groups capable of solving EEs!
    – Sharing software

• Many new challenges in grids
  – LSU at forefront
  – Opportunities to work in projects

• Look forward to tackling them with you!
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Thanks

- NCSA & environs
  - Larry Smarr, Paul Walker, Joan Massó, John Shalf, Wai-Mo Suen (WashU), Ian Foster (ANL/UC)

- AEI, ZIB, RZG
  - Gabrielle Allen, Werner Benger, Thomas Drahlitsch, Tom Goodale, Ralf Kaehler, Hartmut Kaiser, Ian Kelley, Thomas Radke, Gerd Lanfermann, Andre Merzky, Bernard Schutz, Oliver Wehrens, Michael Russell, Jason Novotny, Christian Ott, many others...

- GridLab
  - Jarek Nabrzyski, Giovanni Aloisio, Peter Kacsuk, Thilo Kielmann, Ludek Matyska, Alexander Reinefeld, Ian Taylor...

- LSU
  - CCT family (esp. Peter Diener, Erik Schnetter), Gov. Blanco

- NSF, DOE, DFN-Verein, EU, MPG, DFG

- Microsoft, Intel, SGI, Cisco, IBM, Sun, HP