Scientific Computing Group

Presented by

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Scientific Computing
National Center for Computational Sciences

Scientific Computing

Scientific Computing facilitates the delivery of leadership science by partnering with users to effectively utilize computational science, visualization, and work flow technologies on LCF resources to

Port, tune, augment, and develop current and future applications at scale	Provide visualizations to present scientific results and augment discovery processes	Automate the scientific computational method

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Deputy Project Director

K. Boudwin

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K. Dempsey

Hardware Acquisition
A. Bland*

Test and Acceptance Development
S. Canon

Commissioning
A. Baker

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Project R&D
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Cray Project Director
K. Kafka[4]

LCF System Architect

S. Poole

Chief Technology Officer

A. Geist

Cray Supercomputing Center for Excellence

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D. Kiefer[4]
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Scientific Computing

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M. Henley
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D. Levy[5]
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B. Whitten
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High-Performance Computing Operations

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[#]Technical Coordinator

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Visualization and data analytics

Visualization

Once users have completed their runs, the Visualization task group helps them make sense of the sometimes overwhelming amount of information they generate.

- Viewing at a 30′ x 8′ PowerWall
- Cluster with GPUs for remote visualization

End-to-End Solutions

Researchers must analyze, organize, and transfer an enormous quantity of data. The End-to-End task group streamlines the work flow for system users so that their time is not eaten up by slow and repetitive chores.

- Automate routine activities, e.g., job monitoring at multiple sites

Oak Ridge National Laboratory

Scientific computing user support model

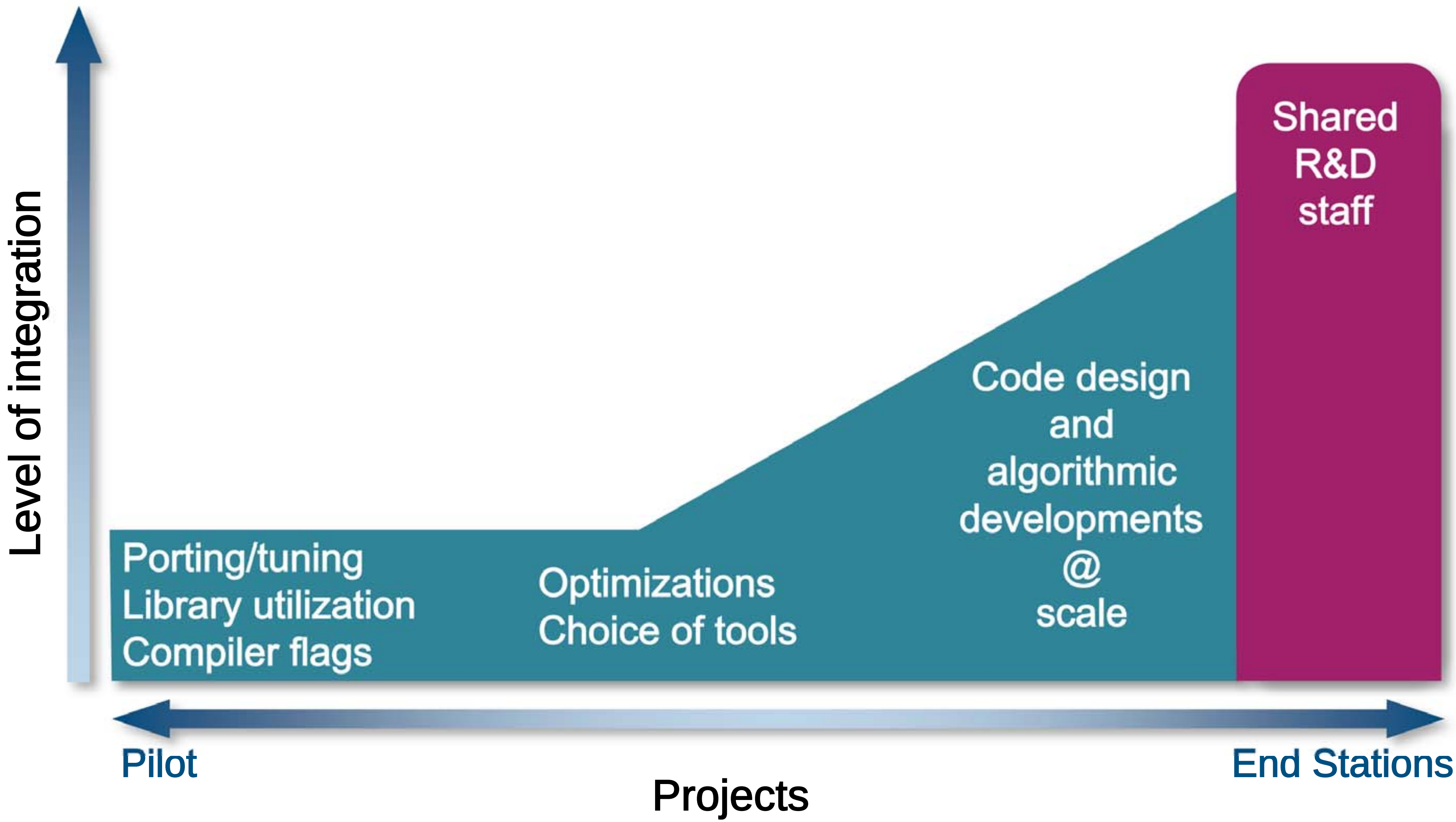
- “Whatever it takes” is the motto.
- Share expertise in algorithms and application-development strategies.
- Provide porting, tuning, optimization.
- Help users in running applications, using application development tools and libraries.
- Ensure application readiness by partnering with users to develop current next-generation applications.
- Represent users’ needs in LCF planning and reporting exercises:
  - application requirements,
  - scientific progress and highlights,
  - issues with current resources.

Expertise

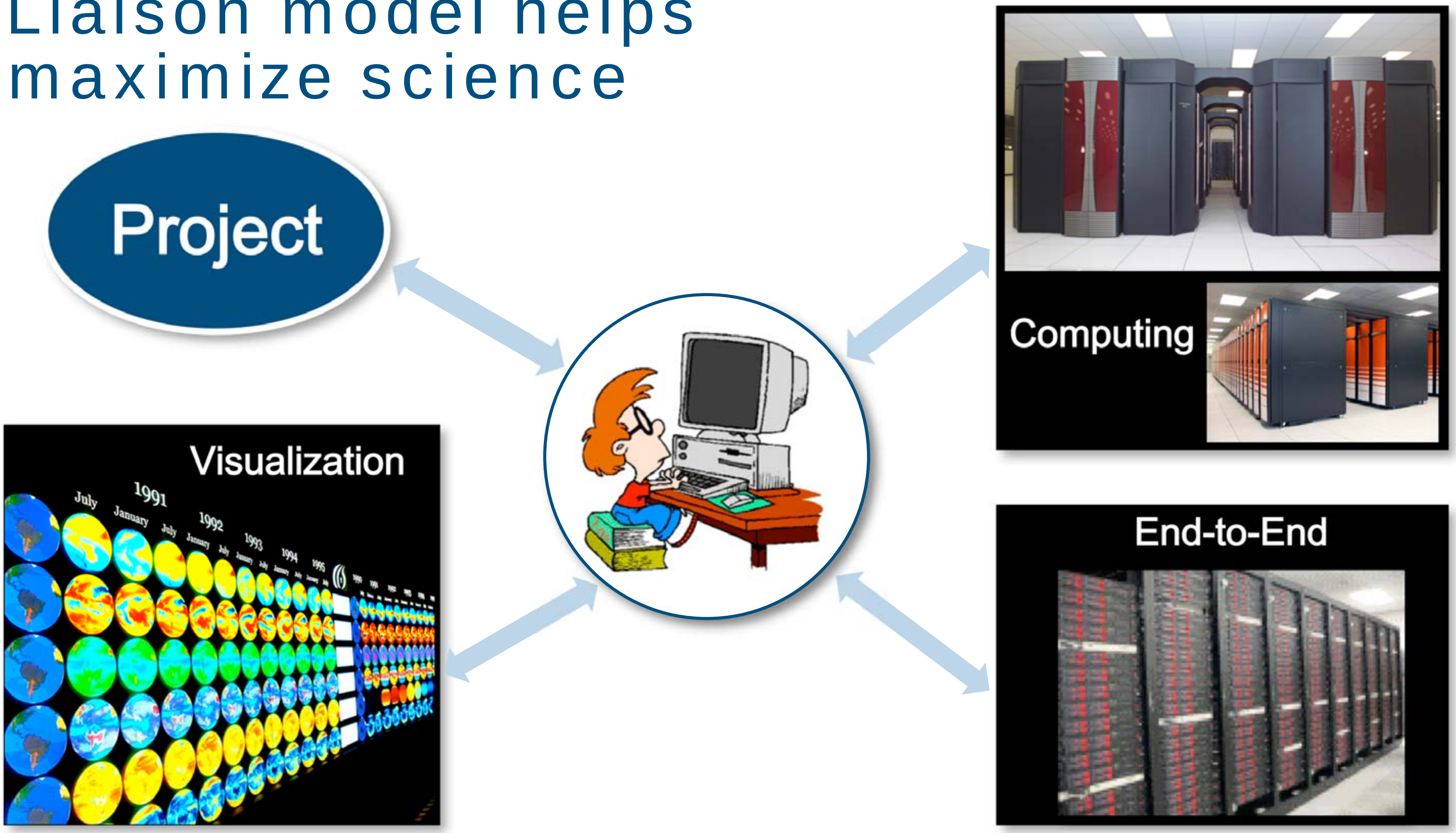
The LCF provides experts in user support, including Ph.D.-level liaisons from fields such as chemistry, climate, physics, astrophysics, mathematics, numerical analysis, and computer science—who are also experts in developing code and optimizing it for the LCF systems.

Large projects are assigned liaisons to maximize opportunities for success on the leadership computing resources.

Partnership with projects on LCF resources



Liaison model helps maximize science

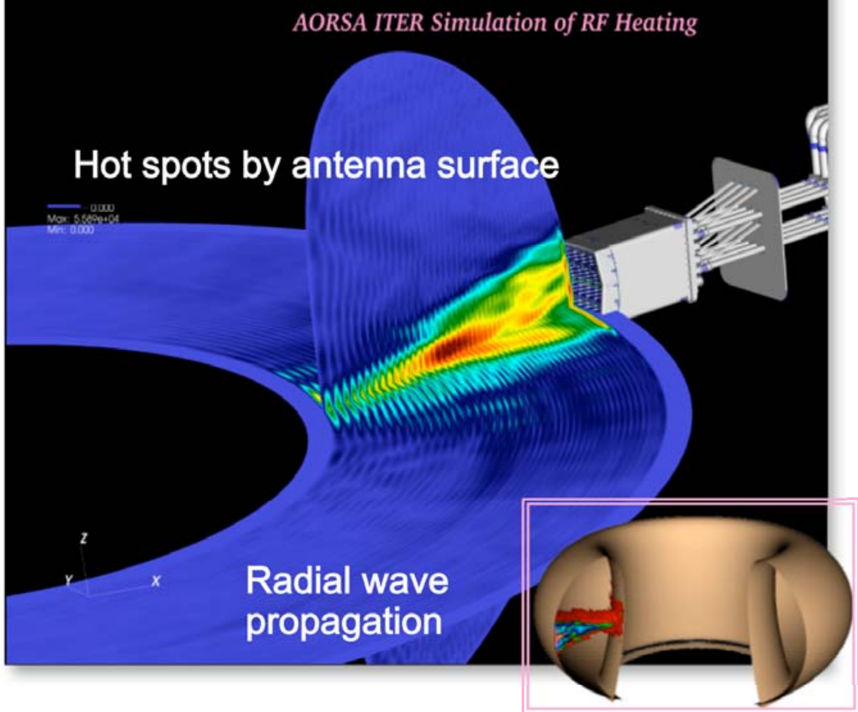


Whatever It Takes!

Producing new insights for RF heating of ITER plasmas

Fully 3-dimensional simulations of plasma shed new light on the behavior of superheated ionic gas in the multibillion-dollar ITER fusion reactor.

"Until recently, we were limited to two-dimensional simulations. The larger computer [Jaguar] has allowed us to achieve three-dimensional images and validate the code with observations." – Fred Jaeger, ORNL



- 3D simulations reveal new insights:
  - "hot spots" near antenna surface,
  - "parasitic" draining of heat to the plasma surface in smaller reactors.
- Work pushing the boundaries of the system (22,500 processor cores, 87.5 TF) and demonstrating
  - radial wave propagation and rapid absorption,
  - efficient plasma heating.
- AORSA's predictive capability can be coupled with Jaguar power to enhance fusion reactor design and operation for an unlimited clean energy source.

LCF liaison contributions

- Converted HPL from double real to double complex and replaced Scalapack
  - 45 TF to 75 TF!
- Acquired new version of BLAS from TACC
  - 75 TF to 87 TF!
- Net performance gain of almost a factor of 2

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Climate scientists on cloud 9 (or 3.5)

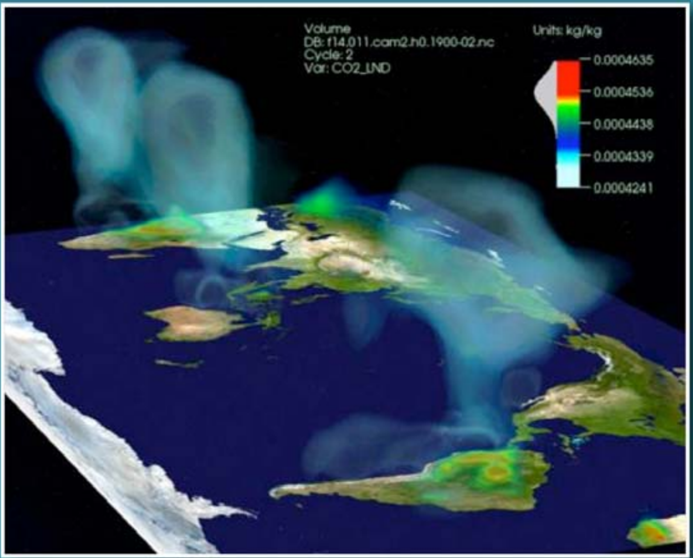
- **First-ever control runs of CCSM 3.5 at groundbreaking speed**

  "[On Jaguar,] we got 100-year runs in 3 days. This was a significant upgrade of how we do science with this model. Forty years per day was out of our dreams."– *Peter Gent of NCAR, Chairman of CCSM Scientific Steering Committee, during keynote address at CCSM Workshop, June 19, 2007*

- **Major improvements in CCSM 3.5**
  - Arctic and Antarctic sea ice: Will the Arctic be ice free in summer of 2050?
  - Surface hydrology of land, critical for predictions of drought

- **Positioned to test full carbon-nitrogen cycle**

Simulated time evolution of the atmospheric CO_2 concentration originating from the land's surface



"The most impressive new result in 10 years." – Peter Gent, NCAR, on El Ninõ/Southern Oscillation

LCF liaison contributions

- New preconditioner for barotropic solver
- Visualization of CO_2 transport
- Contributed bug fixes to POP 2.0
- Represented needs at OBER/ESNET meeting

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Turning vehicle exhaust into power

Researchers simulate materials that turn heat into electricity

- Waste heat claims 60% of the energy generated by an automobile engine.
- Team led by Jihui Yang of General Motors simulates materials that turn that heat into electricity.
- General Motors, largest-ever simulation—1,000-plus atom supercell—made possible by NCCS leadership computing resources.
- Exploring thermodynamic properties of promising lead-tellurium-based material.

"Only at a place like the LCF can such an expensive calculation be done. We're very lucky that LCF has been very supportive."

– *Jihui Yang, General Motors*

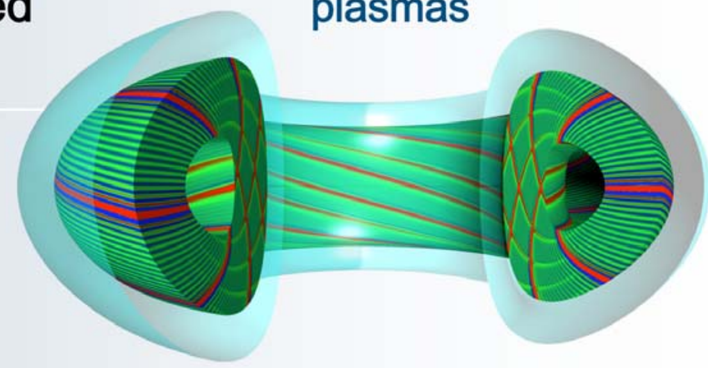
LCF liaison contributions

- Forged new relationships with DOE/EERE Program Office
- Pointed GM researchers to more scalable and capable version of VASP ab initio code

Finding the right balance of plasma turbulence for fusion energy

Plasma creates energy when hydrogen atoms collide	• Resulting high-energy alpha particles heat the plasma, but can be ejected by turbulence of the gas.
Turbulence is necessary for a tokamak reactor	• The GYRO code computes "optimal turbulence," finding the perfect balance of heat and alpha-particle production and loss.
LCF liaison contributions	• Doubled performance of GYRO application on Cray X1E. • More effective use of MPI communication; bug finds and fixes. • Imported new sparse solver for decreased memory size and B/W requirements.

Cutting-edge research explores tokamak plasmas



GENERAL ATOMICS

" I just want to repeat that Mark Fahey of ORNL has been a crucial person in this effort, especially for code optimization. He sees things we sometimes don't. I have nothing but great things to say about him."– *Jeff Candy, General Atomics*

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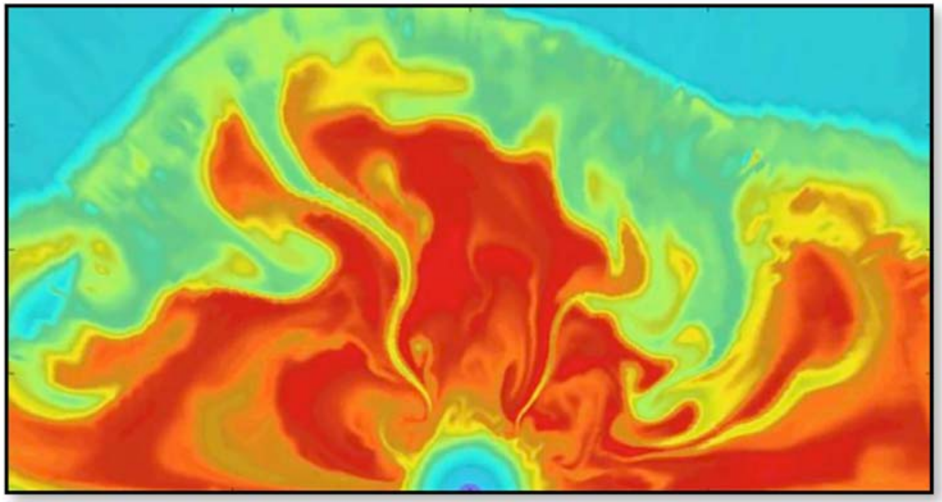
Discovering the elusive core-collapse supernova explosion mechanism

Researchers glean unprecedented insight into the shock waves that blow apart a 10- to 20-Solar-mass star.



The upgraded Jaguar allows researchers to double the time simulated to 0.8 second "post-bounce." Petascale systems will allow longer simulations. Tens of seconds after the explosion, heavy elements such as uranium are produced by the fiery storm of the supernova.

LCF liaison contributions

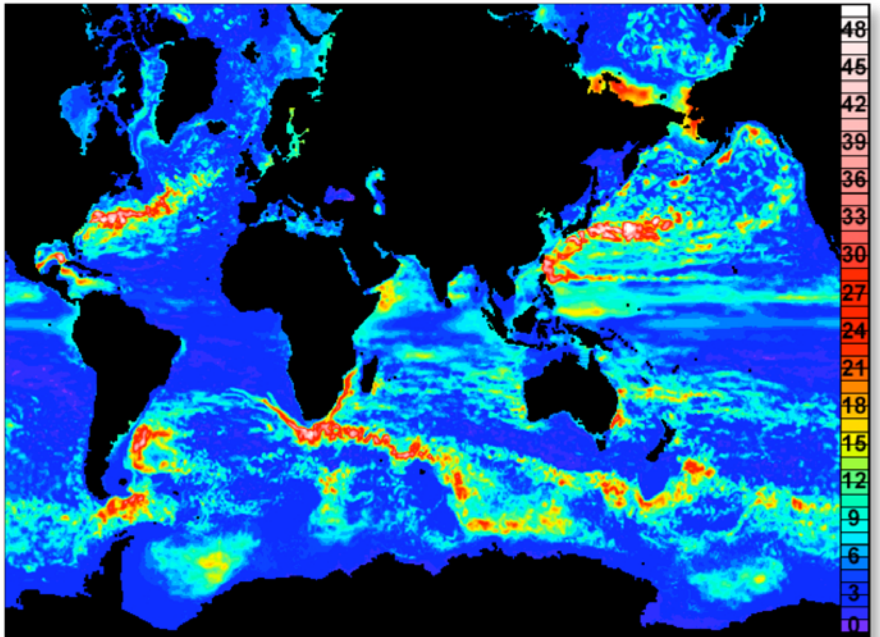
- Implementing efficient, collective I/O
- Pencil decomposition of 3D flow algorithm
- Preconditioning of the neutrino transport equation

- Investigators achieved longer run simulations and, 0.8 seconds after explosion, saw the initial shock wave revived by turbulence of infalling material.
- CHIMERA code to investigate multiple stellar models, the effects of both Newtonian and Einsteinian gravity, and the impact of recently discovered subatomic physics.
- Simulations achieved a 256 x 256 spatial mesh (2- to 4-fold increase over the state of the art).

High-fidelity modeling of ocean CO_2 uptake

Project looks into the fate of trapped heat and greenhouse gases

- First-ever 100-year simulation of the ocean at a fine enough scale to include the relatively small, circular currents known as eddies. Until recently researchers lacked the computing power to simulate eddies directly on a global scale.
- The most fine-grained, global-scale simulations ever of how the oceans work.
  - New knowledge of the currents and processes at work in the oceans.
  - Details of possible transport of gases and chemicals released into the ocean.



Simulation promises to increase understanding of the ocean's role in regulating climate, as a repository for greenhouse gases

LCF liaison contributions

- New preconditioner for barotropic solver
- Contributed bug fixes to POP 2.0; represented needs at OBER/ESNET meeting

Gaining understanding of cause and effect of core plasma turbulence

- A team led by Dr. W. W. Lee is using NCCS supercomputers to explore heat and particle loss in tokamak reactors.
- Tokamaks are doughnut-shaped devices that house the ionized gas responsible for sparking the fusion reaction necessary to produce the energy.
- Temperature must be regulated to create a proper environment for reactions.
- Device must be large enough to facilitate the reactions.
  - 2006 allocation: 2 million hours on Jaguar and 225,000 hours on Phoenix.
  - 2007 allocation: 6 million hours on Jaguar and 75,000 hours on Phoenix.

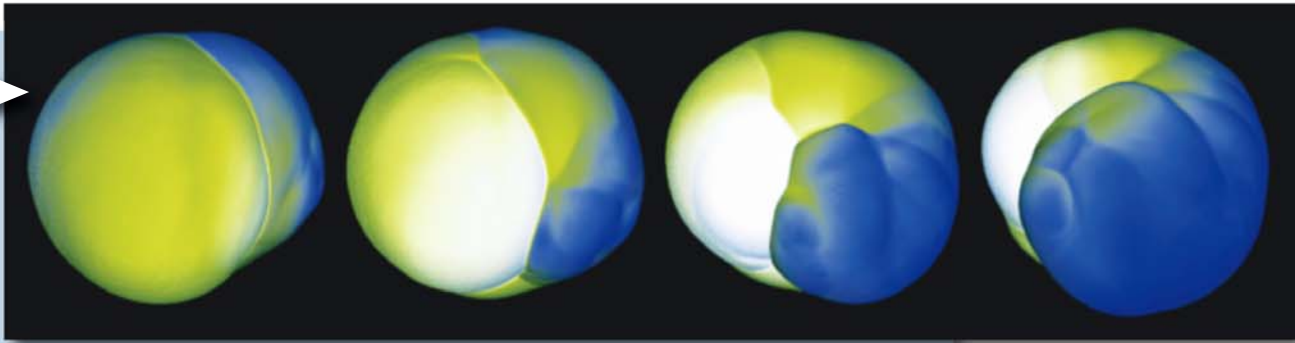
LCF liaison contributions

- Asynchronous I/O
- Automated end-to-end workflow
- Porting/scaling new shaped plasma version

Small eddies created by plasma turbulence in cross section along with the magnetic field lines threading the simulated tokamak

Researchers spin better pulsar explanation

- **Pulsars are left over from core-collapse supernovas.**
  - Conventional wisdom: Pulsar spin comes from the spin of the original star.
  - Better explanation: The core-collapse shockwave creates two rotating flows, with pulsar spin created by the inner flow.
  - Why it's better: It explains the range of observed pulsar spins, while the conventional wisdom explains only the fastest spins.
- **Three-dimensional simulations run on the Cray X1E (Phoenix).**
- Tony Mezzacappa, **ORNL, and** John Blondin, **North Carolina State, published their findings in the January 4, 2007 issue of *Nature*.**



This visualization shows the propagation of a stationary-accretion-shock-instability wave in a core-collapse supernova. The leading edge of a spiral flow near the surface of the supernova shock is marked by the blue area in the figure. It is accompanied by a second flow spinning in the opposite direction underneath. This second spinning flow is responsible for imparting the pulsar spin, according to three-dimensional simulations performed at Oak Ridge National Laboratory.

Image Courtesy of John Blondin

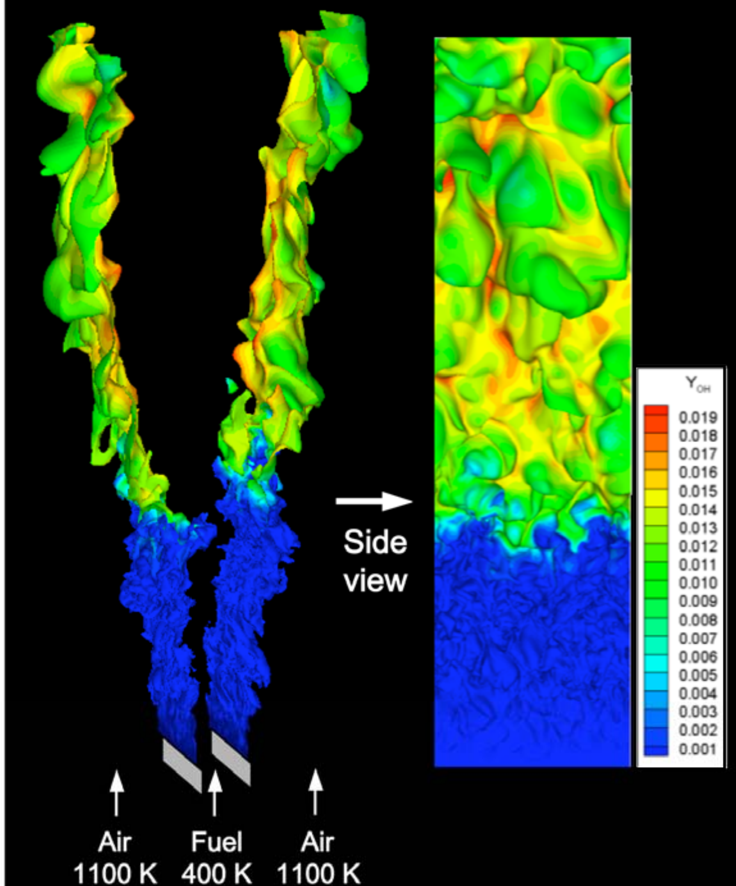
OAK RIDGE National Laboratory

New results in flame stabilization in an auto-ignitive jet

- First fully resolved simulation of a 3D lifted flame in heated co-flow with detailed chemistry.
- Lifted flames occur in diesel engines and gas turbine combustors.
  - Flame stabilized against fuel jet and recirculating hot gases.
- Direct numerical simulation of a lifted flame in heated co-flow:
  - ~1 billion grid points and 14 degrees of freedom per grid point,
  - H_2/air detailed chemistry,
  - jet Reynolds number = 11,000,
  - largest DNS at the highest Reynolds number,
  - 2.5 M hours on Jaguar at the LCF.
- Simulation reveals source of stabilization:
  - upstream auto-ignition,
  - vorticity generation at flame base due to baroclinic torque.

LCF liaison contributions
- Cray X1E loop vectorization of S3D
- Identified and fixed X1E MPI bottleneck
- Lagrangian tracers; I/O rework with NW University
- Jaguar scaling studies helped to identify processors burdened by memory corrections

Instantaneous OH radical concentration on a stoichiometric mixture fraction iso-surface shows flame liftoff



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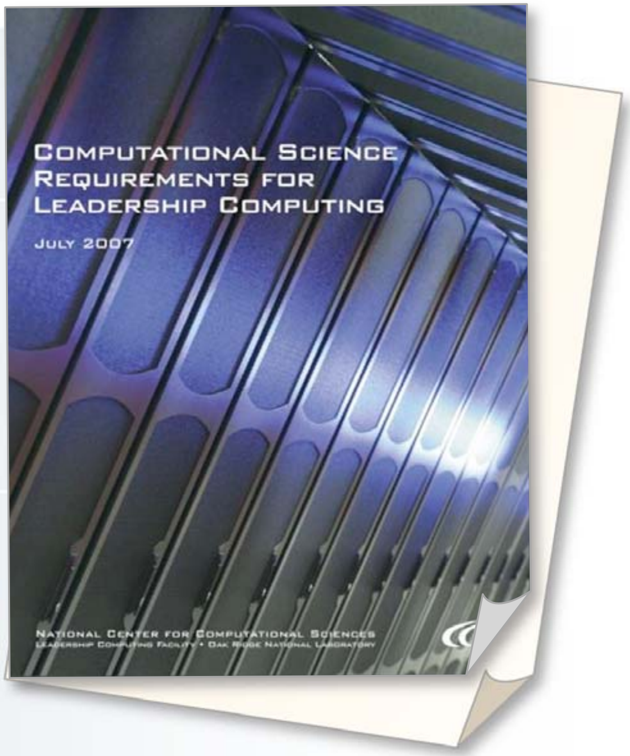
Preparing for the future

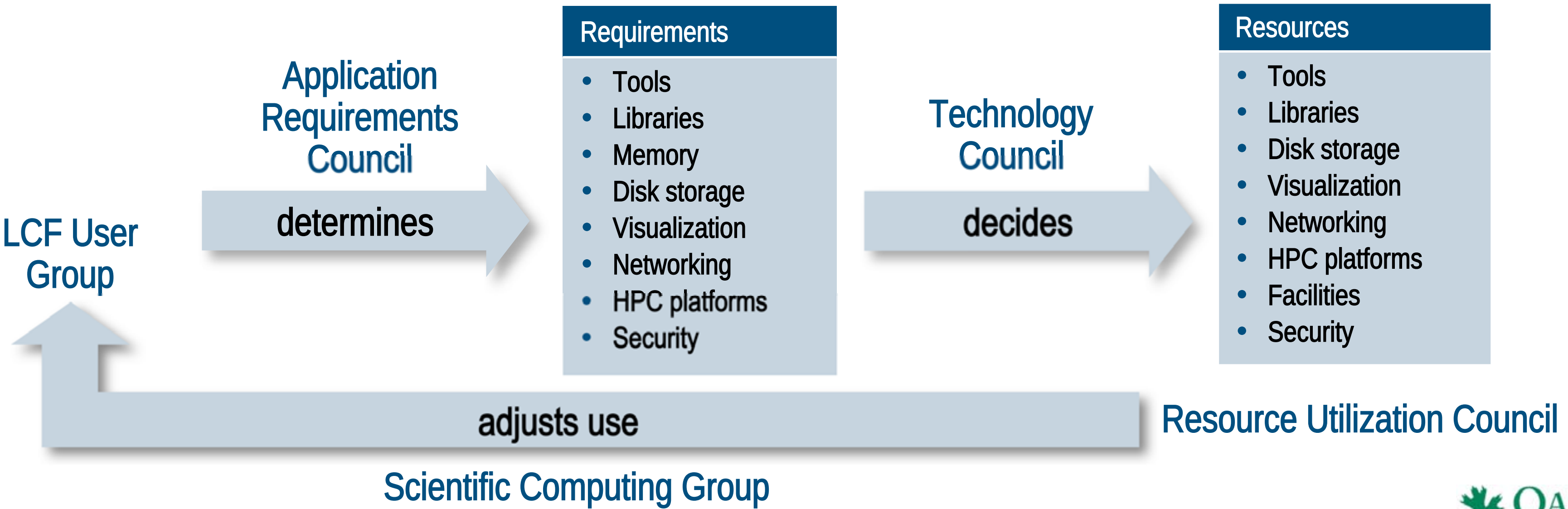
Application requirements: Process and actionable results

LCF Application Requirements Council (ARC)	• Stood up in 2006 • Established ARC charter and requirements management process
LCF elicits requirements in many ways	• INCITE proposals • Questionnaires devised by LCF staff • One-on-one interviews • Existing publications/documentation • Analyzing source code
Application categories analyzed	• Science motivation and impact • Science quality and productivity • Application models, algorithms, software • Application footprint on platform • Data management and analysis • Early access science-at-scale scenarios
Results	• First annual 100+ page application requirements document published: September 2007 • New methods for categorizing platforms and application attributes devised and utilized in analysis: guiding tactical infrastructure purchase and deployment • Best practice: Process being embraced and emulated by others



Innovation
Feedback loop for ensuring application readiness

Scientific Computing Group	Liaisons to application project teams
Application Requirements Council	Identification of application requirements
Technology Council	Decide how to best meet future application resource needs
Resource Utilization Council	Takes into account Science Team time constraints, e.g., upcoming meeting



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