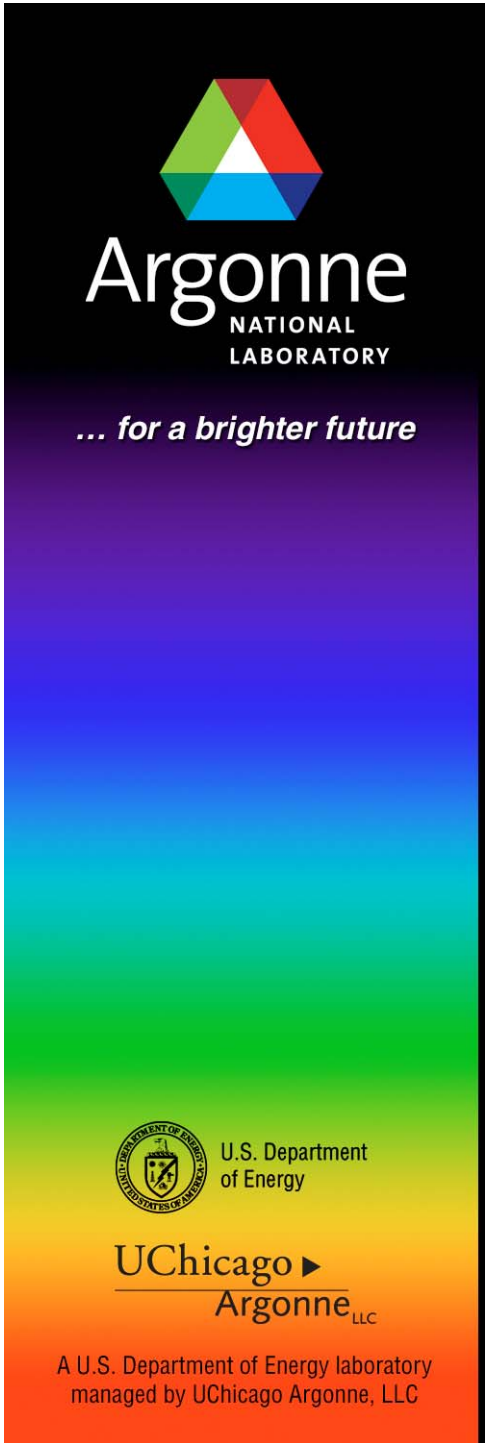


An Overview of High Performance - "Leadership" - Computing at Argonne National Laboratory

Robert Rosner

Laboratory Director

HPC Users Forum
Norfolk, VA

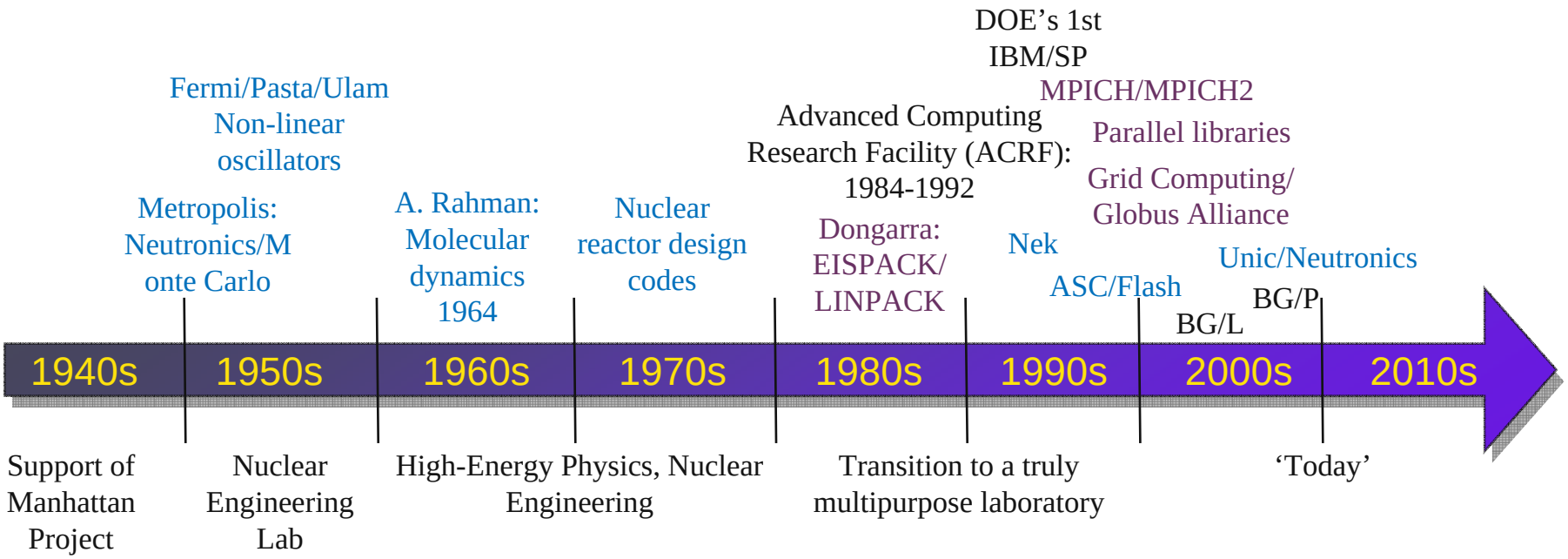
15 April 2008

QuickTime™ and a
decompressor
are needed to see this picture.

Outline

- Time line for computing at Argonne
- Status report: Argonne Leadership Computing Facility & IBM BG/P
- ‘Early science’ results from BG/L and BG/P …
- Where are we going - comments from a ‘user/provider’ perspective …

Argonne has been in HPC since its beginnings …



'The trouble with computers is you play with them . . . and it interferes completely with the work" - R. Feynman (1988)

ANL status report: Argonne Leadership Computing Facility: Part 1

- *Established 2006*
- *Dedicated to breakthrough science & engineering*

In 2004 DOE selected the ORNL, ANL and PNNL team based on a competitive peer review

- ORNL to deploy a series of Cray X-series systems
- ANL to deploy a series of IBM Blue Gene systems
- PNNL to contribute software technology

Blue Gene/P

2007-8 Blue Gene/P Installation

- 556 Teraflops computer
- 80 Terabytes of memory
- 8 Petabytes of disk storage
- 10,000 volume tape archive

ANL status report: Argonne Leadership Computing Facility & BG/P: Part 2

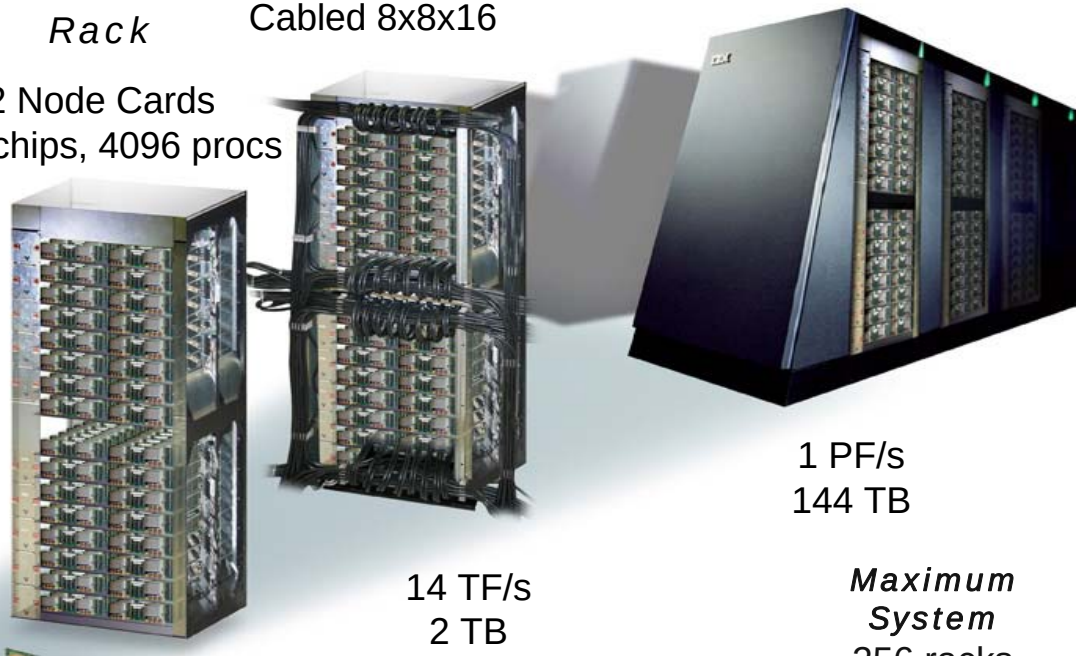
292,914 CPUs
Petaflops System
72 Racks

4,096 CPUs
Rack

Cabled 8x8x16

32 Node Cards
1024 chips, 4096 procs

1 petaflops =
1,000,000,000,000,000 (10^{15})
arithmetic operations per second



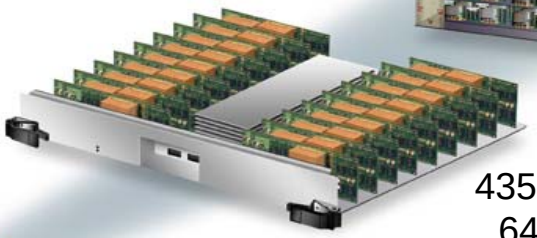
1 PF/s
144 TB

Node Card
(32 chips 4x4x2)
32 compute, 0-2 IO cards

14 TF/s
2 TB

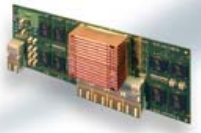
Maximum System
256 racks
3.5 PF/s
512 TB

Compute Card
1 chip, 20 DRAMs



435 GF/s
64 GB

Chip
4 processors



13.6 GF/s
2.0 GB DDR
Supports 4-way SMP

13.6 GF/s
8 MB EDRAM

Front End Node / Service Node
System p Servers
Linux SLES10

HPC SW:
Compilers
GPFS
ESSL
Loadleveler

Now: the Interim Supercomputer Support Facility (ISSF)
Coming soon: the Theory and Computational Sciences Building (TCB)

- ISSF:
  - Constructed to meet the interim needs of ALCF and future needs of ANL
  - 6000 SF within an existing high bay building
  - 2.5 MW Installed Power
  - 600 Tons Total Cooling Capacity
  - 300,000 CFM air volume
- TCB:
  - 3rd-party financed, construction starting next month (May), completion 2009
  - 200,000 ft^2 (30,000 ft^2 labs, 25,000 ft^2 computing)

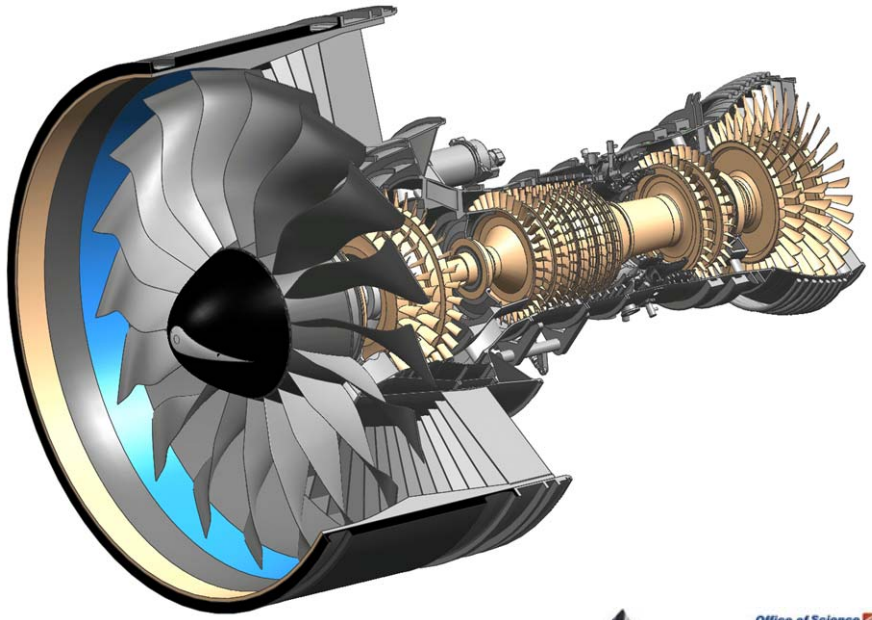
'Early science' results … a sampler

Early science results sampler: Reactive Hydrodynamics

High Fidelity Simulation of a Jet Engine Combustor

Peter Bradley, PI (Pratt & Whitney)

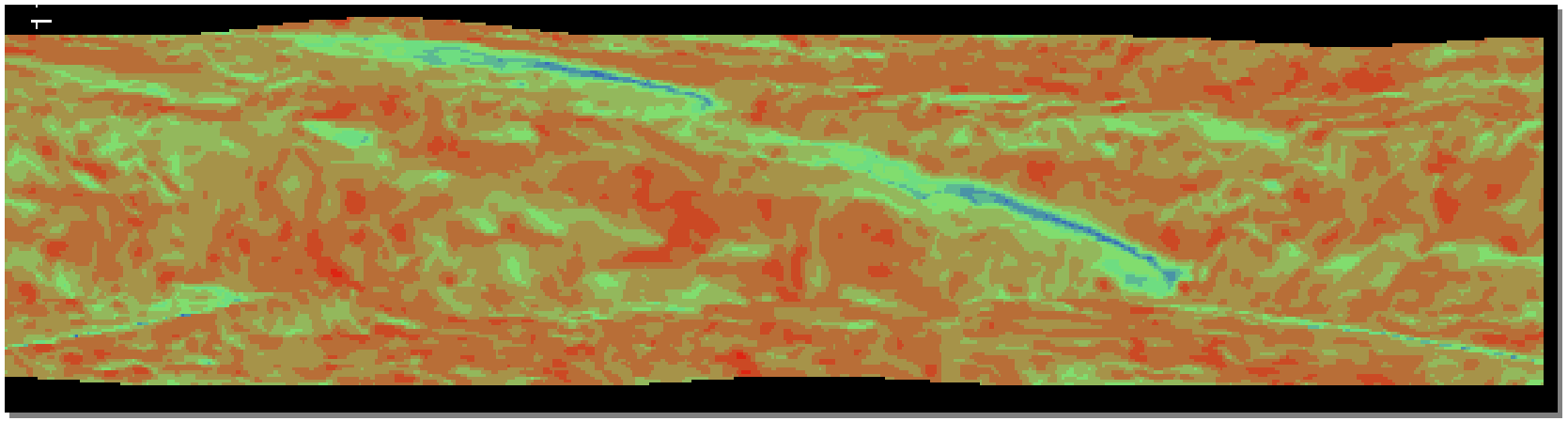
- **High-fidelity analysis of highly unsteady reacting flows**
  - **Critical to next-generation fuel efficiency, emissions**
  - **Develop scalable algorithms to enable rapid turnaround of traditionally long-running problems**
- **Leverage BlueGene to break (constructively) traditional design tools**
  - **Model**
  - **Grid partitioning**
  - **Solution**
  - **Visualization/interrogation**



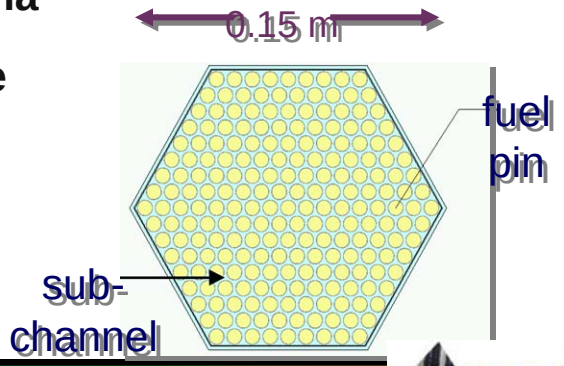
Early science results sampler: (Nuclear) Thermal Hydraulics

High-Resolution Fluid Dynamics and Heat Transfer

Paul Fischer (PI), Argonne National Laboratory



- **By recycling spent nuclear fuel, advanced burner reactors reduce nuclear waste in geological repositories by up to 100x.**
- **Large-scale numerical simulations of turbulent thermal transport in sodium-cooled reactor cores reveal thermal mixing phenomena**
- **Single-pin and 7-pin subassembly computations have identified key-flow features in interior and peripheral flows within wire-wrapped fuel bundles**
- **Bypass-flow peaks migrate around the perimeter of the subassembly and may influence uniform cooling**

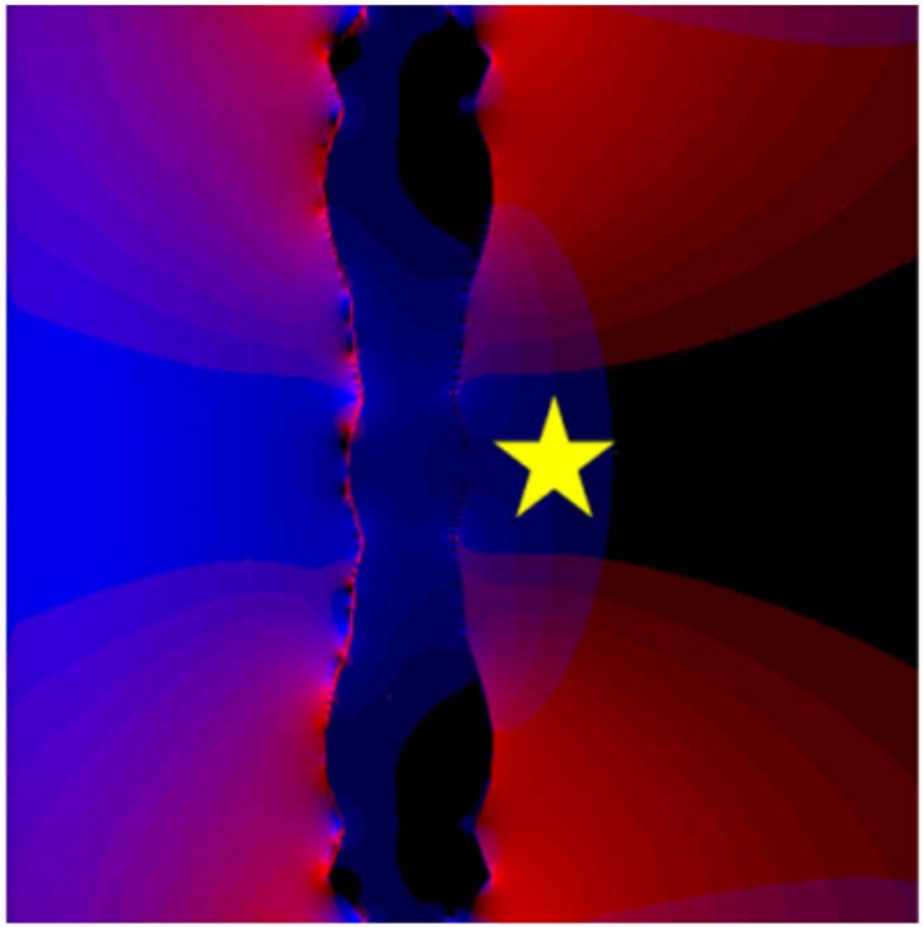


Early science results sampler: Simulations at the nanoscale

Numerical Approach Guides Light in the Nanoscale

Tamar Seideman (PI), Northwestern University

- Optimal control theory is applied as a numerical design tool to produce nanophotonics with desired functionalities.
- Applications range from novel sensors and medical diagnostics through sub-diffraction waveguides to tip-enhanced molecular spectroscopy and dynamics.
- Figure illustrates the design of a metallic ‘nano-lens’ by optimization of a metal slab to focus electromagnetic radiation to a pre-specified point (shown as a star on the output side).

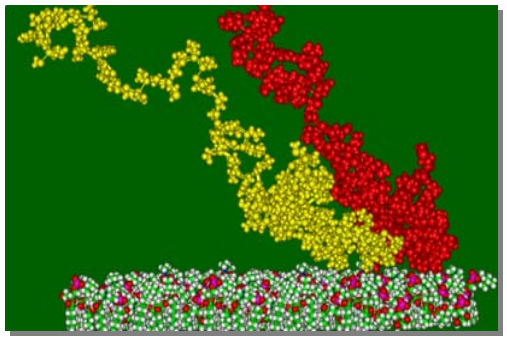


Early science results sampler: (Biological) molecular modeling

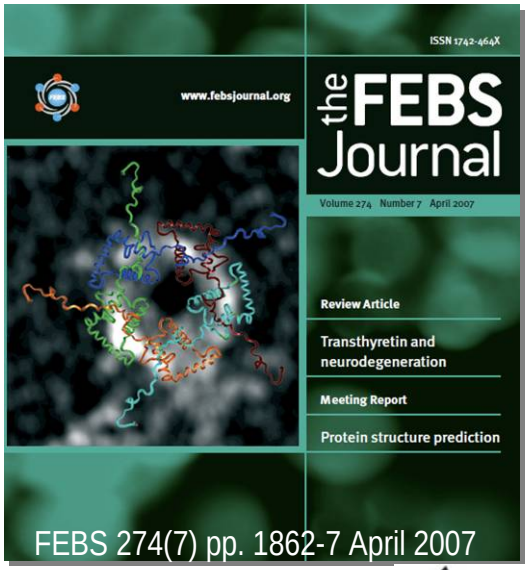
Modeling of Protofibril Structures Provides Insight into Molecular Basis of Parkinson's Disease

Igor Tsigelny (PI), UC San Diego

- Parkinson's Disease is the 2nd most common adult neurological disease
- Increased aggregation of *alpha-synuclein* protein is thought to lead to harmful pore-like structures in human membranes
- UCSD - SDSC team used molecular modeling and molecular dynamics simulations in combination with biochemical and ultrastructural analysis to show that *alpha-synuclein* can lead to the formation of pore-like structures on membranes
- Used NAMD and MAPAS on Blue Gene/L at ALCF and SDSC



alpha-synuclein forming a dimer (above) and a completed pentamer (below) attached to a membrane

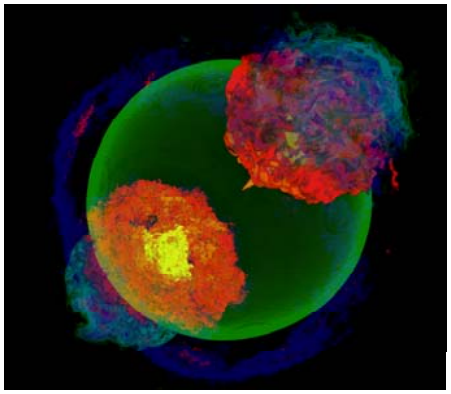


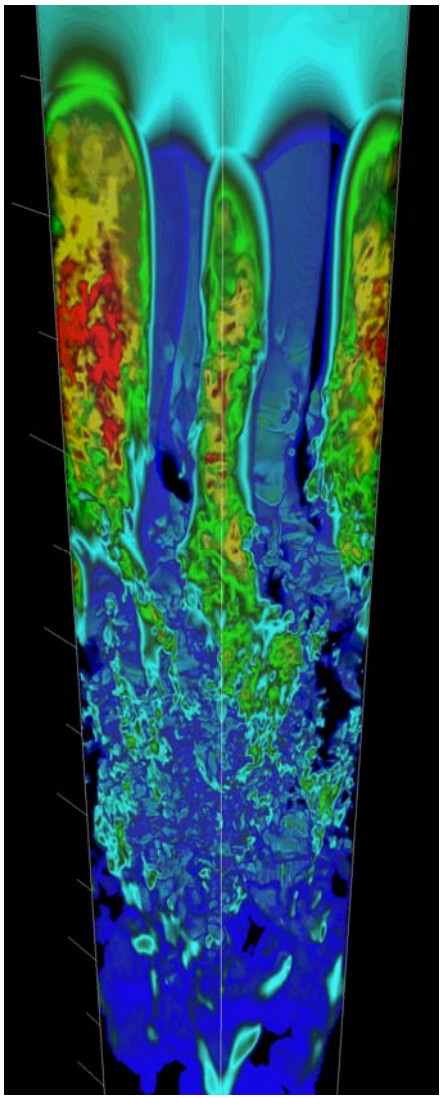
Early science results sampler: Nuclear astrophysics & CFD

Buoyancy-Driven Turbulent Nuclear Burning and Validation of Type Ia Supernovae

Don Lamb (PI), University of Chicago

- Type Ia Supernovae are the *standard candles* of the universe
- Observations of Type Ia SNe revealed the universe is accelerating and led to the discovery of dark energy
- FLASH is working on two of the major challenges in the Type Ia SNe field
  - Understanding of the key physical process
  - Furthering the limited simulations of the four primary models of Type Ia

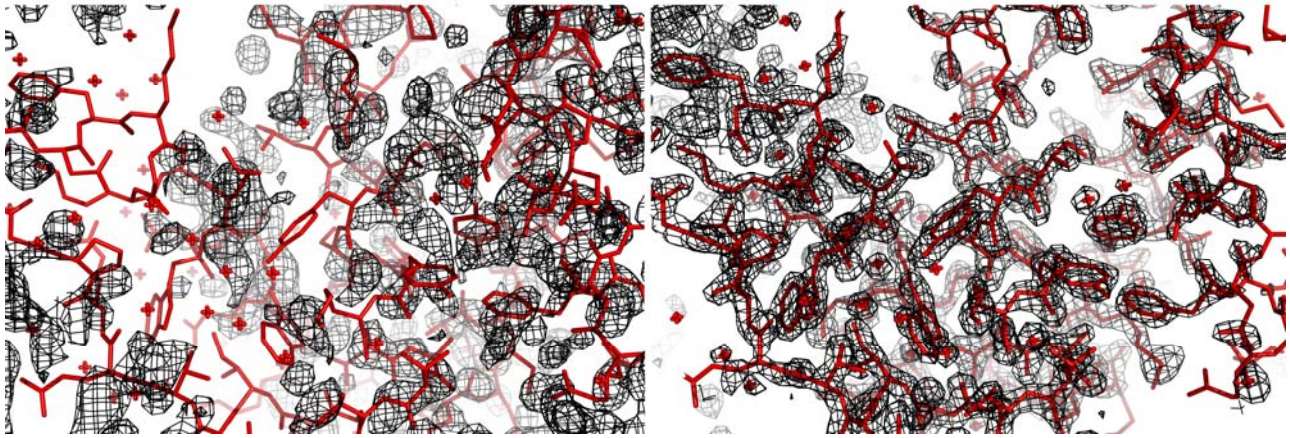


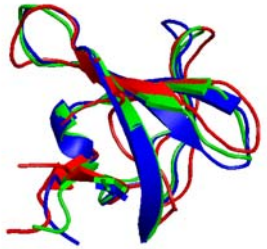


Early science results sampler: Biomolecules by design

High Resolution Protein Structure Prediction
David Baker (PI), University of Washington

- Goals:
  - Understand the structure and functionality of amino acids in a protein
  - Create new proteins by removing undesired functionality and replacing it with desired features
  - Design better drugs and new biological organisms by computationally engineering proteins with new functions





Blue : Native structure

Red : Starting low-resolution NMR model

Green : Rosetta prediction

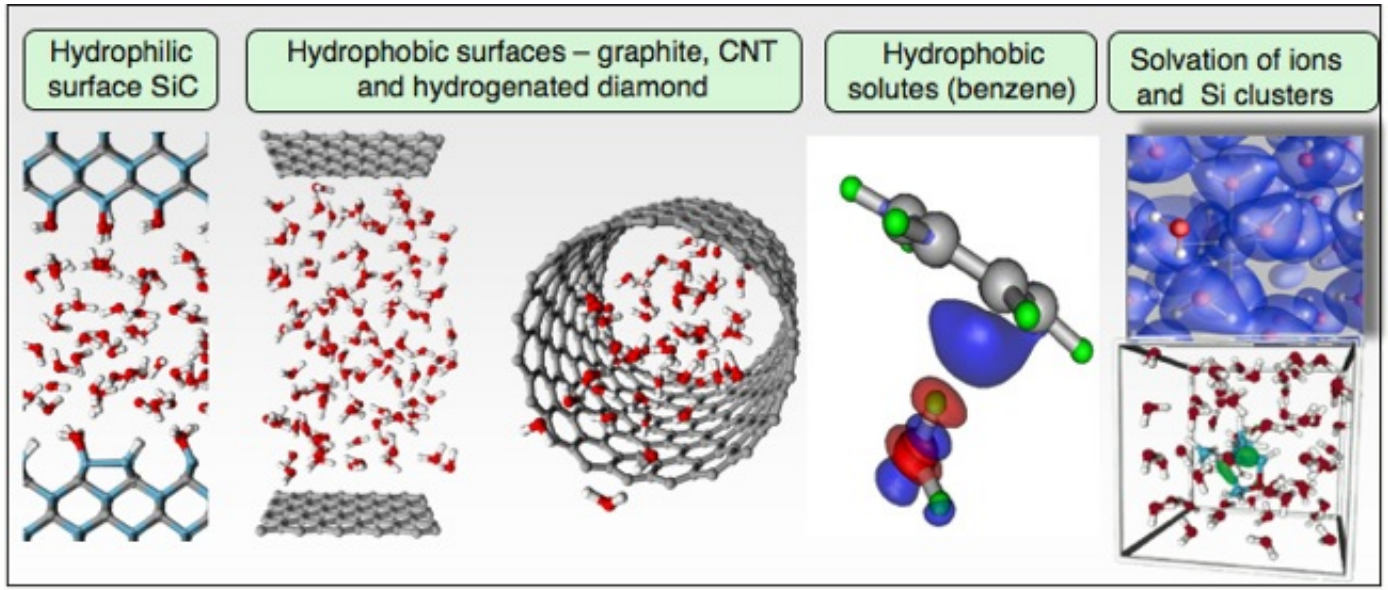
Electron density map generated from phases determined from the starting low-resolution model (left panel) and the map generated from phases determined from Rosetta refined model (right panel). The red model is the deposited native structure fitting the calculated density.

Early science results sampler: Materials by design

Computational Material Design with Nano-Building Blocks

Giuila Galli and Francois Gygi

- Advance the field of custom designed materials through the understanding how to control nanostructure assemblies
- Impact includes
  - protein folding
  - cell-membrane flow
  - materials in confined media
  - nanofluidic devices

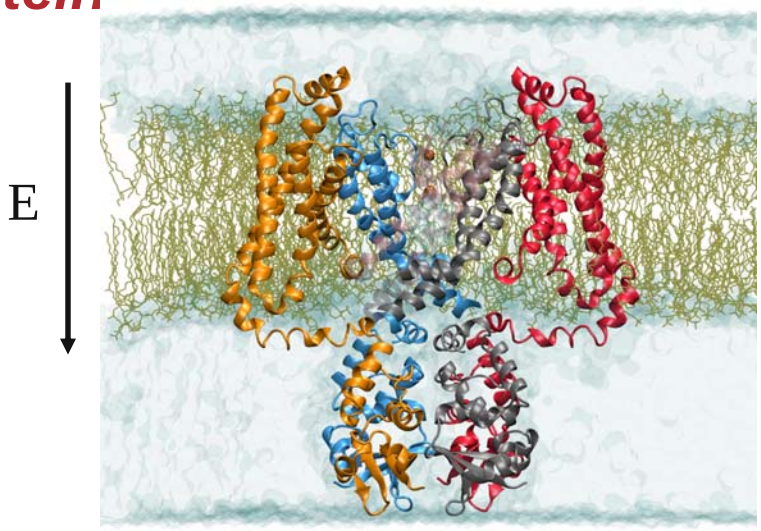


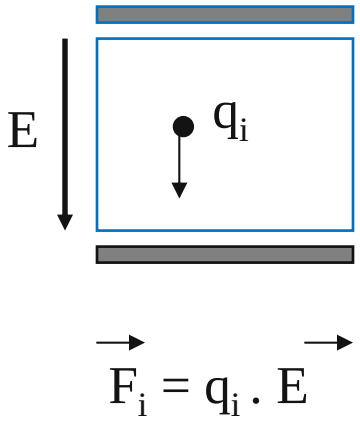
Early science results sampler: Modeling cells

Gating Mechanism of Membrane Proteins

Benoit Roux (PI), UofC/ANL

- The cell membrane represents the physical and functional boundary between living organisms and their environment.
- Membrane associated proteins play an essential role; truly "molecular machines"
- How is an external energy source, the membrane voltage, is converted into molecular motion
- Encode information-carrying physiological signals by a membrane protein





$$\vec{F}_i = q_i \cdot \vec{E}$$

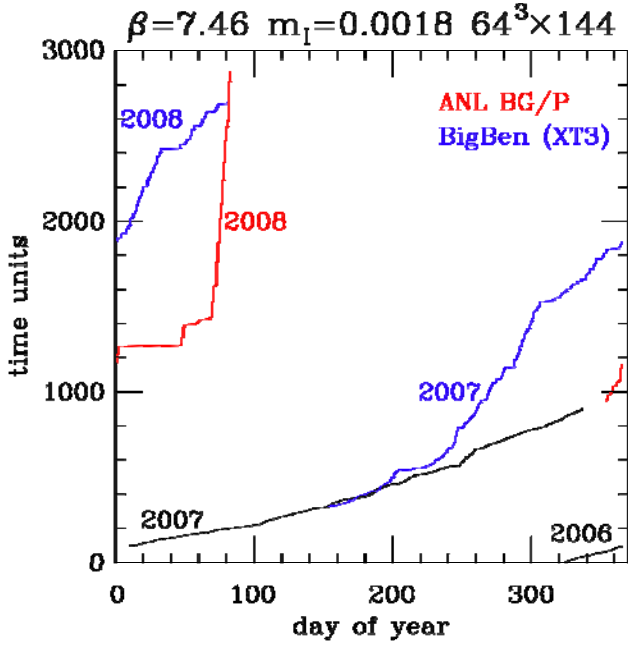
Early science results sampler: QCD by computer …

Lattice-QCD
Bob Sugar (PI), et al., USQCD

- Precisions tests of the fundamental theory of matter
- Calculate weak interaction matrix elements of strongly interacting particles to the accuracy needed to make precise test of the standard model
- Determine the properties of strongly interacting matter at high temperatures and densities, such as those that existed immediately after the Big Bang

Configuration Generation Plans

QCD Action	Lattice Spacing (Fermi)	m_l/m_s	Lattice Dimensions	Lattice Size (GB)	TF-Years
ASQTAD	0.060	0.10	$60^3 \times 144$	9.0	2.0
ASQTAD	0.045	0.20	$56^3 \times 192$	9.7	1.9
ASQTAD	0.045	0.10	$80^3 \times 192$	28.3	13.7
ASQTAD	0.060	0.05	$84^3 \times 144$	24.6	23.2
DWF	0.094	0.27	$32^3 \times 64$	0.6	1.2
DWF	0.094	0.19	$48^3 \times 64$	2.0	7.8
DWF	0.094	0.11	$48^3 \times 64$	2.0	25.2
CLOVER	0.100	0.22	$32^3 \times 128$	1.2	0.8
CLOVER	0.100	0.15	$40^3 \times 128$	2.4	4.1
CLOVER	0.080	0.18	$40^3 \times 128$	2.4	4.5
CLOVER	0.080	0.15	$48^3 \times 128$	4.1	22



The basic message …

- **BG/P works great!**
- **Come join us computing!**

Some final comments from a user/provider …

- Potential computing power is currently outpacing our algorithmic capabilities of exploiting this power
  - Relatively few application codes are currently able to take full advantage of the largest computing systems
  - But: building 'capable' codes is both demonstrably possible AND is not cheap
  - **Conclusion**: **SciDAC-type/ASC-type investments are sorely needed**
- The vastly increase in computer power over the past 5 years has led some disciplines to surmount a crucial barrier - transforming the discipline
  - In CFD, astrophysics and nuclear physics, it is now possible to carry out physically meaningful (= no longer 'toy') direct numerical simulations
    - *New generations of state-of-the-art thermal hydraulics/neutronics codes for reactor design; new coupled N-body/hydro/MHD cosmological evolution codes; new capabilities for nuclear structure codes; …*
  - In biology, metagenomics is no longer just a concept …
  - **Conclusion: Computing/simulation is proving to be transformative!**
- In other disciplines, this transition has not yet occurred - but is finally in sight (!!)
  - Example: Intelligent agent modeling of complex non-equilibrium economic systems that can be V&V'd (!!)

Which brings us to … questions and discussion