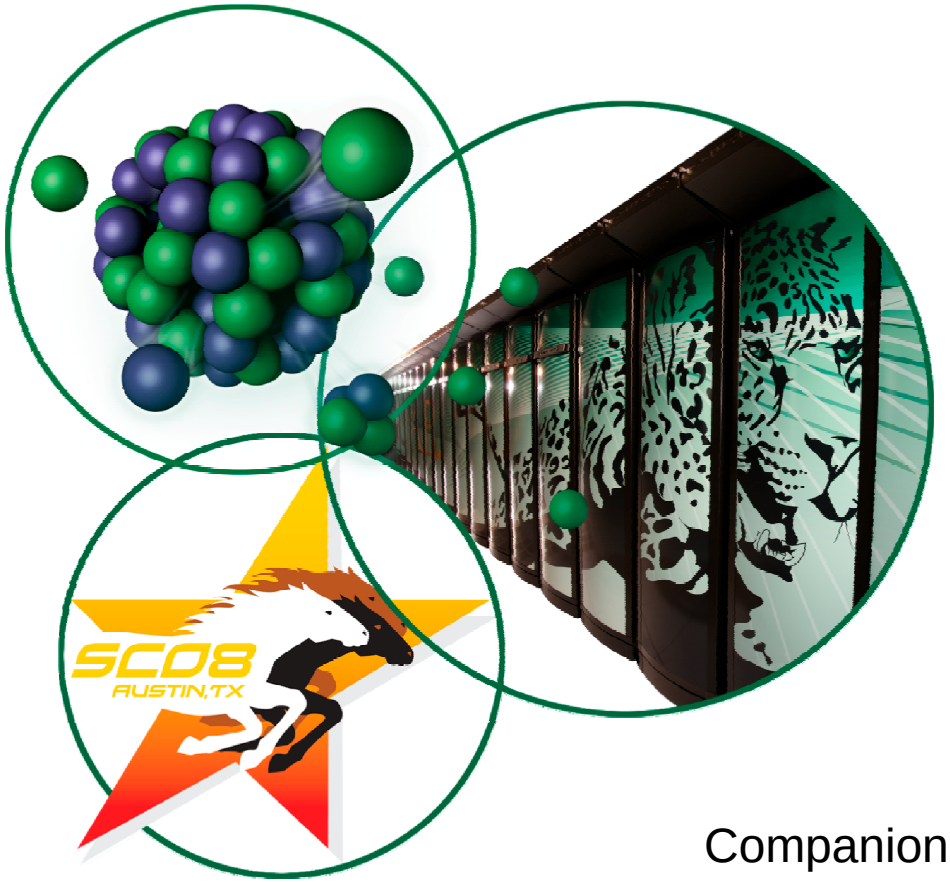
ORNL Leadership Computing Facility: Preparing for the Exascale



Presented by

Douglas B. Kothe

National Center for Computational Sciences

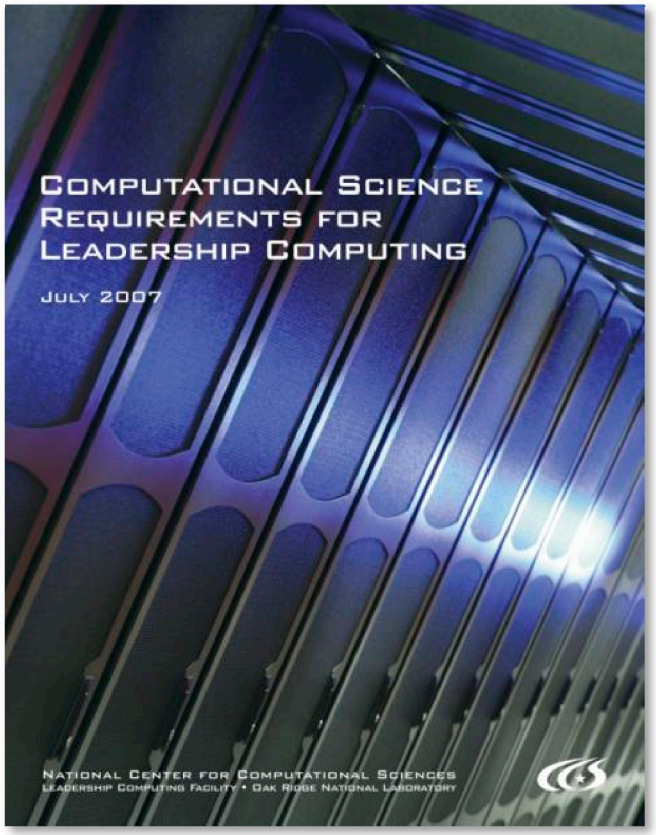
Companion presentations:

"Overview of Science at the ORNL Leadership Computing Facility"

"Breakthrough Science in the 2008 INCITE Program at ORNL"

Preparing for the petascale

LCF petascale applications document published in September 2007



- 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 used in analysis: guiding tactical infrastructure purchase and deployment
  - Best practice: Process being embraced and emulated by others

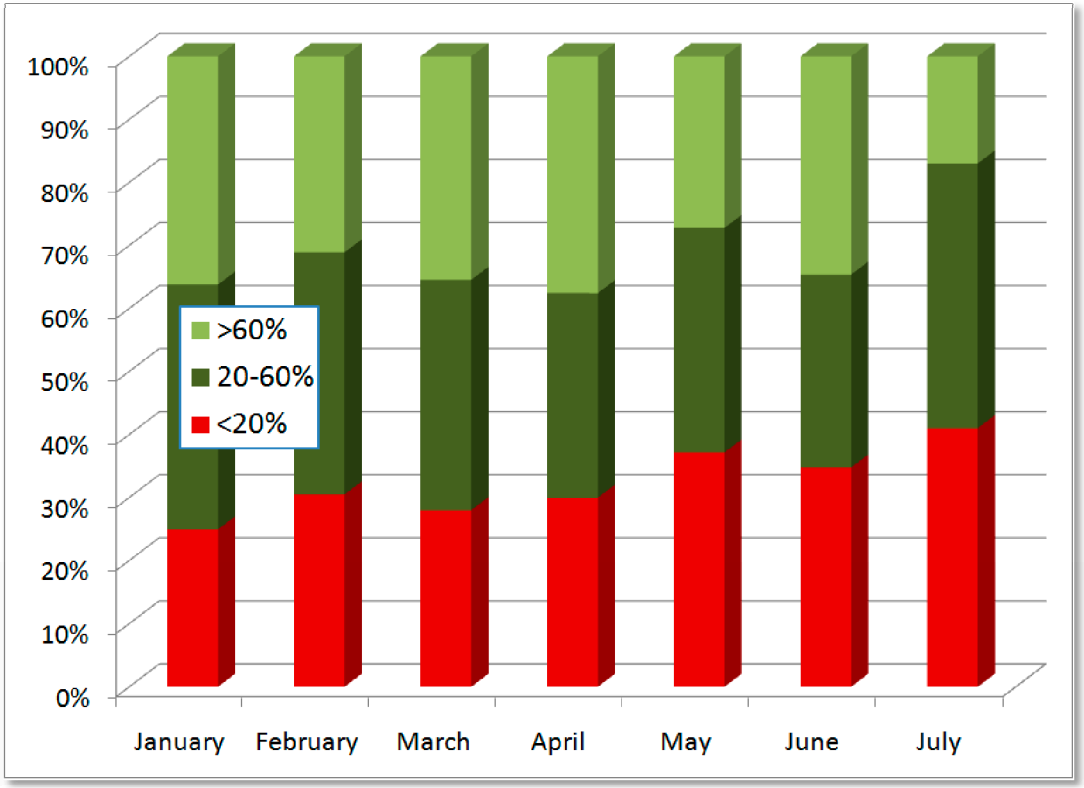
Capability usage

LCF goals

- **In the first year, 35% of the CPU time will be used by jobs using 20% or more of the available processors**
- **In subsequent years, 30% of the CPU time will be used by jobs using 30% or more of the available processors**

Jaguar is greatly exceeding this metric (everything above the red)

Jobs that use >60% (light green) (about 18,000 cores) account for about 30% of the total core-hours consumed



In 2007, Jaguar (dual-core) capability usage was 30% and rising. CY 2008 capability usage on Jaguar (quad-core) systems is 67%

Sample LCF INCITE application codes

Astrophysics	CHIMERA, GenASiS, 3DHFEOS, Hahndol, SNe, MPA-FT, SEDONA, MAESTRO, AstroGK, PKDGRAV2
Biology	NAMD, LAMMPS
Chemistry	CPMD, CP2K, MADNESS, NWChem, Parsec, Quantum Expresso, RMG, GAMESS
Nuclear Physics	ANGFMC, MFDn, NUCCOR, HFODD
Engineering	Fasel, S3D, Raptor, MFIX, Truchas, BCFD, CFL3D, OVERFLOW, MDOPT
High Energy Physics	CPS, Chroma, MILC
Fusion	AORSA, GYRO, GTC, XGC
Materials Science	VASP, LS3DF, DCA++, QMCPACK, RMG, WL-LSMS, WL-AMBER, QMC
Accelerator Physics	Omega3P, T3P
Atomic Physics	TDCC, RMPS, TDL
Space Physics	MK-FLUKSS
Climate and Geosciences	MITgcm, PFLOTRAN, POP, WRF, CCSM (CAM, CICE, CLM, POP)
Computer Science	Active Harmony, IPM, KOJAK, mpiP, PAPI, PMaC, Sca/LAPACK, SvPablo, TAU

LCF is executing its 250 TF transition to operations

An overview of the pioneering application codes selected		
CHIMERA	**Astrophysics**	Core-collapse supernova explosion mechanism
S3D	**Turbulent combustion**	Lifted flame stabilization in diesel and gas turbine engines
GTC	**Fusion**	Analyze and validate CTEM and ETG core turbulence
POP	**Global ocean circulation**	Eddy-resolved flow with biogeochemistry
DCA++	**High-temperature superconductivity**	Effect of charge and spin inhomogeneities in the Hubbard Model superconducting state
MADNESS	**Chemistry**	Neutron and X-ray spectra of cuprates; dynamics of few-electron systems; metal oxides surfaces in catalytic processes

LCF is executing its 250 TF transition to operations

We are carrying out an aggressive set of science-at-scale simulations

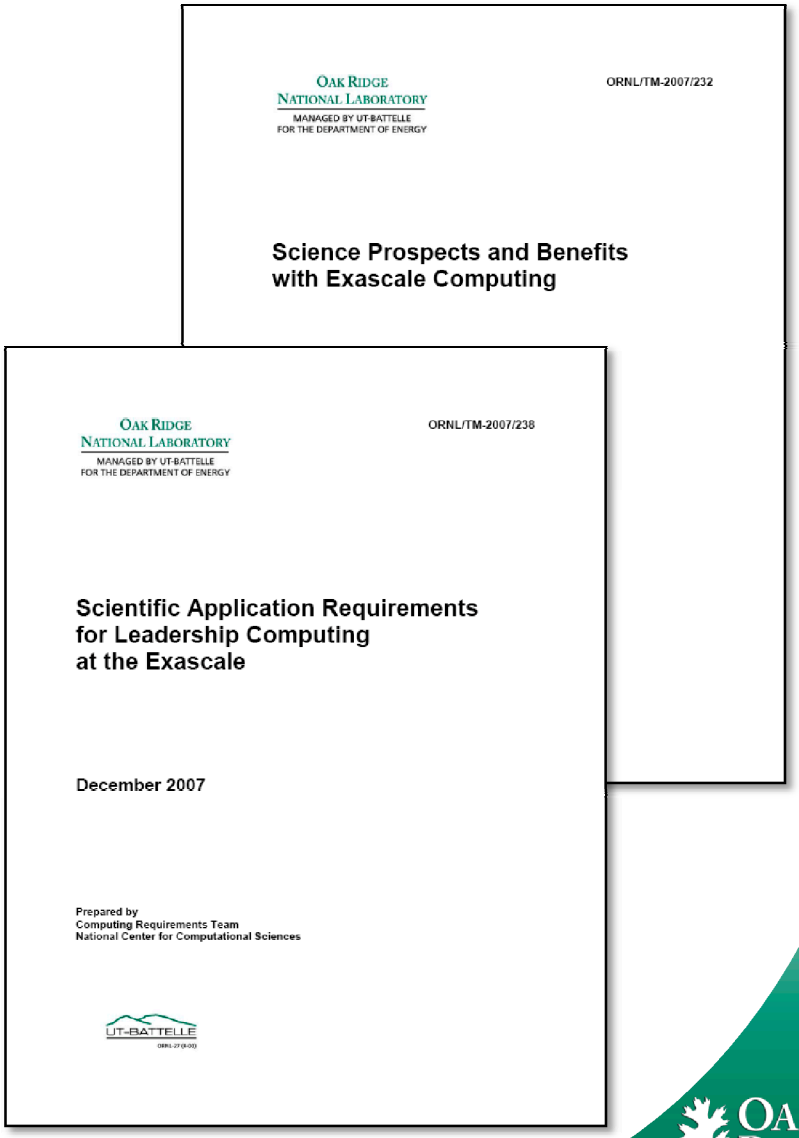
Code	Quad-Core Nodes	Global Memory Reqm (TB)	Wall-Clock Time Reqm (hours)	Number of Runs	Local Storage Reqms (TB)	Archival Storage Reqms (TB)	Resolution and Fidelity
CHIMERA	7824 4045	16 8	100 100	1 1	13	50	256×128×256 or 256×90×180 20 energy groups, 14 alpha nuclei
GTC-S GTC-C	3900 3900	40 60	36 36	2 2	350	550	600M grid points, 60B particles 400M grid points, 250B particles
S3D	7824	10	140	1	50	100	1B grid points, 15 μm grid spacing 4 ns time step, 23 transport vars
POP	2500	1	400	1	1	2	3600×2400×42 tripole grid (0.1°) 20-yr run; partial bottom cells; first with biogeochemistry at this scale
MADNESS	7824	48	12 2	10 12	5	50	600B coefficients
DCA++	2000 6000	16 48	12 to 24	20	1	1	Lattices of 16 to 32 sites 80 to 120 time slices $O(10^2–10^3)$ disorder realizations

- **Weekly (Saturday) full-system simulations with goal of 27M hours consumed by end of year**
- **12.5M hours utilized YTD with average job size of 20.9K cores**
- **59% of usage has been at >30K cores**
- **Over 70 TB of data generated to date**

Preparing for the exascale

Long-term science drivers and requirements published in December 2007

- **The LCF surveyed, analyzed, and documented the science drivers and application requirements envisioned for exascale leadership systems in the 2020 timeframe**
- **These studies help to**
  - **Provide a roadmap for the ORNL Leadership Computing Facility**
  - **Uncover application needs and requirements**
  - **Focus our efforts on those disruptive technologies and research areas in need of our and the HPC community's attention**


OAK RIDGE NATIONAL LABORATORY
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Science Prospects and Benefits with Exascale Computing

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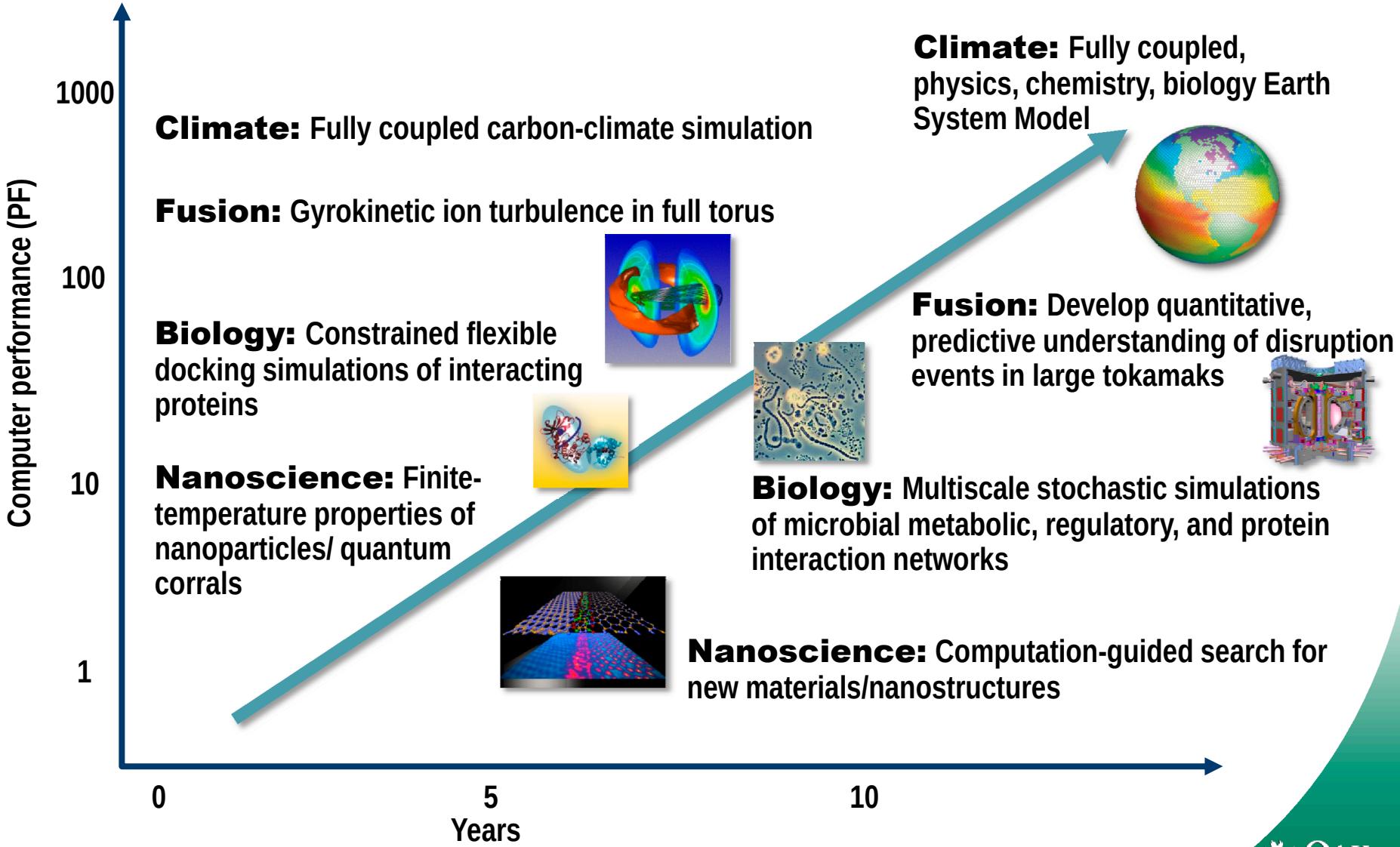
Scientific Application Requirements for Leadership Computing at the Exascale

December 2007

Prepared by
Computing Requirements Team
National Center for Computational Sciences

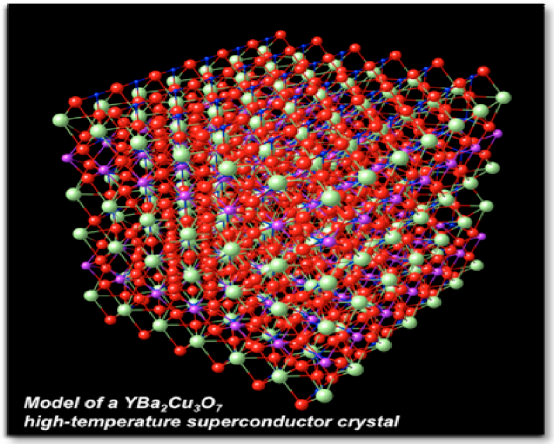
UT-BATTELLE

Science advances over the next decade require leadership computing

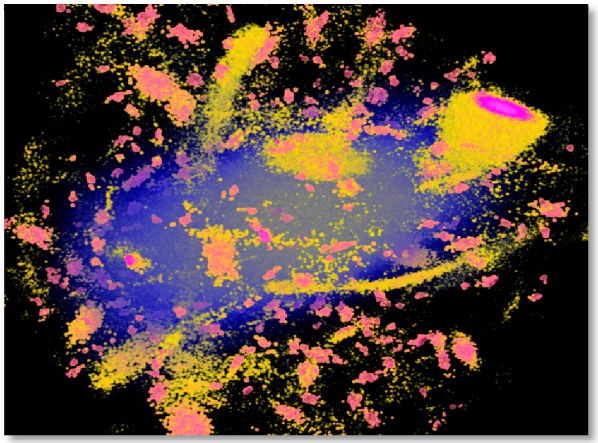


Advancing scientific discovery

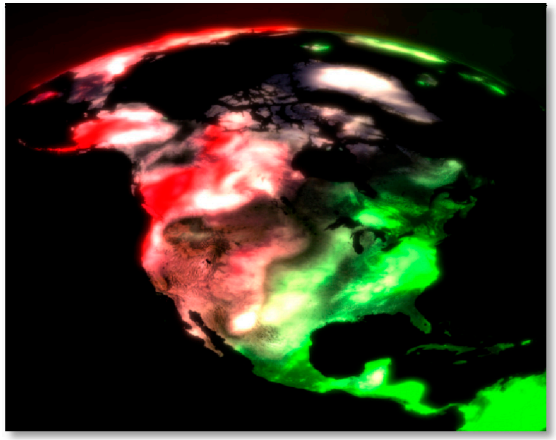
Five of the top 10 ASCR science accomplishments over the past 18 months used ORNL LCF resources and staff



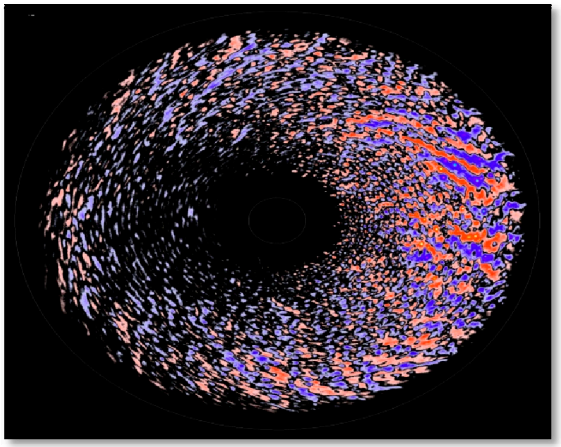
Electron pairing in HTC cuprates*
The 2D Hubbard Model emits a superconducting state for cuprates and exhibits an electron pairing mechanism most likely caused by spin-fluctuation exchange. *PRL* (2007, 2008)



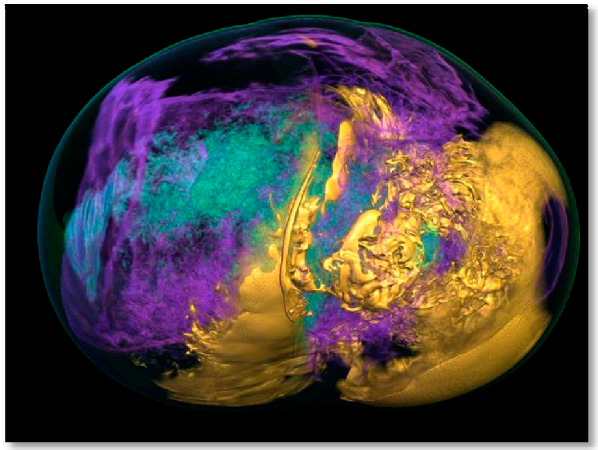
Shining the light on dark matter*
A glimpse into the invisible world of dark matter, finding that dark matter evolving in a galaxy such as our Milky Way remains identifiable and clumpy. Upcoming issue of *Nature*



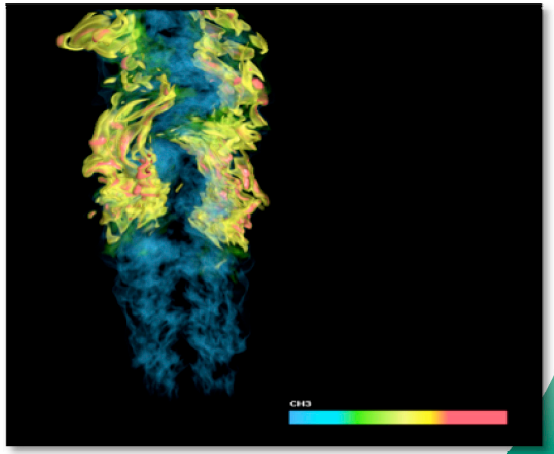
Modeling the full Earth system
Simulated time evolution of the atmospheric CO_2 concentration originating from the land's surface



Taming turbulent heat loss in fusion reactors*
Advanced understanding of energy loss in tokamak fusion reactor plasmas. *PRL* (**99**) and *Physics of Plasmas* (**14**)



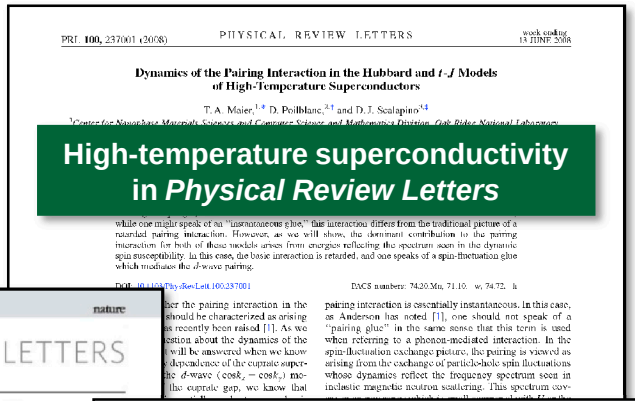
How does a pulsar get its spin?*
Discovery of the first plausible mechanism for a pulsar's spin that fits observations, namely the shock wave created when the star's massive iron core collapses.
Jan 4 2007 issue of *Nature*



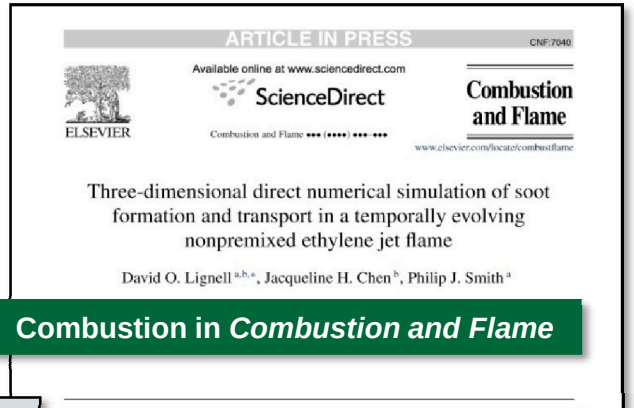
Stabilizing a lifted flame*
Elucidation of the mechanisms that allow a flame to burn stably above burners, namely increasing the fuel or surrounding air co-flow velocity
Combustion and Flame (2008)

*Used ORNL LCF computers

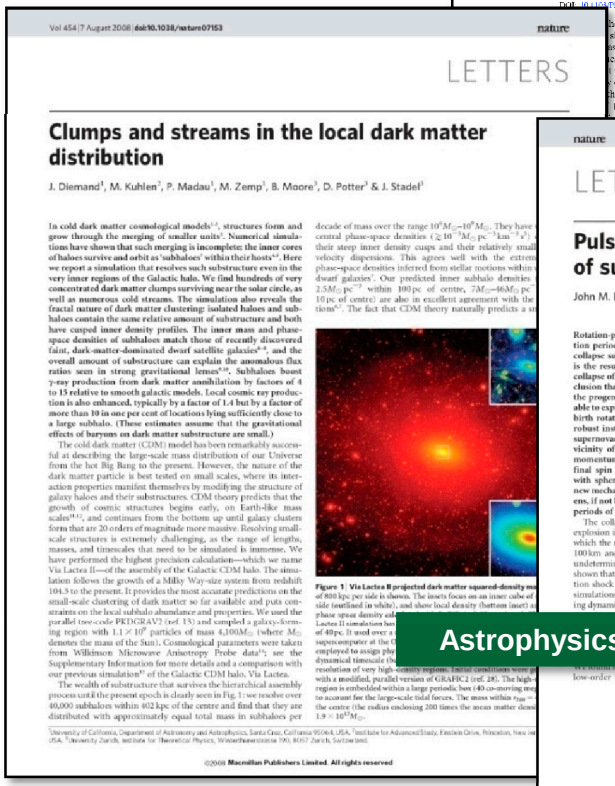
Recent and highly visible science output at the ORNL LCF

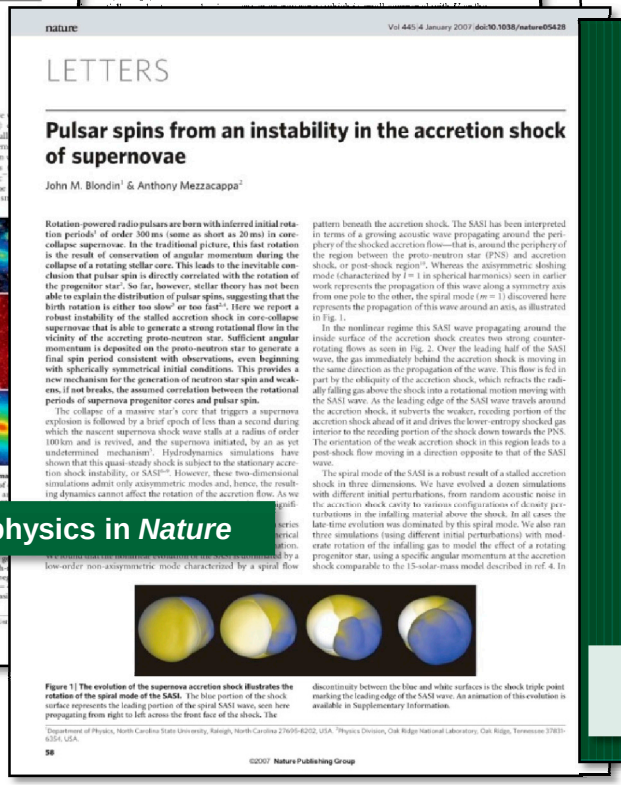


High-temperature superconductivity in *Physical Review Letters*

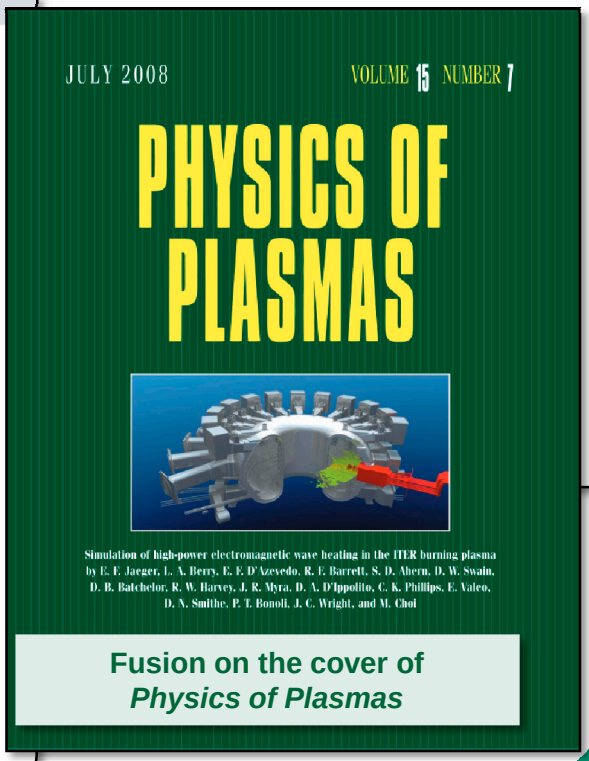


Combustion in *Combustion and Flame*





Astrophysics in *Nature*



Fusion on the cover of *Physics of Plasmas*

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