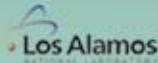




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# Computer Science and Mathematics Division

Jack C. Wells

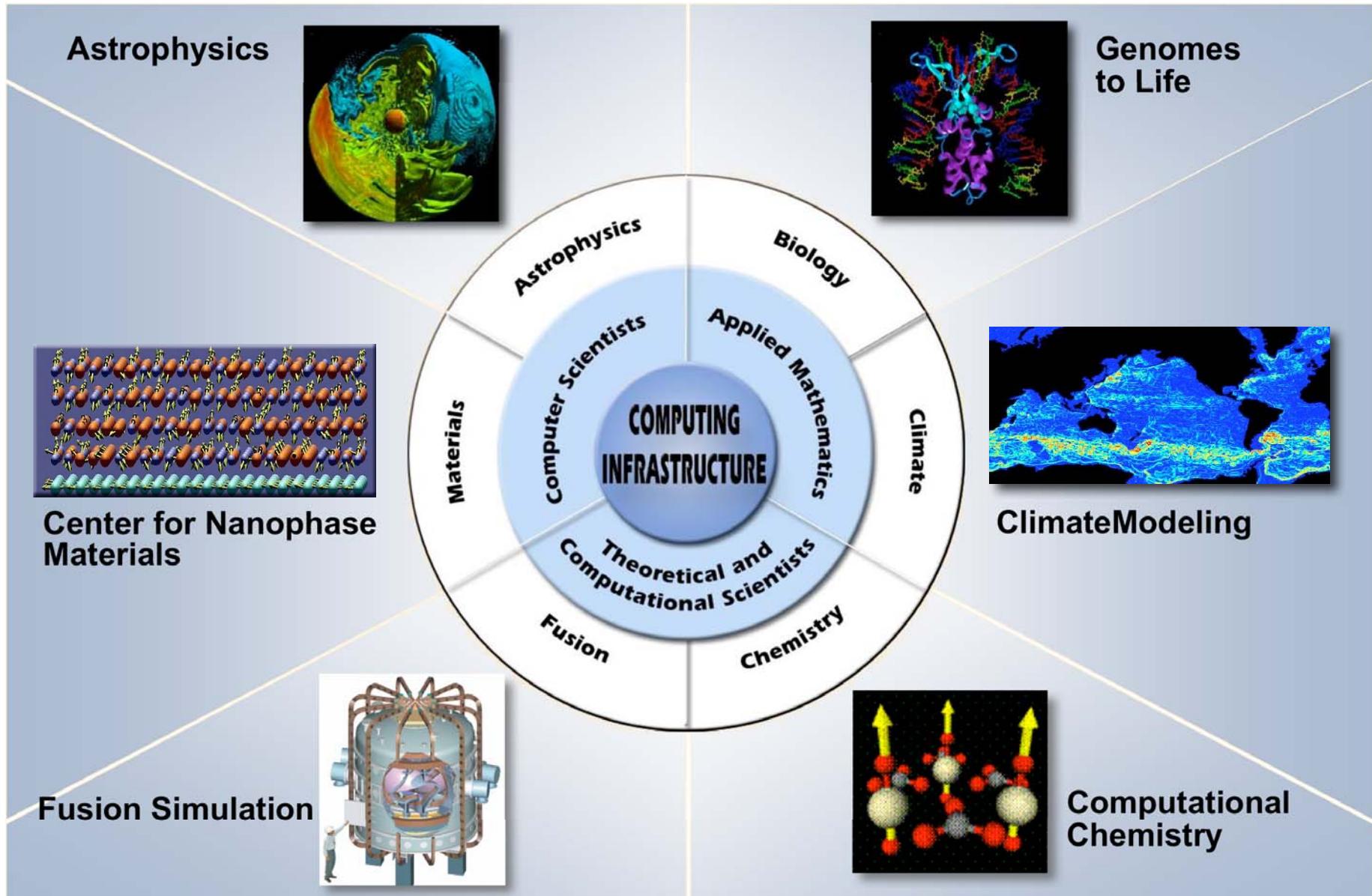
**Computer Science and Mathematics Division &  
Center for Nanophase Materials Science  
Oak Ridge National Laboratory**

**RAMS Workshop  
December, 2005  
Oak Ridge**

**THE CENTER FOR  
COMPUTATIONAL SCIENCES**

**OAK RIDGE NATIONAL LABORATORY  
U. S. DEPARTMENT OF ENERGY**

# Focused on grand challenge scientific applications



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ESH/Safety Officer
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5600 Labs Manager
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CSB Computing Center Manager
<b>M. W. Dobbs<sup>6</sup></b>
Quality Assurance
<b>R. W. Counts<sup>6</sup></b>

<sup>1</sup>Student/<sup>1a</sup>Faculty

<sup>2</sup>Joint Faculty

<sup>3</sup>Wigner Fellow

<sup>4</sup>Householder Fellow

<sup>5</sup>Postdoc/<sup>5a</sup>Postmaster

<sup>6</sup>Dual Assignment

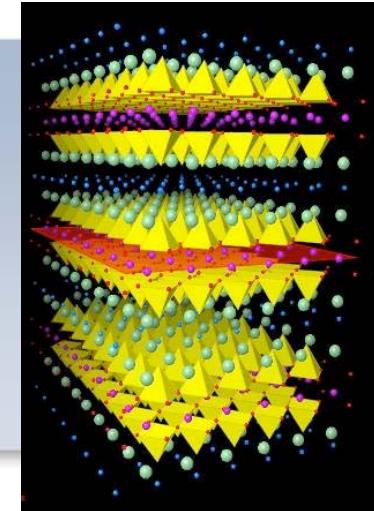
<sup>7</sup>Part-time

# Our Motivation: *Opportunities for Breakthrough Science*

Two recent examples:

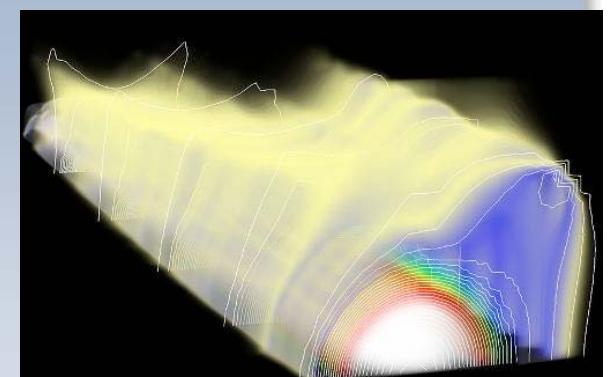
High-T<sub>C</sub> superconducting materials:

- First solution of 2D Hubbard Model  
(T. Maier, *PRL*, accepted 10/2005)



Fusion plasma simulation:

- Largest simulation of plasma behavior  
in a tokamak  
(F. Jaeger, APS-DPP invited  
presentation, 10/2005)

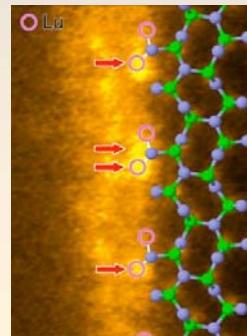
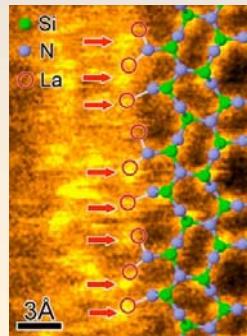


# Advancing scientific discovery through computing

## Design of ceramic materials

### A New Second Variational Binding Energy Model

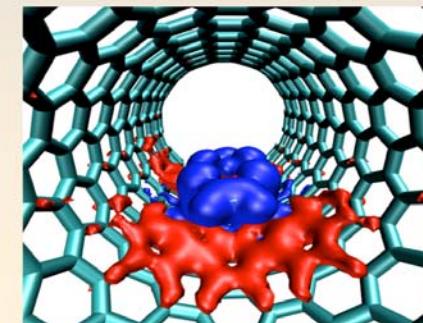
- Interprets observed properties in terms of chemical bonding
- Control of the microstructure and mechanical properties
- Correctly predicts interface positions of sintering additives
- Simulations led experiment!
- N. Shibata et al., *Nature* 428, 730–733 (2004)



## Computational Nanoscience

### Design and Control of Nanoscale and Molecular Electronic Devices

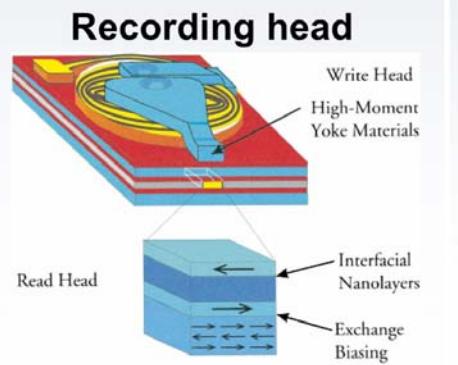
- Practical nanotube devices demand air stable, controllable, large-scale doping
- Recent experiments suggest organic doping is viable
- Simulations confirm experiment and enable detailed understanding & design
- Large-scale quantum conductance calculations on Cray-X1 and SGI-Altix
- Meunier and Sumpter, *Journal of Physical Chemistry* (2005, accepted)



# Prediction and discovery of giant tunneling magnetoresistance (TMR) for spin valves

## Magnetoresistance applications today:

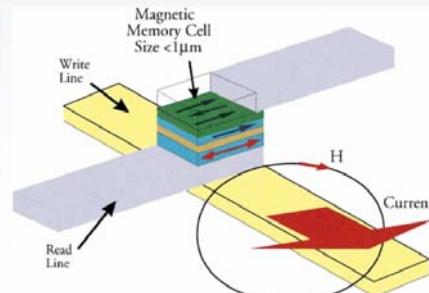
- Recording head in computer hard discs
- Magnetic random access memory



## Typical TMR for amorphous aluminum oxide barrier:

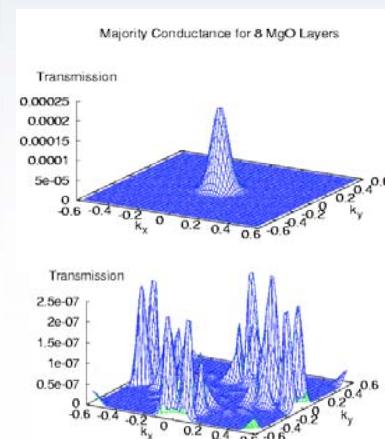
- 1995: ~10% (discovery @ MIT)
- 2005: ~70% (after a big experimental effort)

## Magnetic Random Access Memory



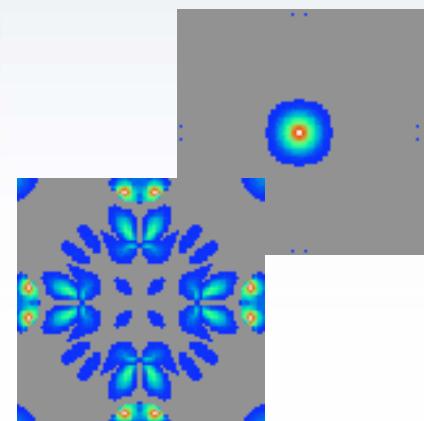
Computational prediction: TMR of 1000% is possible for crystalline MgO barrier, if interfaces are good enough

- Butler, Zhang, Schulthess, and MacLaren (ORNL), *Phys. Rev. B* (2001)

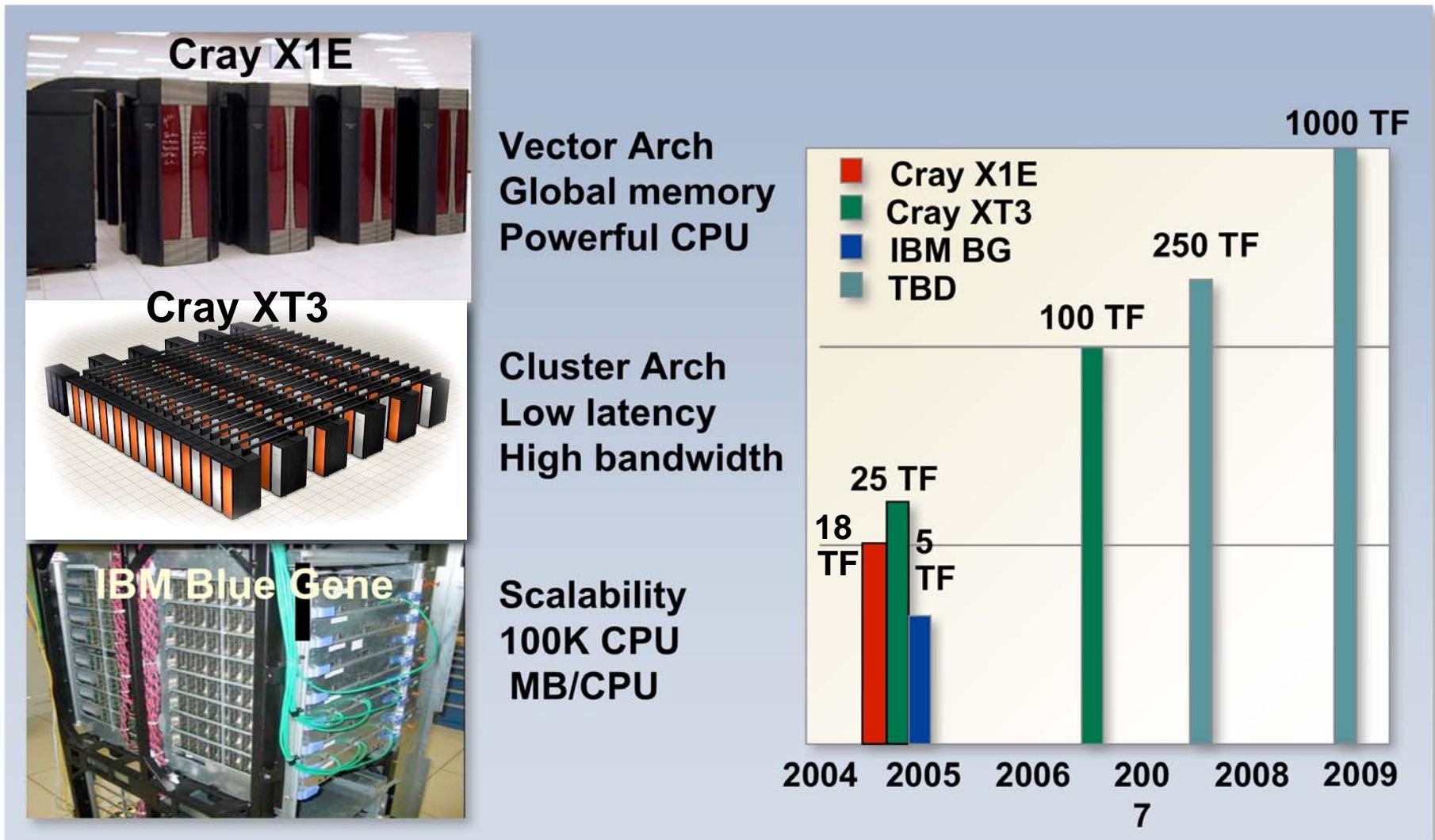


By 2004, MgO-based heterostructures with >300% TMR discovered experimentally

- Parkin *et al.*, *Nature Materials* (2004)
- Yasa *et al.*, *Nature Materials* (2004)

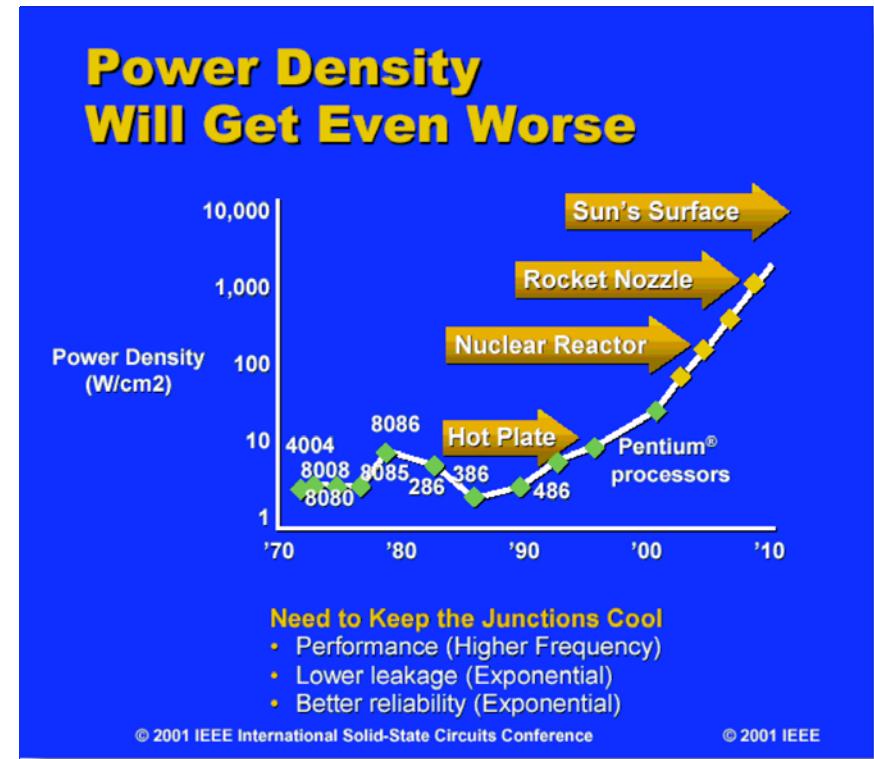


# NLCF plan for the next 5 years:



# Observations

- **Memory-processor performance gap leading to low sustained performance on important applications**
- **ITRS predicts that Moore's Law will be coming to an end in 2012-2015**
- **Practical considerations (power, cooling, floor space) are forcing architects to change their designs now**



Source: Pat Gelsinger, CTO, Intel



Intel's CTO: "Pentium PC May Need the Power of a Nuclear Reactor"

## Intel Cancels Top-Speed Pentium 4 Chip

1 hour, 42 minutes ago  
October 15, 2004

By Daniel Soria

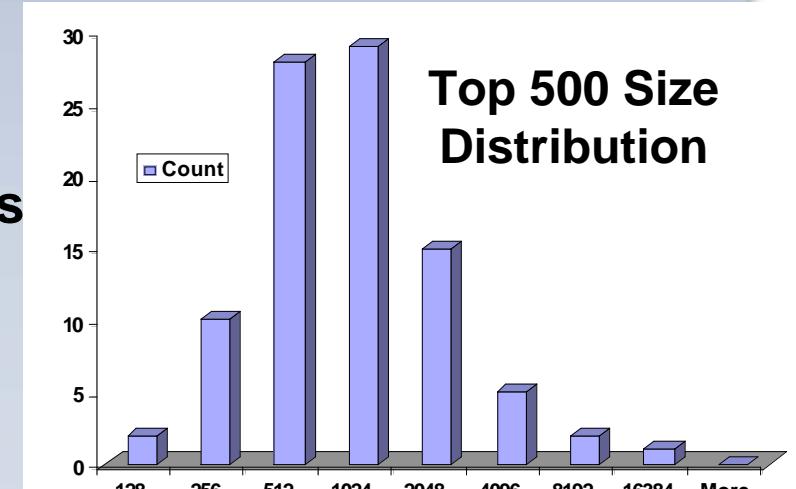
SAN FRANCISCO (Reuters) - Intel Corp. (Nasdaq:INTC - news) on Thursday canceled plans to introduce its highest-speed Pentium 4 chip for desktop computers, marking another in a string of unexpected product changes, cancellations and recalls at the world's largest computer chip maker.

REUTERS

has become a widely discussed issue. probably something the industry is of heat dissipation, which rises difficulty very well, as the now.

# How Big Is Big?

- **Every 10X brings new challenges**
  - 64 processors was once considered large  
It hasn't been “large” for quite a while.
  - 1024 processors is today's “medium” size
  - 2048-16192 processors is today's “large”  
We are struggling even here.
- **100K processor systems**
  - are being designed/deployed
  - have fundamental challenges ...  
... and no integrated research programs
- **Petascale data archives**
  - the “personal petabyte” very near
- **See recent PITAC report**
  - [www.nitrd.gov](http://www.nitrd.gov)



# Preparing for Big: *Math and CS challenges*

- **Theoretical Models (existing)**

- May not perform well on petascale computers
- May not have needed fidelity
- May be inadequate to describe new phenomena revealed by experiment or simulation

- **Scientific Modeling and Simulation Codes (existing)**

- Do not take advantage of new architectures (5%-10% of peak)
- New computing capabilities lead to new simulation possibilities and, thus, new applications codes

- **Systems Software**

- Vendor operating systems do not provide needed functionality
- Systems software for petascale applications non-existent
  - Software to manage and visualize massive (petabyte) data sets
  - Software to accelerate development and use of petascale scientific applications
  - Techniques for porting software to the next generation inadequate
- Few mathematical algorithms scale to thousand-million processors

# People and partnerships



**Thomas Maier**  
Wigner Fellow



**Jennifer Ryan**  
Householder Fellow



**Gonzalo Alvarez**  
Wigner Fellow



**Elbio Dagotto**  
Distinguished Scientist



**Jeff Vetter**  
Future Technologies

We have methodically hired  
122 research staff in 5 years  
in support of computing

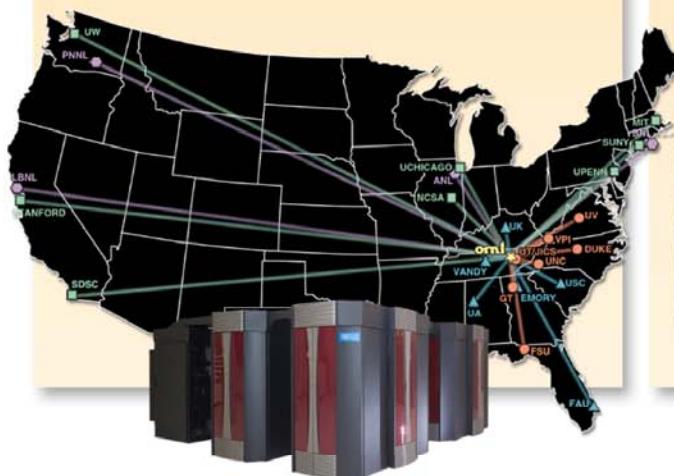
- Strong partnerships with sister labs (ANL, LBNL, PNNL) and other centers
- Interagency partnerships with NSF, NSA, NNSA, NASA, DHS
  - Key resource for Intergovernmental Panel on Climate Change (IPCC)
- Joint Institute for Computational Sciences/core universities
  - Graduate program in computational Sciences
  - Distinguished Scientists/ Joint faculty appointments
- Cray Center of Excellence

	2002	2003	2004	2005
S&T	15	21	31	23
Postdocs	58	40	56	30
Students	34	41	46	43

# Our Aspirations

**World leader  
in scientific computing**

**“User facility providing leadership-class computing capability to scientists and engineers nationwide independent of their institutional affiliation or source of funding”**



**Intellectual center in  
computational science**

**Create an interdisciplinary environment where science and technology leaders converge to offer solutions to tomorrow's challenges**



## Transform scientific discovery through advanced computing

**“Deliver major research breakthroughs, significant technological innovations, medical and health advances, enhanced economic competitiveness, and improved quality of life for the American people”**

