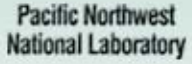


Computer Science and Mathematics Division

Jack C. Wells

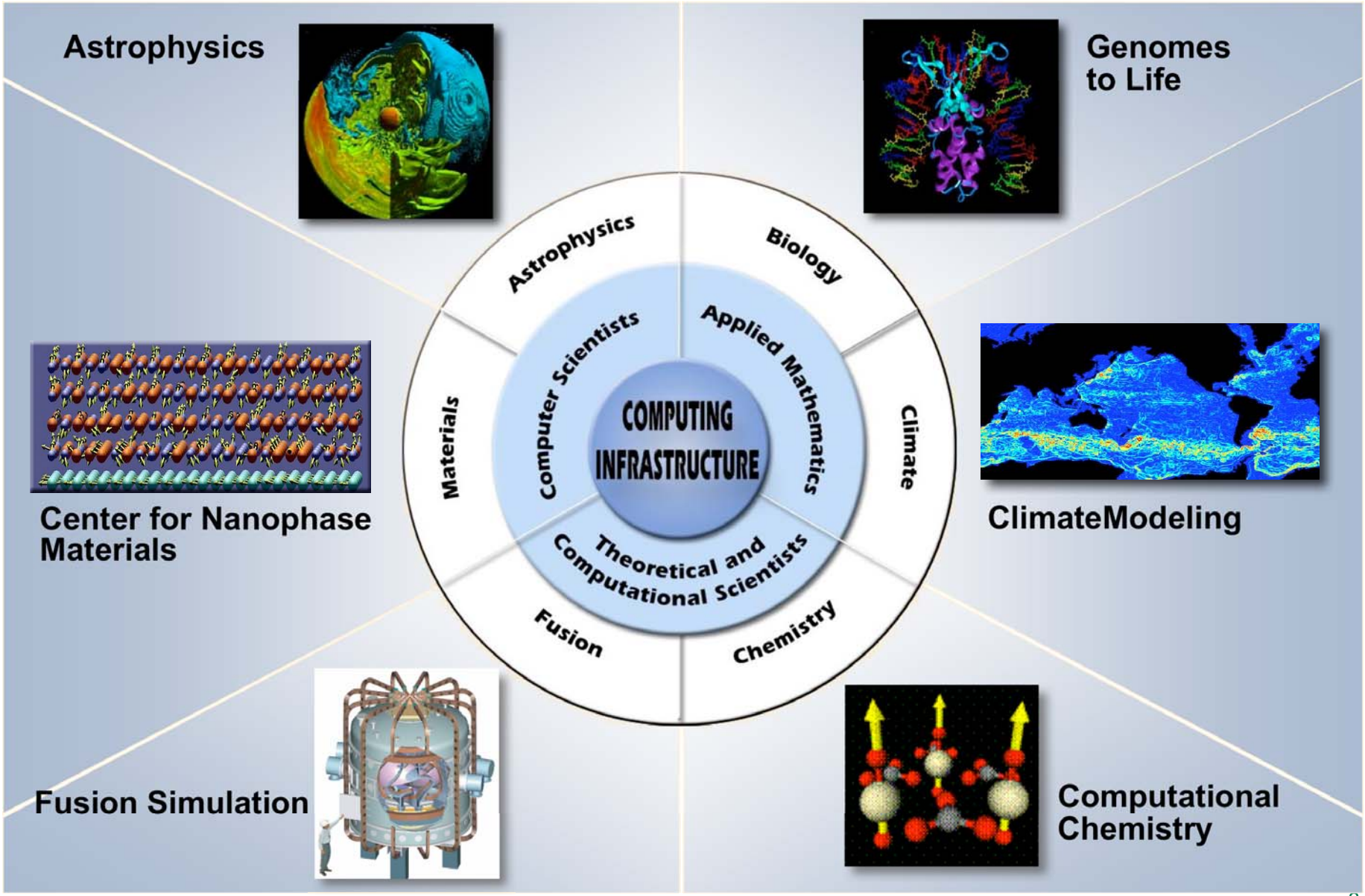
Computer Science and Mathematics Division &

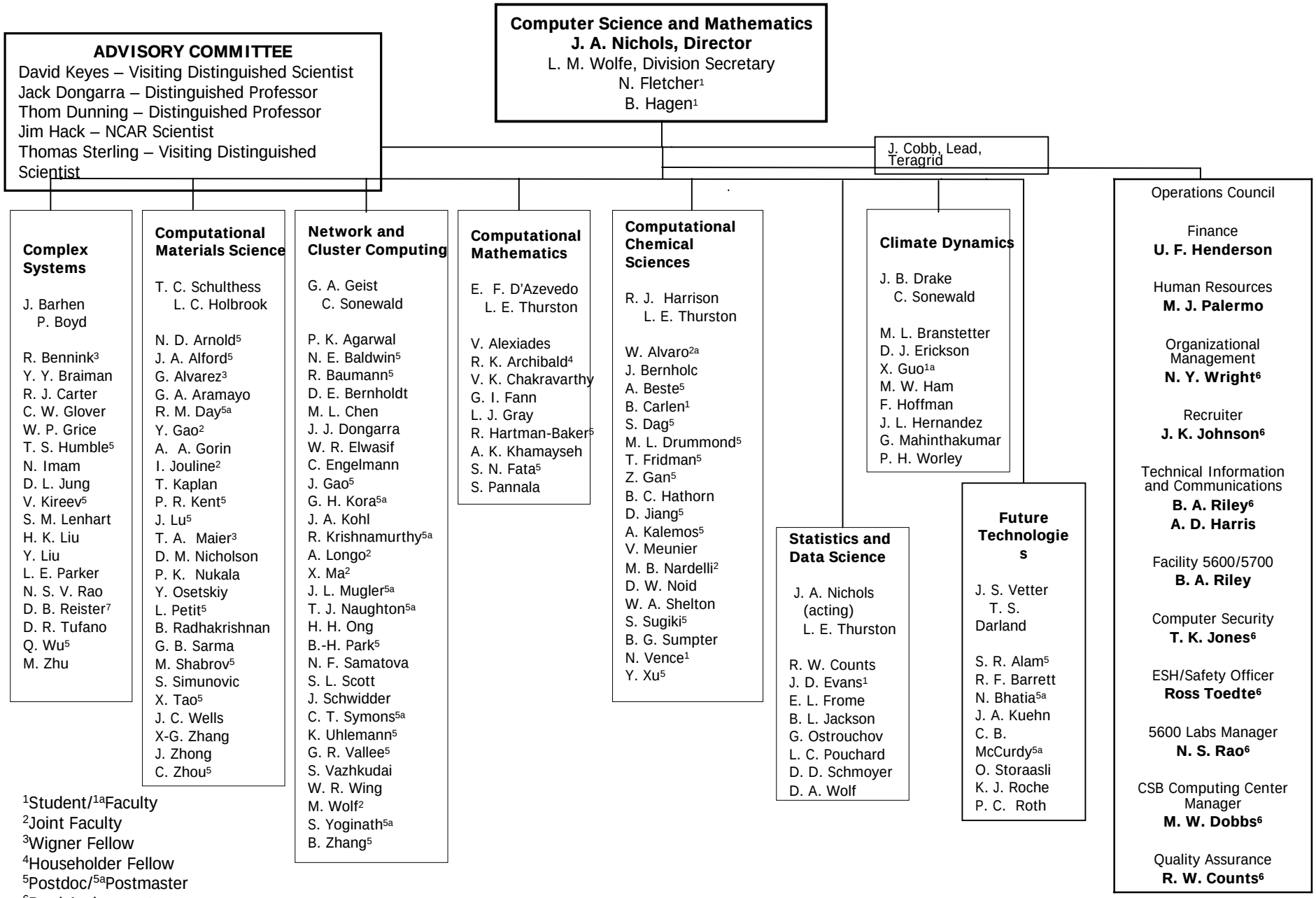
Center for Nanophase Materials Science

Oak Ridge National Laboratory

RAMS Workshop
December, 2005
Oak Ridge

Focused on grand challenge scientific applications





[1]Student/[1a]Faculty
[2]Joint Faculty
[3]Wigner Fellow
[4]Householder Fellow
[5]Postdoc/[5a]Postmaster
[6]Dual Assignment
[7]Part-time

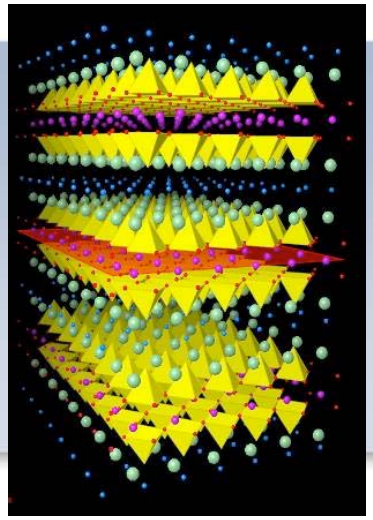
11/15/05

Our Motivation:
Opportunities for Breakthrough Science

Two recent examples:

High-T_C superconducting materials:

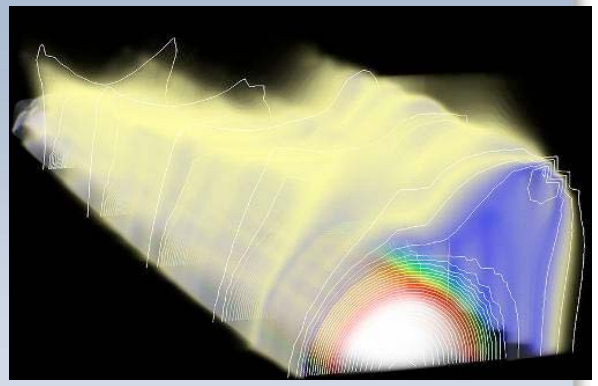
- First solution of 2D Hubbard Model (T. Maier, *PRL*, accepted 10/2005)



Fusion plasma simulation:

- Largest simulation of plasma behavior in a tokamak

  (F. Jaeger, APS-DPP invited presentation, 10/2005)

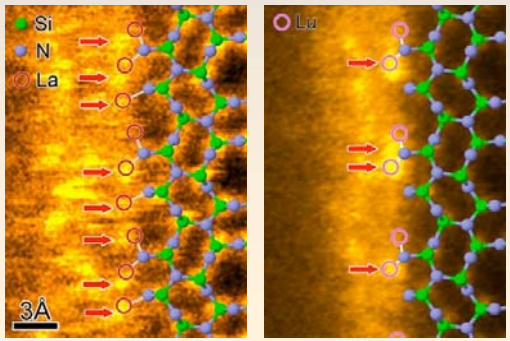


Advancing scientific discovery through computing

Design of ceramic materials

A New Second Variational Binding Energy Model

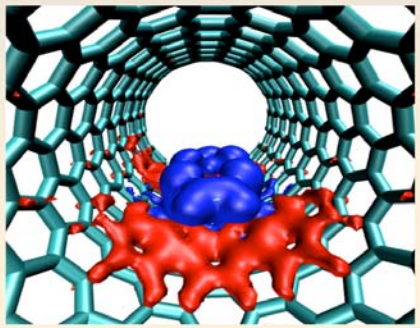
- **Interprets observed properties in terms of chemical bonding**
- **Control of the microstructure and mechanical properties**
- **Correctly predicts interface positions of sintering additives**
- Simulations led experiment!
- **N. Shibata et al., *Nature* 428, 730–733 (2004)**



Computational Nanoscience

Design and Control of Nanoscale and Molecular Electronic Devices

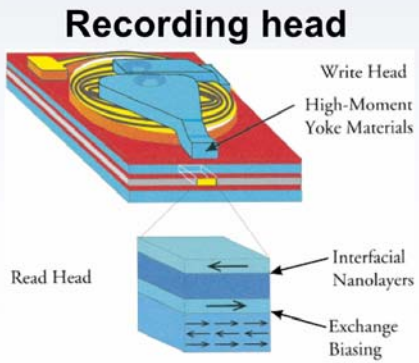
- **Practical nanotube devices demand air stable, controllable, large-scale doping**
- **Recent experiments suggest organic doping is viable**
- **Simulations confirm experiment and enable detailed understanding & design**
- **Large-scale quantum conductance calculations on Cray-X1 and SGI-Altix**
-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



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

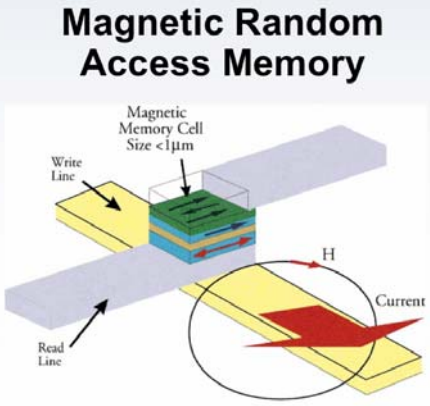
Magnetoresistance applications today:

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



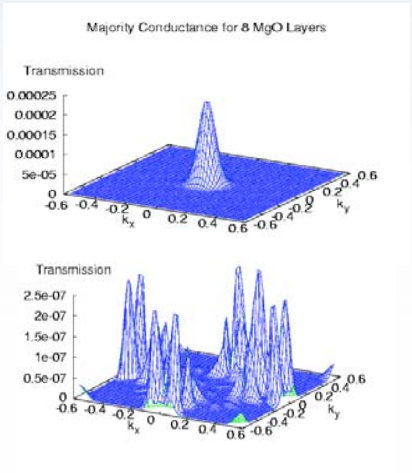
Typical TMR for amorphous aluminum oxide barrier:

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



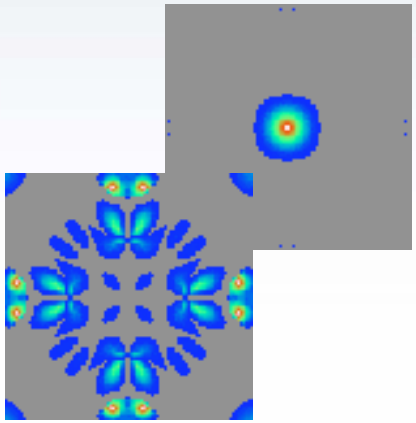
Computational prediction: TMR of 1000% is possible for crystalline MgO barrier, if interfaces are good enough

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

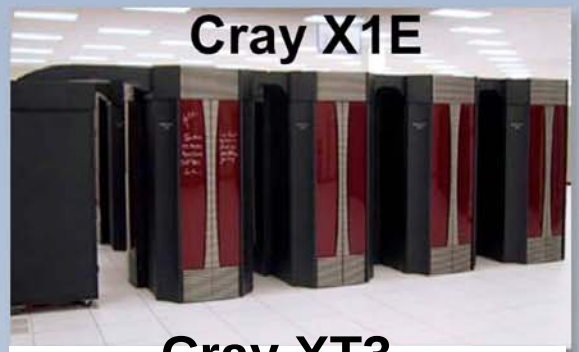


By 2004, MgO-based heterostructures with >300% TMR discovered experimentally

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



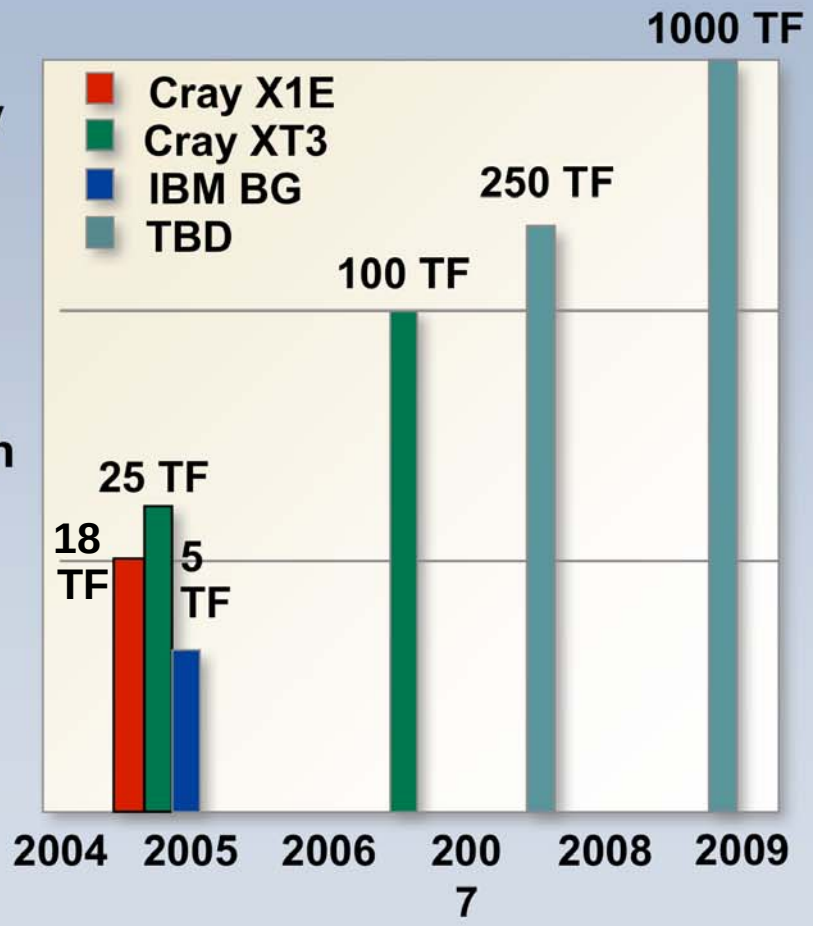
NLCF plan for the next 5 years:



Vector Arch
Global memory
Powerful CPU

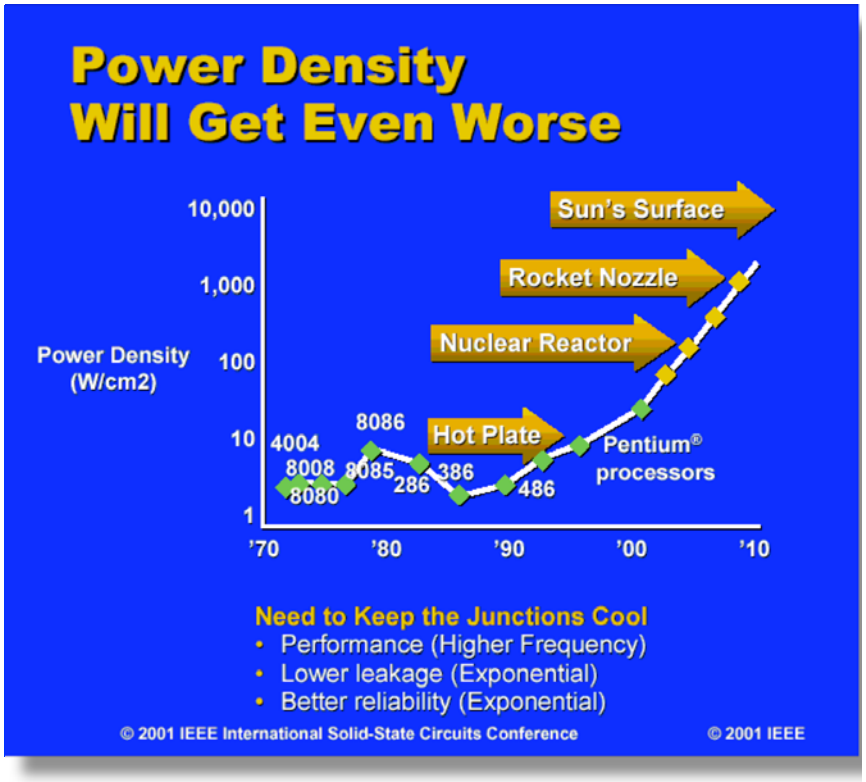
Cluster Arch
Low latency
High bandwidth

Scalability
100K CPU
MB/CPU

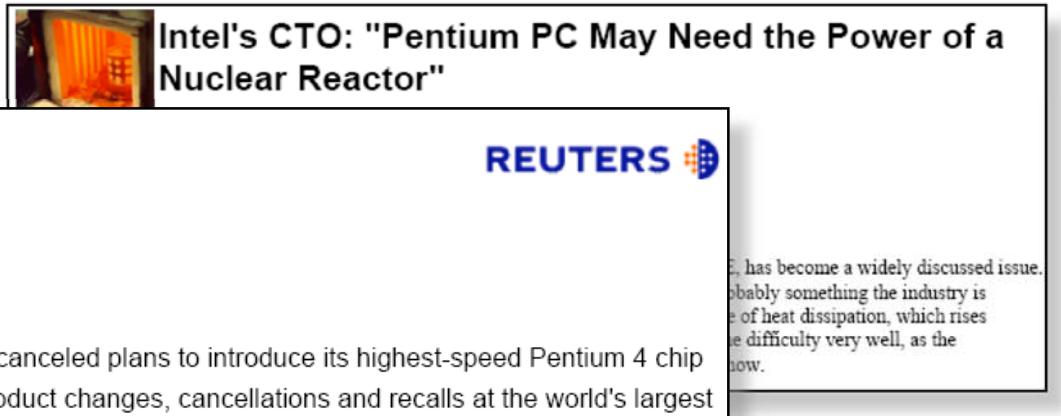


Observations

- **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"

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

Intel Cancels Top-Speed Pentium 4 Chip

REUTERS

1 hour, 42 minutes ago
October 15, 2004

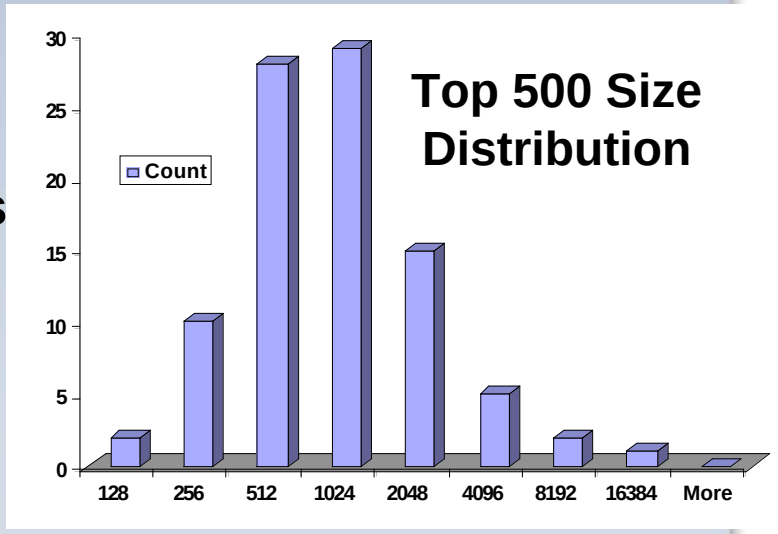
By Daniel Sorid

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.

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**



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

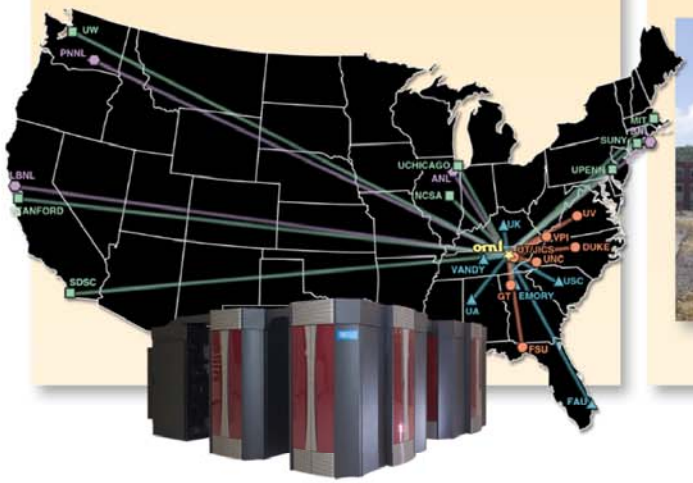
	2002	2003	2004	2005
S&T	15	21	31	23
Postdocs	58	40	56	30
Students	34	41	46	43

- **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**

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"