DMR ITR Computational Review and Workshop:
ITR and beyond

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June 17-19, 2004
Urbana, IL

Objectives of Program Overview
What brings us together today ?

- **Diverse group representative of computational Materials Theory**
- **Opportunity to present your research to NSF and peers**
- **Encourage "cross-communication" & "cross fertilization"**
- **Student and postdoc participation**
- *Opportunity to provide your input to NSF*

Objectives of Program Overview
The Burning Issues

- **Participants represent research projects supported under ITR (FY01 to FY03)**

- **This is the last year of ITR (FY04)**

- **ITR in DMR has been managed by Materials Theory for the past 4 years**
    - *Separate activity; not part of MT's budget*
    - *Significant part of DMR ITR is Materials-Theory-related research*

Materials Theory

- **Provides support for theory, modeling and simulation which spans DMR (theoretical condensed matter physics, theoretical materials science and solid state chemistry)**

- **Provides support for theoretical topics funded in other DMR programs, i.e., if it is supported in DMR, MT will support the theory**

- **Does not explicitly fund experimental research, although experimental connections are important**

- **Advances methodologies and techniques. e.g., algorithms, formal methodologies, mathematical methods**

- **Nurtures an integrated 'Materials Theory' community**
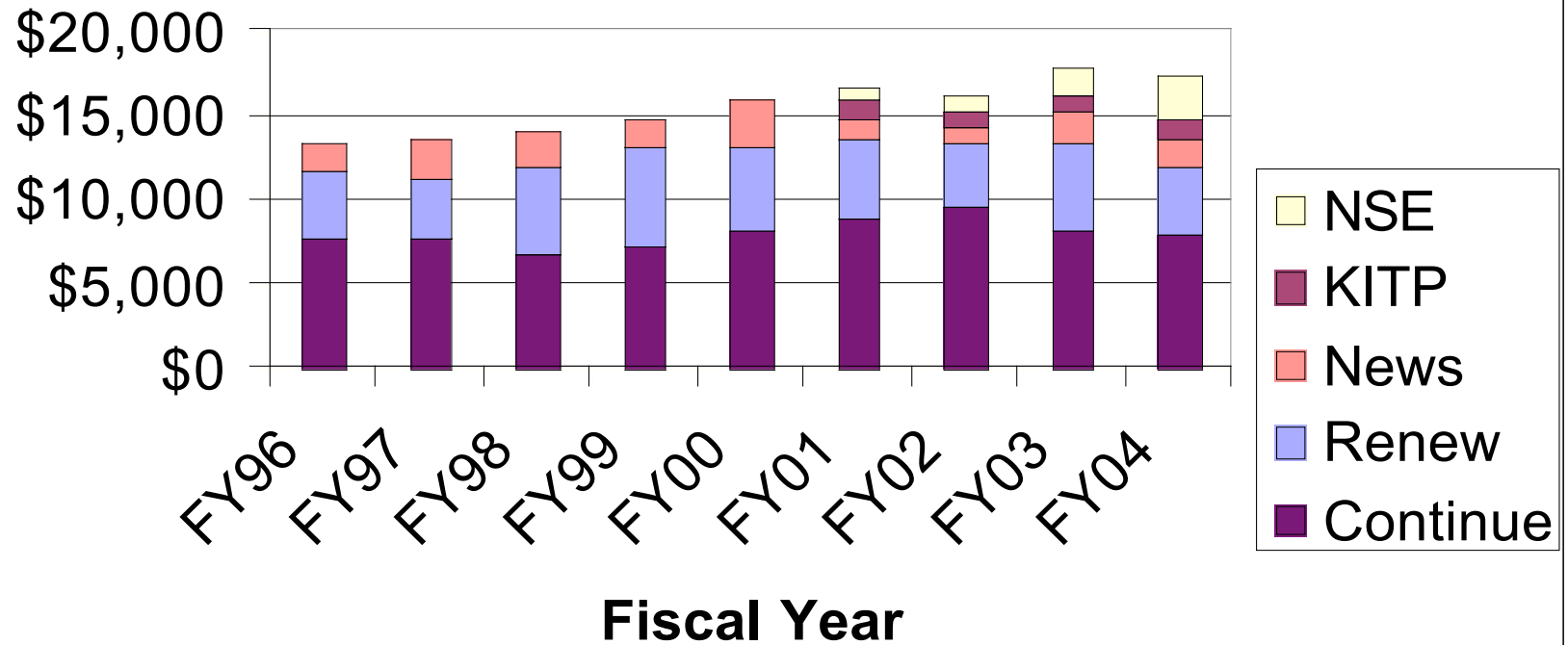
ITR Initiative

	FY00	FY01	FY02	FY03	FY04
DMR budget (Millions)	$0 [all in CISE]	$7.28	$9.24	$9.93	$10
Awards Medium [MT-related]		5 [3]	3 [2]	7 [3]	No Size Categories
Awards Small [MT-related]		5 [5]	9 [7]	17 [15]	5-8 ?

DMR has used this opportunity to enhance computational research at *all levels*

Objectives of Program Overview
The Burning Issues

- *What is the future of research in DMR supported under ITR?*
  - *Science opportunities ?*
  - *Funding?*

Objectives of Program Overview
The Burning Issues: What's next?

- ## Cyberinfrastructure [CI] from the ACP

    Historically, infrastructure was viewed largely as raw resources like compute cycles or communication bandwidth. As illustrated by many activities in the current PACI centers and by the recent NSF middleware program, the scope of infrastructure is expanding dramatically beyond this narrow definition. *For purposes of the ACP, infrastructure will comprise of a diverse set of technologies, facilities, and services and intangibles like design processes and best practices and shared knowledge. A major technological component is software that participates directly in applications and software tools that aid in the development and management of applications. A critical non-technological element is people and organizations that develop and maintain software, operate equipment and software as it is used, and directly assist end-users in the development and use of applications.*

    The ACP seeks to bring about dramatic and beneficial change in the conduct of science and engineering research. Applications will greatly expand their role and become increasingly integral to the conduct of science and engineering research.

Objectives of Program Overview
The Burning Issues: What's next?

- ## Cyberinfrastructure [CI]

    – **Vague:** *A shared integrated system of interconnected computation, communication, and other information technology that supports a range of activities in a research community.*

    – **Elements:** *Advanced computing hardware, networks, software, data storage, data management, digital libraries ...*

    – **What does CI mean …**

        - for the computational materials research community?
        - for the broader materials research community?

Objectives of Program Overview
The Burning Issues: What's next?

- ## MPS view: Science drives Cyberinfrastructure
  - ### Workshop at NSF in April – MPS wide
  - ### *What is the science that requires CI?*
  - ### *What are the cyberinfrastructure needed to do the science?*
  - ### Common themes across MPS? Unique needs? … stay tuned for Saturday!
    #### *What are the priorities ?*

CYBERSCIENCE WORKSHOP

Identifying Major Scientific Problems in the Mathematical and Physical Sciences and Their CyberInfrastructure Needs

WEDNESDAY, APRIL 21, 2004
8:00 AM – ROOM 110
National Science Foundation

INVITED SPEAKERS

Dr. Brent Fultz, California Institute of Technology

Dr. David Keyes, Columbia University

Dr. Vijay Pande, Stanford University

Dr. Dan Reed, University of North Carolina

Dr. Larry Smarr, University of California, San Diego

Dr. Alex Szalay, Johns Hopkins University

AFTERNOON BREAKOUT SESSIONS

I. Algorithms and Software; II. Software Infrastructure; III. Hardware, Facilities; IV. Network Infrastructure; V. Data Management and Analysis

Information
Morris L. Aizenman, Senior Science Associate, MPS Directorate, 703-292-8807

Credit: © Eric J. Heller, Harvard University

Objectives of Program Overview
The Burning Issues: What's next?

- ## Our concern here:

  Computational Materials Research Community (Condensed Matter Physics, Materials Science, & Solid State Chemistry)

  – *What is the science that the computational materials research community aspires to do? ("Cyberscience")*

  – *What are the cyberinfrastructure needs of the computational materials research community to do the science?*

  What are the priorities ?

DMR ITR Computational W & R
Where are we and where do we want to go?

Web/Paper Survey: (http: ???)

- **Thursday-Friday**
  - **What is the science we *are* doing?**
  - **What CI *are* we using?**
  - **What CI could have made a difference?**
- **Saturday**
  - **What science *will* we engage at our frontiers?**
    - **5 years? 10 years?**
  - **What CI *will* we need to make advances?**
    - **5 years? 10 years?**
- **What is high priority? What is lower priority but still important?**

DMR ITR Computational W & R

Where are we and where do we want to go?

Please complete the survey before Saturday morning

Please participate in the Saturday session

There will be a written summary of this workshop

- **Mark Novotny, Todd Martinez, David Ceperley, Chakram Jayanthi, Richard Martin, …**

- **Please help these folks any way you can**

Your input is important

It is your future!

For more information ...

- **Atkins report**

  http://www.cise.nsf.gov/sci/reports/toc.cfm

- **Information Technology Research**

  http://www.itr.nsf.gov

DMR involvement in Computation-related Solicitations

- **HPCC/CARM 1992 & 1995**

- **KDI 1998 & 1999**

- **ITR 2000-2004 (Small, Medium and Large)**

- **?**