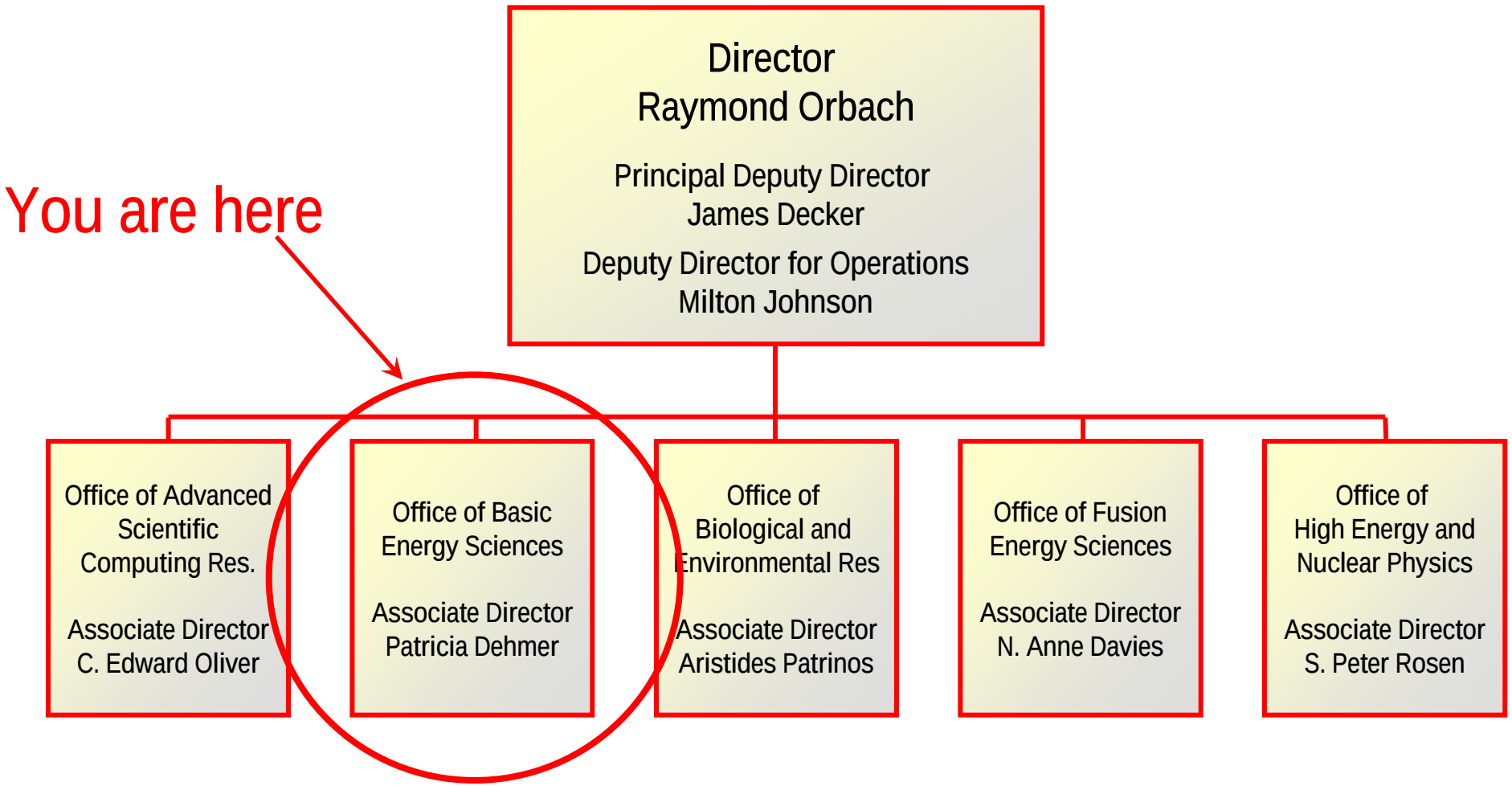
What's New in DOE's Neutron Scattering Program

Helen Kerch

Program Manager
X-ray and Neutron Scattering

SENSE workshop
Tallahassee, FL September 25, 2003

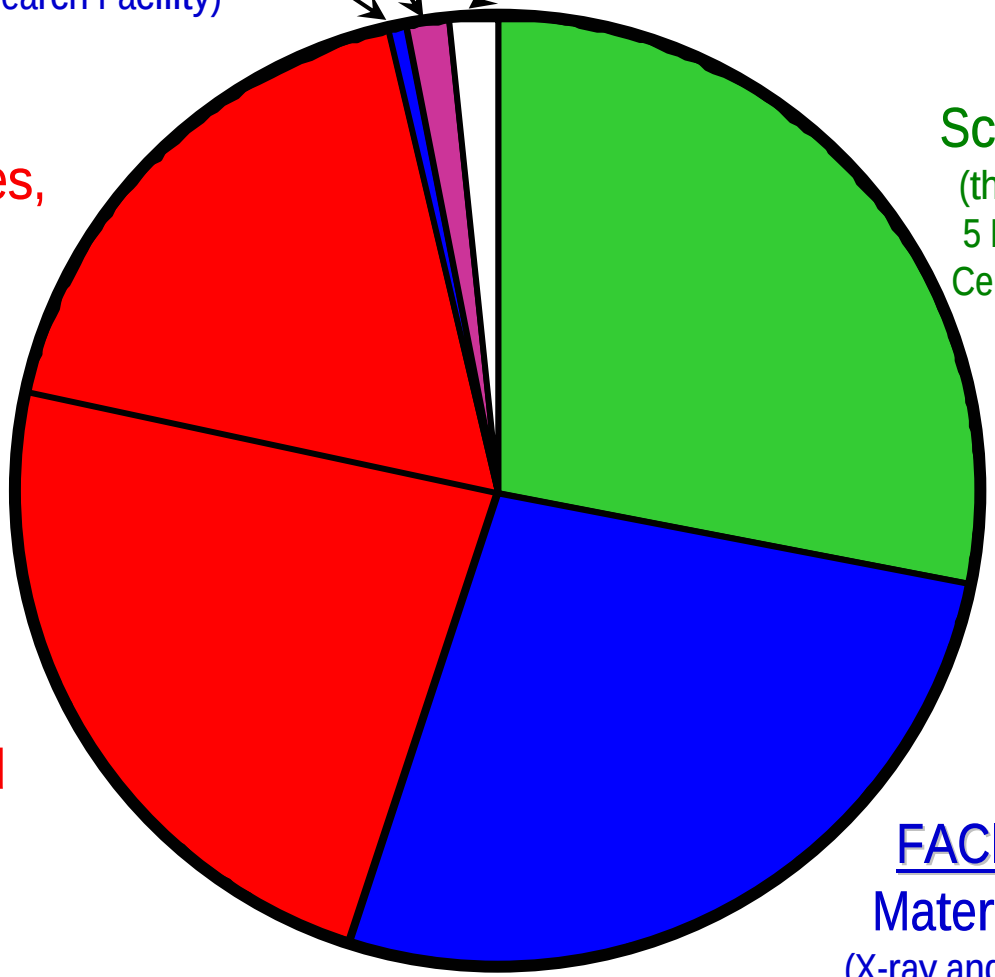
DOE's Office of Science



"... to foster and support fundamental research to expand the scientific foundations for new and improved, environmentally conscientious energy technologies"

"... to plan, construct, and operate major scientific user facilities for the Nation"

BES – Where Does the $1 Billion Go?



FACILITY OPERATIONS
CS,G,B
(Combustion Research Facility)

GPP/GPE

SBIR/STTR

RESEARCH
Chemical Sciences, Geosciences, Biosciences
(~$200M)

CONSTRUCTION
Scientific User Facilities
(the Spallation Neutron Source, 5 Nanoscale Science Research Centers, and the Linac Coherent Light Source)
(~$225)

RESEARCH
Materials Sciences and Engineering
(~$250M)

FACILITY OPERATIONS
Materials Sciences & Eng.
(X-ray and Neutron Scattering Facilities)
(~$300M)

~$1 Billion

FY04 Pres. Req.

BES Facilities for X-ray and Neutron Scattering

Advanced Light Source

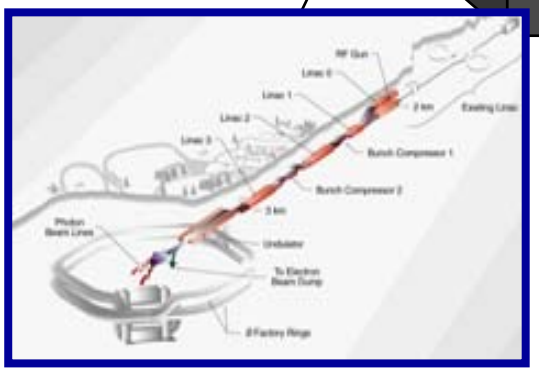
Advanced Photon Source

National Synchrotron Light Source

Stanford Synchrotron Radiation Laboratory

Intense Pulsed Neutron Source

Spallation Neutron Source



Linac Coherent Light Source

Manuel Lujan Jr. Neutron Scattering Center

High-Flux Isotope Reactor

Office of Basic Energy Sciences

Patricia Dehmer, Director

Mary Jo Martin, Administrative Specialist

http://www.sc.doe.gov/production/bes/BESjobs.html

Director's Office Staff

Robert Astheimer
F. Don Freeburn
Stanley Staten
Sharon Long
Financial Management Specialist (Vacant)

Materials Sciences and Engineering Division

Patricia Dehmer, Director (Acting)
Christie Ashton, Program Analyst
Anna Lundy, Secretary

- Materials and Engineering Physics
  - Robert Gottschall
  - Terry Jones, Prog. Asst.
  - Structure & Composition of Materials — Altaf (Tof) Carim
  - Mechanical Behavior of Materials & Rad Effects — Yok Chen; ● Michael Kassner, OR State
  - Physical Behavior of Materials — Harriet Kung
  - Synthesis & Processing Science — Jane Zhu; ◆ Darryl Sasaki
  - Engineering Research — Timothy Fitzsimmons
- Condensed Matter Phys and Materials Chemistry
  - X-Ray & Neutron Scat.
  - William Oosterhuis
  - Melanie Becker, Prog. Asst
  - Experimental Condensed Matter Physics — James Horwitz
  - Theoretical Condensed Matter Physics — Dale Koelling
  - Materials Chemistry & Biomolecular Materials — Dick Kelley; Aravinda Kini
  - X-ray & Neutron Scattering — Helen Kerch
  - Experimental Program to Stimulate Competitive Research (EPSCoR) — Matesh Varma

Scientific User Facilities Division

Patricia Dehmer, Director (Acting)
Support Staff (Vacant)

- X-ray & Neutron Scattering Facilities — Pedro Montano; Vacant
- Spallation Neutron Source (Construction) — Jeffrey Hoy
- Nanoscale Science Research Centers (Construction) — Kristin Bennett; Altaf (Tof) Carim
- Linac Coherent Light Source (Construction) — Jeffrey Hoy
- SNS, LCLS, and X-ray&Neutron Scattering Instrument MIEs — Kristin Bennett

Chemical Sciences, Geosciences, and Biosciences Division

Walter Stevens, Director
Karen Talamini, Program Analyst
Secretary (Vacant)

- Fundamental Interactions
  - Eric Rohlfing
  - Sharon Bowser, Prog. Asst
  - Atomic, Molecular, and Optical Science — ◆ David Ederer
  - Chemical Physics — William Kirchhoff; ◆ Frank Tully, SNL
  - Photochemistry & Radiation Research — Mary Gress
  - Computational and Theoretical Chemistry — Vacant
- Molecular Processes and Geosciences
  - William Millman
  - Diane Marceau, Prog. Asst
  - Catalysis and Chemical Transformation — Raul Miranda; ◆ Detailee (Vacant)
  - Separations and Analysis — John Miller
  - Heavy Element Chemistry — Lester Morss; □ Norman Edelstein, LBNL
  - Chemical Energy and Chemical Engineering — Paul Maupin
  - Geosciences Research — Nicholas Woodward; ● IPA (Vacant)
- Energy Biosciences Research
  - James Tavares
  - Patricia Snyder, Prog. Asst
  - Plant Sciences — James Tavares
  - Biochemistry and Biophysics — Sharlene Weatherwax

● IPA
◆ Detailee
□ Detailee, 1/4 time, not at HQ

August 25, 2003

Two Division Director Position Openings within BES

- BES has recently undergone a reorganization to form two Divisions from its existing Materials Sciences and Engineering Division.

- DOE is now seeking applications;
  - •Director, Materials Sciences and Engineering Division (Open till 10/22/03)
  - •Director, newly established Scientific User Facilities Division.

- http://www.sc.doe.gov/production/bes/BESjobs.html

Short Tutorial on Applying for BES Research Funds

One-page Information Sheet for Grant Applicants is Available

Some information that may be of interest to grant applicants

Division of Materials Sciences and Engineering
Office of Basic Energy Sciences
Office of Science
U.S. Department of Energy

Please note that many of the suggestions and procedures below are specific to the Division of Materials Sciences and Engineering, and pertain only to applications submitted under our "core" research program - not to special initiatives or other announced program opportunities.

Fundamental science is the primary concern in the work that our Division supports. Studies that are directed primarily towards engineering, demonstration, or development goals, such as producing specific devices or identifying optimal processing for a particular application, are less likely to compete successfully. However, our portfolio does include scientific instrument development that enables fundamental materials research.

Practical details:

Electronic Submission: The Office of Science has now fully implemented a secure, web-based electronic proposal submission system. All formal applications must now be electronically submitted by an authorized institutional business official through this system. Further information is available at DOE's Grants and Contracts web site: http://www.science.doe.gov/grants/.

A pre-proposal (2 pages or less) may be submitted but is not required, and in general (for our core program) it will be used mainly to establish whether the topic area falls within our purview. If you do wish to submit a pre-proposal, electronic submission as an e-mail attachment is preferred. We will respond to pre-proposals by phone or e-mail.

Proposal handling: Most new proposals are examined by most of the program managers within our Division, with one taking the lead on handling it. Some may be declined without external peer review. On the other hand, we are required to obtain outside peer reviews for any that we intend to fund.

Timing of submissions and awards: Proposals may be submitted at any time, but we recommend that they be sent to us between April 1st and September 30th. This allows sufficient time for completion of the peer review process prior to the annual cut-off date for new award decisions. Proposals that arrive later run the risk of being turned down regardless of the quality of reviews because all funds for the fiscal year may be committed prior to completion of the review process. Decisions on new proposals are usually made early in the following calendar year.

Typical term of support: Usually three or four years for a new proposal and three years for subsequent renewals. Renewal applications should be submitted at least nine months in advance of the scheduled termination date.

Names of reviewers: Within our Division, we do not ask applicants to suggest reviewers, and typically do not use anyone so suggested. We will honor any request to not use a specific reviewer; no reason is needed.

Sabbaticals or other leaves of absence during the grant should be discussed with us in advance.

Conferences, symposia, workshops, and meetings, other than those we initiate, are rarely supported.

Contacts within our Division, including phone and e-mail information, are available on the second web site listed below. The corresponding organization chart can be reached via a click button on this site. For further inquiries, please contact the program manager whose areas of expertise and/or responsibility most closely match the topic area.

Web sites with further information:
http://www.science.doe.gov/bes (Office of Basic Energy Sciences)
http://www.science.doe.gov/bes/besstaff.html (BES staff contacts and directory; click to org chart)
http://www.science.doe.gov/bes/dms/dmshome.html (Division of Materials Sciences & Engineering)
http://www.science.doe.gov/grants/ (sponsored research details)
http://www.science.doe.gov (Office of Science)
http://www.energy.gov/scitech/index.html (science and technology across the Dept. of Energy)

- General information
- Comments on:
  - Electronic Submission
  - Submission Timing
  - Pre-proposals
  - Proposal Handling
  - Grant Lengths
- Listing of Web Sites (including staff contacts, submission details, etc.)

Peer Review Guidelines are on the Web

BES Merit Review - Microsoft Internet Explorer provided by - The Office of Science -

File Edit View Favorites Tools Help

Back Search Favorites Media

Address http://www.er.doe.gov/production/bes/peerreview.html Go Links

Office of Basic Energy Sciences

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Review and Selection of Research Projects

All research projects supported by the Office of Basic Energy Sciences (BES) undergo regular peer review* and merit evaluation based on procedures set down in 10 CFR Part 605 for the extramural grant program and in an analogous process for the laboratory programs and scientific user facilities. The BES peer review process evaluates the following four criteria, which are listed in order of decreasing importance:

1) **Scientific and/or technical merit of the project;**

- for example, the influence that the results might have on the direction, progress, and thinking in relevant scientific fields of research; the likelihood of achieving valuable results; and the scientific innovation and originality indicated in the proposed research.

2) **Appropriateness of the proposed method or approach;**

- for example, the logic and feasibility of the research approaches and the soundness of the conduct of the research.

3) **Competency of the personnel and adequacy of proposed resources**; and

- for example, the background, past performance, and potential of the investigator(s); and the research environment and facilities for performing the research.

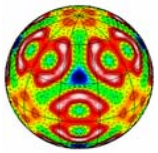
4) **Reasonableness and appropriateness of the proposed budget**.

The criteria for a review may also include other appropriate factors established and announced by the Office of Basic Energy Sciences. The BES peer review and merit evaluation procedures are described within the following documents:

- Office of Science (SC) Merit Review System
  - SC Grant Application Guide
  - 10 CFR Part 605
- BES Merit Review Procedures for Projects at DOE Laboratories
  - BES Guide for Preparation of Review Documents
  - DOE Order 412.1, "Work Authorization System"

For more information about SC's merit review system, please browse the Grants and Contracts Division homepage.

The Construction Management Support Division within the Office of Science (SC) conducts independent technical, cost, schedule, and management peer reviews of SC construction projects and large experimental equipment. These reviews are known as "Lehman Reviews" after the Division Director, Dan Lehman. Lehman Reviews are widely known in DOE, other agencies, and abroad. Dan Lehman has briefed OMB and other agencies on the process, which has been adopted by other parts of DOE.

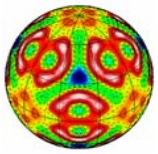


Grant applications: timing and submission

- For core program, applications accepted at all times, but recommend submission April 1 through September 30
  - Federal fiscal year runs October 1 through September 30
  - Permits ample time for reviews by mail before next fiscal year decisions are made, typically January through June
- Special programs have specific submission deadlines
- Most research grants are approved for an initial or renewal 3 or 4 year period, assuming annual progress is acceptable
- We now require electronic submission; http://e-center.doe.gov/

SBIR/STTR Topic In Neutron Instrumentation

- 14a. NEUTRON AND ELECTRON BEAM INSTRUMENTATION
  - •neutron detectors
  - •neutron optics
  - •neutron scattering instrumentation
- Release date: October 7, 2003
- Solicitation closing date: January 6, 2004
- Phase I awards are up to 100K for 9 months
- Phase II awards are up to 750K for 2 years
- For more information: www.science.doe.gov/sbir

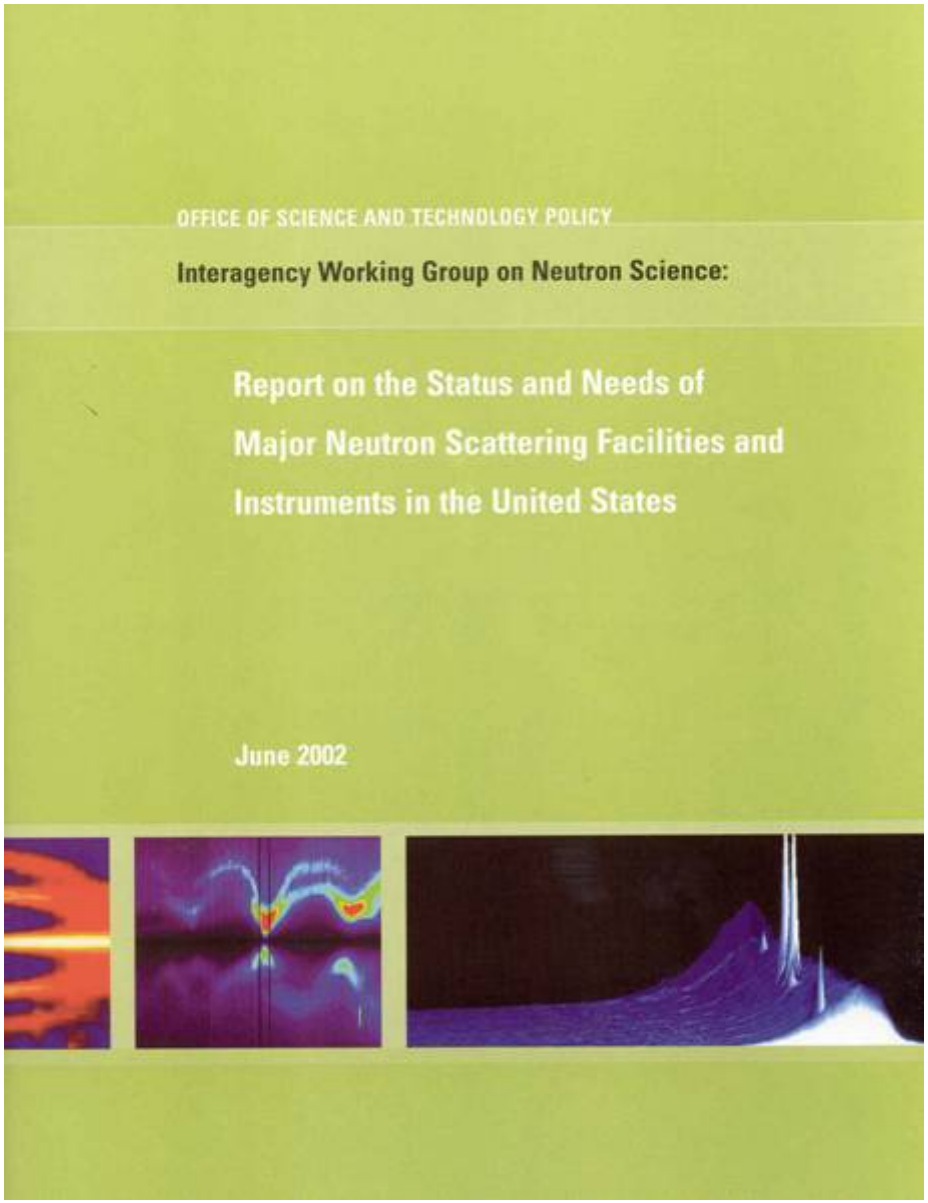


Assessing the Status and Needs of the Nation's Neutron Scattering Facilities and Instruments

The OSTP Interagency Working Group on Neutron Science

"… make recommendations to maximize the availability, use and impact of these facilities to the US science program. The IWG should consider, but not be limited by, the following questions:

1. Are existing neutron facilities scheduled to operate at the maximum extent possible and do they have the resources to meet that schedule?
2. What are the available opportunities to provide needed state-of-the art scientific capabilities at these facilities?
3. What are the issues facing users of neutron facilities and what can be done to maximize the scientific impact of these facilities?"



http://www.ostp.gov/html/NeutronIWGReport.pdf

Recommendations

Support robust user facility operations

"… The highest priority for federal investments in neutron scattering is to fully exploit the best U.S. neutron source capabilities – including the SNS – for the benefit of the broadest possible scientific community.

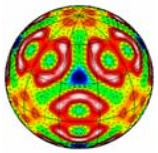
Specifically:

Fully develop at least 85% of available beam lines with neutron instrumentation that exceeds, or is at least competitive with international best-in-class instruments;

Maximize the amount of beam time made available to the the scientific community through an independent, peer-reviewed based general user program;

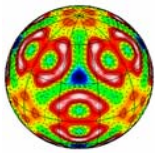
Provide resources to fully staff and support the high productivity operation of the instruments;

Provide additional support for research using neutron techniques.



Implementation Priorities

- Spallation Neutron Source
  - –develop Federal partnerships - DOE & NSF – to support state-of-the-art instrument suite
- NIST Center for Neutron Research
  - –seek increased support for user and research program
- High Flux Isotope Reactor
  - –support cold neutron and instrument upgrade projects

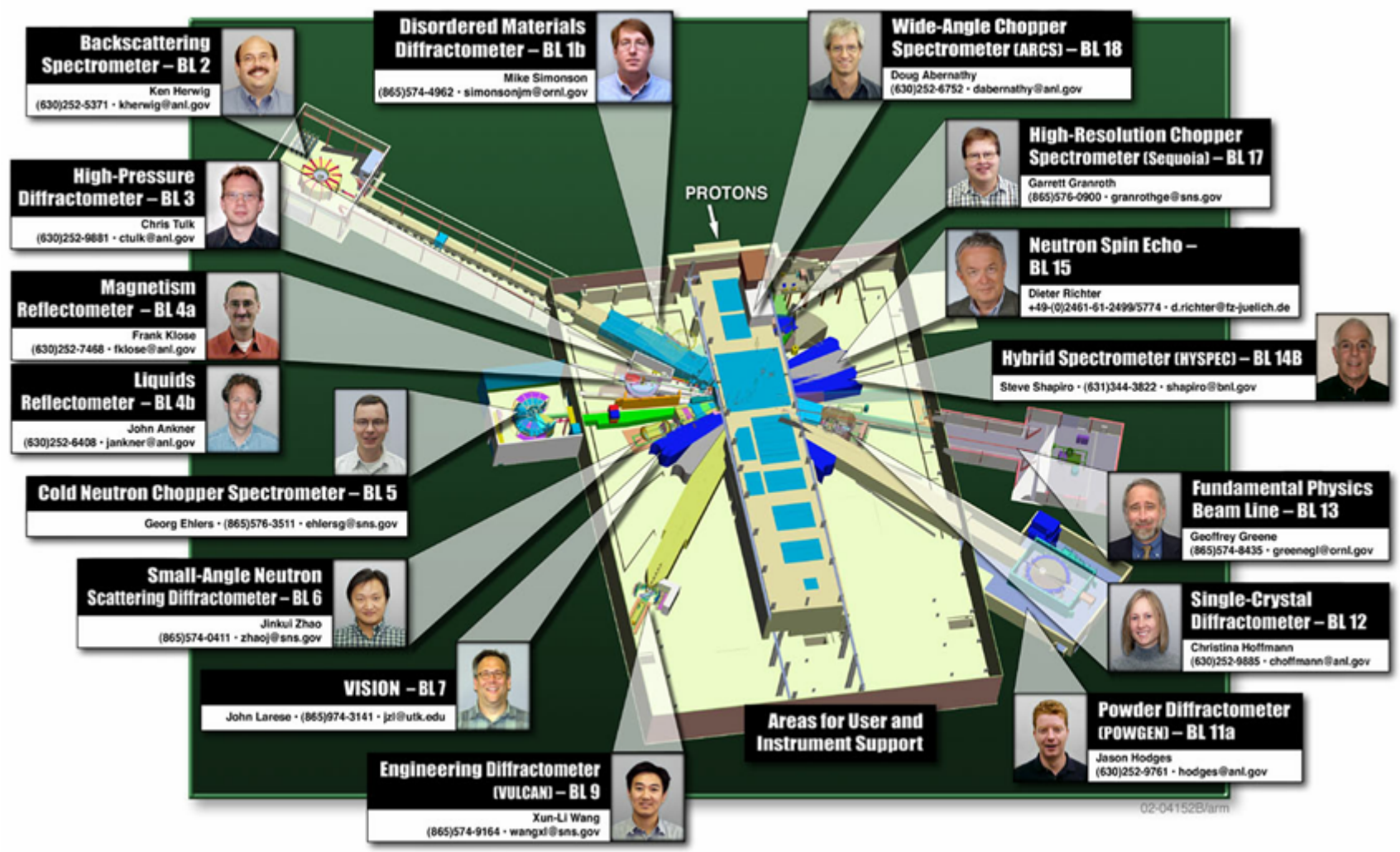


BES has committed to 5 additional SNS instruments

- Ultra High Pressure Diffractometer (SNAP)
  - –Atomic structure at pressures up to 100 GPa
- High Resolution Thermal Chopper Spectrometer (SEQUOIA)
  - –Atomic-scale dynamics at thermal and epithermal energies, with emphasis on magnetic scattering from single crystals
- Single Crystal Diffractometer (SCD)
  - –Rapid atomic structure in moderate-unit-cell single-crystal samples
- Disordered Materials Diffractometer (NOMAD)
  - –Atomic scale structure of liquids, glasses, and disordered crystals
- Hybrid Spectrometer (HYSPEC)
  - –Inelastic and elastic neutron spectroscopy of single crystals with polarization analysis capability

Plus Instrument concepts for SERGIS and DSD

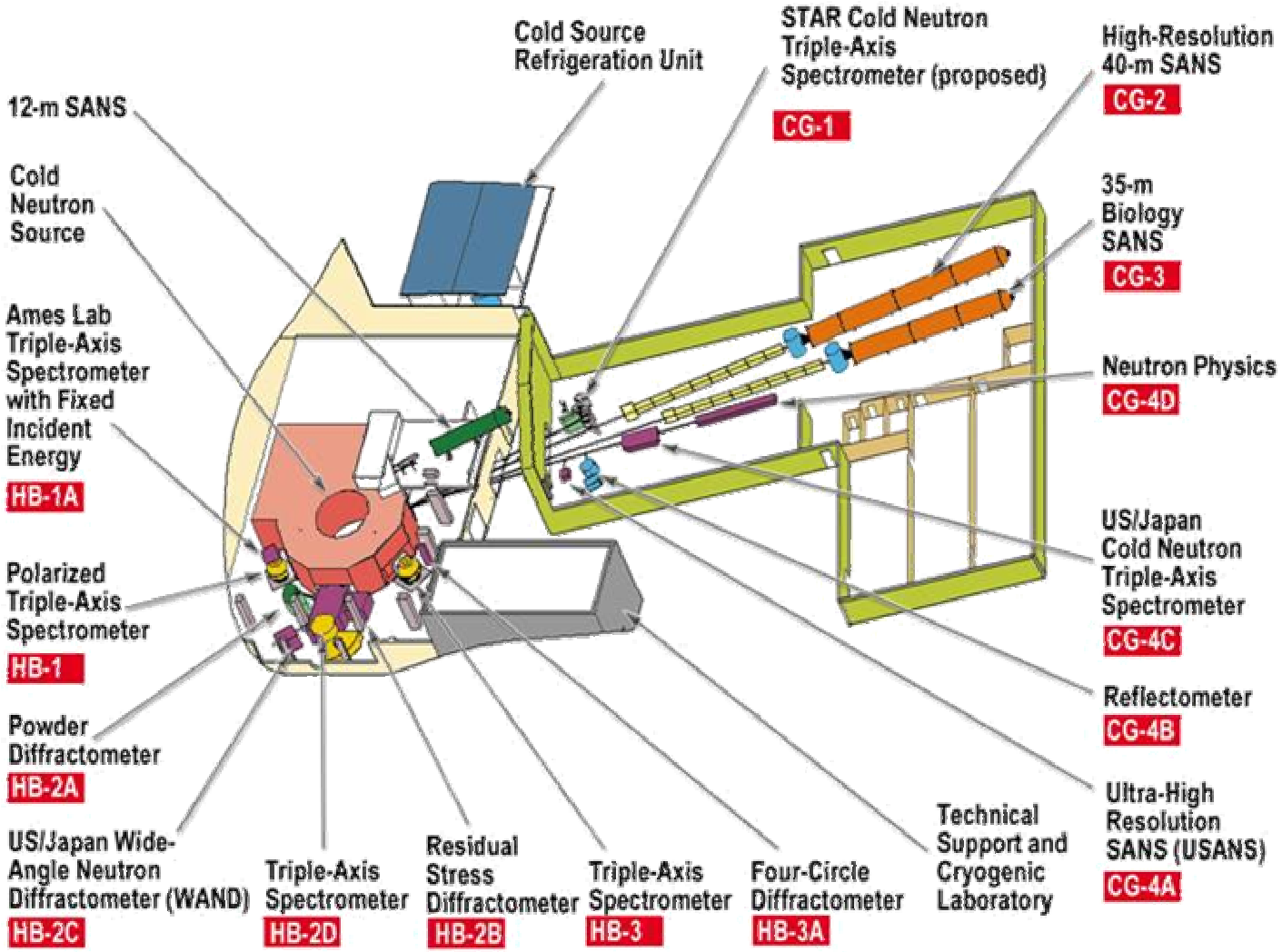
16 Instruments Now Formally Approved



Neutron Scattering Upgrades at HFIR

The upgraded HFIR will include 15 state-of-the-art instruments on some of the world's most intense steady-state neutron beams

- New SANS cold guide hall
- Cold source brightness comparable to the world's best
- New and upgraded instruments
- Thermal neutron intensities 2-3 times world's best for many experiments
- Formal user program instituted, which is the same as the SNS
- 3 thermal instruments on-line



The DOE fully supports the cold source and instrument upgrade project

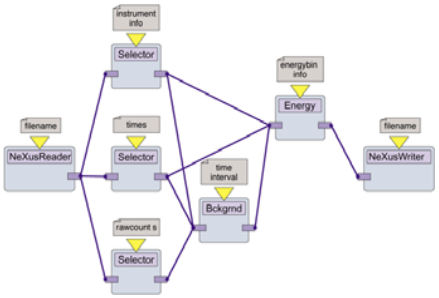
Partnerships Mechanisms and Activities

- American Neutron Scattering Conferences
  - –First conference held June 2002 with over 400 participants
  - –Next conference June 2004 in College Park, MD
- North American Neutron Facility Director Interactions
  - –First meeting Jan. 16-17, 2003
  - –best practices, forum for collaboration and coordination
- Joint Inter-Facility Workshops in Enabling Technologies
  - –co-funding by NSF, DOE and NIST
  - –polarized neutrons, detectors, sample environment, software

Development of Supporting Technologies

- **Detectors**
  - –White paper
  - –2nd US workshop held May 29-30 (DOE/NSF supported)
  - –Executive committee formed
  - –Proposals to BES/NSF
  - –In-house development

- **Polarized Neutrons**
  - –PPN workshop held in February (DOE/NSF funded)
  - –Term position at SNS
- **Sample Environment**
  - –SENSE workshop planned for September (NSF supported)
  - –High Field Magnet proposal sent to NSF
- **Software**
  - –DANSE white paper (CalTech)
  - –NSF proposal “Bringing Neutrons to the Teragrid”



Coordinating efforts with European and Japanese development programs