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Argonne Scattering, Imaging and Spectroscopy Institute

(ASISI)

Raymond Osborn
*James W. Richardson**
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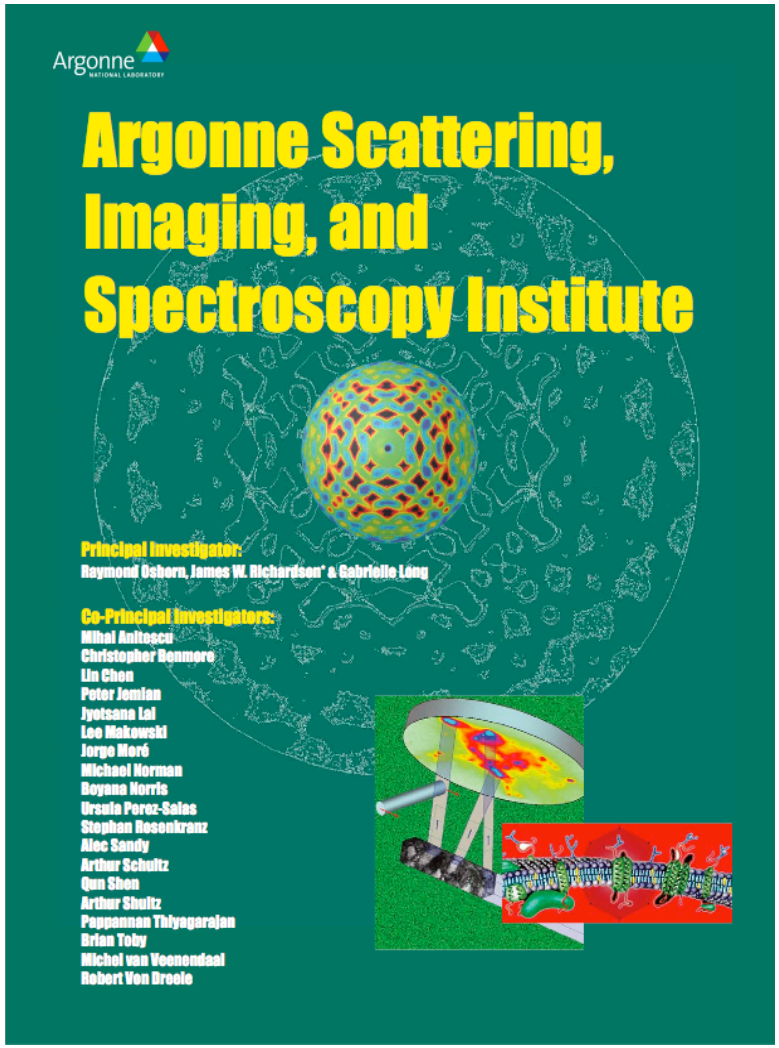
MSD	*SNS*
(PNS)	*Lujan*
CSE	*ESRF*
BIO	*NSLS*
XSD	*ALS*
MCS	*SSRL*
AES	*LCLS*
. . .	*. . .*

**deceased*



The proposal to build ASISI at ANL

- Institute sited at Argonne in support of US Scattering, Imaging and Spectroscopy

- "***The goal of the Argonne Scattering, Imaging and Spectroscopy Institute is to address grand challenges in materials science that involve the use of x rays, neutrons, and electrons and build a theoretical and computational infrastructure that will benefit the entire materials science community.***"

- Project orientation (4 - 6 projects, 2 - 3 new/year)
  - General community initiation and participation
- Holistic approach to scientific problems
  - Linking theory/simulation more closely with scattering, imaging, spectroscopy
  - New algorithms that incorporate constraints from x ray, neutron and electron scattering
  - New algorithms for new science with new instrumentation
  - Visualization
- Establish stronger ties with large-scale computing
  - Resources for theory/simulation calculations
  - Eventually, on-line analysis during measurements (semi-continuous access)
- Develop professional software for the general community
  - Large group of professional programmers working closely with scientists

Brief history of ASISI

- Presentation by Ray Osborn (MSD) to Pat Dehmer and Pedro Montana. With Pat's encouragement, we sent in a white paper, and then were invited to submit a full **ASI** proposal.

- Jim Richardson and Ray Teller visited the US neutron facilities, and Ray Osborn, Jim Richardson, Gabrielle Long, George Crabtree visited the x-ray facilities. We also shared the **ASII** proposal with Bill Stirling and Sine Larsen.
  - good discussion
  - endorsements

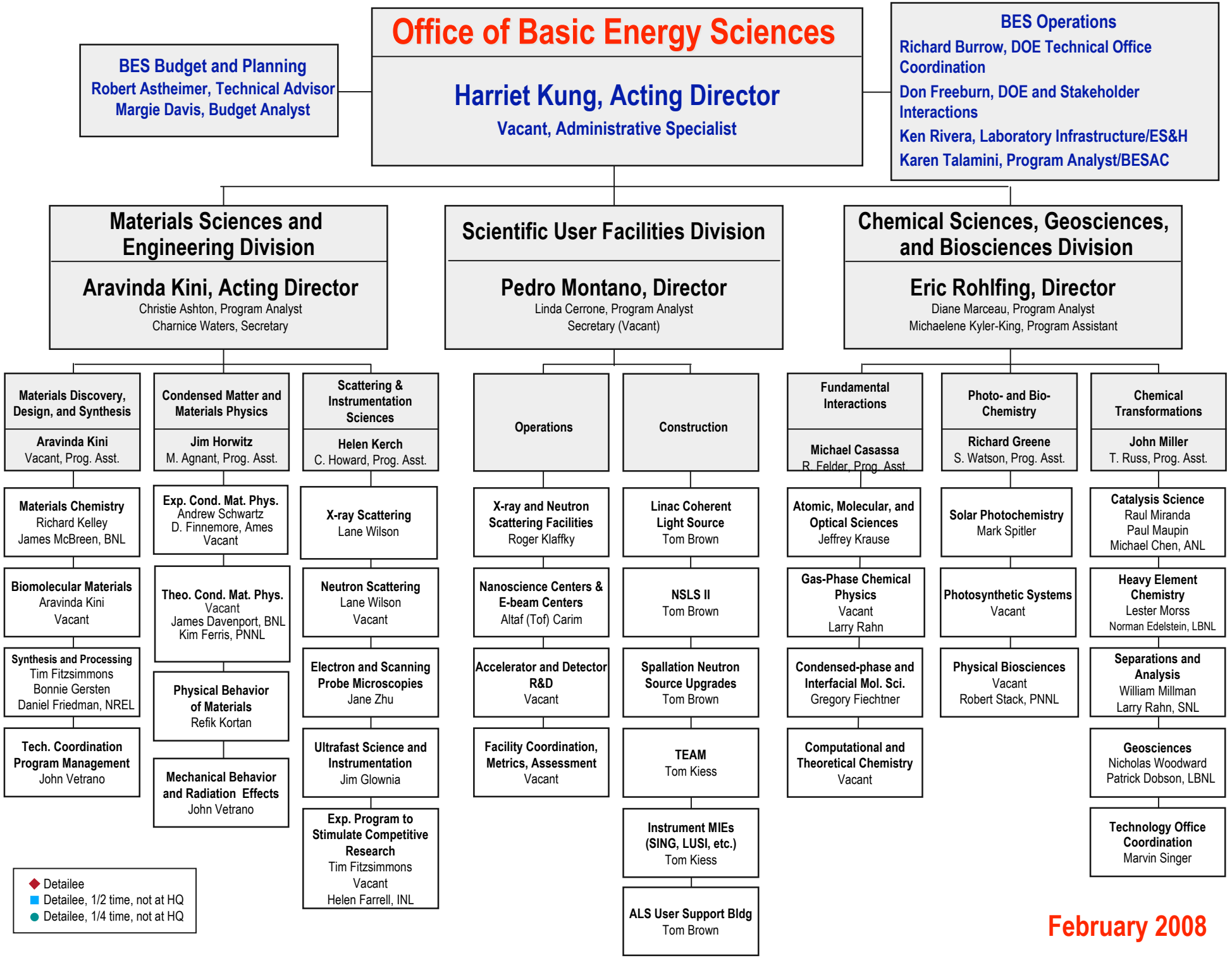
- At over **$18M**, the first proposal was regarded as too costly, so a second version **ASISI** was prepared.
  - improved focus on the connections between the APS, MCS and the research divisions
  - greater detail on the proposed organization
  - cost now just over **$12M**

- Next steps are to bring together the community outside the facilities with a series of workshops
  - draw endorsements from broader scientific base

The landscape in the US and in the world

- Examples in the US
  - Joint Institute for Neutron Science (JINS) adjacent to the SNS at ORNL
  - Joint Photon Sciences Institute (JPSI) adjacent to NSLS-II (in planning) at BNL
  - Photon Ultra-fast Laser Science and Engineering (PULSE) associated with the LCLS at Stanford
  - DANSE (Data Analysis for Neutron Scattering Experiments) $11M over 5 years from the NSF

- Example in Germany
- Current and future activities at DESY in Hamburg
  - Doris III
  - PETRA III
  - FLASH
  - euro-XFEL
  - CFEL
    - *50 M€ from the City of Hamburg for the CFEL building (to be completed 2010)*
    - *Space for ≈ 300 people*
    - *Four experimental core groups (Max Planck Gesellschaft and the University of Hamburg) and one theory core group plus . . .*
    - *Three independent Junior Research Groups from MPG and Advanced Study Groups from MPG and the University of Hamburg*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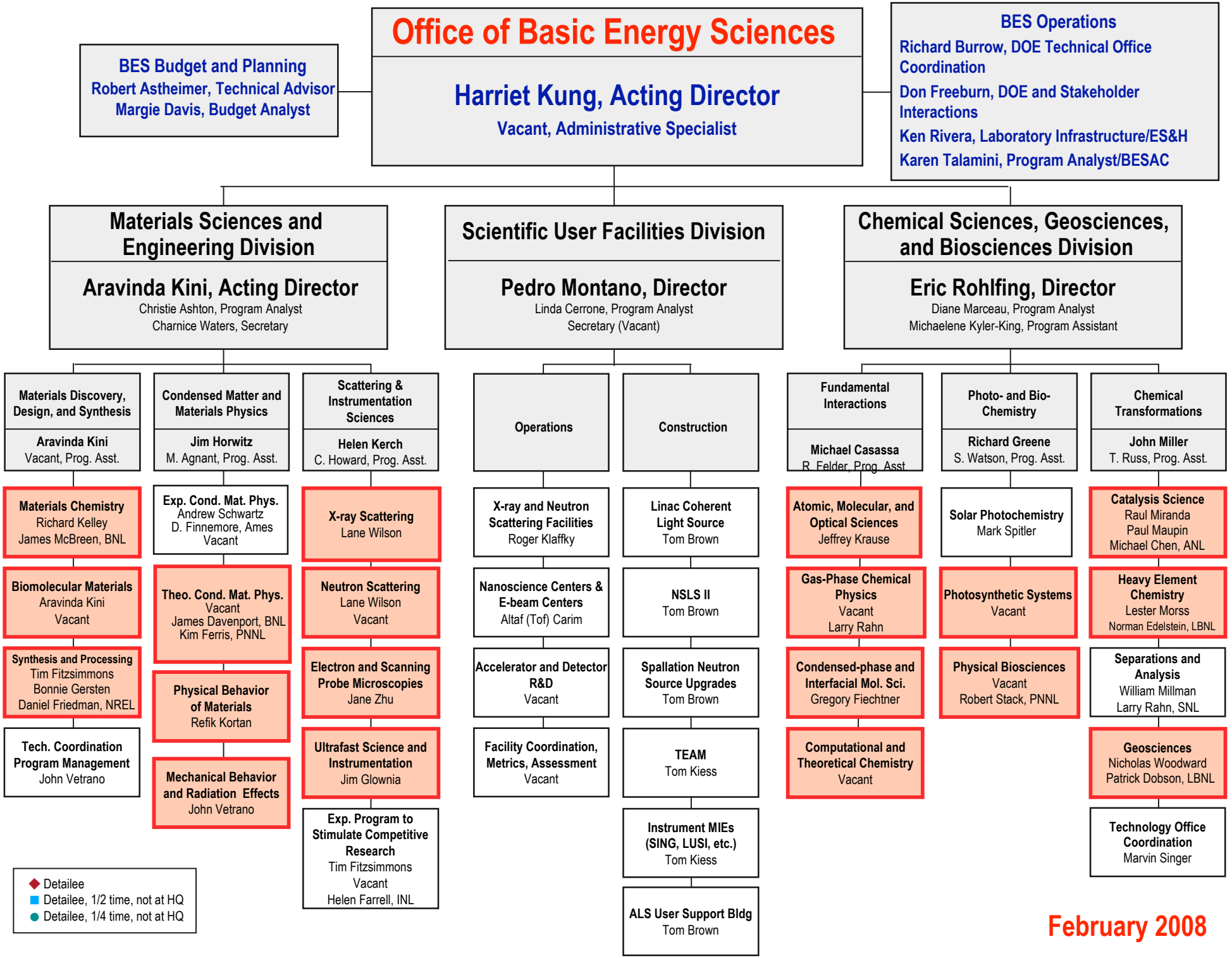
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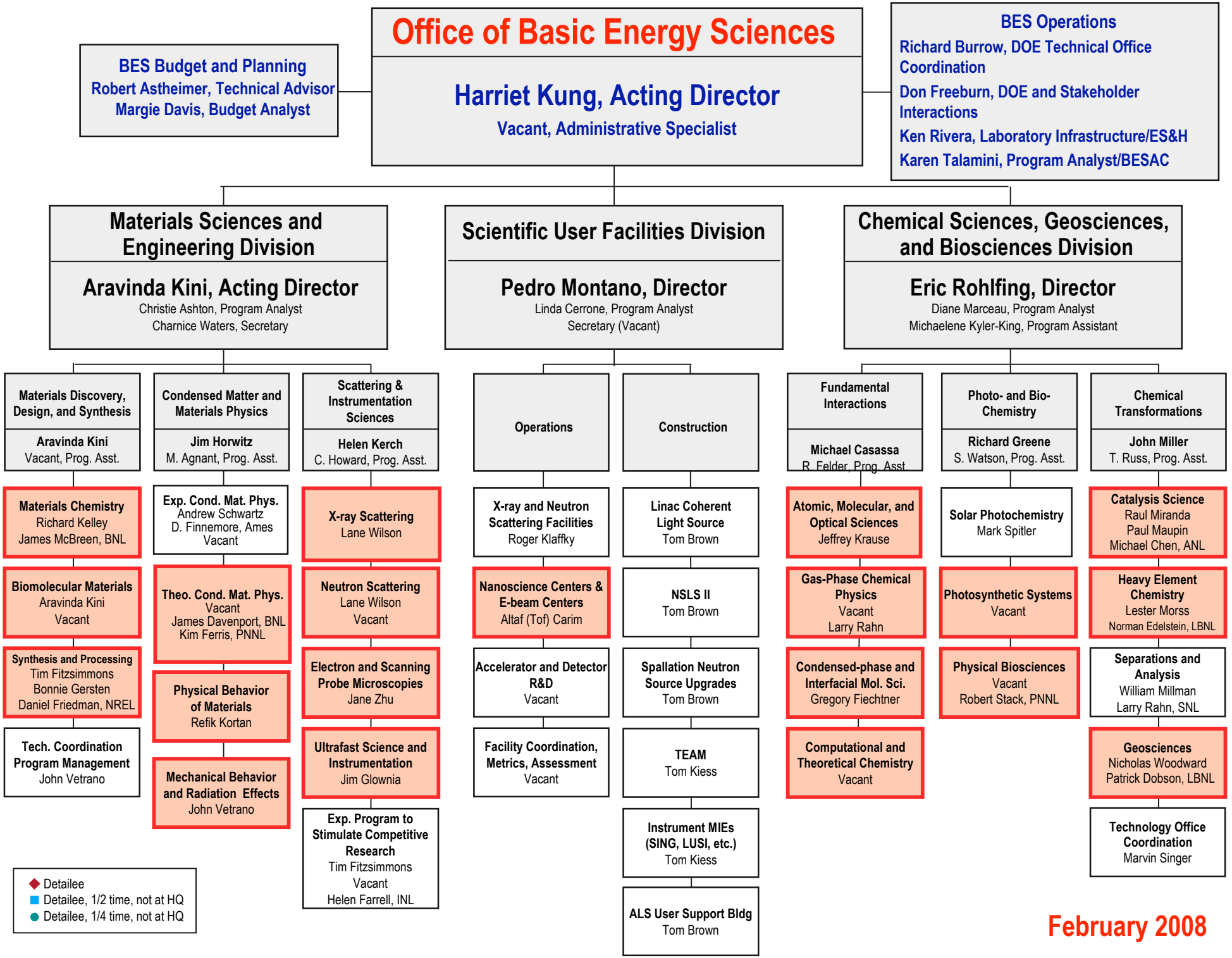
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ASISI operation

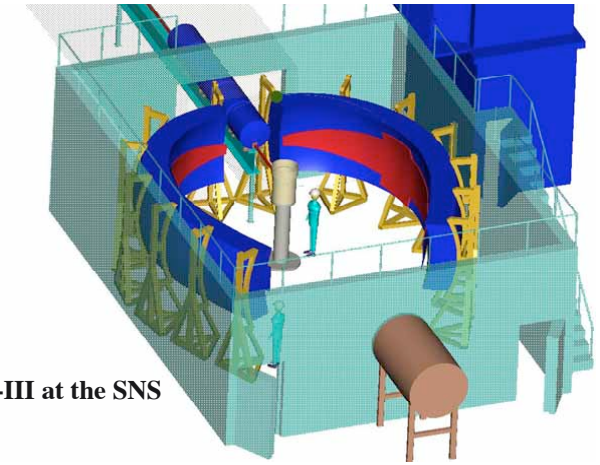
- ***"The goal of the Argonne Scattering, Imaging and Spectroscopy Institute is to address grand challenges in materials science that involve the use of x rays, neutrons, and electrons and build a theoretical and computational infrastructure that will benefit the entire materials science community."***

- ASISI will invite proposals for limited-term projects to tackle scientific "grand challenges."
- Proposals will go to a broadly based Evaluation Committee that will rank the projects using three criteria:
  - The importance of the scientific problem.
  - The need for multidisciplinary support.
  - The breadth of the community that would benefit.

- ASISI will then set up teams to work with the PI's and provide
  - **Theory, numerical analysis and visualization expertise, and computational support**

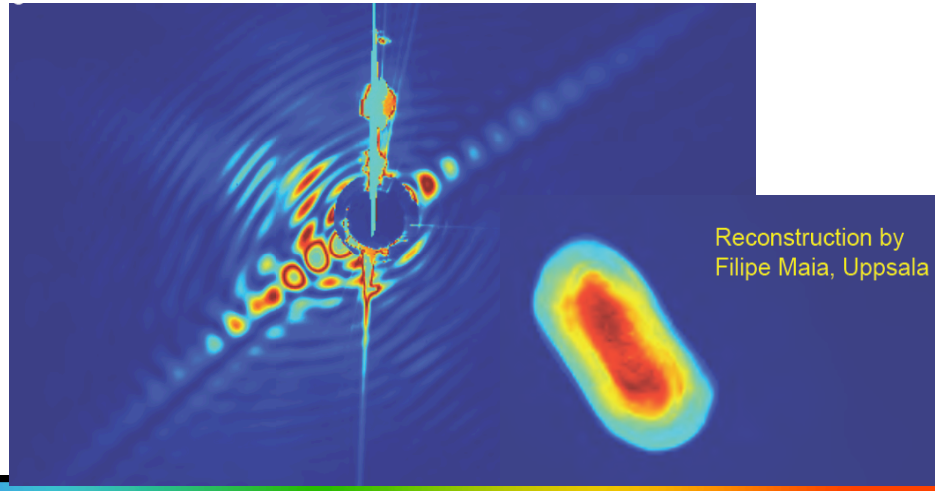
Project Matrix

- Multidisciplinary teams will be assigned to each project drawn from three groups:
  - Scattering, Imaging, Spectroscopy Theory Group
  - Numerical Analysis and Visualization Group
  - Software Engineering Group
- Core programs will be established to maintain existing code and ensure the longevity of the software that is developed



POWGEN-III at the SNS

- GSAS-II core program
  - Converting GSAS to a modern component-model codebase
  - Combining crystallography and PDF
  - Adding constraints from XAFS, NMR, . . .
- Coherent Diffraction Imaging
  - Establishing a unified platform for
  - experiments
  - Encoding phase retrieval algorithms
  - Solving the missing data problem



live picoplankton - A Barty, H Chapman

Community Interactions

- ASISI should have the resources to play a significant role in promoting software development within the community.
  - All software will be open source, multi-platform, and well documented.

Professor David Bish using GSAS (& EXPGUI) north of the Arctic Circle. Adjacent to his left shoulder is a prototype of an x-ray diffractometer (CheMin IV) that will fly on the 2009 Mars Rover; above his right shoulder is a rifle for protection from polar bears. [David Bish, University of Indiana]

- ASISI will establish lines of communication with the major facilities
  - in the US
  - around the world
- The plan is for ASISI to stimulate more investment in scientific software at facilities
- ASISI will support emerging standards
- Stay tuned for the upcoming ASISI workshops !

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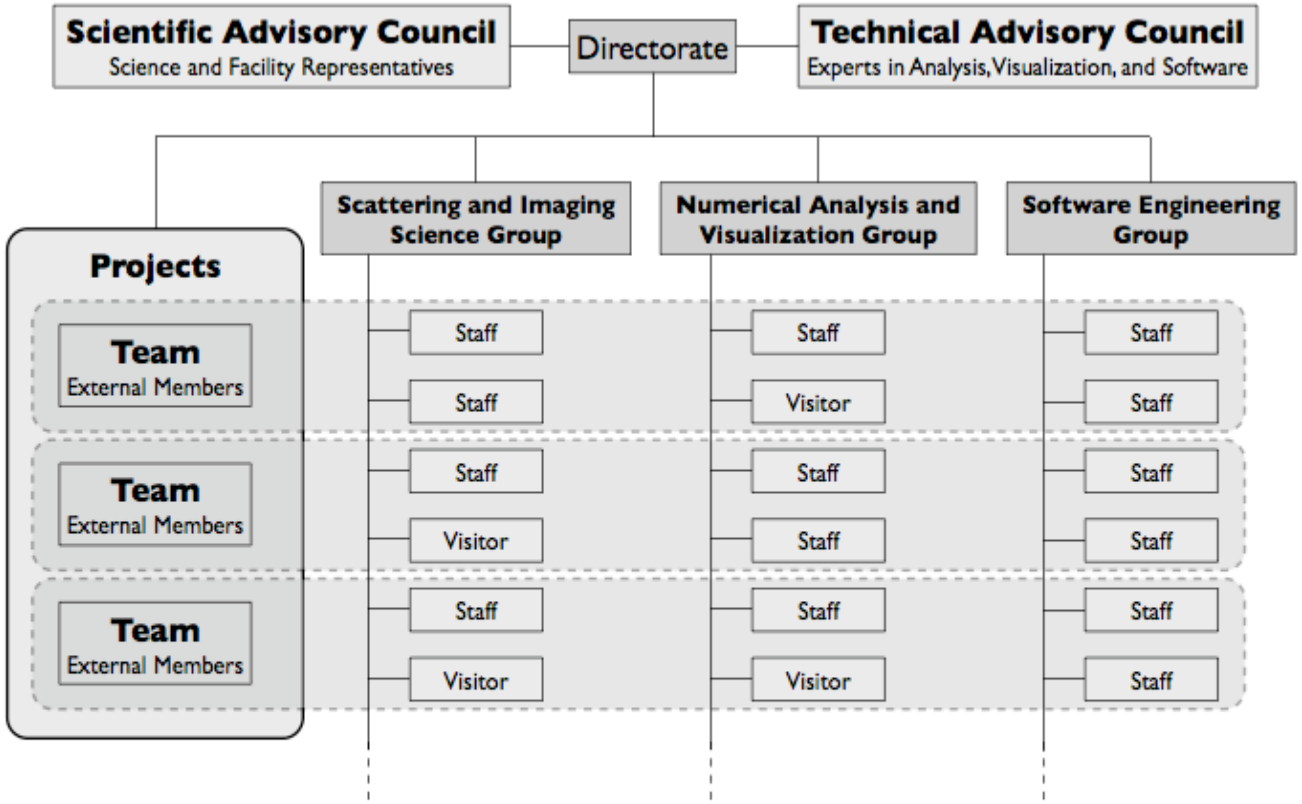
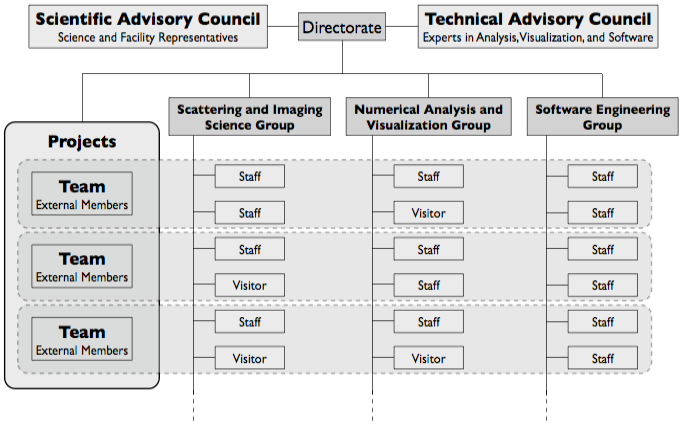


Numerical Analysis and Visualization Group

- Allows ASISI to take advantage of the latest developments in numerical analysis and advanced visualization.
- Enhances interaction between the major DOE facilities.
- Responsible for developing:
  - new algorithms
  - optimization techniques
  - advanced statistical analysis
  - methods of automated data mining
  - multi-dimensional histogramming
  - data inversion
  - image reconstruction
  - integrating sparse data
  - visualizing embedded dispersion surfaces and E
  - parallelization



- The group will have a combination of
  - computational scientists with research responsibilities
  - non-research staff with primary responsibilities for software and technique development.
- This group will receive high-level advice from the Technical Advisory Council.

Software Engineering Group

- ASISI will provide advanced software engineering support
  - required software is computationally intensive
  - it requires advanced code parallelization or grid computing techniques
- The software will be developed within a coherent framework using the best practices of software engineering so that it is
  - easy to maintain
  - compatible with modules developed by other projects
  - platform-independent
  - user friendly
  - well documented.
- This group will consist of professional software engineers, who will be responsible for developing and maintaining the “community code” developed through the projects.
- They will ensure that the computational infrastructure developed by ASISI will serve the needs of the overall U.S. scattering and imaging community, and not just the immediate needs of each project.