Argonne NATIONAL LABORATORY

... for a brighter future

IPNS Status Update

including the Argonne Scattering and Imaging Institute (ASI^2) initiative

Raymond Teller
Director
Intense Pulsed Neutron Source
Argonne National Laboratory

Argonne User's Meeting, May 2007

U.S. Department of Energy

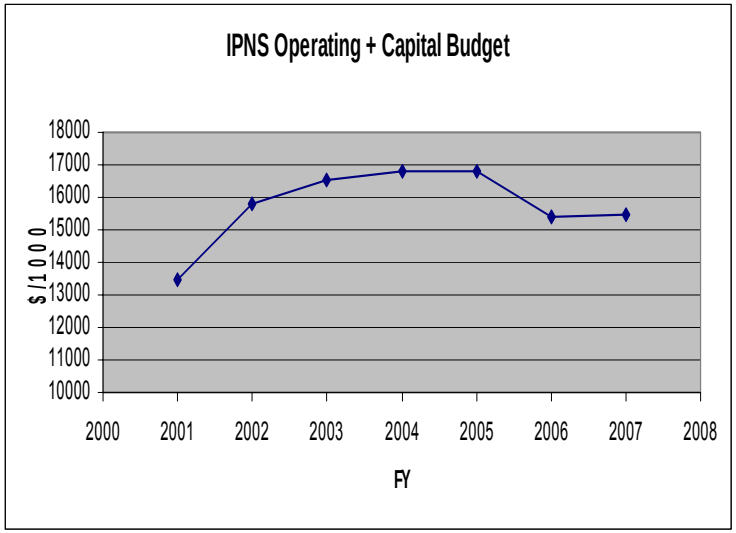
UChicago Argonne LLC

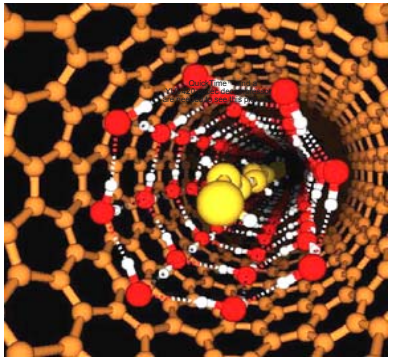
Office of Science
U.S. DEPARTMENT OF ENERGY

A U.S. Department of Energy laboratory managed by UChicago Argonne, LLC

IPNS operating status

- **Neutron operations**
  - Reliable and efficient
  - 8 of 13 instruments in user program
  - Most instruments improved-5 years-ave gain ~x7
- **FY06 user program statistics**
  - 24 weeks of operation at 96.5% accelerator reliability
  - ~350 experiments performed by 328 users (including visiting and remote access users)
- **FY07 and FY08 user program**
  - 18 weeks scheduled for FY07 and FY08
- **IPNS remains scientifically productive**
  - FY06: ~140 peer-reviewed publications
  - 2003-2005: 124 different journals
  - ~10% in journals with Impact Factor ≥ *Phys. Rev. Letters*
  - >35% in journals with ISI Impact Factor ≥ *Phys. Rev. B*
  - Top twenty publications: 318 citations; average = 16 (10 IPNS instruments represented)

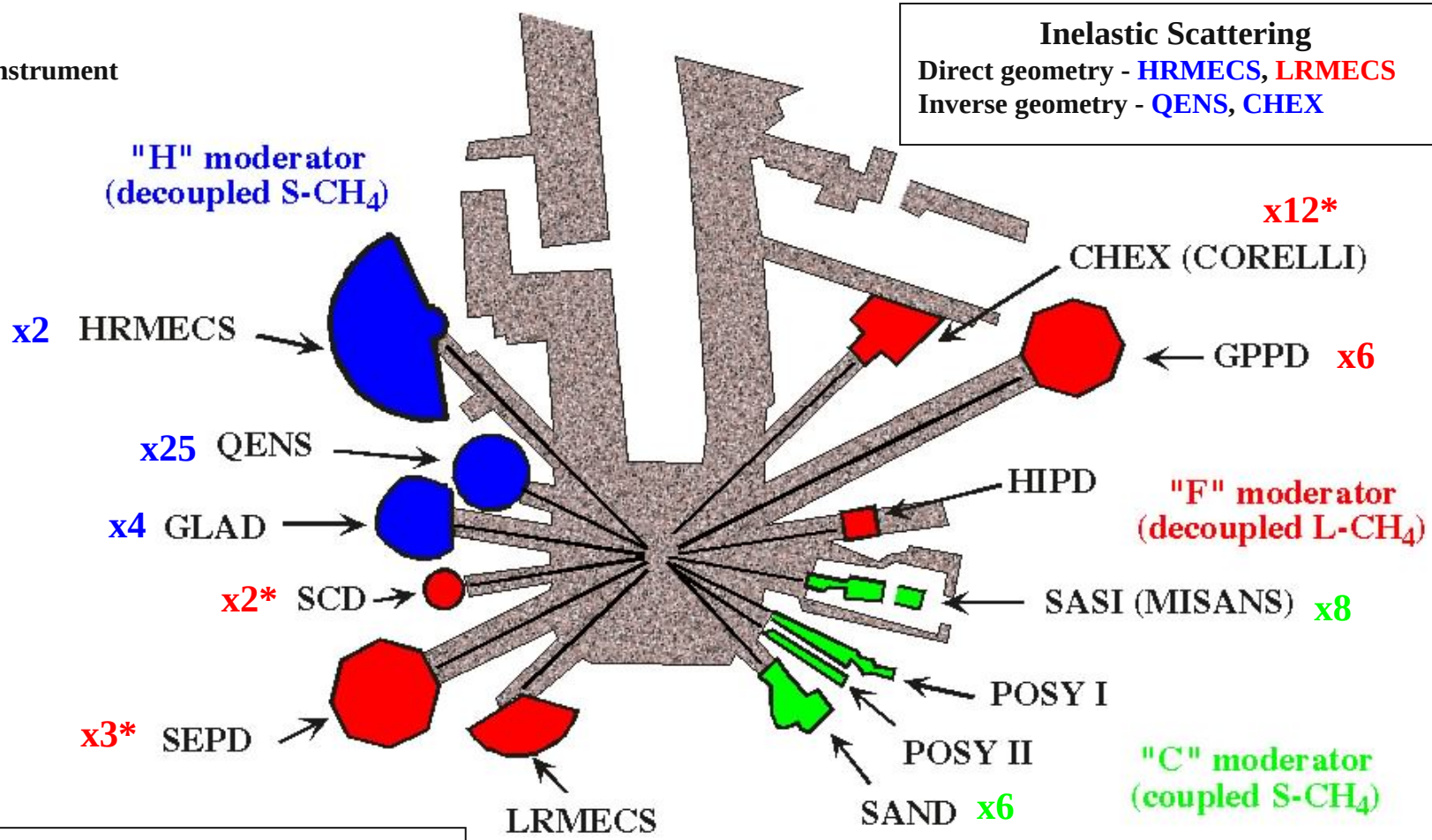




IPNS Instrument Suite

* New instrument

Inelastic Scattering
Direct geometry - HRMECS, LRMECS
Inverse geometry - QENS, CHEX

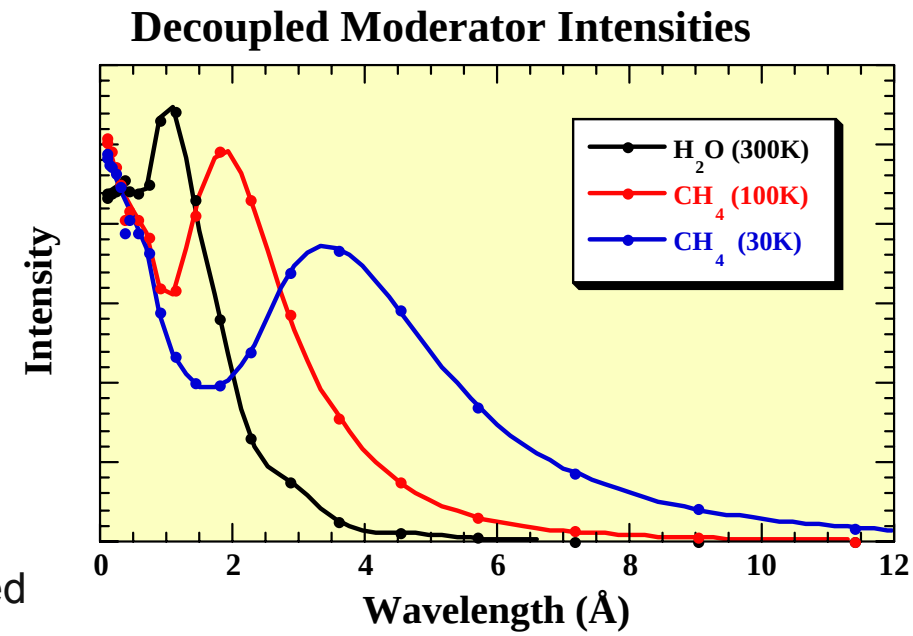


Diffraction
Powder diffraction - SEPD, GPPD, HIPD
Single crystal - SCD
Liquids and Amorphous Materials - GLAD

Large Scale Structures
Small Angle Scattering - SAND, SASI
Reflectometry - POSY I, POSY II

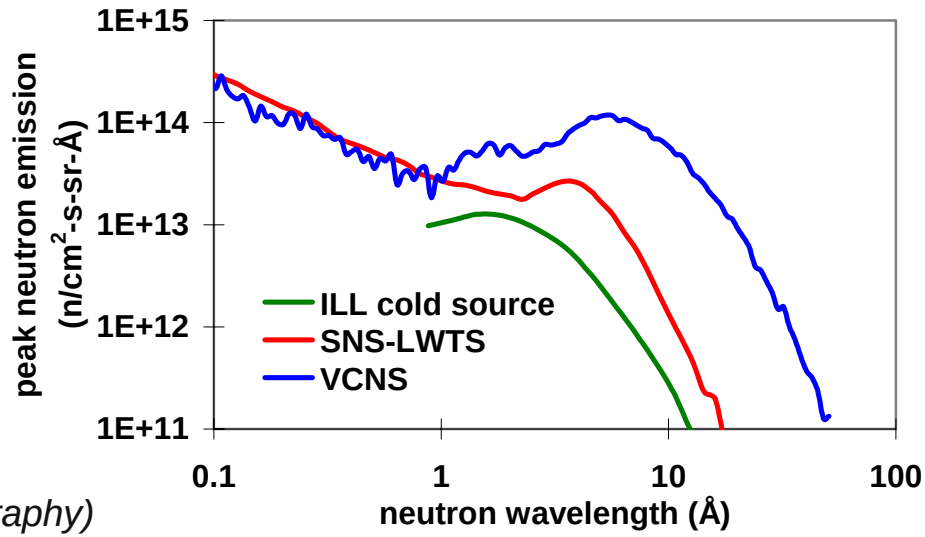
Instrumentation - unique in US

- **Cold moderators**
  - Coupled and decoupled S-CH_4 (~30K) and decoupled L-CH_4 (~100K)
- **Inelastic scattering**
  - QENS - Broad Q-range spectroscopy with diffraction
- **Small-angle scattering**
  - SAND - broad Q-range: 0.0035 - 2 $Å^{-1}$
  - SASI / MISANS - combined SANS and spectroscopy
- **Reflectometry**
  - POSY I - xyz magnet
- **Diffraction**
  - GLAD - only diffractometer in US dedicated to amorphous materials
  - GPPD - with bandwidth chopper, capable of accessing long wavelengths (12A) with high resolution
  - Christina (under construction) - elastic diffuse scattering



New ANL-inspired instrument and source concepts

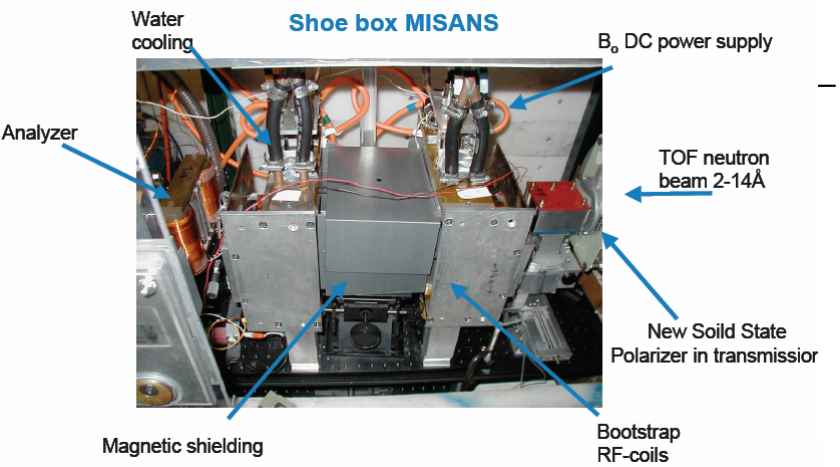
- **Possible future SNS instruments**
  - MaNDi - Large-scale structures (IPNS-ANL)
  - SERGIS - Spin-echo resolved grazing incidence neutron scattering (MSD-ANL, IUCF)
  - MISANS - Small angle scattering with MIEZE (IPNS-ANL)
  - CORELLI - Elastic diffuse scattering (MSD-ANL)
  - USANS - Ultra-small angle scattering (IPNS-ANL, SNS-ORNL, HFIR-ORNL)
- **Possible future neutron scattering source - VCNS**
  - The goal of the VCNS is an intense neutron source with peak flux around 20 Å and usable flux extending out to 100 Å)
  - A VCNS would:
    - *Address problems in fundamental nuclear physics (neutron half-life, EDM)*
    - *Study spin dynamics in magnetic nanostructured materials*
    - *Image the motion in proteins and molecular motors within living cells*
    - *Characterize hydrogen transport in storage and photoproduction materials*
    - *Exploit direct-imaging neutron techniques (microscopy, tomography, holography, radiography)*

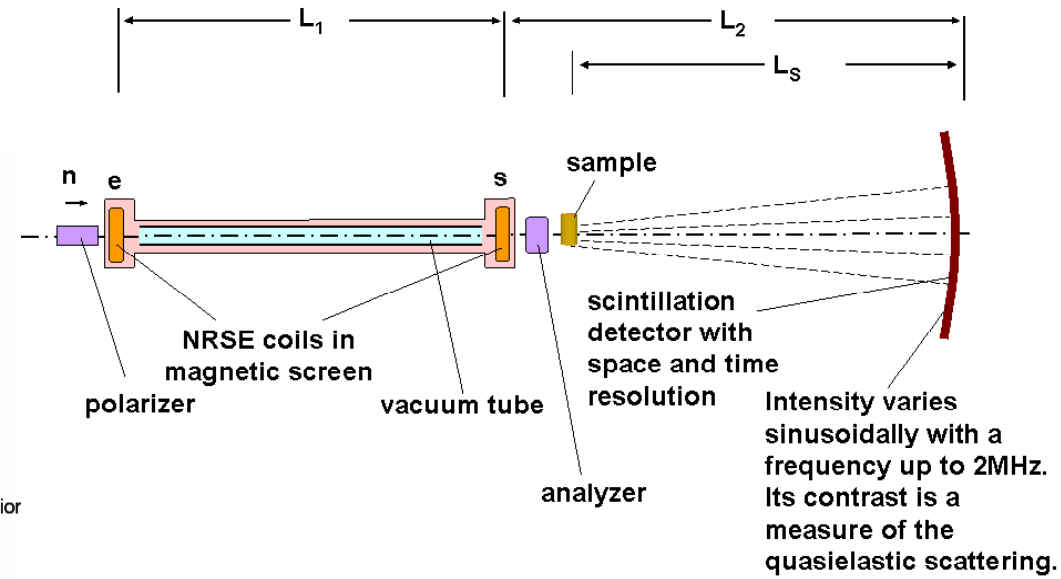


MISANS (Modulated Intensity Small Angle Neutron Spectrometer)

Effort led by Jyotsana Lal (Inst. Sci.), Ed Lang (SA), Markus Bleuel (post doc)

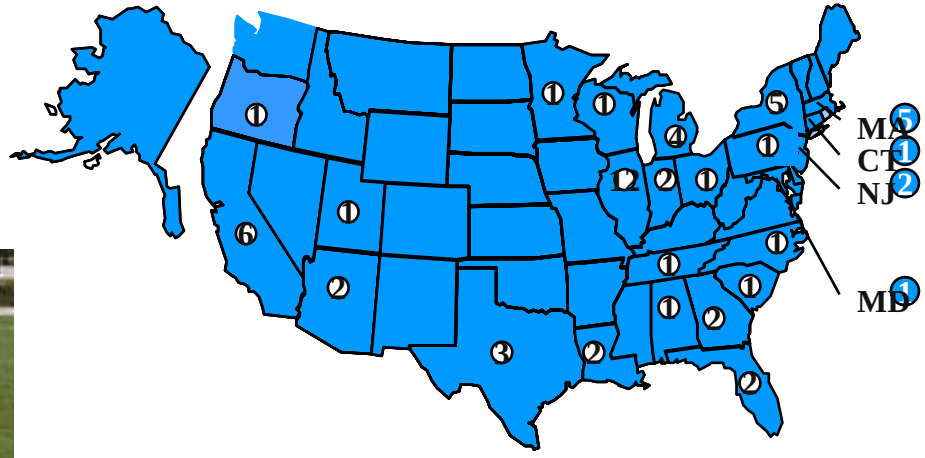
- **Prototype instrument at IPNS**
  - Polarizing capability added to SAD instrument (new name: SASI)
  - Adding neutron spin echo capability and test concept (1st of it's kind in the world)
  - Development of instrument for SNS (will require detector development)
- **Status:**
  - Polarization and modifications to beamline to accommodate optics complete
  - Prototype rf system in place
  - Proof of principle experiments: FY07-08

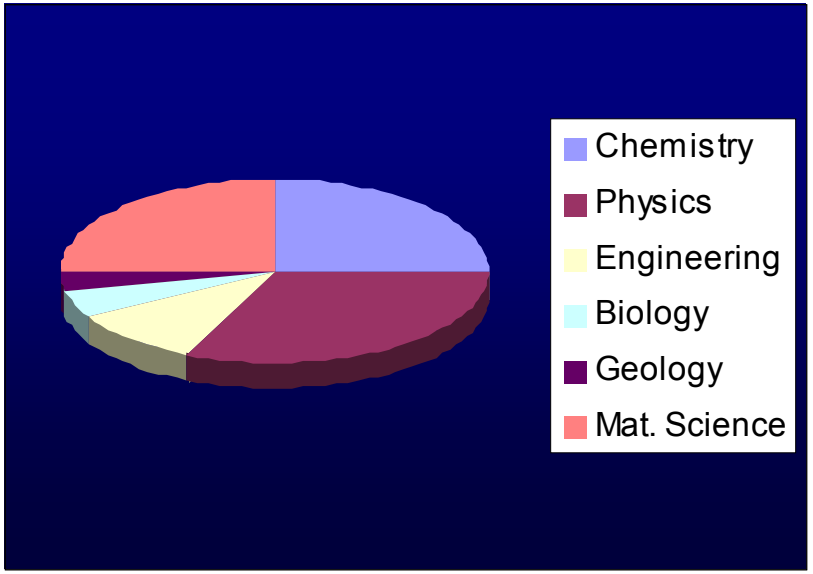




n-x School at ANL

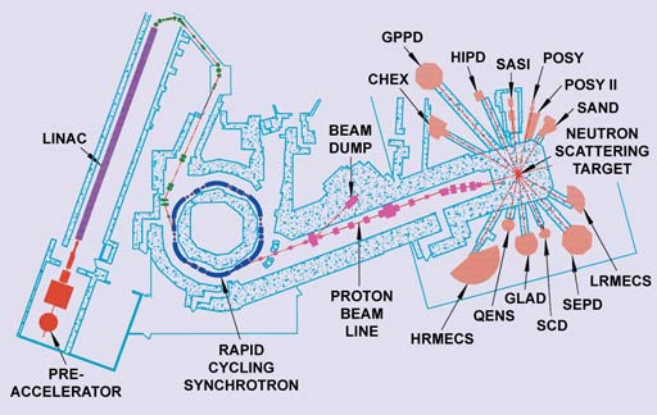
- **A model for educating students in the utility of neutrons and x-rays – 60 students/yr held August every year**



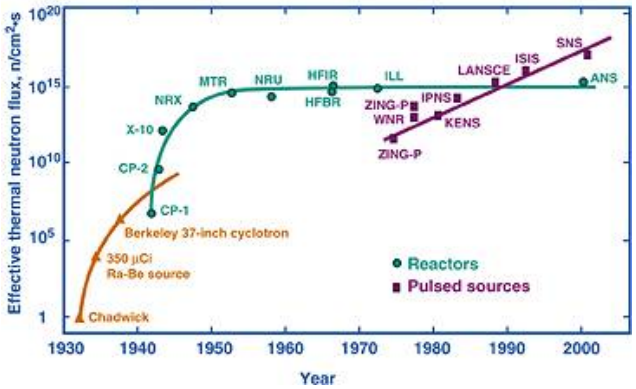


Summary

- **Instruments performing at highest capacity ever**
  - Enhancements for all major instruments completed over past 5+ years
  - World-class special environment capabilities, reasonably well-integrated
  - But, no funding for further improvements
- **Future operations**
  - Uncertain beyond FY08-09
- **Desired outcomes**
  - Retain key personnel for the benefit of Argonne
    - *: beamline staff, accelerator expertise*
    - *Transitions to APS - accelerator group moved Feb. 2007*



Something Completely Different: Argonne Scattering and Imaging Institute (ASI^2) Initiative

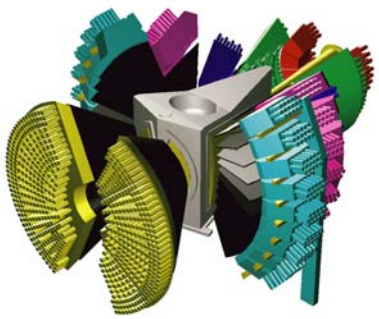


- **ASI^2 aspires to:**
  - Become a driver for new discoveries through more effective use of scattering data
  - Become a leading innovator in scattering theory, simulation and analysis, data visualization, and instrumentation design
  - Host community scattering data analysis development through creation of large group of dedicated scientists and programmers
  - Create strong but flexible interfaces with major US facilities and scattering research groups at DOE laboratories and universities

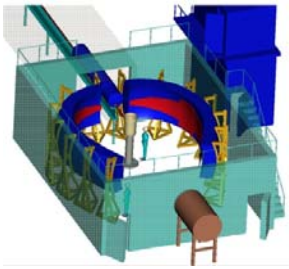
D1a (ILL) 1978

12 detectors
0.1m^2

GEM (ISIS) 2000



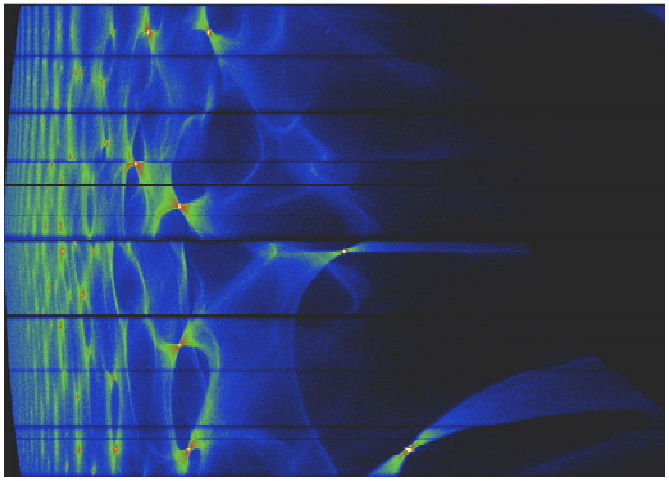
10,000 detectors
10m^2



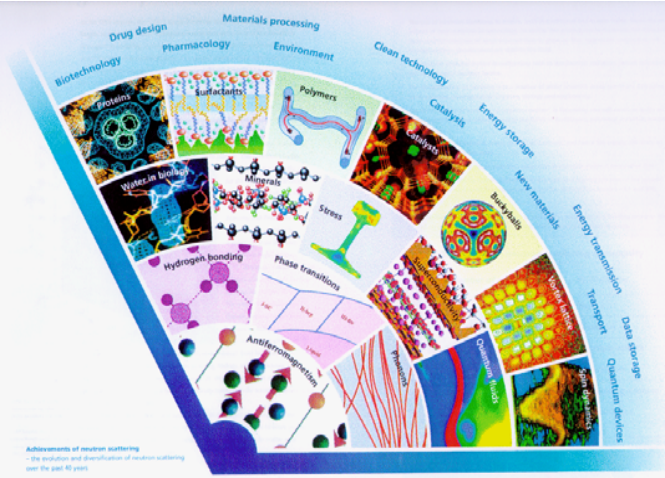
POWGEN3 (SNS) 2006

240,000 detectors
47m^2

Si single crystal on GPPD - 1.8 Mpixels



Motivations for ASI^2 (why ANL is interested)



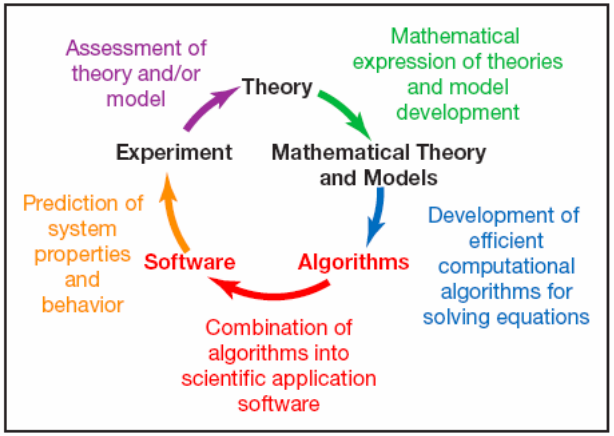
- **Sustain strong scattering presence in Midwest**
  - Needed to leverage opportunities at US facilities
  - Many ANL programs rely on scattering resources
- **Relevant to highest priority missions at DOE**
  - Hydrogen, solar, catalysis, nano-technology, nuclear
  - Facilities development
  - Large-scale computing - LCF (Leadership-class Computing Facility)
- **Partnerships with SNS/HFIR, APS - common needs, requirements**
  - ~60% of US neutron scattering instrumentation at ORNL in ~2020
  - ~50% of US neutron/x-ray instrumentation and funding at SNS+APS
  - Explore ways to make collaborative scattering science at facilities more efficient and effective
  - Simultaneous measurements with multiple probes
- **Time is right**
  - APS taking responsibility of more instruments and beginning to focus seriously on software needs
  - SNS has DANSE project (NSF funded), but minor emphasis at SNS for many years

How ASI² will operate

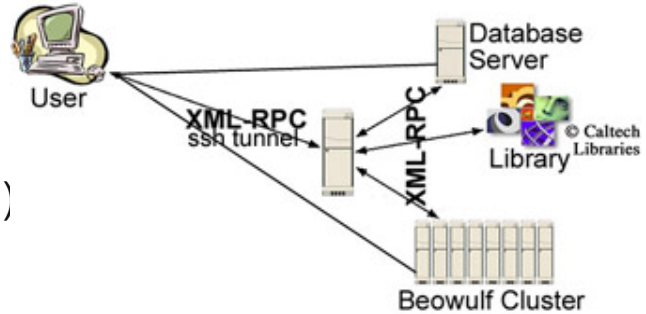
- **Staffing**
  - Scientists – experimental scatterers, theory, simulation, numerical analysis
  - Software engineers - simulation, analysis, visualization, porting to parallel computing
- **Project orientation**
  - Analysis and visualization for immediate facility needs
  - Theory and simulation to match expanding experimental scope - eventually on-line
- **Three imperatives:**
  - ***Guidance*** from BES user facilities to insure compatibility and integration of the institute with facility goals
  - ***Science-driven*** as defined by DOE grand challenges and in BES workshop reports
  - ***Software*** development and maintenance as required by the scattering community and to meet DOE grand challenges
- **ASI² scientific portfolio - much already defined by DOE/BES**
  - *Can we transform data collection at BES user facilities into "**discovery**" experiments?*
  - *Can we understand the details of **catalytic processes**?*
  - *Can we develop the tools to routinely solve structures of **nano-materials**?*
  - *Can we finally understand **correlated electron systems**?*
  - *Can we understand the limitations of current and future **hydrogen storage** devices?*
  - *Can the fundamentals of **solar energy** conversion be understood?*

Benefits of ASI^2 to the whole scattering community

- **Development of an integrated computational infrastructure**
  - ASI^2 will provide a scalable data analysis architecture for combining scattering and imaging experiments
    - *from laptops to advanced computing facilities (LCF, Grid,...)*
- **Leadership role in the scattering community**
  - DANSE is a project with similar goals to ASI^2 but insufficient resources
    - *NSF-funding to multiple institutions ($2.4M/yr over five years)*
- **Vertical integration**
  - Starting from the ground up means never building higher than the 1st floor
- **Professional software development**
  - Scattering scientists determine and guide project goals
  - Software engineers ensure well-structured, well-documented solutions
- **Principal investgators**
  - Ray Osborn (MSD-ANL), Jim Richardson (IPNS-ANL) Gabrielle Long (APS-ANL)



from Opportunities for Discovery: Theory and Computation in Basic Energy Sciences, January, 2005



Summary

- **ASI^2 will:**
  - Enable more efficient and effective scattering experiments
  - Serve common needs of neutron and x-ray scattering communities
  - Help insure close coordination between facilities and scattering community
  - Produce world-class science
- **Status**
  - DOE requested an ASI2 White paper (Mar ’07)
  - White paper accepted, full proposal requested (May ’07)