

The Role of Software at Scientific User Facilities

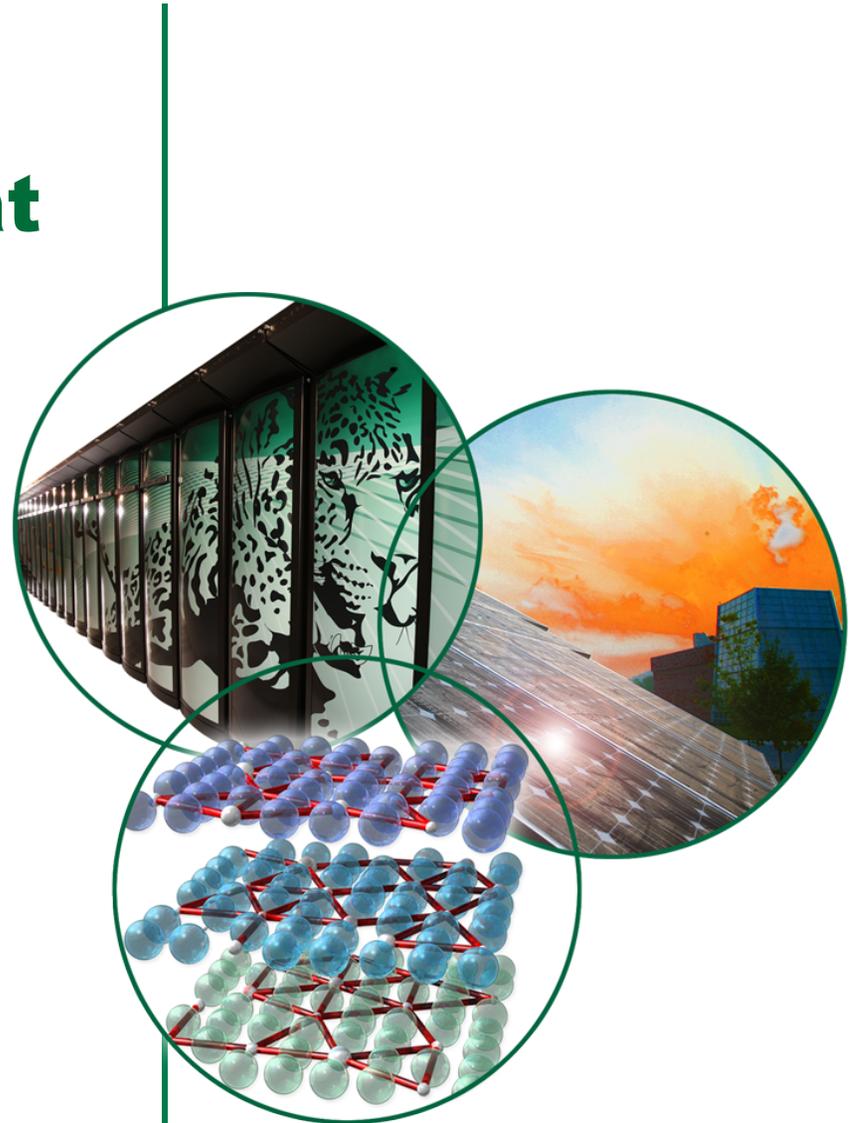
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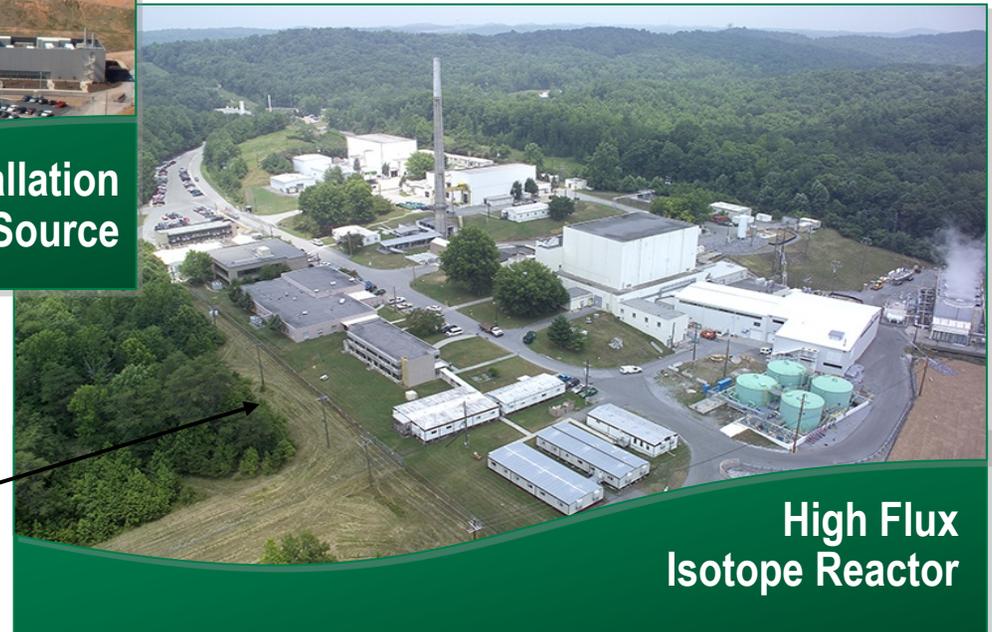
U.S. DEPARTMENT OF
ENERGY

 **OAK RIDGE NATIONAL LABORATORY**
MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY

ORNL's two world-leading facilities for neutron science



422 Unique Users in FY 2010



375 Unique Users in FY 2010

Department of Energy Scientific User Facilities
Unique Capabilities Available through Peer Review

A world leading science center and user facility for neutron scattering research

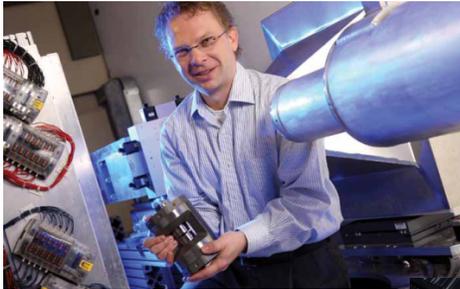
- Carry out world class research
- Provide an outstanding User Science Program
- Develop cross cutting signature science programs and partnerships
- Stay at the leading edge of neutron science by developing new capabilities, instruments, and tools



Delivering Infrastructure, Instruments, and an outstanding User Science Program

Neutron Scattering Instruments

- SNS – 13 operational, 7 fully in user program, 6 commissioning, 2 more in 2011
- HFIR – 11 operational, 9 fully in user program, 1 commissioning, 1 more in 2012

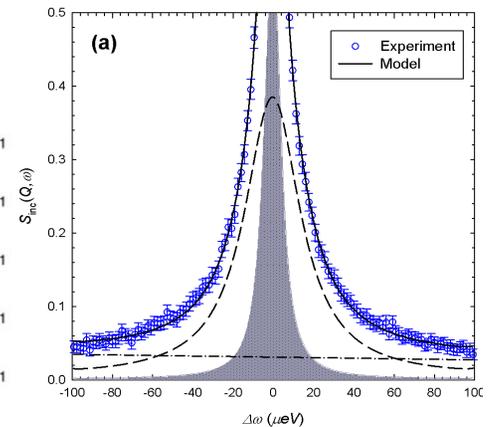
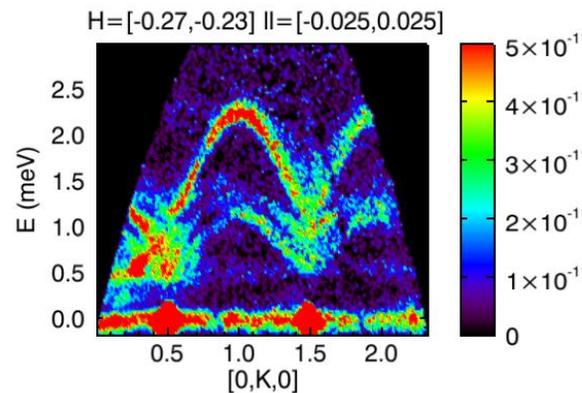
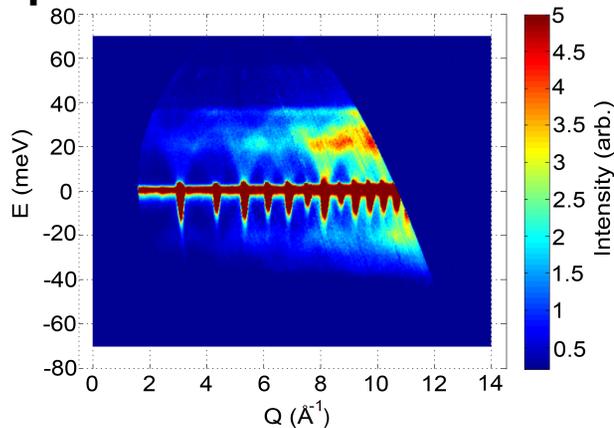
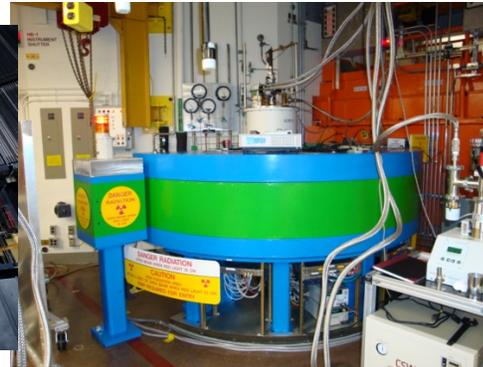


User Program

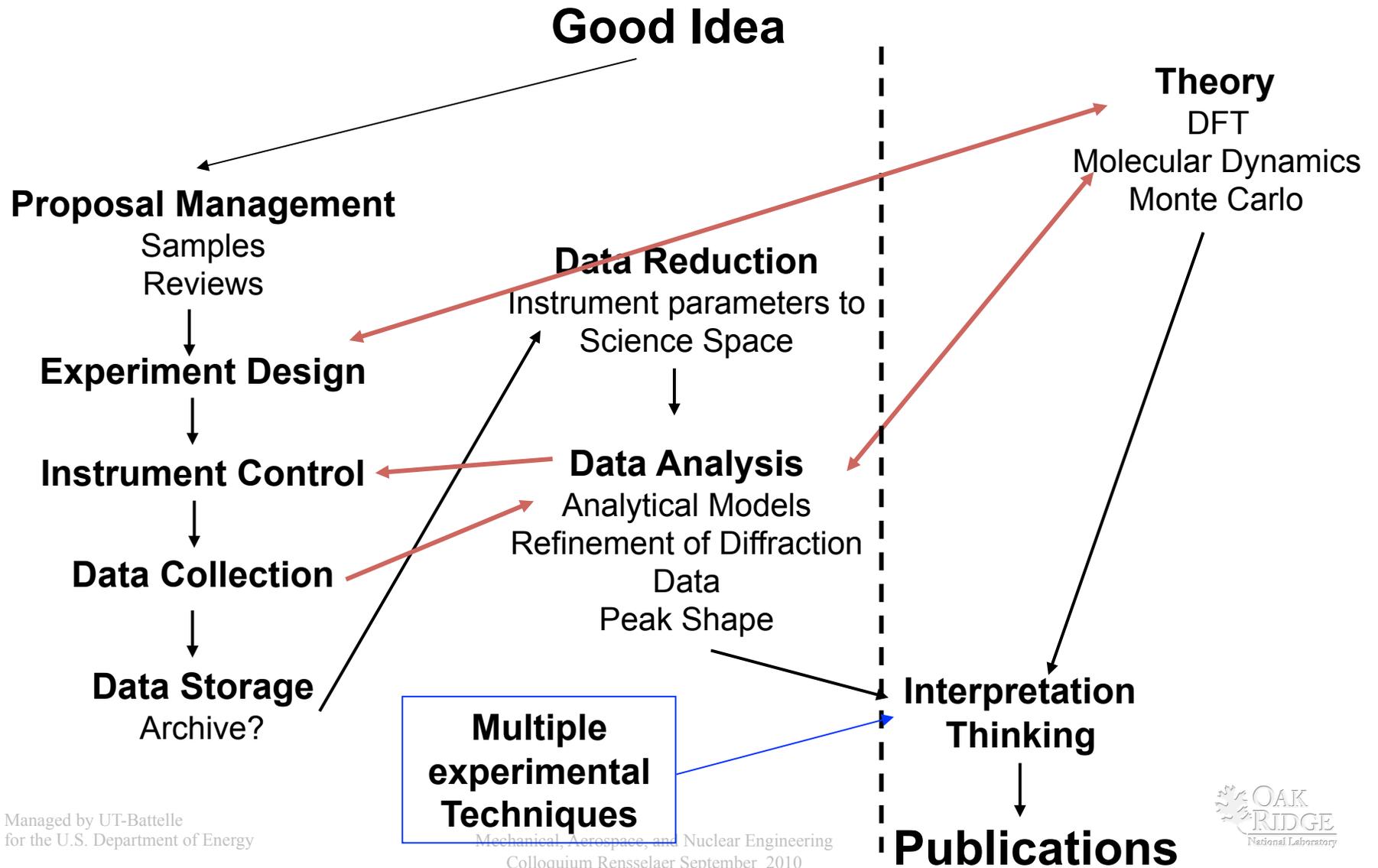
Current call

420 SNS proposals

224 HFIR proposals



Computing at User Facilities



How does Scientific Software get produced?

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Individual Research Groups

- Adaptive/dynamic
- Students/postdocs
- Narrow focus/Specific Science Drivers
- Programming Standards?
- Maintenance/Support?

Centrally-led Collaboration

- Defined Scope
- Students/postdocs/staff
- Several to many modest scale projects
- Single Unifying Theme
- Defined development framework
- Maintenance/Support?

Software Center

- Resources to tackle large scale development
- Partnerships – multiple themes, cross-disciplinary
- Professional Scientific Programmers
- Broad focus – multiple Science Drivers
- Service to Community
- Maintenance/Support built into operations plan

Longevity

Summary

- **User Facilities**
 - Major capital investments
 - Serve a diverse and changing user base
 - Bottom Line – deliver science
- **Modern Facilities could not operate without the major advances in computing infrastructure**
- **Traditional Approaches - linear**
- **Opportunities – Maximize scientific impact through development of better computational tools**
 - More closely couple data collection and analysis
 - Optimize use of instrument time through more intelligent control of experiment
 - Couple theory to experiment design
 - Need tool sets that can map theoretical calculations into “data”
 - Couple theory to data analysis
 - Flexible optimization engines that provide robust interface to sophisticated (computationally expensive) theoretical modeling
 - Refine theoretical parameters?
 - Integrate “data” from multiple experimental techniques