



... for a brighter future

Scientific Software Section

Kenneth Evans, Jr., Project Leader

*(presented by Pete Jemian, Group Leader,
Beam line Controls & Data Acquisition)*

*APSUO Steering Committee Meeting
2007 January 11*



U.S. Department
of Energy

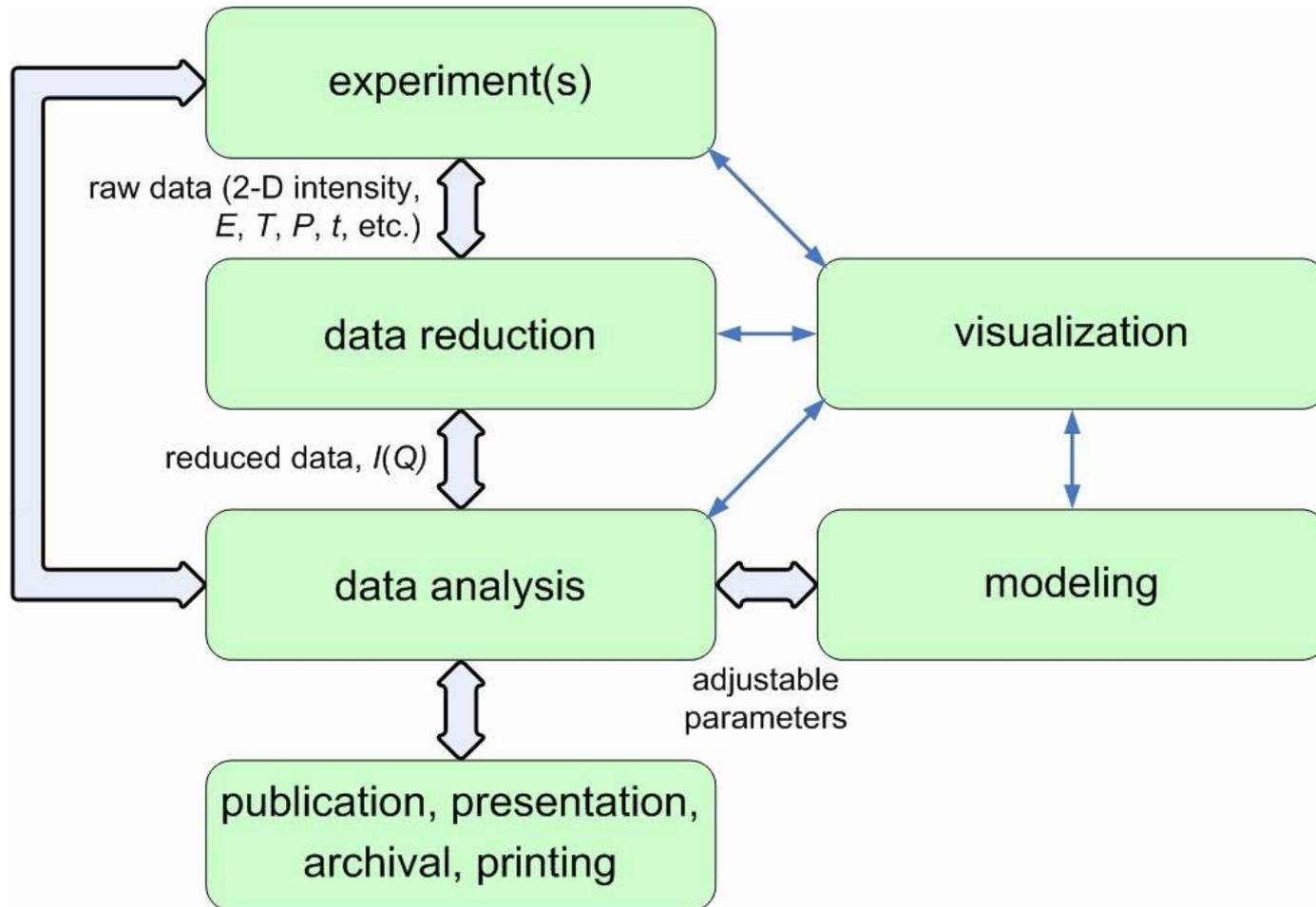
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Improving the scientific efficiency of the APS

- The APS management has stated that “Attaining our goal of maximizing the scientific productivity and impact will demand not only changes in beamline configuration but also improved detectors and software for data reduction and analysis.... Providing robust data reduction, data analysis, modeling and simulation software to our users is an important enabler to increase the volume of high-impact APS results. This program has very high priority, and will be pursued simultaneously with the highest priority beam line upgrades.”
- The Scientific Software Workshop Committee reports that “*It is essential for the APS to take a more concerted and focused approach to the development of real-time analysis and data visualization software than has been done to date.*”
- The purpose of creating the Scientific Software Section is to establish a coordinated software development program at the APS

Scientific Workflow Diagram



The Committee is now the Working Group

- [Kenneth Evans, Jr.](#), chair
 - [Francesco De Carlo](#)
 - [Pete Jemian](#)
 - [Jonathan Lang](#)
 - [Ulrich Lienert](#)
 - [John Maclean](#)
 - [Matt Newville](#)
 - [Brian James Tieman](#)
 - [Brian H. Toby](#)
 - [Michel A. Van Veenendaal](#)
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- Committee formed in fall 2005 from the APS User Community
 - Survey of APS User Community in summer 2006: ANL-APS-TB-52
 - Workshop held 2006 August 29: ANL-APS-TB-51
http://www.aps.anl.gov/News/Conferences/2006/APS_Upgrade/XSD-SciSoftware.html
 - This diverse, eclectic committee continues as a working group
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- If you want to join, please contact Ken Evans
 - If you want to give input, contact any committee member
 - They will be glad to help
 - Your input is important

Quick Overview of Scientific Software Section

- Scientific Software Section Created 2006 October 1
 - Positioned into APS Engineering Support Division under BCDA
 - As staffing level grows, could become stand-alone group
- Ken Evans transferred from Controls group to be Project Leader
- Goals for this year
 - Create the Scientific Software Section
 - Project proposal for visiting scientist program to advance theory and analysis – will leave behind codes to be converted into APS user software
 - Project proposal for two staff positions this year
 - Continue to grow the staff in future years (PhDs, career software engineers, postdocs, students)
 - Extend our effort through outside collaborations

Goals - continued

- Collaborations
 - Tony Lam – ANSTO
 - Andy Goetz – ESRF
 - Tom Swain – UTK
 - Peter Peterson - SNS (Steve Miller's DANSE group)
 - Matthias Clausen - DESY

- Continue to grow the staff in future years
(PhDs, career software engineers, postdocs, students)

- Want a complete example from start to finish
- Looking for those who want to work with us
(several candidates already identified)
- We are open to ideas, please contact Ken Evans

Activities

- Exploring existing software packages, especially visualization, that have potential for scientific software.
- Attending DANSE, NeXus, and NOBUGS meetings, keep aware of the community
 - DANSE Developers' meeting at SNS/ORNL, Jan. 22-23
- We are also working to establish collaborative relationships with people responsible for x-ray and neutron scattering software at other organizations, including ESRF, ANSTO, and DESY, as well as the University of Wisconsin and IPNS. Given the hiring situation and small current size of the Scientific Software Section, we feel it is essential to foster such collaborative relationships in order to leverage our limited resources.
- Working with beam line 1-ID to make a pilot visualization application for their data analysis
- Major thrust at this time is to establish the foundation, including collaborations, for what needs to be done to provide coordinated scientific software development rather than to work on specific applications.
 - For that we need more people.
 - We are exploring the possibility of postdoctoral appointments to help with this need.