DANSE

Brent Fultz
California Institute of Technology

Software Construction for Neutron Scattering Science

B. Fultz, Caltech

Directions for computing and neutrons

Tasks and goals of DANSE

Procedures, Status and Challenges

DANSE Software will enable:

New Science

Better Science

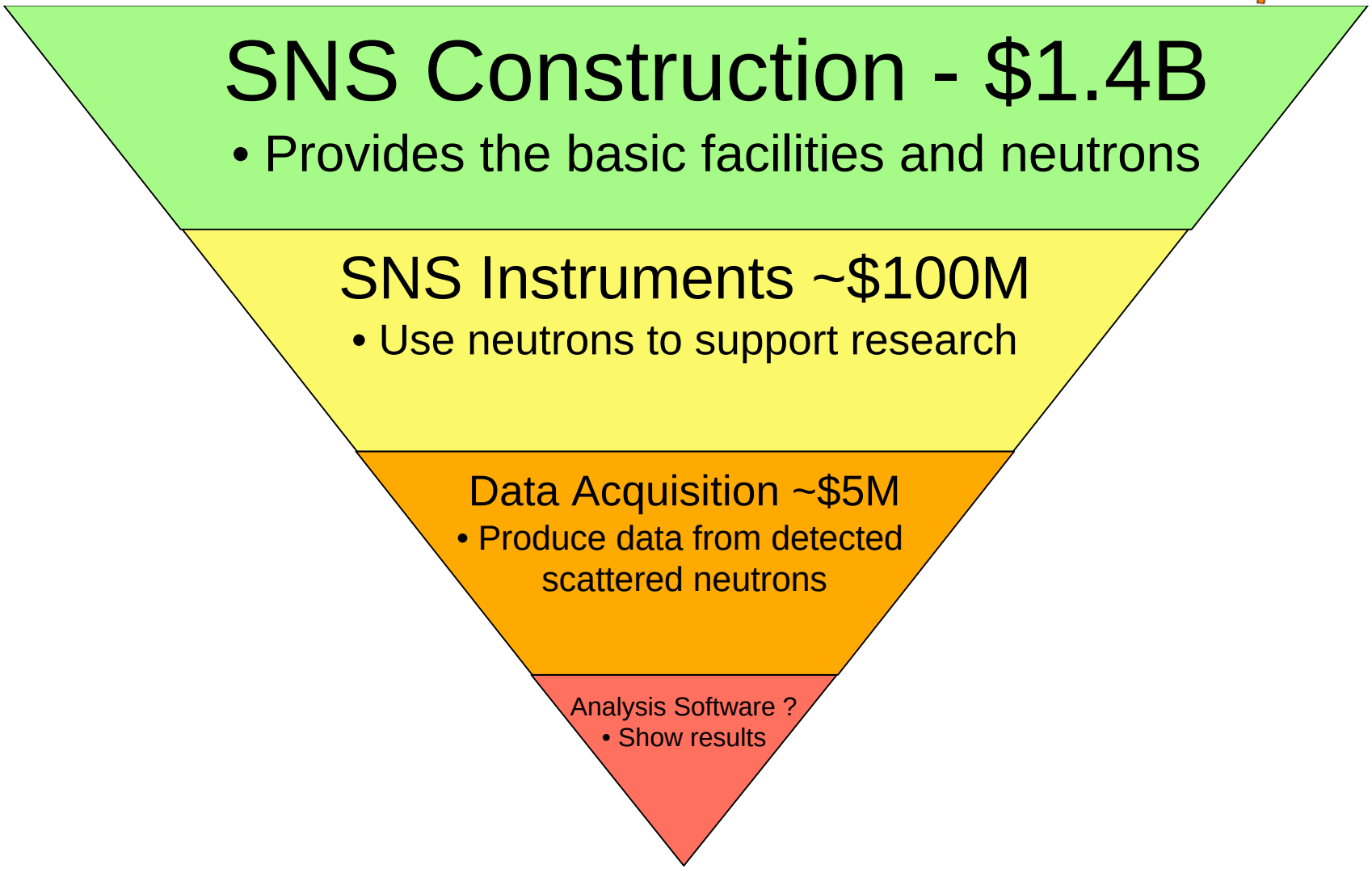
Ease of Use

Software Stability and Reuse

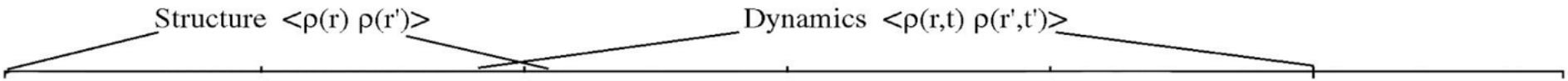
Support Early Operations of the SNS

DANSE Project: Big Picture

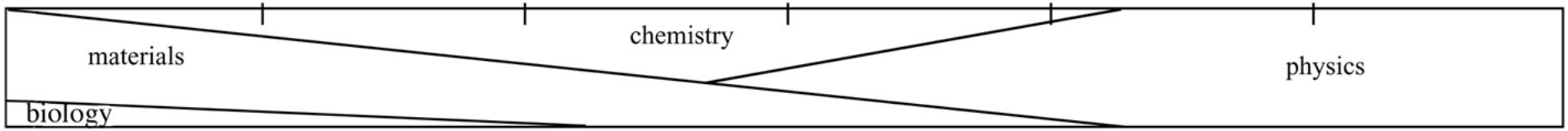
- Enable new neutron scattering science by scientific computing.
- Build enough important and quality pieces to make DANSE the choice of future developers.
- Detailed WBS, development process, and Earned Value Management
- M$ 12 over 5 years (Award announced June 1, 2006)


SNS Construction - $1.4B
• Provides the basic facilities and neutrons
SNS Instruments ~$100M
• Use neutrons to support research
Data Acquisition ~$5M
• Produce data from detected scattered neutrons
Analysis Software ?
• Show results

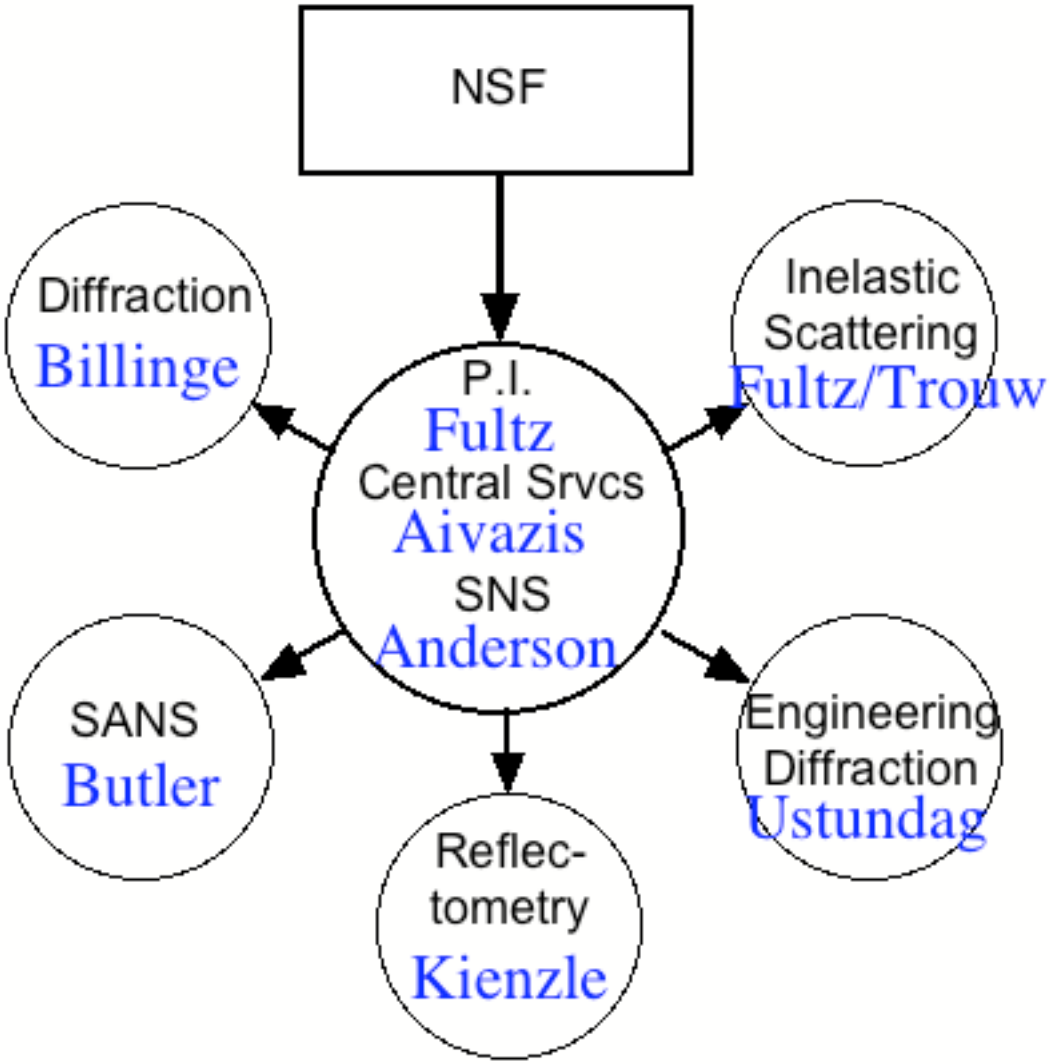
Neutron Science



Microstructure	Crystal Structure	Diffusion	Vibrations	Excitations	Nuclear/Particle
Small-Angle Scattering, q – polymers – nanostructures – macromolecules *Reflectometry* , **q** – soft matter – magnetic surfaces *"Engineering" Diffraction*, **q** – micro-mechanics – residual stress – environmental	*Powder Diffraction*, q – Rietveld (order) – pair distribution function (disorder) – pressure,temperature *Single Crystal Diffraction*, **q** – atom structures – magnetic structures – proteins	*Quasielastic*, ε *Backscatter*, ε, q – molecular motions and rotations – diffusion – hydrogen dynamics	*Chopper*, *3-axis*, ε, **q** – phonon entropy – interatomic forces – soft modes – e^- -phonon coupling – liquids (classical, quantum)	*Chopper*, *3-axis*, ε, **q** – Spin fluctuations - paramagnetic - spin waves - colossal magnetoresistance – Charge fluctuations - crystal fields - valence fluctuations - correlated electrons - Hi-Tc – Quantum Phase Transitions	*Beams*, ε – Resonance cross sections *Bottles*, ε, t – Ultra-cold neutrons – Tests of Standard Model

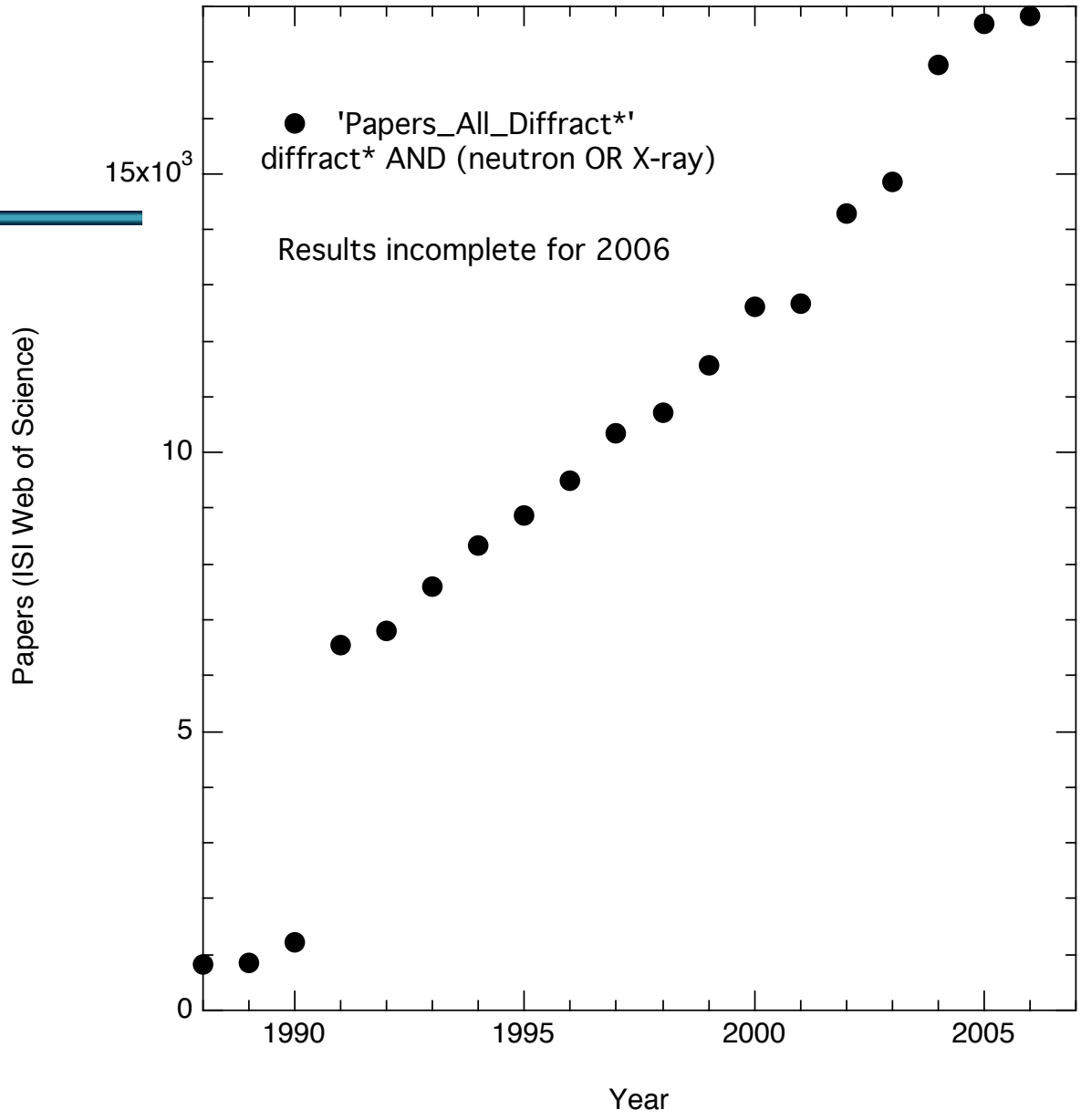


The DANSE Project



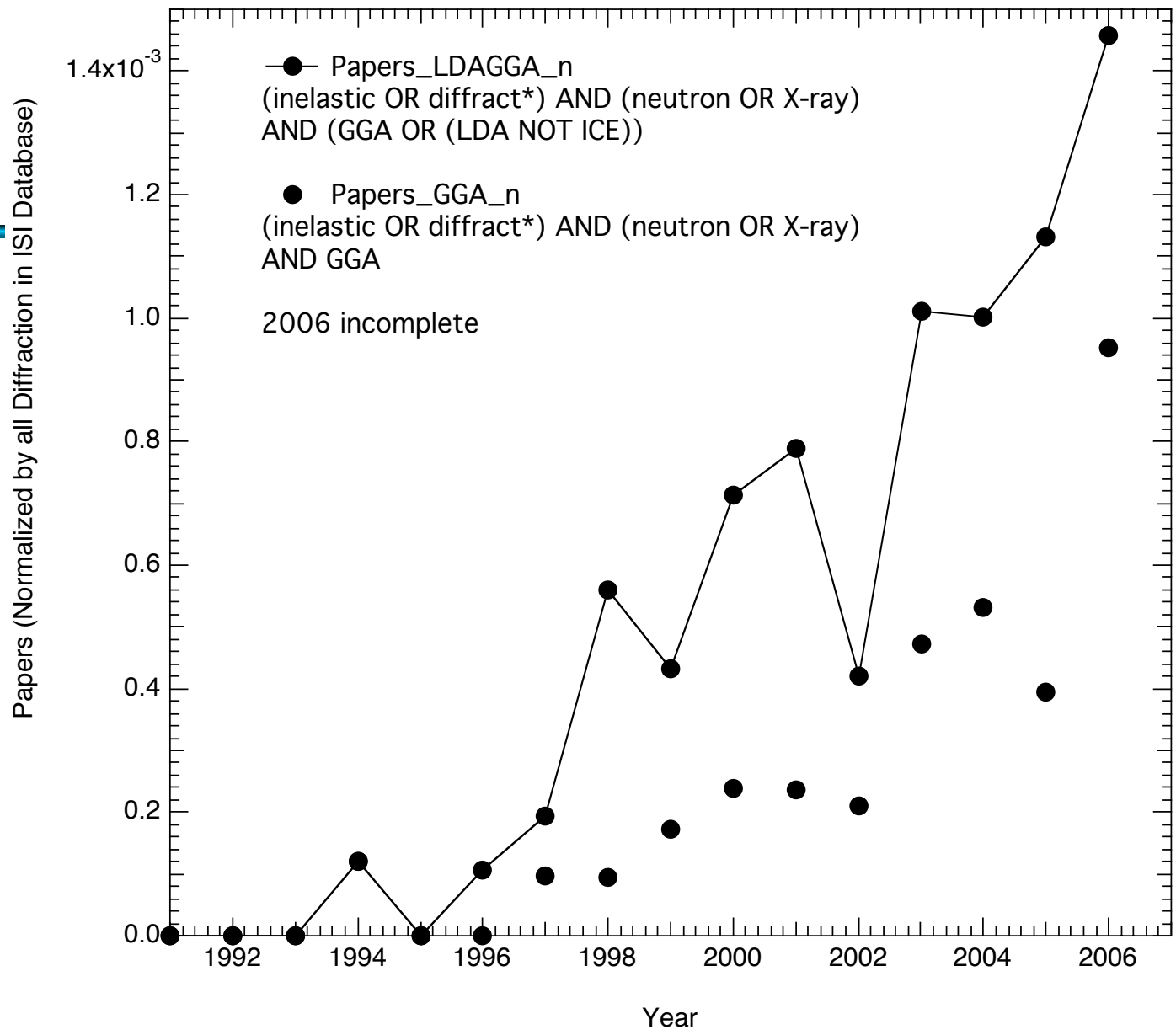
Publication Trends

All Diffraction



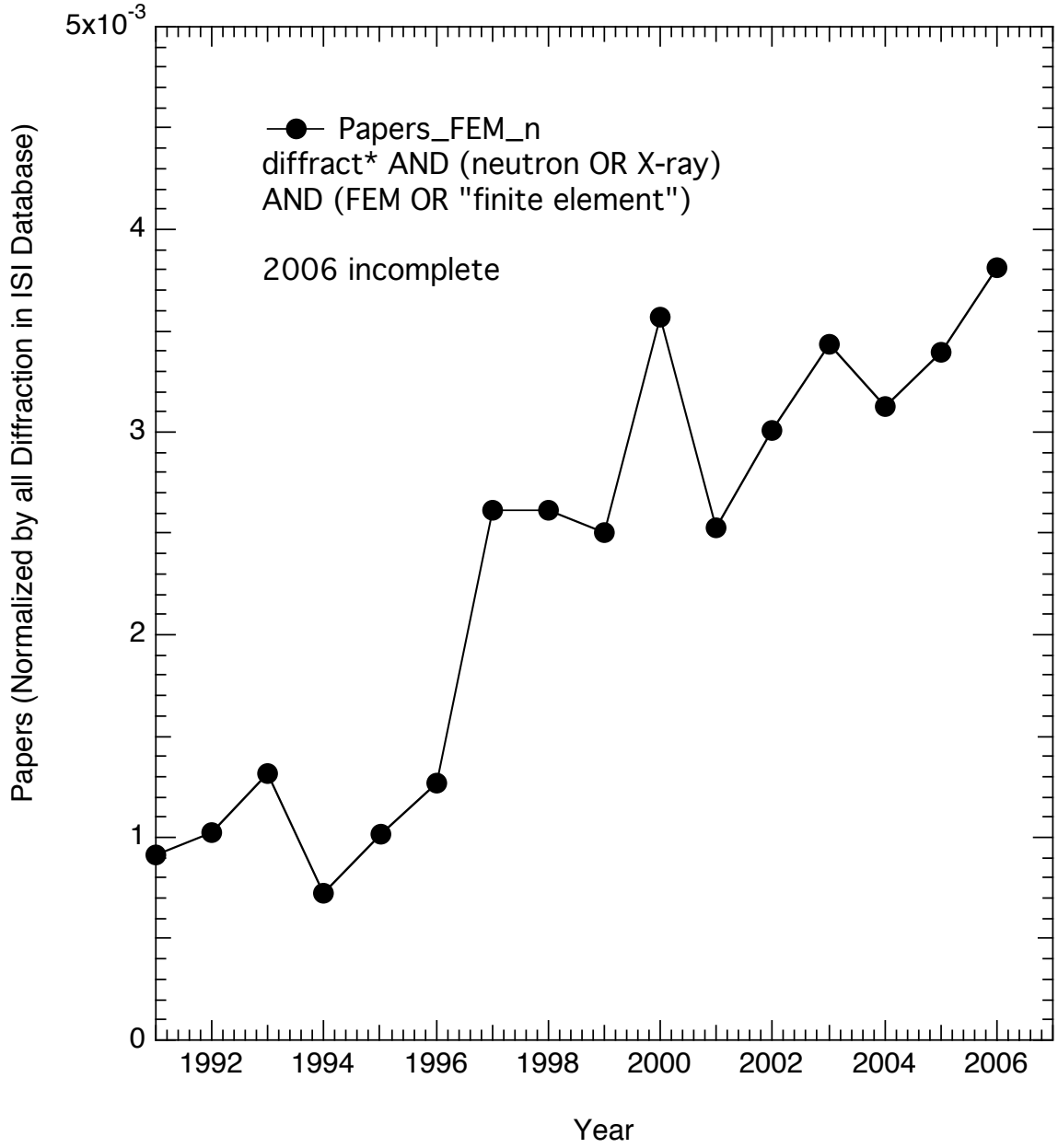
Publication Trends

Density Functional and Scattering



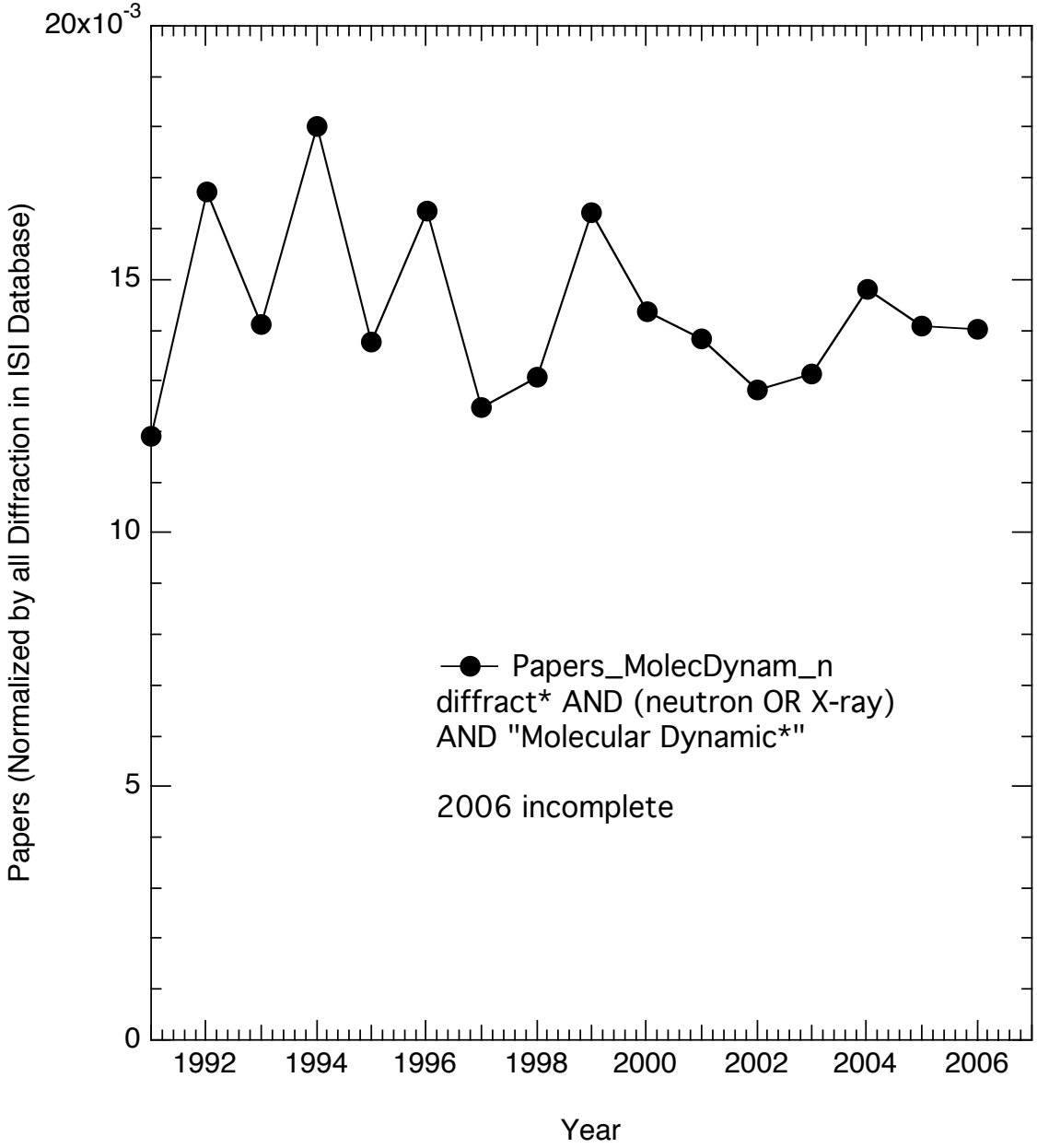
Publication Trends

Finite Element and Diffraction



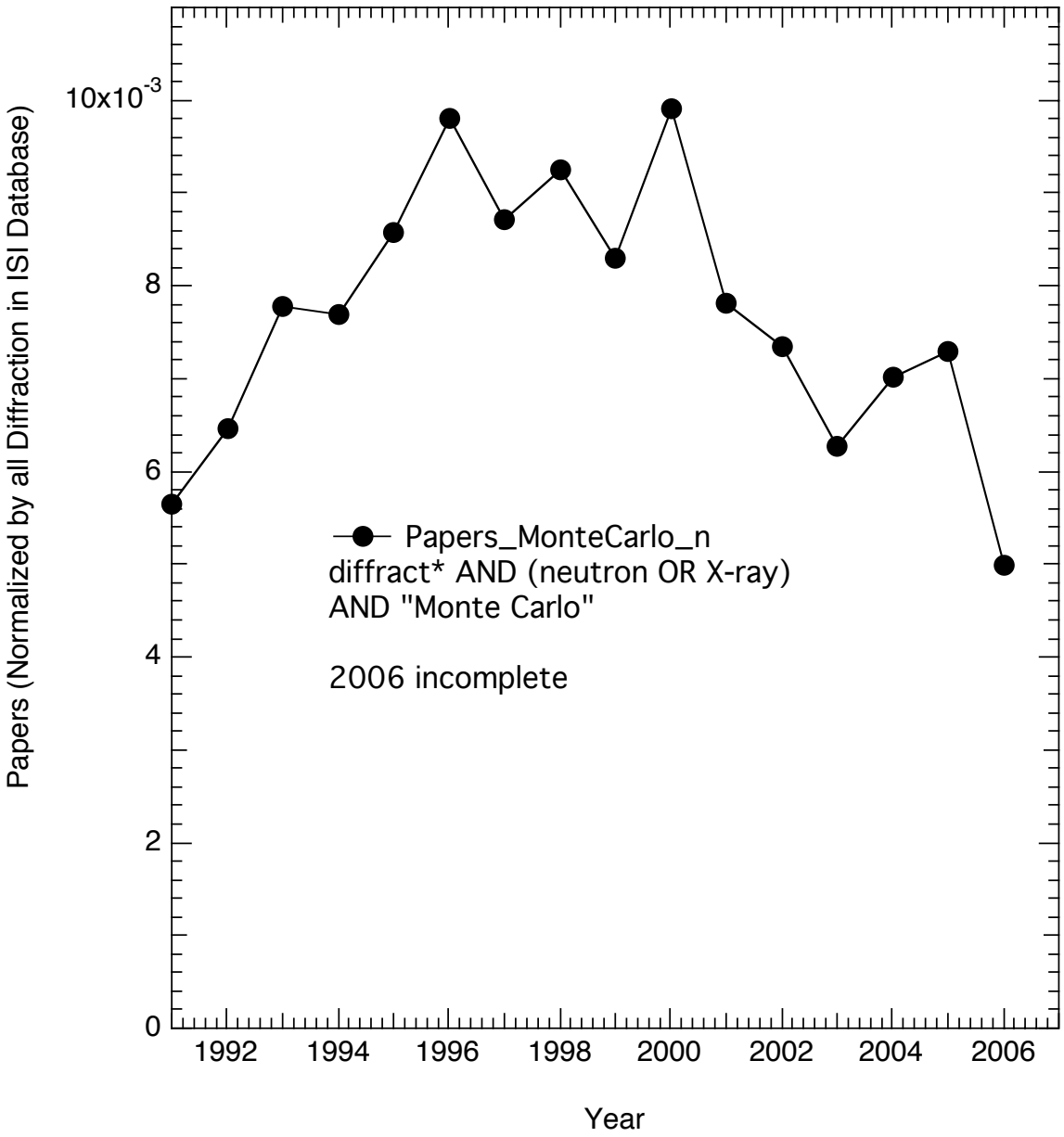
Publication Trends

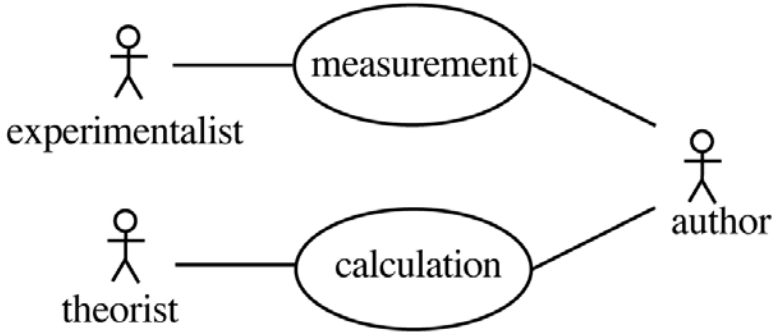
Molecular Dynamics (not all computing) and Diffraction



Publication Trends

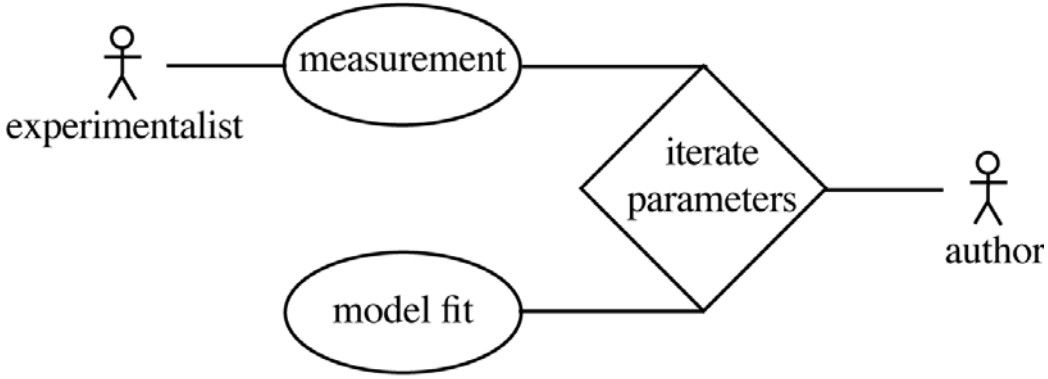
Monte Carlo and Diffraction

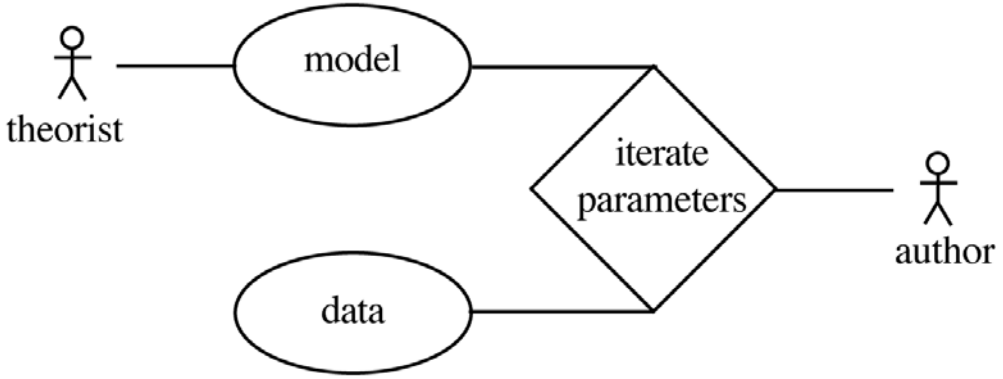




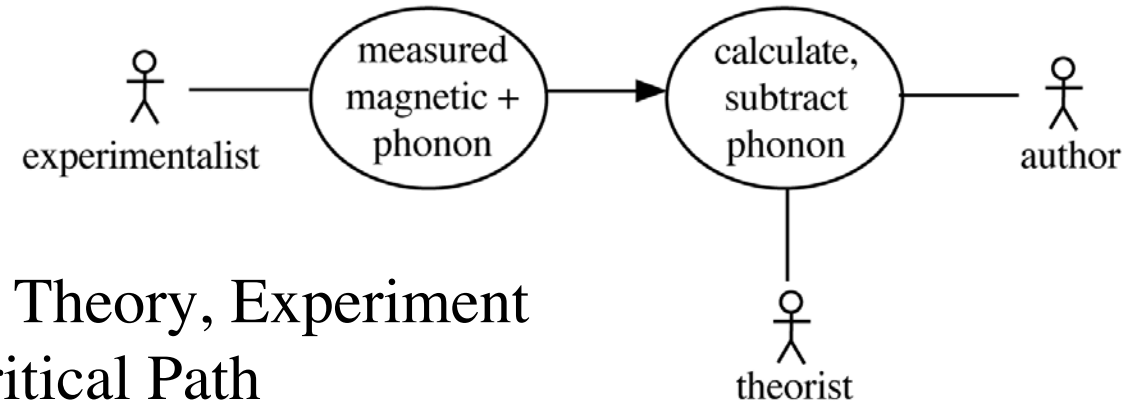
Dominant style of today

Natural Extensions

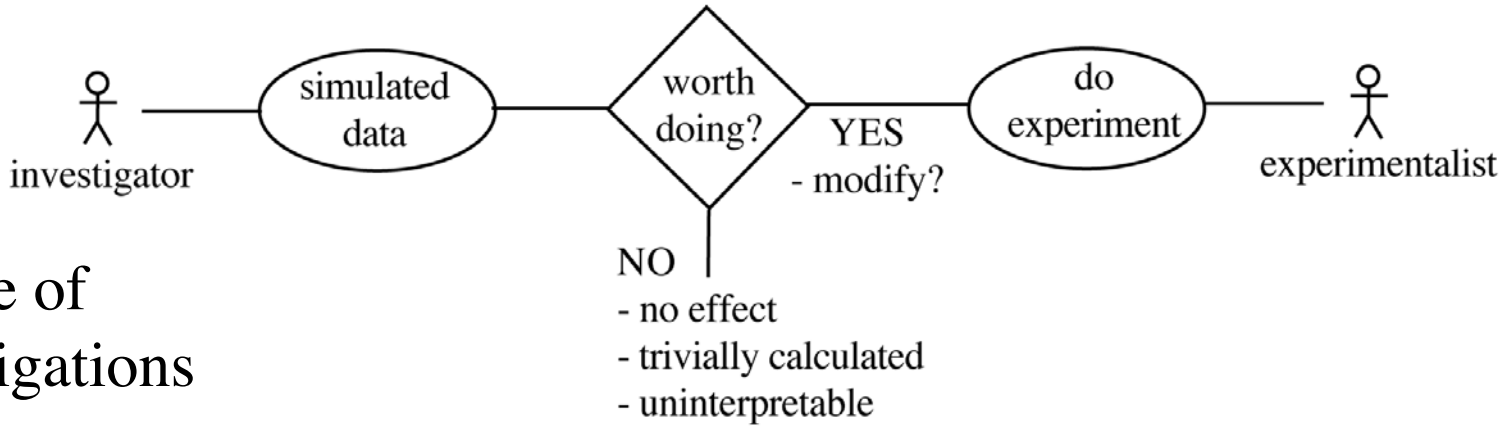




Near Future



Both Theory, Experiment in Critical Path

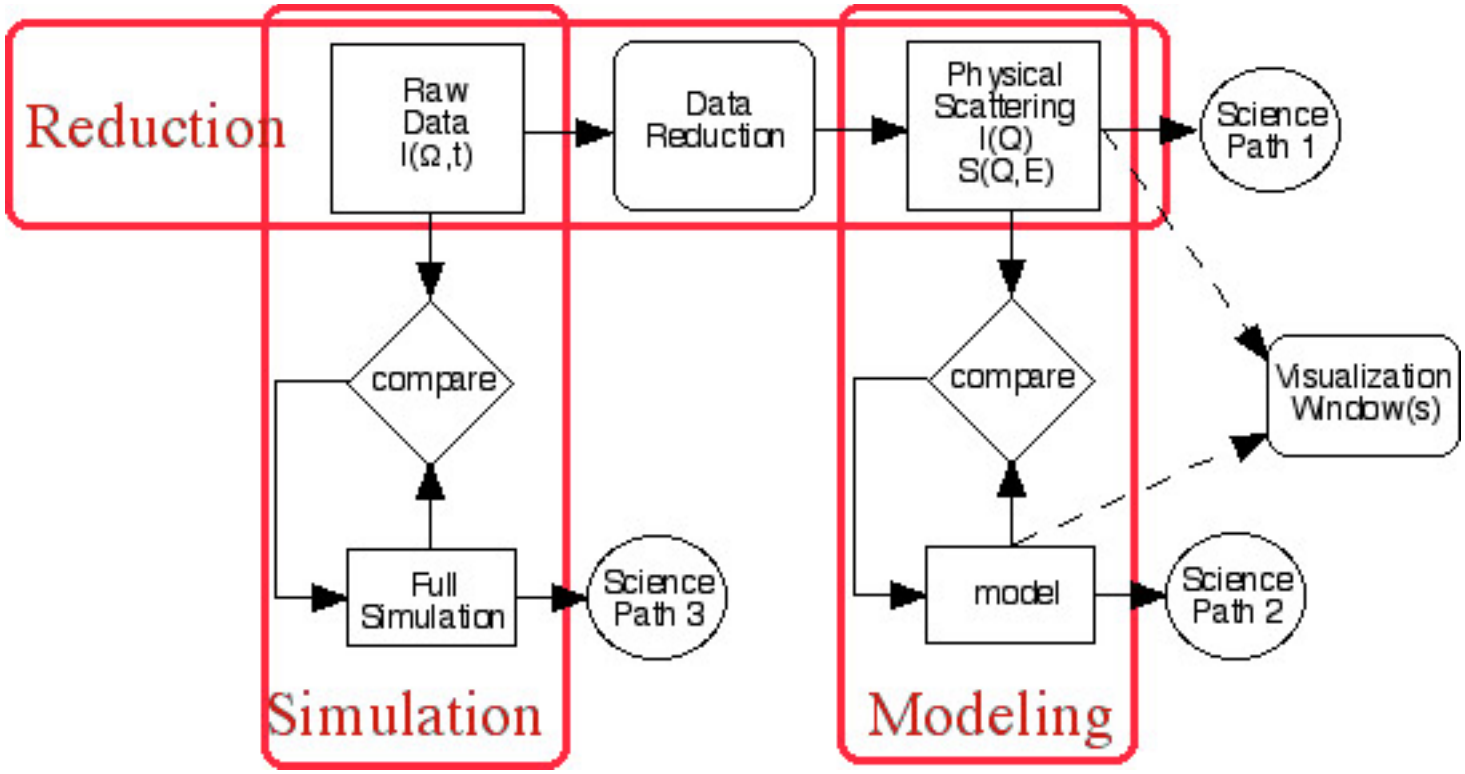


Choice of Investigations

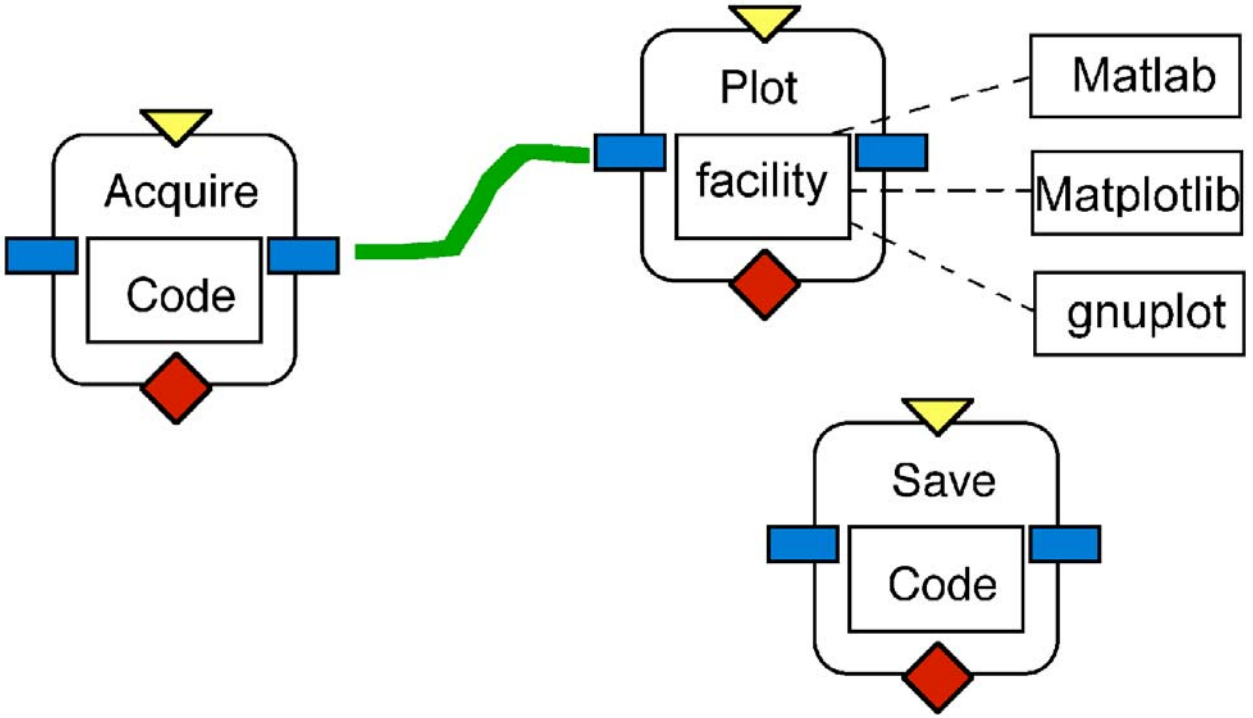
Facilitate discovery in neutron scattering science by enabling computation at a higher level of abstraction.

Is there a career path for scientists who add value at this higher level?

The Three-Fold Way to Science



Component Framework



Encapsulate scientist's code within component.

A component inherits methods from the framework, user communicates properties through framework.

Runtime Components on a Framework

1) Accommodates new analysis networks
   - useful components provided by DANSE
   - low barrier to making new components

2) Allows national coordination of DANSE Project
   - common algorithms
   - quick adaptation of new ideas
   - helps configuration management
   - uniformity of quality and performance

3) Framework - framework coordination?
   - Python - Java?

Design and Development Process

- Vision for component, function, behavior
- Object-oriented programming allows early selection of design patterns
- Review, document review, archive
- Prototype. Review the design and costs
- Build to specifications, revise specs, testing plan
- Release

Planning of Reviews

- Beware: 200 components x 4 reviews = 10^3 reviews
- Reviews must help developers, not hinder them
- Priorities for Reviews:
  - Any Flagship Application
  - A component used by many developers
  - A component interfacing to many components
  - Regular schedule for all subgroups

attendees: linjiao, mmckerns, swain, delaire, patrickh

JL> We can describe histogram as a mapping from a rectangular area in phase space to R2. Of course, we need an axis that is descretized into bins, and also R2 represents the 2-tuple of data and error.

PH> So does that mapping do interpolation?

JL> No.

PH> What if asks for point that is not part of defining list?

JL> It throws an exception.

PH> What if x is floating point, and you have a precision problem, is it smart to throw a exception?

JL> That's an implementation detail that we must talk about with DiscretizedAxis and GenuineDiscretizedAxis. If a GenuineDiscreteAxis has ticks of floating numbers, than I should not allow a rounding-error. If we are talking a bout DiscretizedAxis with ticks only (on bins), then the rounding error should be allowed. For an axis with bins, then we should return a value whenever the input value is inside one of the bins.

PH> Where do you put interpolation?

JL> I do not put in interpolation... if you want to do interpolation of

WBS and Earned Value Management System

- WBS is nearly up-to-date today
- Changes are expected, but must be approved and documented. This should be agile for software development.
- Monthly report forms are generated from WBS
  - tasks (WBS level 4)
  - effort (man months)
  - percent complete (WBS “level 5”)
  - highlights
- Challenge to keep WBS up with design changes
- EVMS requires either
  - stable plan (we are doing this first)
  - agility

Times and Time Scales for Development

Stability 1/(Rate of Change)		Process for Software Development	
Low	Coding	First	Project Plan
↓	Documented Design	↓	Documented Design
	Reviewed Design		Coding
	Project Plan (PCRs)		Reviewed Design
High	Science Applications	Last	Science Applications

Accommodation of Practices

Management Should Support Developers	Developers Should Help Management
• Agile project management • Room for prototypes • EVMS criteria - rolling wave of components - keep sight on science applications	• More up-front effort on design, documentation, planning • Focus on early deliverables to help tune the system

DANSE Effort Today (Personnel)

- All senior personnel together since early 2003
  - scientific and technical leadership
  - assessment of what is practical to deliver
- Professional staff
  - managed carry-over of personnel from CED award
  - new personnel in place, or coming soon
- Postdoc Software Developers
  - new personnel in place, or coming soon
- Graduate Students
  - can leverage DANSE in thesis research
  - A little development, but testing and some development
- Undergraduate Students
  - mostly in computer science
- External collaborators

DANSE Effort Today (Technical)

- Scientific capabilities defined
- Flagship applications selected
- Common components for I/O, interface, and numerics
- Software development process is running
- Releases:
  - ARCS inelastic software in production, pyre framework
  - Reflectometry software in production, moving to framework
  - Diffraction prototype (PDFGUI)

DANSE Effort Today (Management)

- Earned value management ready to try with a Project Baseline
- Change, risk, configuration control plans are ready
- Infrastructure tools in place (svn, trac, build/release, gui)
- Development processes are in place
- Project management in place

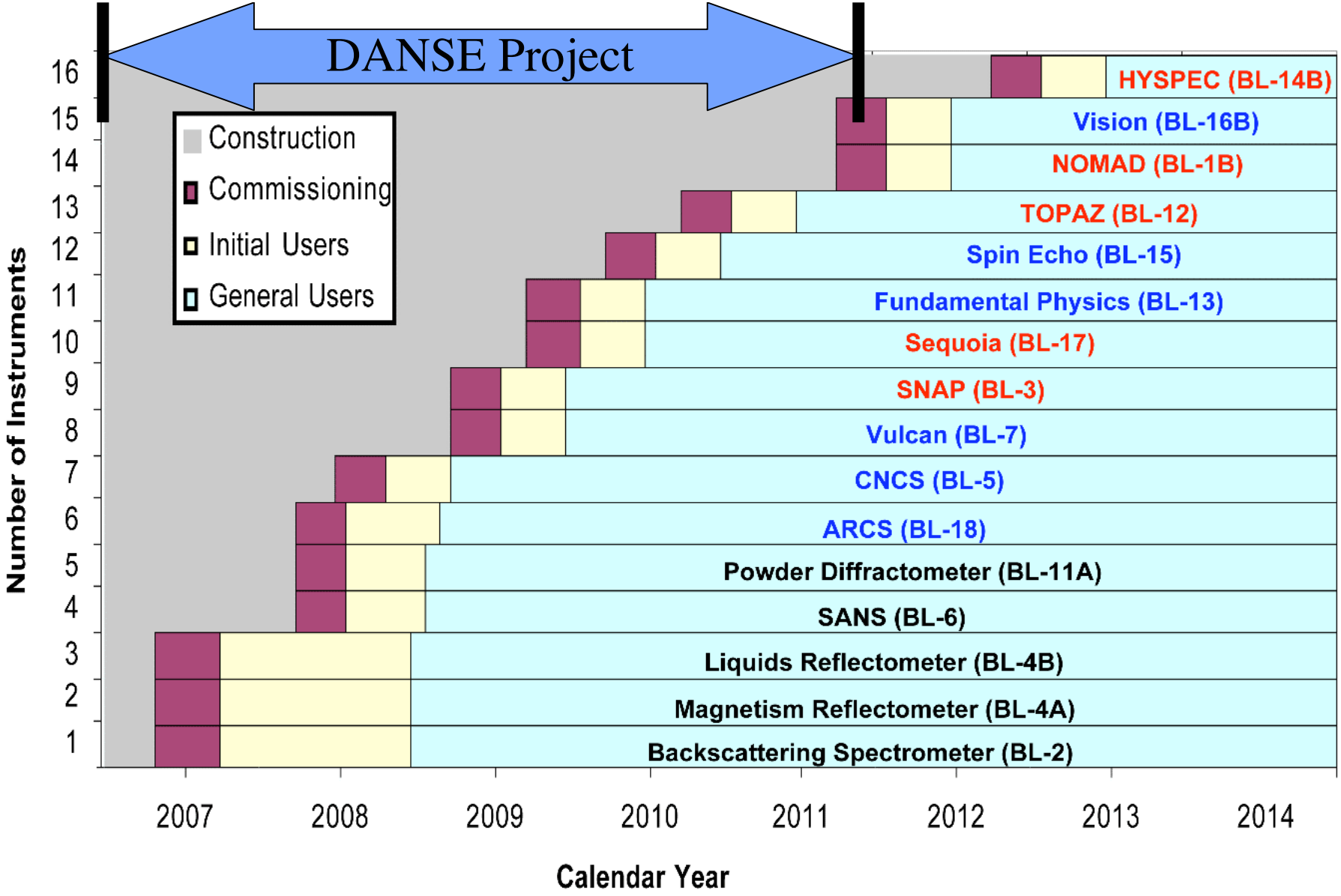
DANSE Project Execution Plan (draft)

DANSE functionalities
Milestones
Reviews
Management structure
Project Baseline
Project contingency
EVMS
Release Management
QA
SNS transition

License
Components
Flagship Applications

DANSE and the SNS

- DANSE will facilitate new science from the SNS, especially in the early years of operations
- Good communication channels between SNS and DANSE
- Complementarity of software efforts
  - DANSE emphasis on advanced data analysis (modeling and simulation)
  - SNS emphasis on data services (acquisition, curation, reduction)
- Engineering consistency: SQRL consults for the SNS, subcontract with DANSE


DANSE Project
Construction
Commissioning
Initial Users
General Users
HYSPEC (BL-14B)
Vision (BL-16B)
NOMAD (BL-1B)
TOPAZ (BL-12)
Spin Echo (BL-15)
Fundamental Physics (BL-13)
Sequoia (BL-17)
SNAP (BL-3)
Vulcan (BL-7)
CNCS (BL-5)
ARCS (BL-18)
Powder Diffractometer (BL-11A)
SANS (BL-6)
Liquids Reflectometer (BL-4B)
Magnetism Reflectometer (BL-4A)
Backscattering Spectrometer (BL-2)
Number of Instruments
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
2007
2008
2009
2010
2011
2012
2013
2014
Calendar Year

Education

- Plan for pre-service teacher education at ISU (NSF RET)
  - develop K-12 lesson plans using content from subprojects
  - adoption by young teachers
- Nanoscience program at MSU
- Student involvement
  - minority student funds
  - testers of software and documentation
  - some in computer science
- Textbooks

Outreach to Broader Community

- Open source (BSD license) facilitates collaborations and interactions

  SNS ASG, NeXus/NIAC, McStas, NumPy, SciPy, cctbx, NAMD, VMD, MMTK, gnuplot, ISAW, matplotlib, CEDS Berkeley component

- Workshops and Organizations

  M. McKerns to Australian Research Council NCRIS [National Collaborative Research Infrastructure Strategy], XSD Software Workshop, Paul Kienzle elected DANSE representative to NIAC.

Challenges and Risks

- Optimizers for modeling -- we don't understand the math.
- A large amount of legacy code is not documented well.
- Microsoft Windows (builds, user expectations, multiple configurations)
- User science expertise sometimes needs to be high.
- How will we support friendly users?
- How much testing can we afford?
- Coordinating project-wide releases.
- Learning curves of new personnel.

Philosophy and Summary

- We wished carefully, and the DANSE Project has come true.
- Good morale – let's keep it this way.
- Lots of low-lying fruit for computation and neutron science.
- Roles of DANSE and SNS have evolved naturally:

  - SNS software affects the quality of the data from the facility.

  - DANSE does data analysis at a higher level of abstraction.
- Integration of Design, Development, QA, Release Management is running now.
- We will present our detailed plans at this meeting. These plans have been aired many times in their scientific communities, but there is still room for ideas and prioritization.