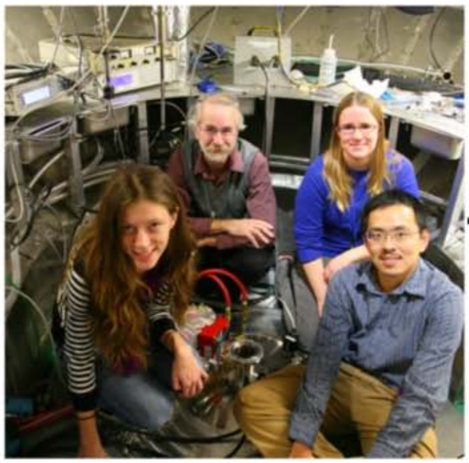
Computational Workflows in Scattering Science

Brent Fultz, Caltech



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Positive Vibrational Entropy of Chemical Ordering in FeV

J. A. Muñoz,[1] M. S. Lucas,[2,3] O. Delaire,[2] M. L. Winterrose,[1] L. Mauger,[1] Chen W. Li,[1] A. O. Sheets,[3] M. B. Stone,[2] D. L. Abernathy,[2] Yuming Xiao,[4] Paul Chow,[4] and B. Fultz[1]

[1]*California Institute of Technology, W. M. Keck Laboratory 138-78, Pasadena, California 91125, USA*
[2]*Oak Ridge National Laboratory, 1 Bethel Valley Road, Oak Ridge, Tennessee 37831, USA*
[3]*Air Force Research Laboratory, Wright-Patterson AFB, Ohio 45433, USA*
[4]*HPCAT, Geophysical Laboratory, Carnegie Institution of Washington, Argonne, Illinois 60439, USA*
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Inelastic neutron scattering and nuclear resonant inelastic x-ray scattering were used to measure phonon spectra of FeV as a *B2* ordered compound and as a bcc solid solution. The two data sets were combined to give an accurate phonon density of states, and the phonon partial densities of states for V and Fe atoms. Contrary to the behavior of ordering alloys studied to date, the phonons in the *B2* ordered phase are softer than in the solid solution. Ordering increases the vibrational entropy by $+0.22 \pm 0.03 k_B$/atom, which stabilizes the ordered phase to higher temperatures. First-principles calculations show that the number of electronic states at the Fermi level increases upon ordering, enhancing the screening between ions, and reducing the interatomic force constants. The effect of screening is larger at the V atomic sites than at the Fe atomic sites.

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At finite temperatures T, the entropy S of a material is dominated by the contribution from atom vibrations. Nevertheless, the relative stabilities of alloy phases depend on differences in their free energies, $F = E - TS$, and understanding differences in vibrational entropy is an active topic of research [1]. For chemical ordering transitions in alloys, the changes of vibrational entropy can be comparable to the large decrease in configurational entropy that accompanies ordering [2]. Stronger bonds between unlike pairs of atoms lead to ordering, and it is generally expected that such bonds would also be stiffer, reducing the vibrational entropy of the ordered phase [3]. For alloy

energy of phonons in the ordered phase. At the Fermi energy, the projected electronic density of states (DOS) at the V atoms undergoes a larger increase with ordering than the projected DOS at the Fe atoms, and the phonon partial DOS of V shows a larger softening with ordering than the phonon partial DOS of Fe.

Samples were prepared by arc-melting vanadium slugs of 99.8% purity and iron lumps of 99.98% purity in equiatomic ratios under a high-purity argon atmosphere. For inelastic neutron scattering (INS) measurements, ingots of the arc-melted FeV, along with pieces of elemental iron and elemental vanadium, were cold rolled

- Goals for the workshop, some administrative matters
- Community organizing around workflow needs
- Issues in Computational Scattering Science

Who are you, the attendees?

- You all were invited based on reputation.
- 65 registrants, each working on 2 topics.
- Ten topics, average of 13 persons per topic.
- Topic leaders picked for willingness to write.
- Speakers and posters today to give context.
- Thanks in advance for your thoughtful work.

Topics – Pick one from Group A and one from B
Vote with your feet – room numbers listed on Agenda.

Group A

- Simulations of Experiments – John Rehr
- Microstructure – Tony Rollett
- Hardware Trends in Computing – Mark Stalzer
- Excited Electrons – David Prendergast
- Human Resources – Sven Vogl

Group B

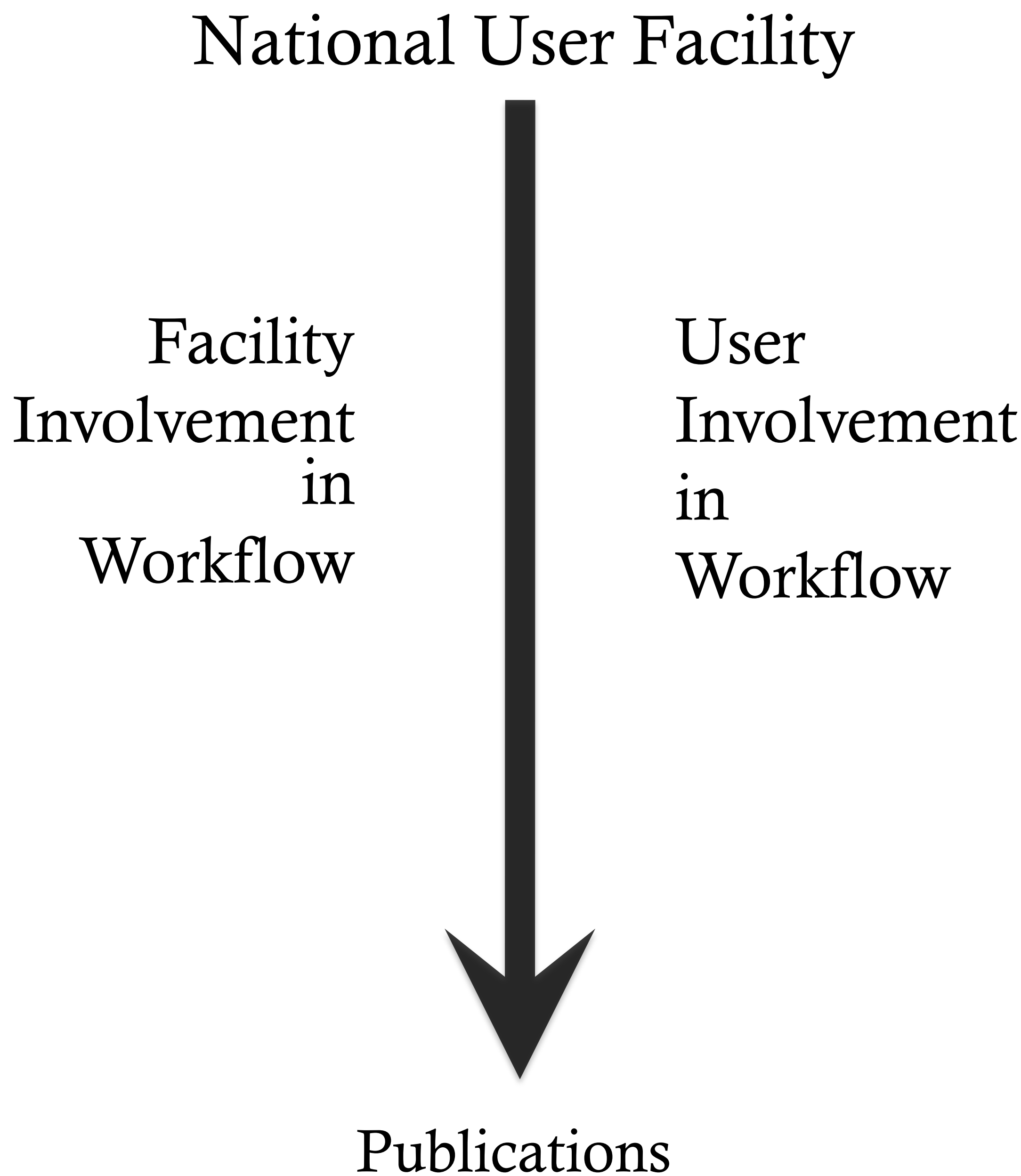
- Software Design – Thomas Proffen
- Electronic Structure – Olivier Delaire
- Software Institute – Brent Fultz
- Uncertainty Quantification – Simon Billinge
- Fast Dynamics – Ercan Alp

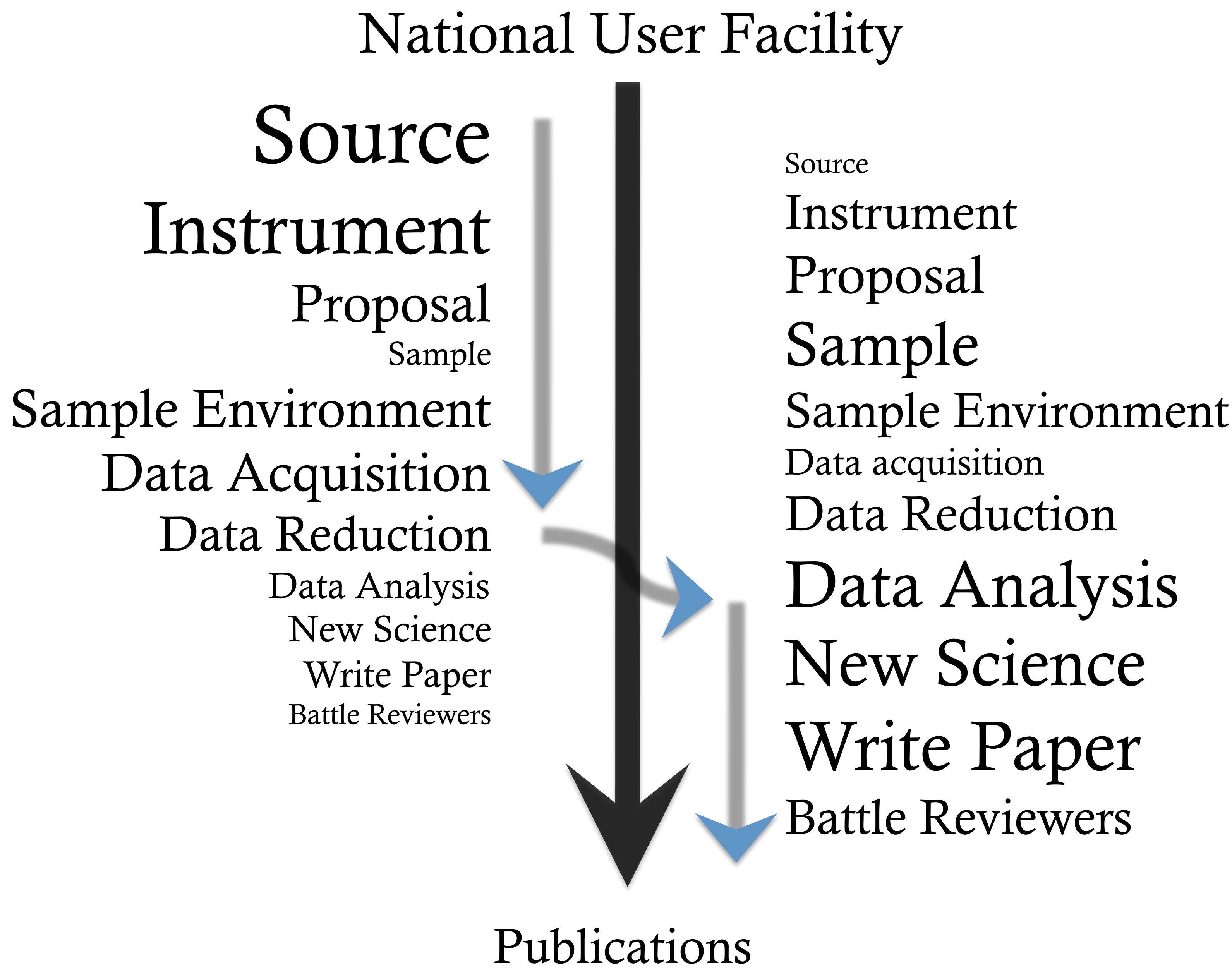
Beams of neutrons or X-rays from big facilities are used in many “small science” investigations

- Numerous instruments, experiments, and science goals
- Most of the 14,000 annual users are experimentalists in small research groups
- Diverse user expectations about computing

X-rays at Advanced Photon Source
(Argonne IL)

Neutrons at Spallation Neutron Source
(Oak Ridge TN)


National User Facility
Facility Involvement in Workflow
User Involvement in Workflow
Publications


National User Facility
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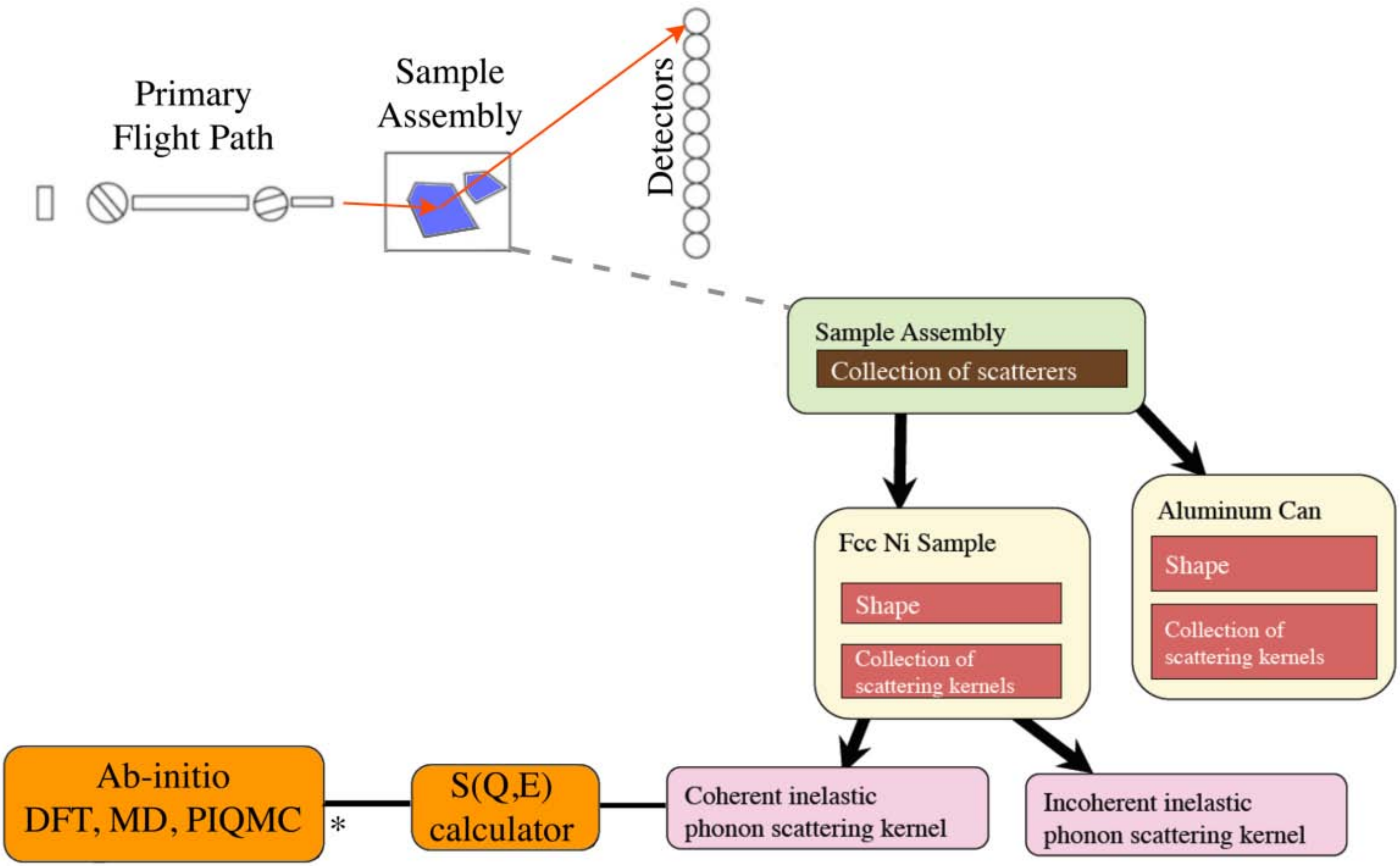
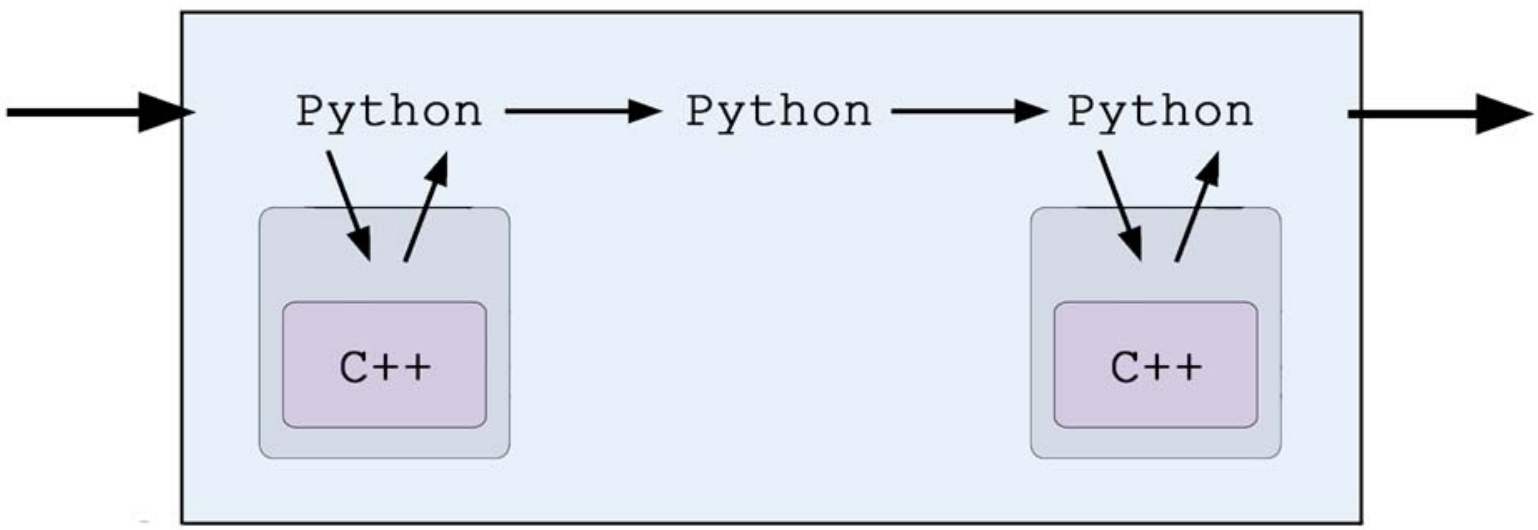
Virtual Neutron Facility (vnf.caltech.edu)



Implementation of Software Modules (Components)

- Higher level — Python
- Lower level — bindings to C++ code or FORTRAN packages



When analysis components
are building blocks,
what will scientists build?

Phonon Thermodynamics

Partition function, Z_{ph}, from phonon density of states, $g(\varepsilon)$

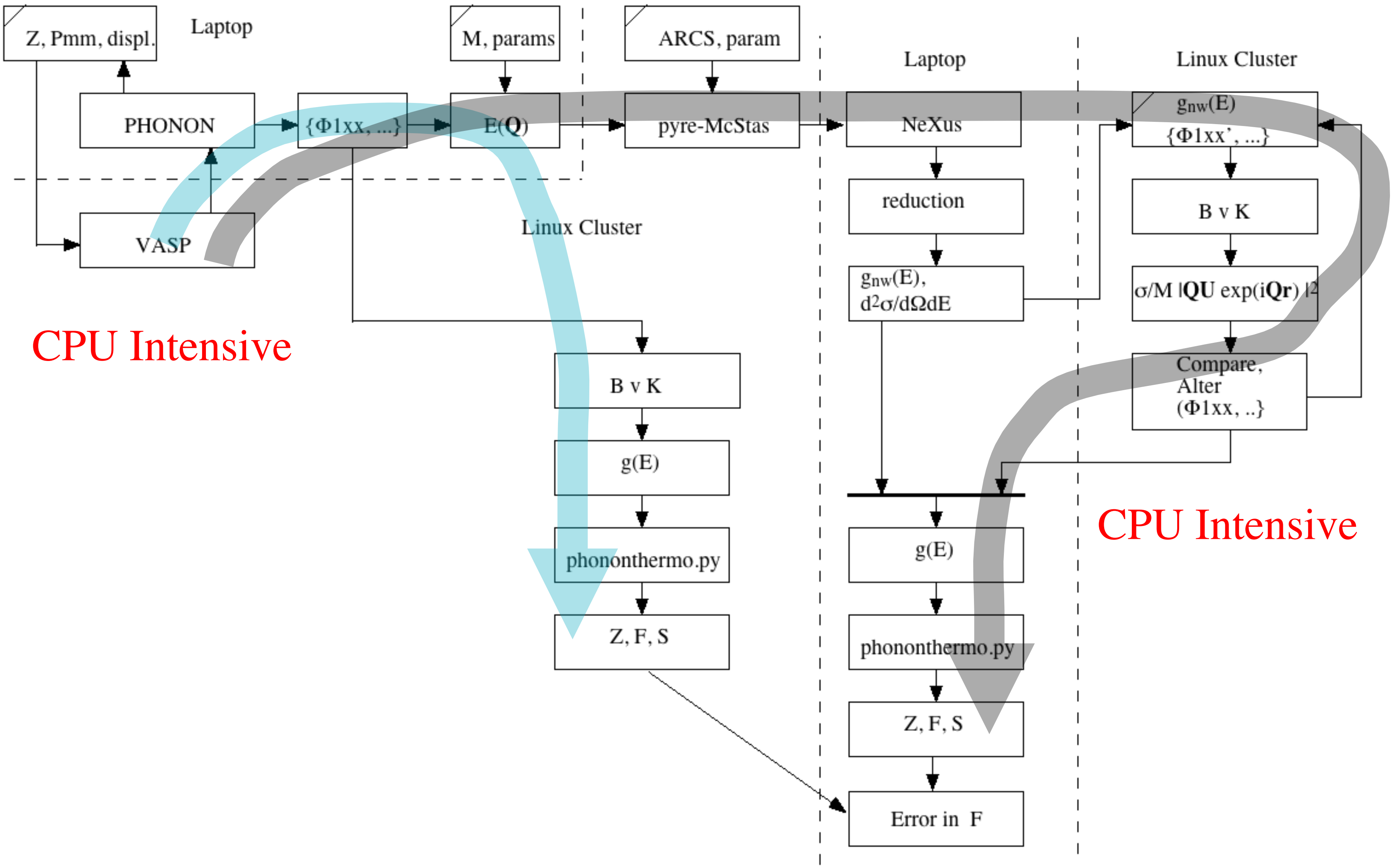
$$Z_{\mathrm{ph}}(T) = \mathrm{e}^{3N\int_0^\infty g(\varepsilon)\ \ln\left(z(\varepsilon,T)\right)\,\mathrm{d}\varepsilon}$$

Free energy

$$F_{\mathrm{ph}} = -k_{\mathrm{B}}T\ \ln Z_{\mathrm{ph}}$$

…and other quantities.

Estimating Uncertainty in Phonon Thermodynamics



Issues for Math and Computer Science (1)

Uncertainty Quantification with Multiple Data Sources

- Bayesian approach can mislead if priors are unreliable -- what is the divergence/convergence on the truth?
- Extracting maximum value from multiple models.
- What is the uncertainty of the uncertainty?

Optimization

- Rates of convergence of iterative calculations
- Finding and classifying both local and global minima

Issues for Math and Computer Science (2)

Algorithms for emerging hardware architectures.
• Huge number of cores with little memory per core.
• Penalties for moving data.

Designs for software architecture
• Appropriate component framework?
• Data structures for workflows tend to be aggregations – can they follow science hierarchies?

For big data sets, what is balance between early reduction and later flexibility?

Community Organization Requires:

Shared Vision

Stable Expectations

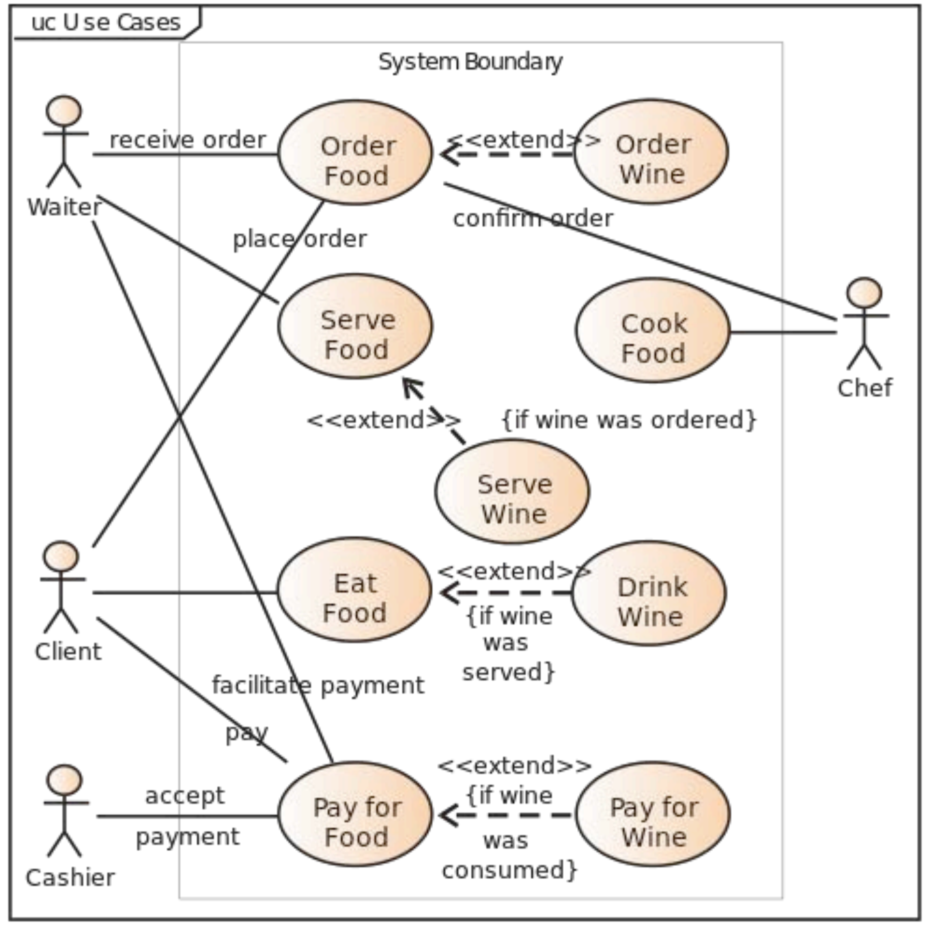
Realistic Estimates

Architectural Coherence

Must Agree On Proposed Work…

Workflows and Use Cases

A **use case** is a list of **steps** defining interactions between an “**actor**” and a **system** to achieve a **goal**.



Don’t forget headcount for dinner tonight

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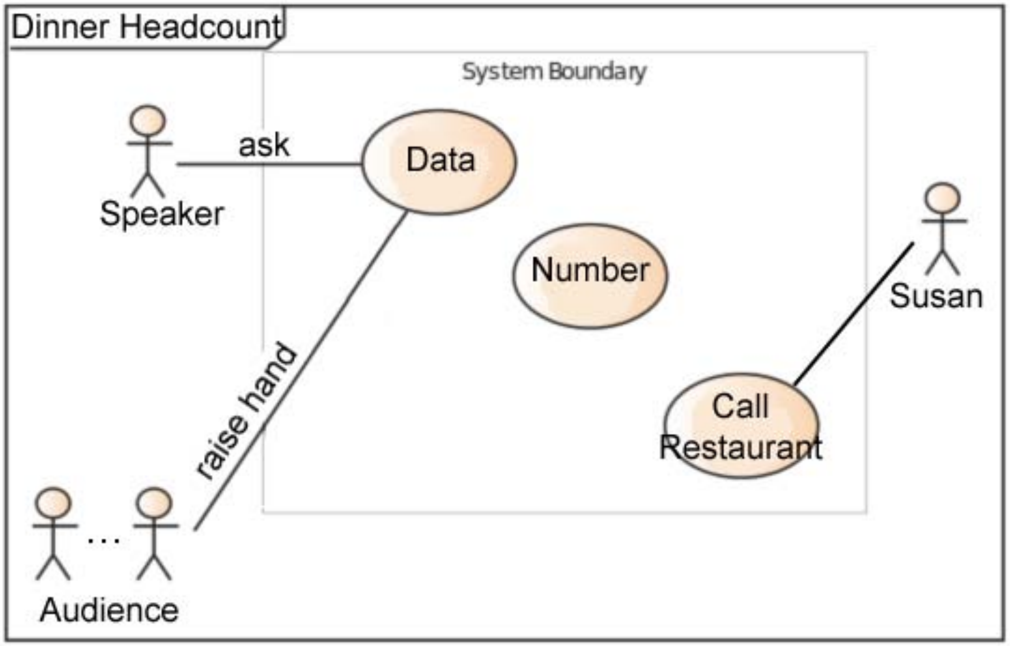

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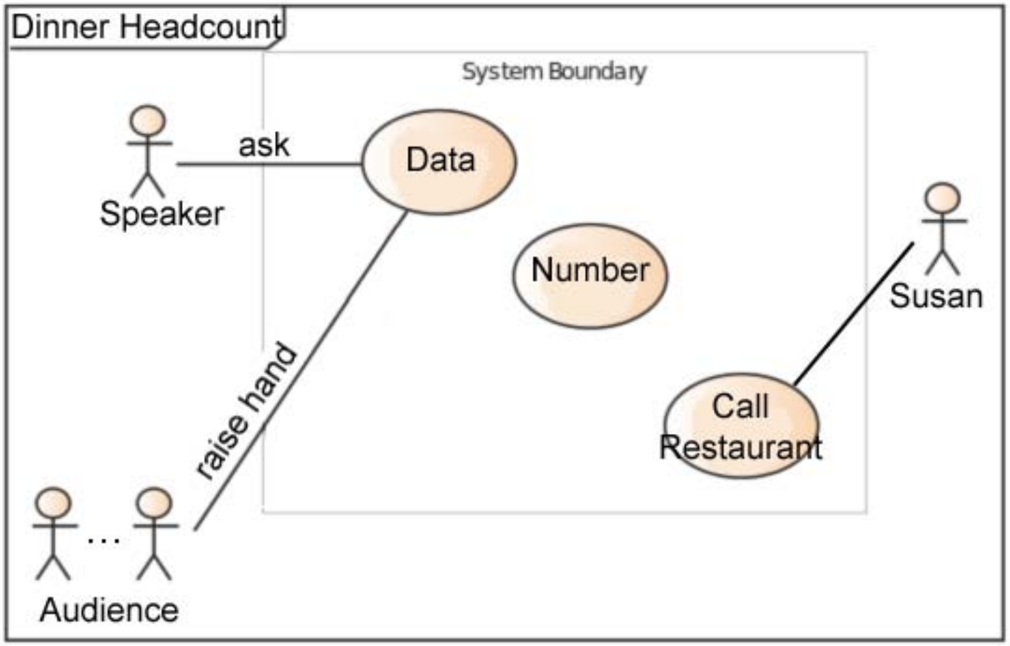

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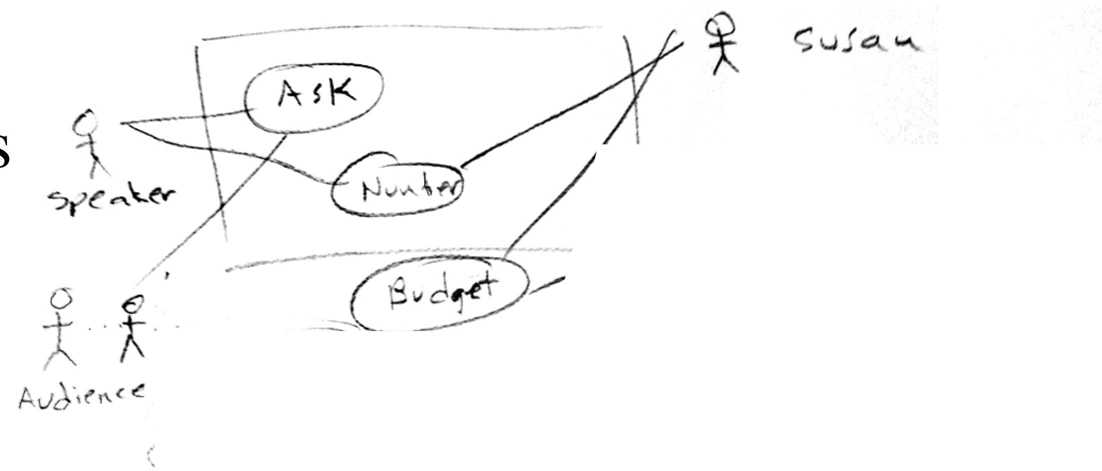


Develop a Strategic Plan For Computational Scattering Science

- **Situation** - evaluate the present situation and history.
- **Target** - define goals and/or objectives (sometimes called ideal state)
- **Path** - map a route to the goals/objectives, preferably with steps and milestones.

Computational Scattering Science Today

- Who: Individuals, cooperation varies
- What: Specialized software packages
- Why: Get more science from measurements
- When: Steady state in U.S. over the past three decades
- How: Cottage industry

Where can we go in principle?

- What is the low-lying fruit for computational materials science to elevate scattering experiments?
- What does the scattering community need to better utilize modern computational methods?
- What are the appropriate interfaces -- technical, organizational, and social -- to best interconnect theory and experiment?
- How can we measure progress and impact?

How do we get there expediently?

- If we make 1,000 users happy, will 13,000 be unhappy?
- How best to survey the community and engage it?
- How to supervise and coordinate technical efforts?
- Who will do the work of development and support?

Estimate: 4,000 persons

Resources (*sine qua non*)

Hardware

Data, bandwidth (okay: TB/day neutrons, PB/day X-rays)
CPU (never enough)

Software

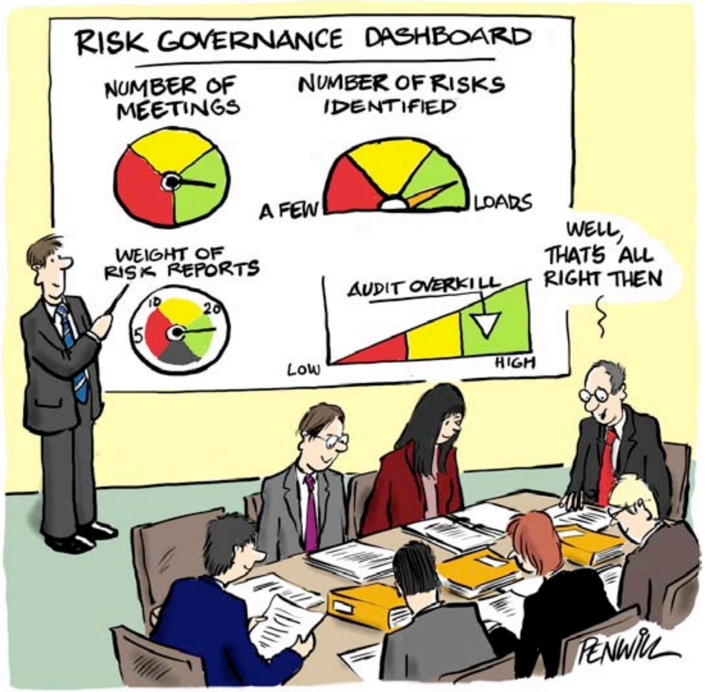
Easy-to-use computational workflows for new science
Development and support need tools from the software industry

People

Good people are critical: factors of >100 in productivity
What is the career path for this work?

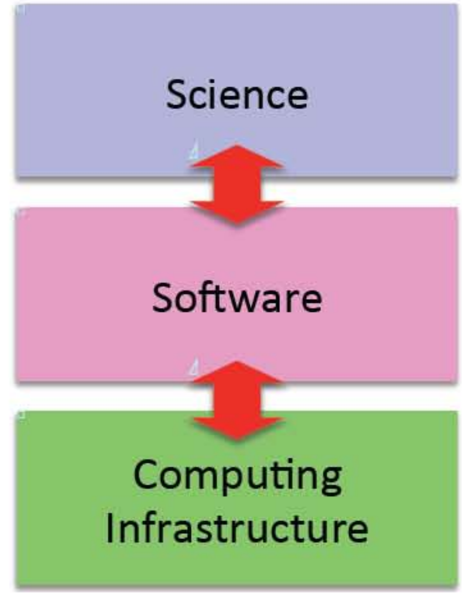
Ideas about an Institute

- Project–based activities (earned value management?)
- User support (may be 35-50% of effort)
- Metrics for success?
- Governance:
  - NSF point of contact needs to make firm decisions
  - Need for community involvement



Software is Infrastructure

- Software (including services) essential for the bulk of science
  - About half the papers in recent issues of Science were software-intensive projects
  - Research becoming dependent upon advances in software
  - Significant software development being conducted across NSF: NEON, OOI, NEES, NCN, iPlant, etc



These three slides are presented with the courtesy of Dan Katz.
Opinions expressed in them are Dan’s and do not reflect the policy of the NSF.

Institute Funding

- Goal: Institutes start in FY15
- Process for recommending FY15 budget request starts soon
- In order to set aside funds for full institutes in FY15 budget, NSF needs expectation that good institute proposals will be submitted, meaning:
  - Strong team, strong ideas, etc.
  - Very strong community recognition of need, including acceptance that this must be funded to enable many science awards to progress
  - Program officers in discipline unit(s) and OCI agree that the community is behind this effort
  - Administrators in discipline unit(s) and OCI are convinced directly (by community) or indirectly (by program officers) of the need

Role of S2I2 PIs

- Now: Get "community" behind an institute
  - Define community
  - Understand what they need
  - Convince them that an institute will help them
    - That they need an institute
  - Bring them in to your vision, or even in to the institute (engage to the point of shared leadership)
  - Build word of mouth that gets to NSF
- End of project: write institute plan as final report
- Later: Write a good proposal