



## DANSE: “Facility Update”

M. McKerns, B. Fultz Caltech

---

- Goals and Issues
  - Schedule, Cost, and Quality
  - What will be delivered?
- Project Management
  - Management Practices

# Why DANSE ?

---

*New Science*

*Better Science*

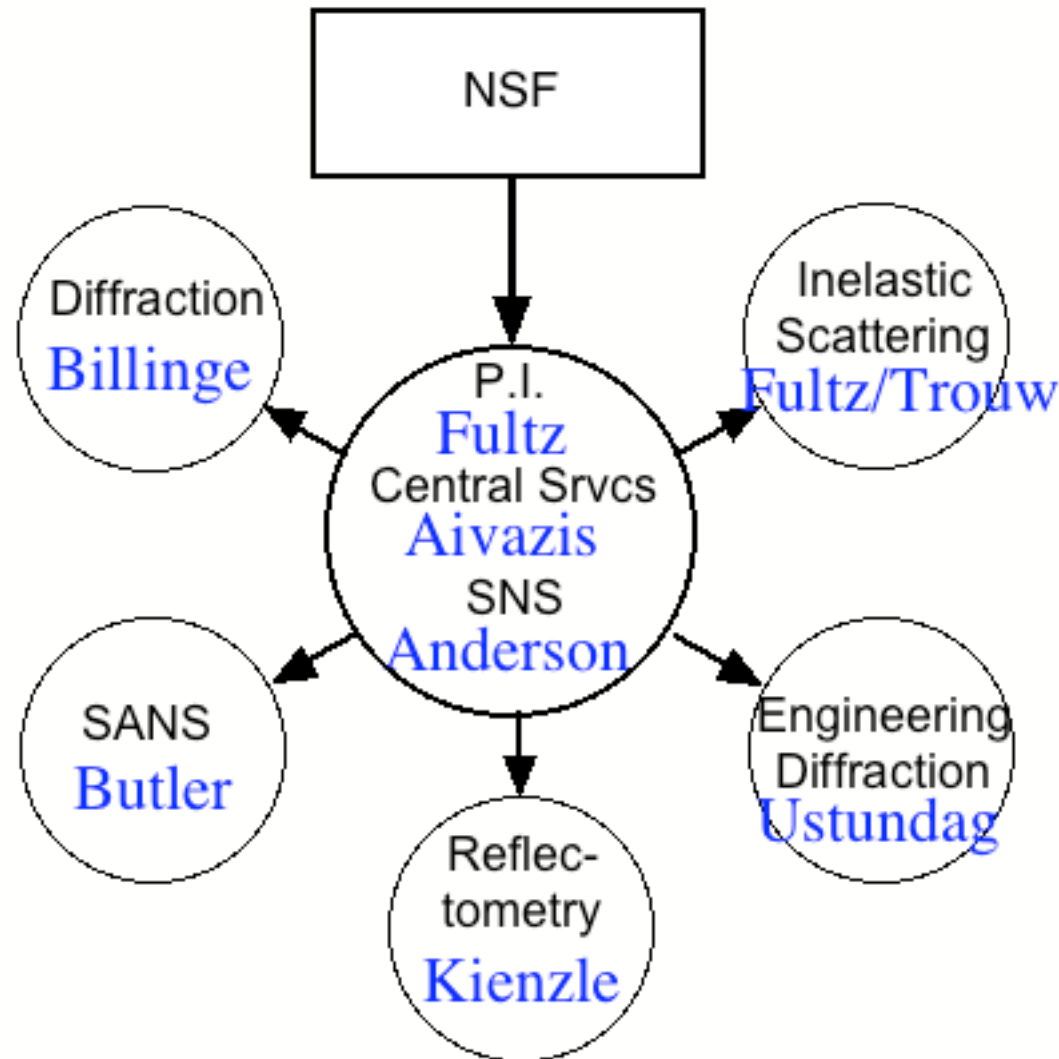
*Ease of Use*

*Software Stability and Reuse*

*Support Early Operations of the SNS*

---

# The DANSE Project



---

*Develop computing methods  
for new types of discovery in  
neutron scattering science.*

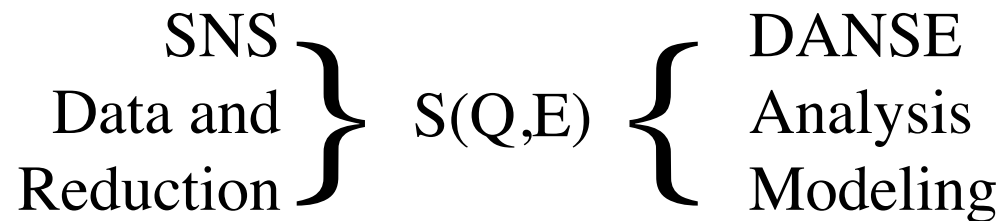
---

*Ensure a career path for scientists who add  
value at this higher level.*

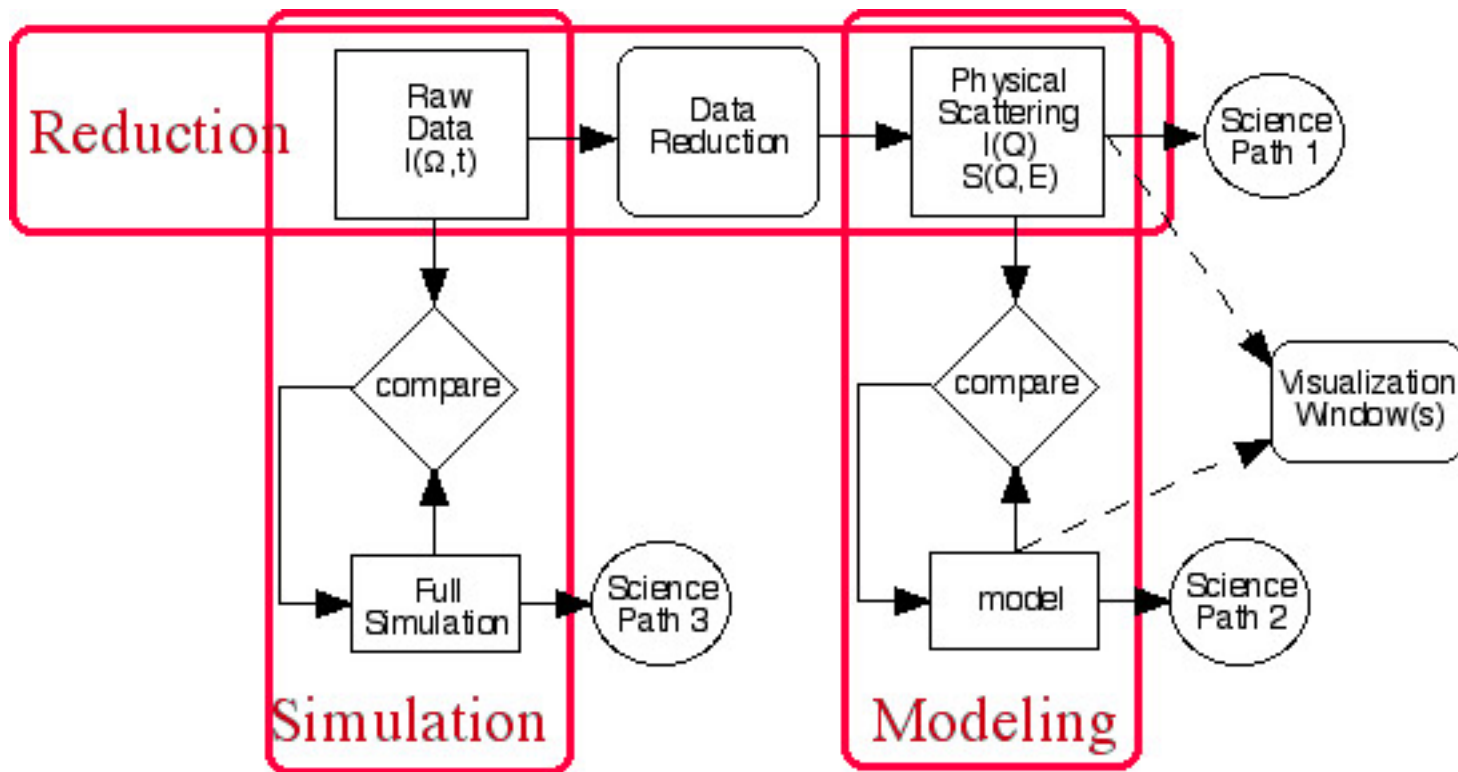
# DANSE focus is higher-level analysis tools

---

Approximately, the responsibilities of DANSE and SNS meet at  $S(Q,E)$  or  $I(Q)$



# Three Paths to Discovery



# Users Differ in Expertise

---

1. Beginning Student
2. Senior Student or Postdoc
3. Young Scientist
4. Established Researcher
5. Instrument Scientist
6. Software Developer
7. System Maintainer



***REQUIREMENT***  
*One application must serve everybody. Support for different user interfaces*

# Project Metrics: Schedule, Cost, Quality

---

- All are critical
- Reality: pick 2 of 3
- NASA Management emphasis on  
“Faster, Cheaper, Better” proved a disaster
- DANSE is doing well on Cost and Quality  
Schedule is a personnel issue

# What Will DANSE Produce?

---

- Science-specific packages in Diffraction, Engineering Diffraction, SANS, Reflectometry, Inelastic
- Deliverables are at the discretion of project leaders, and vary by community needs
- SANS, reflectometry, diffractometry, have large numbers of users who need fast data visualization and manipulation
- Inelastic, engineering diffraction have focus on developments in materials theory (DFT, FEA) -- deployment as a web service.

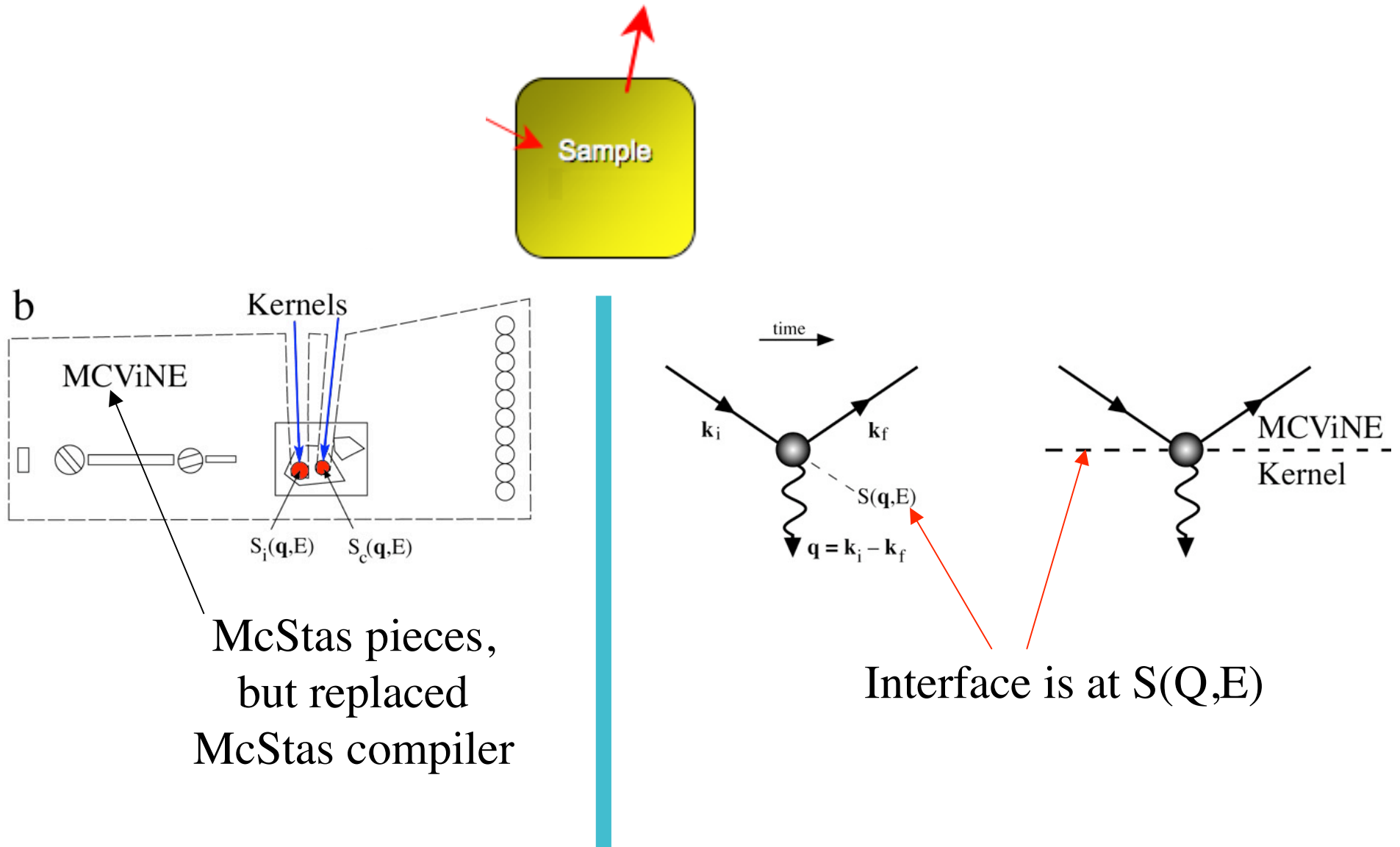
# Data Reduction for Chopper Spectrometers (DRCS, or “DrChops”)

- Installed on the ARCS cluster, to be adapted to SEQUOIA, CNCS
- Modular structure allows quick production of diagnostic tools
- Performance scales almost linearly with the number of processors.
- In use now.



# Virtual Neutron Facility: vnf

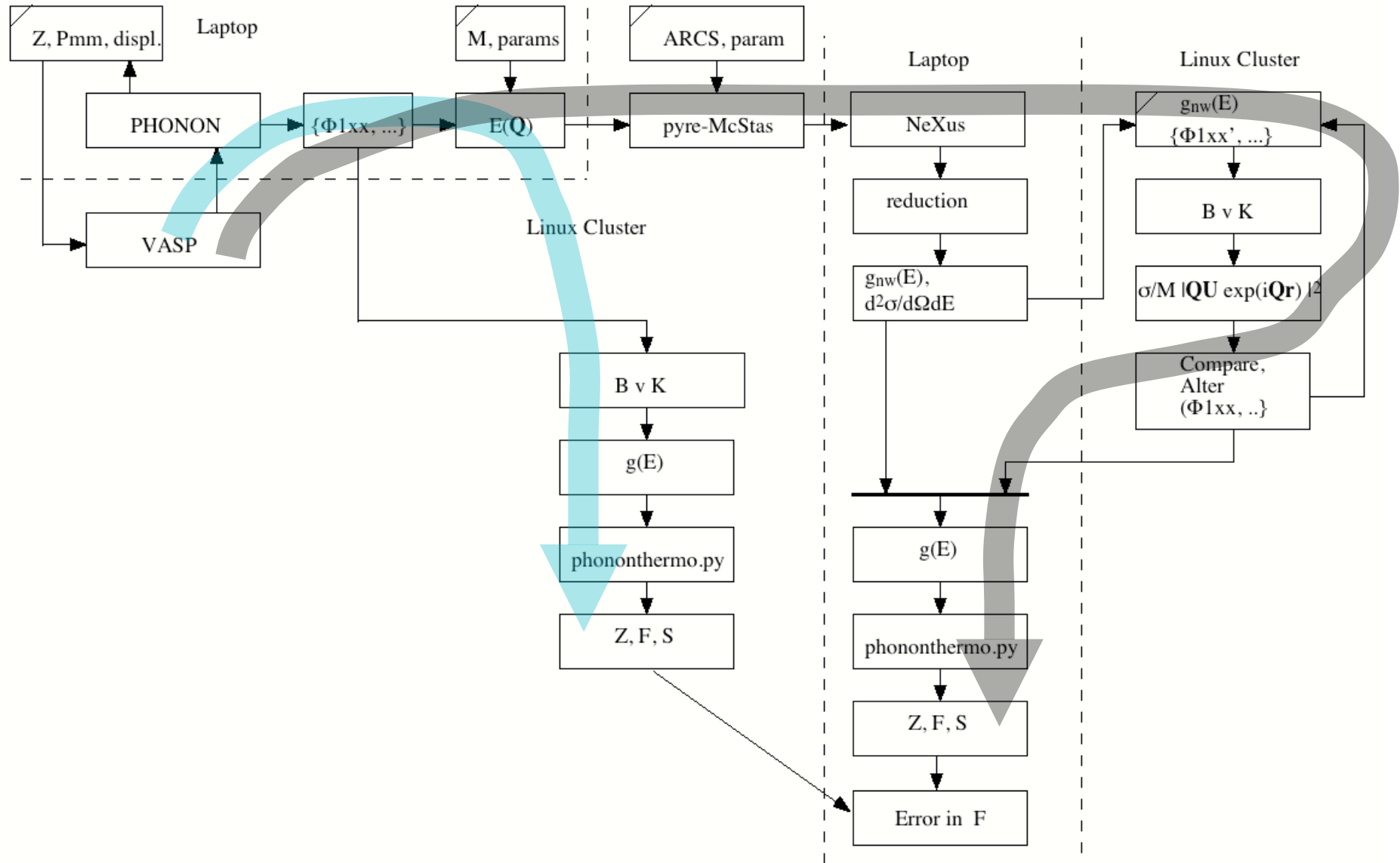
## Monte Carlo Instruments + Scattering Kernels



# Demo of vnf web service

<http://vnf.caltech.edu>

# Error Bars in Phonon Thermodynamic Quantities



# Summary

---

- Lots of low-lying fruit for computation and neutron science.
  - Laptop-friendly focus for SANS, reflectometry
  - Computational science focus for inelastic, engineering diffraction
- Misperceptions of specifications are the biggest risk in software projects, but DANSE developers are users.
- Subproject leaders know what science they want. Roles of DANSE and SNS have evolved naturally.
- The DANSE Project is initiated, and path forward is clear.