Neutron Scattering Experiments and Data Analysis

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- Big Facilities are Needed to Make Neutron Beams
- Neutron Beams are used for “Small Science”
  - Numerous instruments, experiments, and science goals
  - Wide variety of user needs and sophistication in computing
  - Most data analyses today use linear data flow
  - New software can elevate the science of neutron scattering

SNS

Accelerator + Target + Instruments = B$ 1.411

NSF IMR-MIP: Distributed Data Analysis for Neutron Scattering Experiments (DANSE)

- DANSE will Deliver
  - Today's basic capabilities for data analysis
  - Software for new types of science in major subfields of neutron scattering
- Uses a Python-based runtime interpretive framework
  - scientists can rearrange software components
  - scientist/developers can add components

Opportunities in Experiment Execution

- Experiment planning. User training with unexpected events.
- Data-driven reduction and display of incoming data.
- Sample environment control in loop.
  - Today:
```
for T in [110,120,130,140]:
    "do standard acquisition"
```
  - Preferred:
```
while interesting:
    "do better resolution"
```
- Instrument hardware in loop.
  - acquire data to appropriate statistics for pre-selected model(s).
  - change instrument hardware during run (shutters, choppers…)

Opportunities in Data Analysis

- Analysis networks customized at runtime for each experiment.
- Dynamic data driving of inverse problem computations.
  - Dynamical selection of parameters
  - Optimizer packages interchanged dynamically for complex fitting landscapes.
  - Dynamic model selection for data analysis.
- Refine physical models (or identify models) using simultaneous analysis of multiple types of experimental data.
- Identify additional data that would reduce ambiguity.

Infrastructure

Applications Infrastructure

- DANSE today supports dynamical selection of runtime components and component life-cycle management.
- Algorithms for streaming data rather than full data arrays.
- Algorithms to identify features in data are pre-requisites for intelligent experiment control.
- Interactions between concurrent threads.

Systems Infrastructure

- Databases of physical data (think “CRC Handbook”)
- Computing on demand is necessary
- “Reservations” for anticipated resources

Challenges for DDDAS in Neutron Scattering

- How to verify, validate, and certify software having data-driven dynamics
  - appropriate suites of regression tests
  - statistical testing of applications and networks, using sampling of execution paths
  - end user testing
- New algorithms often required
- Consistency with user expectations (community acceptance?)

Summary of Key Points

- Neutron scattering community includes many independent groups with different physical models and many types of data.
- DDDAS opportunities for neutron scattering research
  - Convenient with DANSE software and SNS hardware
  - Data-driven selection of physical models during analysis
  - Beamtime decisions based on acquired data (sample environment control, maybe instrument hardware)