OAK RIDGE National Laboratory

AGENDA

MANAGED BY UT-BATTELLE FOR THE US DEPARTMENT OF ENERGY

Second Target Station/Computer Science & Math Workshop

8600, Room C-156, June 23-24, 2022

8:30am – 4:00pm (EDT)

https://conference.sns.gov/event/332/

Time (EDT)	Event/Activity	Lead
June 23, 2022		
Virtual link for plenary and working lunch talks: click HERE / On site : 8600, Room C-156		
8:30am – 8:50am	Welcome & Introduction to STS	Ken Herwig, Jeff Vetter, John Hetrick and Jiao Lin
8:50am – 10:35am	**Scientific software needs for Second Target Station session**	**Chaired by Jon Taylor**
8:50am – 9:20am	Future direction and current capabilities of FTS	Thomas Proffen/Pete Peterson
9:20am – 9:40am	STS Software needs	Shuo Qian
9:40am – 9:50am	STS experiment automation needs	Yaohua Liu
9:50am – 10:30am	STS data acquisition system	Matt Pearson
10:30am – 10:50am	Break	
10:50am – 12:10pm	**State of art scientific computing tools session**	**Chaired by John Hetrick**
10:50am – 11:10am	Inverse and Data Analytic Methods for Experimental Facilities	Rick Archibald
11:10am – 11:30am	AI/ML	Pradeep Ramuhalli
11:30am – 11:50am	INTERSECT	Ben Mintz
11:50am – 12:10pm	HPC and AI Convergence in Edge-to-Exascale Science Infrastructures	Malikarjun Shankar (Arjun)
12:10pm – 1:00pm	**Working Lunch:** Towards Autonomous Hyperspectral Computed Tomography (CT) Instruments	Singanallur Venkatakrishnan

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Time (EDT)	Event/Activity	Lead
1:00pm – 3:30pm	**4 Parallel breakout sessions. Each session starts with 15min talks followed by 5 min discussions. Details are attached to the end of the agenda.**	**Breakout session chairs**
8600, Room AG06 Click HERE to join	Unique software needs by STS Jamboard link	Shuo Qian and Lipeng Wan
8600, Room C-156 Click HERE to join	Experiment automation Jamboard link	Yaohua Liu and Steve Hartman
8600, Room C-152 Click HERE to join	Overall system architecture Jamboard link	Stuart Campbell
8600, Room AG05 Click HERE to join	Strategy for STS software development Jamboard link	Mathieu Doucet and Jon Taylor
3:30pm – 4:00pm	Recap	John Hetrick and Jiao Lin
June 24, 2022		
Virtual link for plenary and working lunch talks: click HERE		
8:30am – 10:30am	**4 Parallel Breakout writing sessions**	**Session chairs**
8600, Room AG06 Click HERE to join	Unique software needs by STS Jamboard link	Shuo Qian and Lipeng Wan
8600, Room C-156 Click HERE to join	Experiment automation Jamboard link	Yaohua Liu and Steve Hartman
8600, Room C-152 Click HERE to join	Overall system architecture Jamboard link	Stuart Campbell
8600, Room AG05 Click HERE to join	Strategy for STS software development Jamboard link	Mathieu Doucet and Jon Taylor
10:30am – 10:40am	Break	
10:40am – 12:00pm	4 Parallel breakout sessions Further discussion and summarize	Session chairs
12:00pm – 1:00pm	Working Lunch: AI-guided experimentation in multi-dimensional transmission electron microscopy	Maxim Ziatdinov
1:00pm – 2:40pm	Summary from all sessions	Session chairs

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Time (EDT)	Event/Activity	Lead
2:40pm – 3:00pm	Break	
3:00pm – 4:00pm	Discussion on planning for STS software strategy and concluding remarks	Ken Herwig, Jeff Vetter, John Hetrick and Jiao Lin

Breakout sessions

Unique software needs by STS -- chaired by **Shuo Qian** and **Lipeng Wan**
Onsite location: Building 8600, Room AG06
Virtual: Click HERE to join
Jamboard: https://jamboard.google.com/d/1MROS4ZJsJ4LWQO8Vh2v5_QeEbdHHrPbbx4mX1pWrDZ0/edit?usp=sharing
Discussion on unique software needs by STS instruments and answer the following charge questions

- What are the current workflows when running experiments on those instruments at SNS? How is the experimental data generated/transferred/stored/processed/analyzed, etc.? Is there a particular bottleneck that hampers the timeliness of getting the scientific results and affects scientists' productivity?
- What algorithms need to be developed to enable the unique capabilities of the selected STS instruments?
- What gaps in current data analysis and reduction packages will need to be addressed to enable STS instrument?
- What software do your user community need but underdeveloped/not developed?

Talks to inspire the discussion

- "Reduction and analysis challenges across the STS instrument suite", Garrett Granroth
- "Scientific machine learning tools for neutron scattering data", Guannan Zhang
- "Atomistic modeling and machine learning for neutron scattering data analysis", Yongqiang Cheng

Experiment automation – chaired by **Yaohua Liu** and **Steven Hartman**
Onsite Location: Building 8600, Room C-156
Virtual: Click HERE to join
Jamboard: https://jamboard.google.com/d/1Kfp6pW0tHnfB5GktLYf2tg6gBFbFV33BXZSO9OLDP24/edit?usp=sharing
Discussion on unique software needs for experiment automation for STS instruments with the following topics

- Current experiences in neutron/x-ray user facilities.
- Trends in data acquisition
- Impacts on STS instrument design

Talks to inspire the discussion

- "Using Bluesky for Data Acquisition", Tom Caswell (NSLS II)
- "Autonomous X-ray Scattering Experiments at NSLS-II", Masafumi Fukuto (NSLS II)
- "Automatic high data-rate macromolecular crystallography", Alexei Soares (NSLS II)
- "Autonomous Discovery of the Magnetic Oder Parameter with ANDiE, the Autonomous Neutron Diffraction Explorer", Austin McDannald (NIST)

Overall system architecture. – chaired by **Stuart Campbell**

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Onsite Location: Building 8600, Room C-152
Virtual: Click HERE to join
Jamboard: https://jamboard.google.com/d/1TXEFngmhN1tuw1Bmub7GN5mAJS1VDLFSET8hxoYaKMw/edit?usp=sharing
Learn from system architectures for scientific computing systems in neutron/x-ray user facilities worldwide and discussion on guidelines for designing STS system architecture. Topics include

- Integration of DAQ, data management, data reduction, and data analysis
- Interfaces between components

Talks to inspire the discussion

- "FTS architecture", Pete Peterson
- "NSLS-II architecture", Stu Campbell (NSLS II)
- "DAQ Architecture for Instruments at the European Spallation Source", Tobias Richter (ESS)

Strategy for STS software development. – chaired by **Mathieu Doucet** and **Jon Taylor**
Onsite location: Building 8600, Room AG05
Virtual: Click HERE to join
Jamboard: https://jamboard.google.com/d/1EK6YRDXOLu2oeWlcBLvG8SlCY8aWlQp7Zh80-4t4zEQ/edit?usp=sharing
Discussion on timeline and strategy for STS software development. Topics include

- How to "future proof" software?
- What are the critical decisions for STS software, and when should they be made (timeline)?
- Lessons learned in software development in neutron/x-ray user facilities worldwide

Talks to inspire the discussion

- "ESS software strategy", Jon Taylor
- "FTS software strategy", John Hetrick
- "NSLS-II software strategy", Stuart Wilkins (NSLS II)