

Second Target Station/Computer Science & Math Workshop

June 23-24, 2022

8:30am – 4:00pm (EDT)

Draft

Time (EDT)	Event/Activity	Lead
June 23, 2022		
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	Chair: Jon Taylor
8:50am – 9:10am	Current software stack and future direction of FTS	Thomas Proffen/Pete Peterson
9:10am – 9:30am	STS Software needs	Shuo Qian
9:30am – 9:50am	Autonomous experiments for STS	Yaohua Liu
9:50am – 10:35am	STS data acquisition system	Matt Pearson
10:35am – 10:50am	Break	
10:50am – 12:10pm	State of art scientific computing tools session	Chair: John Hetrick
10:50am – 11:10am	Inverse and Data Analytic Methods for Experimental Facilities	Rick Archibald
11:10am – 11:30am	AI/ML	TBD
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 Venkatakrisnan

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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
3:30pm – 4:00pm	Recap	John Hetrick and Jiao Lin
June 24, 2022		
8:30am – 10:30am	4 Parallel Breakout writing sessions	Session chairs
	Unique software needs by STS	Shuo Qian and Lipeng Wan
	Experiment automation	Yaohua Liu and Steve Hartman
	Overall system architecture	Stuart Campbell
	Strategy for STS software development	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
2:40pm – 3:00pm	Break	
3:00pm – 4:00pm	Discussion on planning for STS software strategy	John Hetrick and Jiao Lin

Breakout sessions

Unique software needs by STS -- chaired by **Shuo Qian** and **Lipeng Wan**

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**

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 Order Parameter with ANDIE, the Autonomous Neutron Diffraction Explorer", Austin McDannald (NIST)

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

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**

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

- "FTS software strategy", John Hetrick

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- “ESS software strategy”, Jon Taylor
- “NSLS-II software strategy”, Stuart Wilkins (NSLS II)