



WORKSHOP ON
**SOFTWARE INFRASTRUCTURE
FOR ADVANCED
NUCLEAR PHYSICS
COMPUTING** JUNE 20-22, 2024

Workshop introduction

Amber Boehnlein and Peter Jacobs

For the Organizing Committee:

Amber Boehnlein (JLab), co-chair

Peter Jacobs (LBNL), co-chair

Joe Carlson (LANL)

Ian Cloet (ANL)

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Robert Edwards (JLab)

Raphael Hix (ORNL)

Thomas Papenbrock (UTK)

Brad Sawatzky (JLab)

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Software and computing have become drivers in Nuclear Physics (NP) due to the **explosive growth of scientific data and exascale facilities**. Exploitation of these opportunities **requires new hardware architectures and new algorithmic approaches at exascale**, including those based on Artificial Intelligence and Machine Learning.

New collaborative efforts have emerged to capitalize on such opportunities, bringing **NP theorists and experimentalists together with data and computer scientists**. A common focus of these collaborative efforts is the development of **robust, large-scale Software Infrastructure frameworks** to carry out their complex scientific programs. **Such frameworks require long-term support**; however, establishment of suitable support mechanisms is challenging. The curation and long-term preservation of data is an important related issue.

The 2023 NSAC Long Range Plan incorporates a vision for the future of advanced computing for NP research. **This workshop will bring together NP computing practitioners** to discuss the implementation of this vision, with a focus on **identifying mechanisms to achieve long-term, sustainable Software Infrastructure**. A key output of the workshop will be a **White Paper documenting community consensus on critical research directions, concerns, and opportunities in this area**.

The workshop program will cover a broad range of current software and computing projects in the Nuclear Physics domain. Discussions will include general issues such as the **role of research vs. infrastructure software, development of common software ecosystems, software sustainability best practices, and workforce development**. Consideration of new opportunities will be carried out in the context of **existing and currently planned DOE and NSF programs** that support advanced NP computing and cyber-infrastructure.

Workshop is in response to a request from the Agencies for guidance

- opportunity to help shape the future NP program in Advanced Computing

Product of the Workshop: White Paper

Workshop structure:

1. Survey of the field: funded collaborations, open mic, discussion with agencies
2. Parallel sessions: unstructured discussion to develop White Paper bullets and supporting text in main sub-areas
3. Plenary: White Paper draft of bullets and supporting text

Agenda Thursday 6/20

Timetable

Main Session
 Open Mic Plenary

09:00	Welcome; Safety; Conference Logistics Auditorium, Cebaf Center	09:00 - 09:05
	Introduction to SANPC <i>Amber Boehnlein et al.</i> Auditorium, Cebaf Center	09:05 - 09:20
	MUSES <i>Andrew Manning et al.</i> Auditorium, Cebaf Center	09:20 - 09:40
	ENAF <i>W Raphael Hix</i> Auditorium, Cebaf Center	09:40 - 10:00
10:00	NUCLEI <i>Thomas Papenbrock</i> Auditorium, Cebaf Center	10:00 - 10:20
	Break Atrium, Cebaf Center	10:20 - 10:50
	BAND <i>Kyle Godbey</i> Auditorium, Cebaf Center	10:50 - 11:10
11:00	JETSCAPE <i>Abhijit Majumder</i> Auditorium, Cebaf Center	11:10 - 11:30
	QuantOm <i>Ian Cloet</i> Auditorium, Cebaf Center	11:30 - 11:50
	SciDAC FastMath <i>Todd Munson</i> Auditorium, Cebaf Center	11:50 - 12:10
12:00	Infrastructure for Nuclear Nonproliferation Data Science Res <i>Paul Adamson</i> Auditorium, Cebaf Center	12:10 - 12:30
	Lunch Cebaf Center	12:30 - 13:30
13:00	Exp - Collider (RHIC, LHC, EIC) <i>Mateusz Ploskon</i> Auditorium, Cebaf Center	13:30 - 13:55
	Exp - JLab/FRIB <i>Sean Liddick</i> Auditorium, Cebaf Center	13:55 - 14:20
14:00	Computing for Neutrino Physics <i>Jason Brodsky</i> Auditorium, Cebaf Center	14:20 - 14:45
	Break Atrium, Cebaf Center	14:45 - 15:15
15:00	JLab Angular Momentum (JAM) <i>Wally Melnitchouk</i> Auditorium, Cebaf Center	15:15 - 15:35

Funded collaborations

Adjacent agencies

Experiments

15:00	Atrium, Cebaf Center	14:45 - 15:15
	JLab Angular Momentum (JAM) <i>Wally Melnitchouk</i> Auditorium, Cebaf Center	15:15 - 15:35
	LQCD <i>William Detmold</i> Auditorium, Cebaf Center	15:35 - 16:05
16:00	IQUS <i>Martin Savage</i> Auditorium, Cebaf Center	16:05 - 16:25
	Community-driven repositories of knowledge <i>Kyle Godbey</i> Auditorium, Cebaf Center	16:25 - 16:35
	Sharing simulation data with community <i>Chun Shen</i> Auditorium, Cebaf Center	16:35 - 16:45
	Maintaining and Refactoring Legacy Code <i>Abraham Flores</i> Auditorium, Cebaf Center	16:45 - 16:55
17:00	Challenges in non-equilibrium many-body dynam <i>Aurel Bulgac</i> Auditorium, Cebaf Center	16:55 - 17:05
	HPC and Quantum Computing in Nucle <i>Joseph Carlson</i> Auditorium, Cebaf Center	17:05 - 17:15
	QMC calculations of nuclear responses: beyond Carbon <i>Lorenzo Andreoli</i> Auditorium, Cebaf Center	17:15 - 17:25
	ML for [high-energy] Nuclear Physics <i>Mateusz Ploskon</i> Auditorium, Cebaf Center	17:25 - 17:35
	Neural Network for low-energy nuclear structure <i>Alex Gnech</i> Auditorium, Cebaf Center	17:35 - 17:45
	Optimization with Correlated Errors <i>Ron Soltz</i> Auditorium, Cebaf Center	17:45 - 17:55
18:00	TListSpectrum: toolset for spectroscopic analysis <i>Heather Garland</i> Auditorium, Cebaf Center	17:55 - 18:05
19:00	Welcome Event	
20:00	Atrium, Cebaf Center	18:15 - 20:15

Funded collaborations

Open mic

Agenda Friday 6/21



Parallel session convenors

Theory: Claudia Ratti, Kostas Originos

Experiment: Markus Diefenthaler, Mateusz Ploskon

Joint Theory+Experiment: Kyle Godbey, Ron Soltz

Agenda Saturday 6/22

09:00	Main Session: Writing	
10:00	<i>Auditorium, Cebaf Center</i>	09:00 - 10:30
	Break	
	<i>Atrium, Cebaf Center</i>	10:30 - 11:00
11:00	Main Session: Writing	
	<i>Auditorium, Cebaf Center</i>	11:00 - 12:00
12:00	Wrap Up Discussion	
	<i>Auditorium, Cebaf Center</i>	12:00 - 12:30

Writing session

Goal: consensus draft of White Paper main bullets + supporting text

Final comments

This workshop is an experiment. It is up to us collectively to figure out how to make it work efficiently and productively

- aim for open and in-depth discussion
- but there is a lot to cover: agenda is (necessarily) packed

Plenary session chairs should let discussion run within reason, but extended discussion should be tabled for the parallel sessions

- charge to parallel convenors: keep track of such discussions and incorporate into parallels as appropriate

Goal for Saturday noon: workshop consensus of main bullets and (brief) supporting text

Post-workshop: writing of full White Paper

- Overleaf, structured and delegated as needed
- Time scale ~2 months (?)
- Last point of discussion on Saturday: next steps

Thanks for support:



Office of Nuclear Physics and ASCR

