Minority Serving Institution Partnership Program (MSIPP)
National Nuclear Security Administration (NNSA)
Nuclear Security Advanced Manufacturing Enhanced by Machine Learning
2025 NSAM-ML Annual Workshop
February 24-25, 2025, Southern University at Baton Rouge

Zoom link login for remote access:
(Meeting ID: 910 2870 9618; Passcode: 285363)

Day 1: **February 24, 2025**

8:15 am **Central Time**	Arrival, Breakfast on the 2nd floor and nametag pick-up/meeting in **Room 313 Allain**
8:50 – 9:10 am	Welcome by Dr. Abdennaceur Karoui, Consortium Director and PI Welcome and opening remarks by Dr. Martin, Dean of College of Sciences and Engineering; Dr. Kourouma, Chair of Computer Science (SUBR)
9:10 – 9:30 am	Keynote Speaker: Dr. Michael Pettes Center for Integrated Nanotechnology Deputy Group Leader at LANL (Virtual)
9:30 – 10:30 am	**NSAM-ML programs**
15 min	Abdennaceur Karoui: NSAM-ML Consortium Mission and Progress
15 min	Bijandra Kumar: Advancements in NSAM-ML Research at ECSU for Electrochemical CO_2 Conversion
15 min	Branislav Vlahovic: Overview of the NSAM-ML Research and Academic Program at NCCU and Its Potential Expansion with Manufacturing Using Positron Beams
15 min	Shizhong Yang: Advances in the NSAM-ML research on structural alloys for nuclear reactors
10:30 – 10:50	**Coffee Break**
10:50 – 12:05 pm	**Presentations by SNL and LANL partners**
15min	David Littlewood: Overview of Center for Computing Research at Sandia and Opportunities for Students
15 min	Yongqiang Wang: Ion Beams to Advance Fusion Materials Research and Opportunities for Students
15 min	Ben Derby：Extending interfaces in 3D to enhance strength and ductility under extreme mechanical load
20 min	James Goff: Atomistic structure generation and inverse machine-learning for materials from LAMMPS (SUBR-ECSU-SNL cooperative project)
12:50 – 1:50 pm	**Lunch at 2nd Floor, T. T. Allain Hall** Group picture outside of T. T. Allain

1:50 – 2:50 pm	Parallel Session 1: LANL (Room 313 Allain) https://zoom.us/meeting/91028709618?occurrence=1740492000000&meetingMasterEventId=NR0v0ojPR9-1XVHKC1-nKA&amp_device_id=7c960437-683b-4183-a32e-9b6f8731e53b (Meeting ID: 910 2870 9618; Passcode: 285363) SUBR (Face to Face), ECSU(Virtual), NCCU (Virtual)
1: 50 – 2:50 pm	Parallel Session 2: SNL (Room 206, Allian) https://us06web.zoom.us/j/89694530525?pwd=kxtnnHF6etmBw0PCbj1adudIqUx7r7.1 (Meeting ID: 896 9453 0525; Passcode: 716162) SUBR (Face to Face), ECSU(Virtual), NCCU (Virtual)
1:50 – 2:50 pm	Parallel Session 3: Meeting of the PIs and Partners (Room 210, Allain) Planning future work, and summary of the accomplished meeting goals
2:50 – 4:20 pm	**Lab tour (Pinchback, then Fisher, Lee, Thurman, and Allain)**
	Coffee Break at T. T. Allain (2nd floor)
4:20 – 5:00 pm 4:20 – 5:45 pm	**Student poster session** Parallel session with FitSNAP hands-on (on site, recording for consortium) Wrap-Up of day 1 meeting
6:00 pm	Dinner (T. T. Allain Hall, 2nd floor)

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Day 2: February 25, 2025

8:15 – 8:50 am	Arrival, Breakfast on the 2nd floor (meeting at Room 313 T. T. Allain)
8:50 – 9:00 am	Opening (Yang & Vlahovic)
9:00 – 10:00 am	Oleg Starovoytov: Development of the machine learning potential for simulations of CrFe alloys, and applications to other NSAM-ML projects
10:00 – 10:20 am	Coffee Break
10:20 – 12:20 am	Work by Students / Teams
10 min	Yang: Student Projects at SUBR
10 min	Student 1: Raelyn L. Henderson: Behind the Beams: Insights and Experiences from Los Alamos National Laboratory
10 min	Student 2: Lewis Jordin: Prediction of Yield Strength in High-Entropy Alloys Using AI Models
10 min	Student 3: Jebriel Morehouse: ML on interatomic potential building: Pb/Cu(223)
10 min	Flanigan: Student Projects at NCCU

10 min	Student 1: Andrea Joseph: Computational simulation of a chemical detector based on quantum confinement
10 min	Student 2: Manuj Mishra, Machine learning-based optimization of data from silicon photonics detector devices (virtual)
10 min	Karoui: Student Projects at ECSU, CNT Library a collection of student research
10 min	Student 1: Luz, Mechanical Properties and Thermal Properties of CNTs
10 min	Student 2: Quimora, Uncertainty Quantification to improve Solving PDE using Machine Learning
10 min	Student 3: Coreen Mullen, Refactoring New Structure Generation Software (SUBR-ECSU-SNL cooperative project)
12:20 – 12:40 pm	**Joint research with SNL and LANL partners**
10 min	Abdennaceur Karoui: NSAM-ML subprojects requiring collaborative efforts
10 min	Discussion
12:30 – 1:30 pm	Lunch
1:30 – 2:00 pm	ECSU Karoui's Team
15 min	Reactive sputtering for hyperdoping Si and SiGe,
15 min	Rogelio Lopez: Diffusion of Nitrogen in N hyperdoped Silicon
2:20 – 3:20 pm	SUBR Research connected with our SNL and LANL partners
15 min	Shizhong Yang: SUBR research and training linked with SNL and LANL
15 min	Shengmin Guo: Friction stir additive manufacture of AL6061 and stainless steel
15 min	Joshua Hinz: Constructing a near minimum ionic descriptor with principal component analysis for transfer learning of interatomic potentials
15 min	Planned joint work SUBR team with SNL and LANL partners
3:20 – 4:00 pm	Meeting of PIs and Partners; Group Pictures
4:00 – 4:30 pm	Coffee Break
	Closing Remarks and future Agenda
6:00 pm	Group Dinner

Note: If you drive from nearby airport hotels, there are three entrances we may use: 1) Harding Blvd (police gate), 2) Swan Ave, or 3) Mills Ave. The last two have no police gate.
For parking, please pick up a parking permit from the police station across Farm Road, and the close by commute parking lot is in northeastern side of Allain, across the traffic light.