



# Earth & Environmental Systems Modeling

## 2024 EESM PI Meeting

August 6-9, 2024

Bethesda North Marriott Hotel & Conference Center  
Rockville, Maryland, USA

**Date and Time:** Thursday, August 8, 2024, 1:00-4:00 p.m.

**Session Name:** 2. Innovative and Emerging technologies: ML/AI, Digital Earth, Exascale and Quantum Computing, Advanced Software Infrastructures

**Breakout Chairs:** Casey Burleyson, PNNL ([burleyson@pnnl.gov](mailto:burleyson@pnnl.gov)), Peter Caldwell, LLNL ([caldwell19@llnl.gov](mailto:caldwell19@llnl.gov)), Travis O'Brien, Indiana University ([obrienta@iu.edu](mailto:obrienta@iu.edu)), and Patrick Reed, Cornell ([patrick.reed@cornell.edu](mailto:patrick.reed@cornell.edu))

**Topic Leads:** Ethan Coon, Andrew Gettelman, Klaus Keller, Ruby Leung, Brian Medieros, Jennie Rice, Chris Vernon, Hui Wan, Xubin Zeng, Qing Zhu

**Room / Location:** White Flint Room

**Session Organization:** Breakouts 1 and 2 will facilitate discussion organized to explore the following three themes. Our discussions will culminate in a report out on opportunities for the EESM program.

- *Theme 1: Machine Learning for Data Analysis*
- *Theme 2: Machine Learning for Simulation and Uncertainty Quantification*
- *Theme 3: High Performance Computing and Exascale Applications*

Talks: 10-minute perspectives that draw from your research to address a theme and facilitate discussion

### ***Breakout Session Agenda***

#### ***Theme 1: Machine Learning for Data Analysis***

- Moderator: TBD
- Rapporteur(s): TBD
- Zoom Monitor: TBD

1:00 p.m.: Introduce Session Organization, Themes for Discussion, and Goals (TBD)

1:10 p.m.: Theme 1 Talk 1 - Advancing Earth System Modeling using AI/ML – Dan Lu, ORNL

1:20 p.m.: Theme 1 Talk 2 - Strategic Systematic Review and Exploration of the Research Area of MultiSector Dynamics using Natural Language Processing, Graph Machine Learning, and Large Language Models – Chris Vernon, PNNL

1:30-1:50 p.m.: Theme 1 Discussion – EESM Opportunities in ML for Data Analysis

### ***Theme 2: Machine Learning for Simulation and Uncertainty Quantification***

1:50 pm Theme 2 Talk 1 - Huge Ensembles of Weather Extremes using the Fourier Forecasting Neural Network – Bill Collins, LBNL

2:00 p.m.: Theme 2 Talk 2 - Using Machine Learning and Bayesian inference to constrain microphysics in LES and ESMs – Marcus van Lier-Walqui, Columbia

2:10-2:30 p.m.: Theme 2 Discussion – EESM Opportunities in ML for Simulation & UQ

2:30-2:45 p.m.: Break

### ***Theme 3: High Performance Computing and Exascale Applications***

- Moderator: TBD
- Rapporteur(s): TBD
- Zoom Monitor: TBD

2:45 p.m.: Theme 3 Talk 1 - Introduction to the Simple Cloud-Resolving E3SM Atmosphere Model (Peter Caldwell, LLNL)

2:55 p.m.: Theme 3 Talk 2 - Adaptive Mesh Refinement in the age of Exascale Computing (Ann Almgren, LBNL)

3:05-3:25 p.m.: Theme 3 Discussion – EESM Opportunities in HPC and Exascale Applications

3:25-3:45 p.m.: Discussion – Research Opportunities that Bridge ESMD, RGMA, and MSD

3:45-4:00 p.m.: Discussion Period – Session Synthesis & Grand Challenges Plenary Report Out Prep

### ***Wednesday Poster Session***

- #121 Assessing weather impacts on crop yield variability: a ML-based transfer learning approach – Srishti Vishwakarma, PNNL
- #122 Accelerating solver performance for simulations of photosynthesis in the E3SM-ELM model using machine learning – Elias Massoud, ORNL
- #123 When Machine Learning Objectives Compete for Improved Subseasonal Bias Correction, Who Wins? – Maria Molina, U Maryland
- #124 Learning data fusion, improved parameterization and atmospheric forcing corrections using a physics-informed, differentiable hydrologic model – Kamlesh Sawadekar, Penn State
- #125 Causal Discovery in Nonlinear Dynamical Systems using Koopman Operators – Derek DeSantis, LANL
- #126 Using the MSD-LIVE Open Science Platform to Teach New Researchers to Use MSD Models – Casey Burleyson, PNNL
- #127 Use of PETSc and libCEED to achieve algorithmic and hardware portability in developing a river dynamical core for E3SM – Gautam Bisht, PNNL
- #128 Differentiable Modeling and Genes of AI for Water, Climate Risks and Global Sustainability – Chaopeng Shen, Penn State

### *Thursday Poster Session*

- #121 SCREAM: The Simple Cloud-Resolving E3sm Atmosphere Model Running on the Frontier Exascale System – Mark Taylor, Sandia
- #122 Parametric Sensitivities of a Wind-driven Baroclinic Ocean using Neural Surrogates and Automatic Differentiation – Yixuan Sun, Argonne
- #123 Accelerating modeling and discovery with data science and machine learning in Arctic environments – Jon Schwenk, LANL
- #124 Is sea surface salinity the missing subseasonal predictor for U.S. summertime precipitation? – Marybeth Arcodia, Colorado State
- #125 A Fortran-Python Interface for Integrating Machine Learning Parameterization into Earth System Models – Tao Zhang, BNL
- #126 Using Information Transfer Constraint to Improve the Generalizability of Physics-Informed Machine Learning Parameterization – Peijun Li, Penn State
- #127 SCORPIO : An I/O library for Exascale ESMs – Jayesh Krishna, Argonne
- #128 OMEGA-0: Preliminary Performance Results for the Ocean Model for E3SM Applications – Brian O’Neill, LANL
- #129 Efficient testing strategies for modernizing the 4-mode Modal Aerosol Model (MAM4) for global kilometer-scale aerosol simulations – Balwinder Singh, PNNL
- #130 Purpose-built modeling to inform climate impact mitigation – Ethan Coon, ORNL