

## MACHINE LEARNING FOR MOLECULAR SIMULATIONS

TRACK NUMBER 600

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### ABSTRACT

Machine learning (ML) is revolutionizing molecular dynamics (MD) simulations and opening new potential applications in mechanics. Recent advancements such as machine learning interatomic potentials (MLIPs), geometric deep learning, and generative modeling have enabled simulations of unprecedented scale, fidelity, and efficiency. This mini-symposium will provide a platform for researchers across disciplines to present and discuss cutting-edge developments at the interface of ML and molecular simulations, with an emphasis on both methodological innovations and impactful applications in mechanics, materials, and structural design.

### Scope and Themes

The proposed symposium will cover a broad spectrum of themes where ML is pushing the boundaries of molecular modeling and simulation:

- **Machine Learning Interatomic Potentials (MLIPs):** Advances in accuracy, transferability, and scalability for atomistic simulations.[1]
- **Geometric Deep Learning & Graph Neural Networks (GNNs):** Leveraging architectures designed for physical systems to capture long-range interactions, many-body effects, and system symmetries.[2]
- **Generative Modeling for Simulation:** Generation of molecular configurations, reaction pathways, and coarse-grained representations. [3]
- **Enhanced Sampling and Coarse-Grained MD:** ML-driven methods for efficient exploration of high-dimensional energy landscapes and long-time scale dynamics. [4]
- **Particle-Based Fluid Simulation:** ML approaches for multiscale modeling of fluids and soft matter systems.
- **Other applications in Computational Mechanics:** Connecting atomistic insights to macroscopic observables such as density, strain, and stress; Structural and materials des; multiscale modeling approaches.

## **Relevance and Impact**

The proposed symposium aligns closely with the congress mission of advancing computational mechanics by integrating new paradigms and technologies. Machine learning not only accelerates MD simulations but also reshapes how fundamental physical principles are encoded, interpreted, and applied. By gathering researchers working on theory, algorithms, and applications, the symposium will foster cross-disciplinary dialogue and collaboration, accelerating the translation of methodological advances from different fields into practical engineering and scientific tools.

## **Organization**

The symposium will be co-organized by experts from diverse institutions to ensure breadth and inclusivity. We anticipate at least two sessions (4 hours total), with the possibility of a keynote lecture highlighting recent breakthroughs in ML-driven molecular modeling. Contributions will be solicited from a diverse international community, ensuring representation across academia, national laboratories, and industry.

## **Conclusion**

This mini-symposium will provide a timely and impactful venue for presenting advances in machine learning for molecular simulations, bridging computational mechanics with data-driven science, and inspiring the next generation of models and applications.

## **REFERENCES**

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