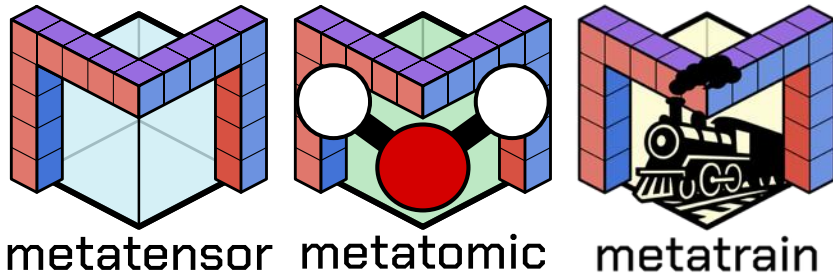
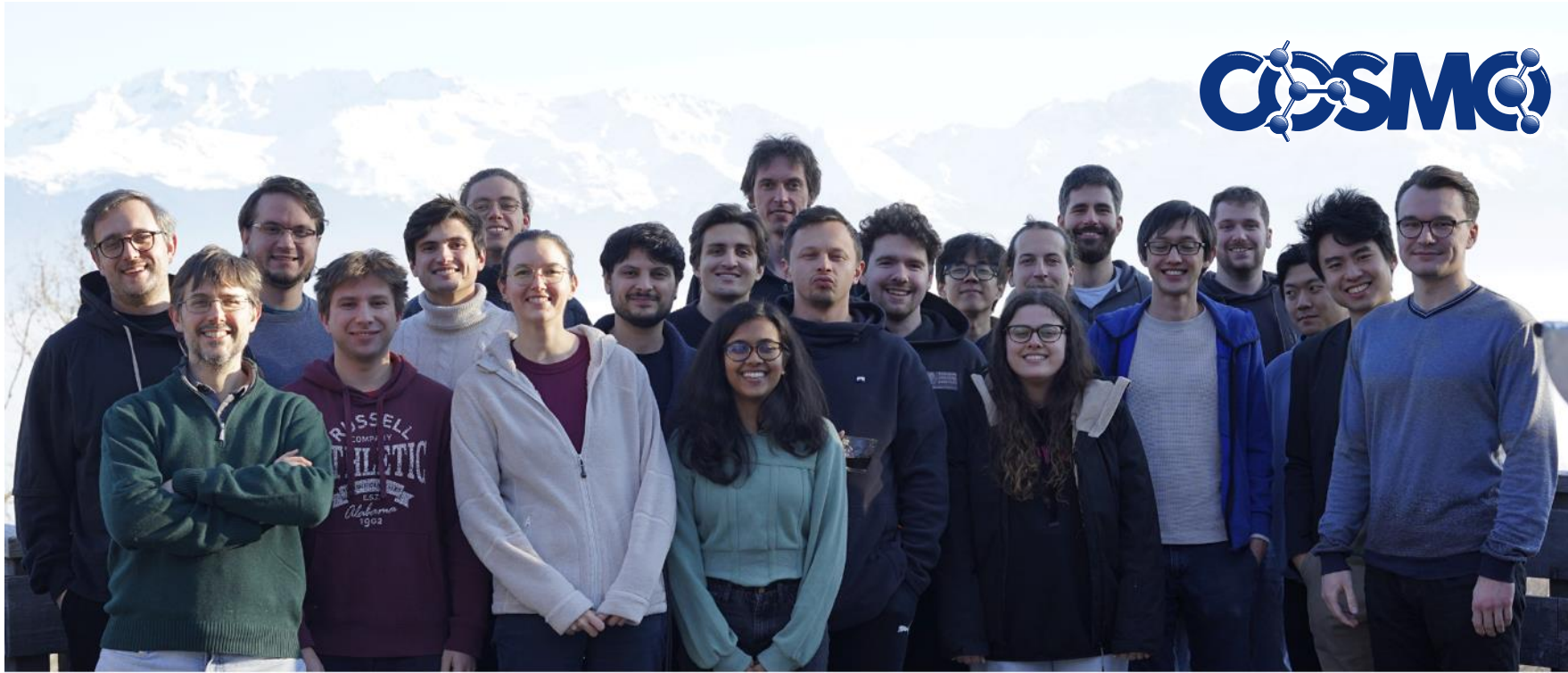


Metatensor Ecosystem Workshop 2025

Welcome & Workshop Overview




Warm Welcome and Acknowledgments





- Software stack to meet the diverse needs of atomistic machine learning
- Developed with support from SNSF, ERC, and ***importantly***: MARVEL



Workshop Schedule

- 09:30-09:40 -- Welcome + workshop overview
- 09:40-10:00 -- Atomistic machine learning: why, what, how
- 10:00-10:45 -- Introduction to **metatensor** and **metatomic**
- 10:45-11:05 -- Coffee break 
- 11:05-11:35 -- **metatrain**, a tool to train your own models
- 11:35-11:55 -- Scientific applications of the **metatensor** ecosystem 
 - ShiftML, DOS, equivariant learning, density/hamiltonian learning, UQ
- 11:55-12:15 -- PET-MAD universal interatomic potential
- 12:15-12:30 -- Pre-tutorial feedback
- 12:30-13:30 -- Lunch 

Workshop Schedule

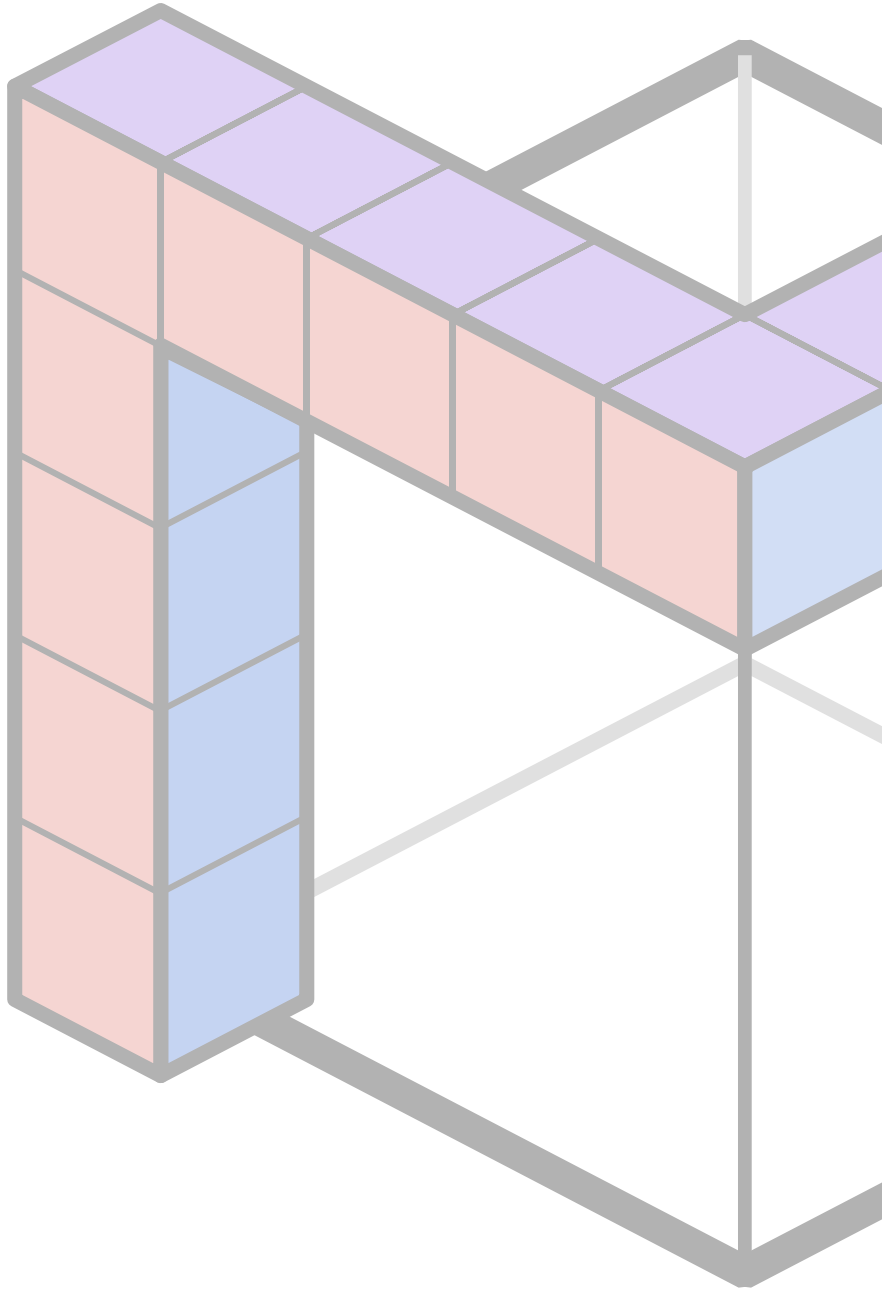
- 13:30-16:45 -- Parallel tutorial sessions 
 - A) A deep dive into **metatensor** for ML model developers
 - B) How to train your model: training custom models on custom datasets
 - C) Fine-tuning the PET-MAD universal model for specific applications
- 16:45-17:00 -- Post-tutorial feedback
- 17:00- -- Apéro  & networking

Workshop Guidelines

- Please save your longer questions
 - Q&A at the end of talks if time permits
 - Otherwise, let's make best use of the breaks and feedback sessions 🙏
- Absolutely no food or drink consumption in CoViz2
 - Don't let the coffee cart fool you ☕
- Let's be patient and respectful
 - We'll do our best to address all your questions and concerns
 - Software may/will fail at some point 💻, tell us and we'll also do our best
- Enjoy your time with us, all feedbacks are welcome 😊
 - We will send out a survey after the workshop to hear from you
 - Send us a mail in case further support is needed

Workshop Repository

<https://github.com/metatensor/workshop-spring-2025>



**We would like to
hear from you!**