

Simulation Workflows in Materials Modelling (CECAM)



Simulation Workflows in Materials Modelling (SWiMM 2021)

15th – 26th March 2021

<https://www.cecamm.org/workshop-details/27>

1. Industrial-accuracy data-driven model parameterization
2. Semantic interoperability and ontology-driven technology
3. Autotuning, load balancing, and task based parallelization
4. Salome and YACS: An integration platform for workflows
5. Simulation workflows with AiiDA and Materials Cloud
6. European Materials and Modelling Ontology
7. The Pyiron IDE for simulation workflows
8. preCICE multi-physics coupling library
9. Atomic Simulation Environment