NSM
NATIONAL SUPERCOMPUTING MISSION

Workshop 2.0

MicroSim

A powerful tool to simulate microstructure evolution using the Phase-Field technique

Mode : Online + Offline

Venue : KPA auditorium , Department of Materials Engg. , IISc Bengaluru

28-29 JULY | 10:00AM - 6:00PM

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EVENT STRUCTURE

10 AM | July 28, 2022

Overview of MicroSim (solvers, tools, updates, website, youtube). Installation and pre-requisities.
(Time: 10AM - 12PM)

Break: 15 mins

Modeling of real alloys. Setting up calculations for single-phase solidfication/precipitation, using different thermodynamic models and strategies for coupling to databases. (Time: 12:15PM - 1:45PM)

Break: 1 hr

Coupling of thermodynamic information from encrypted databases (For binary and ternary alloys).
(Time: 2:45PM - 3:45PM)

Break: 15 mins

OpenFoam solvers for setting up multi-grain solidification.
(Time: 4PM - 5:30PM)

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EVENT STRUCTURE

10 AM | July 29, 2022

OpenCL based solvers for solidifcation in real, binary and ternary alloys.

(Time: 10AM - 11:30AM)

Break: 15 mins

CUDA based solvers for precipitation in a binary alloy with thermodynamic coupling to databases.

(Time: 11:45AM - 1:15PM)

Break: 1 hr

Hands-on experience for getting a calculation running with each solver for a real alloy

(Time: 2:15PM - 4:15PM)

Break: 15 mins

Brief review of the post-processing tools using simulation data available.

(Time: 4:30PM - 5PM)

Micress vs MicroSim (A comparative evaluation)

(Time: 5PM - 6PM)

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MicroSim

(Microstructure Simulator)

MicroSim is a project under the National Supercomputing Mission, Govt of India. The project offers a set of codes that can use high-performance computing to simulate microstructure evolution using the Phase-Field technique. MicroSim is a software stack that consists of phase-field codes that offer flexibility with discretization, models as well as the high-performance computing hardware (CPU/GPU) that they can execute on. Along with this the stack also consists of Multi-physics solver modules that are based on OpenFoam and AMRex libraries (will be added soon). The stack has an integrator interface that is built using python that allows one to create the input and filling files required for the solvers as well as provides a consolidated framework to choose the solver, compile, execute and visualize simulation results. The project is developed and maintained by the consortium of researchers from IISc Bangalore, IIT Hyderabad, IIT Bombay, IIT Madras, Savitribai Phule Pune University, and C-DAC Pune. This is the first release of our phase-field software stack consisting of different phase-field models utilizing separate discretization strategies as well as the flexibility to run on different computing hardware (CPUs and GPUs). The phase-field models include the Grand-potential formalism, Kim-Kim Suzuki as well as the Cahn-Hilliard descriptions. The discretizations include FDM, FVM and FFT.

GitHub Repo | nsmmicrosim.github.io

CONTRIBUTORS

- Tanmay Dutta, Swapnil Bhure, Ravi Kumar, Bikramjit Karmakar, Umate Kartik (IISc, Bangalore) (OpenFoam solvers and documentation)
- Ajay Sagar (IISc, Bangalore) (Python wrapper and infile generator)
- Dasari Mohan, M.P. Gururajan, Gandham Phanikumar (IIT Bombay, IIT Madras) (KKS OpenCl and FFTW codes)
- Saurav Shenoy, Pankaj and S. Bhattacharyya (IIT Hyderabad) (KKS Nvidia-CUDA)
- Abhik Choudhury (IISc, Bangalore) (Grand-potential based solvers)
- Swaroop Sampad, Ankosh Deshmukh, Abhishek Kalokhe, Abhishek Kumbhar, Nasir