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UGM 2020 Training Series

MedeA LAMMPS: Robust Gateway to Molecular Dynamics

Materials Design

October 13th, 2020

Materials Design UGM

Training & Support Team

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presenter

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moderator

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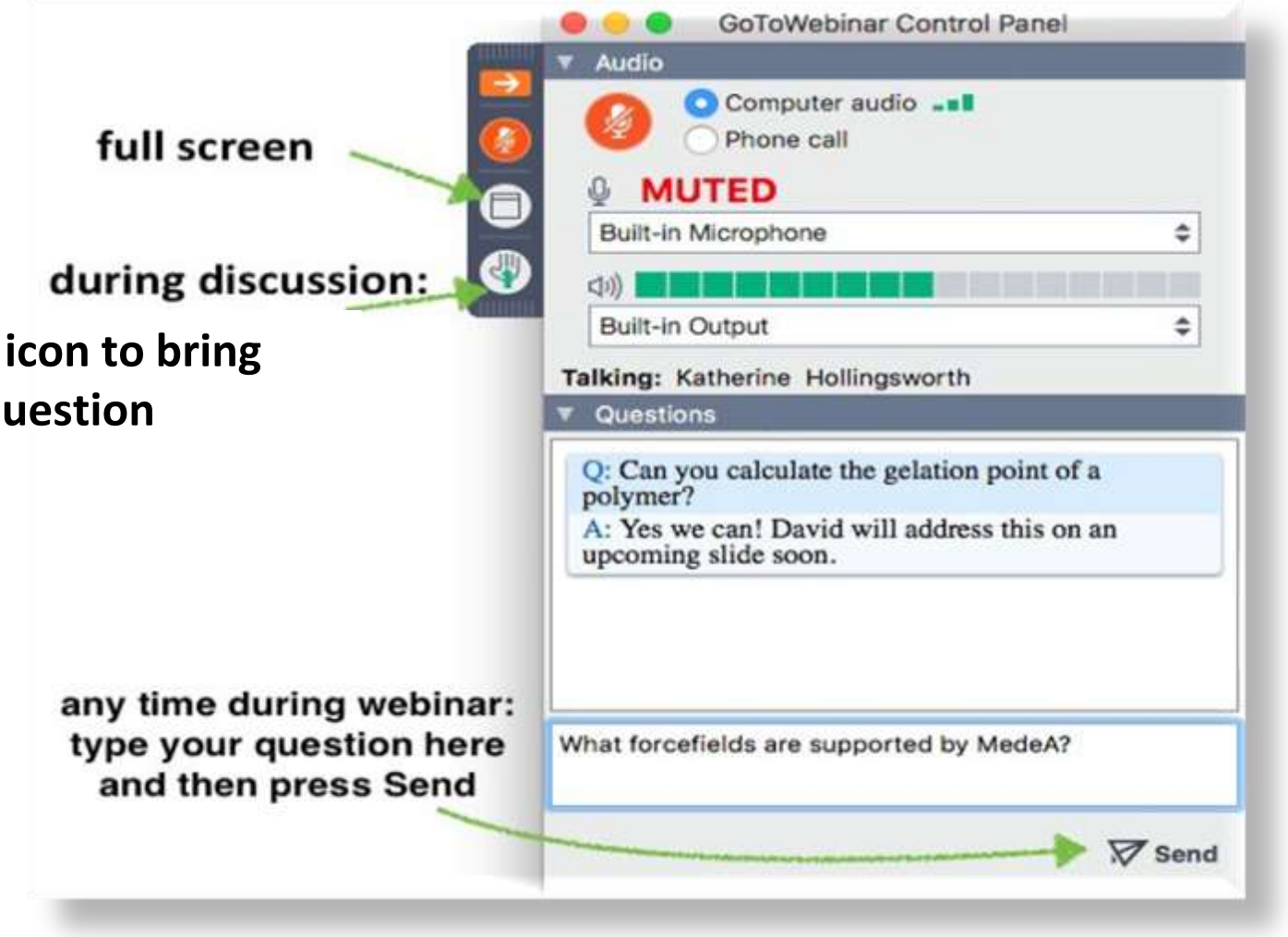
Please Ask Questions!



Use the raise hand icon to bring attention to your question

any time during webinar: type your question here and then press Send

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UGM 2020 Training Series

MedeA LAMMPS: Robust Gateway to Molecular Dynamics

Materials Design

October 13th, 2020

Outline

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- MedeA LAMMPS
- MedeA Forcefields Bundle
- MedeA Mesoscale Simulations
- MedeA Deformation
- MedeA Deposition
- Conclusions

MedeA LAMMPS

MedeA LAMMPS

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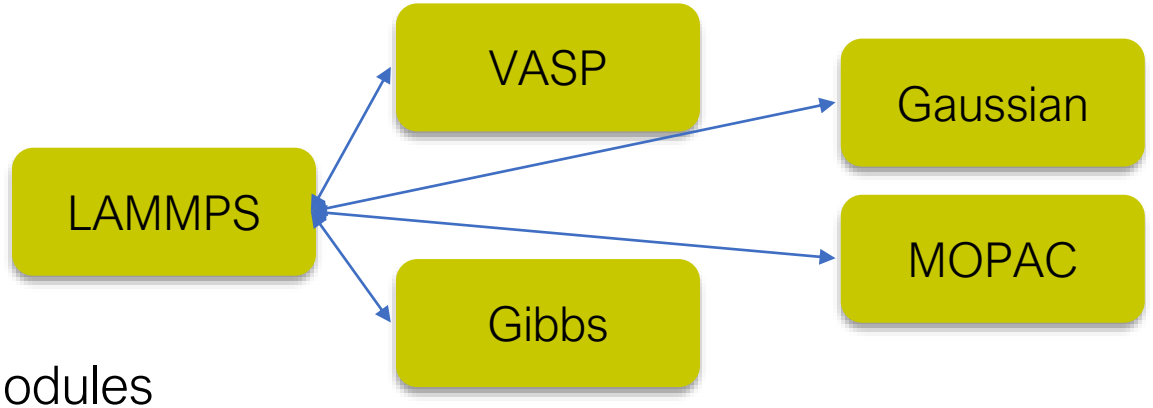
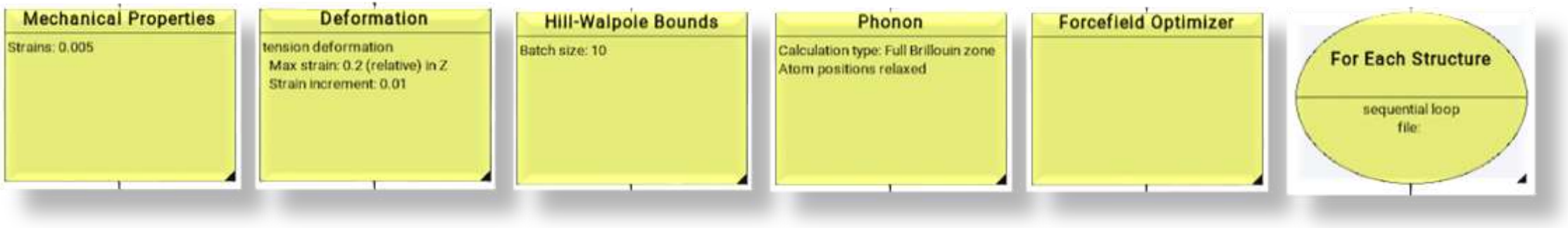
- Integrated with other simulation engines
  - Quantum Methods (VASP, MOPAC, Gaussian) and Monte-Carlo (Gibbs)



- Integrated with other modules
  - Mechanical Properties, Deformation, Hill-Walpole Analysis, Forcefield Optimizer, and High-throughput Launchpad



MedeA LAMMPS

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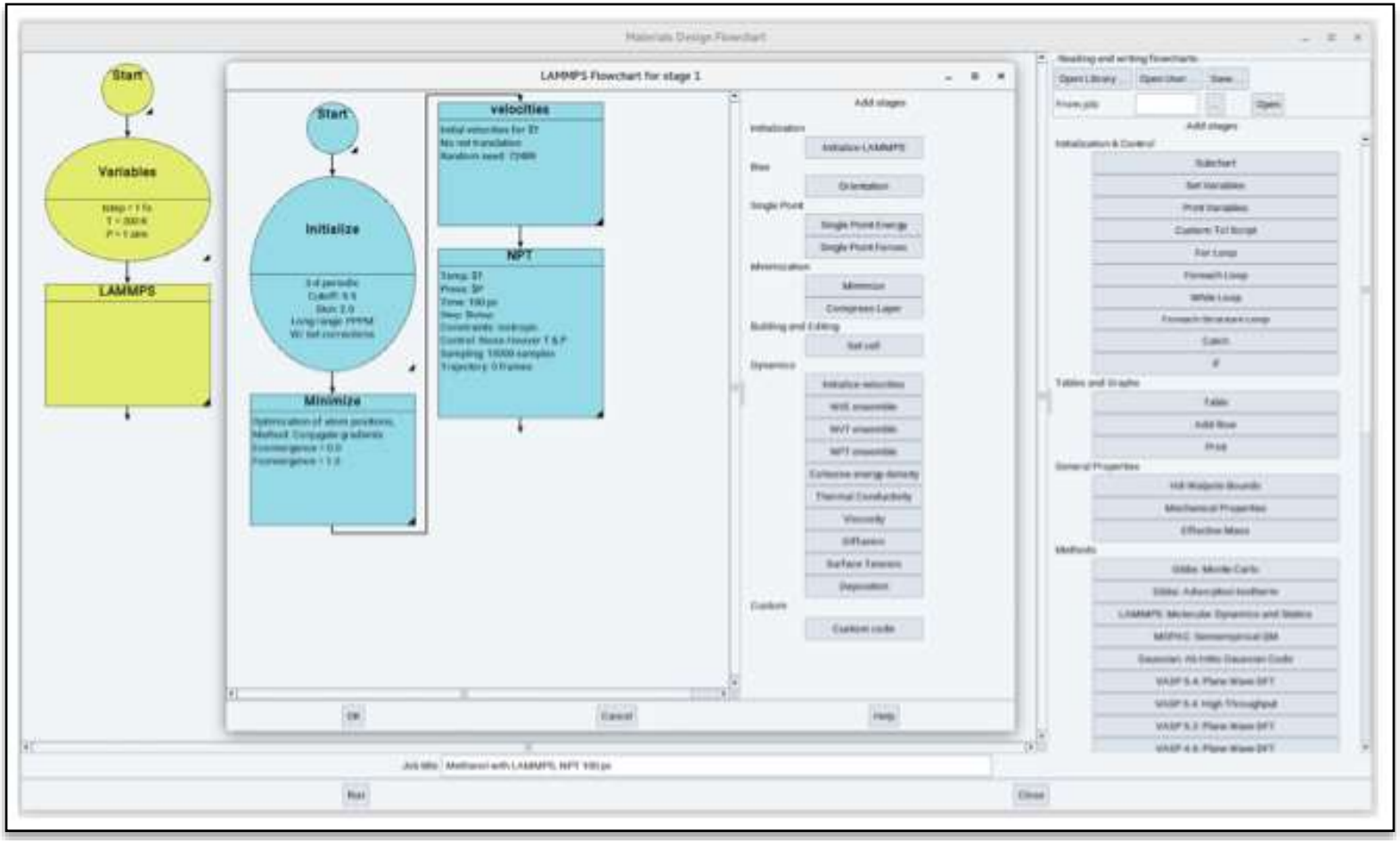
Introduction to MedeA LAMMPS

Release 3.1.0

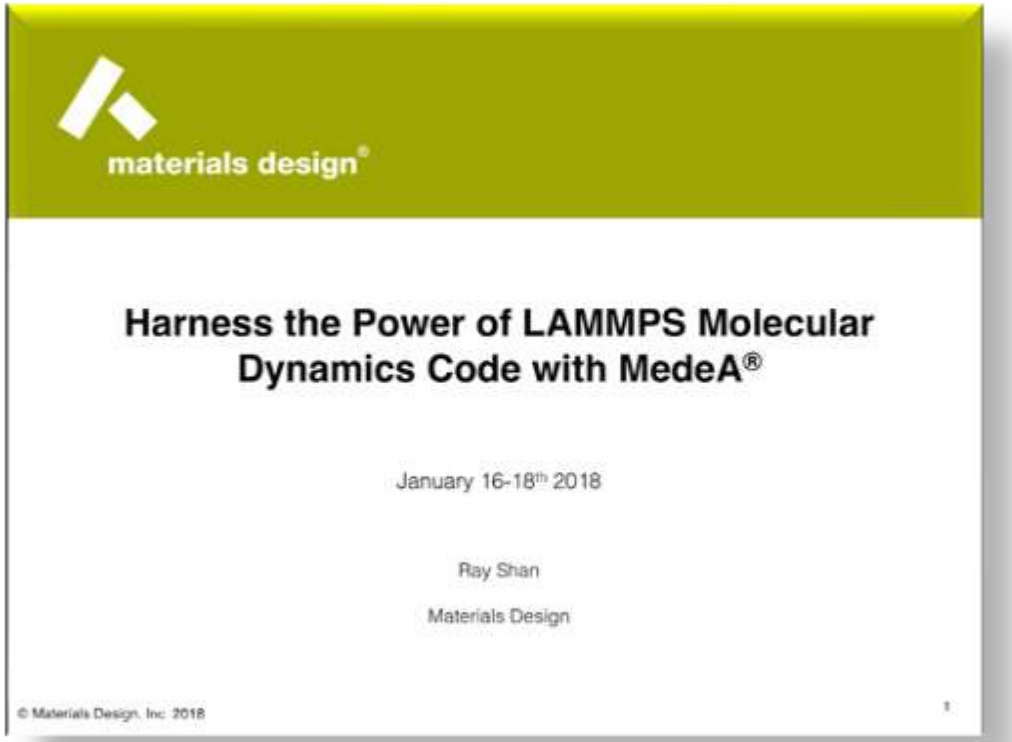
- **Objective:** Learn how to set up and run LAMMPS simulations with MedeA
- **Modules:** *MedeA LAMMPS*, *Supercell Builder*, *Amorphous Materials Builder*

Preparation time	Run time (2 Intel cores)	Level
10 minutes	5 minutes	Beginner



MedeA LAMMPS

- Watch the webinar
  - *Harness the Power of LAMMPS Molecular Dynamics Code with MedeA*
  - http://my.materialsdesign.com/webinar-12



MedeA Forcefield Bundle

Interatomic Potentials in MedeA

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- Metallic
  - EAM *
    - All LAMMPS `eam`, `eam/fs`, and `eam/alloy` variants
  - MEAM
- Inorganic
  - Buckingham (`buck`)
  - BKS (`buck/coul`)
  - Clay-FF (`harmonic` + `lj` + `coul`)
  - CVFF_aug (`class2`)
  - Morse/coul
- Semiconductor
  - Tersoff
  - Stilinger-Weber
  - REBO
- Organic (valence):
  - PCFF/PCFF+ *
  - Compass/Compass+
  - OPLS-AA/OPLS-AA+ *
  - AUA/AUA+ *
  - Trappe+ *
- Mesoscale
  - SPICA
  - Martini
- Variable charge
  - Streitz-Mintmire (`eam + coul + qeq`)
  - COMB3
  - ReaxFF

*** Also available in MedeA®-GIBBS**

Cost of Classical Forcefields

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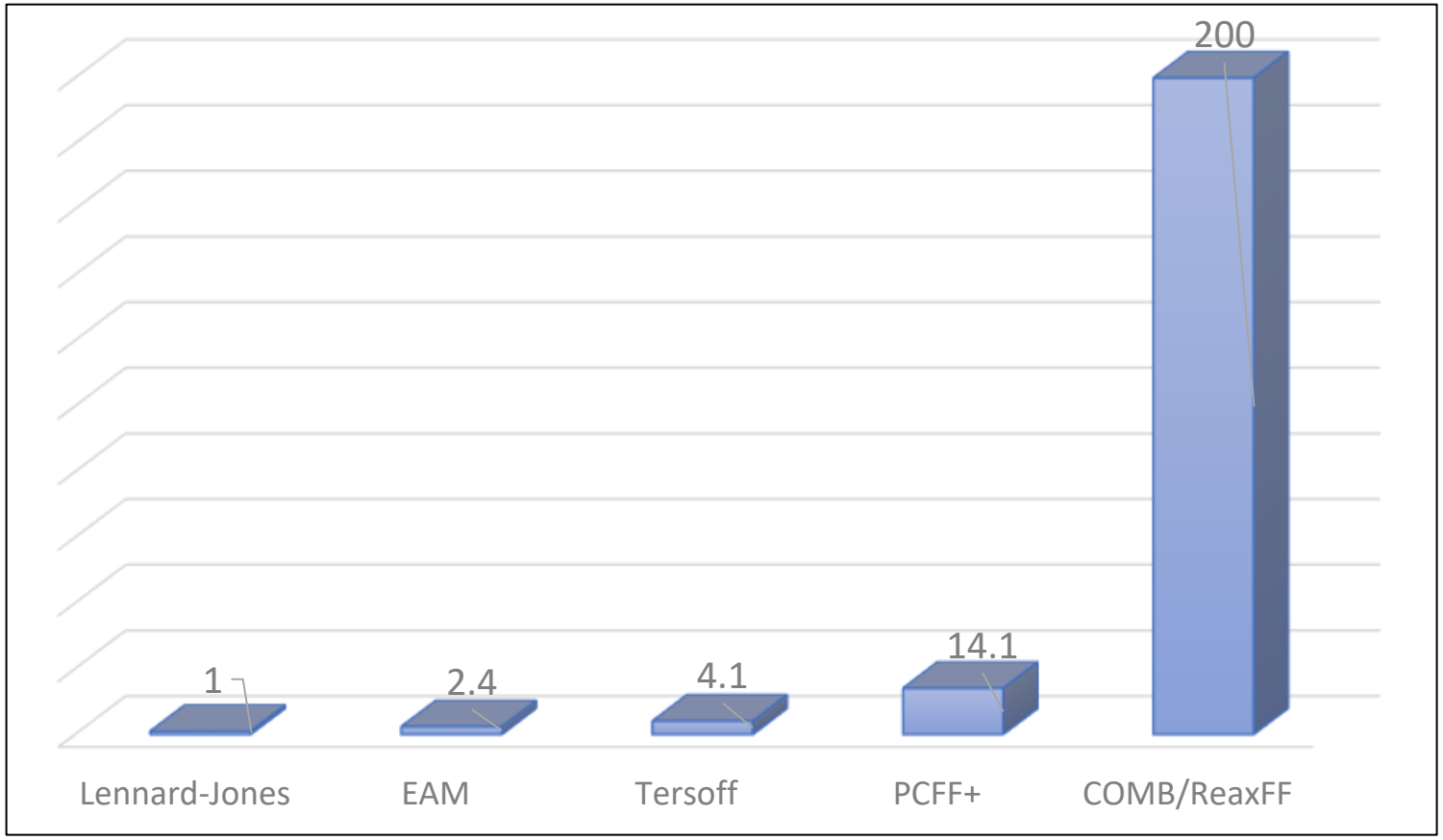
- Long-range electrostatics: 10x more expensive than LJ
- Variable charge equilibration: ~100x more expensive than LJ



Flexibility with MedeA Forcefields

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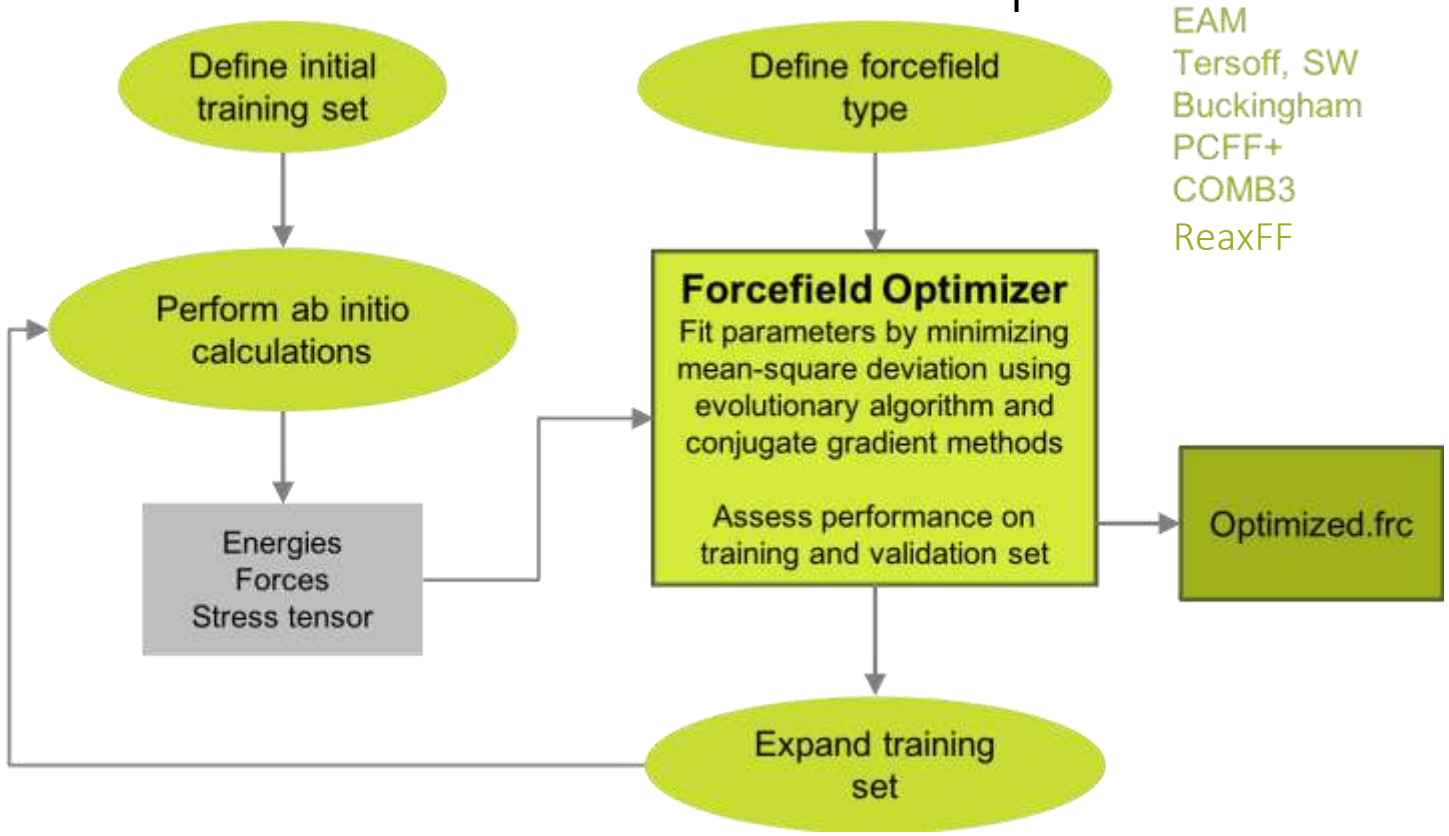
- Import external forcefield parameters
- Import external forcefield parameter files
- Develop new forcefields with MedeA Forcefield Optimizer



Visualize the Optimization

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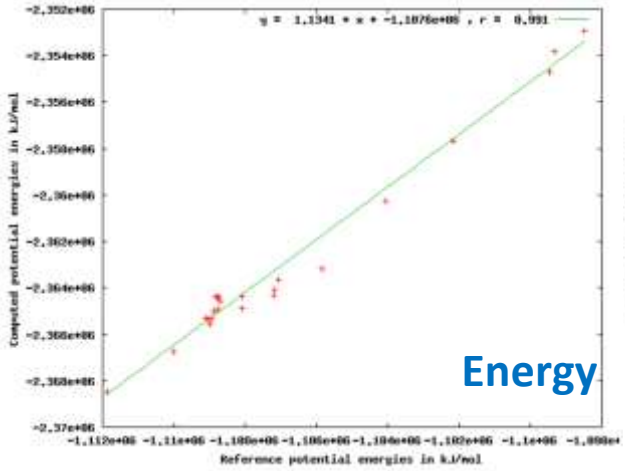
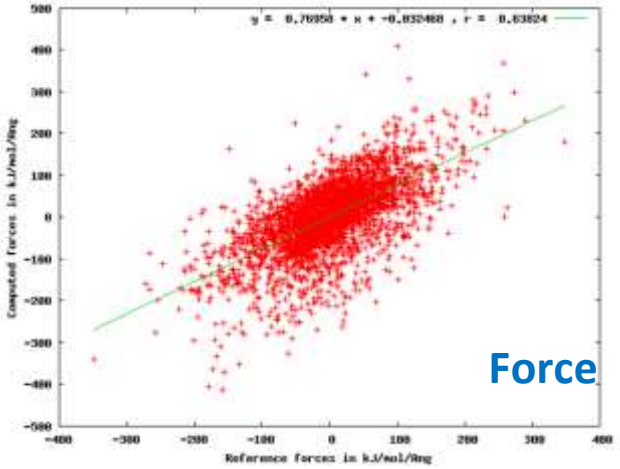
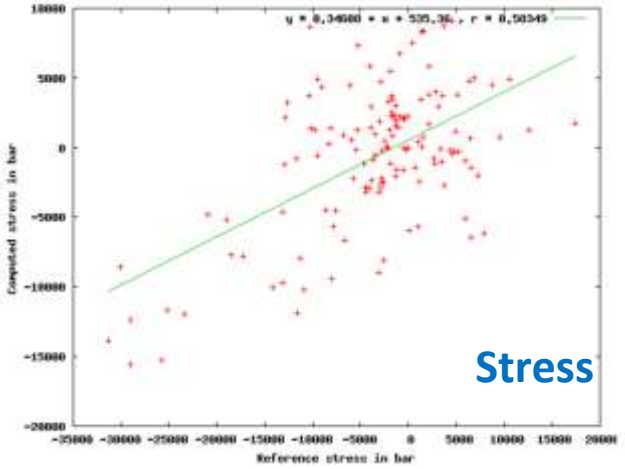
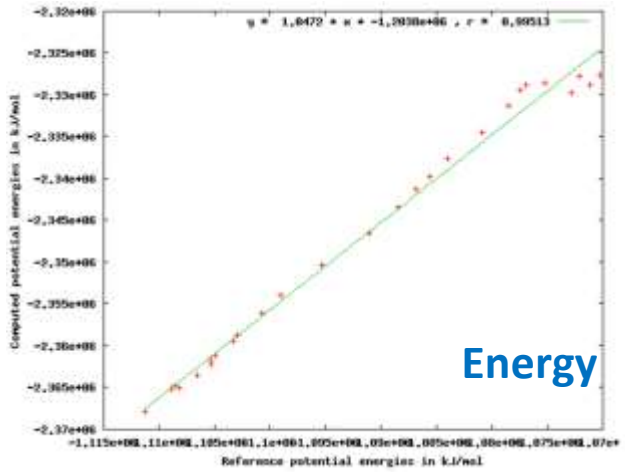
Training

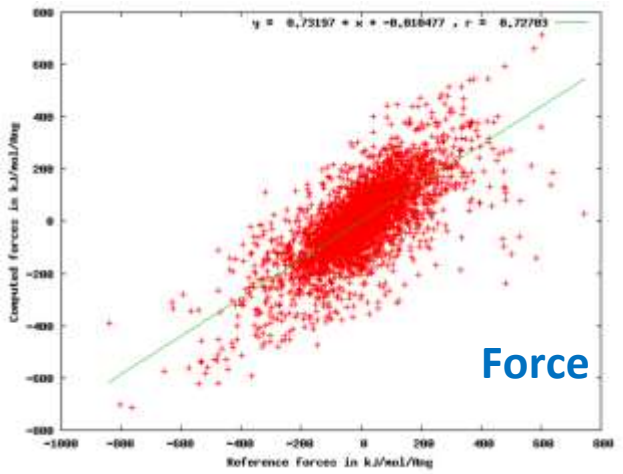


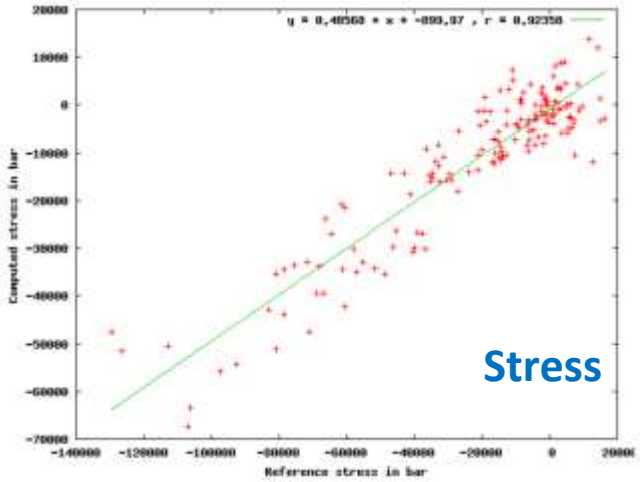




Validation







Interatomic Potentials in MedeA

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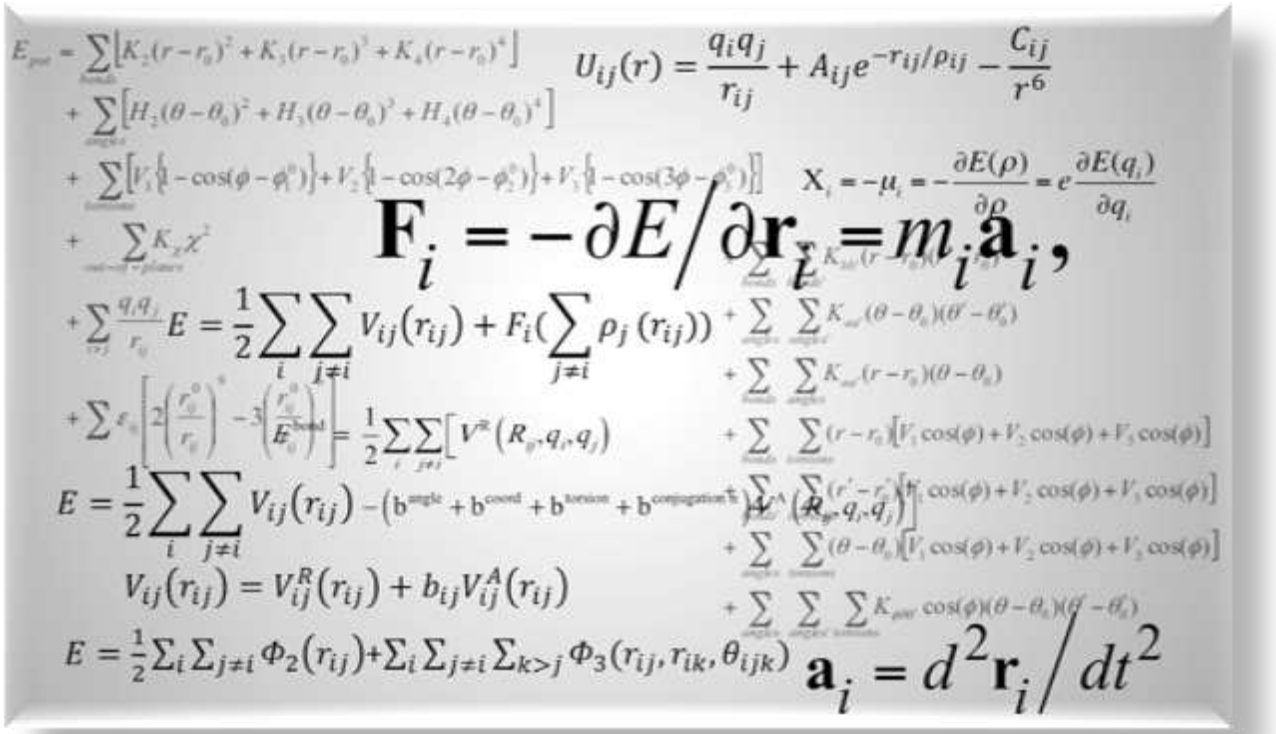
- Watch the webinar:
  - *Classical Forcefields for Modeling Materials on Atomic Scale*
  - http://my.materialsdesign.com/webinar-10



MedeA Mesoscale Simulations

MedeA Mesoscale Simulations

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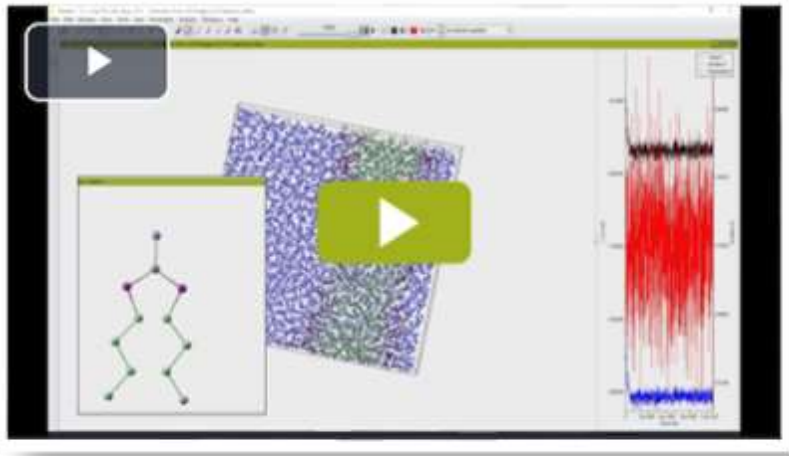
- Watch the webinar
  - *Extending Time- and Length-Scales with Mesoscale Simulations*
  - http://my.materialsdesign.com/webinar-36

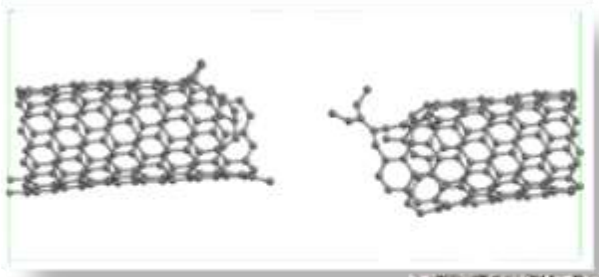
- Demo: DPPC in water, bi-layer self assembly

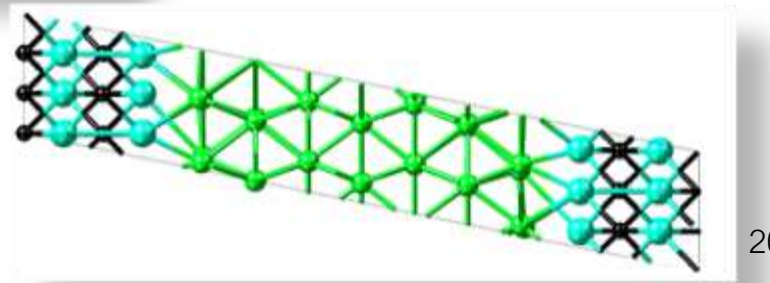


MedeA Deformation

Deformation Simulations

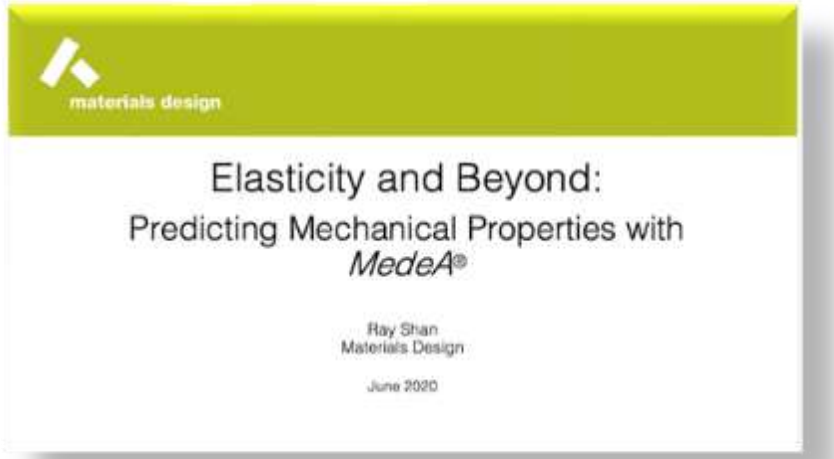
- Tensile deformation of CNT with Tersoff
- Tensile deformation of PE with PCFF+
- Crack propagation of Zr with EAM
- Shear deformation of Co/WC interface

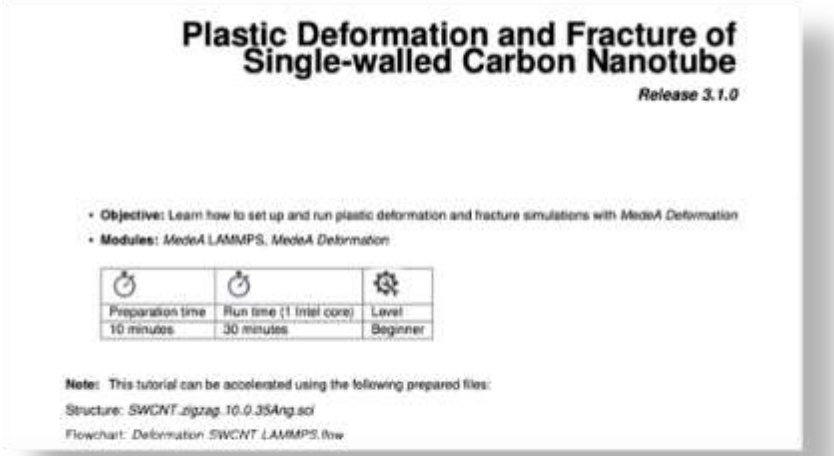




MedeA Deformation

- Watch the webinar
  - *Elasticity and Beyond: Predicting Mechanical Properties with MedeA*
  - http://my.materialsdesign.com/webinar-33
- Demo:
  - http://my.materialsdesign.com/webinar-38

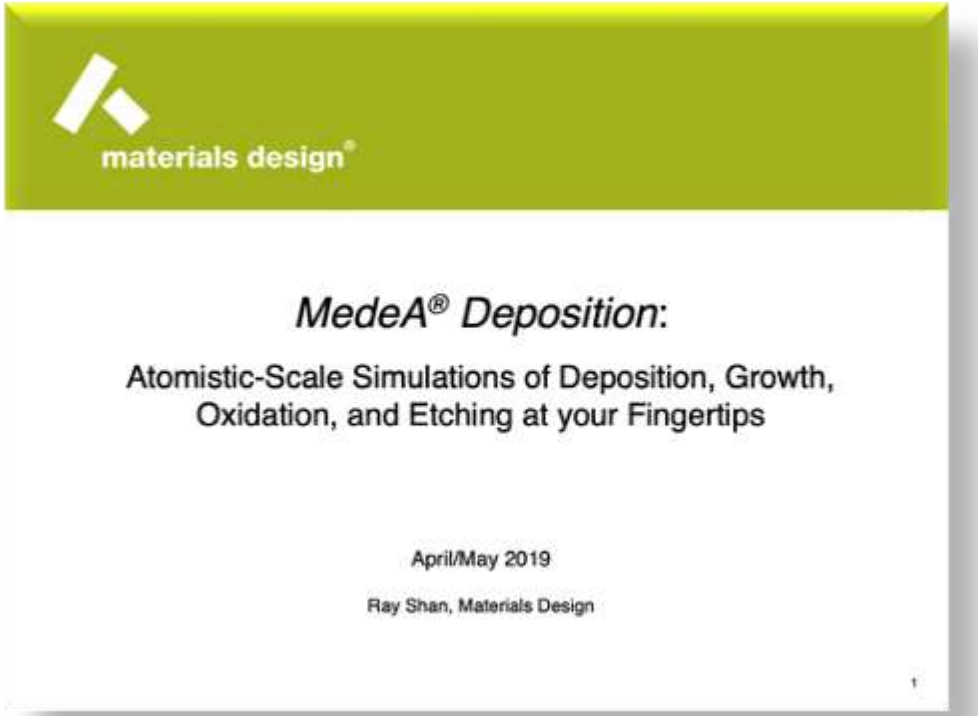




MedeA Deposition

MedeA Deposition

- Watch the webinar
  - *MedeA Deposition: Atomistic-Scale Simulations of Deposition, Growth, Oxidation, and Etching at your Fingertips*
  - http://my.materialsdesign.com/webinar-26



MedeA Deposition Examples

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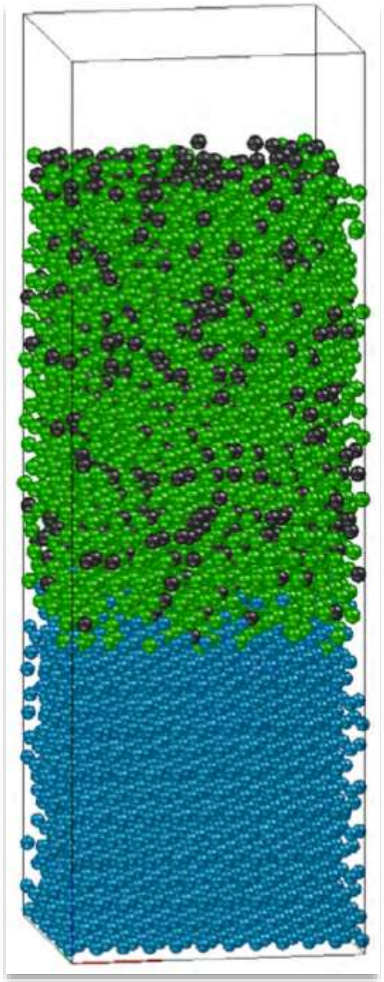
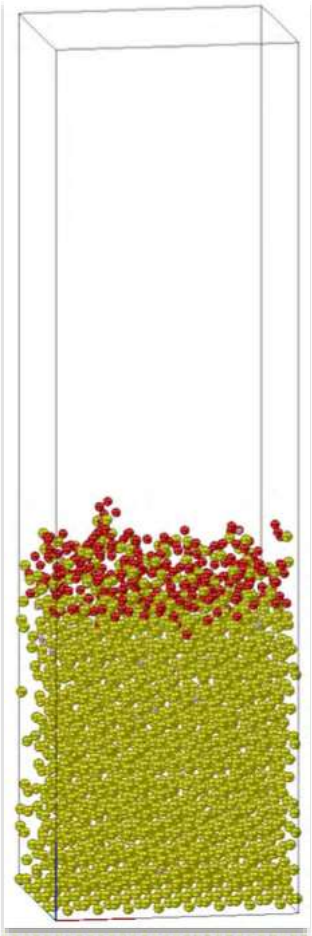
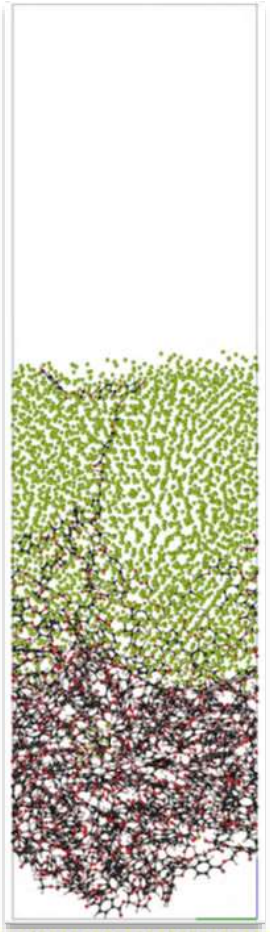
Sputtering of Pd/Ag on Ti



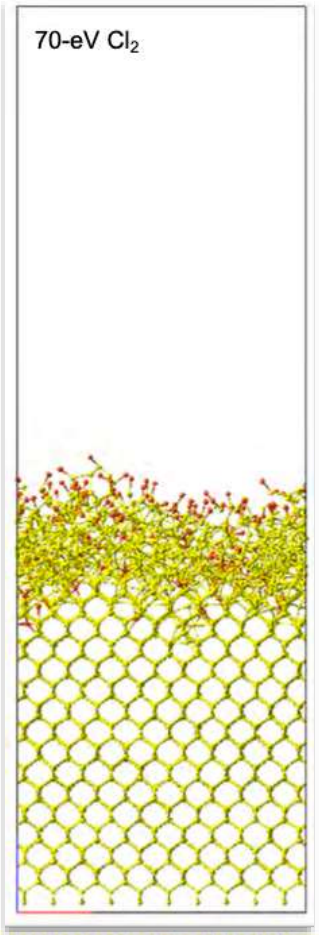
CVD of O_2 on Si



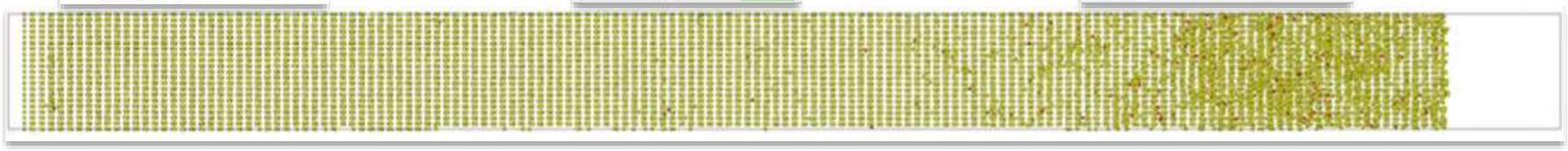
Sputtering of Al on PET



Etching of Si with Cl_2



Ion implantation of O in Si



MedeA Deposition

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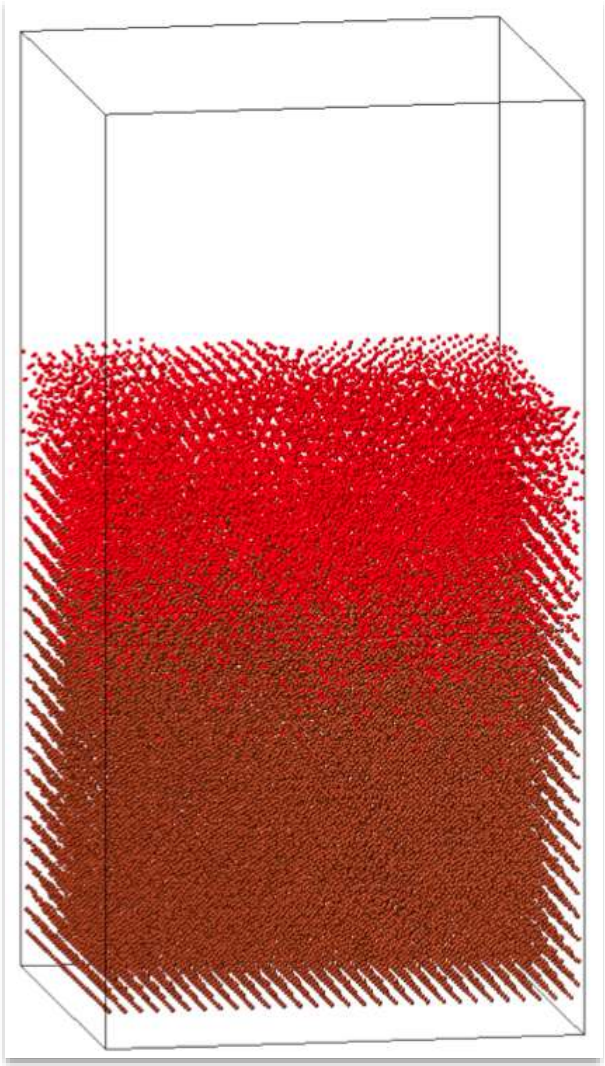

Cold Spray of Cu Nanoparticles on the Cu Surface

Release 3.1.0

- **Objective:** Learn how to simulate the cold spray of metal nanoparticles onto metal surfaces
- **Modules:** *MedeA Deposition*, *MedeA EAM*, *MedeA* LAMMPS

Preparation time	Run time (4 Intel cores)	Level
30 minutes	2 hours	Intermediate

Conclusions

In this live demonstration, we looked at:

- *MedeA LAMMPS*, the robust gateway to classical molecular dynamics simulations
- The collection of interatomic potentials in *MedeA*, including those for metals and alloys, semiconductors, ionic systems, and organic systems, as well as the variable charge potentials
- The steps to export and edit an existing potential (frc) file, and that for importing any external potential parameters into *MedeA*
- The *MedeA Mesoscale*, *Deformation*, *Deposition* modules that employ interatomic potentials for simulating a wide variety of materials processes and properties

List of Resources

- Tutorials:
  - Introduction to MedeA LAMMPS: Learn how to set up and run LAMMPS molecular dynamics simulations with MedeA
  - Importing External Potential Parameters into MedeA: Learn how to import external potential parameters and files into MedeA
  - Deposition of O2 on a Si Surface with Reactive Potentials: Learn how to perform deposition simulation with reactive potentials using MedeA Deposition
  - Cold Spray of Cu Nanoparticles on the Cu Surface: Learn how to simulate the cold spray of metal nanoparticles onto metal surfaces with MedeA Deposition
  - Plastic Deformation and Fracture of Single-walled Carbon Nanotube: Learn how to set up and run plastic deformation and fracture simulations with MedeA Deformation
  - Mesoscale Simulations of Water and Octane: Learn how to set up and run a mesoscale simulation of a mixture with MedeA
  - Self-assembly of Lipid Bilayer: Learn how to run a mesoscale molecular dynamics simulation of self-assembly on a time-scale of a microsecond with MedeA
  - Mechanical Properties of a Thermoset Through Mesoscale Simulations: Learn how to predict mechanical properties of a thermoset through mesoscale simulations
- Webinars:
  - MedeA 3.1: http://my.materialsdesign.com/webinar-38
  - MedeA Mesoscale: http://my.materialsdesign.com/webinar-36
  - MedeA Elastic Properties and Deformation: http://my.materialsdesign.com/webinar-33
  - MedeA Deposition: http://my.materialsdesign.com/webinar-26
  - MedeA ReaxFF: http://my.materialsdesign.com/webinar-17
  - MedeA LAMMPS: http://my.materialsdesign.com/webinar-12
  - MedeA Forcefields: http://my.materialsdesign.com/webinar-10


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October
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Announcements

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Professor Georg Kresse

University of Wien

Dr. David Reith

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Tomorrow's Plenary Speaker

October 14th

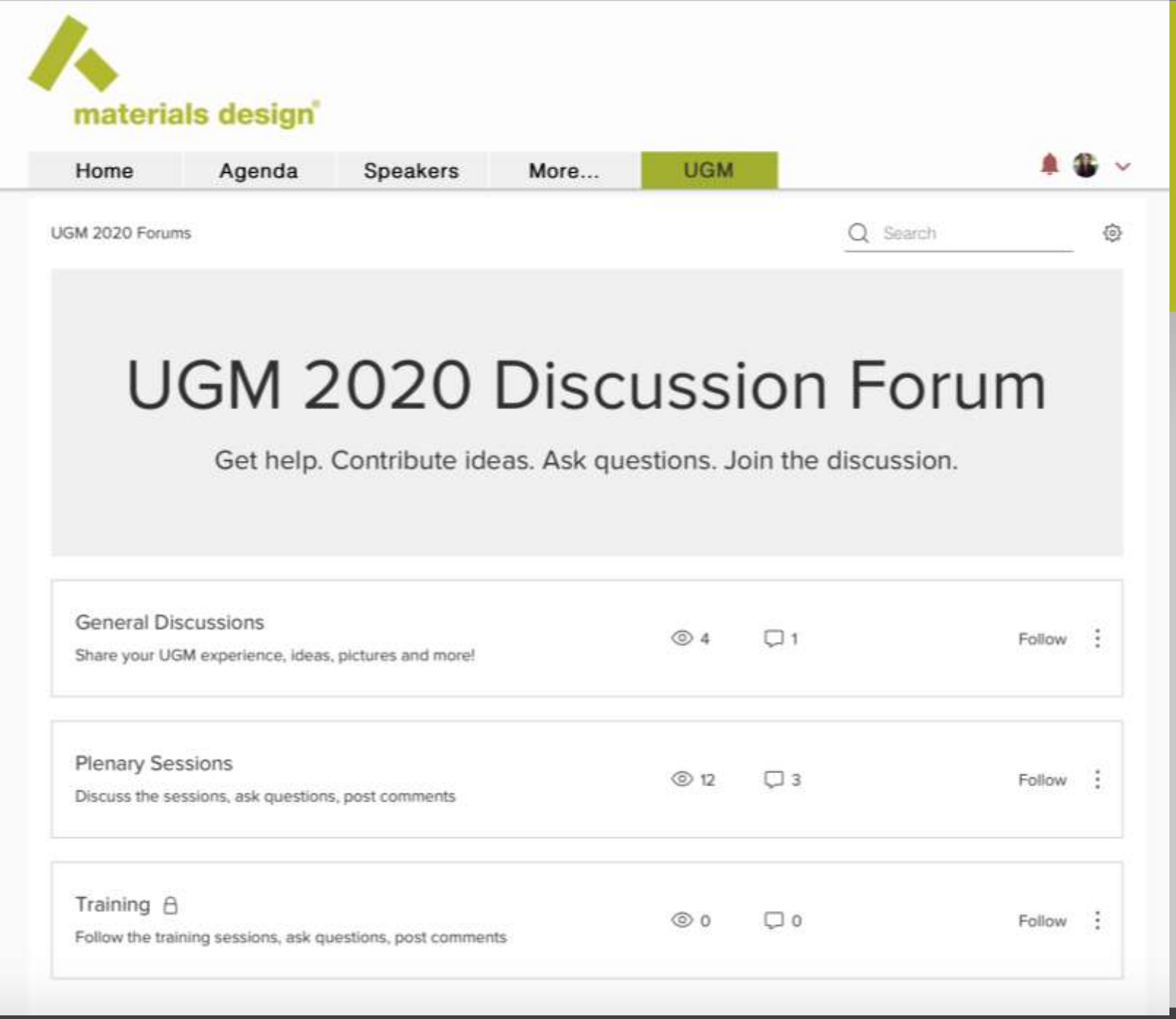
Next Week's MedeA Training

October 20th

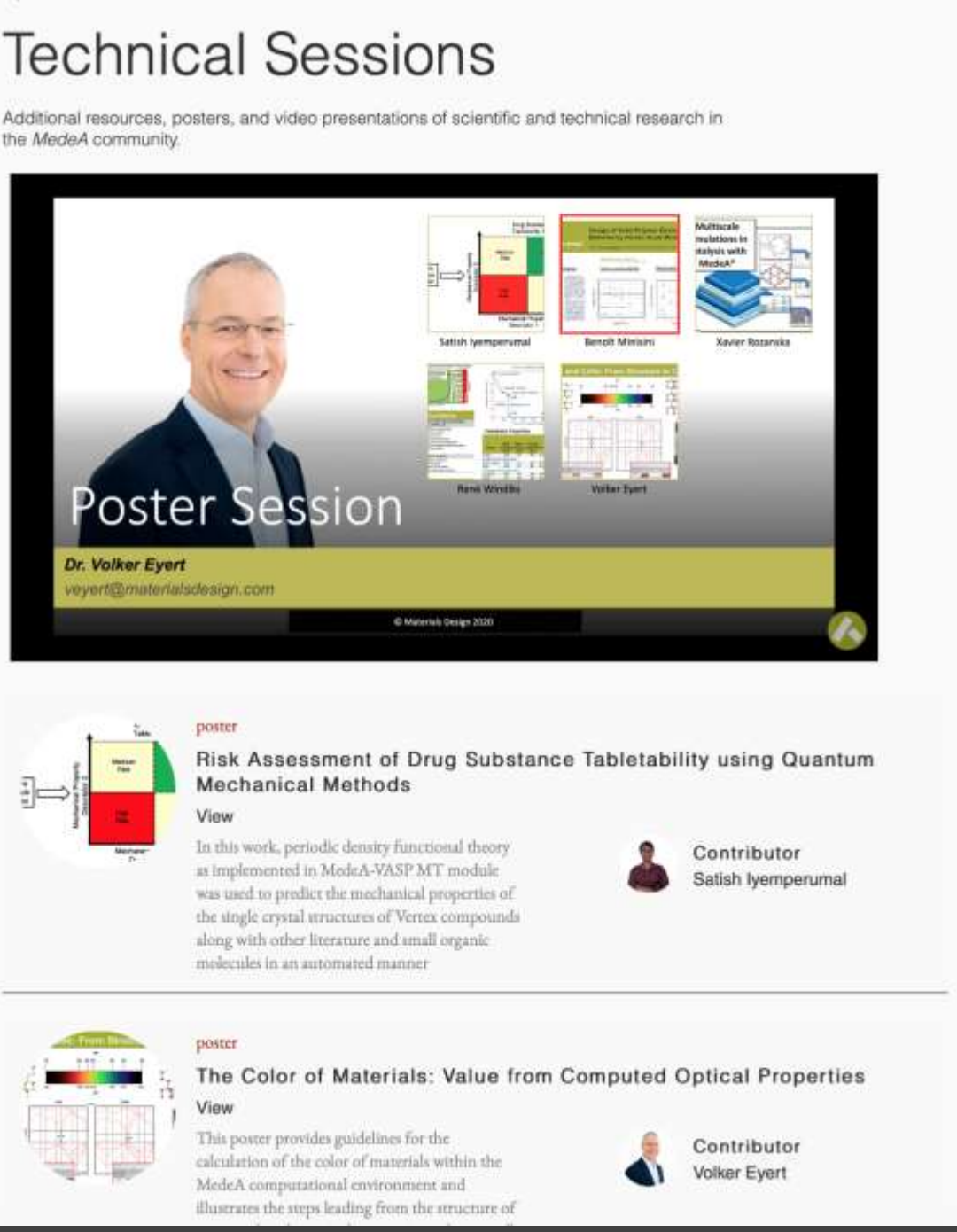
Announcements

Visit the UGM Forum page

https://www.ugm.materialsdesign.com/forum



- Get help on training
- Contribute your ideas
- Discuss the posters and plenary presentations
- Ask questions

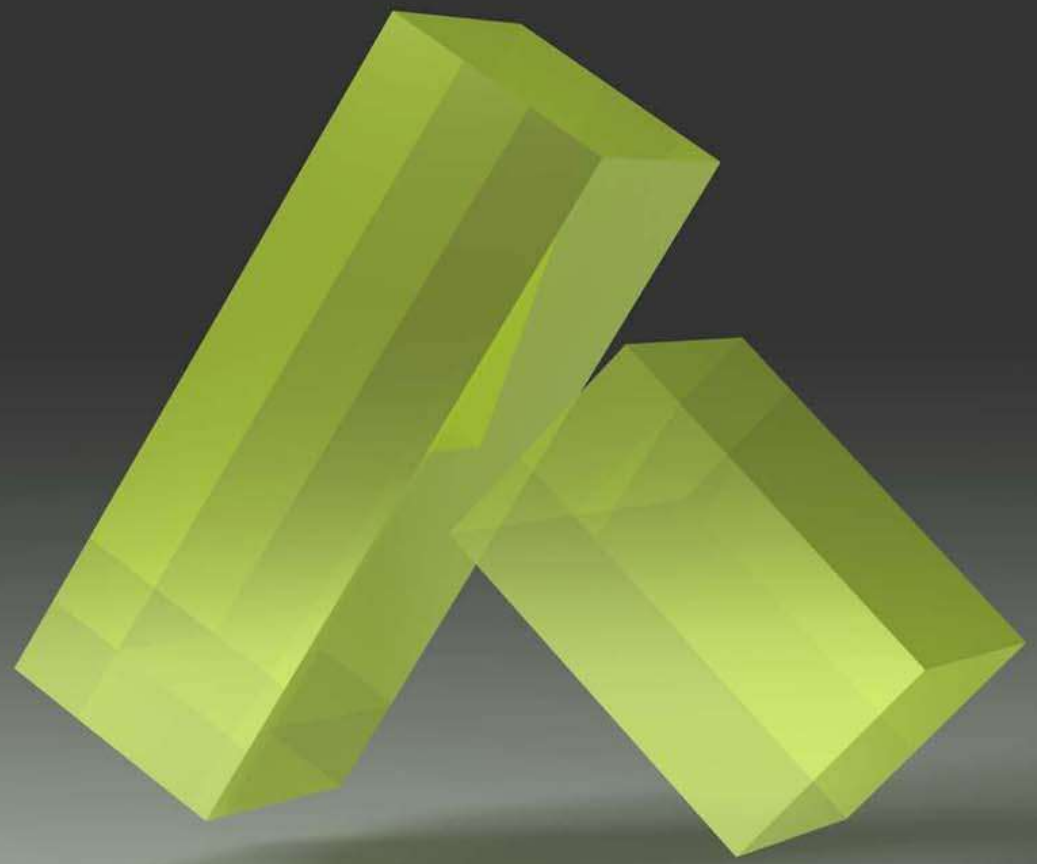


Announcements

Visit the Technical Session page Submitted Talks and Posters

https://www.ugm.materialsdesign.com/posters

- There is still time to submit
- Open to customers under maintenance
- Easily upload on the contributor's page
- Interested? Do you have questions?
  - Contact Volker Eyert
  - UGM@materialsdesign.com



MedeA

Innovation by Simulation