

# Materials Genome Foundation

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<https://materialsgenomefoundation.org/>

# Thank you for participating at the MGF Workshop

Please respond to a survey that will be emailed to you

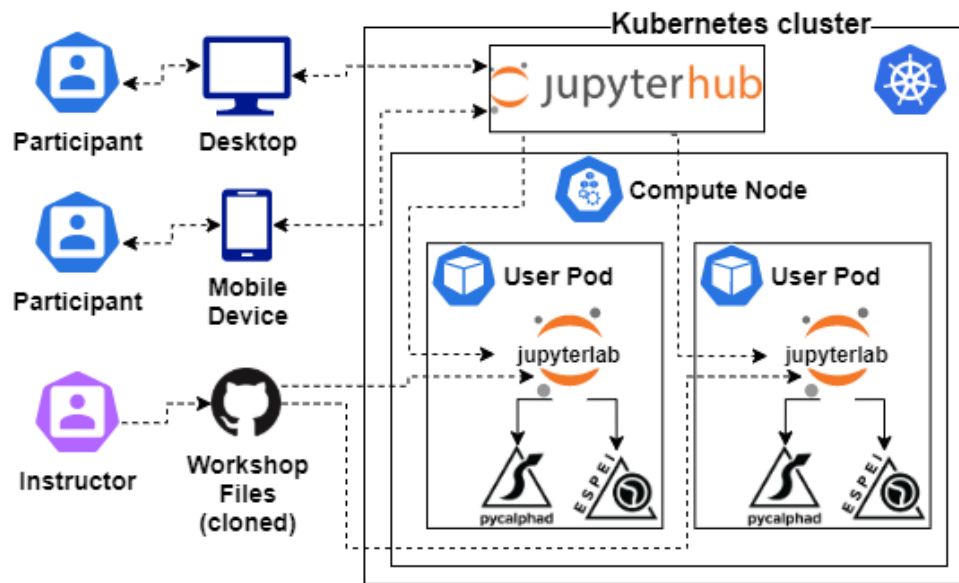
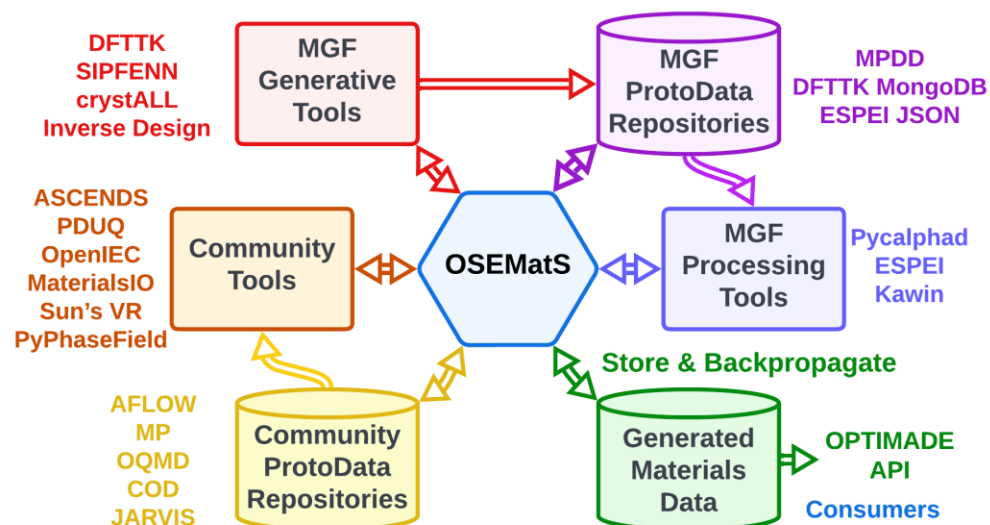
# CALPHAD



- Model properties of individual phases
  - Gibbs energy:  $G_m^\alpha (T, P, x_i, \xi_j)$  and its 1<sup>st</sup> and 2<sup>nd</sup> derivatives
  - Atomic mobility:  $M_k^\alpha (T, P, x_i, \xi_j)$  and tracer/intrinsic/chemical diffusivity
  - Other properties
  - Interfaces between phases?
- Community: [www.calphad.org](http://www.calphad.org)
  - Annual conference: Gordon conference style since 1973, **Plan decade-ahead**
  - CALPHAD, Inc.: Private foundation since 1975, **Scholarships and awards**
  - CALPHAD Journal since 1977
- Tools and databases: CALPHAD, Vol. 26 (2)
  - Commercial: ThermoCalc, Factsage, ComputTherm/Pandat, JMatPro, Matcalc
  - Open Source: OpenCALPHAD, Thermochimica, **PyCalphad/ESPEI (High throughput CALPHAD modeling with uncertainty quantification)**

# MGF Actions

- Open-Source Ecosystem for Materials Science (OSEMatS)
  - Connect and promote community tools and databases: **ASCENDS**
  - Build OSEMatS as a Cloud Native Computing Foundation (CNCF) for materials science
- Provide the cloud-based services for **your workshops**



# Additional links for ASCENDS

- <https://github.com/ornlpmcp/ASCENDS>
- <https://workshop.mgfccloud.org/hub/user-redirect/files/workshop/Example%20Dataset.zip>
- <https://www.energy.gov/eere/vehicles/downloads/accelerated-design-alumina-forming-high-temperature-austenitic-alloys>
- <https://www.energy.gov/eere/vehicles/downloads/machine-learning-and-supercomputing-predict-corrosionoxidation-high-0>
- <https://www.sciencedirect.com/science/article/abs/pii/S0927025621007187>
- <https://www.nature.com/articles/s41529-021-00188-z>

# Future MGF Workshops

- October 4, 2022 as part of [The Structure and Thermodynamics of Oxides/carbides/nitrides/borides \(STOHT2\) conference](#)
- March 18-19, 2023 adjacent to the [TMS 2023 Annual Meeting](#)
- New tools may be added, including
  - Precipitation simulations, kinetics: <https://kawin.org/>
  - DFT Tool Kit for free energy: <https://www.dfttk.org>
  - Machine learning: SIPFENN <https://phaseslab.com/sipfenn>
    - Materials Property Descriptor Database: <https://phaseslab.com/mpdd>, <http://mpdd.phaseslab.com/>
  - Compiled experimental data
    - <https://phaseslab.com/ultera>, for HEA refractory alloys
    - <https://github.com/PhasesResearchLab/ESPEI-datasets>, ESPEI examples