Materials Genome Foundation

PHASES PSU

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Zi-Kui Liu

https://materialsgenomefoundation.org/

Materials Genome Foundation

PHASES PSU

Materials Genome Foundation

- A nonprofit organization incorporated in 2018 in Pennsylvania, USA

- Goals
  - Promote computational approaches in science and engineering
  - Support the development of computational tools and databases

- Actions
  - Organize workshops
  - Provide the cloud-based services for your workshops
  - Develop Open-Source Ecosystem for Materials Science (OSEMatS)

Materials and civilization

- Prehistory and protohistory of humanity
  - Stone Age (~3.4 million years, until 8700–2000 BC), natural materials
  - Bronze Age (3500–300 BC), human-made Cu-12 wt%Sn alloy
  - Iron Age (1200 BC–800 AD), human-made Fe-C alloys
- Industry/Manufacturing/Materials 1.0-3.0
  - Steam power, electricity, and computerization
- Industry/Manufacturing/Materials 4.0
  - Digitization

Digitization of knowledge

- Manufacturing
  - Process of materials to form products that serve one or multiple functions
  - Properties of materials closely related to phases

- Knowledge of phase stability and functionality
  - 1870s: Thermodynamics by Gibbs
  - 1970s: Digitization of thermodynamics by Kaufman
  - 2020s: CALPHAD-based materials design
  - 2070s: Next 50 years

Is thermodynamics for equilibrium only?

- No by 1st Law: $dU = dQ + dW + \sum_{i=1}^{c} U_i dN_i$
- Yes by Gibbs: $dU = TdS - PdV + \sum(U_i - TS_i)dN_i = TdS - PdV + \sum \mu_i dN_i$
- Difference 2nd law

$$dU = TdS - PdV + \sum \mu_i dN_i - \sum D_j \, d\xi_j = \sum Y^a dX^a - \sum D_j \, d\xi_j$$

- Gibbs energy for non-equilibrium: $dG = -SdT + VdP + \sum \mu_i dN_i - \sum D_j \, d\xi_j$

$G(T, P, N_i, \xi_j)$ ← **CALPHAD**

ξ_j: Internal state variables

Examples of internal variables: ξ_j

- Nonstable crystal structure
  - BCC Cu in BCC solid solution between Fe and Cu
- Ordering: Mole fraction in each sublattice
  - $L1_2$: $(Ni, Al)_3(Al, Ni)_1$
- Polarizations: Magnetic spin / Electric dipole configurations
- Defects: Vacancies, dislocations, twins, stacking faults, grain boundaries, phase interfaces, surfaces

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CALPHAD

- Model properties of individual phases
  - Gibbs energy: $G_m^\alpha\ (T, P, x_i, \xi_j)$ and its 1st and 2nd 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
  - 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)

CALPHAD Modeling: Individual phases

Derivatives of Gibbs energy → Thermochemical data: heat capacity, enthalpy, entropy, activity

$D_j d\xi_j = 0$ → Phase equilibrium data: phase stability, phase boundary

Gibbs Energy of Individual Phases

$$G_m^{\alpha}(T, P, x_i, \xi_j)$$

→ Materials Genome®

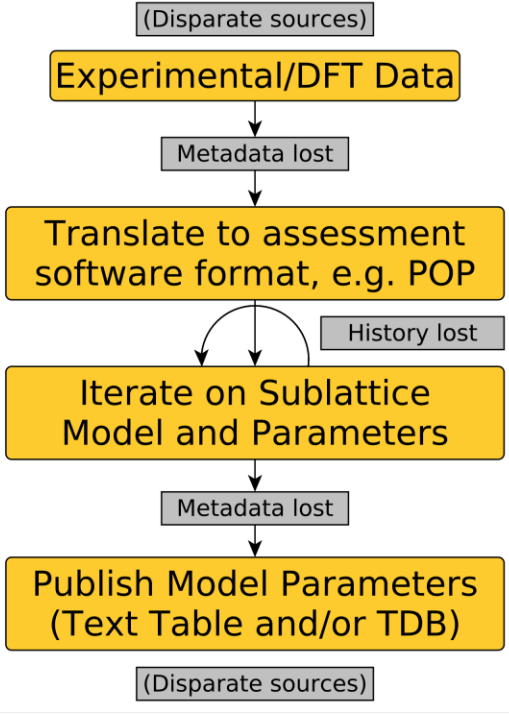
Materials Design: Equilibrium, driving force, physical/chemical properties (1st, 2nd derivatives)

Pure elements → Binary → Ternary → Multicomponent

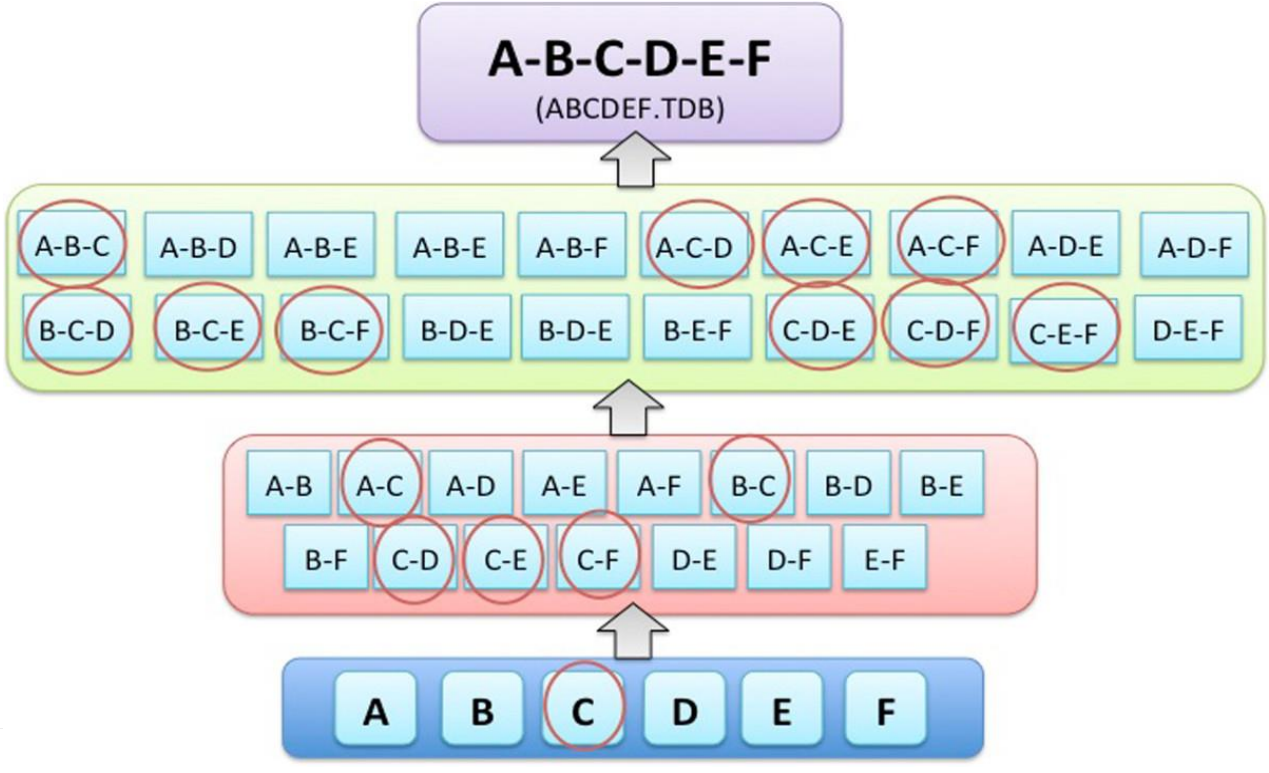
Kaufman & Bernstein: *Computer Calculation of Phase Diagram. 1970*

www.calphad.org

Challenges and Opportunities



Otis, PhD Thesis(2016)



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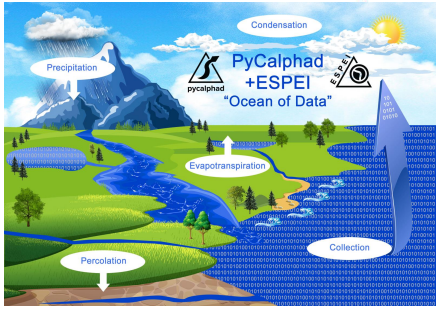
Tool and data: from Penn State



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- Data generation
  - 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
- Data processing
  - pycalphad.org: Thermodynamic and property models
  - espei.org: Evaluation of model parameters & Uncertainty quantification
  - https://pduq.readthedocs.io/: Uncertainty quantification
- Workshops: https://materialsgenomefoundation.org/
  - July 13/14, 2022; October 4, 2022; March 18-19, 2023

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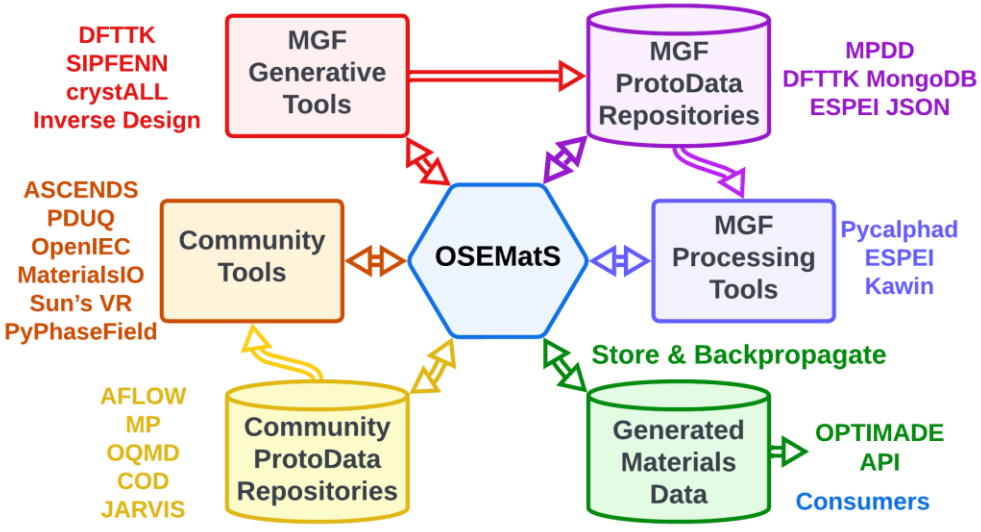
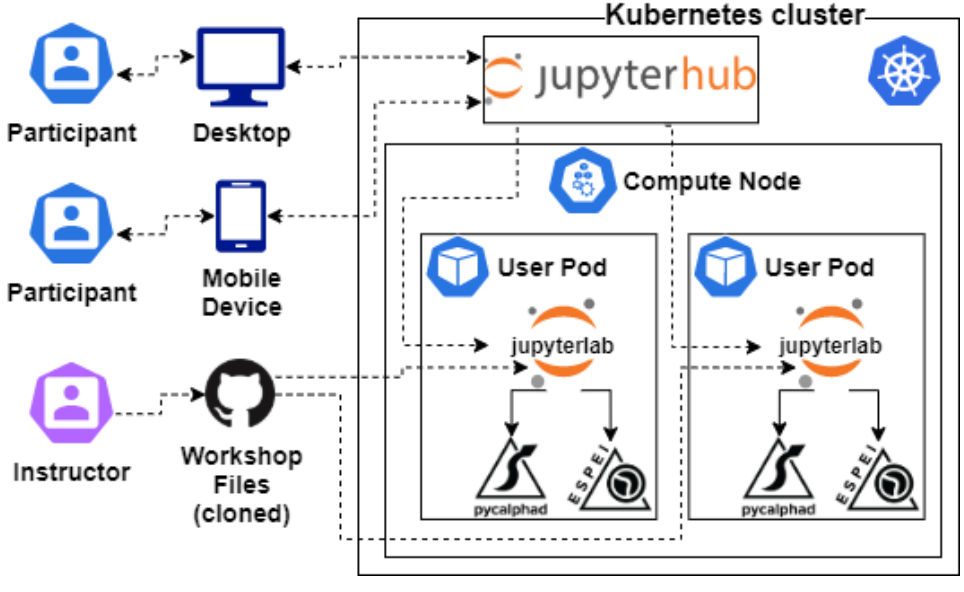
MGF Actions

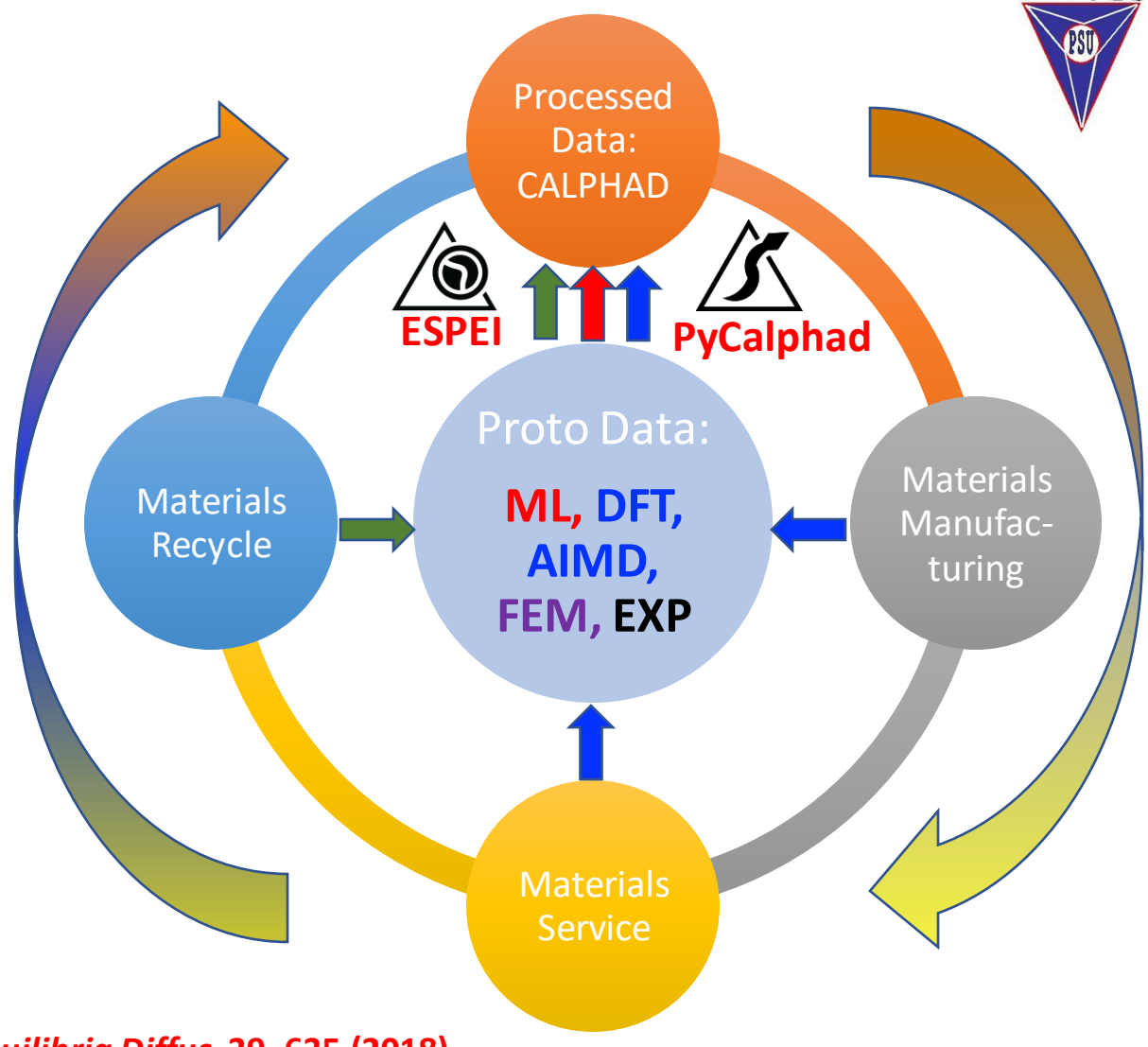
- Open-Source Ecosystem for Materials Science (OSEMatS)
  - Connect and promote community tools and databases: ASCENDS
  - Build OSEMatS as a Cloud Native Computing Foundation (CNCF) for materials science
- Provide the cloud-based services for your workshops





Ecosystem

- Theoretical predictions
  - Machine Learning
  - DFT/AIMD: Density functional theory
  - CPFEM: Mechanical properties
- Experimental measurements



Liu, Ocean of Data, *J. Phase Equilibria Diffus.* 39, 635 (2018)

J. Phase Equilib. Diffus.
https://doi.org/10.1007/s11669-018-0654-z

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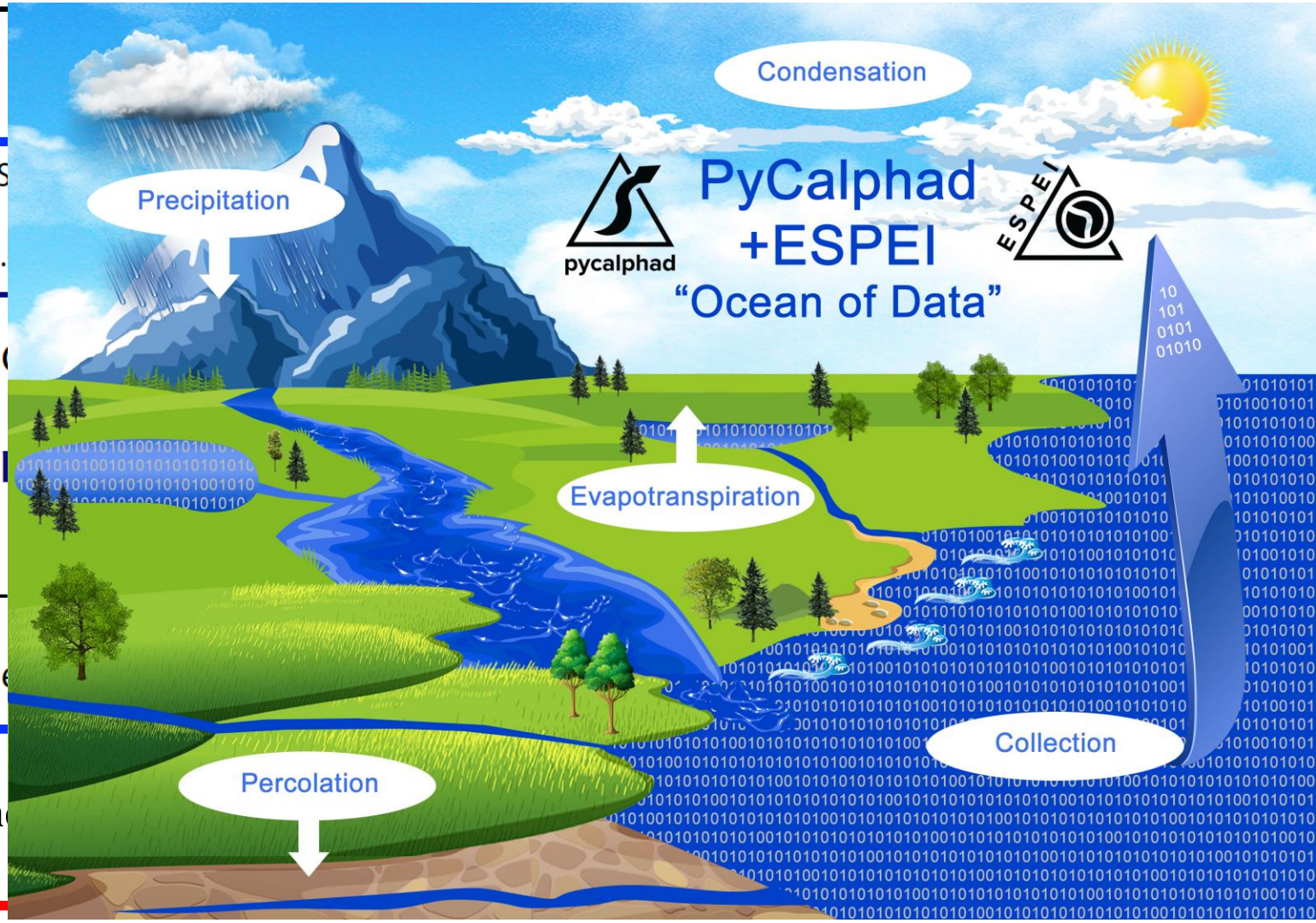
A Data Ecosystem



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Overview article

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