Phase Field Metadata Working Group

2024 MaRDA Meet

https://github.com/marda-alliance/phase-field-schema

Daniel Wheeler, NIST, 02/21/2024

Group Members

- Stephen DeWitt, ORNL
- Trevor Keller, NIST
- Kasra Momeni, U of Alabama
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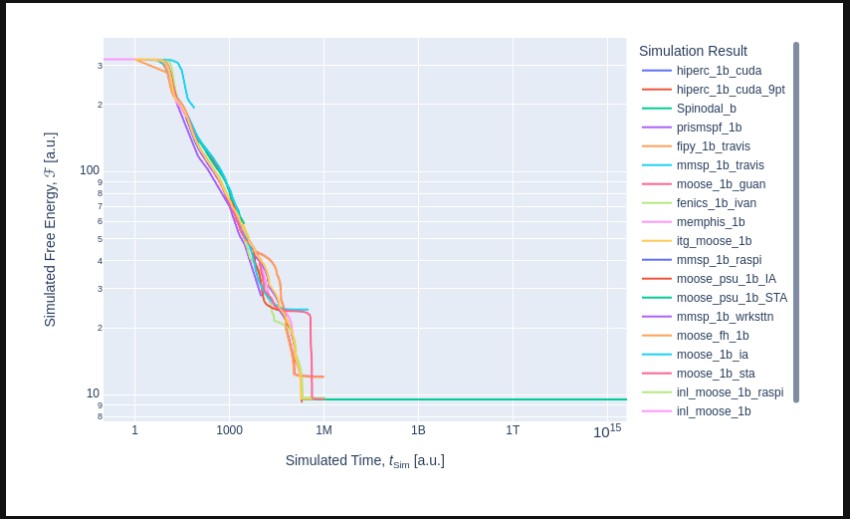
Motivation

- No widely used semantic web standard for materials simulation metadata
- Phase field is a convenient place to start
- Background wrangling data for phase field benchmarks



PFHub Benchmark 1b with data from 20 sources required to be machine readable

Goals

- Generate a metadata standard for phase field data
  - Use current semantic web technologies
- Adopt metadata standard for some published use cases
- *Possibly* provide a template for FAIR metadata standards for materials simulation

data dictionary /
semantic data dictionary /
schema /
ontology

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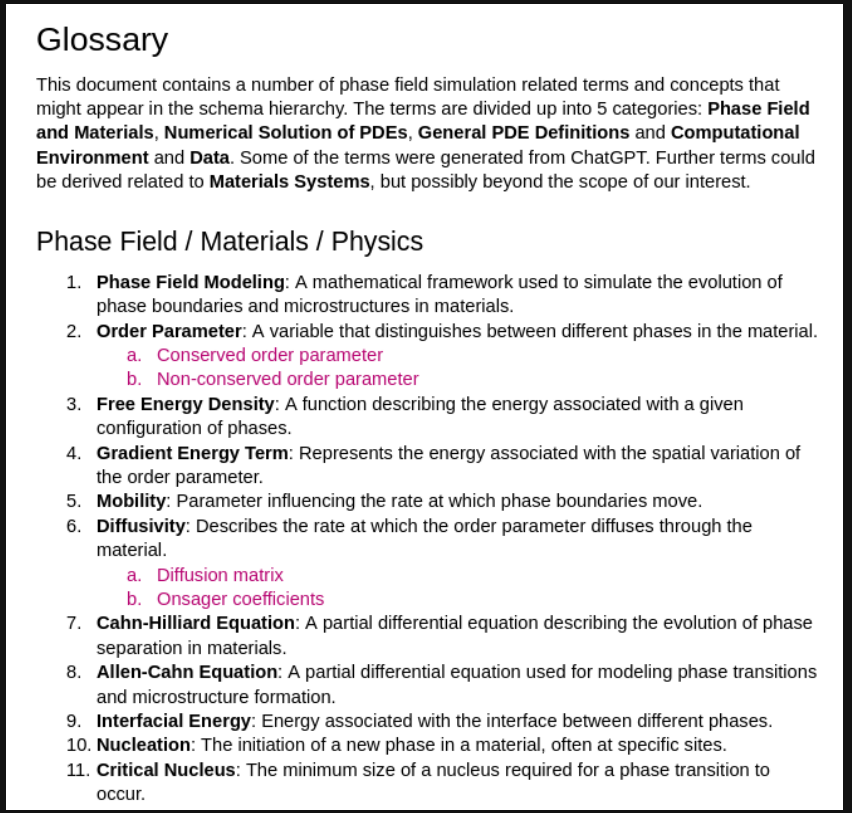
Accomplishments

- Proposal
- 5 use cases
- Literature review
- Glossary
- Loose hierarchy
- Tentative attempts using semantic web tech (schema.org)



Glossary

This document contains a number of phase field simulation related terms and concepts that might appear in the schema hierarchy. The terms are divided up into 5 categories: **Phase Field and Materials**, **Numerical Solution of PDEs**, **General PDE Definitions** and **Computational Environment** and **Data**. Some of the terms were generated from ChatGPT. Further terms could be derived related to **Materials Systems**, but possibly beyond the scope of our interest.

Phase Field / Materials / Physics

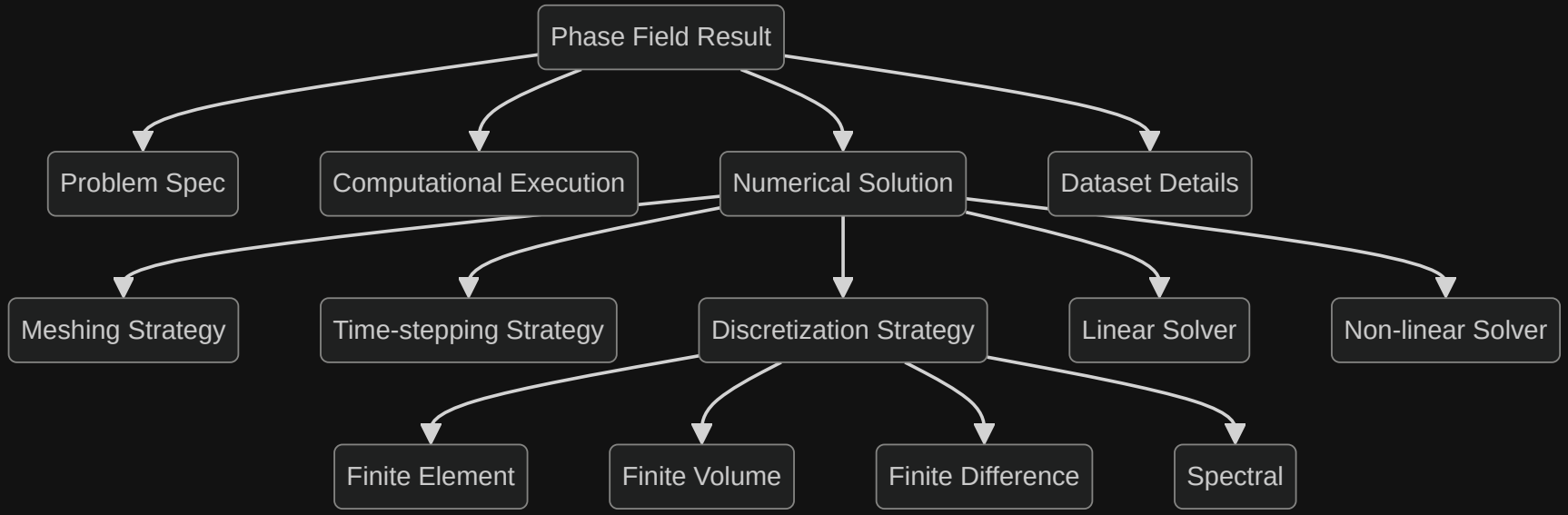
1. **Phase Field Modeling**: A mathematical framework used to simulate the evolution of phase boundaries and microstructures in materials.
2. **Order Parameter**: A variable that distinguishes between different phases in the material.
    a. Conserved order parameter
    b. Non-conserved order parameter
3. **Free Energy Density**: A function describing the energy associated with a given configuration of phases.
4. **Gradient Energy Term**: Represents the energy associated with the spatial variation of the order parameter.
5. **Mobility**: Parameter influencing the rate at which phase boundaries move.
6. **Diffusivity**: Describes the rate at which the order parameter diffuses through the material.
    a. Diffusion matrix
    b. Onsager coefficients
7. **Cahn-Hilliard Equation**: A partial differential equation describing the evolution of phase separation in materials.
8. **Allen-Cahn Equation**: A partial differential equation used for modeling phase transitions and microstructure formation.
9. **Interfacial Energy**: Energy associated with the interface between different phases.
10. **Nucleation**: The initiation of a new phase in a material, often at specific sites.
11. **Critical Nucleus**: The minimum size of a nucleus required for a phase transition to occur.

Initial attempt at a glossary of phase field terms

Use cases

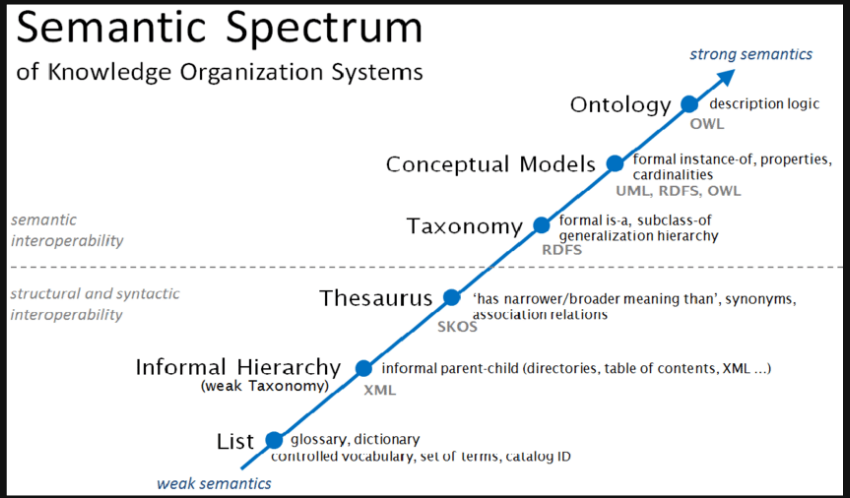
- AI
- Data Management
- Performance Comparison
- Materials Design Workflow
- Phase Field Benchmarks

Metadata Heirachy



Work Plan

- Continue monthly meetings (6 so far)
- Complete metadata hierarchy
- Implement with semantic web tech
- Generate use case / working examples using metadata standard and document
- Publication and disseminate



From "Report on Workshop on Interoperability in Materials Modelling", doi:10.5281/zenodo.1240229

Please join the group if you’re interested in simulation metadata