Ontology-driven computational engineering

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Objectives

- Centralised model repository
- Ontology that captures structure of physics over the scales from sub-molecular to macroscopic mechanical properties
- With data related ontologies for data interoperability
- Recursive generation of surrogate models → making computations feasible on the higher-scale models (curse of scale and dimension)
- Closed stand-alone simulations as well as workflows using a suite of problem solvers

Research/development program

Knowledge repository

- Base semantic network for the generation of an instantiated semantic network for model structure / behaviour, rules and relations.
- Ontology == linked categories for distinctly separate contexts.
- Data description ontologies for interoperability.

Utilisation

- Graphical multi-scale, multi-domain model construction for ultra-fast generation of complex models.
- Recursive internal expansion into the smaller scale physical objects.
- Guided instantiation of the “numerical problem”.
- Time & length-scale motivated model reduction.
- Surrogate identification on the fly and recursive.
- Application factory generating solver task or workflow for specific problems.
- Target: material production process, material being produced and used in the process.

Approach

An environment to generate model ontologies

- Primary ontology structure based on a minimal number of classes and objects:
  - two main categories (i) structure (ii) behaviour.
- Ontology for the equation framework being an instantiated tree of the primary ontology.
- Augment ontology with relations - equations starting with the fundamental state and constants:
  - governing principle - all variables must be a function of existing variables at the time of definition;
  - closure condition for the state.
- Combining multiple domains:
  - intrafaces connect different physical phases,
  - interfaces connect to material models or information processing systems like generic systems for controlling the operations or extracting information.

How does it work ?