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Simulator Design based on Variable Graph for Complex Physical Systems

Motivations

Code Reusability

- When two models have something in common, how can we reuse the code developed for one model for the other?
- What does

  having something in common

  mean for two models?

Model Complexity

- Model complexity **will always grow**.
- It happens when we
  - **couple** models
  - add/replace new physical process in a given model.

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Motivations

Rapid Prototyping

- We target a **couple of weeks** to setup a model
- includes:
  - parameter input
  - control
  - calibration tool

Model Exploration

- What are the **physical variables** that your model knows about?
- How they **relate** with each other?

Interactive Use

- We provide tools for the developer
- The tools **have to be interactive** to help **during** the implementation.

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Variable Graph (VG)

Physical Model

- **Physical quantities**
- **Relationships** between quantities

Physical quantities

- Physical quantities have **names** carefully chosen by the experts
- The relationship between variables can be **explicit** or **implicit**
- implicit relationship gives an equation.

Model = Variable Graph

Variable Graph

- The **nodes** are the variables names
- The **edges** provides the dependence relationship between the variables.
- Directed acyclic graph

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Example

- We have the following chemical systems

$$\mathrm{Li}^{+} + \mathrm{e}^{-} \longleftrightarrow \mathrm{Li}$$

- The equations are

$$\frac{dc_e}{dt} = R \qquad \frac{dc_s}{dt} = -R$$

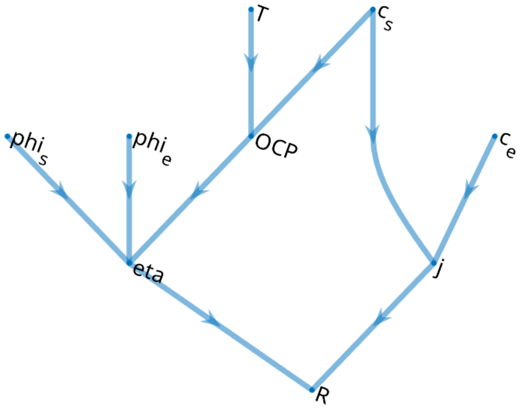
with

$$R = j(c_e, c_s)\sinh(\eta)$$
$$\eta = \phi_e - \phi_s - \mathtt{OCP}(c_e, T)$$

The named variables are

c_e	:	Li concentration in electrolyte
c_s	:	Li concentration in electrode
R	:	reaction rate
j	:	exchange current density
ϕ_e	:	Electric potential in electrolyte
ϕ_s	:	Electric potential in electrode
η	:	overpotential
$\mathtt{OCP}$	:	open circuit potential

Example



(Only the dependency of the reaction term *R*)

Variable graph (VG)

A model development approach based on variable graph enables to

BREAK THE COMPLEXITY

by using a **two-step** approach

First Step	Second Step
Design Variable Graph	Implement Declared Functions

Implementation Requirement

To get a **reusable** code, we need to be able to do the following operations

Import A Model	Add/Remove Variables to a Model	Add/Change Functional Dependencies
Import a VG and use the functions that are defined.	Add/Remove nodes to the VG keeping all the rest.	Add/Change directed edges to VG, keeping all the rest

FULL GRAPH EDITING CAPABILITIES - AT EVERY LEVEL

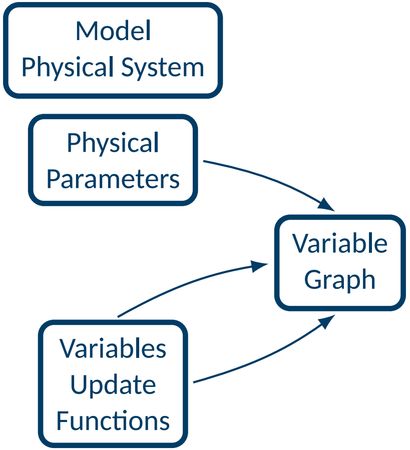
Later, we will go through an example where we see these requirements are met by our implementation

Model Object

```
classdef:

properties:

methods:
```



Model Hierarchy

Model A

nodes: $\{\mathtt{var}_1, \cdots, \mathtt{var}_{n_A}\}$

Model B

nodes: $\{\mathtt{var}_1, \cdots, \mathtt{var}_{n_B}\}$

Graphs are imported as subgraphs at model initialization

Submodel names are used as prefix

Namespace mechanism

Model

`modelA`
`modelB`

nodes: $\{\mathtt{modelA.var}_1, \cdots, \mathtt{modelA.var}_{n_A}$

$\mathtt{modelB.var}_1, \cdots, \mathtt{modelB.var}_{n_B}$

$\mathtt{var}_1, \cdots, \mathtt{var}_n\}$

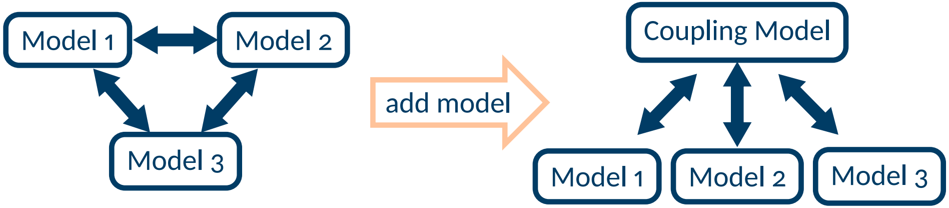
additional edges (always if coupling !)

Model Couplings

- We include **model names**

  model name = namespace for the model variables

- Hierarchical approach : We couple models by adding a coupling model.



VG for Automatic Assembly

automatic assembly setup

roots of the graph ⇒ primary variables

leaves of the graph ⇒ equations

Pre-Processing Step on VG

1. Order the graph using the declared dependency
2. Identify the **primary variables** and the **equations**
3. Setup the **sequence of function call** to update sequentially all variables

Newton Step

1. Instantiate primary variables as **MRST-AD**
2. Run sequence of function calls
3. Extract from the leaves the equations, stab them and send them to the MRST Newton solver

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Graph Setup

Declarative Graph Setup

We do not have to figure out the layout of the graph beforehand.

We use a **declarative** approach : We register the nodes (variables) and the edges (functional dependencies). They can be registered in a **arbitrary order**.

The code **builds the graph** for us and provides **interactive tools** for exploration and visualization.

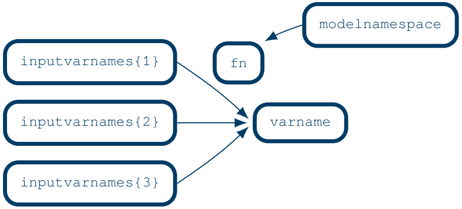
Graphs can be complicated objects...

Simple structures for the architecture implementation

In `BaseModel`, we have the methods

- `registerVarNames` to add variable names
- `registerPropFunction` to add functions

with some **syntactic sugar**



The nodes (variable names)

```
classdef VarName
 properties
  namespace % list of model names
  name      % name of the variable
  index     % if array variables
  dim       % if array variables
 end
end
```

The edges (functional relationships)

```
classdef PropFunction
 properties
  varname         % target variable
  inputvarnames   % list of input variables
  modelnamespace  % model name space
                  % for the parameters
  fn % function handler to update target
 end
end
```

Example

We register the variables

```
classdef ReactionModel < BaseModel
  methods
   function model = registerVarAndPropfuncNames(model)

    model = registerVarAndPropfuncNames@BaseModel(model);

    varnames = {};
    varnames{end + 1} = 'phi_s';
    varnames{end + 1} = 'c_s';
    varnames{end + 1} = 'phi_e';
    varnames{end + 1} = 'c_e';
    varnames{end + 1} = 'eta';
    varnames{end + 1} = 'R';
    varnames{end + 1} = 'OCP';
    varnames{end + 1} = 'j';

    model = model.registerVarNames(varnames);
```

We register the functions

```

    fn = @ReactionModel.updateReactionRateCoefficient;
    inputnames = {'c_e', 'c_s'};
    model = model.registerPropFunction({'j', fn, inputnames});

    fn = @ReactionModel.updateOCP;
    inputnames = {'c_s'};
    model = model.registerPropFunction({'OCP', fn, inputnames});

    fn = @ReactionModel.updateEta;
    inputnames = {'phi_e', 'phi_s', 'OCP'};
    model = model.registerPropFunction({'eta', fn, inputnames});

    fn = @ReactionModel.updateReactionRate;
    inputnames = {'eta', 'j'};
    model = model.registerPropFunction({'R', fn, inputnames});

   end
  end
end
```

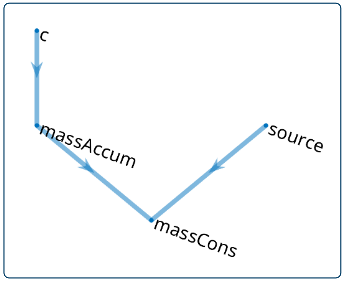
Coupling model - Example

Example from tutorial. We build-up from bottom to top

- `ConcentrationModel`
- `ReactionModel`
- `ThermalModel`
- `ConcentrationReactionModel`
  couples `ConcentrationModel` and `ReactionModel`.
- `ConcentrationReactionThermalModel`
  couples `ConcentrationReactionModel` and `ThermalModel`.

Concentration and reaction model

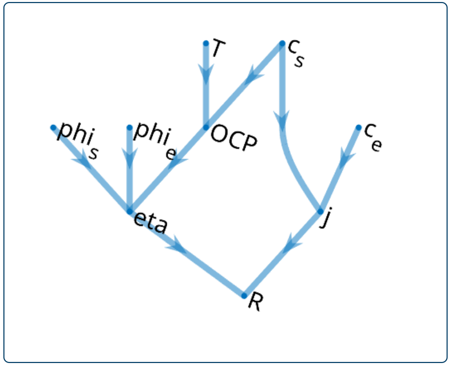
$$\frac{dc}{dt} = S$$



`ConcentrationModel`

$$R = j(c_e, c_s)\sinh(\eta)$$
$$\eta = \phi_e - \phi_s - \mathtt{OCP}(c_e, T)$$

`ReactionModel`



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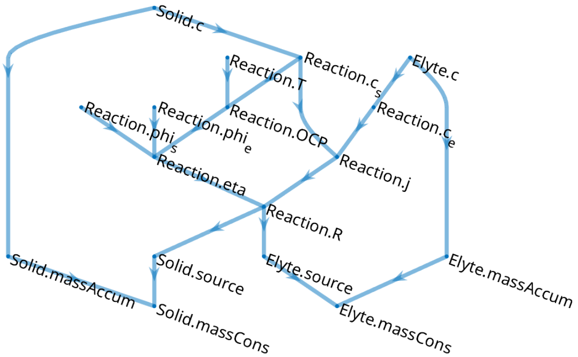
with

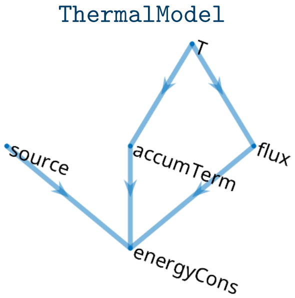
$$R = j(c_e, c_s)\,\sinh(\eta)$$
$$\eta = \phi_e - \phi_s - \mathtt{OCP}(c_e, T)$$

```
ConcentrationReactionModel
⇒ ConcentrationModel (Elyte)
⇒ ConcentrationModel (Solid)
⇒ ReactionModel (Reaction)
```

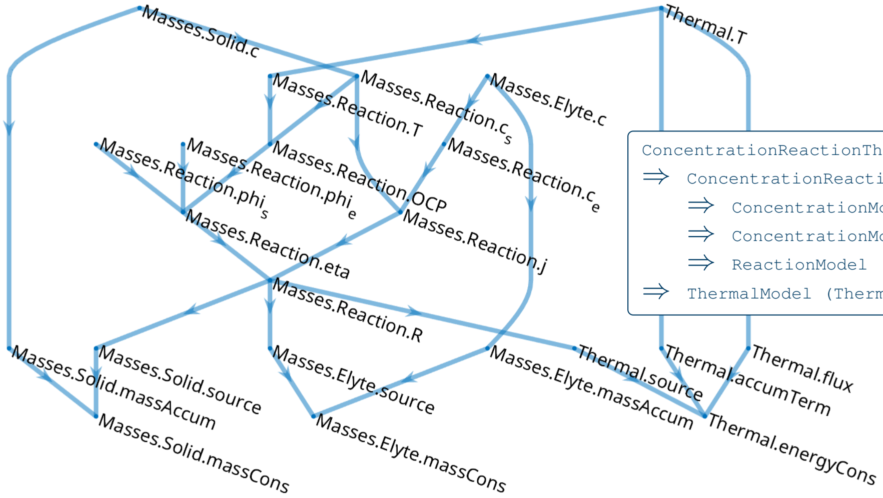


Thermal model

$$\frac{\partial}{\partial t}(cT) + \nabla \cdot (-\kappa \nabla T) = S$$

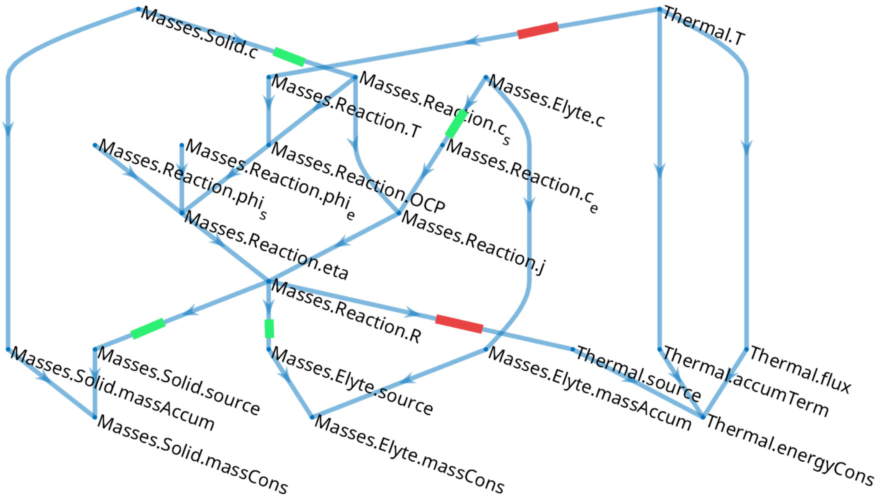


Coupled Thermal Reaction model



```
ConcentrationReactionThermalModel
⟹ ConcentrationReactionModel (Masses)
    ⟹ ConcentrationModel (Elyte)
    ⟹ ConcentrationModel (Solid)
    ⟹ ReactionModel (Reaction)
⟹ ThermalModel (Thermal)
```

Couplings in Thermal Reaction model



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Example

Primary Variables

```
>> cgit.printRootVariables

3 Root Variables:
-----------------
Masses.Solid.c
Masses.Elyte.c
Thermal.T

2 Static Variables:
-------------------
Masses.Reaction.phi_s
Masses.Reaction.phi_e
```

Equations

```
>> cgit.printTailVariables

3 Tail Variables:
-----------------
Masses.Solid.massCons
Masses.Elyte.massCons
Thermal.energyCons
```

Ordered function call list

```
>> cgit.printOrderedFunctionCallList

state.Masses = model.Masses.updateReactionConcentrationS(state.Masses);
state.Masses = model.Masses.updateReactionConcentrationE(state.Masses);
state = model.updateTemperature(state);
state.Masses.Solid = model.Masses.Solid.updateMassAccum(state.Masses.Solid);
state.Masses.Elyte = model.Masses.Elyte.updateMassAccum(state.Masses.Elyte);
state.Thermal = model.Thermal.updateAccumTerm(state.Thermal);
state.Thermal = model.Thermal.updateFlux(state.Thermal);
state.Masses.Reaction = model.Masses.Reaction.updateOCP(state.Masses.Reaction);
state.Masses.Reaction = ...
    model.Masses.Reaction.updateReactionRateCoefficient(state.Masses.Reaction);
state.Masses.Reaction = model.Masses.Reaction.updateEta(state.Masses.Reaction);
state.Masses.Reaction = ...
    model.Masses.Reaction.updateReactionRate(state.Masses.Reaction);
state.Masses = model.Masses.updateConcentrationSource(state.Masses);
state = model.updateThermalSource(state);
state.Masses.Solid = model.Masses.Solid.updateMassCons(state.Masses.Solid);
state.Masses.Elyte = model.Masses.Elyte.updateMassCons(state.Masses.Elyte);
state.Thermal = model.Thermal.updateEnergyCons(state.Thermal);
```

This functions are evaluated **as such** using `eval` in MATLAB, see here.

macro mechanism

(Code that generates code)

Conclusion

Variable Graph based Simulator design enables us to

- Break the complexity
- Build a hierarchy of interacting physical simulation models
- Reuse update-functions which are preferably implemented at lowest scope
- Automate the assembly