

**Preparing input files**

Start with Reactive Transport Model

List geochemical parameters to modify

Choose how to vary parameters

List of values

Randomly distributed

Proportional to other parameters

Evenly spaced

Have rules for all geochemical parameters been defined?

No

Yes

**Running Omphalos**

Submit input file and configuration file

Geochemical parameters are generated from configuration

Input file modified

CrunchTope runs input file

Results are recorded

Have all files run?

No

Yes

Save input files and results

**Data Analysis and Emulation**

Import dataset to Jupyter

Extract geochemical parameters as features

Extract results as labels

Split data into train and test sets

Train a GBT model with the training data

Test model on test data

Is the prediction error over the test data sufficiently low?

No

Yes

Adjust model hyper-parameters

Emulator complete. Finish.