Pruning in RMG-Py

Kehang Han
7/10/2014
Why to Do Pruning

- For complex systems, memory limitation
- Most memory occupied by edge species
- Most edge species won’t be included in final model
- Pruning is trying to get rid of edge species which have least possibility of entering core
Key Params in Pruning

- toleranceInterruptSimulation
- toleranceMoveToCore
- toleranceKeepInEdge
- maximumEdgeSpecies
How Pruning Works
Which Species to Prune

![Graph showing the comparison of different species with respect to their reaction conversion and species flux. The graph highlights three species: A, B, and C, each represented by distinct curves. Species B shows the highest peak in species flux at a certain reaction conversion, indicating it might be the optimal species to prune.]
Which Species to Prune

![Graph showing species conversion and flux](image)

- **Edge Species Flux**
- **Reactant Conversion**

- **A**
- **B**
- **C**

- **toleranceKeepInEdge**
Simulation Runs to Termination

![Graph showing the edge species flux vs. reactant conversion.](image)

- **A**, **B**, and **C** are marked on the graph at specific points.

- The graph indicates the termination conversion.
ToleranceInterruptSimulation

![Graph showing Edge Species Flux vs Reactant Conversion]

- **InterruptSimulation**
- **terminationConversion**

- Species A
- Species B
- Species C
ToleranceMoveToCore

![Graph showing Edge Species Flux against Reactant Conversion with markers for InterruptSimulation, MoveToCore, and terminationConversion.]
ToleranceInterruptSimulation

![Graph showing Edge Species Flux vs Reactant Conversion]

- **Edge Species Flux**
  - A
  - B
  - C

- **Reactant Conversion**
  - 0.2
  - 0.4
  - 0.6
  - 0.8
  - 1

- **InterruptSimulation**
- **terminationConversion**
Normal Rules for Params

- $\text{toleranceInterruptSimulation} \geq \text{toleranceMoveToCore}$
  - Otherwise, always interruption without enlarging core
  - Special cases: equal to each other; Interruption tol$\rightarrow\infty$

- $\text{toleranceKeepInEdge}$ has the unit for flux
  - Not convenient, maybe can do pruning just based on rank

- $\text{maximumEdgeSpecies}$
  - Start deleting species with lowest fluxes if total edge species number exceeds $\text{maximumEdgeSpecies}$
Further Questions to Ask

- How effective it can save memory when dealing with complex kinetics system?
- How it affects model generation/model content?
  - By compare models with and without pruning
  - ....