Model Reduction

RMG Study Group Presentation

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Outline

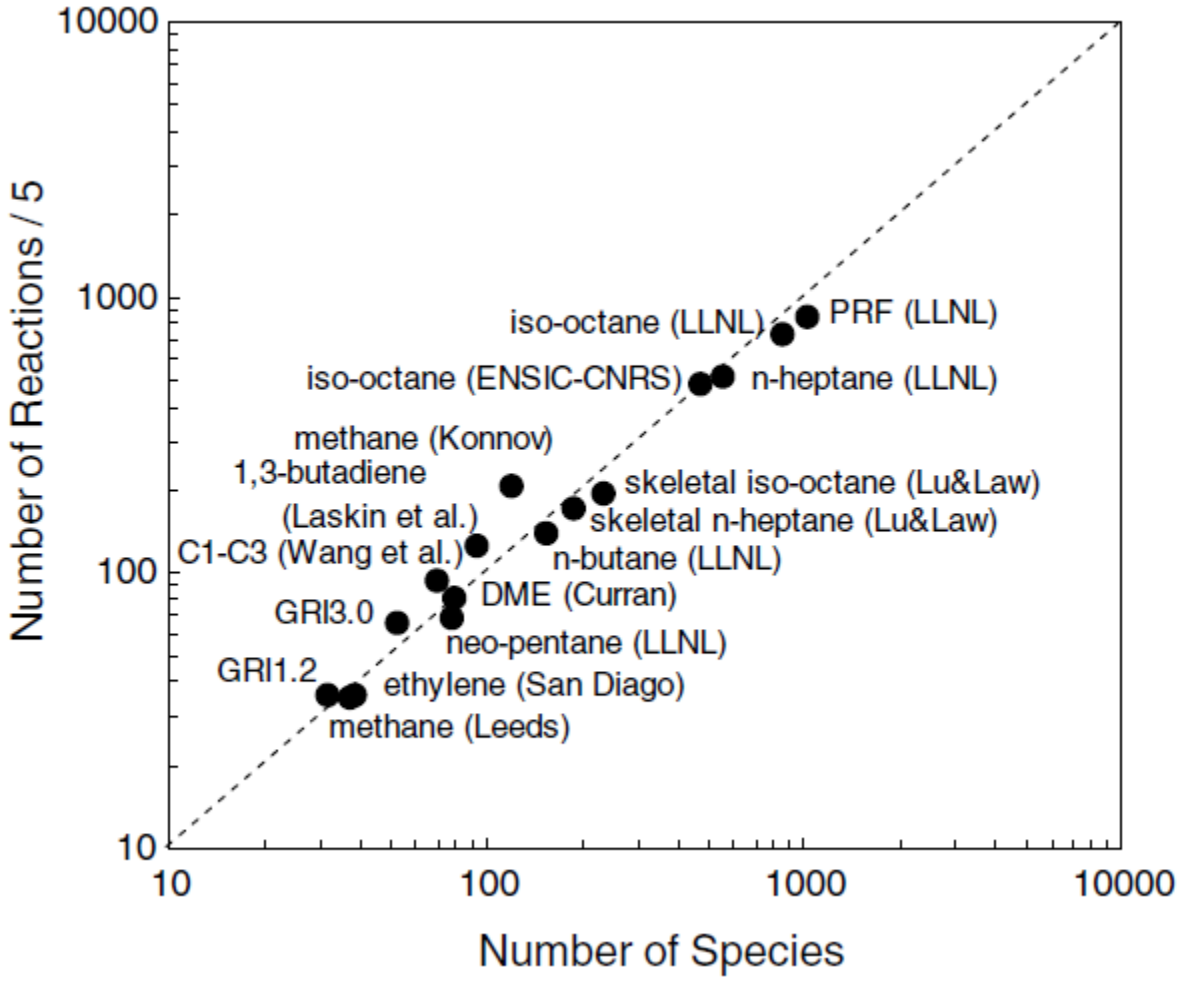
- Why we need model reduction
- Two levels of model reduction
- Most recent methods
- Personal opinion

High CPU time in predictive combustion

- Predictive combustion: detailed model + CFD
- For normal detailed kinetic mechanisms, over 90% of the CPU time of reactive flow simulations is spent solving the ODE systems.[1]
- Why high?
  - Many species and reactions in detailed kinetic models
  - Very different time scales in the models➔ computational stiffness

[1] Long Liang, etc. The use of dynamic adaptive chemistry in combustion simulation of gasoline surrogate fuels (*2009)*

Many species and rxns in detailed models



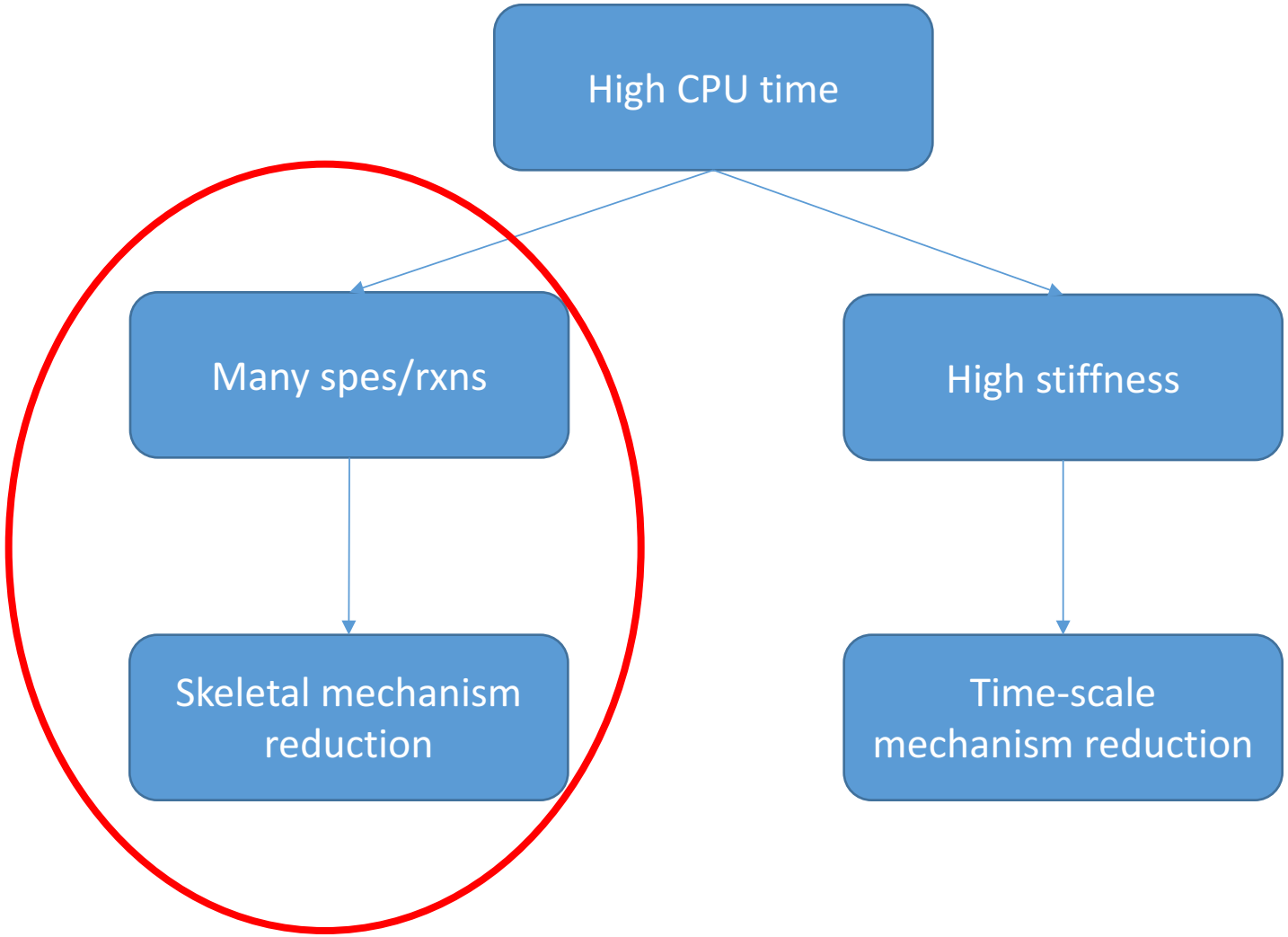
- Tens to hundreds of species
  - Lots of state variables in CFD
  - (x1, x2, x3, …, T, P)
- Hundreds to thousands of rxns [1]
  - RMG gives even more rxns
- Butanol kinetics by Dr. Cai [2]
  - ~90% rxns are insignificant under conditions of his interest

[1] C.K. Law, Proc. Combust. Inst. 31 (2007) 1–29.
[2] Personal conversation with Dr. Jianghua Cai on Apr. 22, 2015

Computational stiffness

- Highly reactive radicals and reactions ➔ very short time scales (usually cause high stiffness ratio*)
- Short time scales ➔ small integration steps➔ long CPU time

Note: $stiffness\ ratio = \frac{\max\ eigen\ value}{\min\ eigen\ value}$


High CPU time
Many spes/rxns
High stiffness
Skeletal mechanism reduction
Time-scale mechanism reduction

Skeletal mechanism reduction

- Identify and eliminate unimportant species and reactions
- Various methods along history
  - Sensitivity analysis
  - Principal component analysis
  - Jacobian analysis
- Most recent methods
  - Directed relation graph (DRG) by Tianfeng Lu (Princeton)
  - Optimization-based approach by Binita Bhattacharjee (MIT)

DRG method

- Being Unimportant: negligible contribution to production rate of every other species [1]

$$R_A = \sum_{i=1,I} \nu_{A,i}\omega_i, \tag{1}$$

$$\omega_i = k_{fi}\prod_{j=1}^{K} C_j^{\nu'_{ij}} - k_{bi}\prod_{j=1}^{K} C_j^{\nu''_{ij}}, \tag{2}$$

$$k_{fi} = [A_i T^{n_i}\exp(-E_i/RT)]F_i, \tag{3}$$

- Dependence of A on B

$$r_{AB} \equiv \frac{\sum_{i=1,I}|\nu_{A,i}\omega_i\delta_{Bi}|}{\sum_{i=1,I}|\nu_{A,i}\omega_i|}, \tag{4}$$

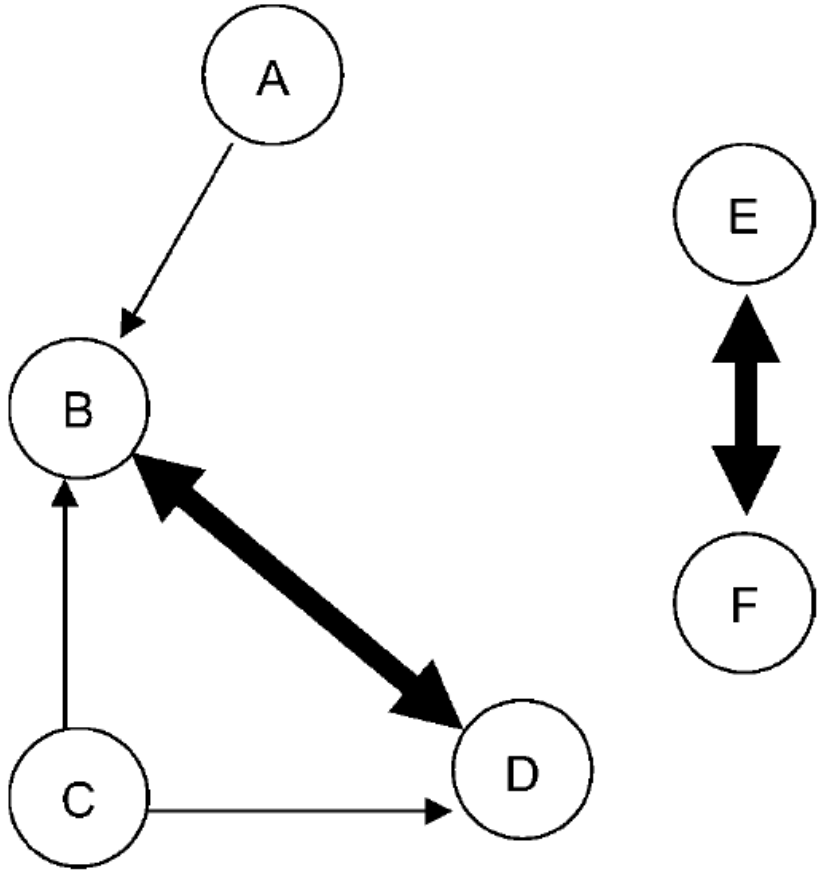
$$\delta_{Bi} = \begin{cases} 1 & \text{if the } i\text{th elementary reaction} \\ & \text{involves species } B, \\ 0 & \text{otherwise.} \end{cases} \tag{5}$$

[1] Tianfeng Lu, Chung K. Law, A directed relation graph method for mechanism reduction 2005

Eliminate negligible dependence

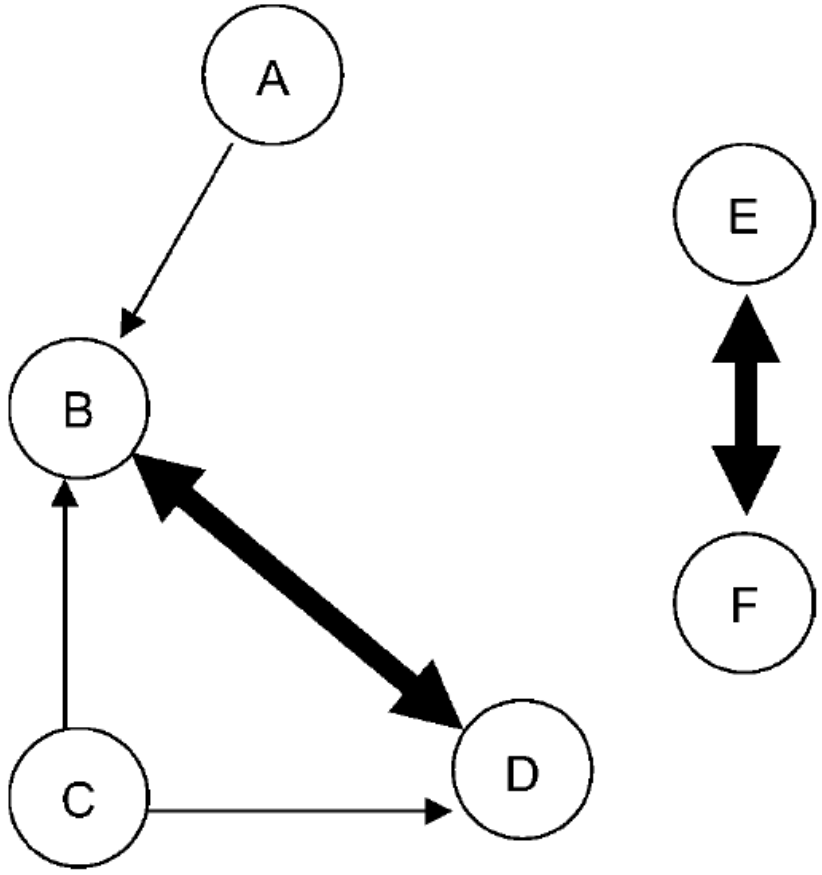
Any r_ij < ε (say, 0.01) would be regarded as negligible dependence

r_ij	A	B	C	D	E	F
A	1	0.2	0.001	0.001	0.002	0.001
B	0.001	1	0.001	0.8	0.002	0.002
C	0.002	0.2	1	0.15	0.002	0.001
D	0.001	0.9	0.002	1	0.001	0.002
E	0.001	0.002	0.001	0.002	1	0.9
F	0.001	0.002	0.002	0.001	0.9	1



Get dependence set of species A

- It seems that A only depend on B
  - To estimate A's flux, B should be included in skeletal model
- But B depends on D heavily
  - To estimate B's flux, D should be included in skeletal model
- So A's dependence set is {B, D}
- Dependence set of A contains all the vertices to which there's at least a path from A



DRG Algorithm

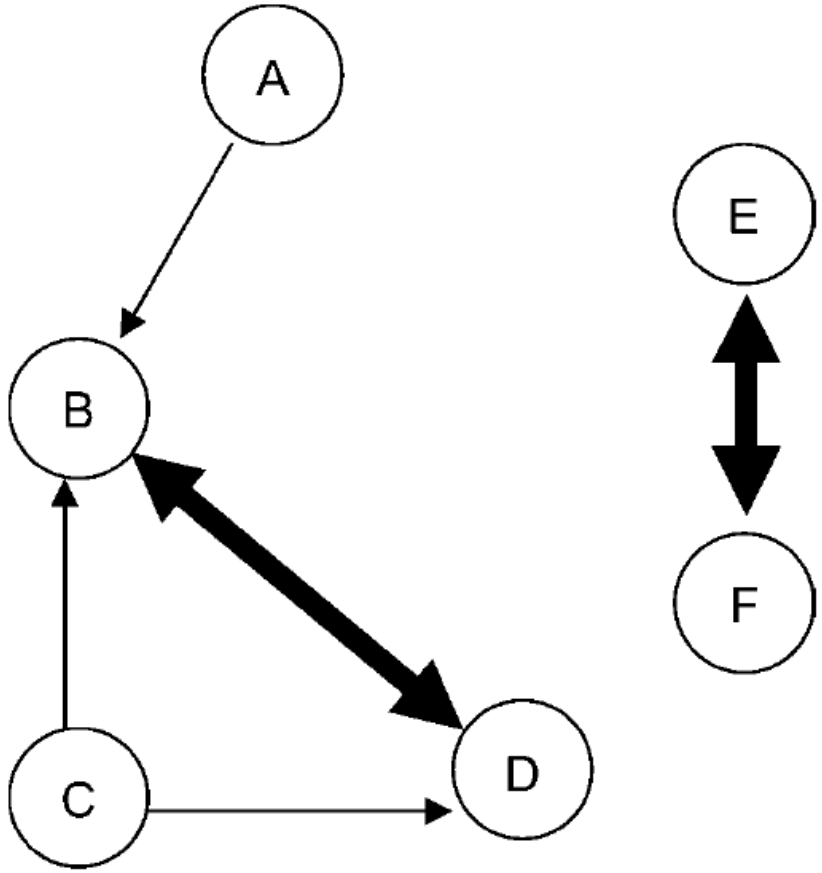
- Step1: select a set of starting species like A
- Step2: calculate r_ij (an N*N matrix where N is the number of species in full mechanism) under selected condition (T, P…)
- Step3: select tolerance ε (there's a paper studying how to choose it [1])
- Step4: draw the dependence graph
- Step5: determine dependence set for each starting species
- Step6: get the final skeletal mechanism by forming union of all the dependence sets f starting species

[1] Xiaolong Gou, Zheng Chen, Wenting Sun, Yiguang Ju. A dynamic adaptive chemistry scheme with error control for combustion modeling with a large detailed mechanism. 2012.

Improved DRG

- Example:
  - Condition: post-ignition
  - Starting species includes CO
  - Skeletal mechanism contains lots of heavy hydrocarbon species
- Reason: strong back propagating connections from CO to heavy HC
- Add search-depth control [1]

$$R_{V_0}(V) = \max_{\Omega}\{\Pi r_{ij}\},$$



[1] Long Liang, John G. Stevens, John T. Farrell. A dynamic adaptive chemistry scheme for reactive flow computations. 2009

Optimization-based reduction

- State variable vector: $x = (x_1, x_2, \ldots, x_n, T, P)$
- The optimization formulation would be

$$\min \sum_{k=1}^{N_R} z_k$$

$$G[x(t, z), x_{ref}(t)] \leq 0$$

$$z_k \in \{0, 1\}$$

$$\left.\begin{aligned} \dot{x}_{j,ref} &= \Gamma_{j,ref}(\boldsymbol{x}_{ref}), \quad x_{j,ref}(t_0) = x_{j,ref,t_0} \\ \dot{x}_j &= \Gamma_j(\boldsymbol{x}, \boldsymbol{z}), \quad x_j(t_0) = x_{j,ref,t_0} \end{aligned}\right\}$$

$$\forall\, j = 1 \ldots N_S + 1 \qquad (3)$$

$$G = \sum_{j=1}^{N_S+1} \alpha_j \left(\int_0^{t_f} \frac{x_j(t, z) - x_{j,ref}(t)}{x_{j,ref}(t)} dt \right)^2 - \delta_1 \leq 0$$

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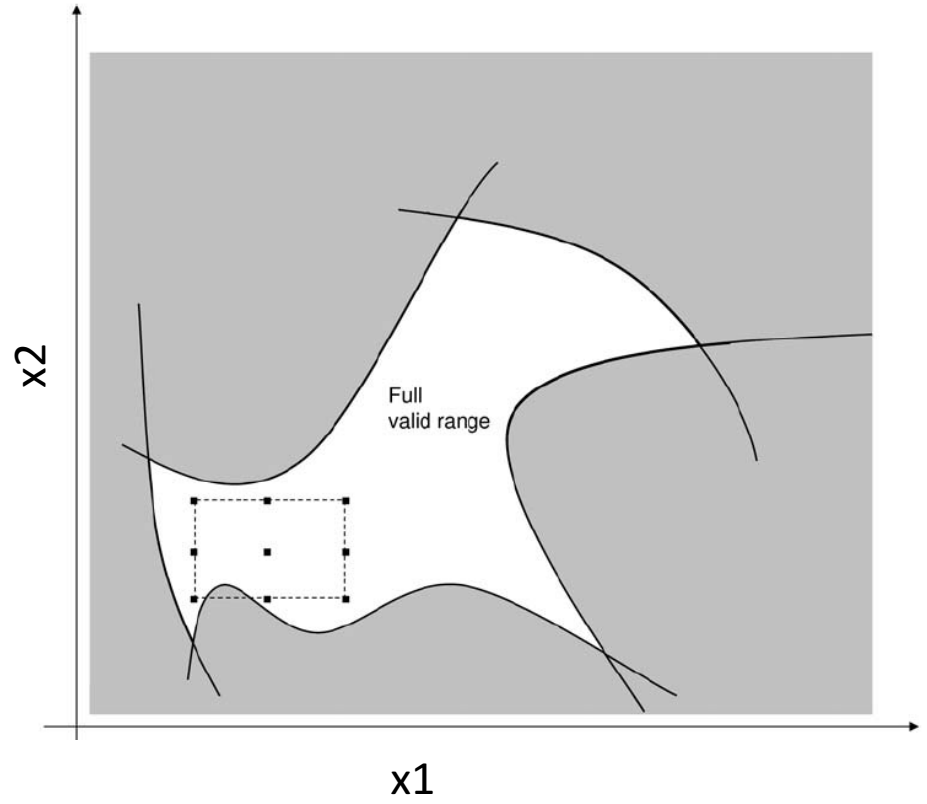
$$G_{j,i} = |\Gamma_j(\boldsymbol{x}_{ref}(t_i), z) - \Gamma_{ref,j}(\boldsymbol{x}_{ref}(t_i))| - (atol_j + rtol_j|\Gamma_{ref,j}|) \leq 0 \quad \forall\, j = 1 \ldots N_S + 1,\ i = 1 \ldots N_t$$

Global minimum is guaranteed!

[1] Oluwayemisi O. Oluwole, Binita Bhattacharjee, John E. Tolsma, Paul I. Barton, William H. Green. Rigorous valid ranges for optimally reduced kinetic models. 2006

Identify valid range for reduced model

- We want to use the reduced model over a range of conditions
- But the reduced model is produced under a single condition



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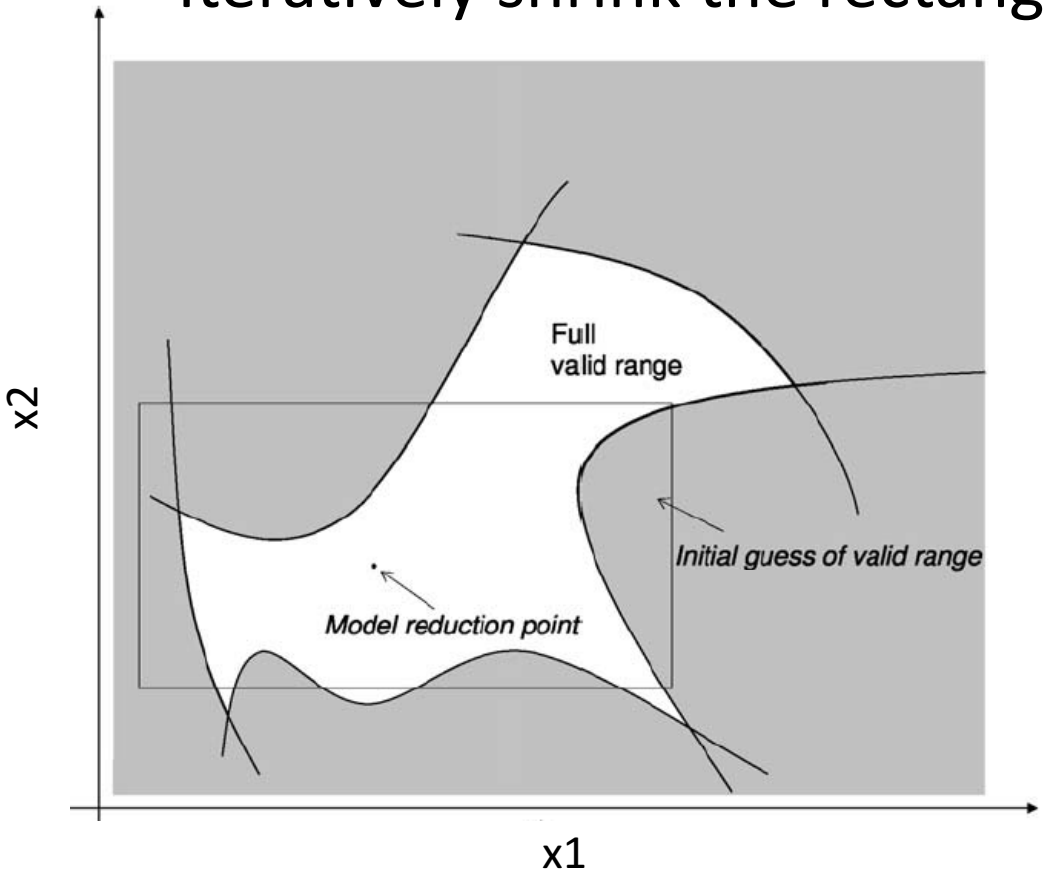
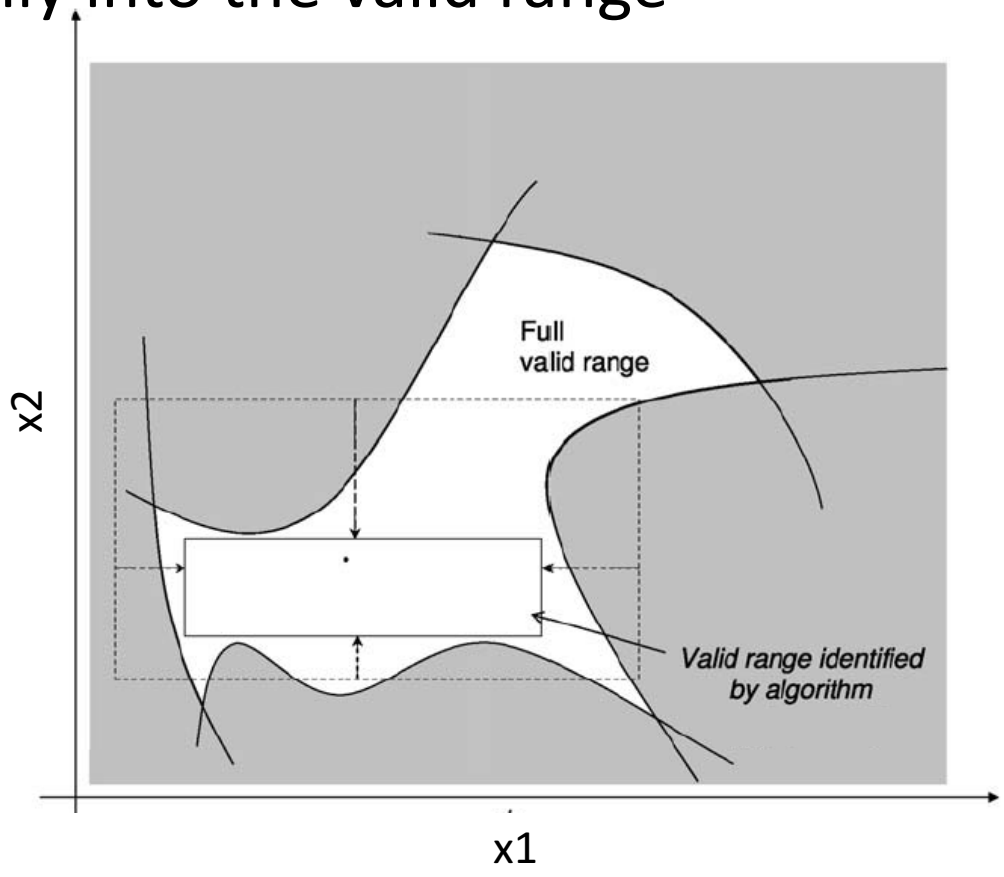
- Fix z*, solve for the range of condition

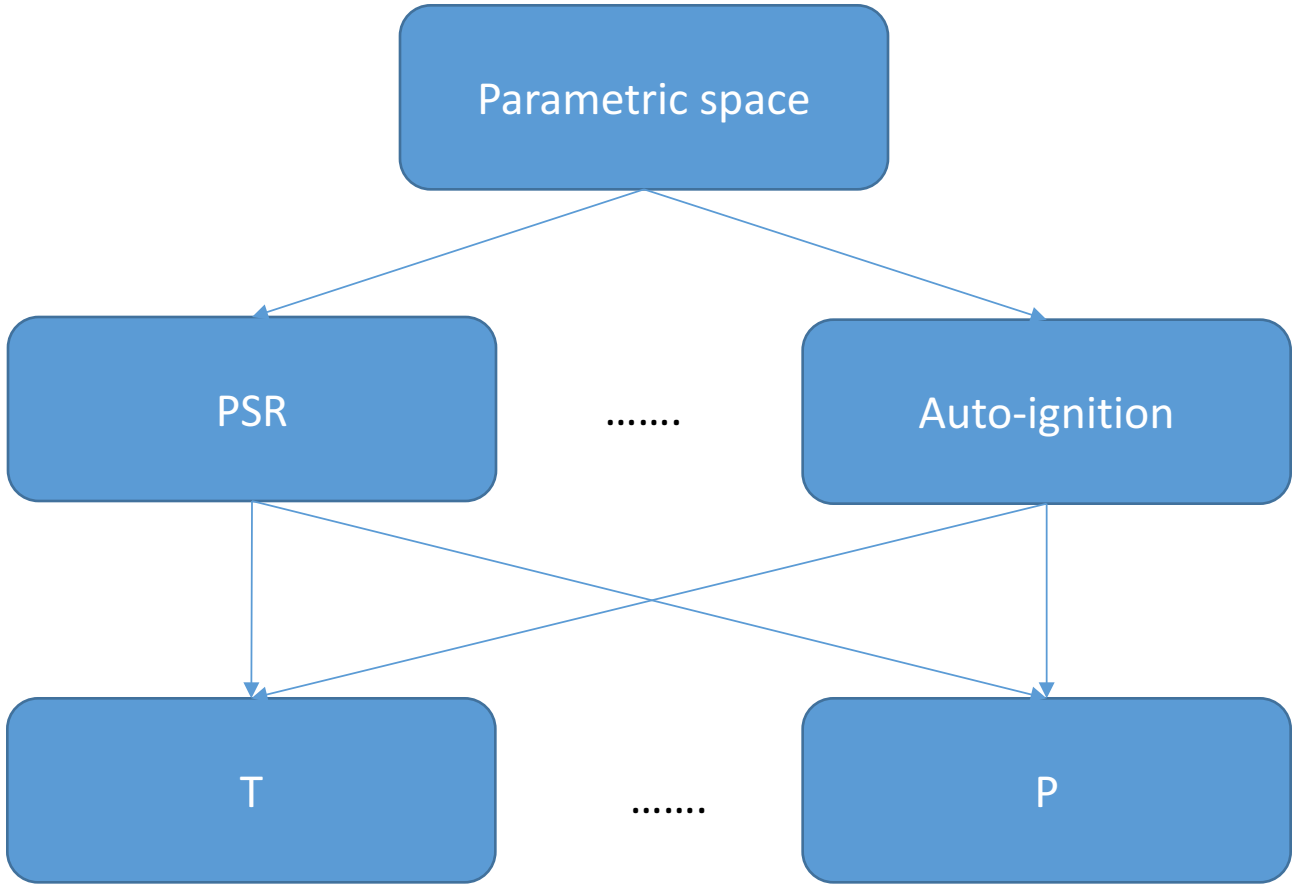
Identify valid range for reduced model

- Initially guess a range ➔ a rectangle
- Iteratively shrink the rectangle fully into the valid range





Make skeletal mechanism valid in a range of parameters



Run model reduction many times under different points in the parametric space and form union of sub-skeletal mechanism

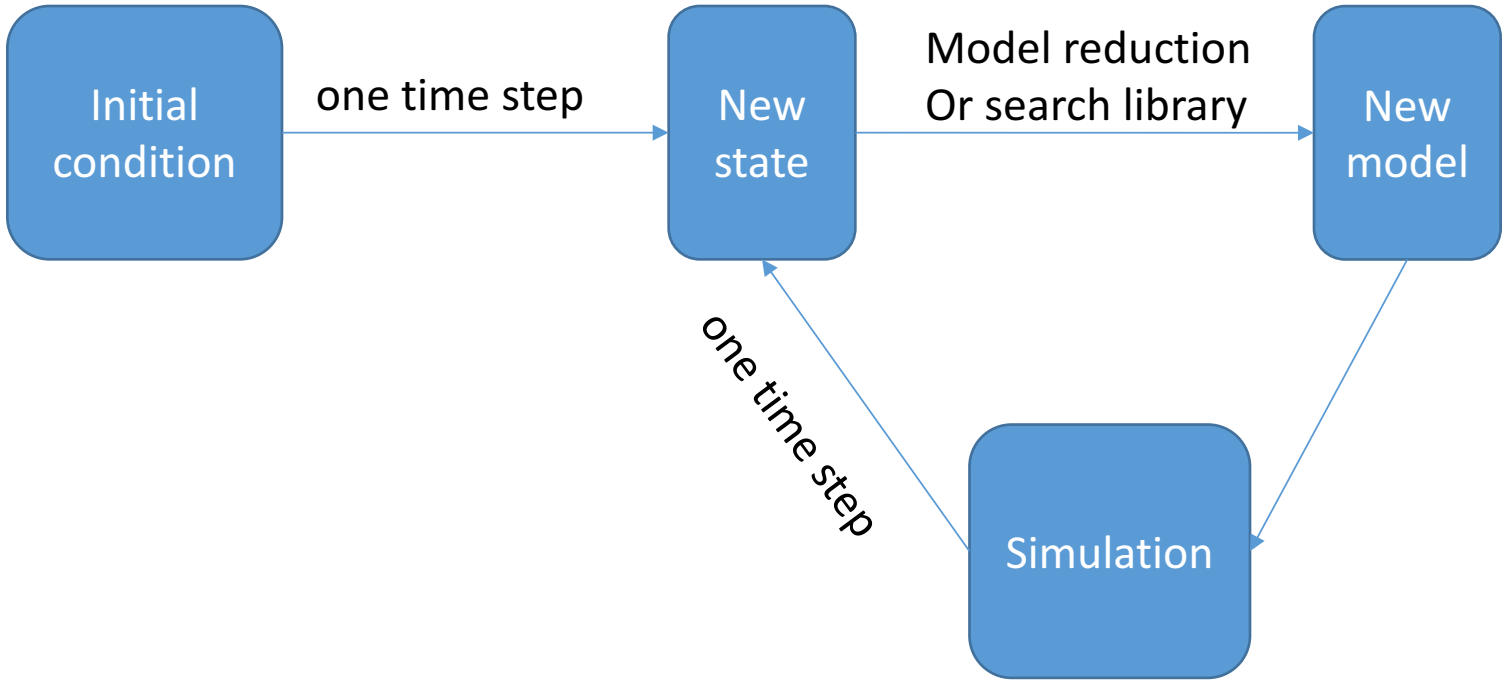
Adaptive chemistry

- Previous union of skeletal mechanisms
  - make big mechanism as well
- An alternative strategy by making use of the nature of local accuracy
- Two approaches to do adaptive chemistry
  - Create a library of reduced models before CFD and choose the most appropriate one during CFD [1]
  - Reduce model on-the-fly [2]

[1] Oluwayemisi O. Oluwole, Binita Bhattacharjee, John E. Tolsma, Paul I. Barton, William H. Green. Rigorous valid ranges for optimally reduced kinetic models. 2006

[2] Long Liang, John G. Stevens, John T. Farrell. A dynamic adaptive chemistry scheme for reactive flow computations. 2009

Adaptive chemistry scheme in CFD



Personal opinion about RMG and model reduction

- RMG is good at generating detailed mechanism over a certain valid condition range [1]
- If we want to add model reduction module,
  - Could use DRG or the optimization-based reduction
- How to pick condition for reduction
  - Single-condition RMG job, directly use that condition and figure out the valid condition range of the reduced mechanism
  - Multi-condition RMG job, run each condition and do union of sub-mechanism
- The reduced mechanism produced by RMG can still use Adaptive Chemistry fashion to conduct CFD

[1] Jing Song, George Stephanopoulos, William H. Green. Valid parameter range analyses for chemical reaction kinetic models. 2002

Backup: Homogeneous reduction→ diffusive applications