Mechanism Reduction via Adjacency Matrix Power

Lásaro Camargos[⋆]
João M. Vedovoto[†]
Ricardo Serfaty[‡]
Aristeu da Silveira N.[†]

⋆Computer Science, Federal University of Uberlândia
†Mechanical Engineering, Federal University of Uberlândia
‡Petrobras

IWMRRF 2015

Problem

Mechanisms that matter are too large to simulate

Problem

Mechanisms that matter are too large to simulate

We must reduce!

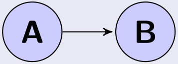
The Direct Relationship Graph Approach

- Build graph from mechanism
- Reduce the graph (prune edges and vertexes)
- Simulate the corresponding reduced mechanism

How do we build the graph?

Species A

B + _ ⇒ A + _



How do we build the graph?

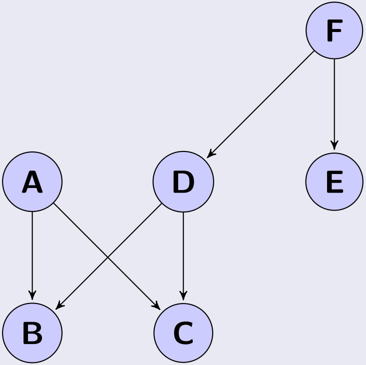
Mechanism

- B + C => A + D
- D + E => F

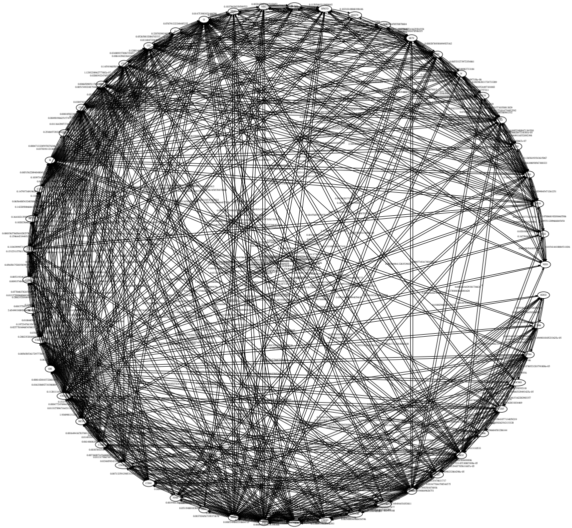
Species

- A
- B
- C
- D
- E
- F

Graph



GRI 3.0 DRG



DRG Approach

- Given a mechanism build corresponding graph
- Reduce the graph (prune edges and vertexes)
- Simulate the corresponding reduced mechanism

How to reduce?

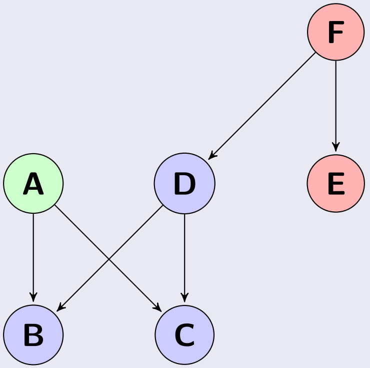
Mechanism

- B + C => A + D
- D + E => F

Species

- A
- B
- C
- D
- E
- F

Graph



How to reduce?

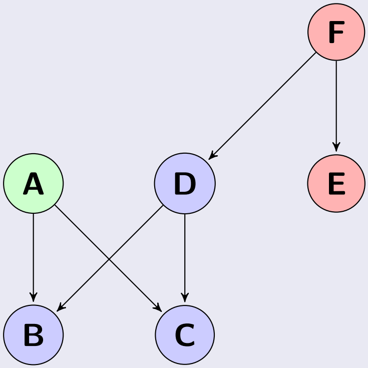
Mechanism

- B + C => A + D
- D + E => F

Species

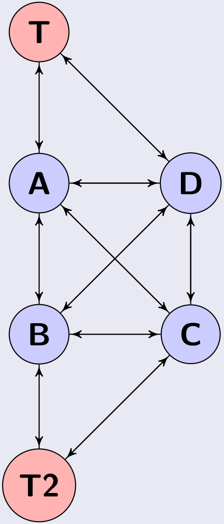
- A
- B
- C
- D
- E
- F

Graph



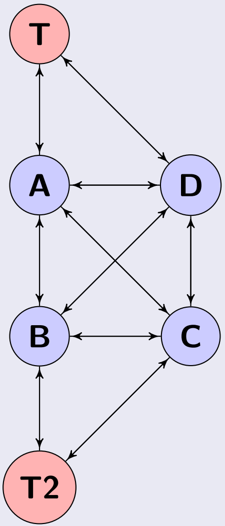
How to reduce?

Clique?

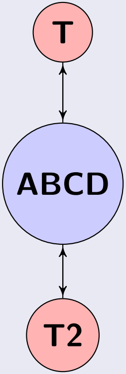


How to reduce?

Clique?



Lump it!



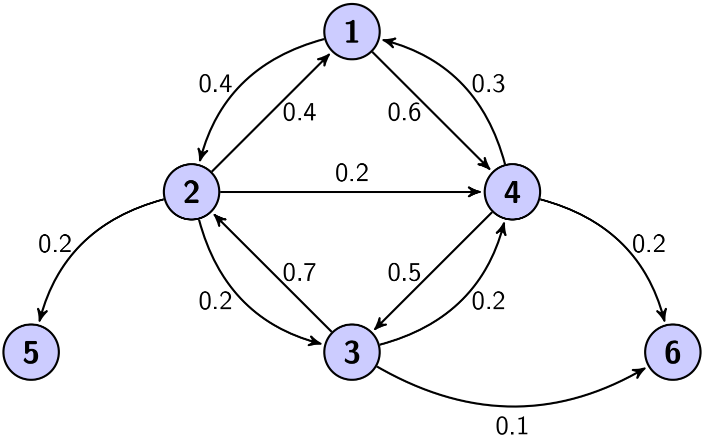
How much effect on each other?

[Nyemeyer 2013, P. Pepiot-Desjardins and H. Pitsch, 2008]

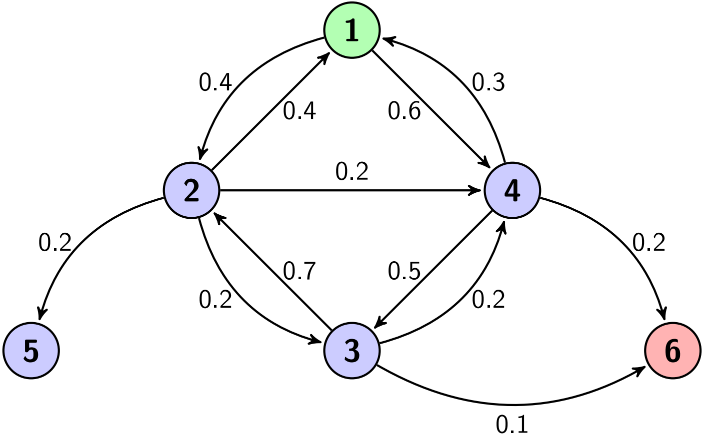
Production of A dependency on B? $r_{AB} = \frac{\left|\sum_{i=1}^{N_R} V_{A,i}\omega_i\delta_B^i\right|}{max(P_A, C_A)}$

- N_R – # reactions
- $V_{A,i} = V''_{A,i} - V'_{A,i}$
- V'' – production stoichiometric coefficient
- V' – consumption stoichiometric coefficient
- ω_i – i-esim reaction rate
- $\delta_B^i = 1$ if reaction i involves B and 0 otherwise
- $P_A = \sum_{i=1}^{N_R} max(0, V_{A,i}\omega_i)$ – Production term
- $P_C = \sum_{i=1}^{N_R} max(0, -V_{A,i}\omega_i)$ – Consumption term

How much effect on each other?



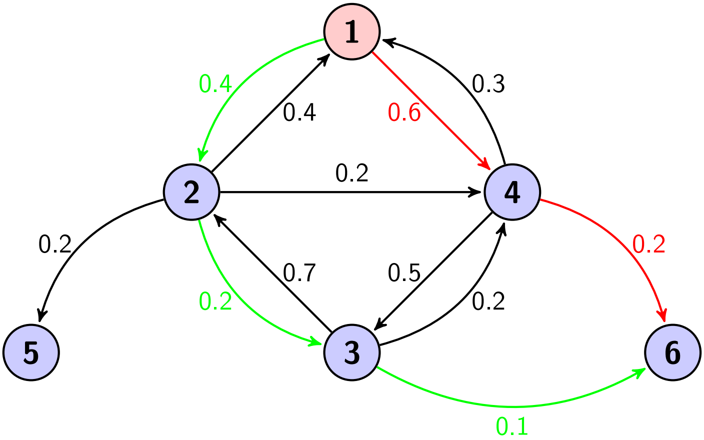
How much effect on each other?



How much effect on each other?

Use paths in the graph to find out!

How much effect on each other?



How to reduce?

Remove the least important reactions/species!

How to reduce?

Remove the least important reactions/species!

But which ones are less important?

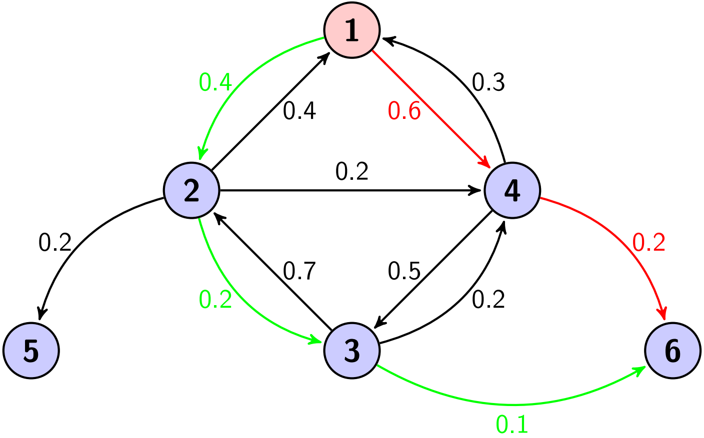
Strategies

- Most important path?
  - Biggest throughput?
    Throughput is smaller edge value
  - Longest path?
    Length is sum)
    DRG with Depth First Search
  - Biggest conditional dependency?
    Dependency is product
    DRG-EP with Dijkstra's shortest path

Strategies

- Most important path?
  - Biggest throughput?
    Throughput is smaller edge value
  - Longest path?
    Length is sum)
    DRG with Depth First Search
  - Biggest conditional dependency?
    Dependency is product
    DRG-EP with Dijkstra's shortest path
- If not important overall, prune

Problem with that?



Strategies

- Most important path?
  - Biggest throughput?
    Throughput is smaller edge value
  - Longest path?
    Length is sum)
    DRG with Depth First Search
  - Biggest conditional dependency?
    Dependency is product
    DRG-EP with Dijkstra's shortest path
- Combination of all paths?

Strategies

- Most important path?
  - Biggest throughput?
    Throughput is smaller edge value
  - Longest path?
    Length is sum)
    DRG with Depth First Search
  - Biggest conditional dependency?
    Dependency is product
    DRG-EP with Dijkstra's shortest path
- Combination of all paths? O(n!)

Proposal: Use all paths of length X.

Adjacency Matrix Power

Adjacency Matrix Power

- All paths of size X are considered
- Large paths include small paths
- Weight is the product of edges' weights
- Multiplication is $O(n^{2.373})$
- x-esim power is $log(x) * O(n^{2.373})$

Adjacency Matrix – M

Spc	1	2	3	4	5	6
1	0	0.4	0	0.6	0	0
2	0.4	0	0.7	0.2	0.2	0
3	0	0	0	0.2	0	0.1
4	0.3	0	0.5	0	0	0.2
5	0	0	0	0	0	0
6	0	0	0	0	0	0

Dependency of i on j

- $M[i,j]$ – directly
- $M[i,k] * M[k,j]$ – via size 2 chain reactions, using k
- $\sum_{k=1}^{N} M[i,k] * M[k,j] = M^2[i,j]$ – via all size 2 chain reactions
- $M^x[i,j]$ – via all size X chain reactions

Now we prune!

Dependency factor (DF): how much target(s) depend(s) on species?

- Cut X% species with the smallest DF
- Cut species with DF smaller than given threshold
- Sum DFs of reactants; cut X% reactions with smallest sums
- Cut reactions with sum smaller than given threshold

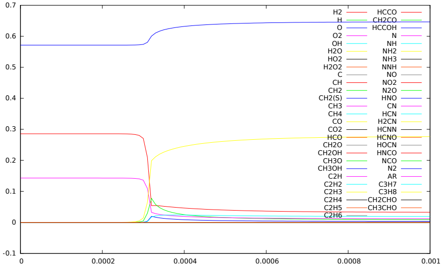
Implementation

- Cantera 2.7
- Boost Graph Library (BGL)
- Dijkstra (from BGL)
- Matrix Power (+ BLAS)
- Full
- Mostly qualitative results so far

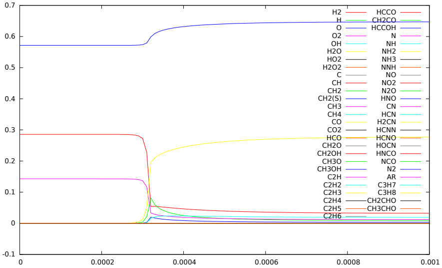
Results

- GRI-MECH 3.0 (53 espécies e 325 reações)
- Initial concentrations: H2:2 O2:1 N2:4
- 1atm
- 1000K
- Prune 25% and 65% less important reactions
- Cut (reactions involving) 25% and 65% less important species

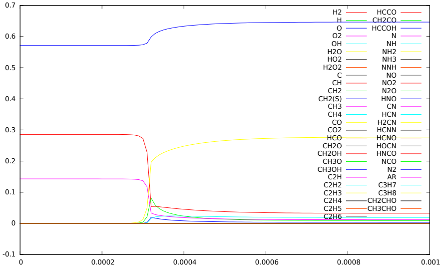
Cut 25% less important reactions



Dijkstra



Matrix Power



Full Mechanism

Mean Squared Error – Full

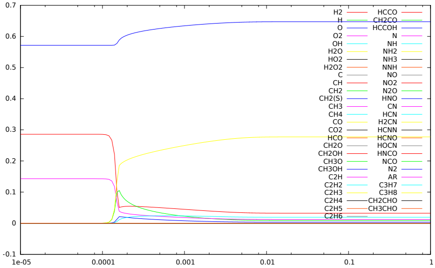
Dijkstra

Temperature (K) Density (kg/m3) Pressure (Pa) H2 H O O2 OH H2O HO2 H2O2 C CH CH2 CH2(S) CH3 CH4 CO CO2 HCO CH2O CH2OH CH3O CH3OH C2H C2H2 C2H3 C2H4 C2H5 C2H6 HCCO CH2CO HCCOH N NH NH2 NH3 NNH NO NO2 N2O HNO CN HCN H2CN HCNN HCNO HOCN HNCO NCO N2 AR C3H7 C3H8 CH2CHO CH3CHO
20.802958 0.001068 0.000000 0.002150 0.001403 0.000382 0.000963 0.000452 0.002752 0.000001 0.000001 0.000000 0.000024 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.001077 0.000000 0.000000 0.000000 0.000000 0.000000

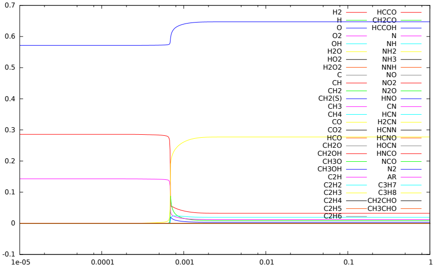
Matrix

Temperature (K) Density (kg/m3) Pressure (Pa) H2 H O O2 OH H2O HO2 H2O2 C CH CH2 CH2(S) CH3 CH4 CO CO2 HCO CH2O CH2OH CH3O CH3OH C2H C2H2 C2H3 C2H4 C2H5 C2H6 HCCO CH2CO HCCOH N NH NH2 NH3 NNH NO NO2 N2O HNO CN HCN H2CN HCNN HCNO HOCN HNCO NCO N2 AR C3H7 C3H8 CH2CHO CH3CHO
16.840980 0.000608 0.000000 0.000807 0.000971 0.000334 0.000518 0.000412 0.001916 0.000001 0.000000 0.000465 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000820 0.000000 0.000000 0.000000 0.000000 0.000000

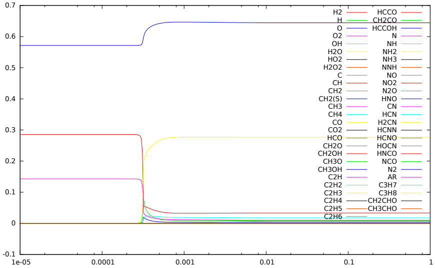
Cut 65% less important reactions



Dijkstra



Matrix



Full Mechanism

Mean Squared Error – Full

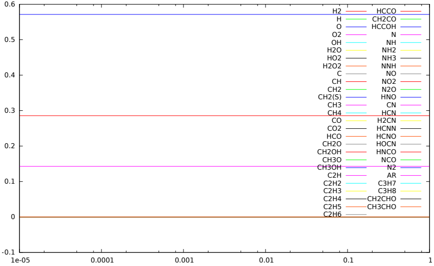
Dijkstra

Temperature (K) Density (kg/m3) Pressure (Pa) H2 H O O2 OH H2O HO2 H2O2 C CH CH2 CH2(S) CH3 CH4 CO CO2 HCO CH2O CH2OH CH3O CH3OH C2H C2H2 C2H3 C2H4 C2H5 C2H6 HCCO CH2CO HCCOH N NH NH2 NH3 NNH NO NO2 N2O HNO CN HCN H2CN HCNN HCNO HOCN HNCO NCO N2 AR C3H7 C3H8 CH2CHO CH3CHO 18.404417 0.001498 0.000000 0.003218 0.001081 0.000509 0.002351 0.001373 0.002879 0.000001 0.000000 0.000001 0.000000 0.000000 0.000000 0.000000 0.005882 0.000001 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.002958 0.000000 0.000000 0.000000 0.000000 0.000000

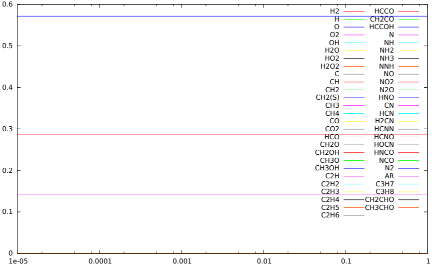
Matriz

Temperature (K) Density (kg/m3) Pressure (Pa) H2 H O O2 OH H2O HO2 H2O2 C CH CH2 CH2(S) CH3 CH4 CO CO2 HCO CH2O CH2OH CH3O CH3OH C2H C2H2 C2H3 C2H4 C2H5 C2H6 HCCO CH2CO HCCOH N NH NH2 NH3 NNH NO NO2 N2O HNO CN HCN H2CN HCNN HCNO HOCN HNCO NCO N2 AR C3H7 C3H8 CH2CHO CH3CHO 31.011686 0.002647 0.000000 0.004804 0.000706 0.000461 0.003023 0.001396 0.004960 0.000004 0.000003 0.000000 0.000001 0.000000 0.000000 0.000000 0.000000 0.005882 0.000001 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.003170 0.000000 0.000000 0.000000 0.000000 0.000000

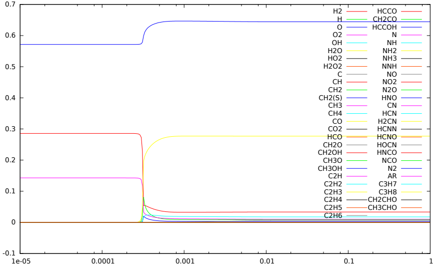
Cut 90% less important reactions



Dijkstra



Matriz



Full Mechanism

Next steps

Real Benchmark

Iso-octane? Ethanol? Others?

Should?

Scaling [Pietot e DesJardins]?

Questions?

Remember: I am a computer scientist! :)