DRGEP-based mechanism reduction strategies: graph search algorithms and skeletal primary reference fuel mechanisms

Kyle E. Niemeyer
Department of Mechanical and Aerospace Engineering
Case Western Reserve University

Chih-Jen (Jackie) Sung
Department of Mechanical Engineering
University of Connecticut

49th AIAA Aerospace Sciences Meeting
January 6, 2010

Introduction

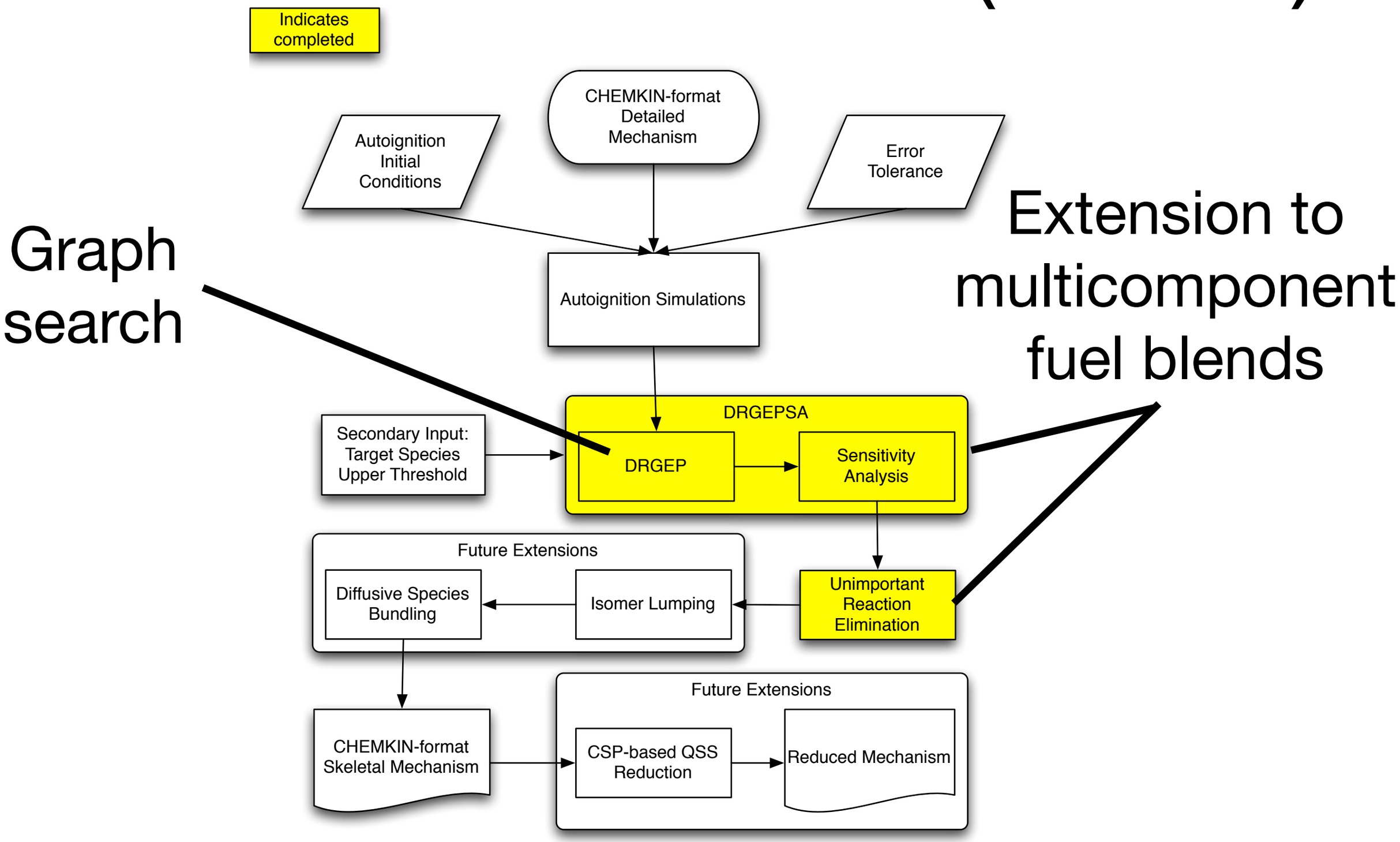
- Why is this research needed?
- Need accurate chemistry model for simulations of engine/burner combustion
- Limited by mechanism size:
  - LLNL gasoline: 1550 species & 6000 reactions
  - LLNL diesel: 2800 species & 11000 reactions
  - LLNL biodiesel: 3300 species & 10800 reactions
  - Jet-A: 2115 species & 8157 reactions (Dooley et al. CNF 2010)

Mechanism Reduction

Skeletal reduction: elimination of unimportant species and reactions

- Directed Relation Graph (**DRG**): Lu and Law 2005
- DRG with Error Propagation (**DRGEP**): Pepiot-Desjardins and Pitsch 2005 & 2008
- DRG-aided Sensitivity Analysis (**DRGASA**): Lu and Law 2007
- DRGEP with Sensitivity Analysis (**DRGEPSA**): Niemeyer, Raju, and Sung 2010
- Path Flux Analysis (**PFA**): Sun et al. 2010

Mechanism Automatic Reduction Software (MARS)



Graph search

Extension to multicomponent fuel blends

Objectives

- Comparison of graph search algorithms for use with DRGEP
- Propose strategies for skeletal reduction of binary PRF using multi-stage approach

DRG/DRGEP

- Graph-theory-based methods to identify unimportant species for removal
- Species are nodes, connections represent species dependencies
- Target species: fuel, oxidizer, important radicals
- Unimportant connections trimmed using error threshold

DRGEP Method

$$r_{AB} \equiv \frac{\left|\sum_{i=1,I} \nu_{A,i}\,\omega_i\,\delta^{i}{}_{B}\right|}{\max\left(P_A, C_A\right)}$$

$$P_A = \sum_{i=1,I} \max\left(0, \nu_{i,A}\,\omega_i\right)$$

$$C_A = \sum_{i=1,I} \max\left(0, -\nu_{i,A}\,\omega_i\right)$$

$$r_{AB,p} = \prod_{i=1}^{n-1} r_{S_i S_{i+1}}$$

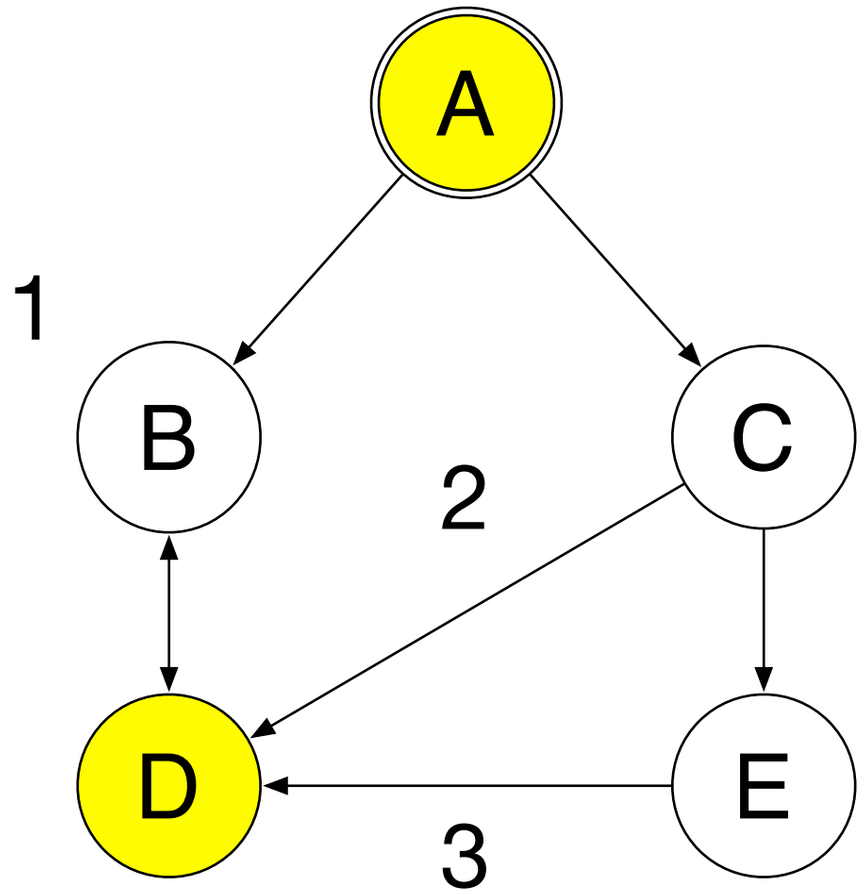
$$R_{AB} = \max_{\text{all paths } p}\left(r_{AB,p}\right)$$

- r_{AB} represents error of removal of B on calculation of A
- Error propagation down pathways determines overall dependence
- For target species A, if $R_{AB} < \varepsilon_{EP}$ then B is removed

$r_{AB,p}$ – path-dependent interaction coefficient for path p between species A and B

R_{AB} – Overall Interaction Coefficient (OIC)

DRGEP Method

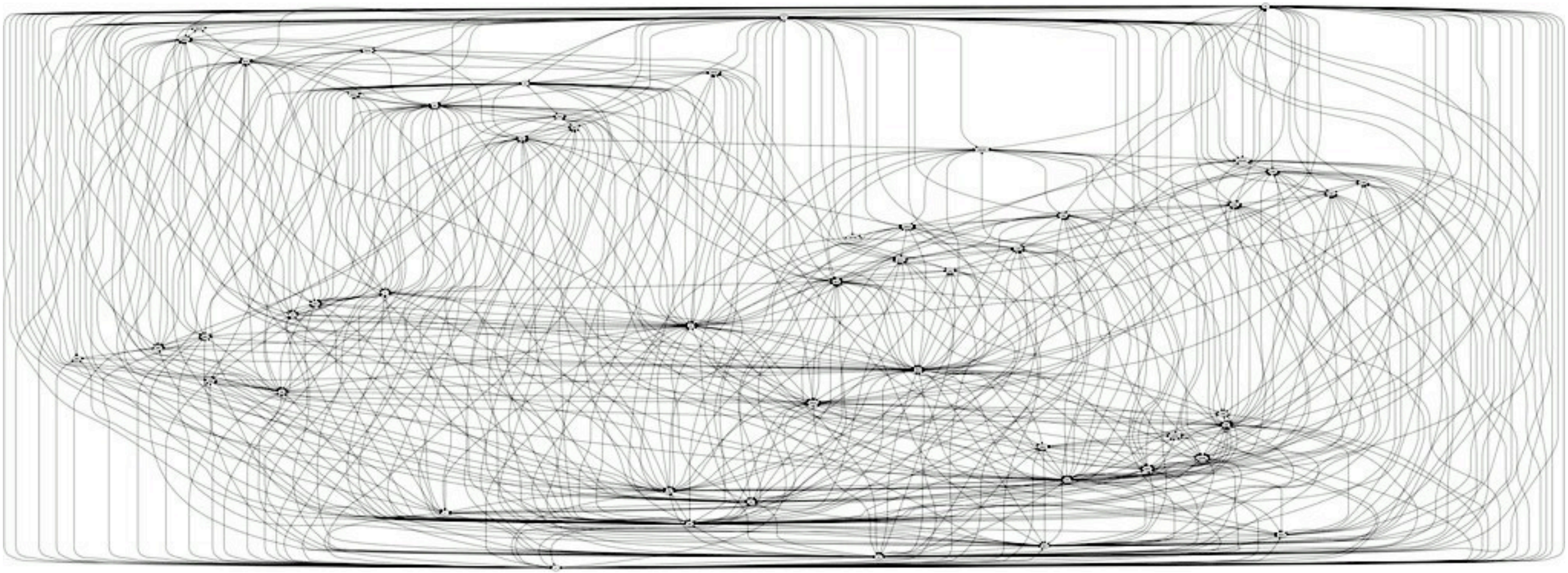


$$R_{AD} = \max\left(r_{AD,1}, r_{AD,2}, r_{AD,3}\right)$$

$$r_{AD,1} = r_{AB} \cdot r_{BD}, \quad r_{AD,2} = r_{AC} \cdot r_{CD}, \quad r_{AD,3} = r_{AC} \cdot r_{CE} \cdot r_{ED}$$

R_{AD} is the overall interaction coefficient of species D to species A

GRI-Mech 3.0 Graph



53 species
1082 connections

Graph Search

- Calculation of OIC requires graph search
- Existing methods:
  - Depth-first search (DFS)
  - Modified DFS (mod. DFS)
  - Breadth-first search (BFS)
  - R-value-based BFS (RBFS)
- New method used here: Dijkstra's algorithm
  - Classical solution to shortest-path problem
  - Compared with various methods

Coefficient Scaling

- Psuedo-production rate of atom *a*

$$P_a = \sum_{\text{all species } S} N_{a,S} \max\left(0, P_S - C_S\right)$$

- Scaling coefficient at time *t*

$$\alpha_{a,T}(t) = \frac{N_{a,T}\left|P_T - C_T\right|}{P_a}$$

- Normalized scaling coefficient at time *t*

$$\alpha_T(t) = \max_{a\in\{\mathcal{E}\}} \left(\frac{\alpha_{a,T}(t)}{\max\limits_{\text{all time}} \alpha_{a,T}(t)} \right)$$

- Importance of species S

$$\overline{R_S} = \max_{\substack{T\in\{\mathcal{T}\} \\ k\in\{\mathcal{D}\}}} \left[\max_{\text{all time, } k} \left(\alpha_T R_{TS}\right) \right]$$

Sensitivity Analysis (SA)

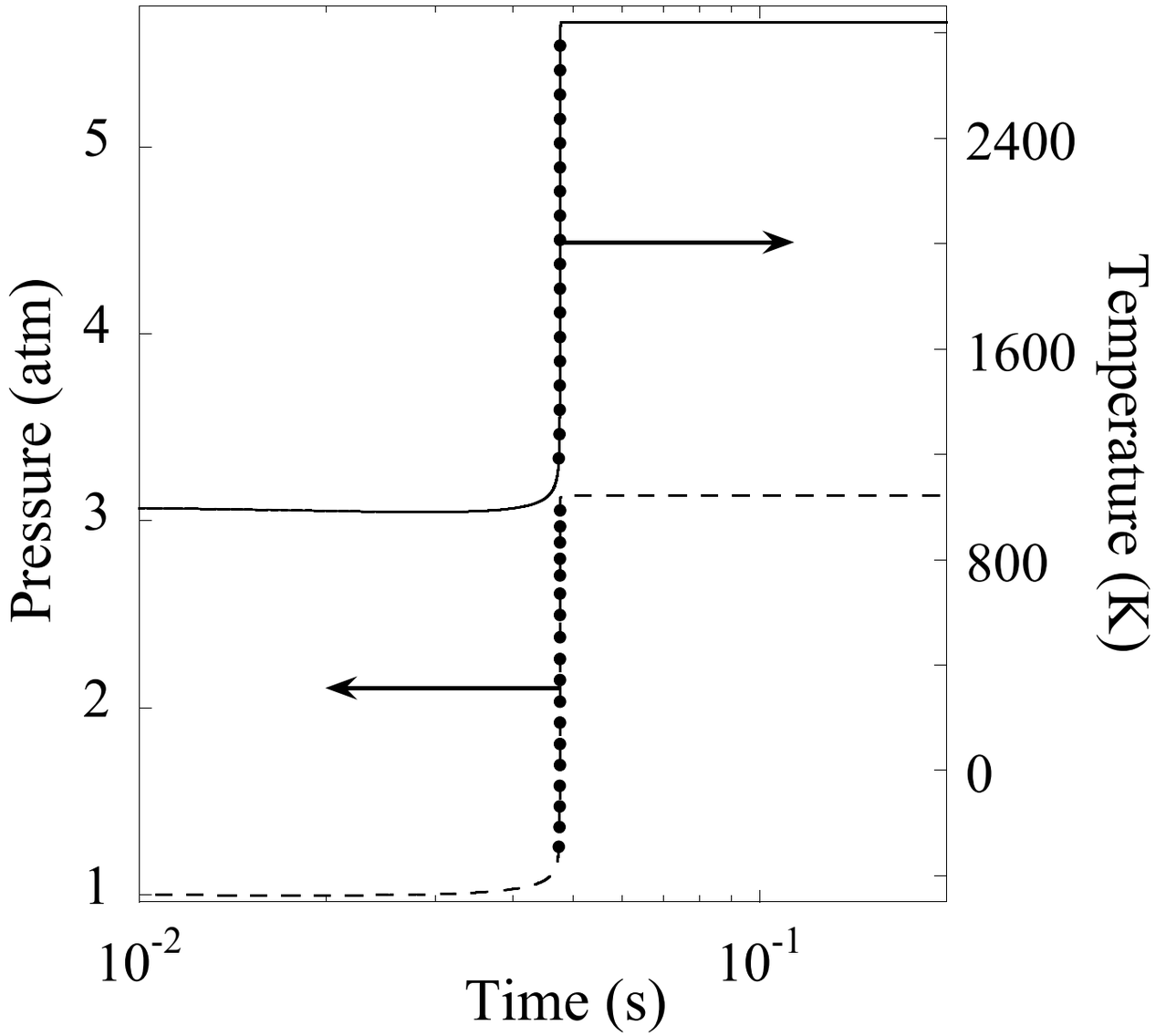
- Retained species: $\overline{R_S} \geq \varepsilon^*$
- Limbo species: $\varepsilon_{\mathrm{EP}} \leq \overline{R_S} < \varepsilon^*$
- Each removed separately, then sorted according to $\delta_S = |\delta_{S,\mathrm{ind}} - \delta_{\mathrm{DRGEP}}|$
- Removed in order until the error reaches the defined limit

Elimination of Unimportant Reactions

- DRGEP & SA stages: reactions removed when participating species removed
- Further reaction elimination:
  - CSP importance index: $$I_{A,i} = \frac{|\nu_{A,i}\omega_i|}{\sum_{j=1,n_R} |\nu_{A,j}\omega_j|}$$
  - Remove reactions where $$\max_{\text{all species } A} I_{A,i} < \varepsilon_{\text{reac}}$$

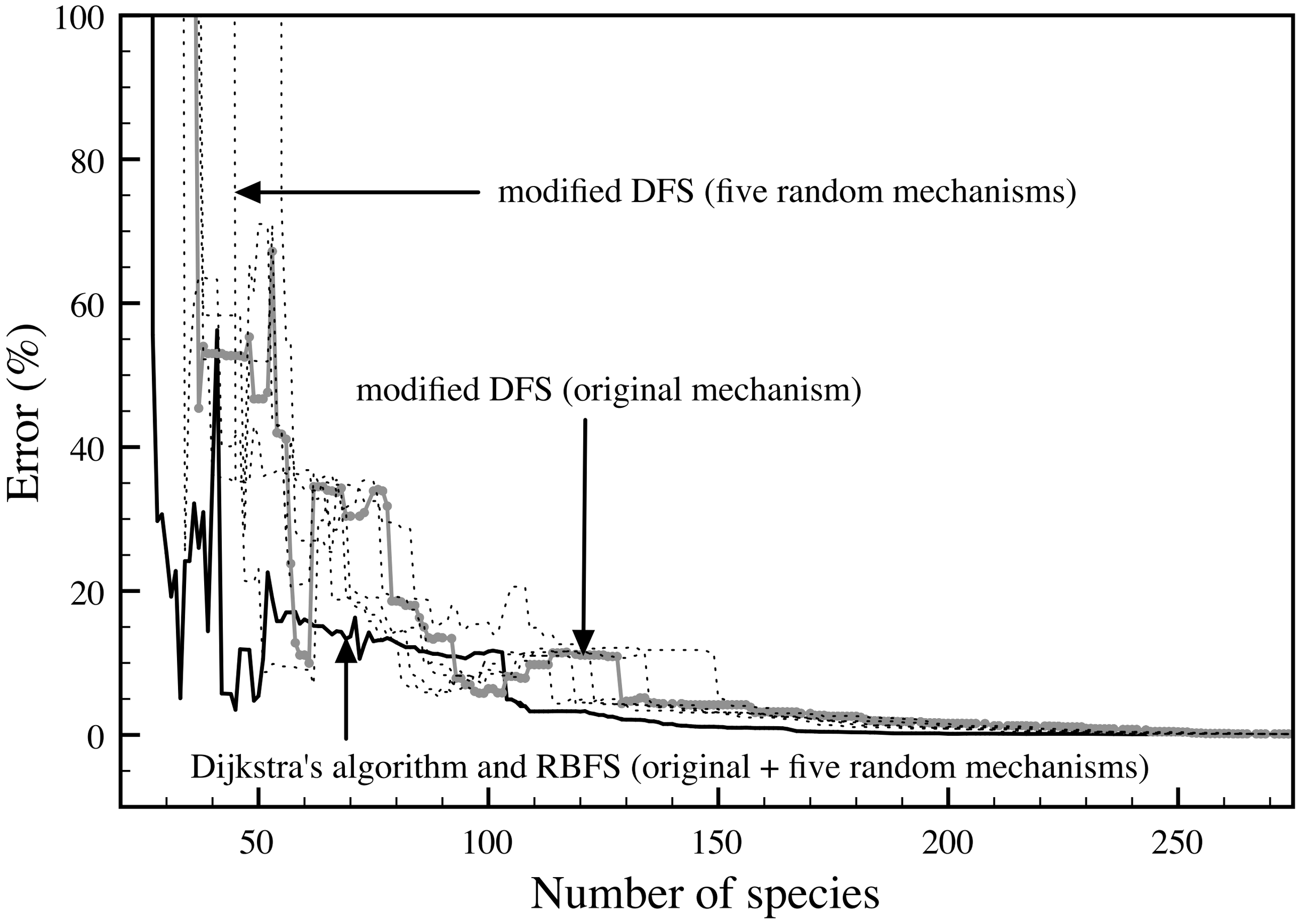
Sampling Procedure

- Constant volume autoignition simulations (SENKIN)
- Chemical kinetics data sampled during ignition evolution



Graph Search Algorithm Reliability

- Search algorithms that produce results dependent on species order do not correctly calculate OIC
- Test by applying DRGEP using different algorithms on mechanism with randomly-shuffled species
- LLNL *n*-heptane (561 species & 2539 reactions), autoignition initial conditions: 1000 K, 1 atm, and Φ = 0.5-1.5


100
80
60
40
20
0
Error (%)
modified DFS (five random mechanisms)
modified DFS (original mechanism)
Dijkstra's algorithm and RBFS (original + five random mechanisms)
50
100
150
200
250
Number of species

Graph Search Algorithm Reliability: Discussion

- DFS and BFS show similar dependence on species order as modified DFS
- Dijkstra's algorithm and RBFS produce results independent of species order

Graph Search Algorithm Effectiveness

- Need to determine effectiveness of DRGEP using various graph search algorithms
  - Dijkstra's, DFS, modified DFS, BFS
    - With and without coefficient scaling
- Generate skeletal mechanisms using DRGEP for LLNL *n*-heptane mechanism (561 species & 2539 reactions)
- Autoignition initial conditions: 600-1600 K, 1-20 atm, & Φ = 0.5-1.5
- Error limit: 30%
- Target species: *n*-heptane, oxygen, nitrogen, and hydrogen radical

Graph Search Algorithm Effectiveness

Algorithm		# species	# reactions	Max. error
DFS	no scaling	461	2304	19%
	scaling	449	2267	19%
mod. DFS		173	868	28%
BFS	no scaling	180	891	29%
	scaling	207	921	25%
Dijkstra	no scaling	178	986	23%
	scaling	**131**	**651**	**17%**

Graph Search Algorithm Effectiveness: Discussion

- Dijkstra's algorithm with coefficient scaling produces most compact skeletal mechanism
- Basic DFS unable to generate skeletal mechanism of comparable size to others
- BFS actually produces slightly larger skeletal mechanism with coefficient scaling

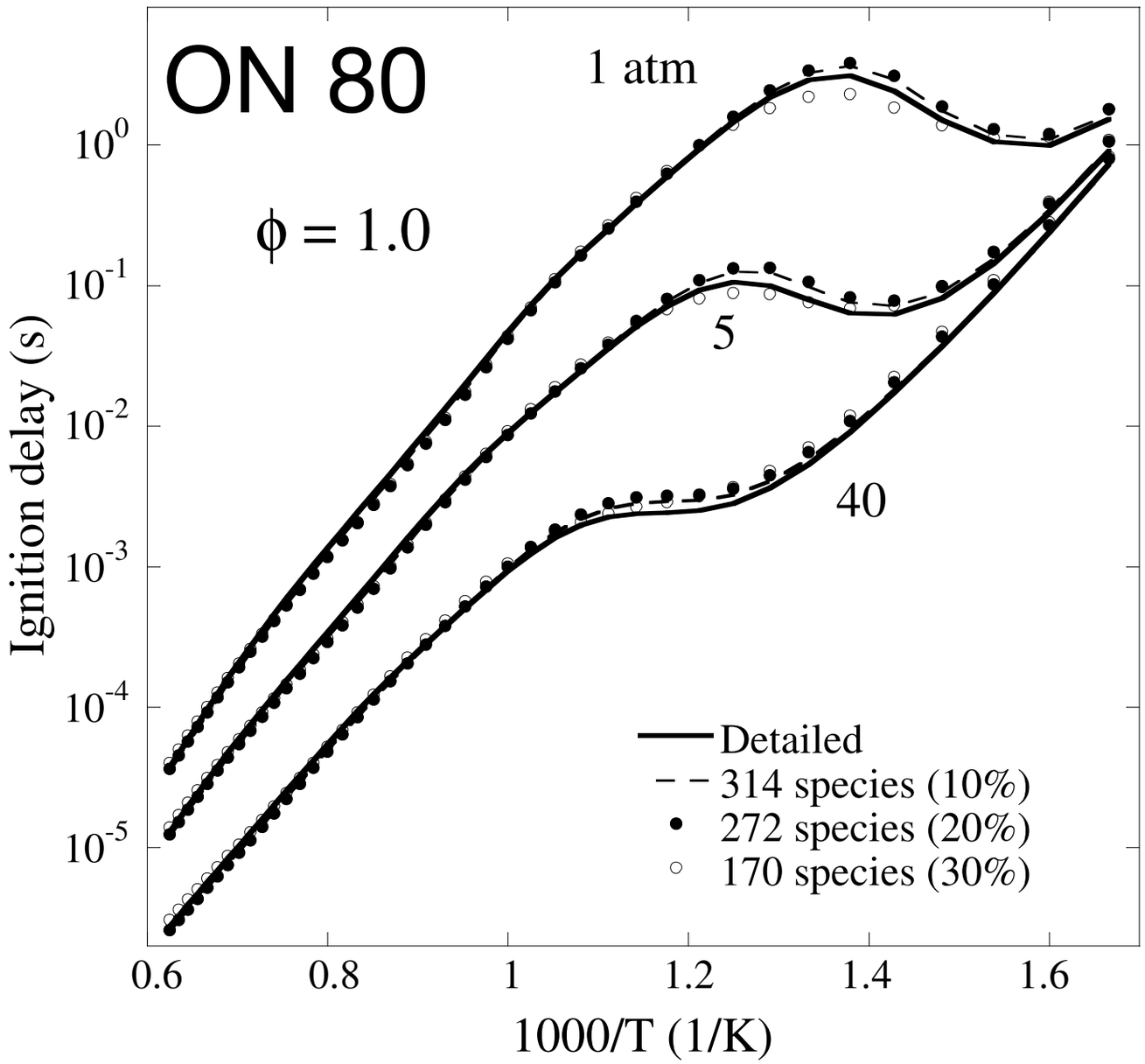
PRF Skeletal Mechanisms

- Ultimate goal: use of multicomponent surrogate mechanisms
- LLNL binary PRF mechanism (*n*-heptane + *iso*-octane): 1034 species and 4236 reactions
- Generate skeletal mechanisms using DRGEPSA + unimportant reaction elimination
  - Error limits: 10%, 20%, 30%
  - Comprehensive-temperature (600-1600 K) and high-temperature (1000-1600 K), 1 atm, Φ=0.5-1.5 (ON 80)
  - Target species: *n*-heptane, *iso*-octane, oxygen, & nitrogen

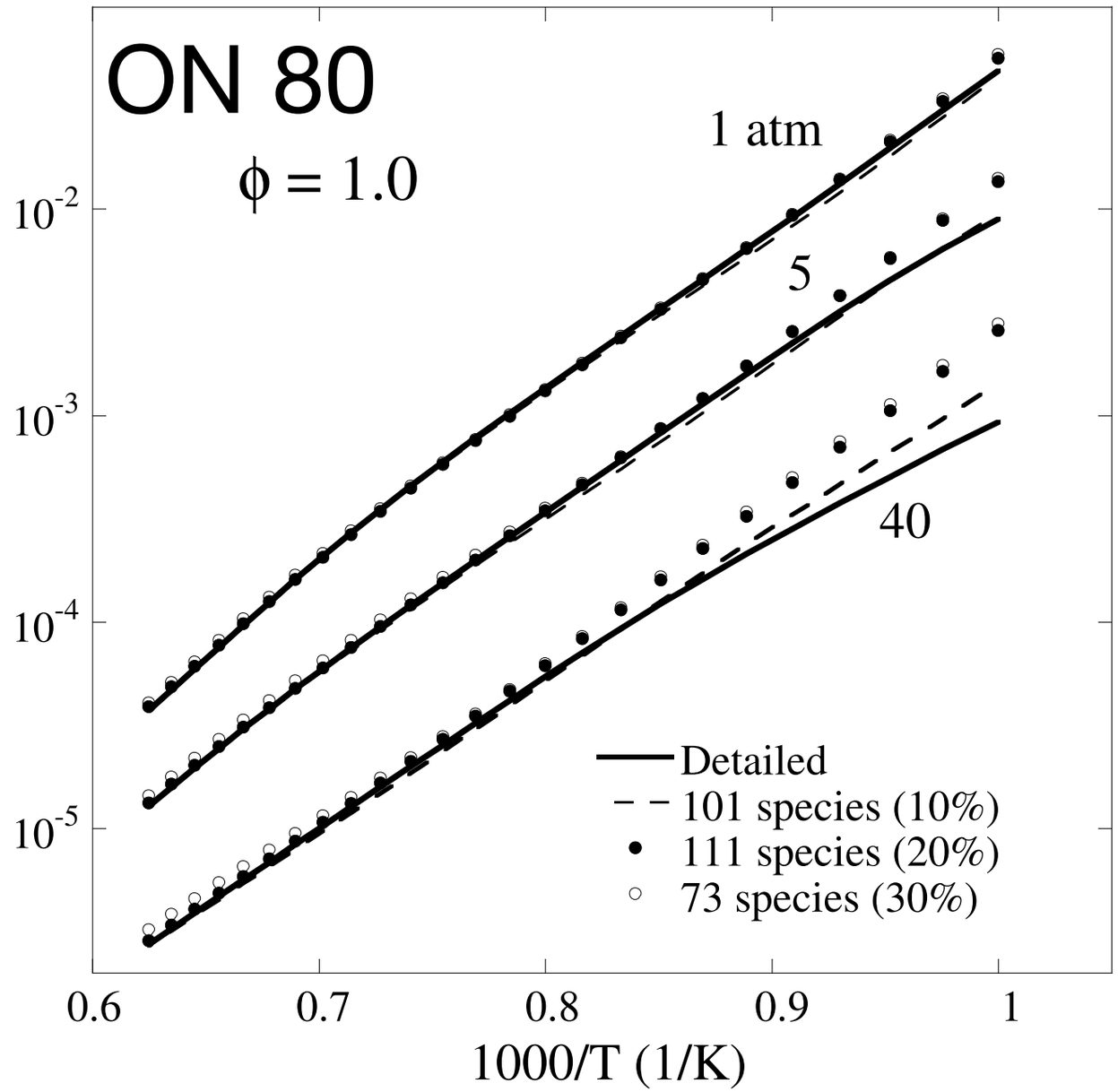
PRF Skeletal Mechanisms

Error limit	Comp-temperature		High-temperature	
	# species	Max. error	# species	Max. error
10%	314	9.6%	101	7.2%
20%	272	19.3%	111	19.2%
30%	170	28.1%	73	28.1%

PRF Skeletal Mechanisms Validation

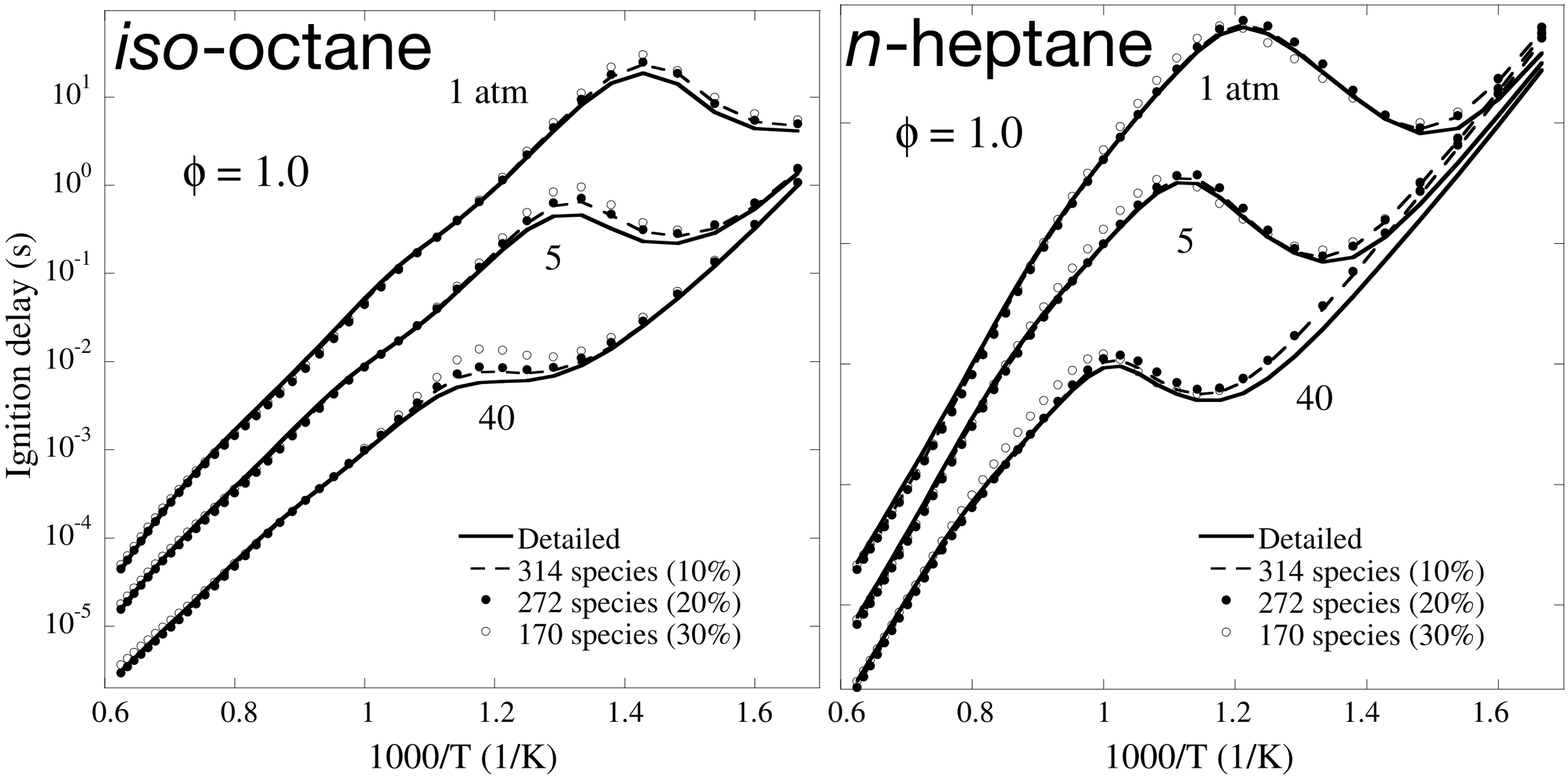


Comprehensive-temp

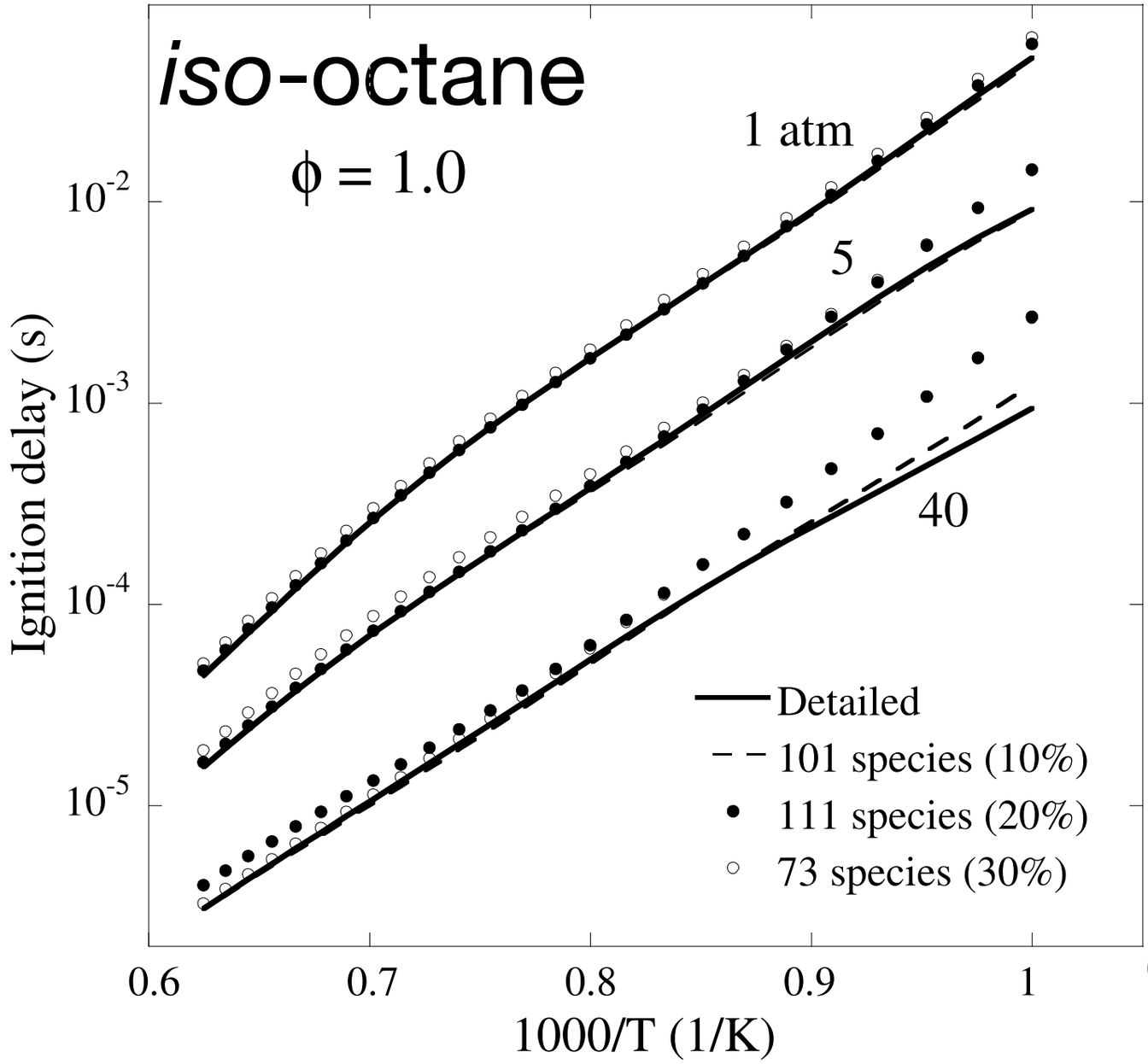


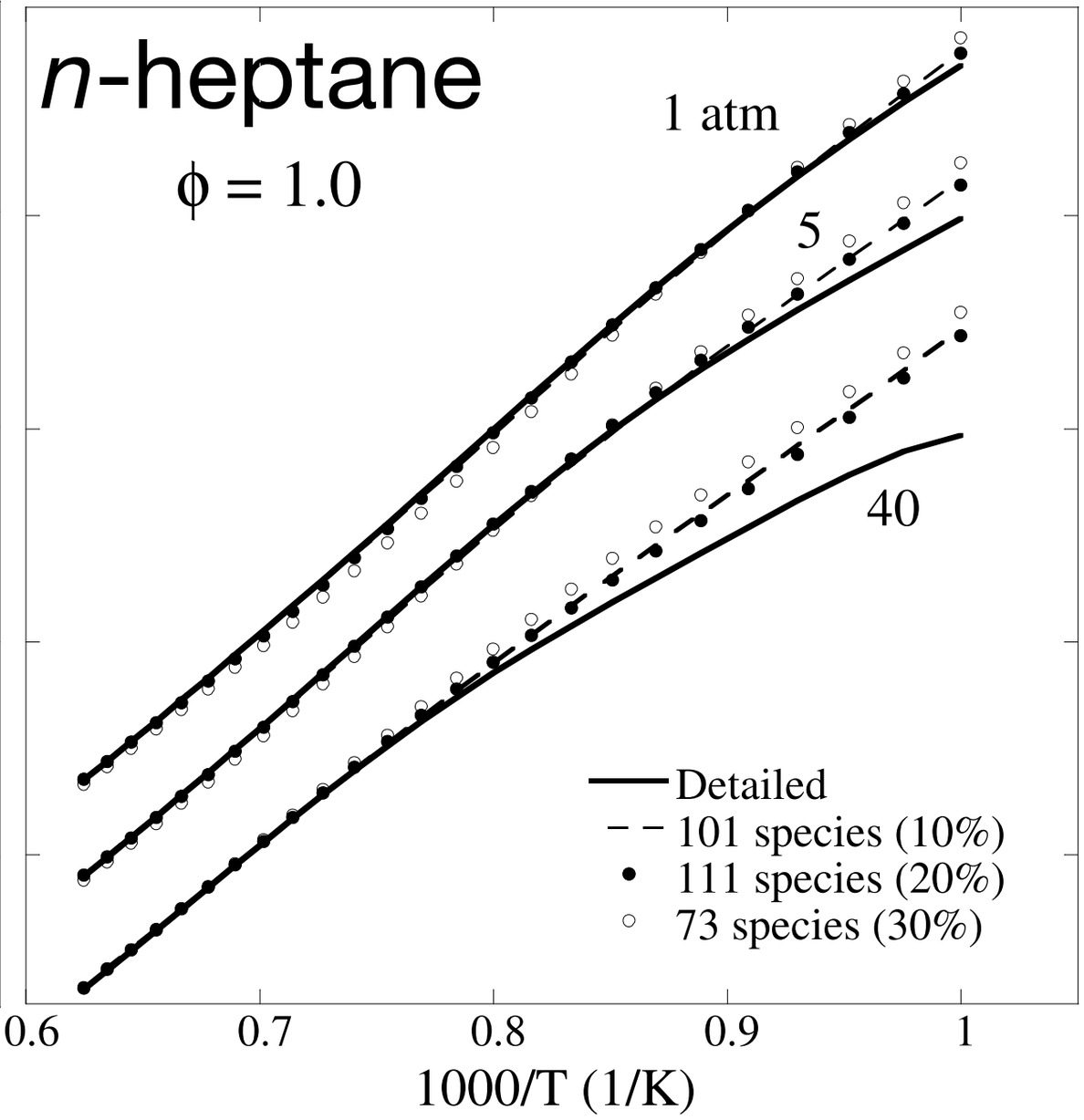
High-temp

Comprehensive-temperature Skeletal Mechanisms

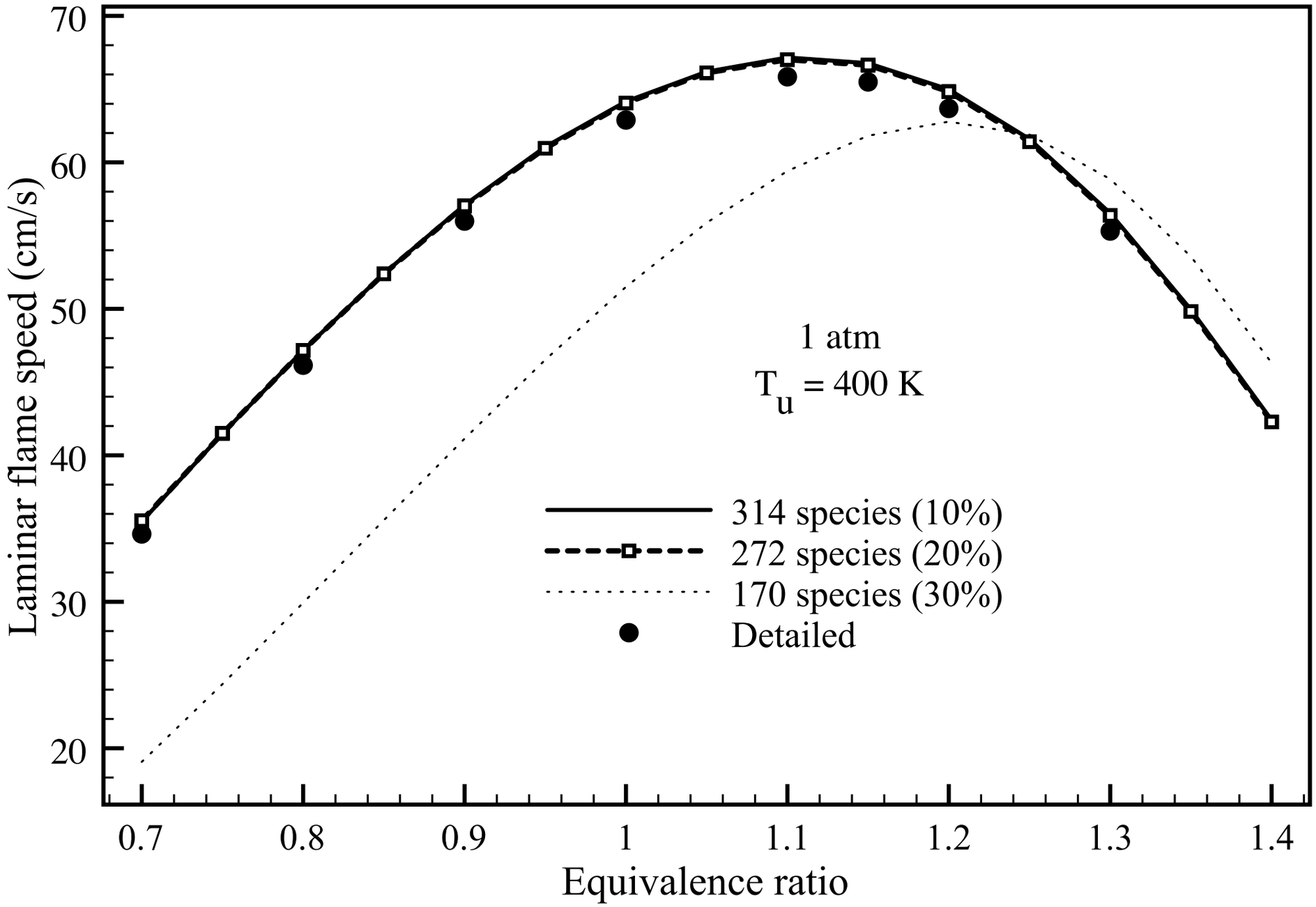


High-temperature Skeletal Mechanisms

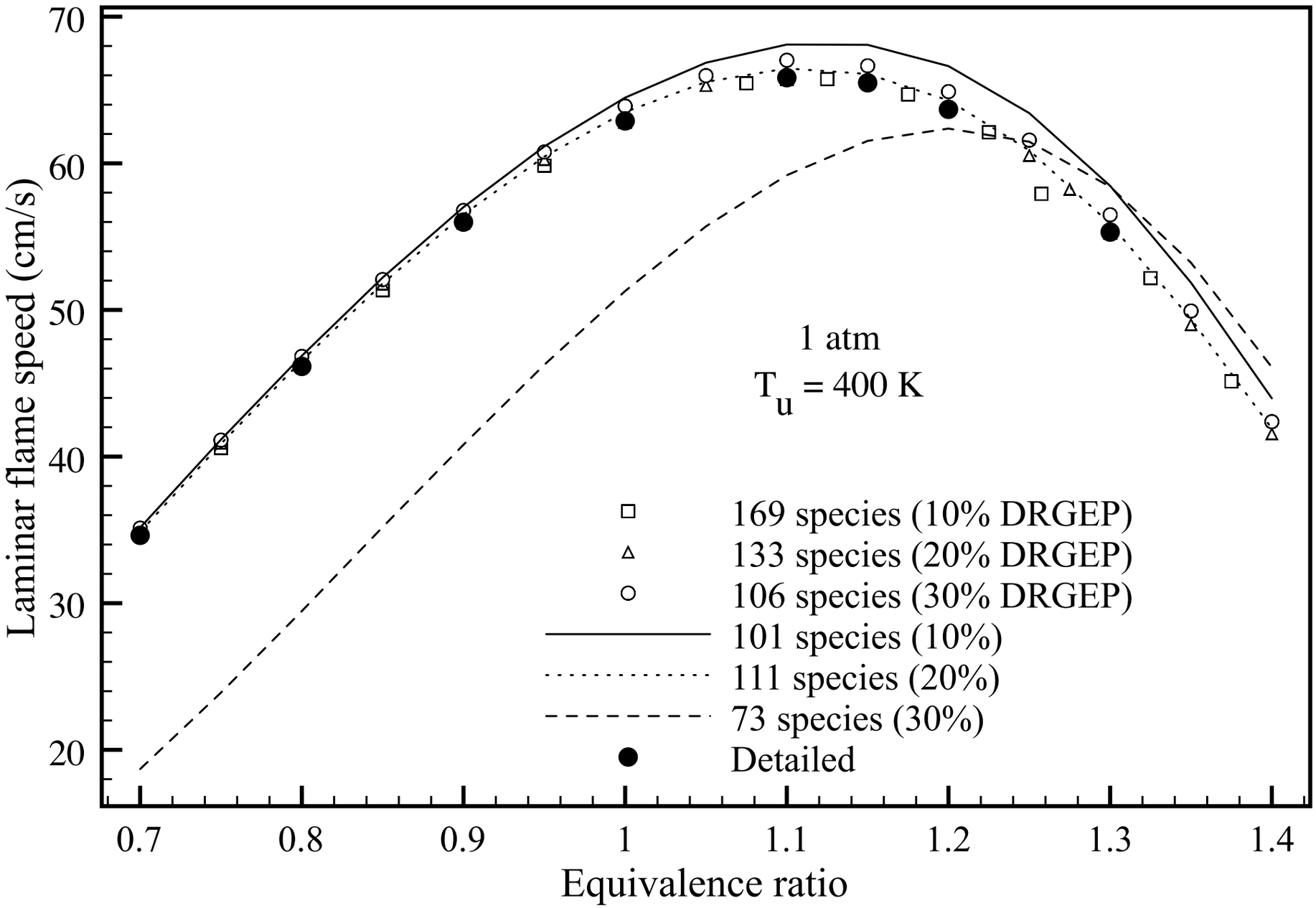




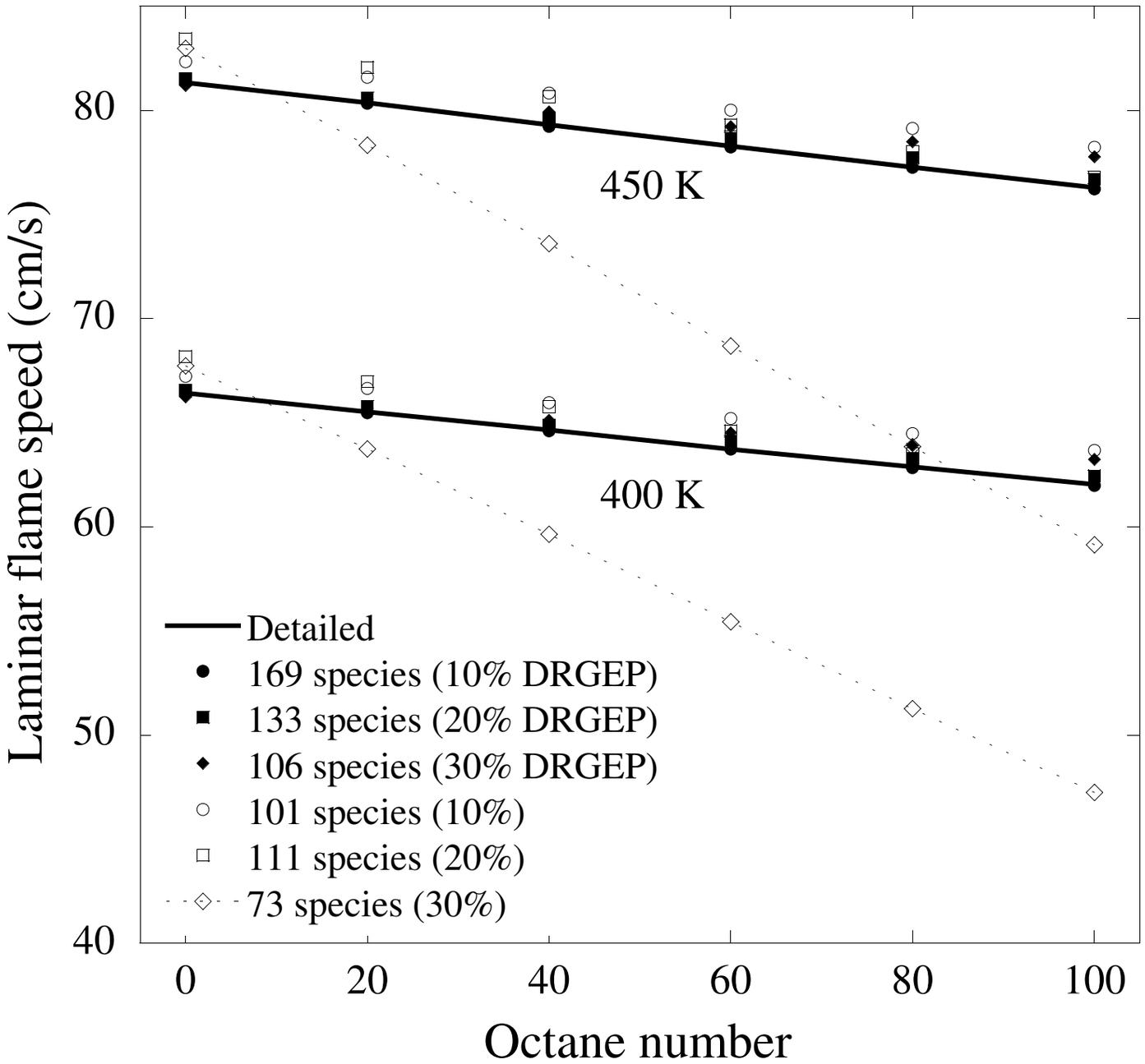
Laminar Flame Speed: Comprehensive-temperature



Laminar Flame Speed: High-temperature



Laminar Flame Speed: ON Variation



PRF Skeletal Mechanisms: Discussion

- Largest error in ignition delay in NTC region and at high pressure, low temperature for high-temperature mechanisms
- Both 30% skeletal mechanisms fail at lean equivalence ratios
  - Analysis of species removed by SA phase of DRGEPSA determined `ic3h5co` as necessary species removed

Conclusions

- Only Dijkstra's algorithm and RBFS produce species-order independent results
- Dijkstra's + coefficient scaling produces most compact skeletal mechanism for given error limit
- Skeletal mechanisms at various levels of detail presented for binary PRF
  - Validated using autoignition and flame propagation
  - Care must be taken at higher error limit

Future Work

- More complex multicomponent blends: toluene reference fuels (TRF)
  - Antagonistic mixture
- Further reduction stages: isomer lumping, diffusive species bundling
- DRGEP-based dynamic reduction

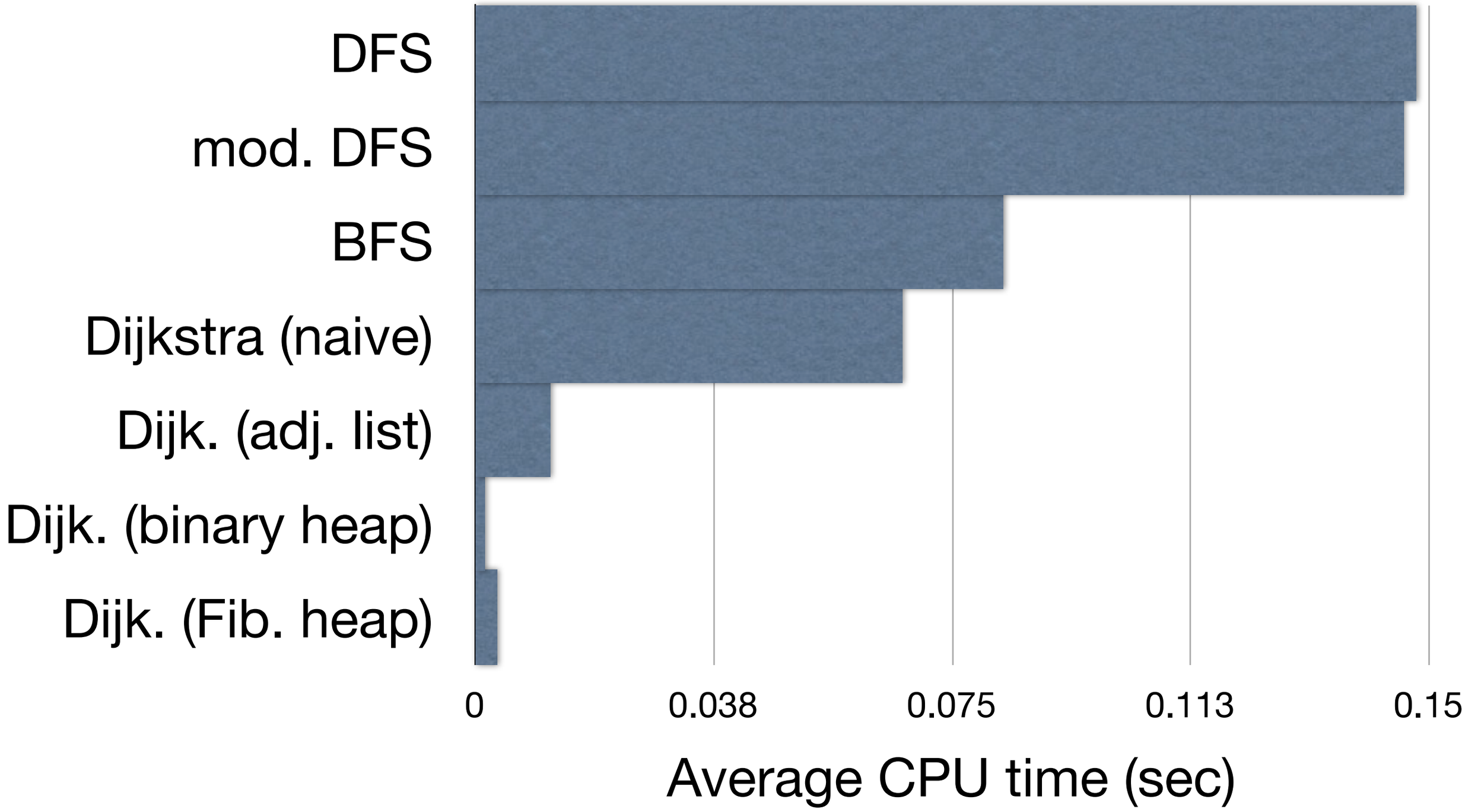
Acknowledgements

Funding sources:

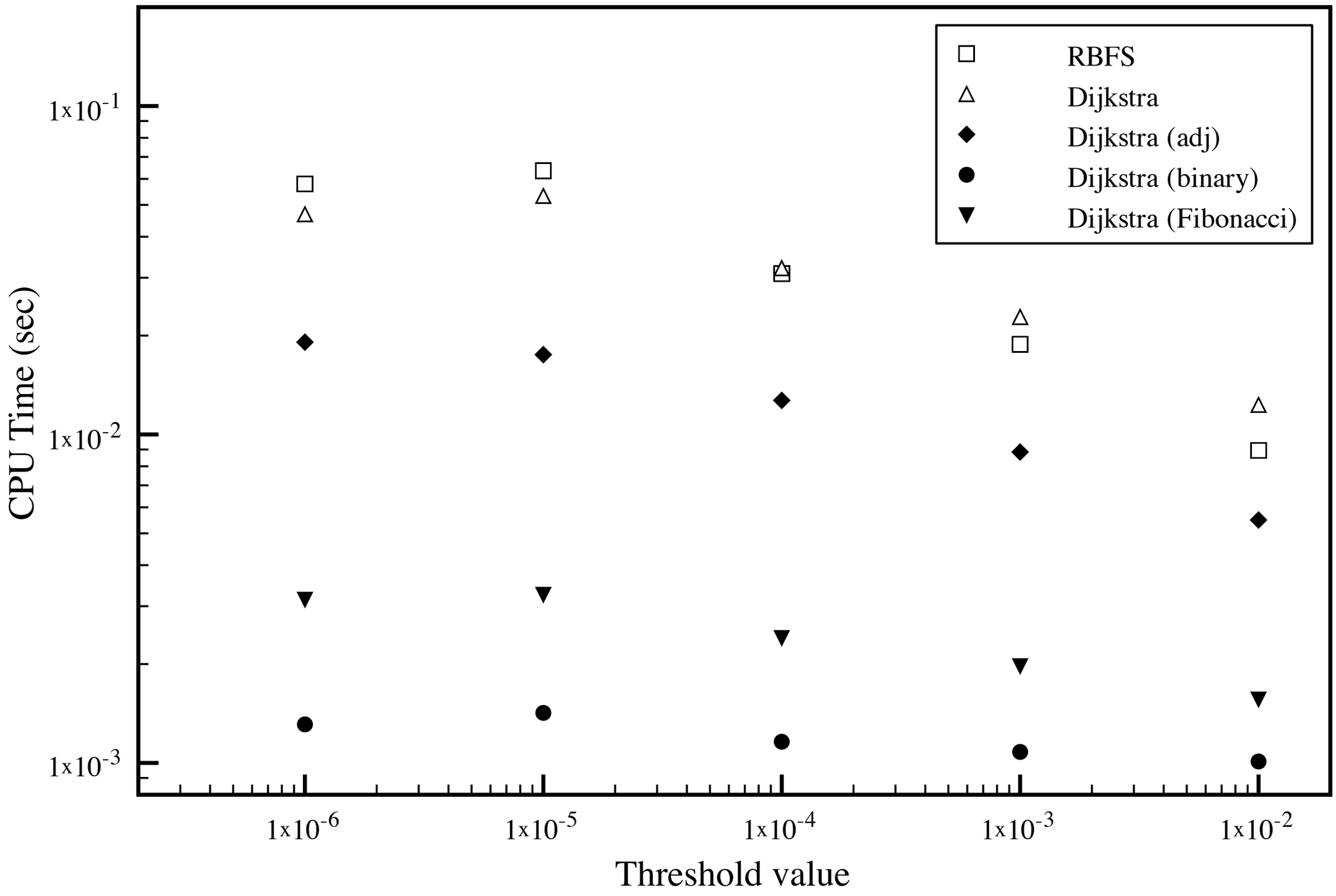
- NSF
- DOD through NDSEG Fellowship

Questions?

CPU Time (1)


DFS
mod. DFS
BFS
Dijkstra (naive)
Dijk. (adj. list)
Dijk. (binary heap)
Dijk. (Fib. heap)
0
0.038
0.075
0.113
0.15
Average CPU time (sec)

CPU Time (2)


RBFS
Dijkstra
Dijkstra (adj)
Dijkstra (binary)
Dijkstra (Fibonacci)
CPU Time (sec)
1x10-1
1x10-2
1x10-3
1x10-6
1x10-5
1x10-4
1x10-3
1x10-2
Threshold value