Enabling next-generation combustion simulations by intelligent integration

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https://git.io/nrg

Today's talk

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- Describe our efforts to reduce associated expense on modern computing architectures
- Summarize other current projects

Acknowledgements

Students

AJ Fillo

Matt Zaiger

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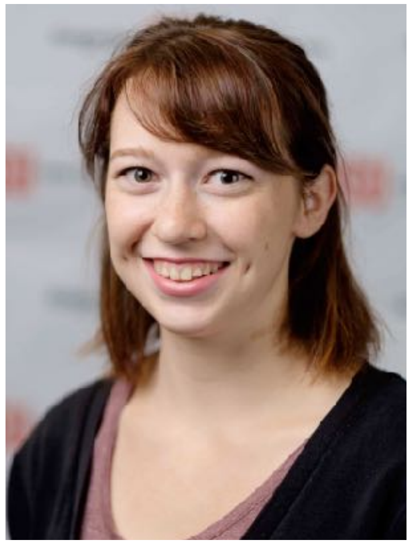
Andrew Alferman

Tejas Mulky



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Collaborators

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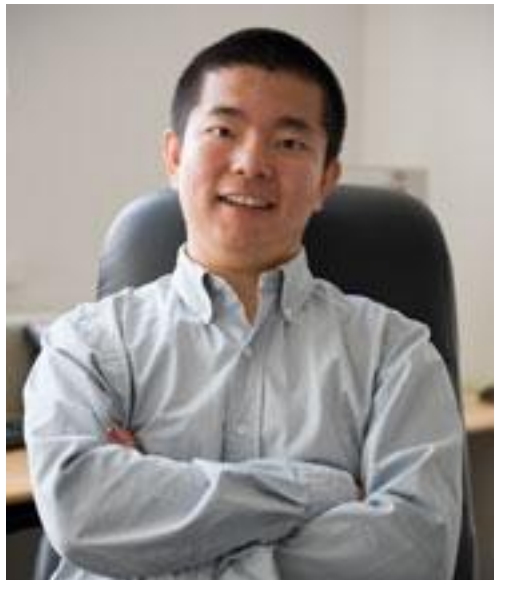
Collaborators

Bryan Weber, UConn

Peter Hamlington, CU Boulder



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DOD · EPA · DOE

Chevron

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DEPARTMENT OF ENERGY · UNITED STATES OF AMERICA ·

NETL

NASA

Challenge

Performing predictive simulations of reactive flows

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... in a **reasonable** amount of time

Challenge

Recent LES of diesel spray with 54-species *n*-dodecane model[1]:

[1]A. A. Moiz et al. *Combust. Flame* 173 (2016): 123–131. doi:10.1016/j.combustflame.2016.08.005

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48,000 CPU core-hours for 2 ms after start of injection

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What drives costs?

What drives costs?

Stiffness

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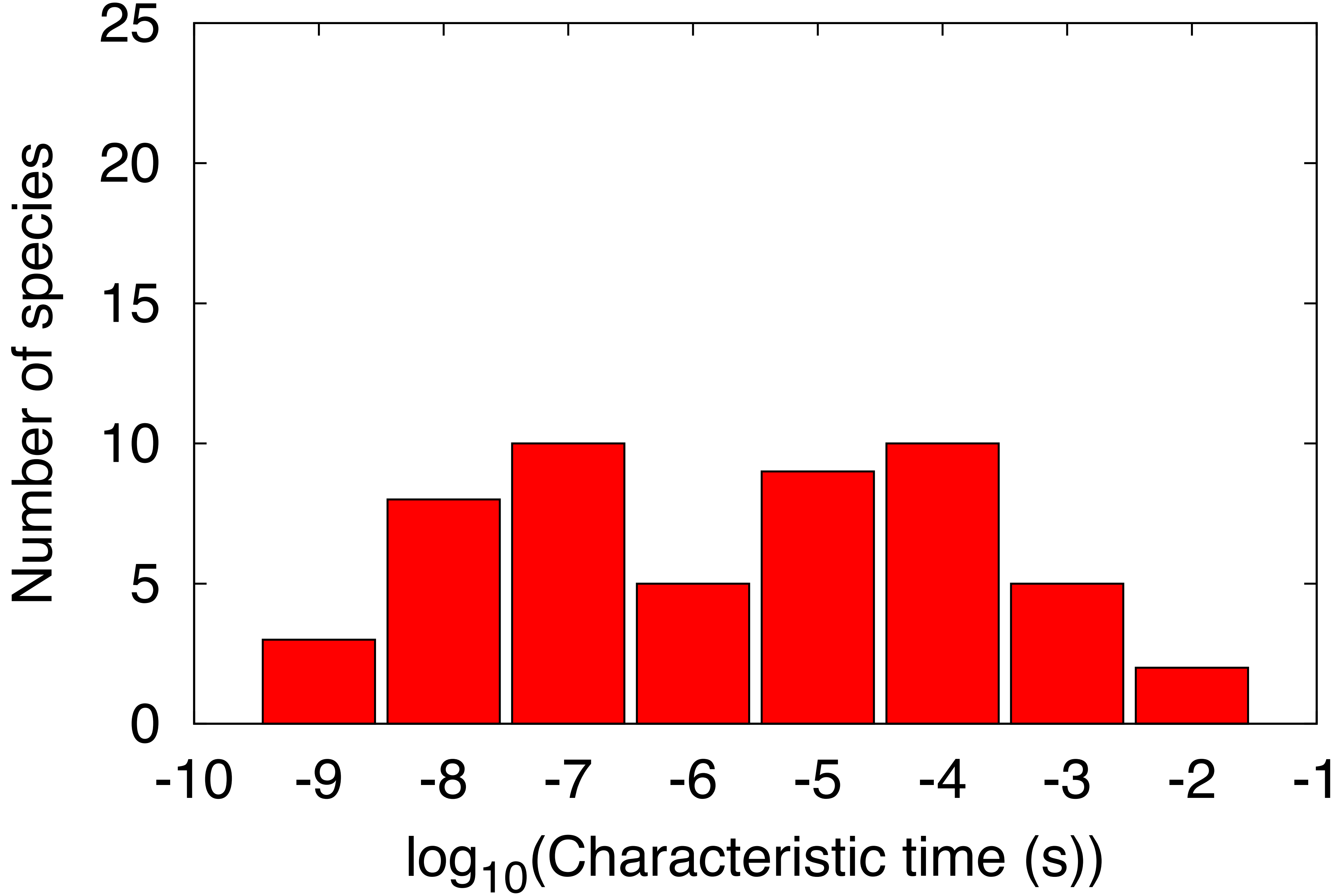
Stiffness

Size

Kinetic models exhibit high stiffness:



Characteristic creation times of methane oxidation[2]

[2]K. E. Niemeyer, N. J. Curtis, & C. J. Sung. Fall 2015 Meeting of the West. States Sect. Combust. Inst. Provo, UT, USA, Oct. 2015. doi:10.6084/m9.figshare.2075515.v1

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- Traditionally requires implicit integration algorithms

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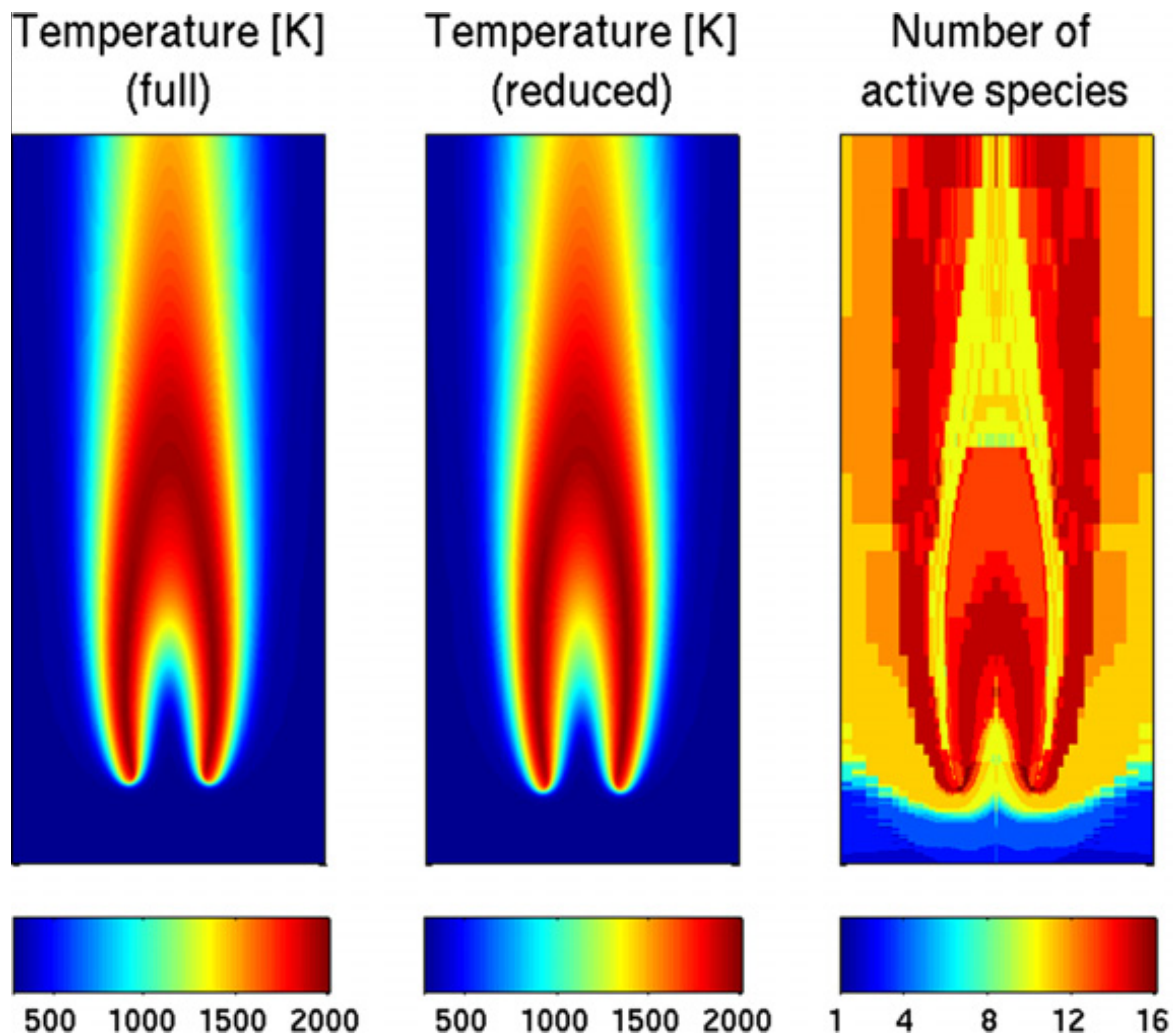

Dynamic adaptive chemistry approach of Tosatto et. al, studying a 2-D diluted JP-8 flame[3]

[3] L. Tosatto, B. Bennett, & M. Smooke. *Combust. Flame* 158.5 (2011):820–835. doi:10.1016/j.combustflame.2011.01.018

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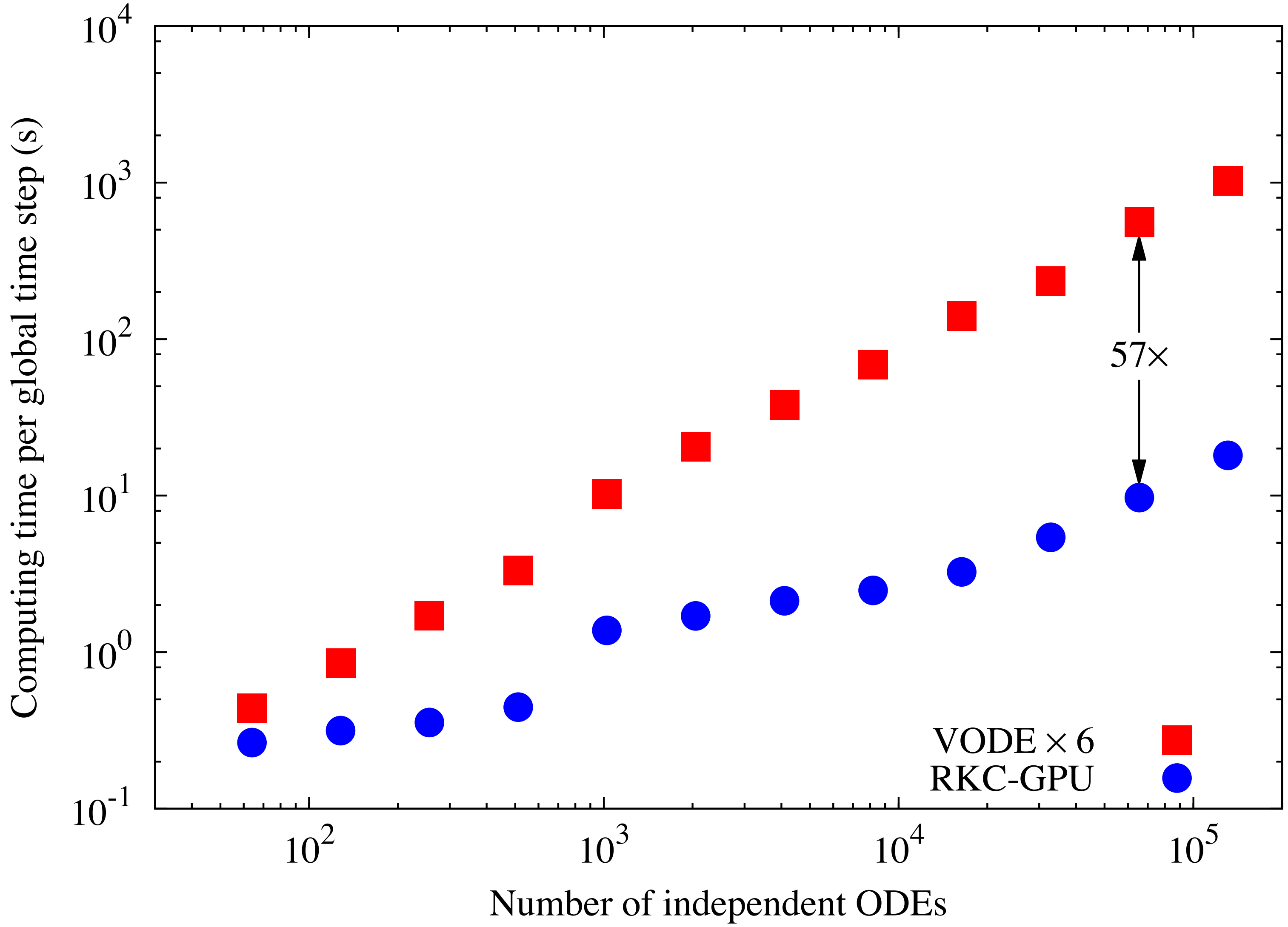

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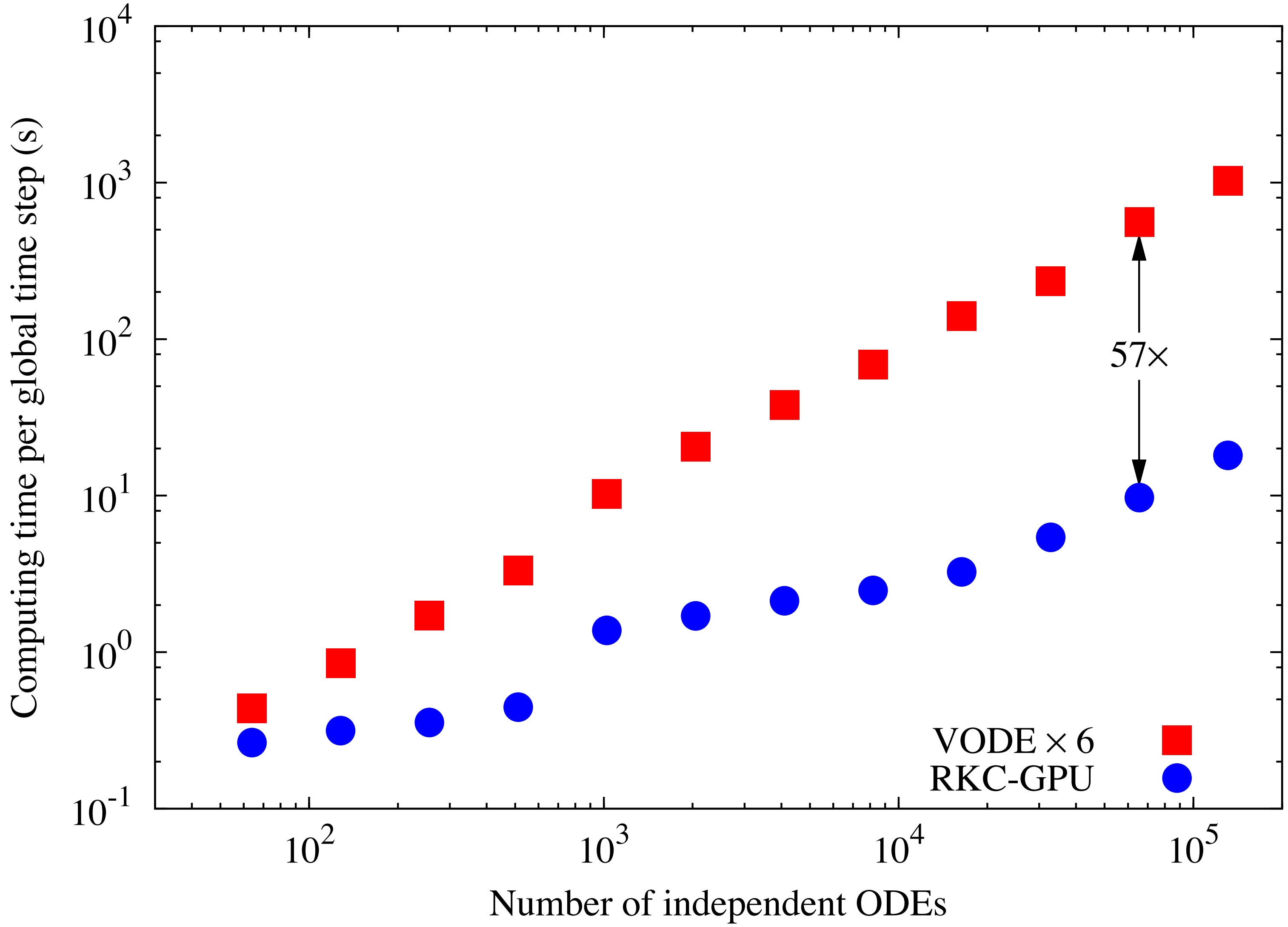

For less-stiff chemistry, stabilized-explicit or semi-implicit solvers may be **much** faster[4]

[4]K. E. Niemeyer & C. J. Sung. *J. Comput. Phys.* 256 (2014), pp. 854–871. doi:10.1016/j.jcp.2013.09.025

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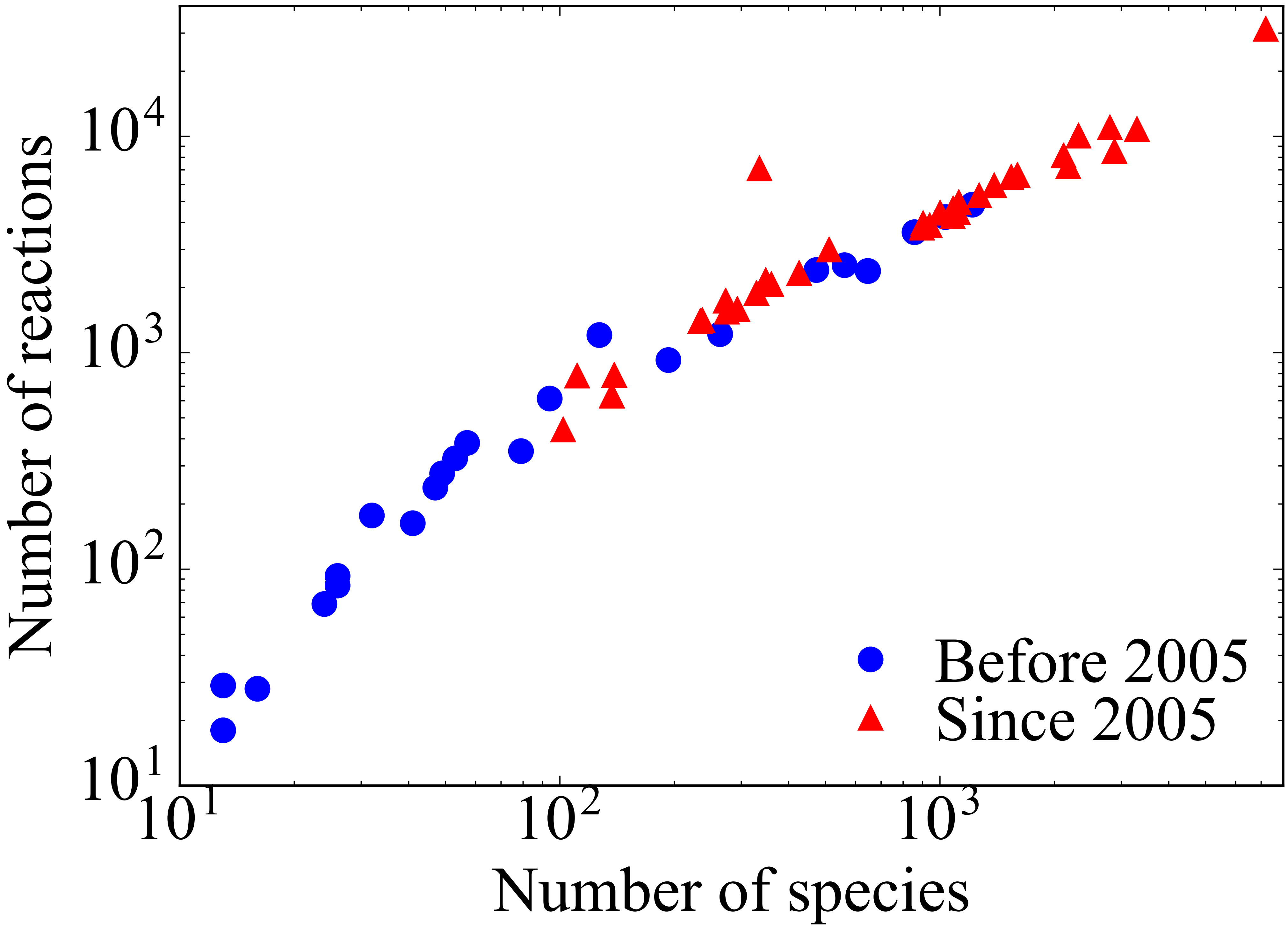
Kinetic model sizes have grown in recent years:



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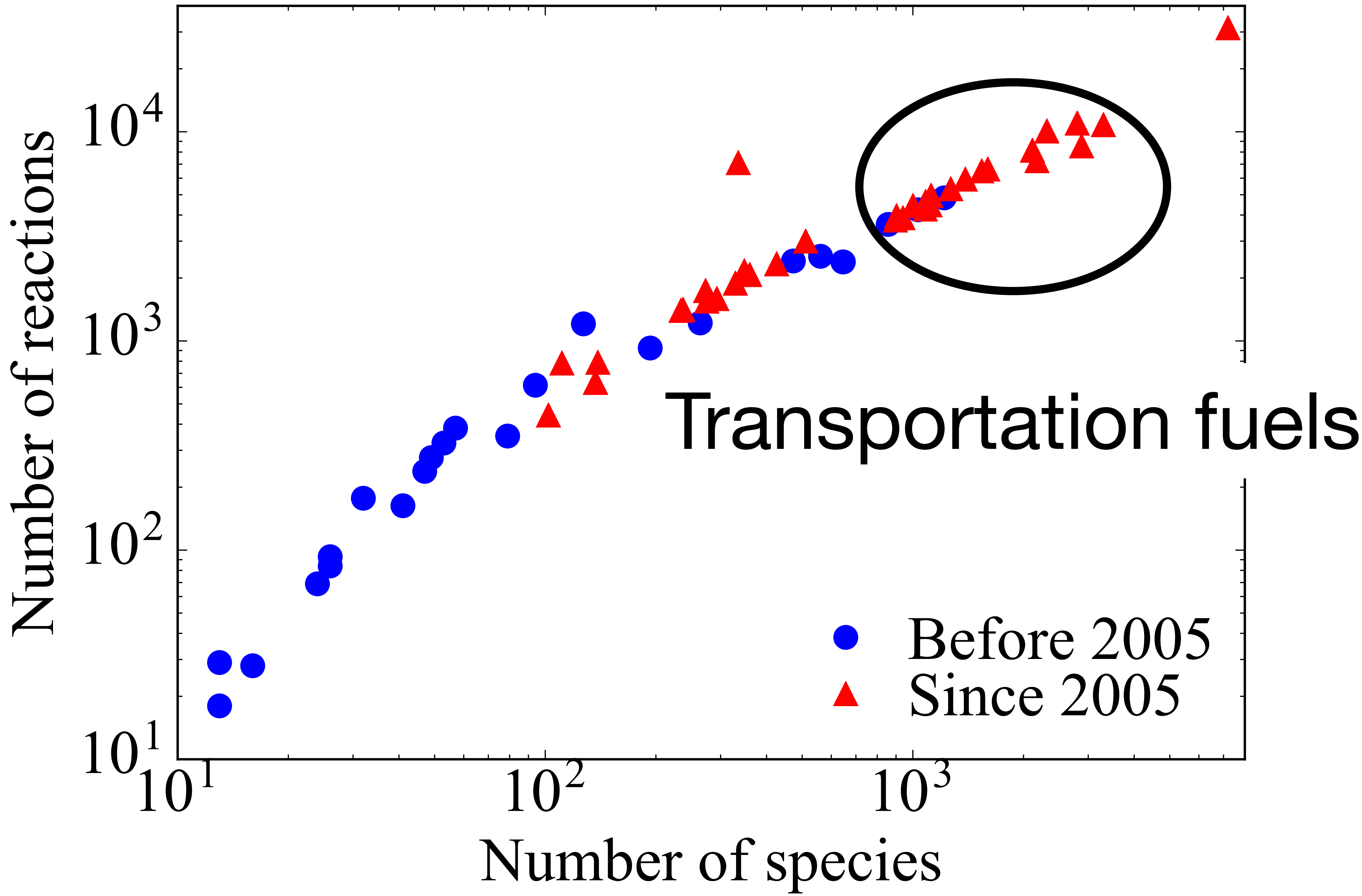

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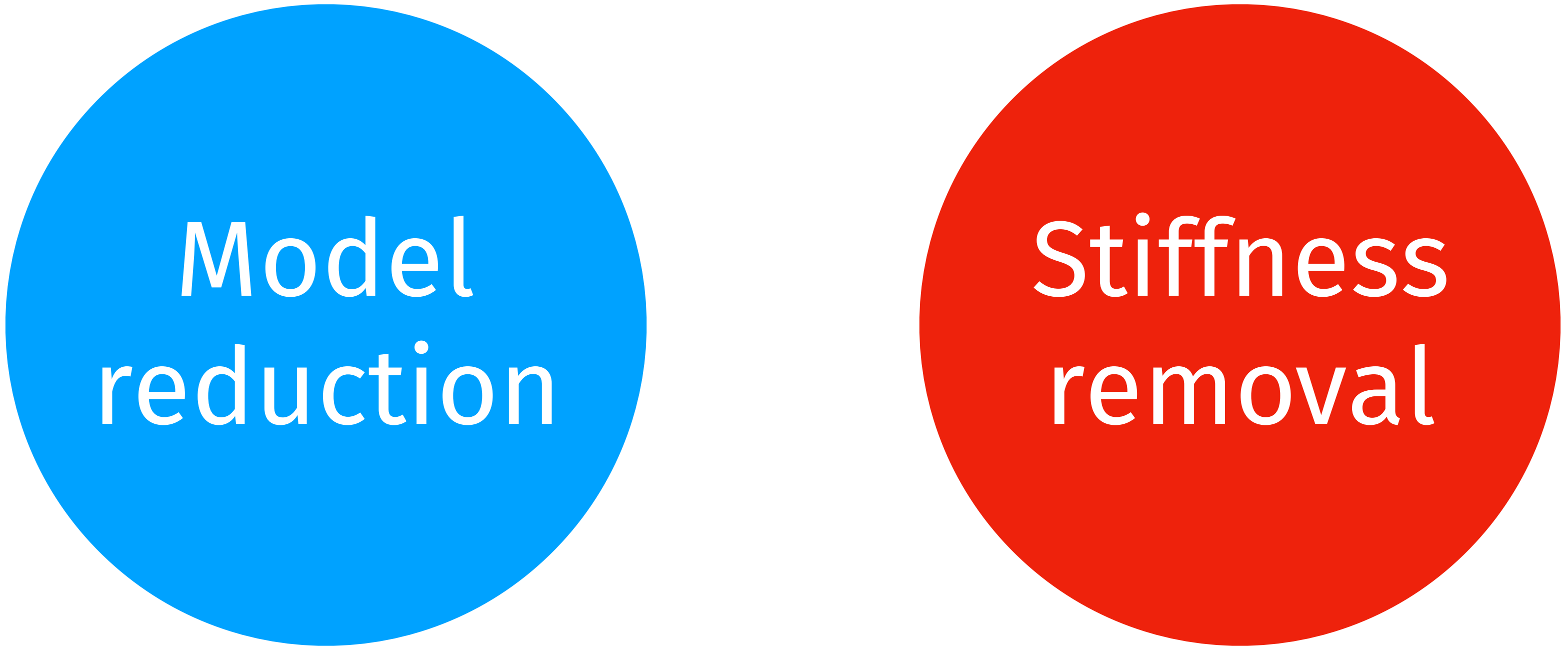

Cost reduction

Model reduction

Stiffness removal

Tabulation

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Integration algorithms

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Speedup may be achieved with a **sparse, analytical** Jacobian formulation

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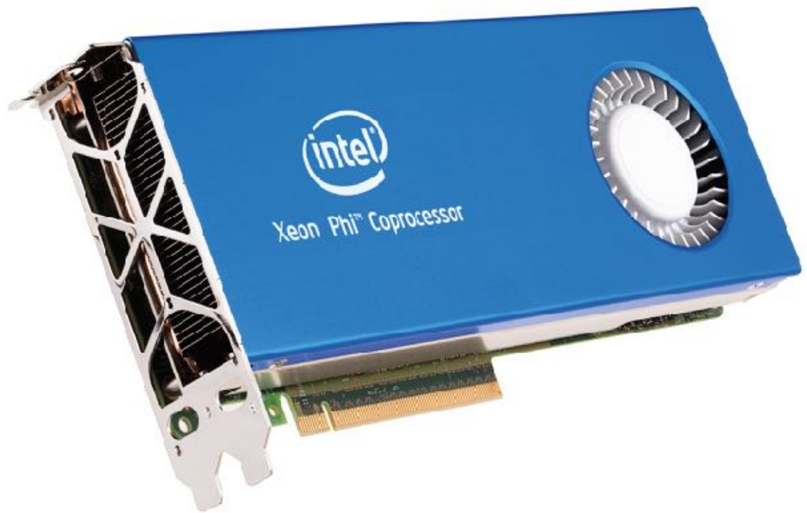

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http://slackha.github.io/

https://github.com/SLACKHA

`pyJac`: analytical chemical kinetic Jacobian generator

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- Python wrapper creation for (relatively) easy access

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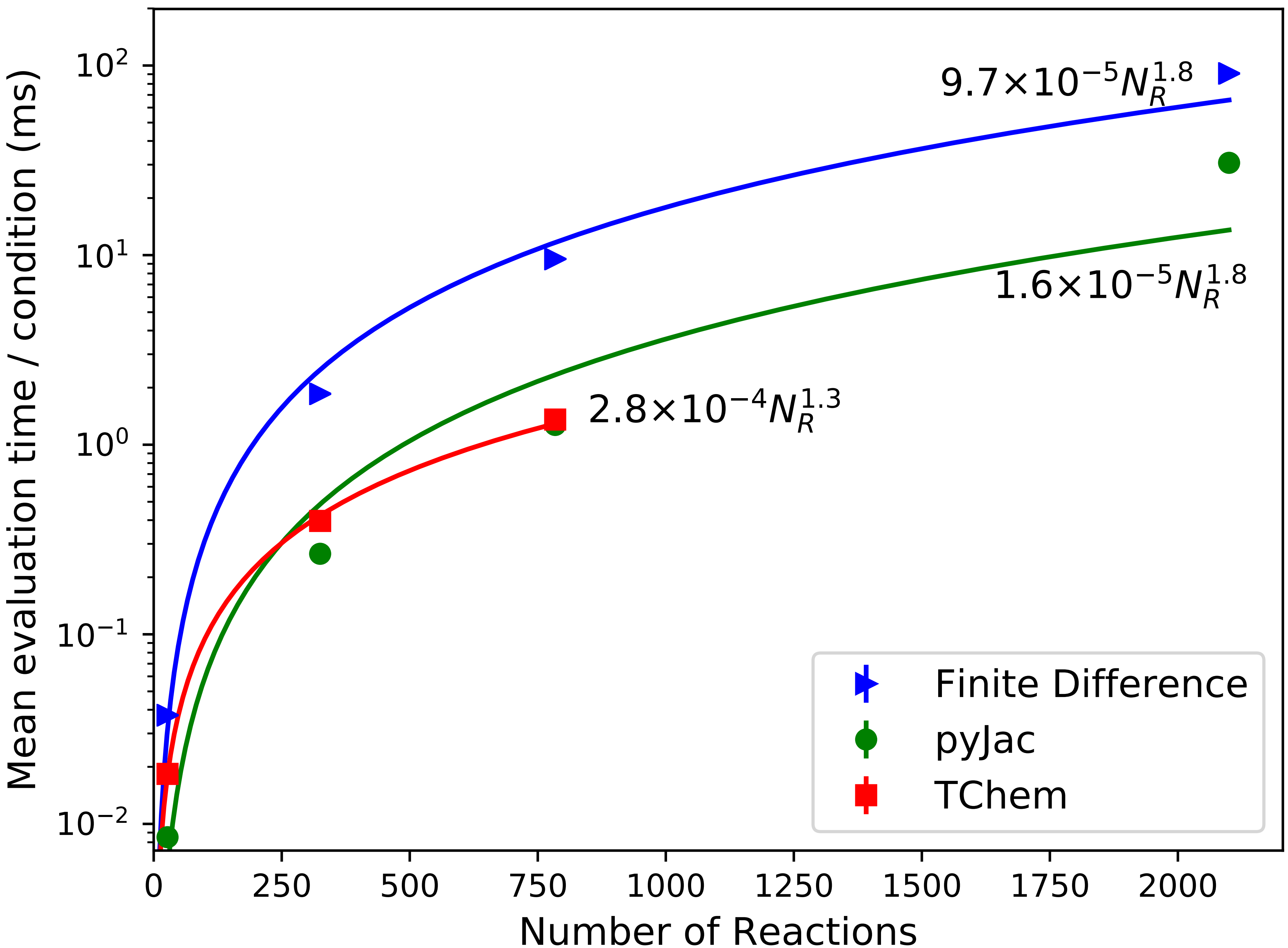

Performance comparison with finite differences and TChem[6]

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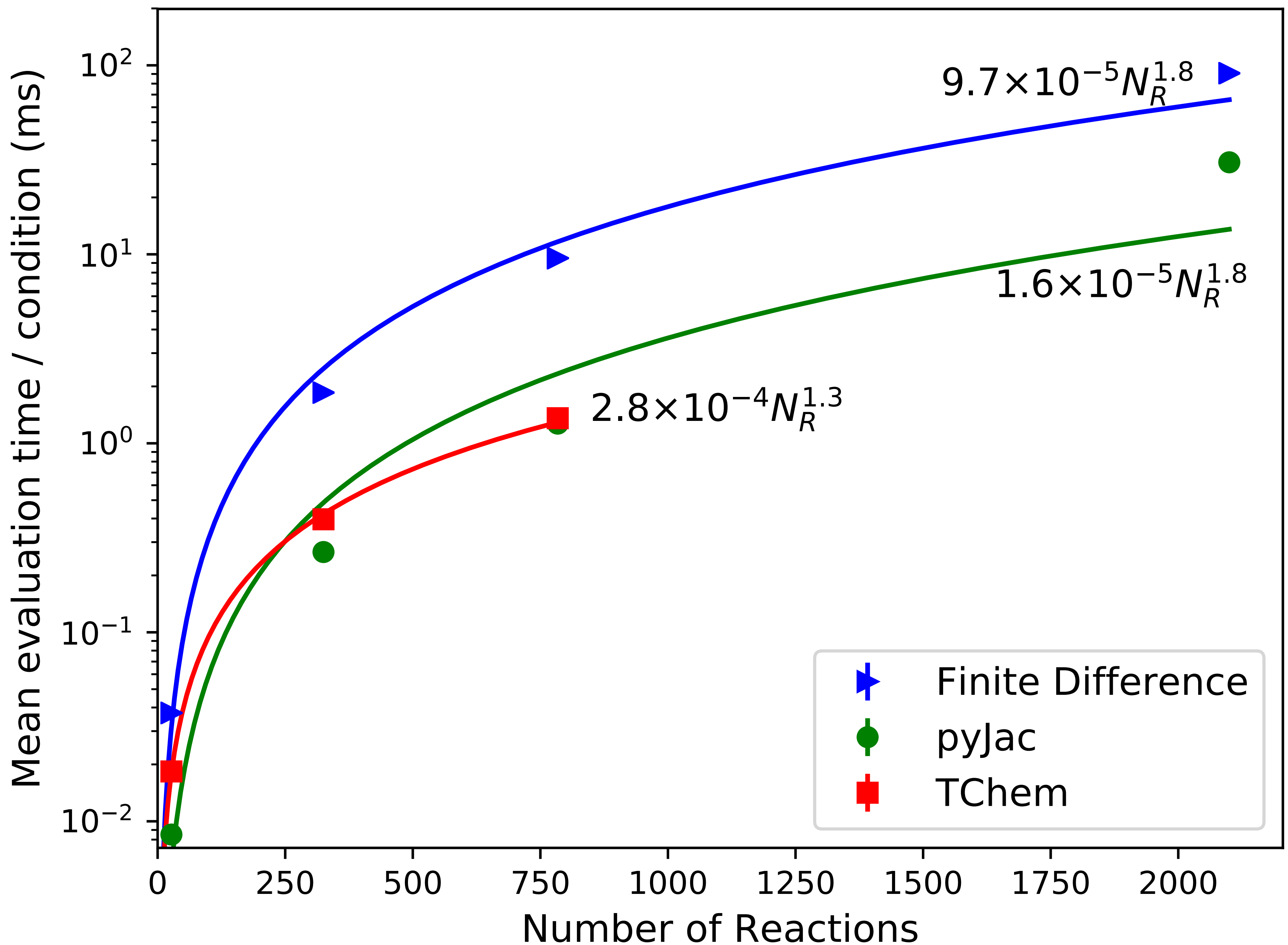

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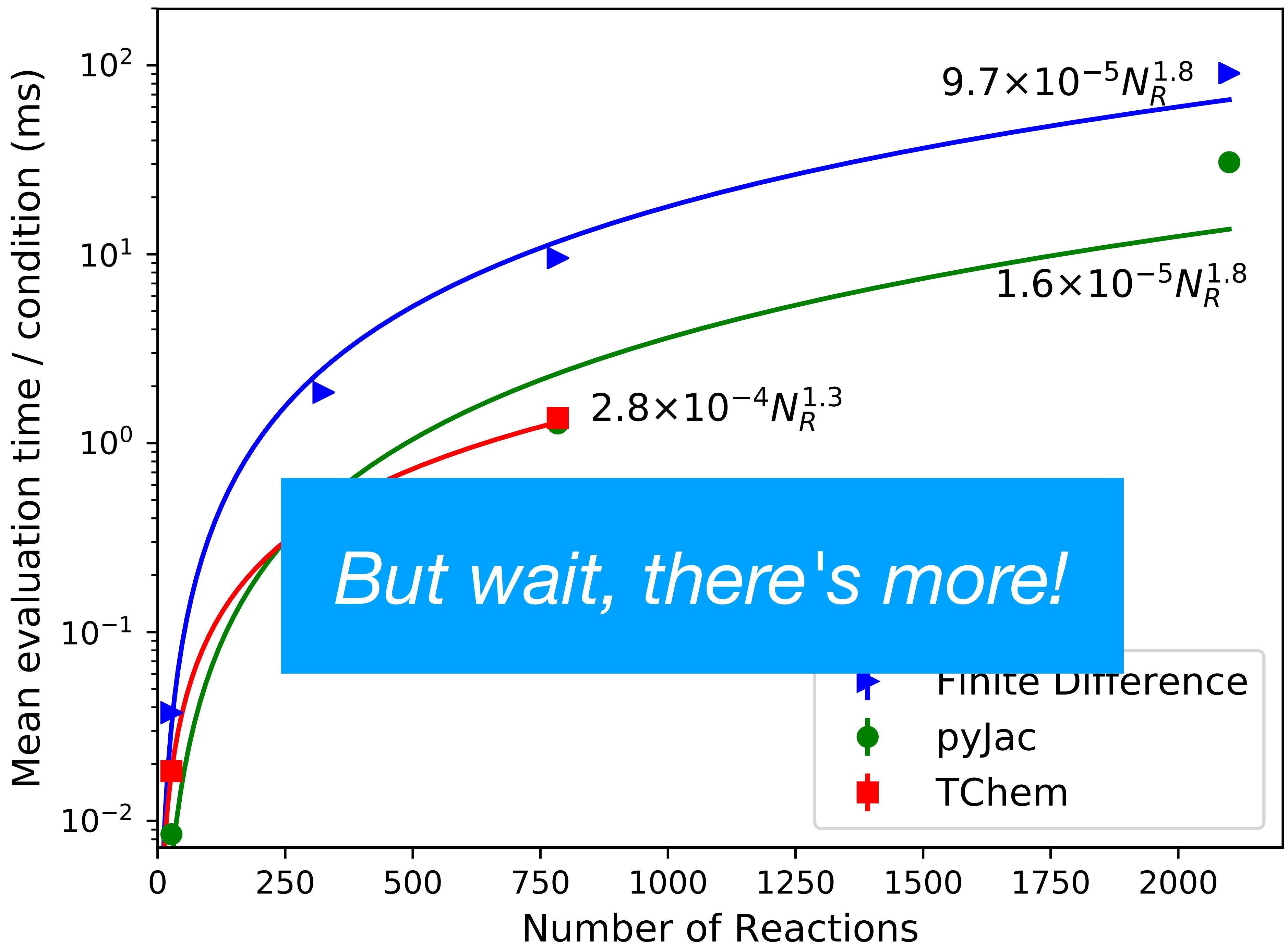

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- Both wide ("per-thread") and deep ("per-block") vectorization pursued to provide more flexible options for ODE integration

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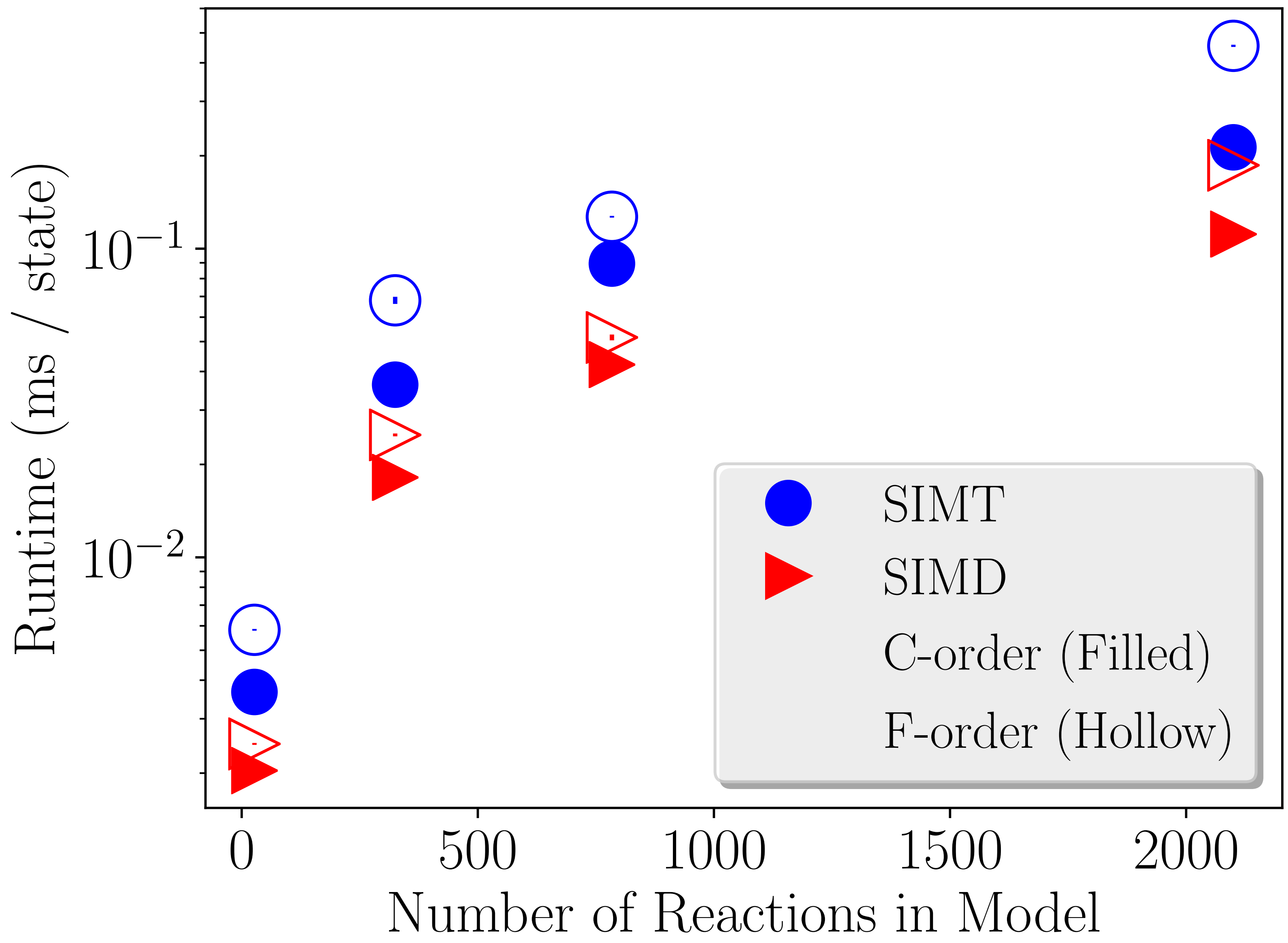
pyJac v2 vectorized rate evaluation



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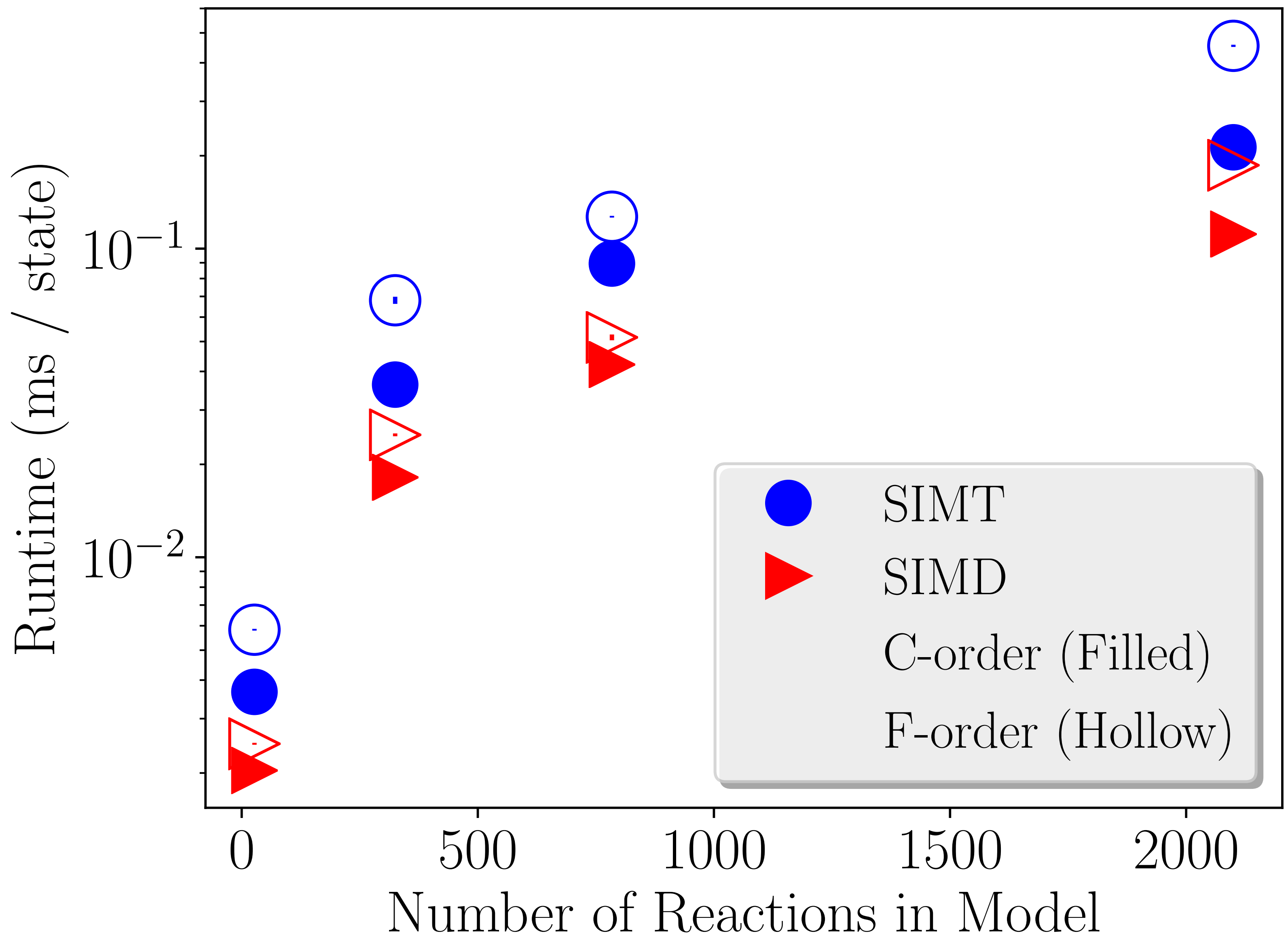

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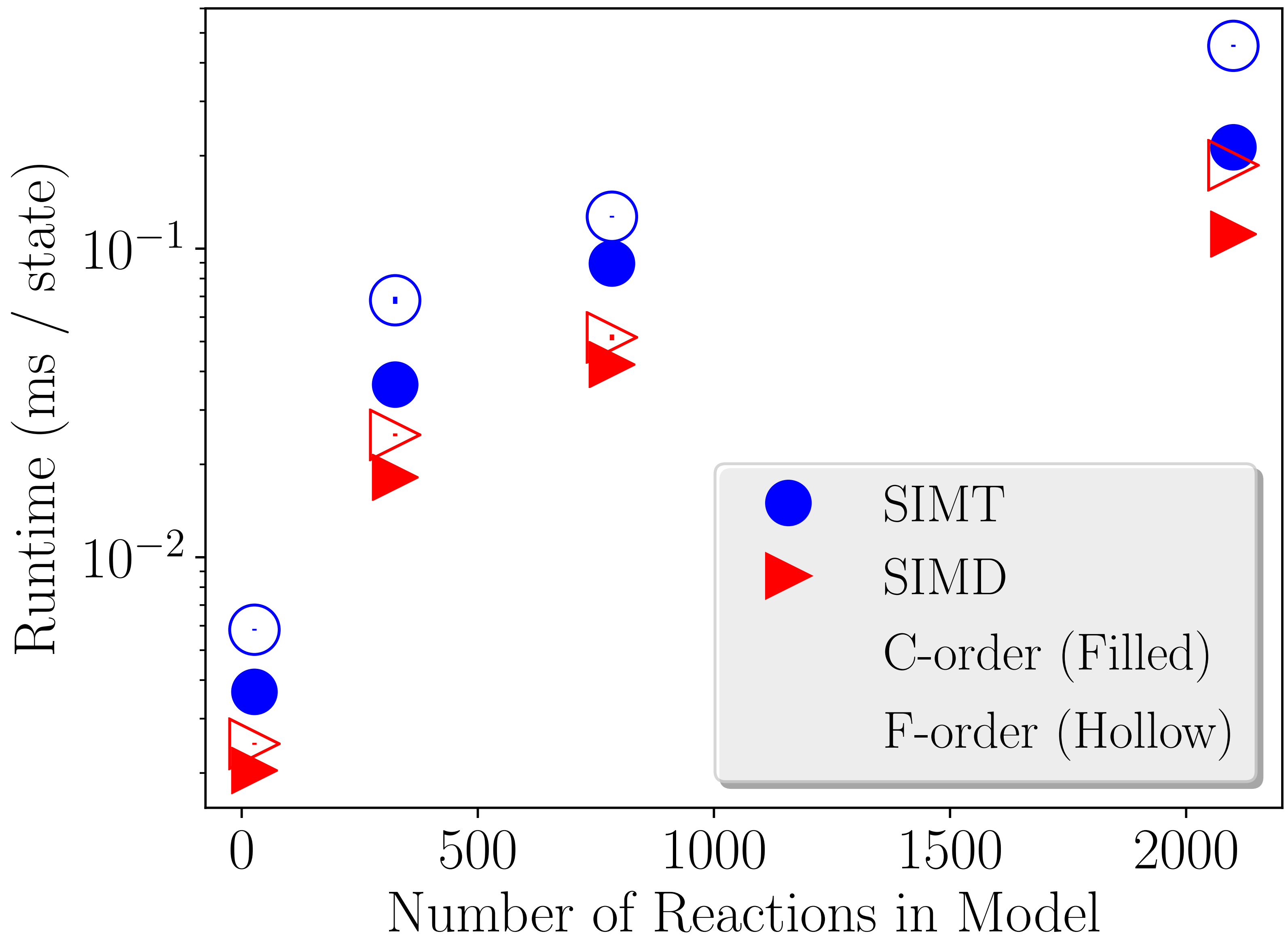

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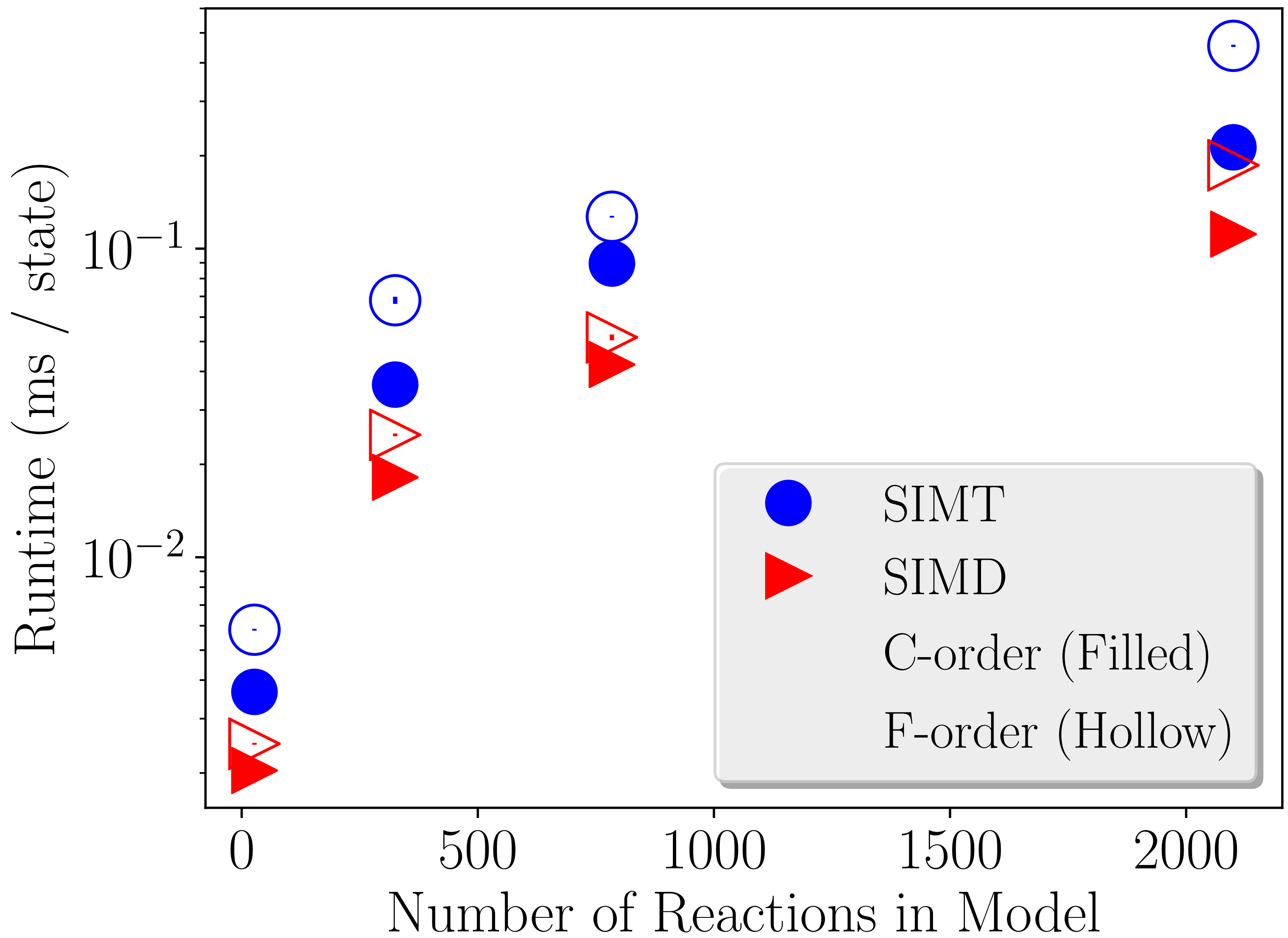

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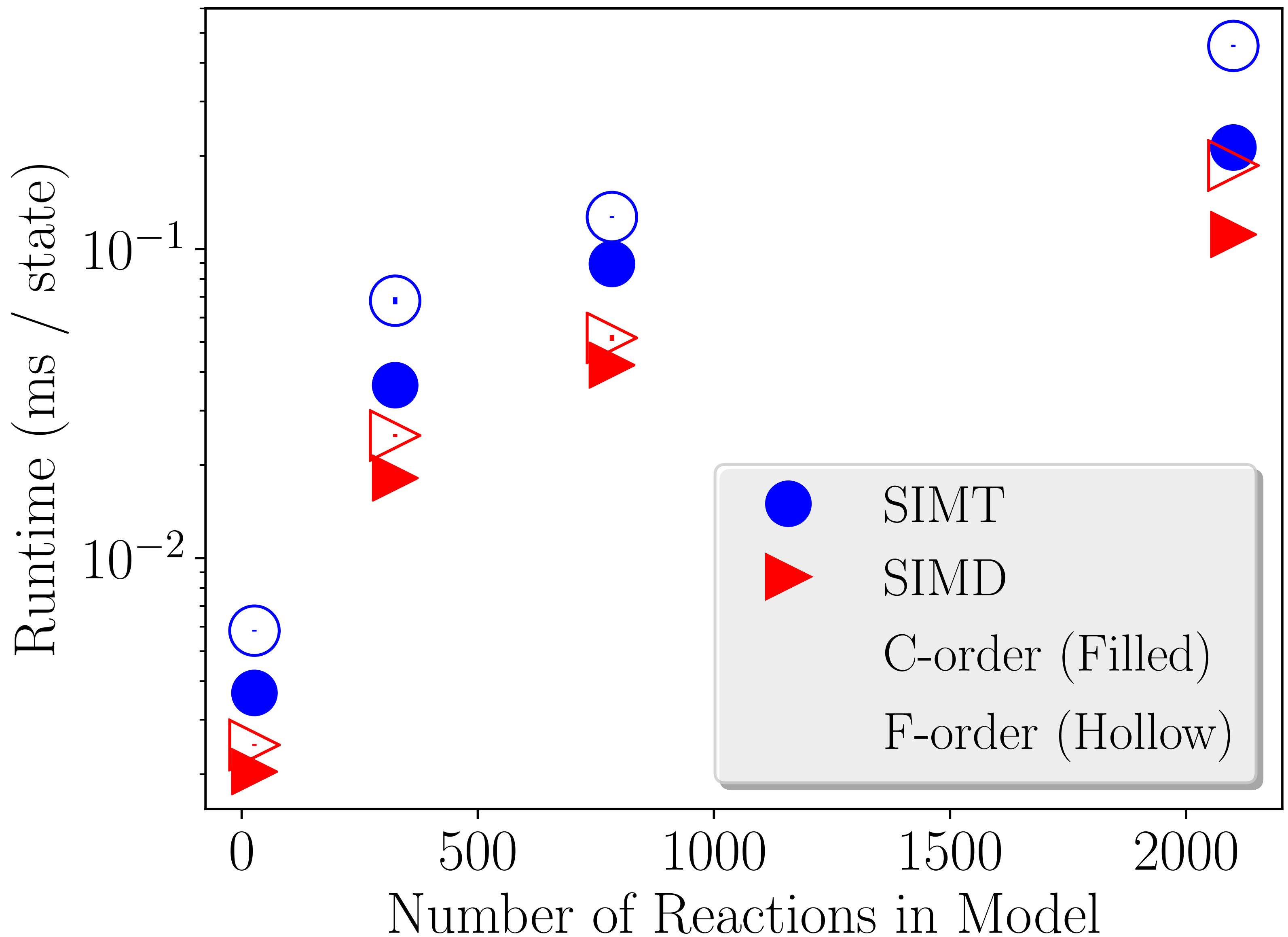

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- SIMD-vectorized code up to 1.99–2.72 × faster than non-vectorized baseline

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[8]N. J. Curtis, K. E. Niemeyer, & C. J. Sung. *Combust. Flame* 179 (2017):312–324. doi:10.1016/j.combustflame.2017.02.005

`accelerInt`: available solvers

Integrator	Type	Order	CPU	GPU
CVODE[9]	Variable-order BDF	Variable (max 5th)	×	–
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[10] G. Wanner & E. Hairer. *Solving Ordinary Differential Equations II*. 2nd ed. Springer-Verlag, Berlin, 1996. doi:10.1007/978-3-642-05221-7

[11] M. Hochbruck, C. Lubich, & H. Selhofer. *SIAM J. Sci. Comput*. 19.5 (1998):1552–1574. doi:10.1137/S1064827595295337

[12] M. Hochbruck, A. Ostermann, & J. Schweitzer. *SIAM J. Numer. Anal*. 47.1 (2009):786–803. doi:10.1137/080717717

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- Addition of linearly-implicit methods (Rosenbrock) and (potentially) hybrid implicit/explicit solvers

Stiffness characterization

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- **Goal**: reliable stiffness metric to switch between integration algorithms based on state & hardware

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- Currently: evaluate existing stiffness metrics using realistic, sampled PaSR state data

Stiffness ratio

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LeVeque, R. J. *Finite Difference Methods for Ordinary and Partial Differential Equations*. (2007)
doi:10.1137/1.9780898717839

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$$\text{ratio} = \frac{\max|\lambda_p|}{\min|\lambda_p|}$$

$$\lambda_p = \text{eigenvalue of Jacobian}$$

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Shampine stiffness index

$$\text{index} = \rho[f_y(x_n, y(x_n))]\|y^{(p+1)}(x_n)\|^{-1/(p+1)}$$

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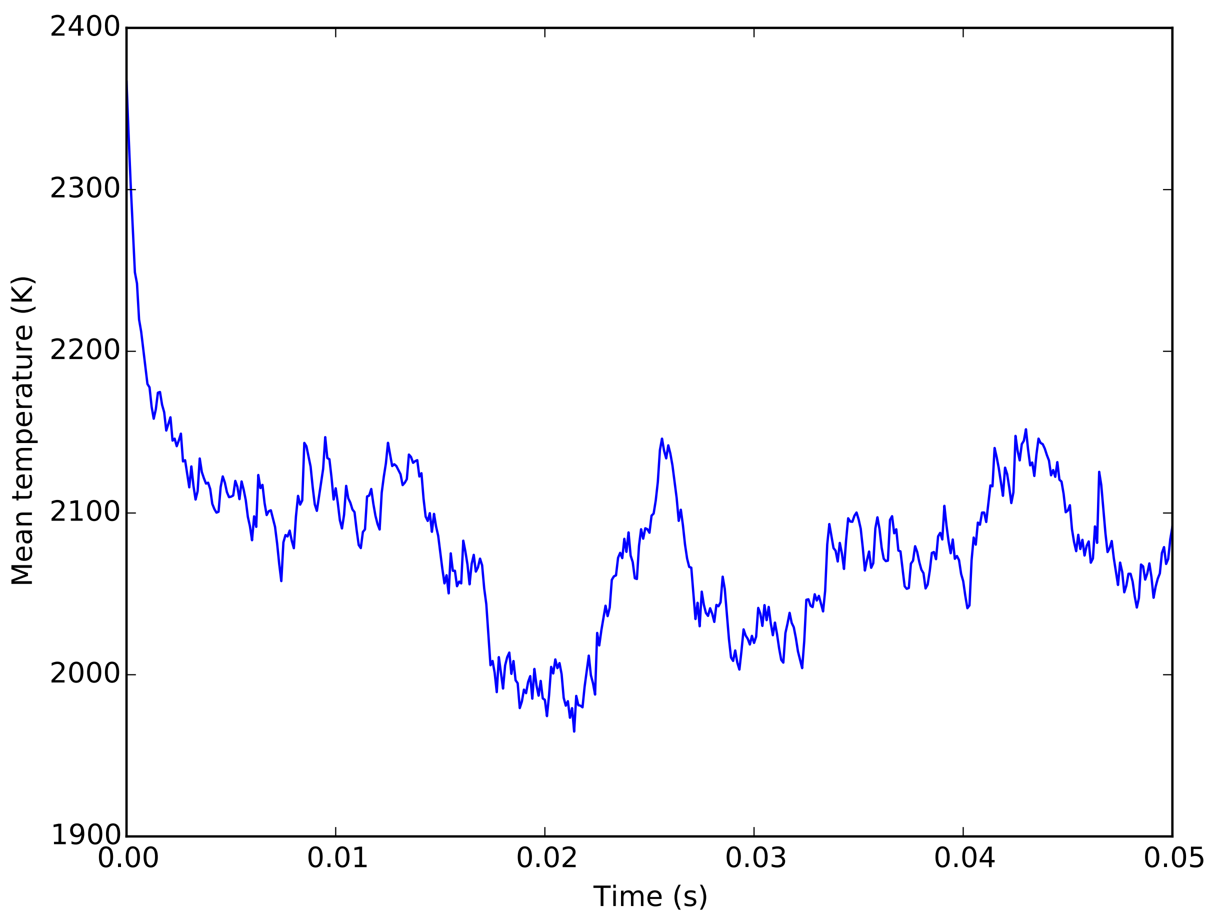
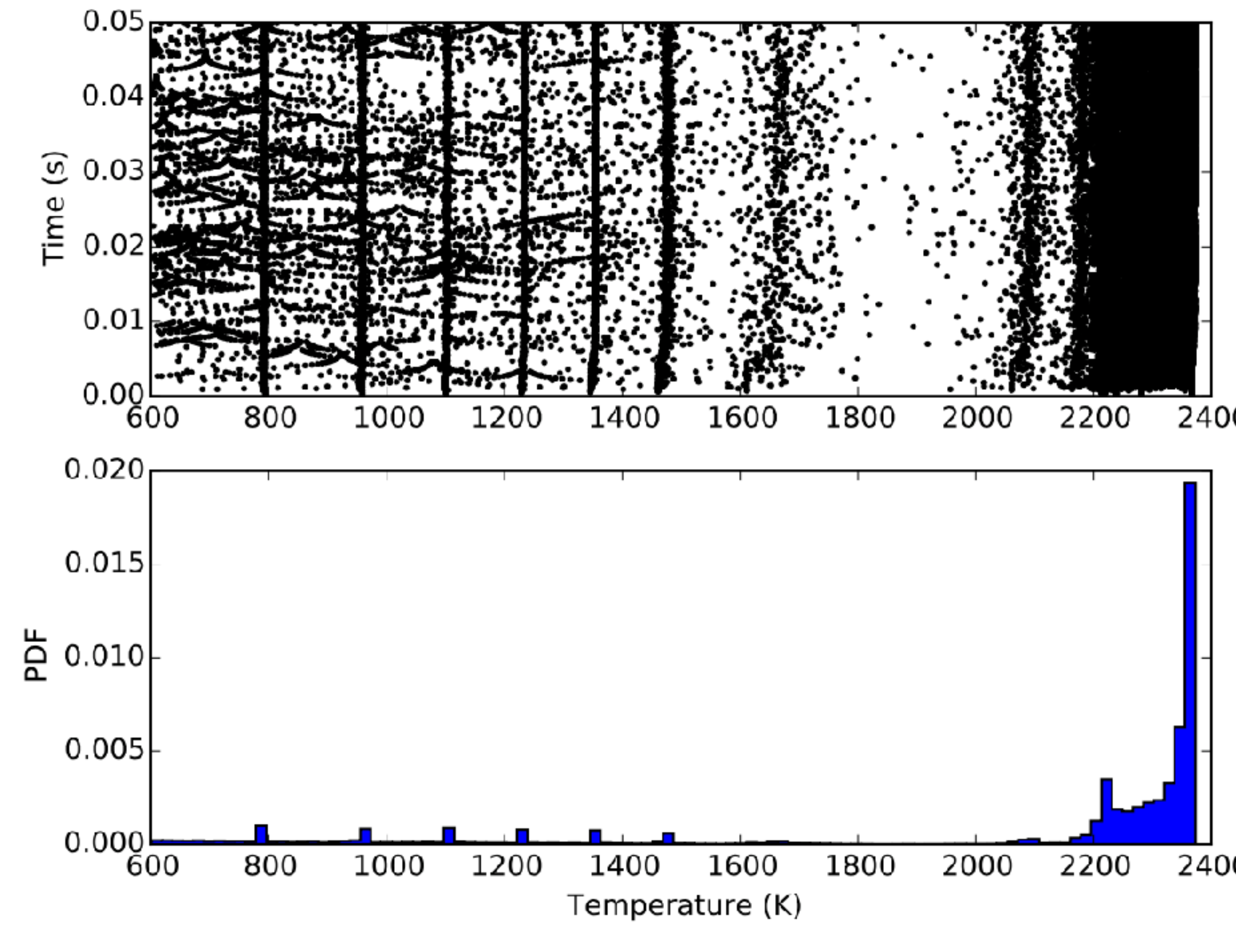
Partially Stirred Reactor (PaSR)





- Cantera-based PaSR implementation; premixed combustion with fresh fuel/air mixture & pilot streams
- Pairwise mixing, reaction fractional steps, inflow/outflow events

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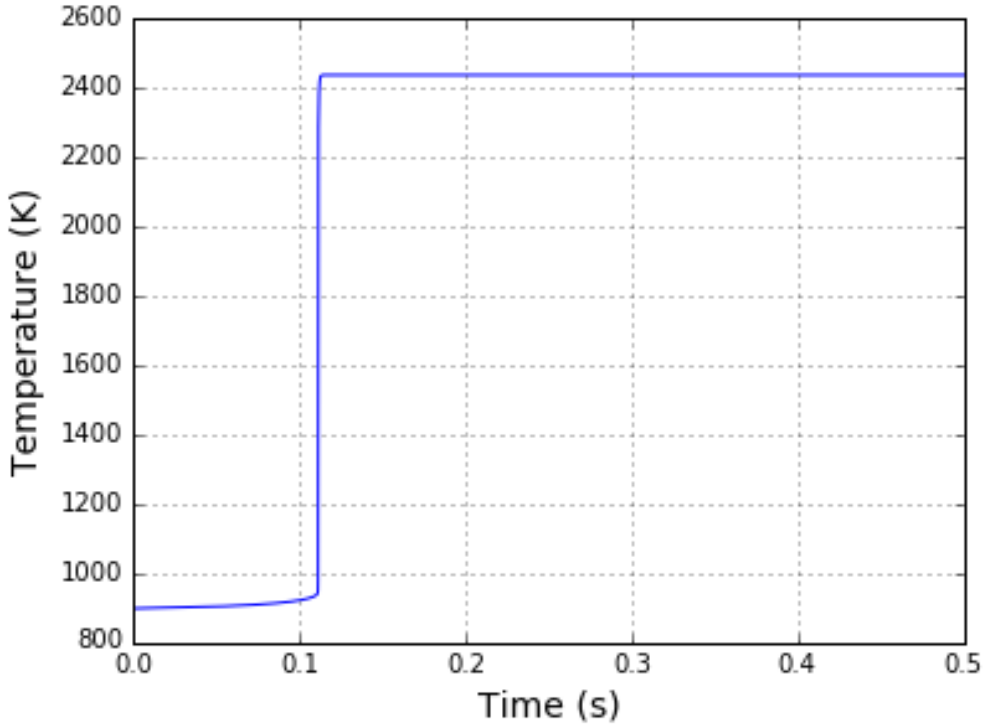
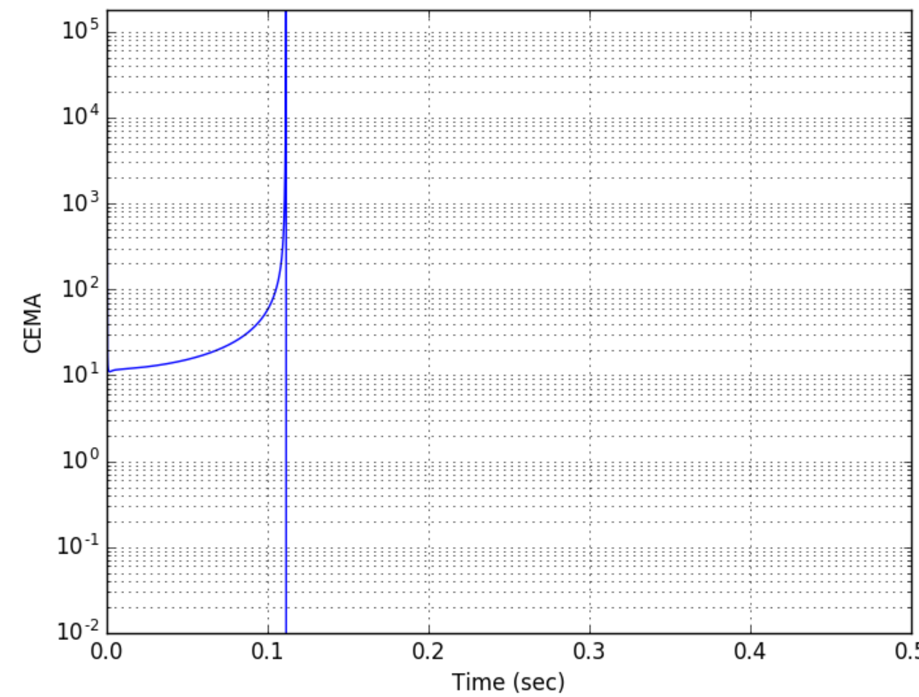
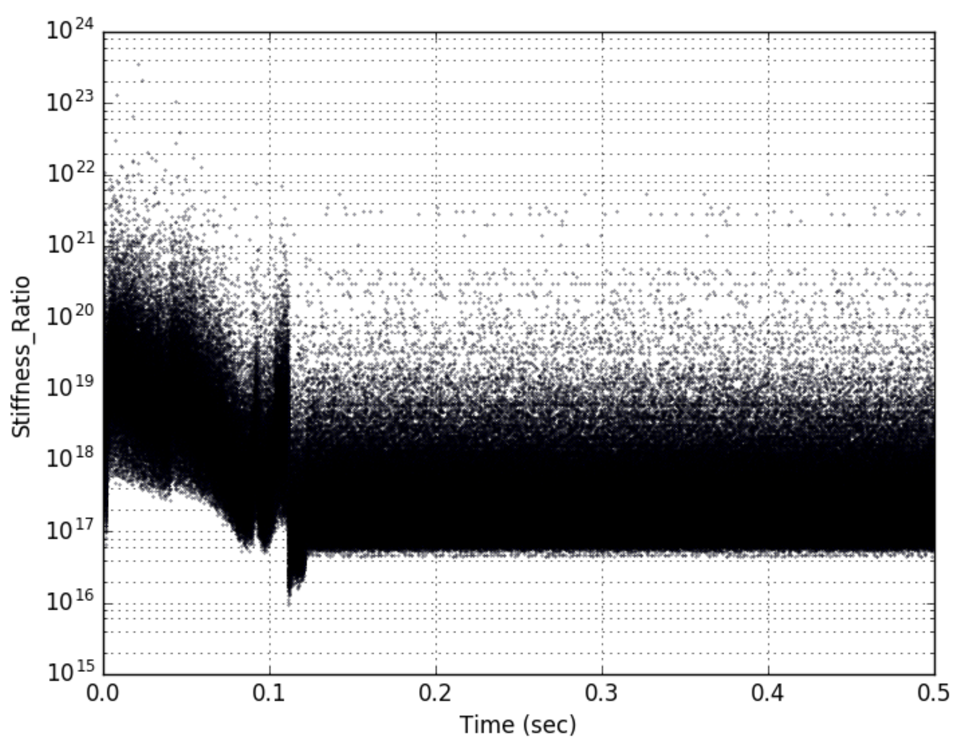


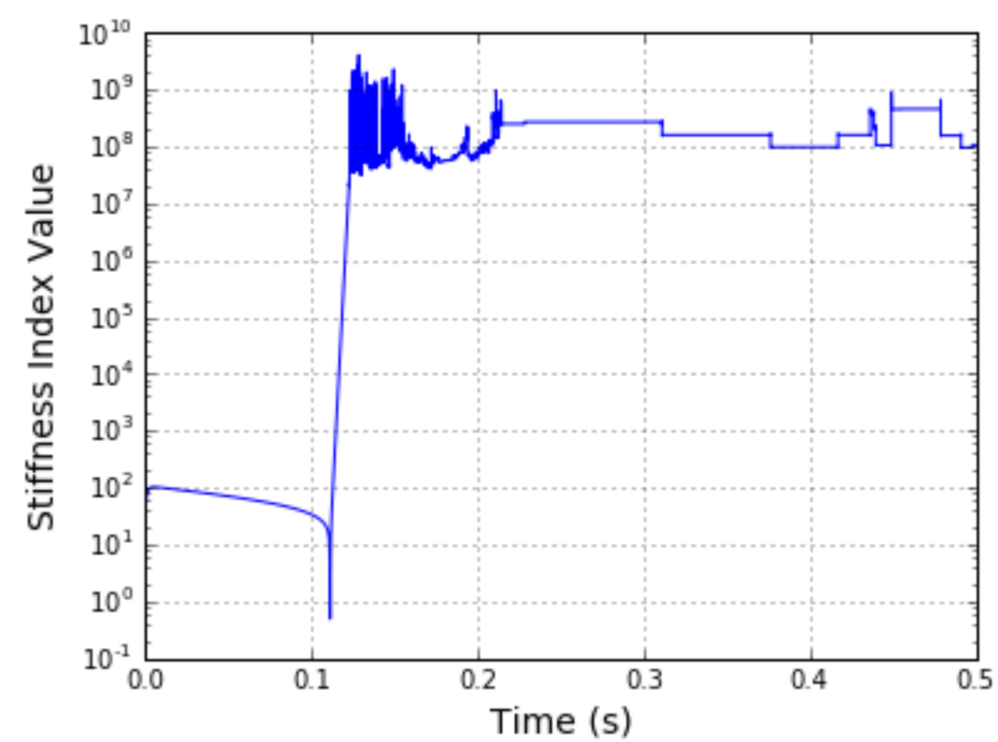
Temperature vs. time



Positive eigenvalue/CEMA

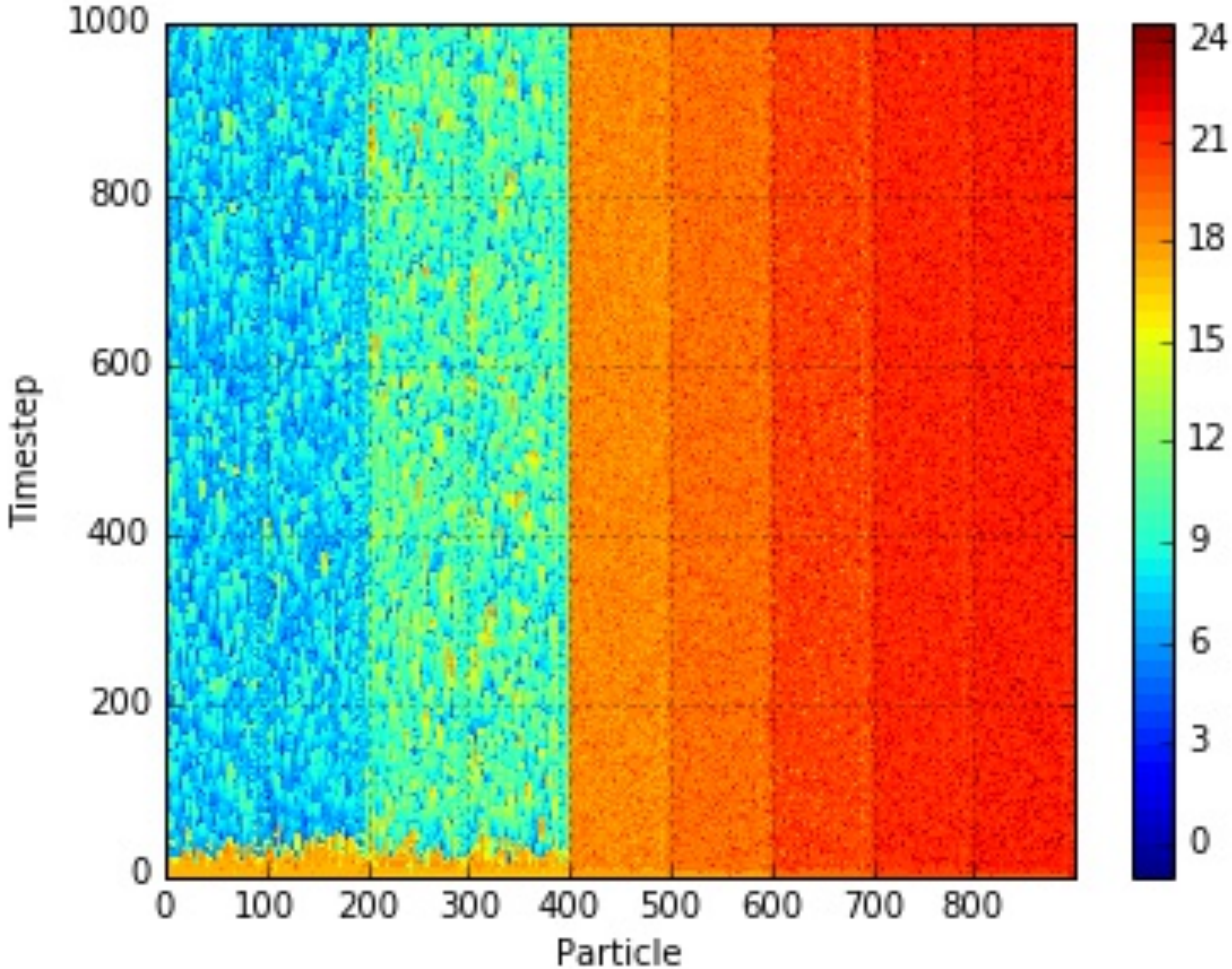


Stiffness ratio vs. time

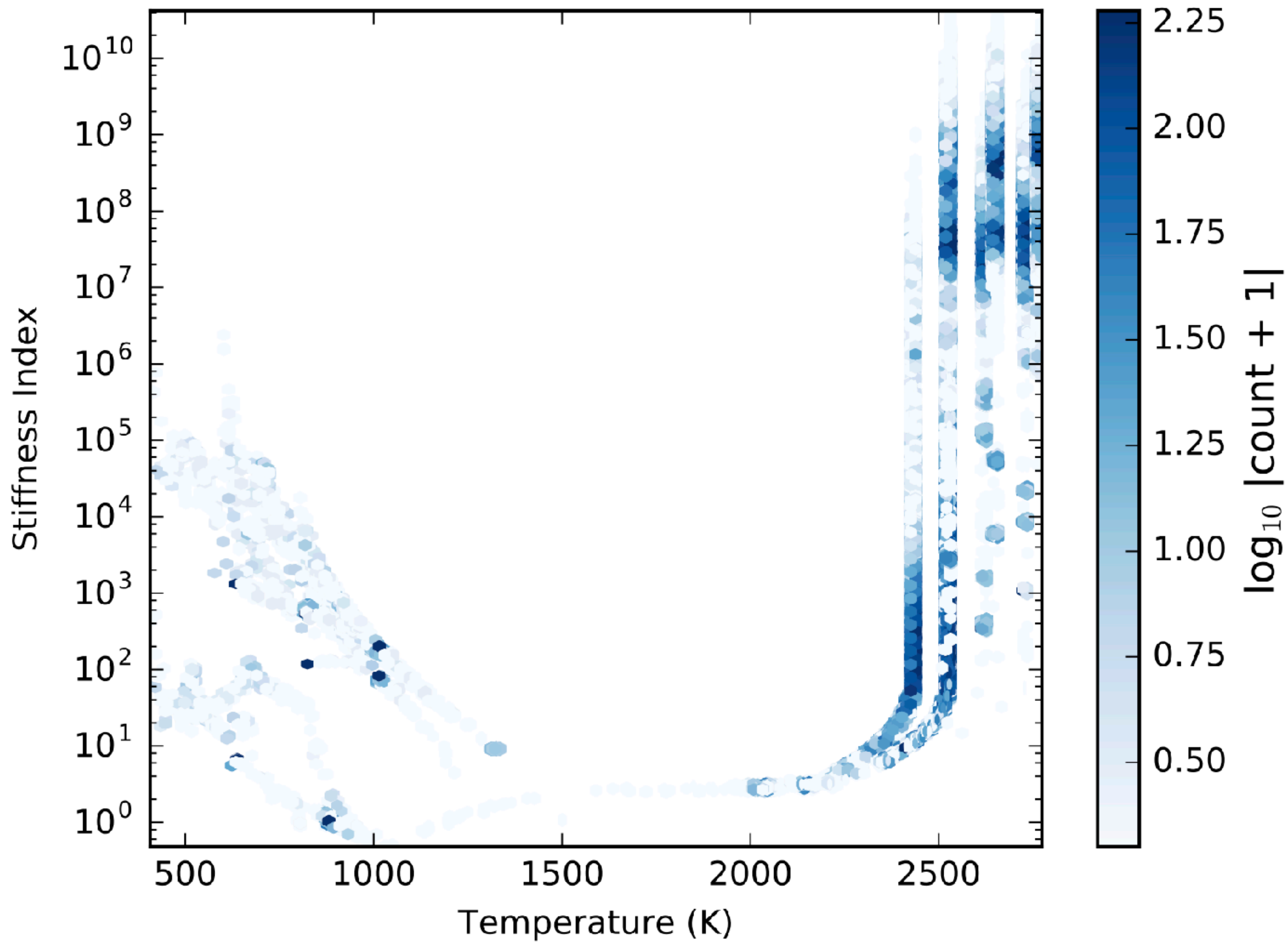


Stiffness index vs. time

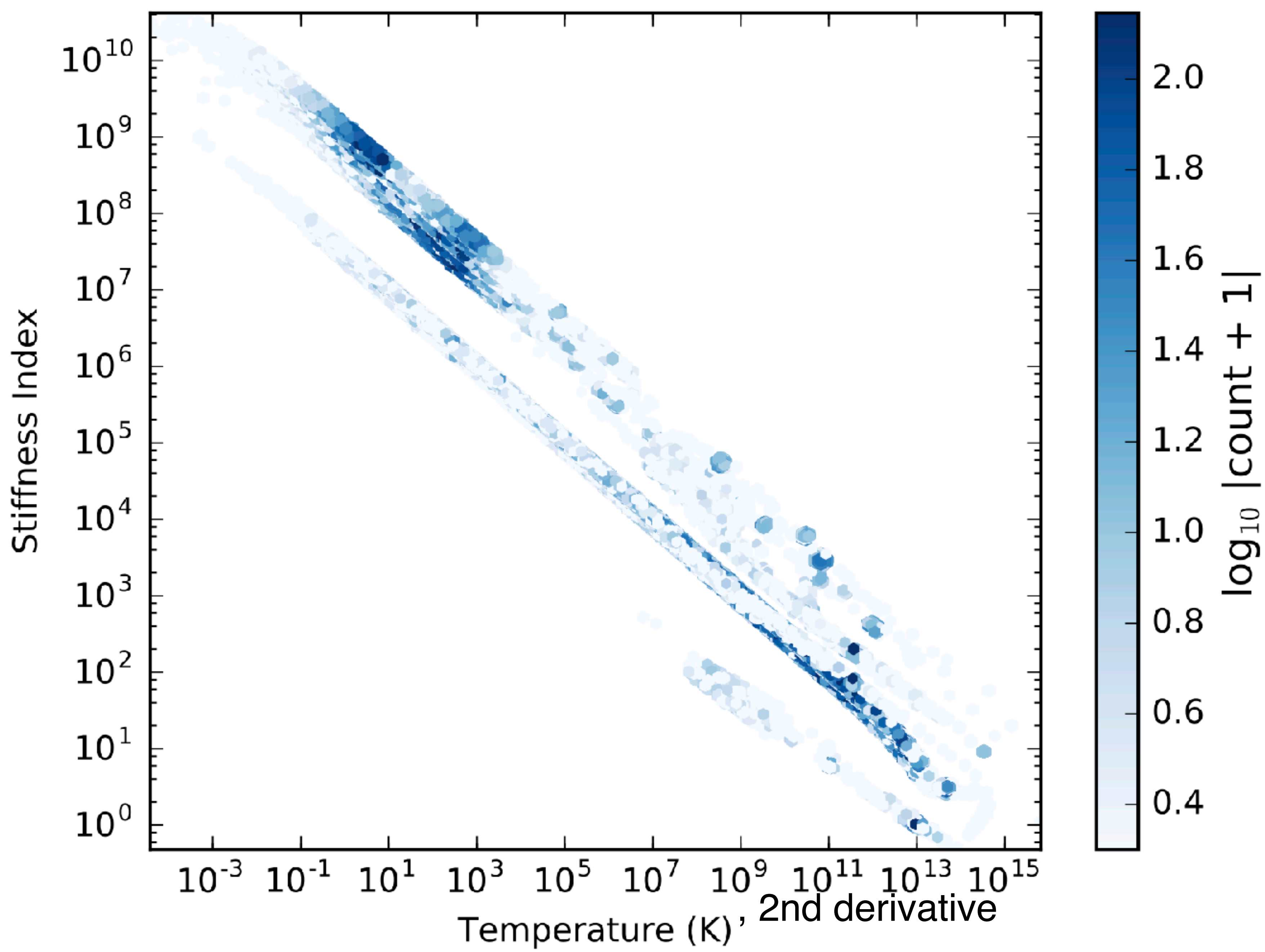
Sampled data



Stiffness index vs. temperature



Stiffness index vs. temperature 2nd derivative



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- Investigating additional metrics (e.g., “stiffness indicator”)
- Also comparing stiffness prediction with “actual” stiffness: computational cost
- Next steps: use metrics to switch integrators, and evaluate improvement in performance

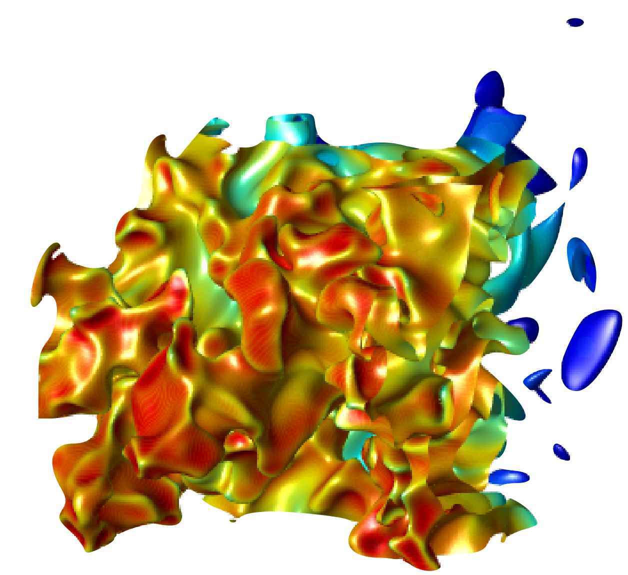
Other ongoing efforts

Group themes

- Combustion/reactive flow modeling
- Numerical methods for CFD
- Ocean biogeochemistry/turbulence
- Smoldering combustion
- Open science

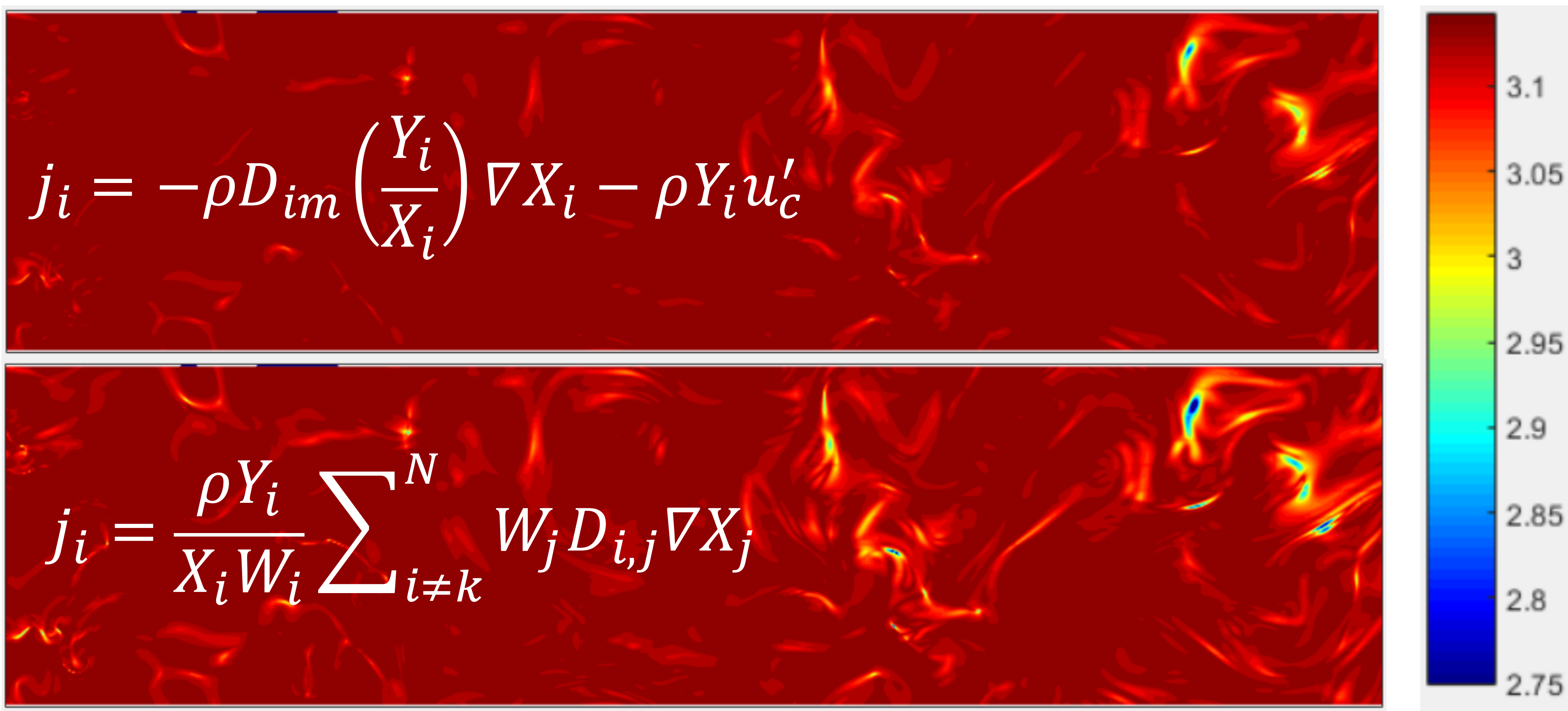
Importance of multicomponent diffusion in turbulent flames

- Student: AJ Fillo; collaboration with Prof. Guillaume Blanquart at CalTech
- DNS supposedly "model-free", but community relies on mixture-averaged (or simpler) approximation for diffusion
- Differences in *laminar* flames have been observed, and recent studies pointed out affect of differential diffusion on *turbulent* flame speed/structure



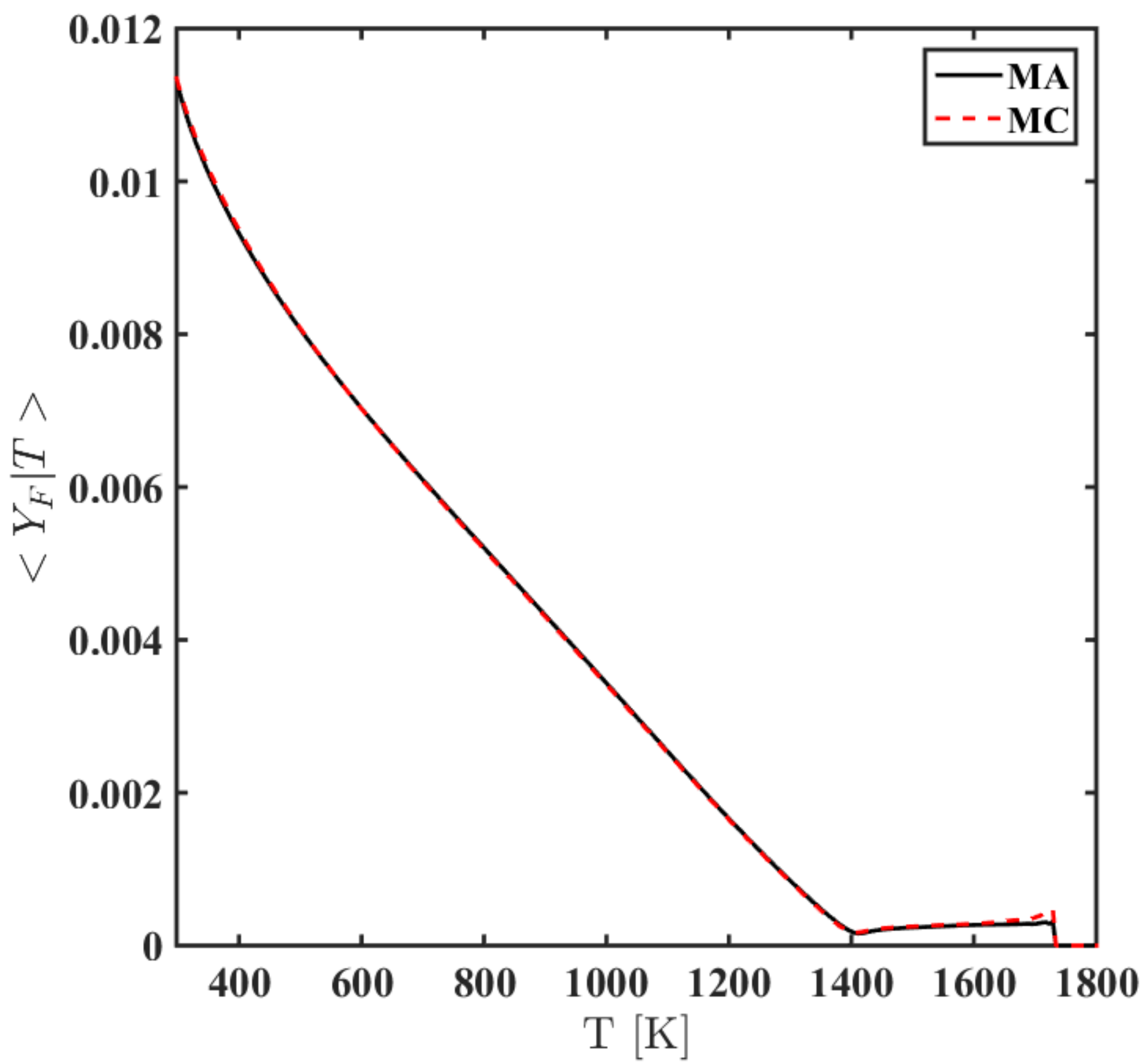
Flux angle contours

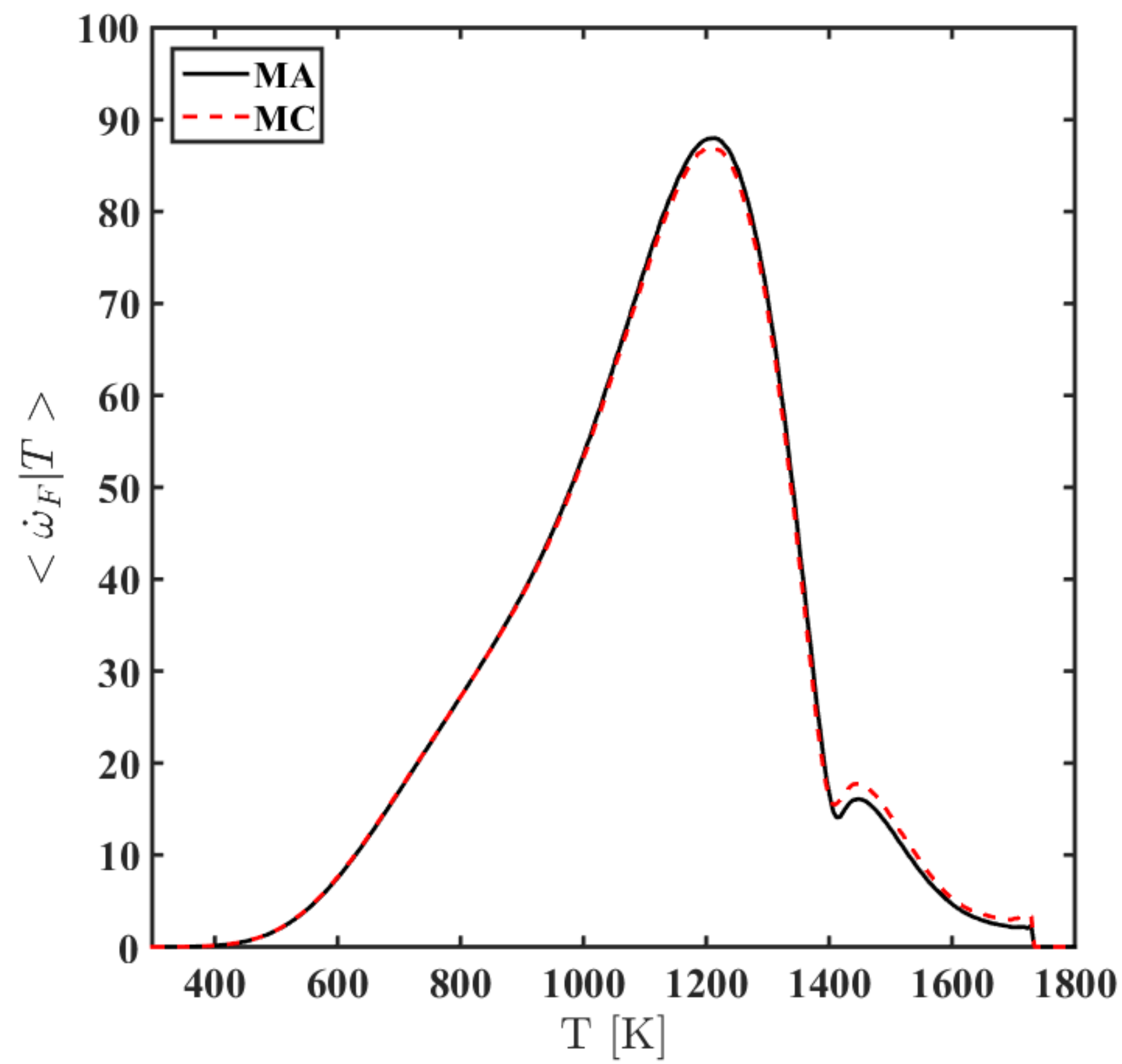
mixture-averaged



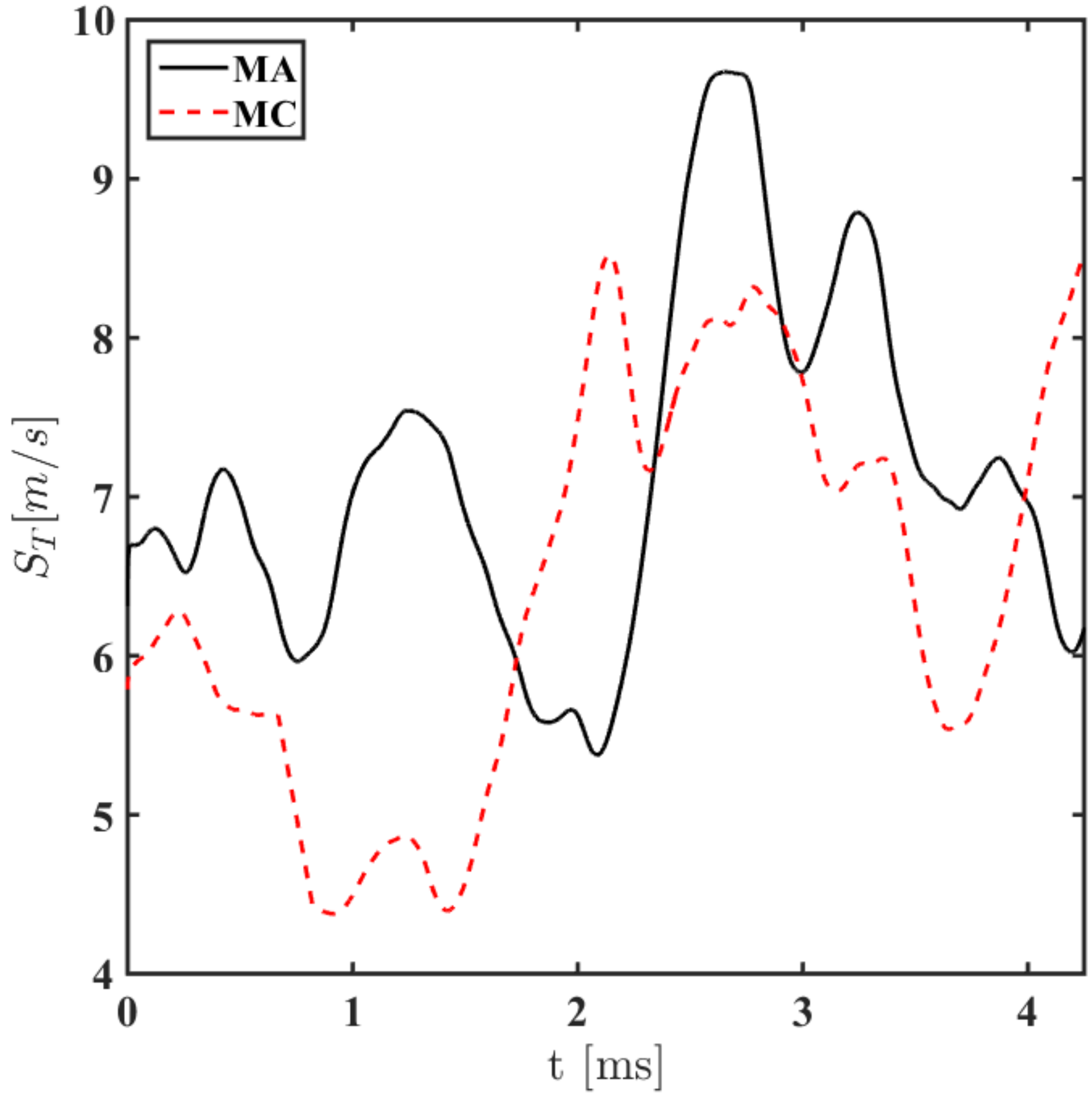
multicomponent

Conditional means

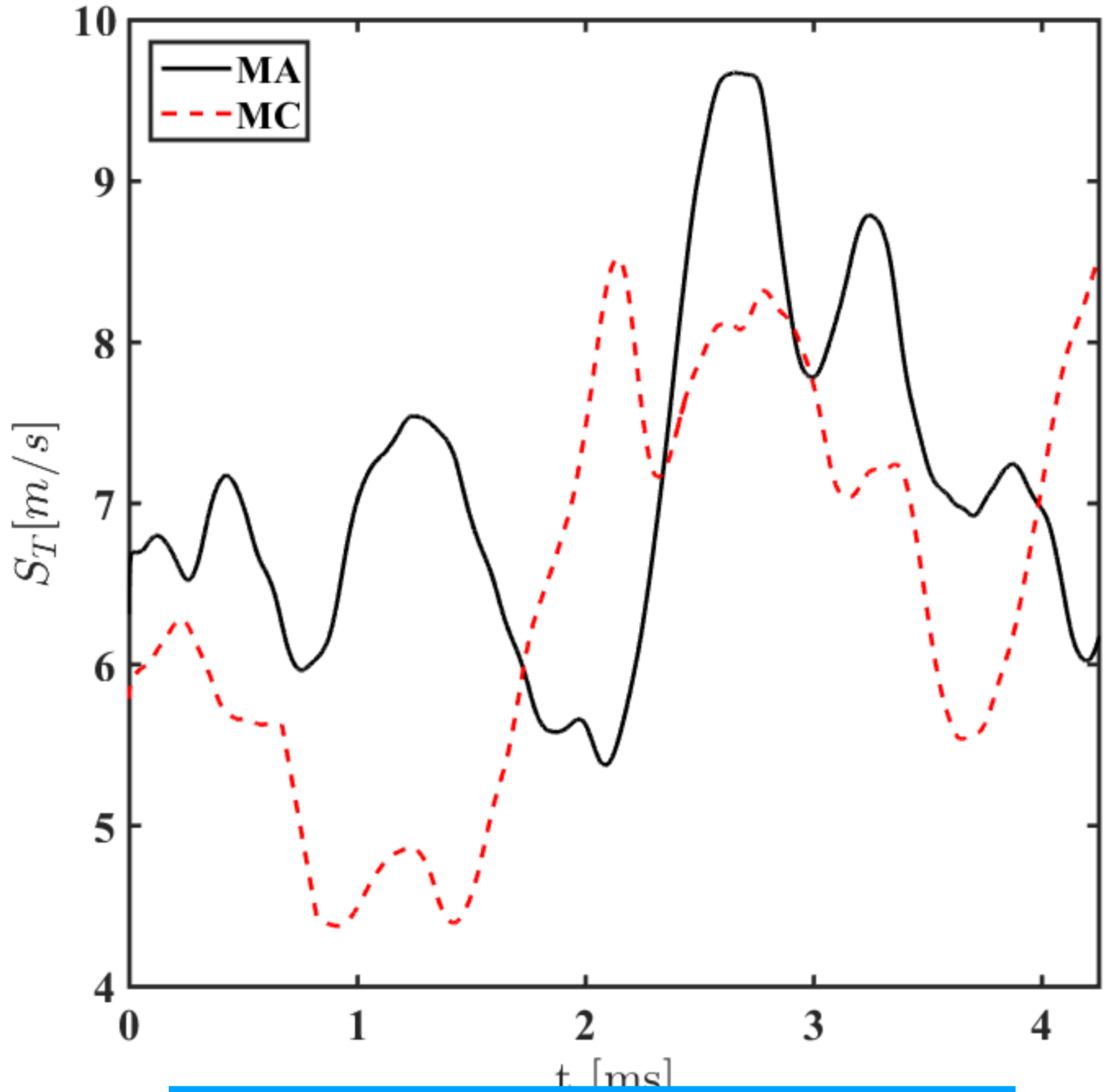




Turbulent flame speed



Turbulent flame speed



~8% difference

Effect of kinetic model reduction on turbulent flame characteristics

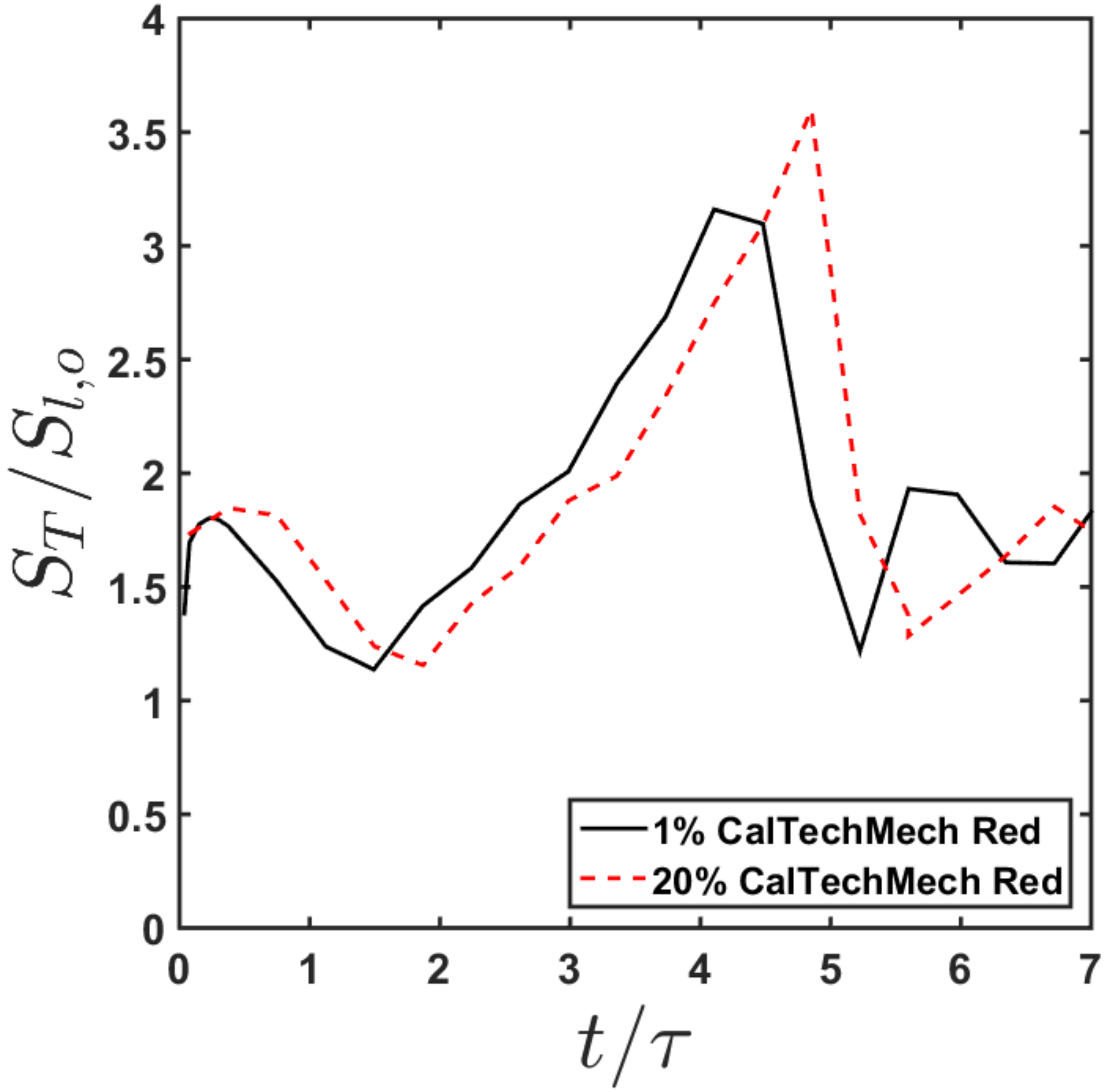
- Student: AJ Fillo

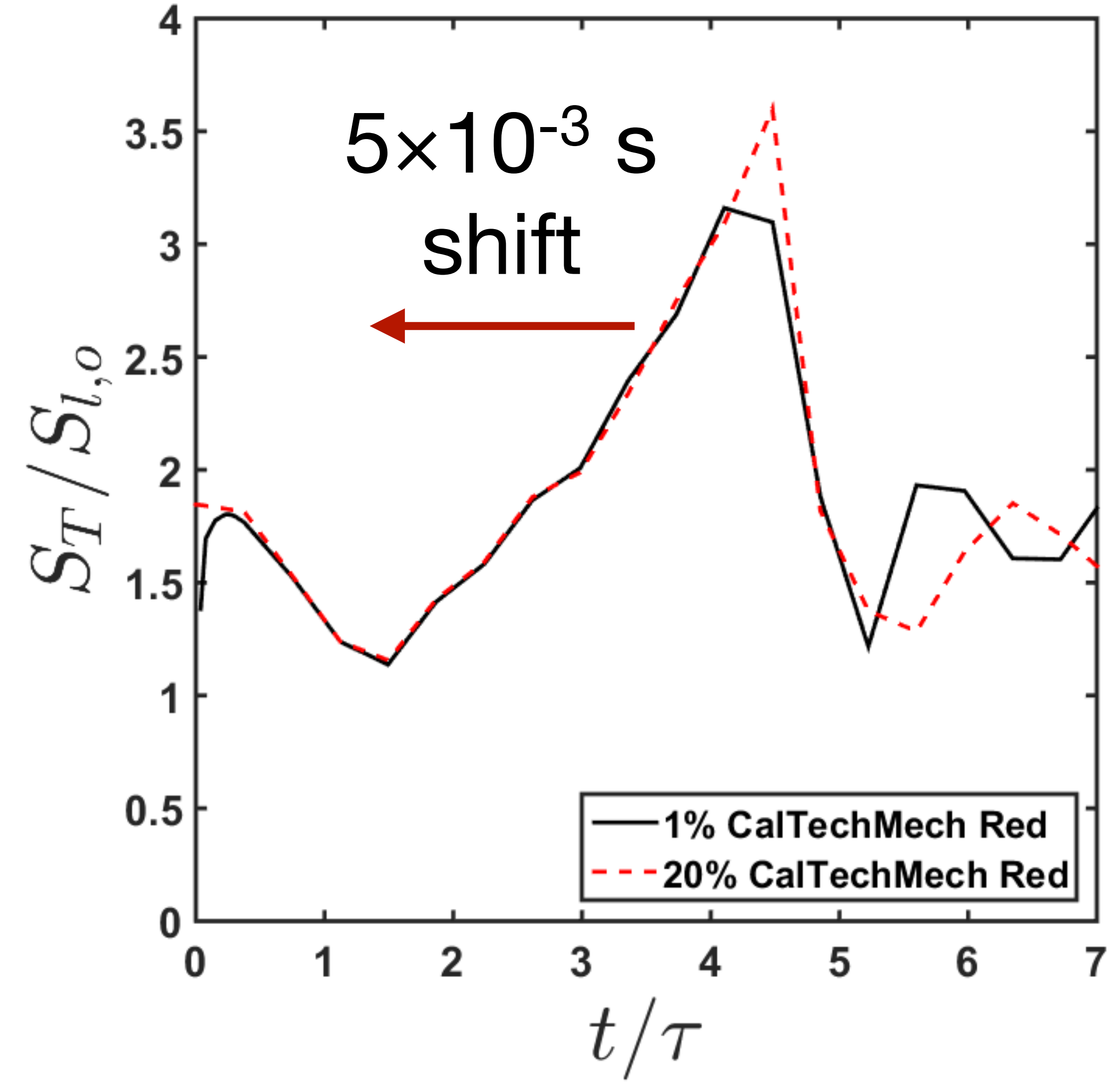
- Common to perform chemical kinetic model reduction and validate against detailed model using homogeneous or laminar phenomena: autoignition, PSR, laminar flame speed

- Assumed that “good” comparison in these implies “good” performance in unsteady, turbulent flames—but this has not been confirmed

- Our work: compare detailed *n*-heptane model (174 species) with reduced models in premixed turbulent flames

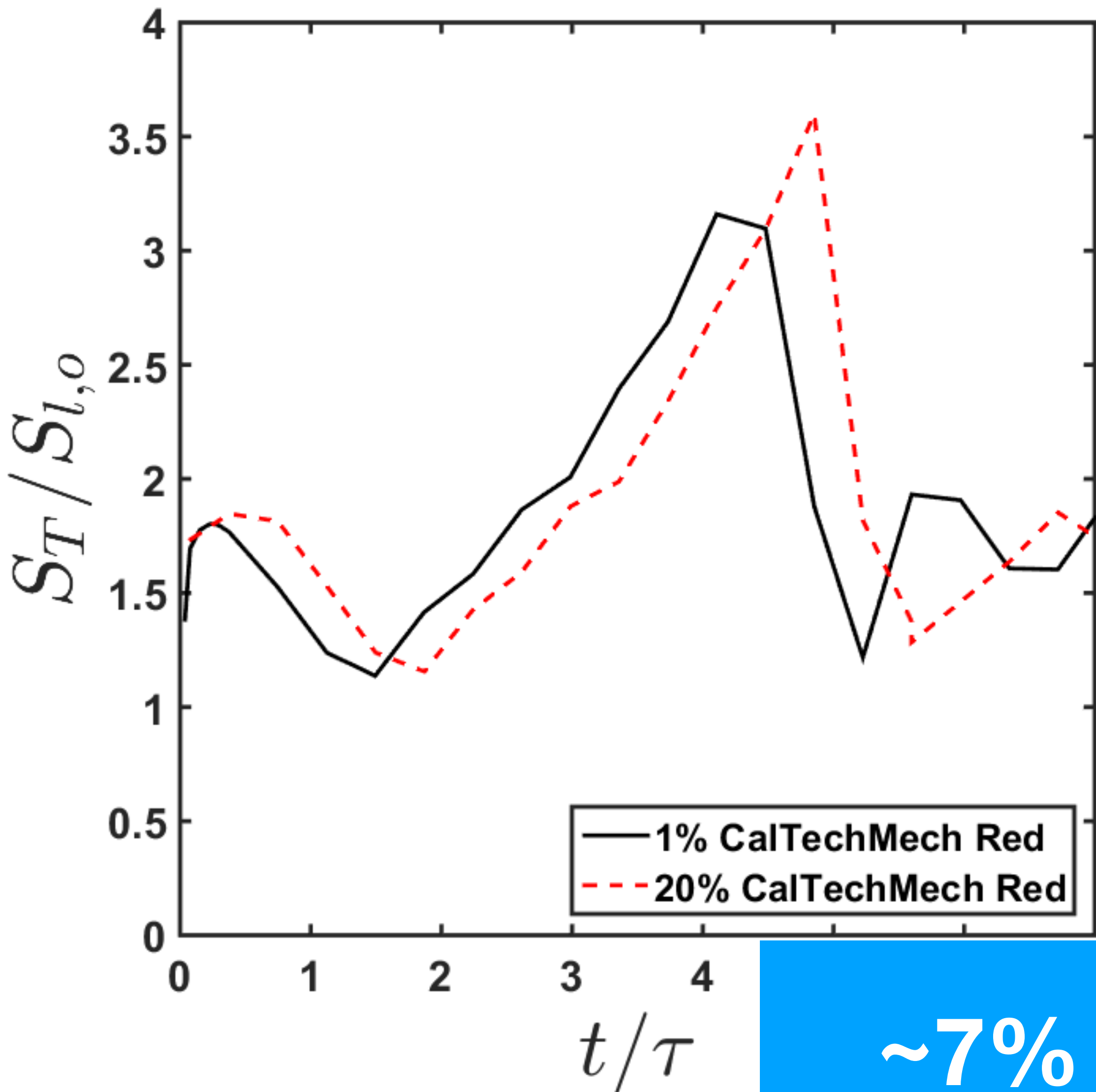
Turbulent flame speed

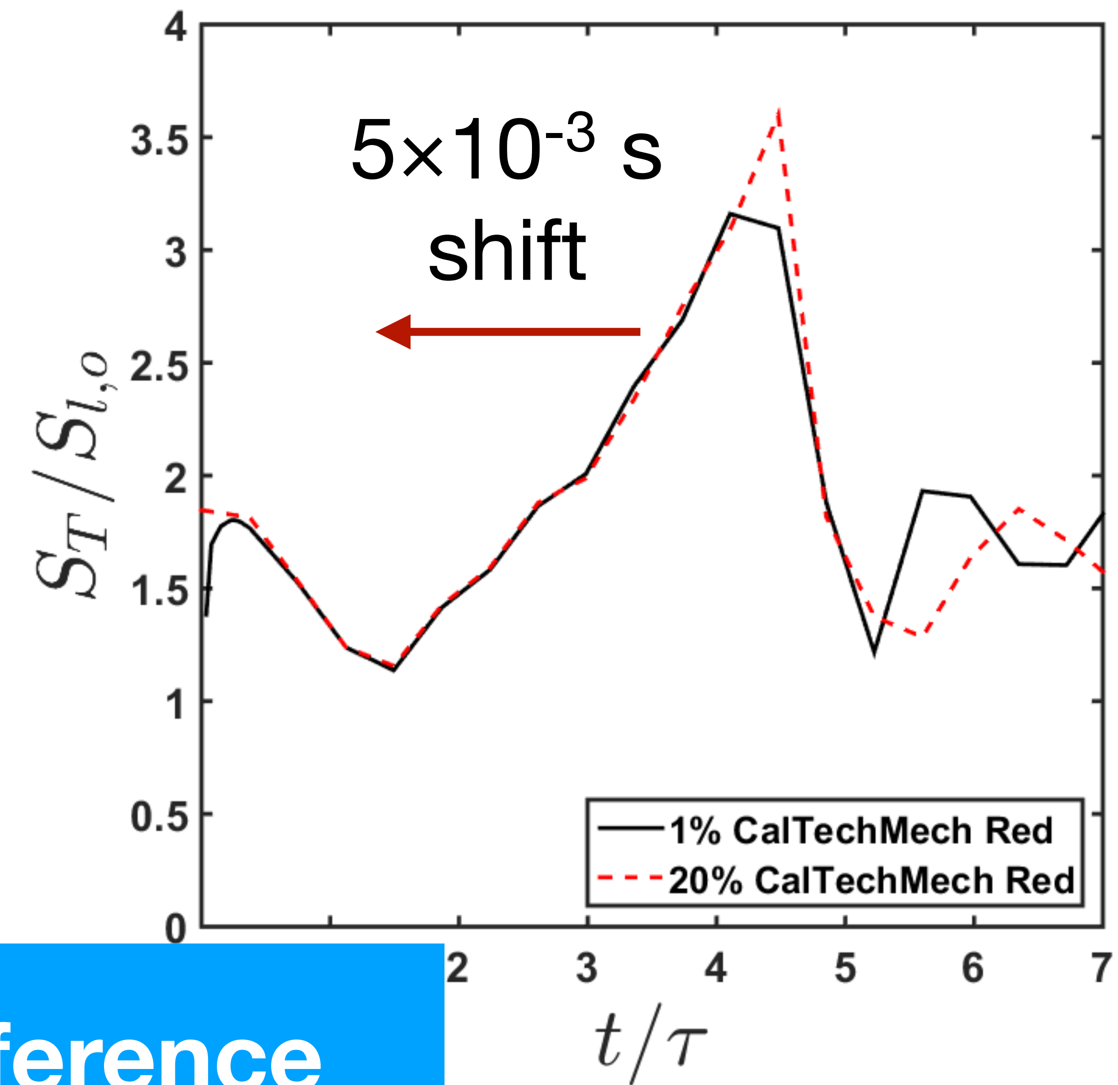




	1% reduction	20% reduction
$S_{L,0}$	37.5 cm/s	36.7 cm/s
S_T	69.3 cm/s	74.04 cm/s

Turbulent flame speed

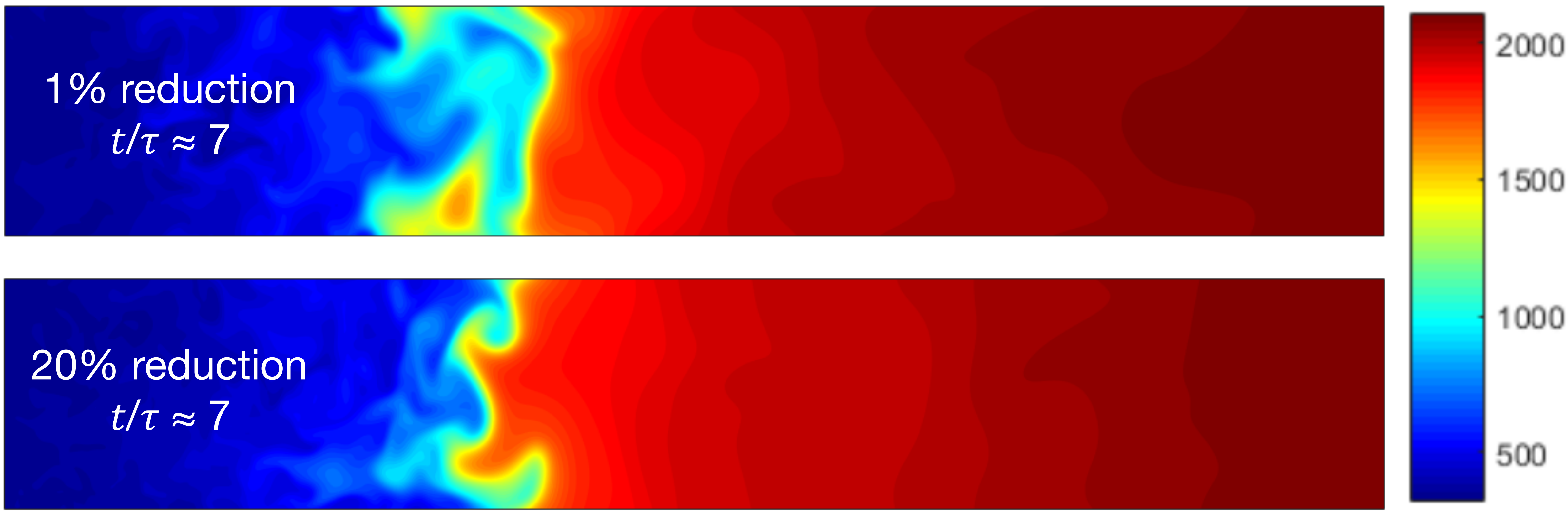




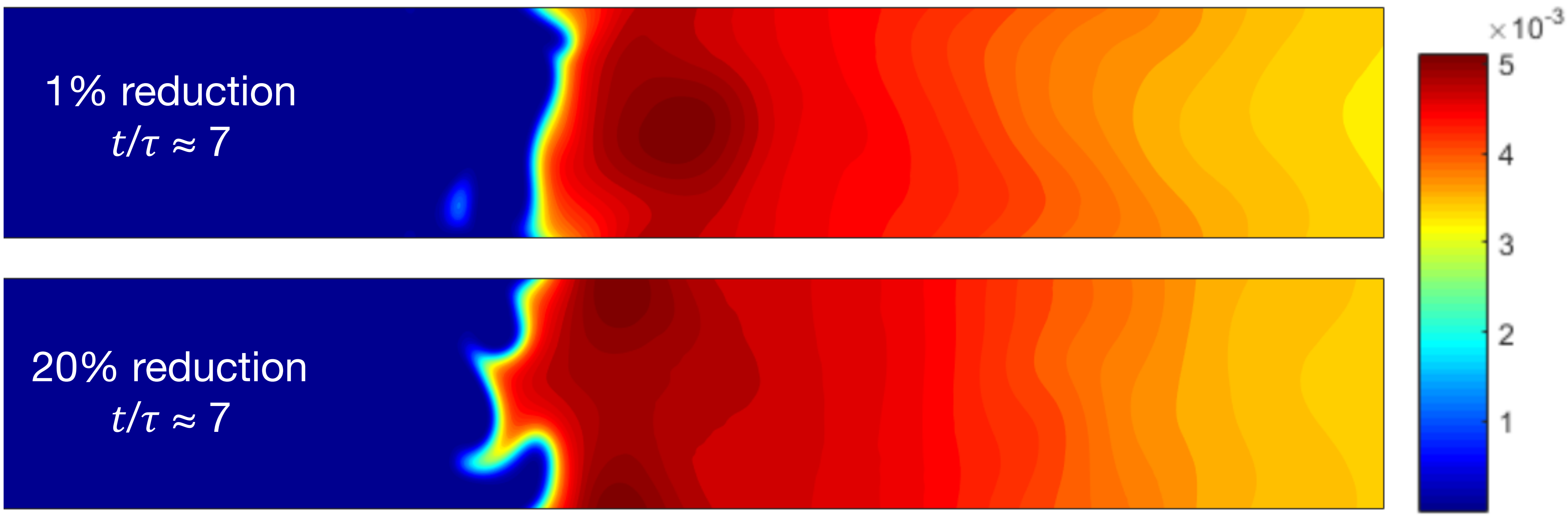
~7% difference

	1% reduction	20% reduction
$S_{L,0}$	37.5 cm/s	36.7 cm/s
S_T	69.3 cm/s	74.04 cm/s

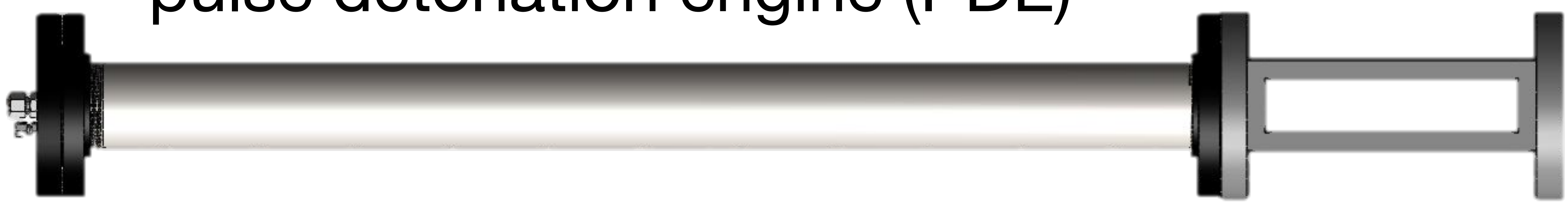
Temperature contour



OH mass fraction contour



PDE-MHD for oxycoal power generation



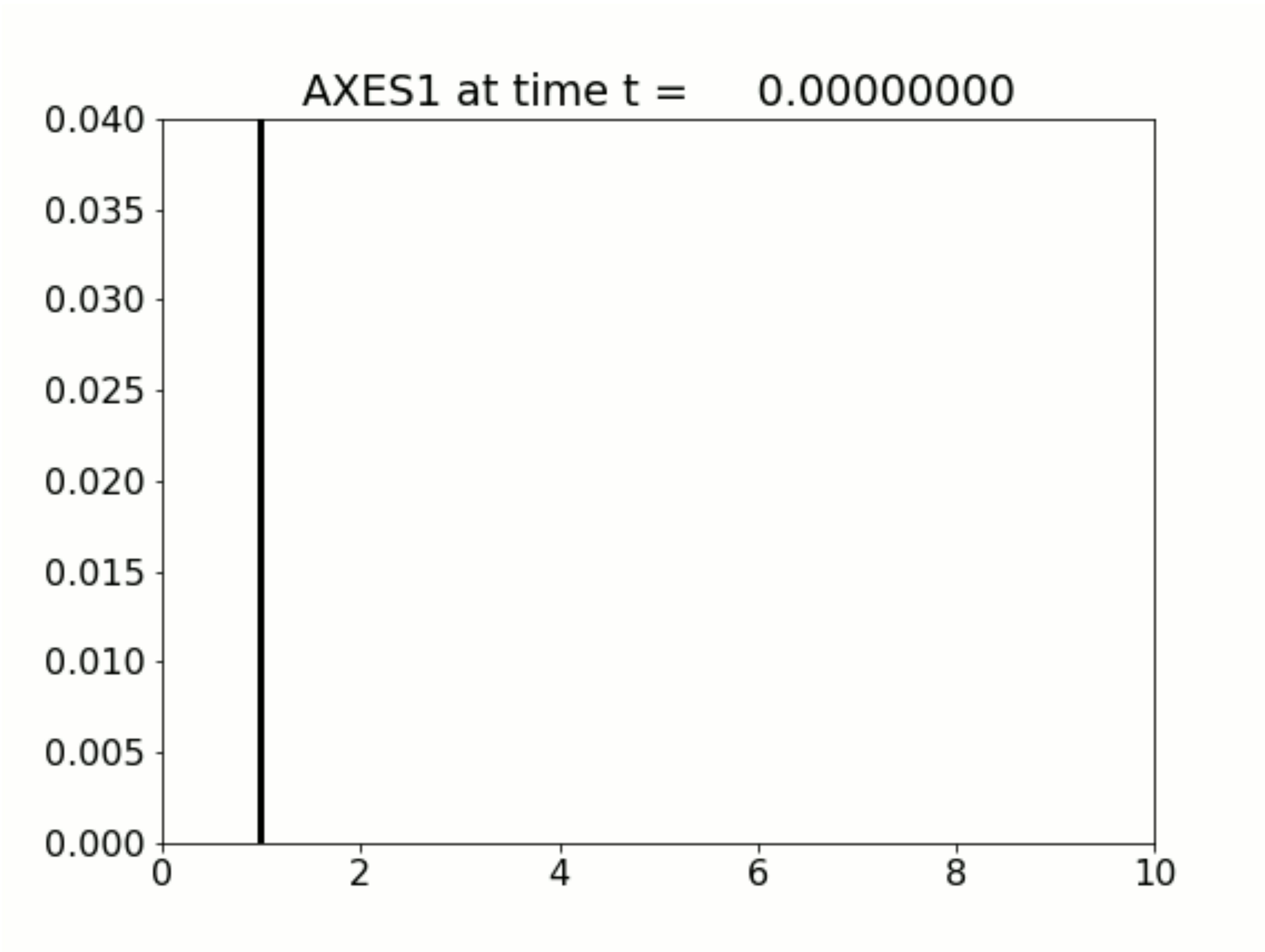
- PDE-MHD potential for oxycoal combustion: high efficiency (topping cycle) & direct power extraction—no moving parts

- Questions about interaction between detonation and MHD/ seed particle ionization, and potential power generation

PDE-MHD for oxycoal power generation

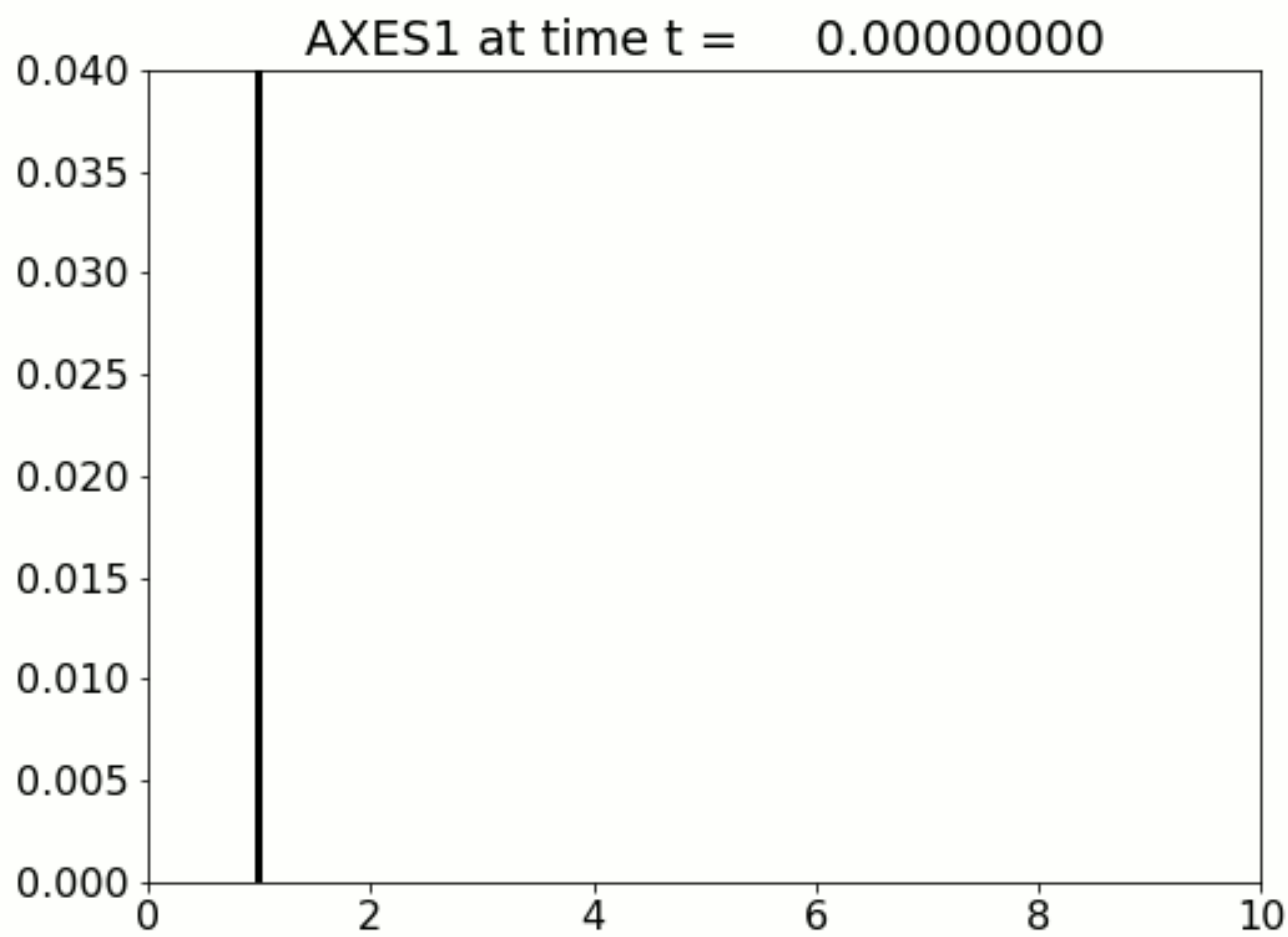
- Student: Matt Zaiger, collaboration with Prof. David Blunck at Oregon State
- Method: use CLAWpack + Cantera to solve reactive Euler equations

PDE: H_2+O_2



AXES1 at time t = 0.00000000
0.040
0.035
0.030
0.025
0.020
0.015
0.010
0.005
0.000
0
2
4
6
8
10

PDE: H_2+O_2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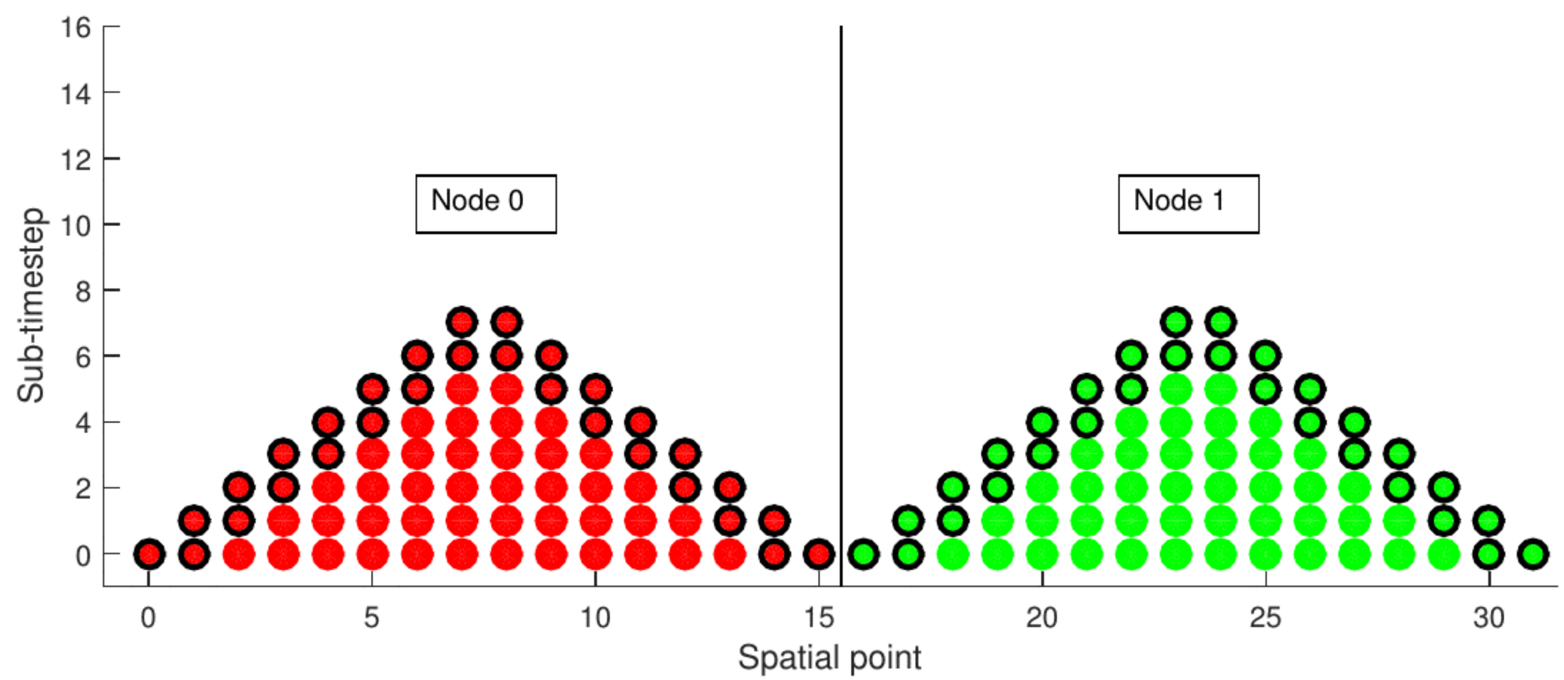
Swept time-space domain decomposition

- Student: Daniel Magee; collaboration with Qiqi Wang (MIT) and David Gleich (Purdue)
- Main idea: reduce communication in distributed parallel PDE solution by performing all possible calculations in subdomain
- Our work: designed GPU-capable version of algorithm, tested with various 1D PDEs



D. J. Magee & K. E. Niemeyer. "Accelerating solutions of PDEs with GPU-based swept time-space decomposition."Under review, 2017. arXiv:1705.03162 [physics.comp-ph]

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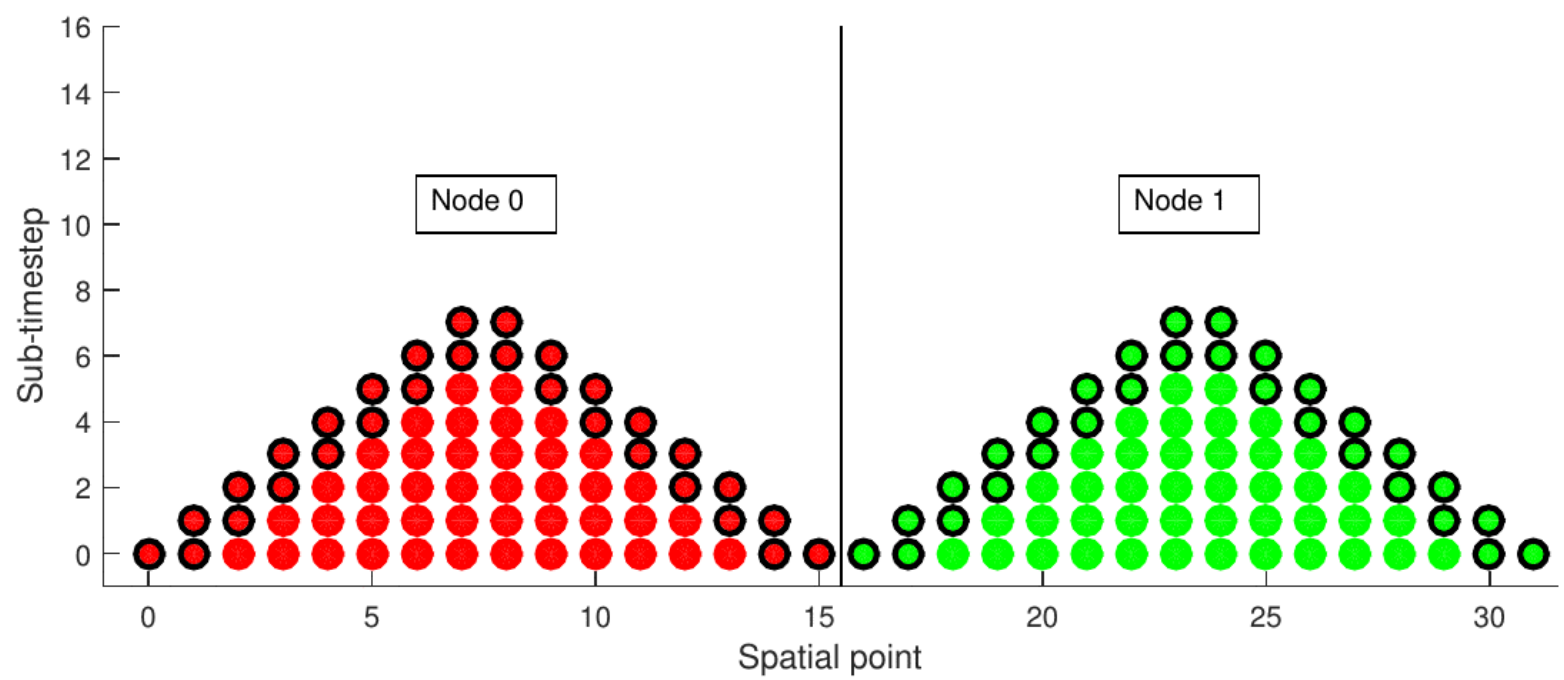

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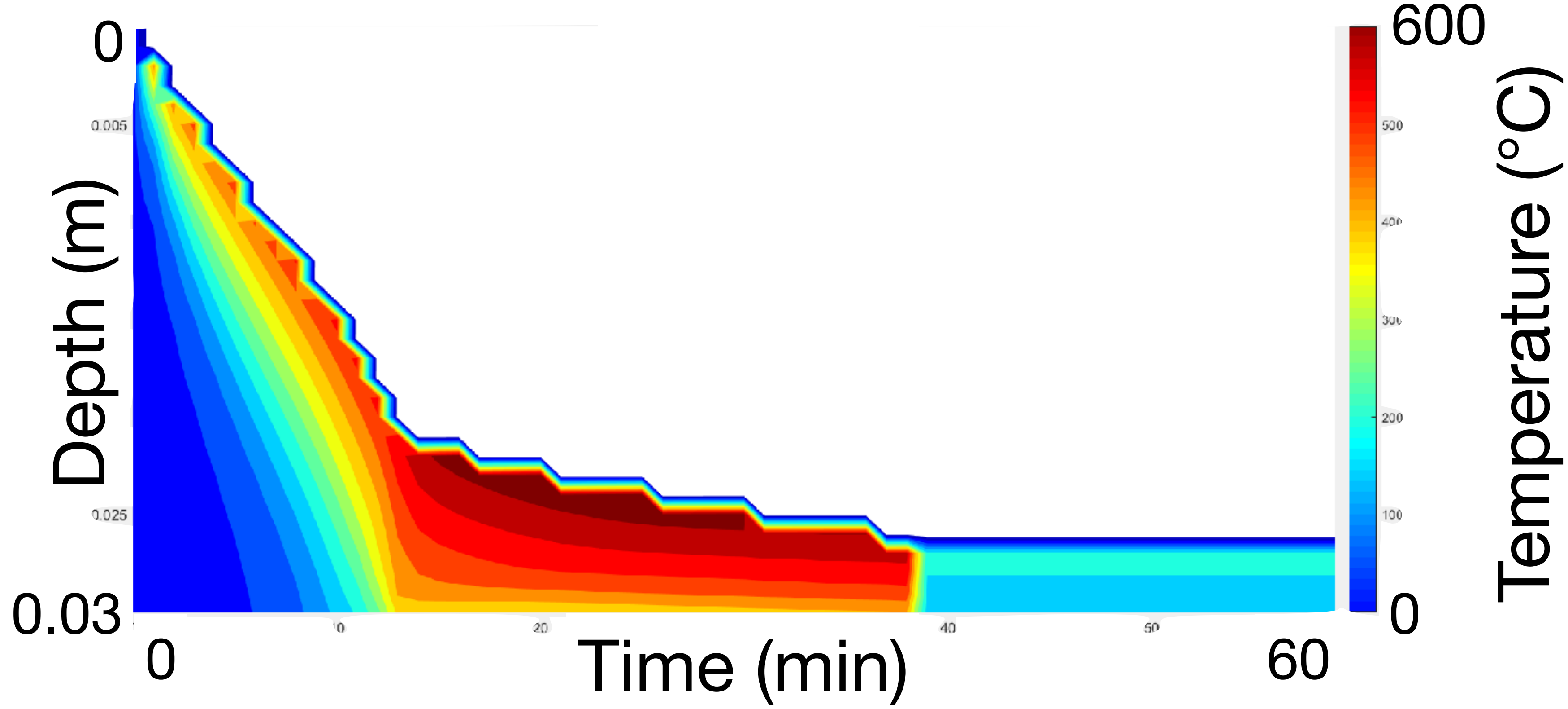
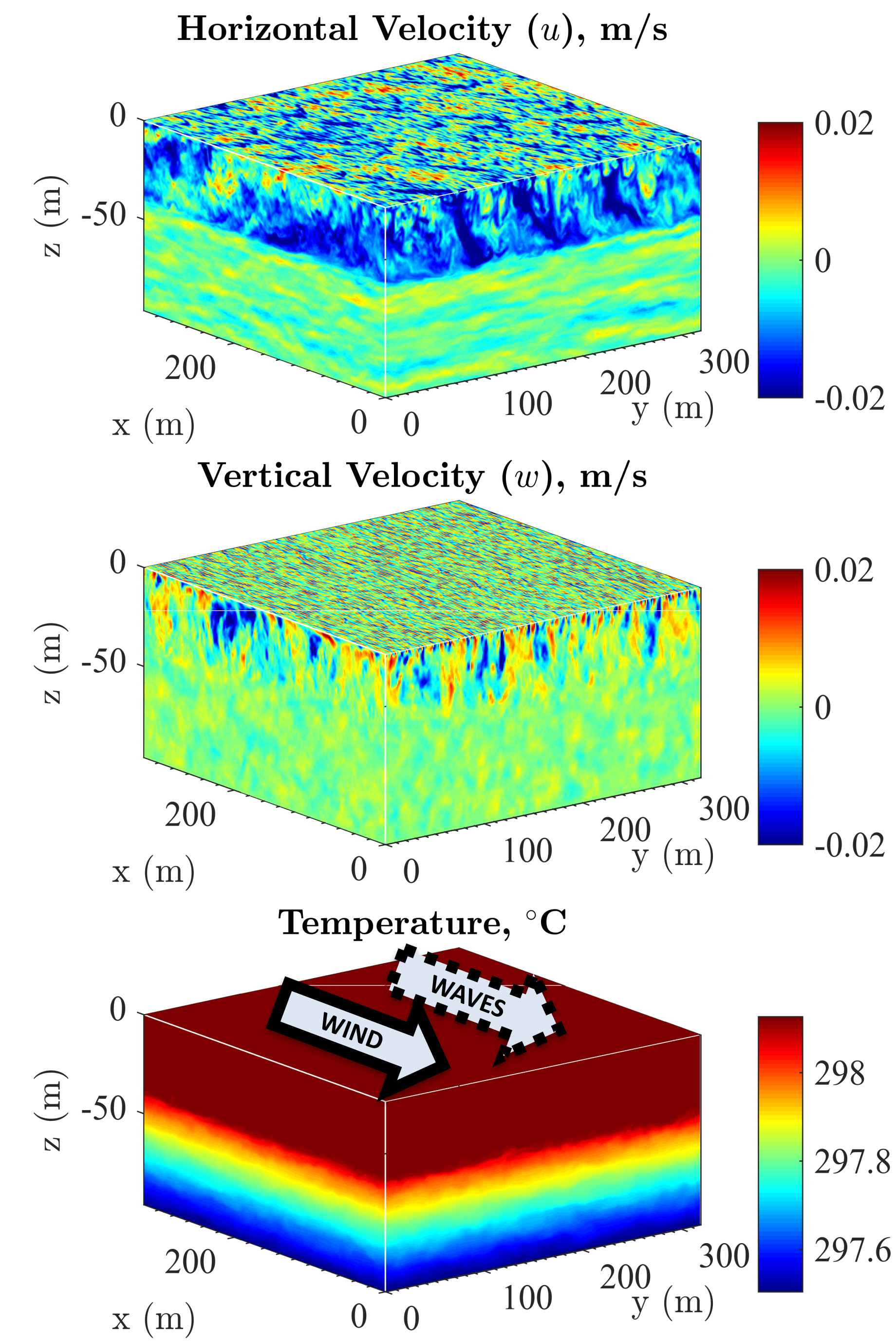
Smoldering combustion of wood fuels

- Smoldering combustion of wood fuels not well understood—what parameters control ignition & propagation?
- Student: Tejas Mulky; collaboration with Prof. David Blunck @ Oregon State
- Fuels of interest: wood-like combinations of cellulose, hemicellulose, & lignin
- Peat smoldering propagation:



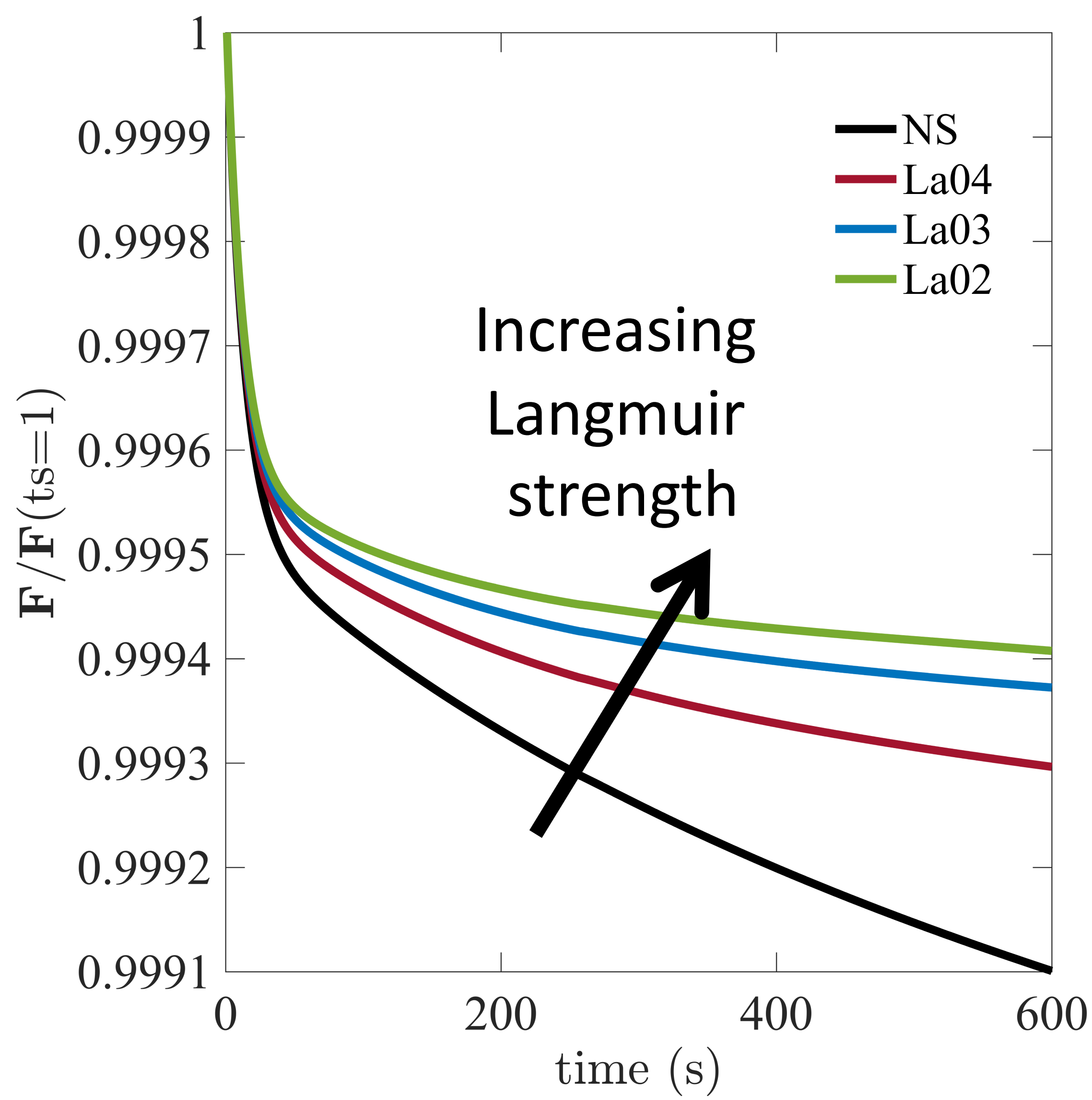
Interaction between ocean biogeochemistry and turbulence

- Student: Luz Pacheco; collaboration with Katherine Smith & Prof. Peter Hamlington @ CU Boulder
- Much like in combustion, in the ocean strong interactions occur between (biogeo)chemistry and turbulence
- Currently: interaction between wave-driven Langmuir turbulence and carbonate chemistry.
- Developing new solver based on FEniCS



K Smith, P Hamlington, K Niemeyer, B Fox-Kemper, & N Lovenduski. "Effects of Langmuir Turbulence on Upper Ocean Carbonate Chemistry", presented at 21st Conference on Atmospheric and Oceanic Fluid Dynamics (2017), Portland OR

Interaction between ocean biogeochemistry and turbulence



Flux rate of CO2 across the air-sea interface as a function of time normalized by initial flux rate

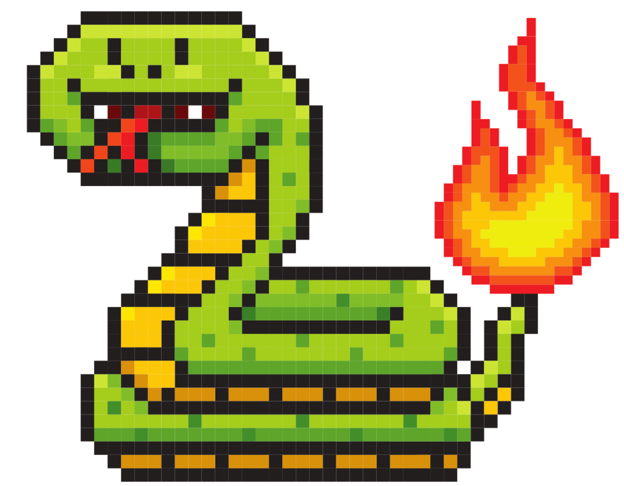
K Smith, P Hamlington, K Niemeyer, B Fox-Kemper, & N Lovenduski. "Effects of Langmuir Turbulence on Upper Ocean Carbonate Chemistry", presented at 21st Conference on Atmospheric and Oceanic Fluid Dynamics (2017), Portland OR

pyMARS: chemical kinetic model reduction software

- Students: Phillip Mestas, Parker Clayton
- **Under development**: Python & Cantera-based, open-source version of MARS for automatically reducing chemical kinetic models
- Currently supports directed relation graph (DRG) method; DRG with error propagation and sensitivity analysis being added

https://github.com/Niemeyer-Research-Group/pyMARS

ChemKED: data format for fundamental combustion measurements



- Student: Morgan Mayer; collaboration with Dr. Bryan Weber @ Univ. Connecticut
- Human- and machine-readable, open standard for describing fundamental combustion experiments—currently, autoignition
- PyKED: Python-based software for validating and interacting with ChemKED files
- Also building database of files: Prometheus

https://github.com/pr-omethe-us/PyKED

JOSS: Journal of Open Source Software

- JOSS publishes (short) software articles
- Peers review article, software, and associated artifacts
- JOSS has an ISSN (2475-9066) and software articles receive Crossref DOI upon publication
- JOSS celebrated its first birthday in May 🎂
- 111 articles published in first year
- Now: 123 published articles and 68 submitted

`http://joss.theoj.org/`

`http://bit.ly/joss-scipy2017`

Group themes

- Combustion/reactive flow modeling
- Numerical methods for CFD
- Ocean biogeochemistry/turbulence
- Smoldering combustion
- Open science

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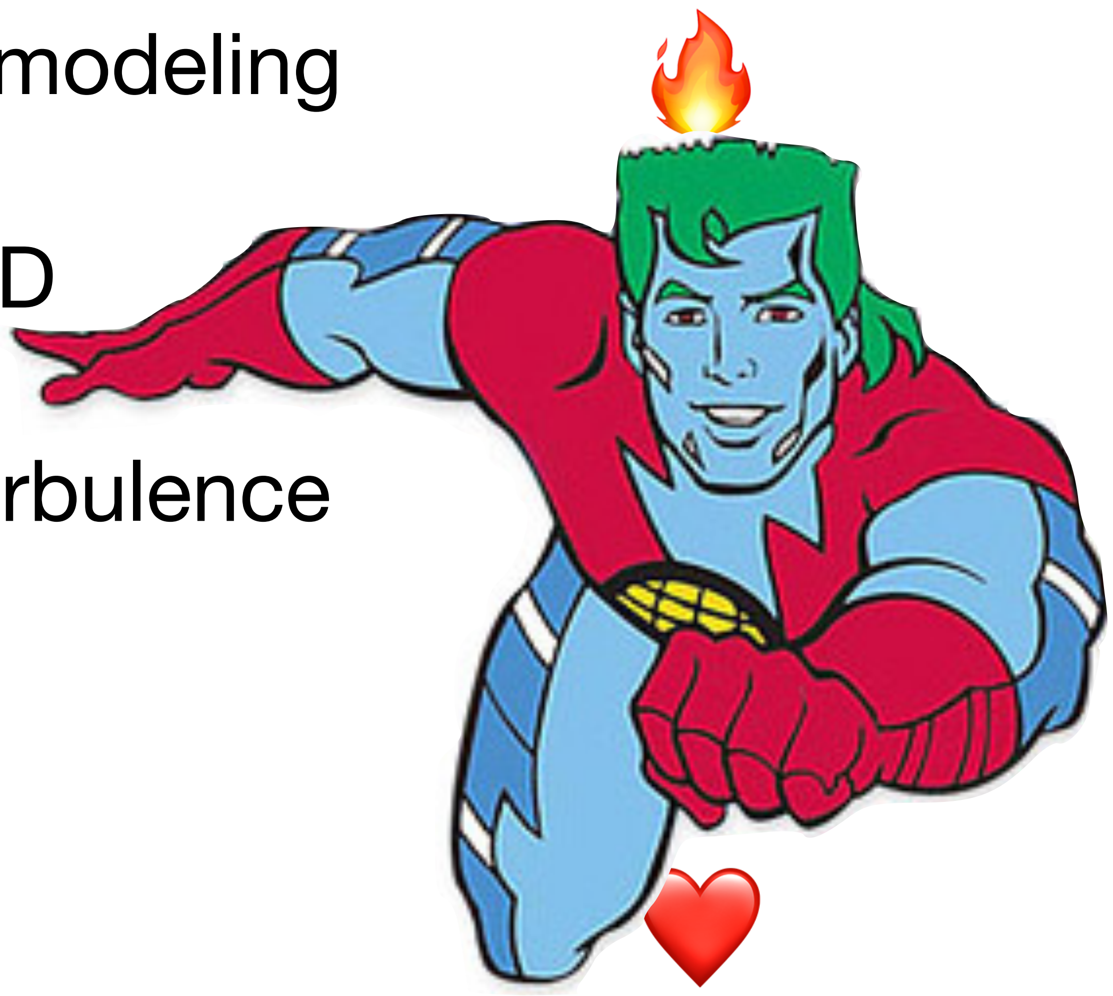

Thank you!
Questions?

https://git.io/nrg

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