Funding: NSF award
ACI-1535065

Investigating stiffness detection metrics for chemical kinetics ODEs

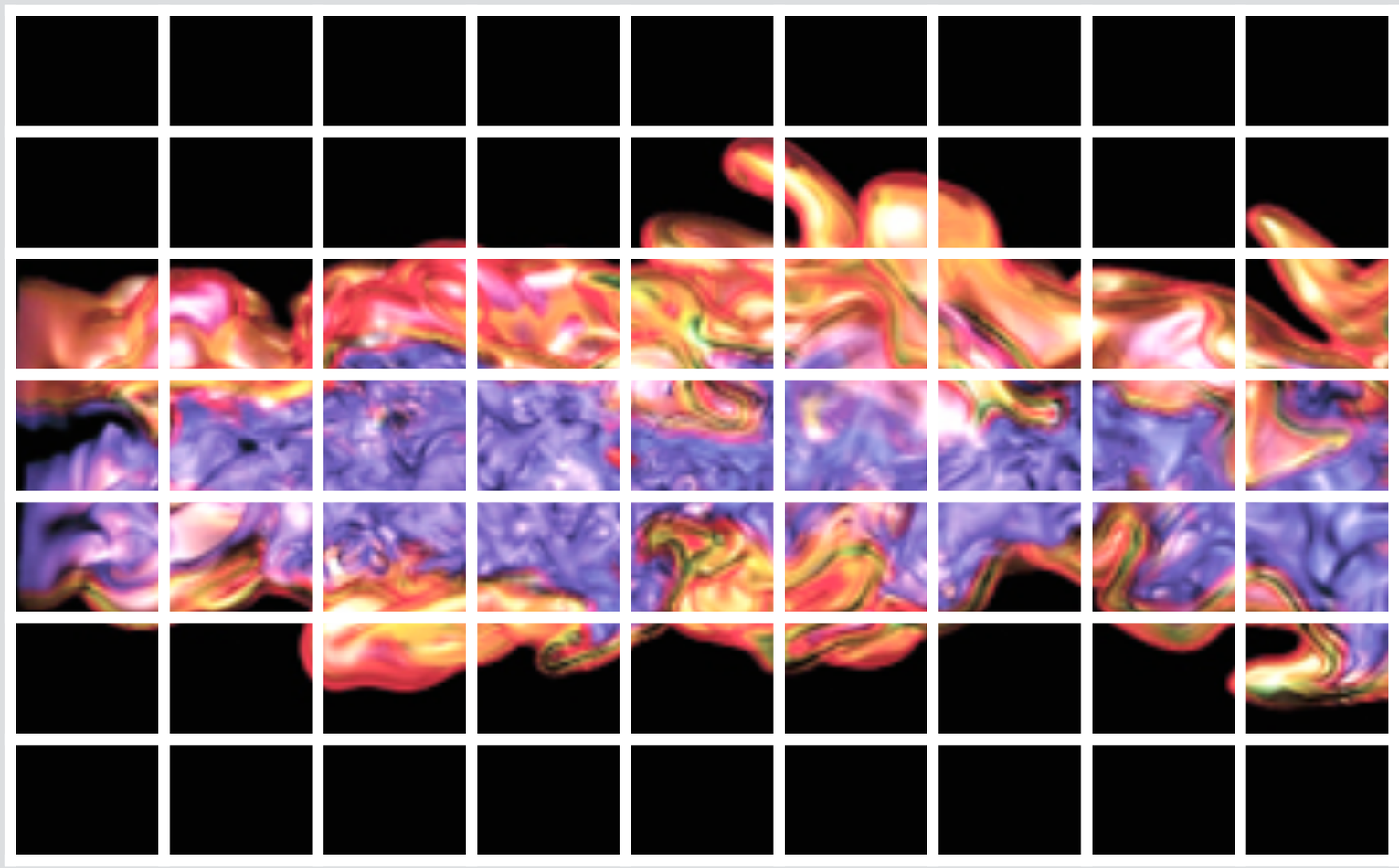
Andrew T Alferman & Kyle E Niemeyer
Oregon State University

SIAM CSE17
3 March 2017

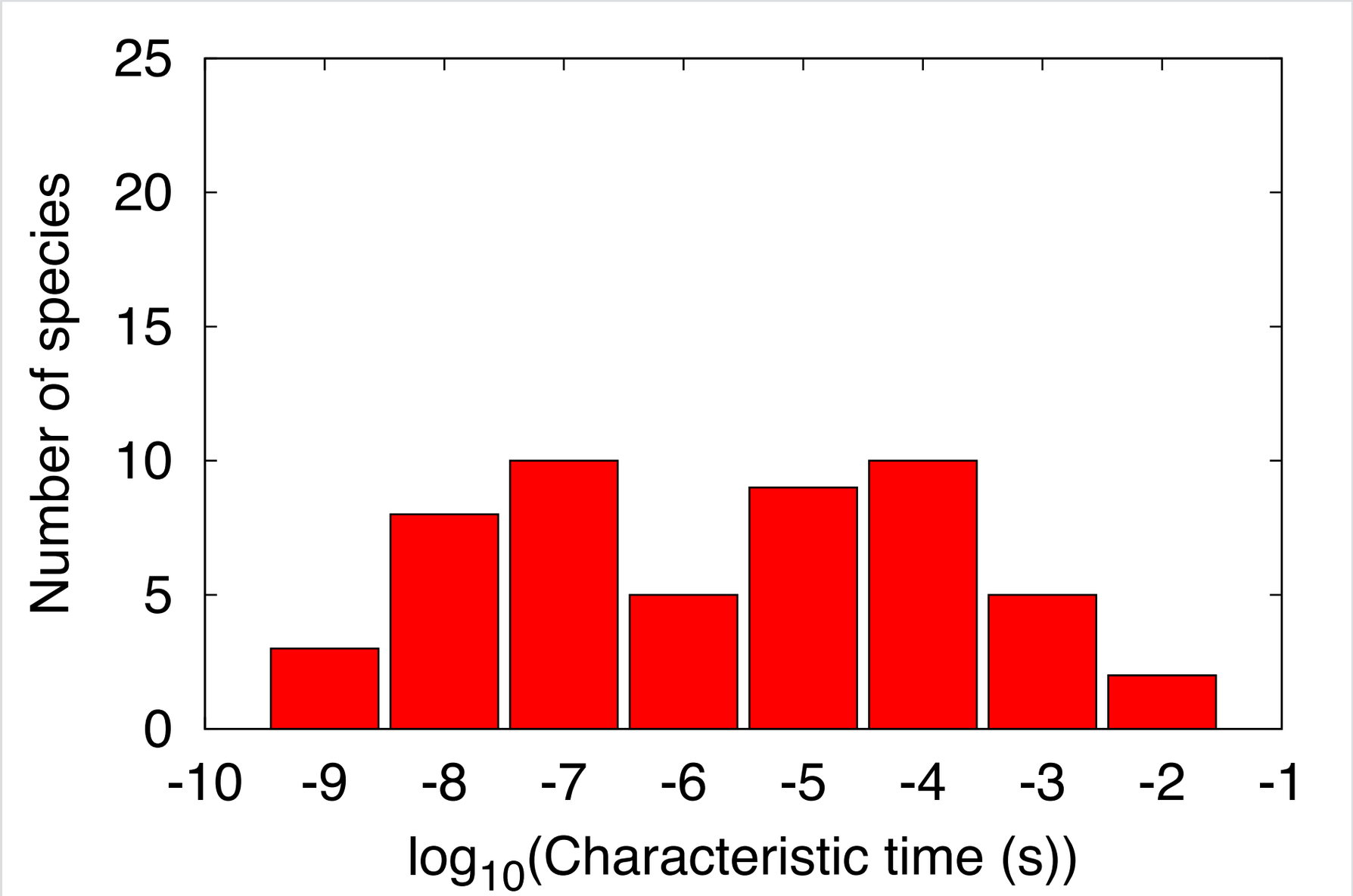
Kyle.Niemeyer@oregonstate.edu
@kyleniemeyer
kyleniemeyer.com

Challenge

Performing predictive simulations of reactive flows
... in a **reasonable** amount of time



Transport + Chemistry



Stiffness of kinetic models

Characteristic creation times of methane oxidation

Stiffness

- Wide range of species/reaction time scales
- Rapidly depleting radical species, fast reversible reactions
- Traditionally requires implicit integration algorithms

Hydrogen Oxidation

$$2H_2 + O_2 \longrightarrow 2H_2O$$

$H_2 + M \longleftrightarrow 2H + M$

$O_2 + M \longleftrightarrow 2O + M$

$H + O_2 \longleftrightarrow O + OH$

$H_2 + O \longleftrightarrow H + OH$

$H_2 + OH \longleftrightarrow H_2O + H$

$2OH \longleftrightarrow H_2O + O$

$O + H + M \longleftrightarrow OH + M$

$H_2O_2 + OH \longleftrightarrow HO_2 + H_2O$

$2H_2O \longleftrightarrow H + OH + H_2O$

$H + O_2 \longleftrightarrow HO_2$

$H_2 + O_2 \longleftrightarrow HO_2 + H$

$HO_2 + H \longleftrightarrow 2OH$

$HO_2 + O \longleftrightarrow O_2 + OH$

$HO_2 + OH \longleftrightarrow H_2O + O_2$

$2HO_2 \longleftrightarrow H_2O_2 + O_2$

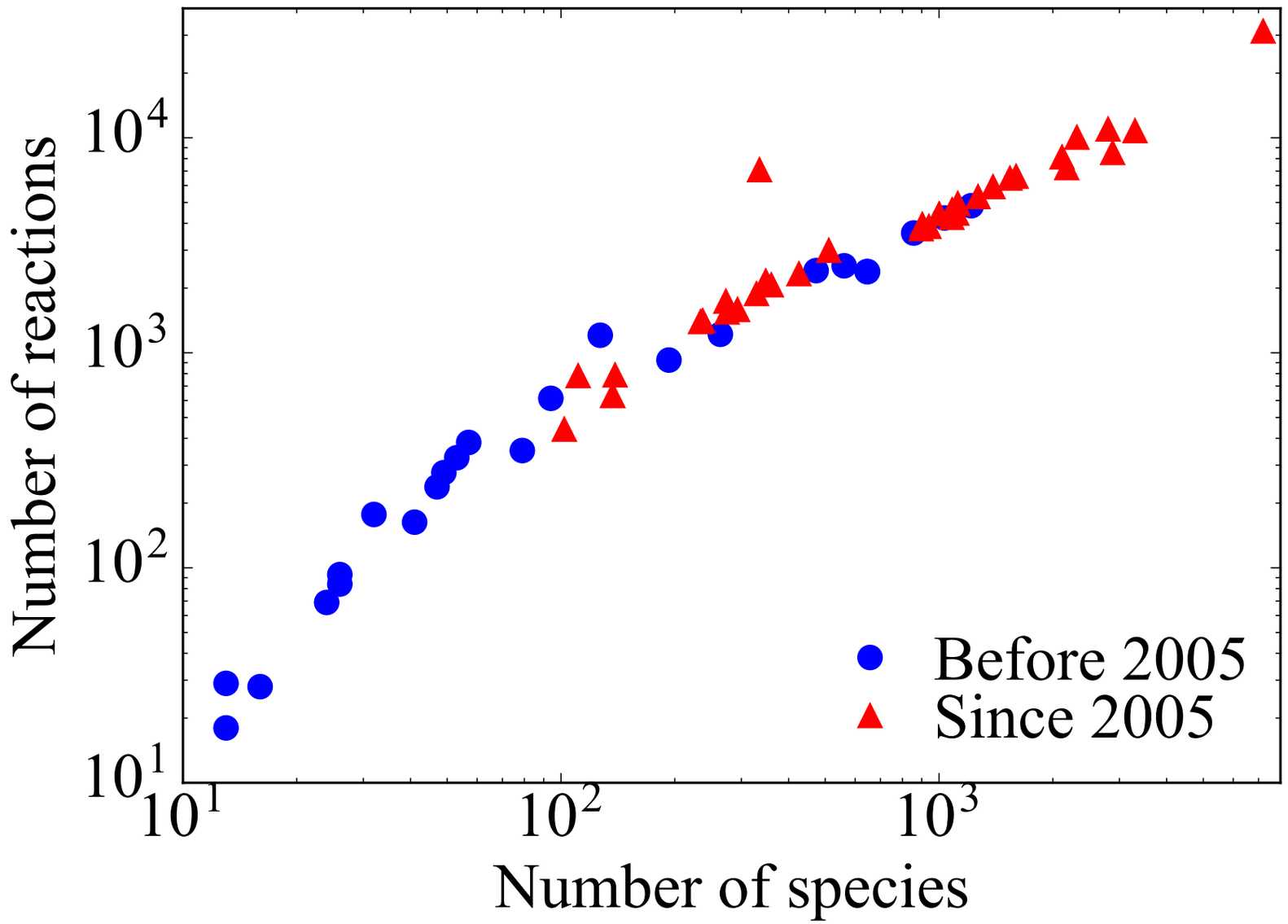
$H_2O_2 \longleftrightarrow 2OH$

$H_2O_2 + H \longleftrightarrow H_2O + OH$

$H_2O_2 + H \longleftrightarrow HO_2 + H_2$

$H_2O_2 + O \longleftrightarrow OH + HO_2$

$H + OH + M \longleftrightarrow H_2O + M$



Size of kinetic models

Hydrocarbon oxidation kinetic models poses challenges even for 0D simulations.

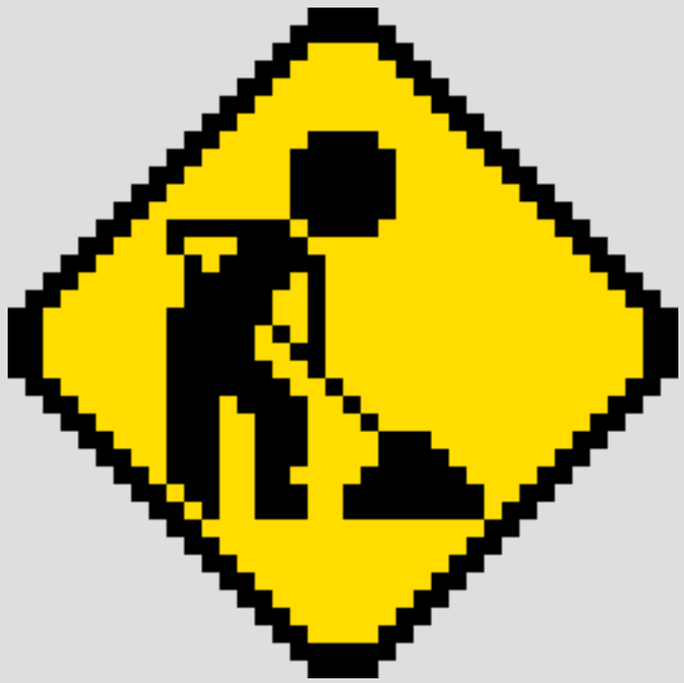
Kyle Niemeyer (2016): Hydrocarbon chemical kinetic model survey. figshare. https://doi.org/10.6084/m9.figshare.3792660

$$\begin{pmatrix} \frac{dY_1}{dt} \\ \frac{dY_2}{dt} \\ \vdots \\ \frac{dY_k}{dt} \end{pmatrix} \qquad \frac{dY_i}{dt} = \frac{W_i}{\rho}\omega_i$$

Today: H_2/CO model of Burke et al. with 13 species and 27 reactions

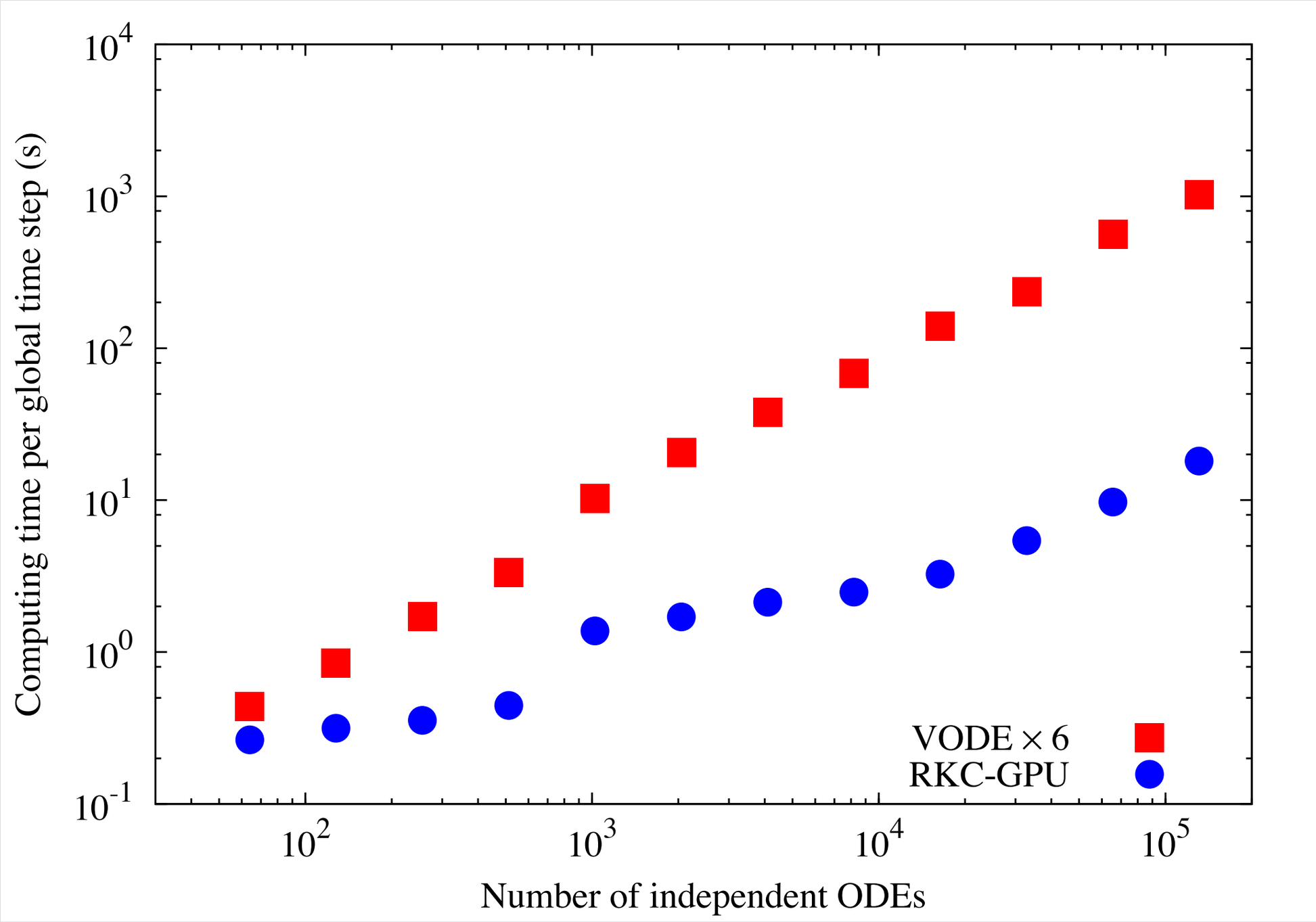
M. P. Burke, M. Chaos, Y. Ju, F. L. Dryer, and S. J. Klippenstein,
Comprehensive H2/O2 kinetic model for high-pressure combustion,
International Journal of Chemical Kinetics 44 (2012) 444–474.
https://doi.org/10.1002/kin.20603

Goals



- Now: Using sampled, realistic state data, evaluate stiffness metrics
- Eventually: use stiffness metric to switch/schedule integration algorithms

Motivation



https://doi.org/10.1016/j.jcp.2013.09.025

Stiffness index

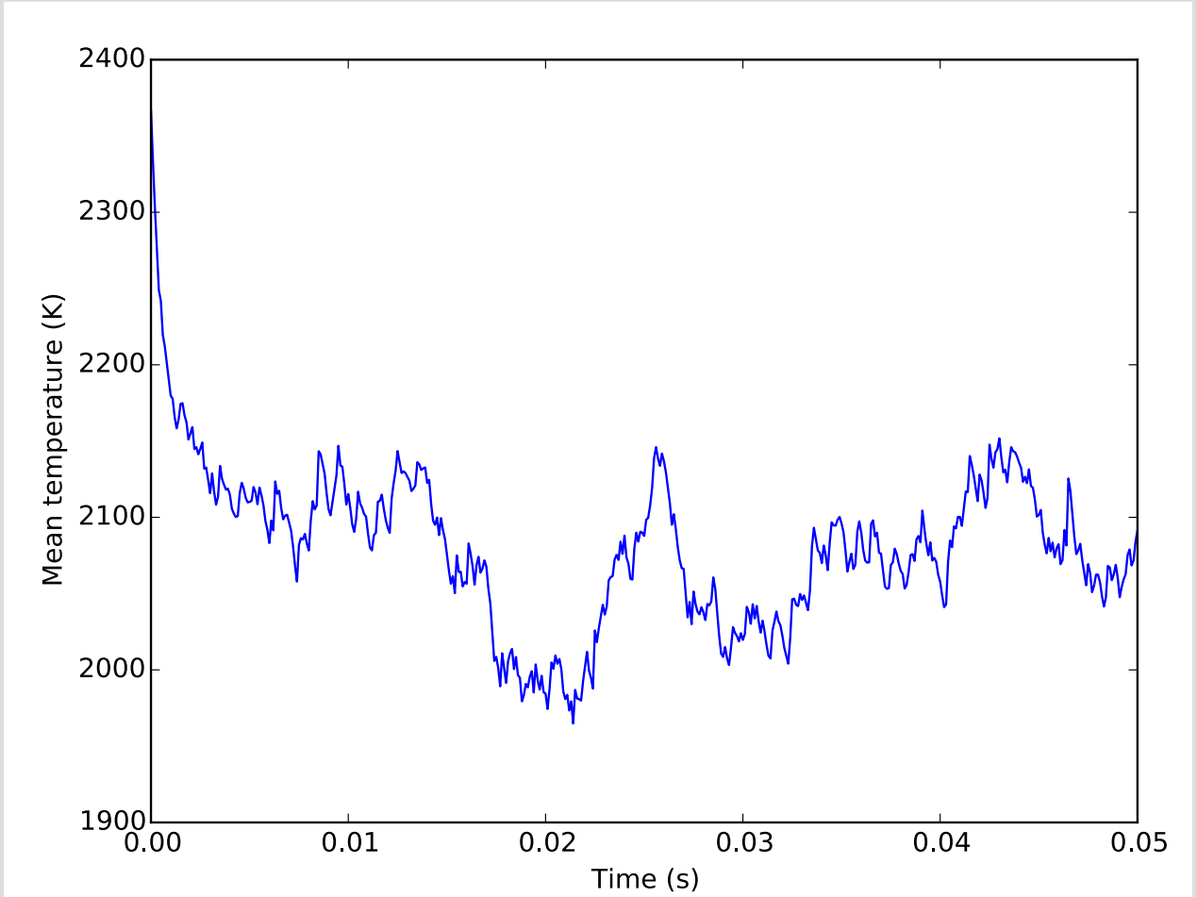
$$\text{index} = \rho[f_y(x_n, y(x_n))] \|y^{(p+1)}(x_n)\|^{-1/(p+1)}$$

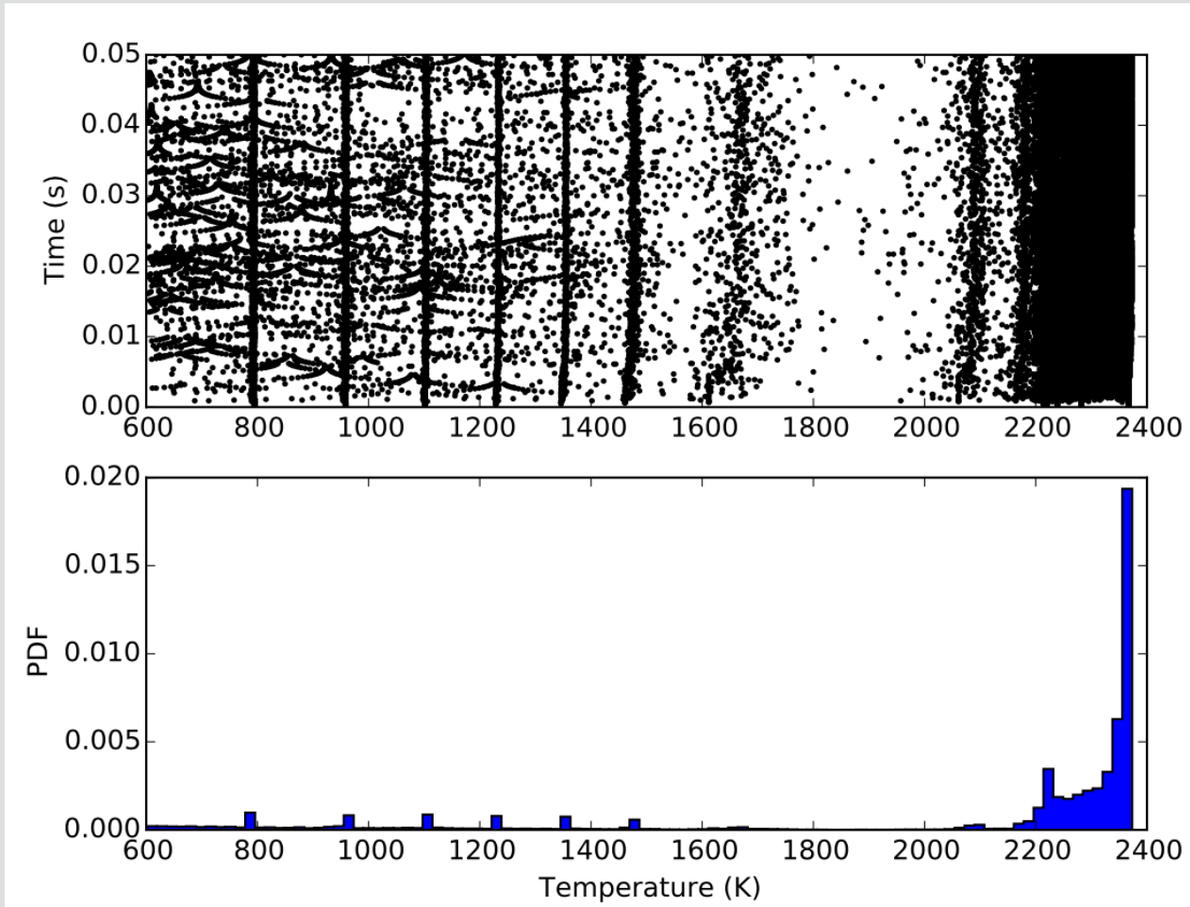
spectral radius of Jacobian

p+1 derivative of solution vector

L. F. Shampine, Type-insensitive ODE codes based on implicit A-stable formulas, *Mathematics of Computation* 39 (1982) 109–123. https://doi.org/10.1090/S0025-5718-1982-0658216-2

Partially Stirred Reactor (PaSR)

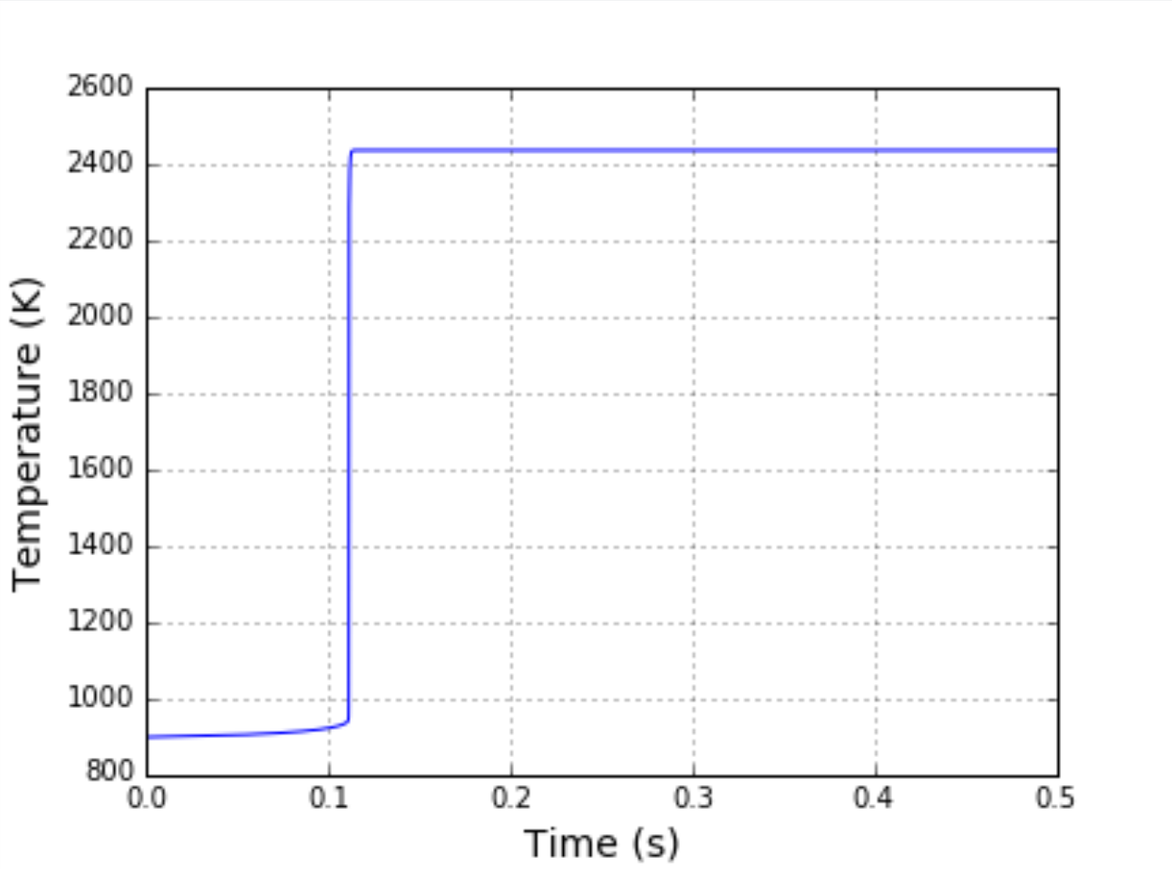




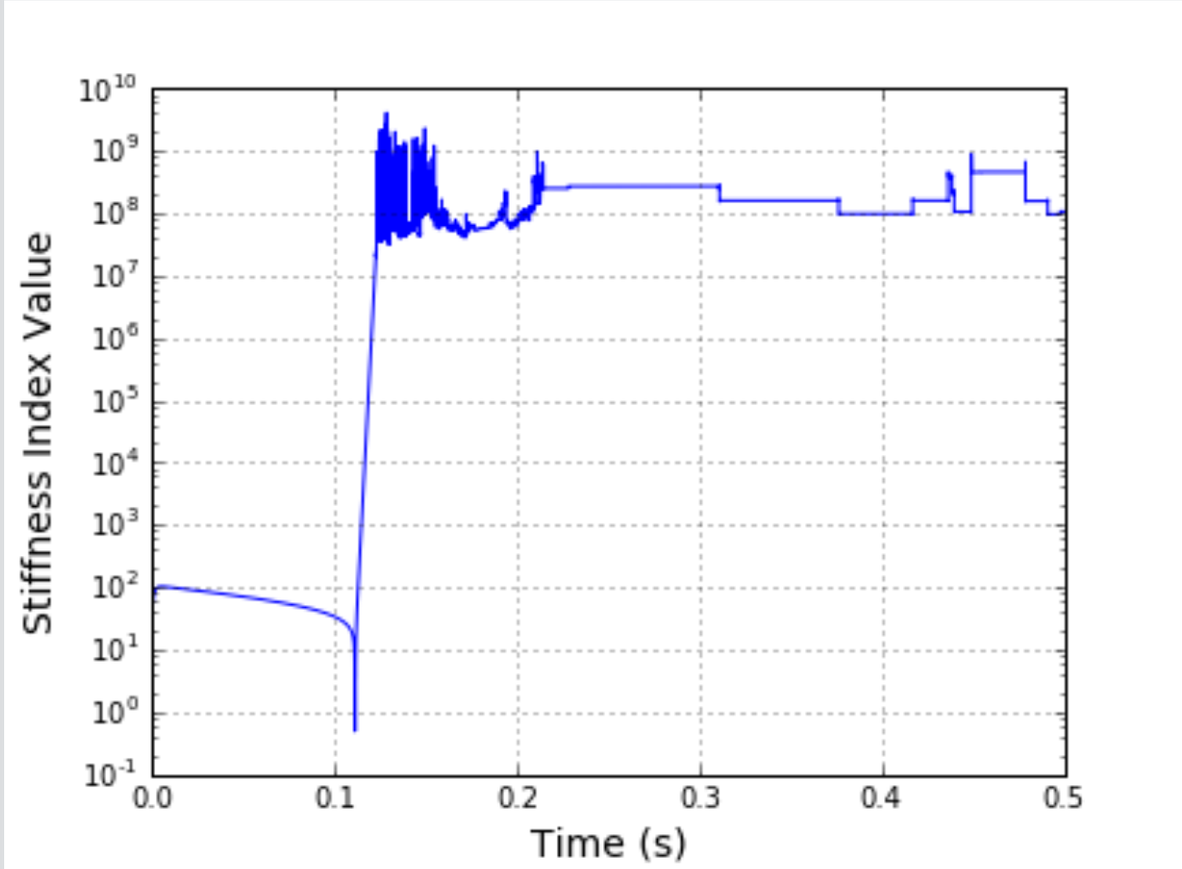
- Cantera-based PaSR implementation; premixed combustion with fresh fuel/air mixture & pilot streams
- Pairwise mixing, reaction fractional steps, inflow/outflow events

https://github.com/SLACKHA/pyJac

Autoignition case

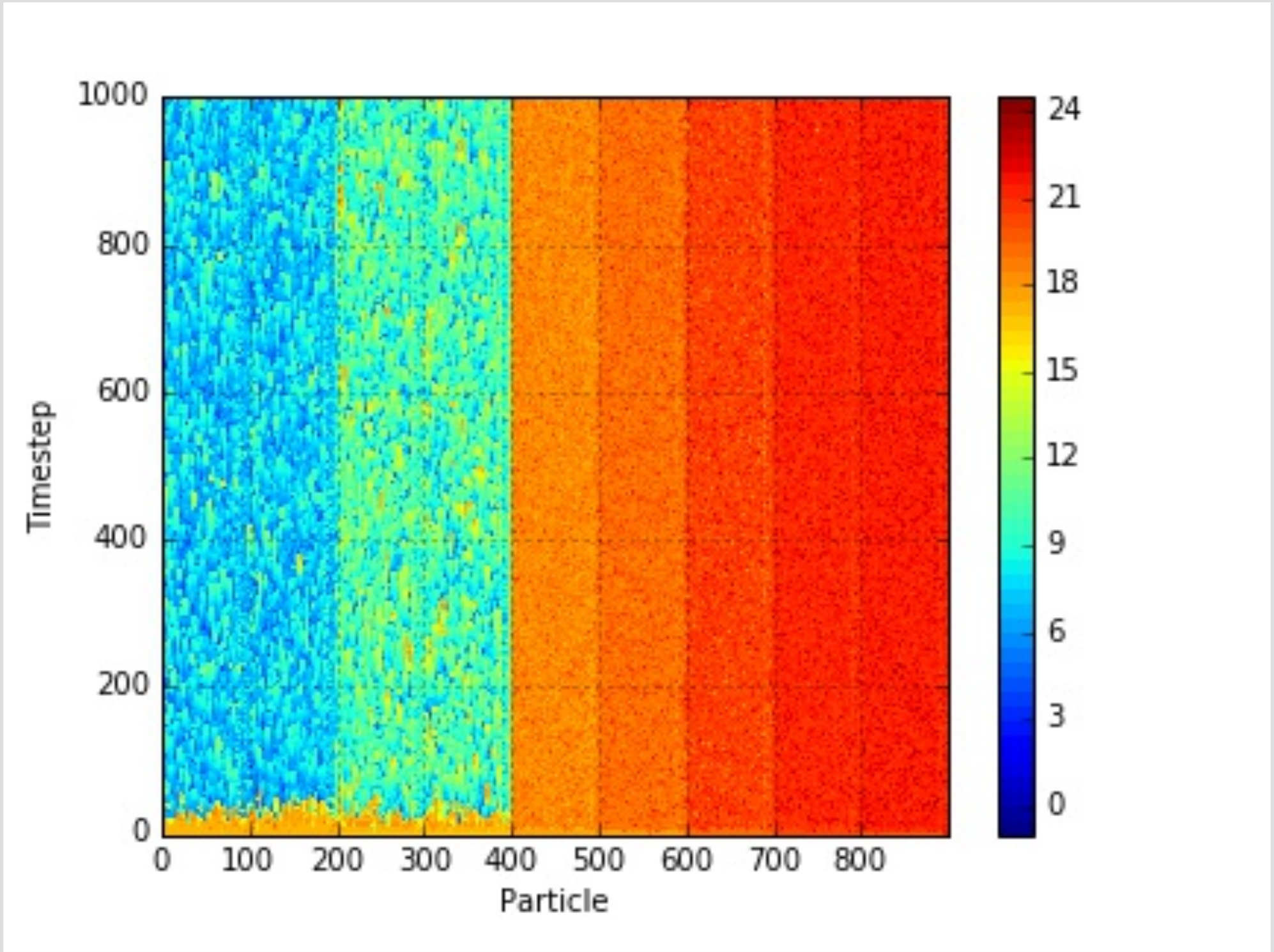


Temperature vs. time

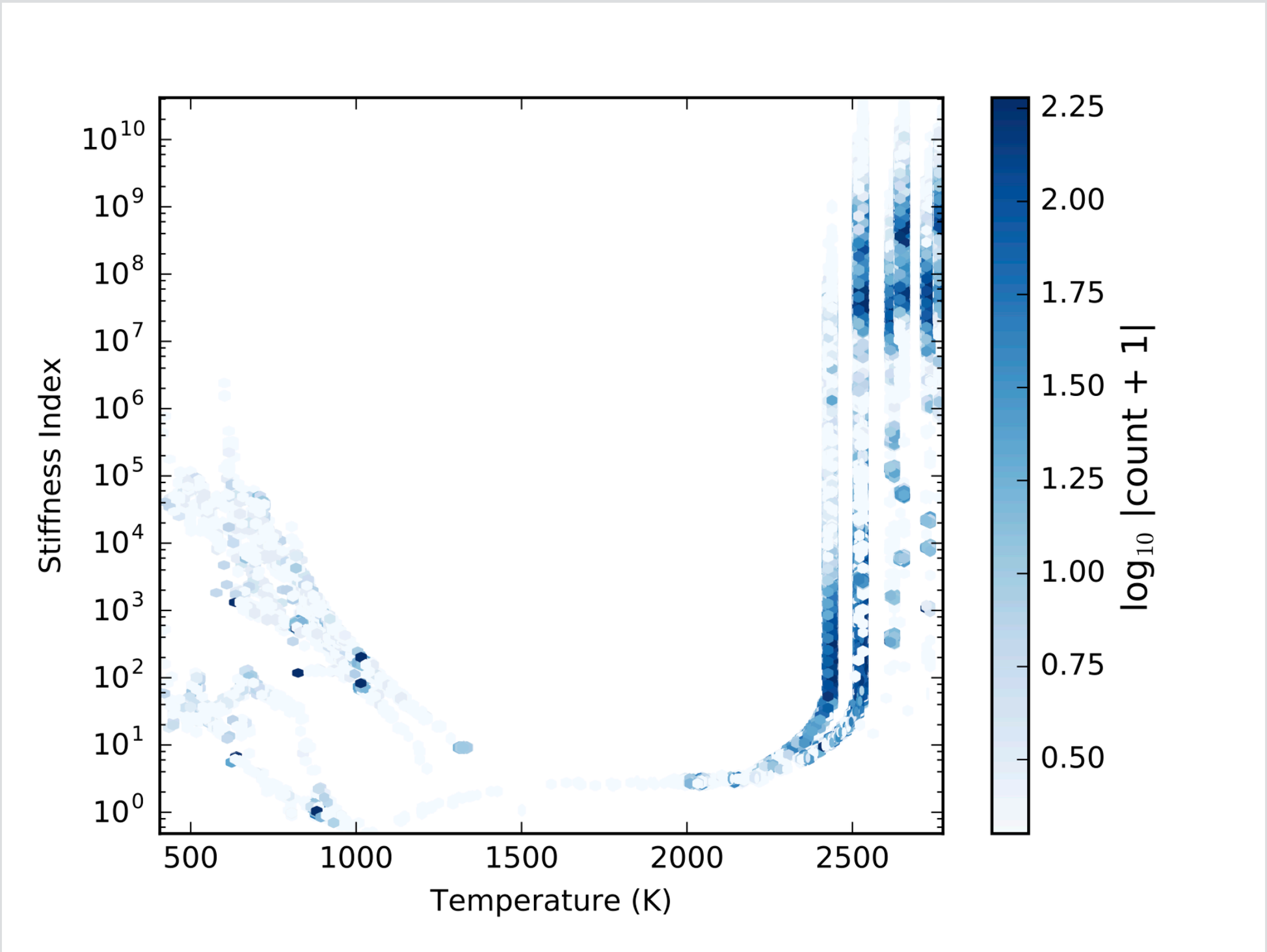


Stiffness index vs. time

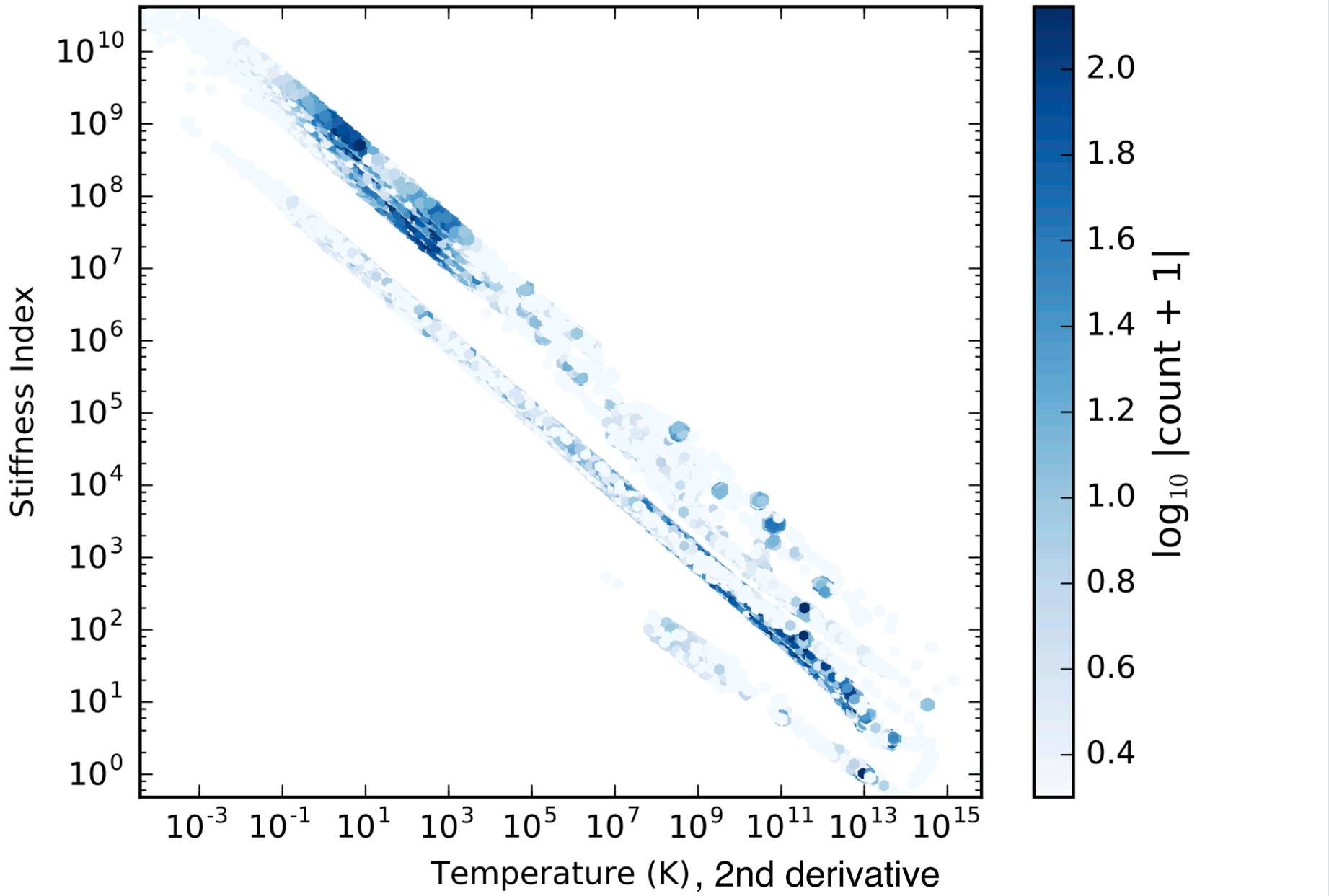
Sampled data



Stiffness index vs. temperature



Stiffness index vs. temperature 2nd derivative



Summary

- Evaluating Shampine stiffness metric for quantifying level of stiffness in chemical kinetic ODEs
- Initial indications: index matches expected/intuitive autoignition behavior
- Future work
  - Evaluate additional metrics
  - Compare with computational cost
  - Create model & scheduler for ODE solver
  - Prosper.

Thank you! Questions?

Project site
http://slackha.github.io

Acknowledgements:
Nick Curtis & Chih-Jen Sung, University of Connecticut
NSF award ACI-1535065