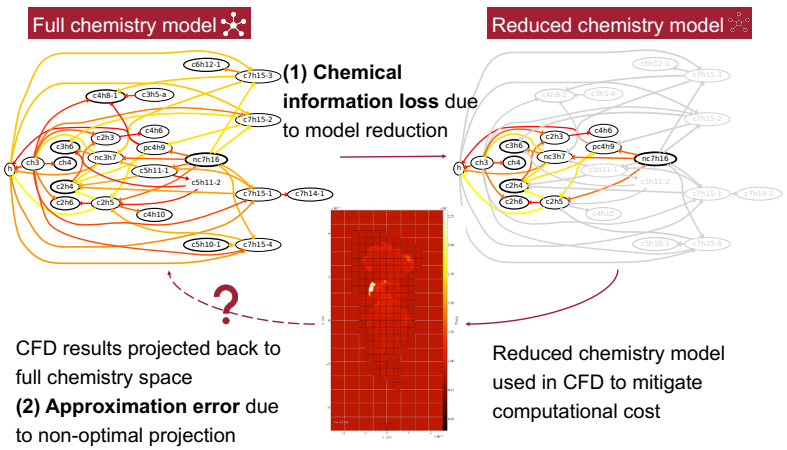
Iterative Workflow for Quantification and Minimization of Reduced Chemistry-Induced Uncertainties in Reacting Flow Simulation

[Hao-Wei Pang](1), Malik Hassanaly[2], Bruce Perry[2], Marc Day[2], William H. Green[1]

1 Massachusetts Institute of Technology

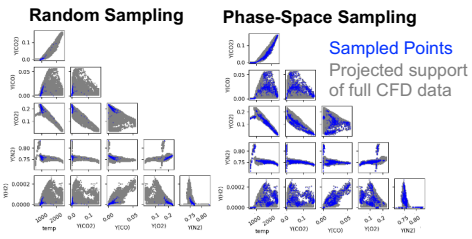
2 NREL Transforming ENERGY

1. INTRO | Reduced chemistry models mitigate computational cost but introduce two sources of uncertainties in reacting flow simulation



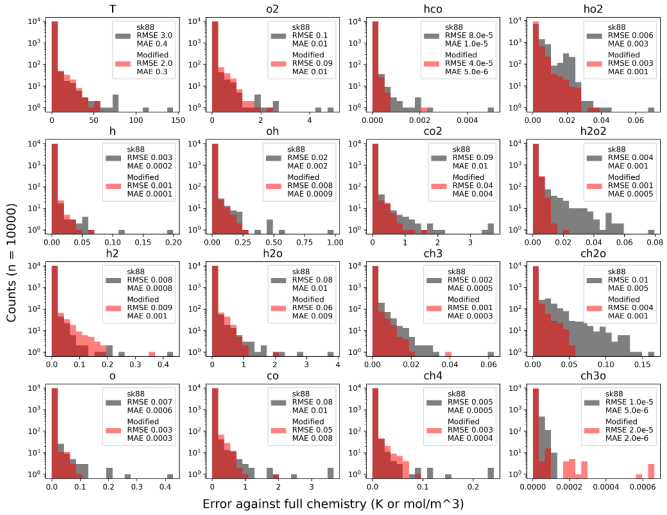
3. CASE STUDY

- Models used for case study
  - Full chemistry model: n-heptane oxidation model w 561 species by Curran et a
  - Reduced chemistry model: skeleton model with 88 species (sk88) by Yoo et al.



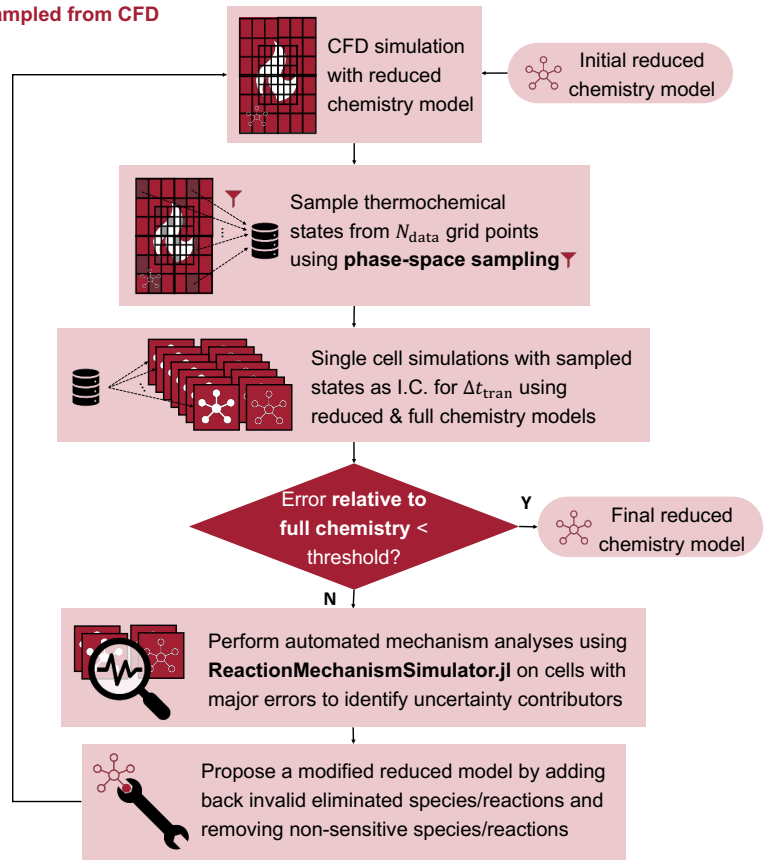
- Aiming to reduce uncertainties in predicted temperature compared to full chemistry
  - Modified model contains 90 species
  - Modified model outperforms sk88 for not only temperature but also many other key species

Error in original & modified reduced chemistry models against full chemistry model



2. WORKFLOW

2.1. Decreases (1) chemical information loss by modifying reduced chemistry model based on error analyses against full chemistry model at thermochemical states sampled from CFD



2.2. Minimizes (2) approximation error by solving for optimal projection using constrained optimization with flux snapshots

$$\underline{Y} = \boldsymbol{L}\underline{Z}$$

$$\frac{d\underline{Z}}{dt} = \underline{\Gamma}\left(\underline{Z}, T, P; \underline{k}_f, \underline{K}_{eq}\right) + \underline{F} \qquad \hat{\underline{Z}} = \boldsymbol{U}\underline{Y} = \boldsymbol{U}(\boldsymbol{L}\underline{Z}) \quad \boldsymbol{U}^* = ? \qquad \frac{d\underline{Y}}{dt} = \underline{\gamma}\left(\underline{Y}, T, P; \underline{k}_f, \underline{K}_{eq}\right) + \underline{f}$$

Integrated over Δt_{tran} to smooth out effects from short-lived reactive intermediates

Collect snapshots of fluxes for both reduced & full chemistry models

$$\boldsymbol{W} = \left(\int_{t_0}^{t_0+\Delta t_{tran}} \underline{\gamma}\left(\boldsymbol{L}\underline{Z}_1, T_1, P_1; \underline{k}_f, \underline{K}_{eq}\right) + \underline{f}\,dt \quad \dots \quad \int_{t_0}^{t_0+\Delta t_{tran}} \underline{\gamma}\left(\boldsymbol{L}\underline{Z}_{N_{data}}, T_{N_{data}}, P_{N_{data}}; \underline{k}_f, \underline{K}_{eq}\right) + \underline{f}\,dt\right)$$

$$\boldsymbol{V} = \left(\int_{t_0}^{t_0+\Delta t_{tran}} \underline{\Gamma}\left(\underline{Z}_1, T_1, P_1; \underline{k}_f, \underline{K}_{eq}\right) + \underline{F}\,dt \quad \dots \quad \int_{t_0}^{t_0+\Delta t_{tran}} \underline{\Gamma}\left(\underline{Z}_{N_{data}}, T_{N_{data}}, P_{N_{data}}; \underline{k}_f, \underline{K}_{eq}\right) + \underline{F}\,dt\right)$$

Minimize differences between projected reduced and full snapshots

Ensure projection back to full chemistry space

$$\boldsymbol{U}^* = \underset{\boldsymbol{\Lambda},\boldsymbol{U}}{\operatorname{argmin}} \frac{1}{2}\left|\boldsymbol{W}^T\boldsymbol{U}^T - \boldsymbol{V}^T\right|_2^2 + \boldsymbol{\Lambda}^T(\boldsymbol{L}^T\boldsymbol{U}^T - \boldsymbol{I}),$$ combining derivative $\frac{\partial \mathcal{L}}{\partial \boldsymbol{U}} = \boldsymbol{W}(\boldsymbol{W}^T\boldsymbol{U}^T - \boldsymbol{V}^T) +$

$\boldsymbol{L}\boldsymbol{\Lambda} = 0$ & constraint, $\boldsymbol{U}^*$ can be solved with $\begin{pmatrix} \boldsymbol{W}\boldsymbol{W}^T & \boldsymbol{L} \\ \boldsymbol{L}^T & \boldsymbol{0} \end{pmatrix}\begin{pmatrix} \boldsymbol{U}^T \\ \boldsymbol{\Lambda} \end{pmatrix}^* = \begin{pmatrix} \boldsymbol{W}\boldsymbol{V}^T \\ \boldsymbol{I} \end{pmatrix}$

ReactionMechanismSimulator.jl

Phase-space sampling

Funding sources

U.S. DEPARTMENT OF ENERGY

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Trust Scholarship

NREL/PO-2C00-83520

This work was authored in part by the National Renewable Energy Laboratory, operated by Alliance for Sustainable Energy, LLC, for the U.S. Department of Energy (DOE) under Contract No. DE-AC36-08GO28308. This research was supported by the Exascale Computing Project (ECP), Project Number: 17-SC-20-SC, a collaborative effort of two DOE organizations, the Office of Science and the National Nuclear Security Administration, responsible for the planning and preparation of a capable exascale ecosystem including software, applications, hardware, advanced system engineering, and early test bed platforms to support the nation's exascale computing imperative. The views expressed in the article do not necessarily represent the views of the DOE or the U.S. Government. The U.S. Government retains and the publisher, by accepting the article for publication, acknowledges that the U.S. Government retains a nonexclusive, paid-up, irrevocable, worldwide license to publish or reproduce the published form of this work, or allow others to do so, for U.S. Government purposes.