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PDF Equations for Propagating Parameter Uncertainty in Reacting Flow CFD

Hemanth Kolla, Michael Hansen

Sandia National Laboratories

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- This presentation describes objective technical results and analysis. Any subjective views or opinions that might be expressed in the paper do not necessarily represent the views of the U.S. Department of Energy or the United States Government.

Motivation: Uncertainty Quantification for CFD

Uncertainty Quantification (UQ) for computational mechanics is challenging

$$\frac{D}{Dt}\phi = \mathcal{R}(\phi, \lambda; x, t)$$

- Inaccurate physics models
- Uncertain parameters
- Initial/Boundary conditions
- Chaotic dynamics

epistemic (reducible)

aleatory (irreducible)

Motivation: Uncertainty Quantification for CFD

Our focus: propagate parameter uncertainty (forward UQ)

$$\frac{\mathrm{D}\boldsymbol{\phi}}{\mathrm{D}t} = \mathcal{R}(\boldsymbol{\phi}, \boldsymbol{\lambda}; \boldsymbol{x}, \boldsymbol{t})$$

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Approach: Solve Evolution Equation for Joint-PDF

The underlying PDE, with uncertain parameters, implies an exact equation for joint PDF [1,2,3]

$$\frac{\mathrm{D}}{\mathrm{D}t}\boldsymbol{\phi} = \mathcal{R}(\boldsymbol{\phi}, \boldsymbol{\lambda}; x, t), \quad p_{\lambda}(\Lambda \qquad \Longrightarrow \qquad \frac{\mathrm{D}\boldsymbol{p}_{\phi}}{\mathrm{D}t} = -\frac{\partial}{\partial}[\boldsymbol{p}_{\phi}\langle\mathcal{R}|_{\phi}, \Lambda; x, t\rangle]$$

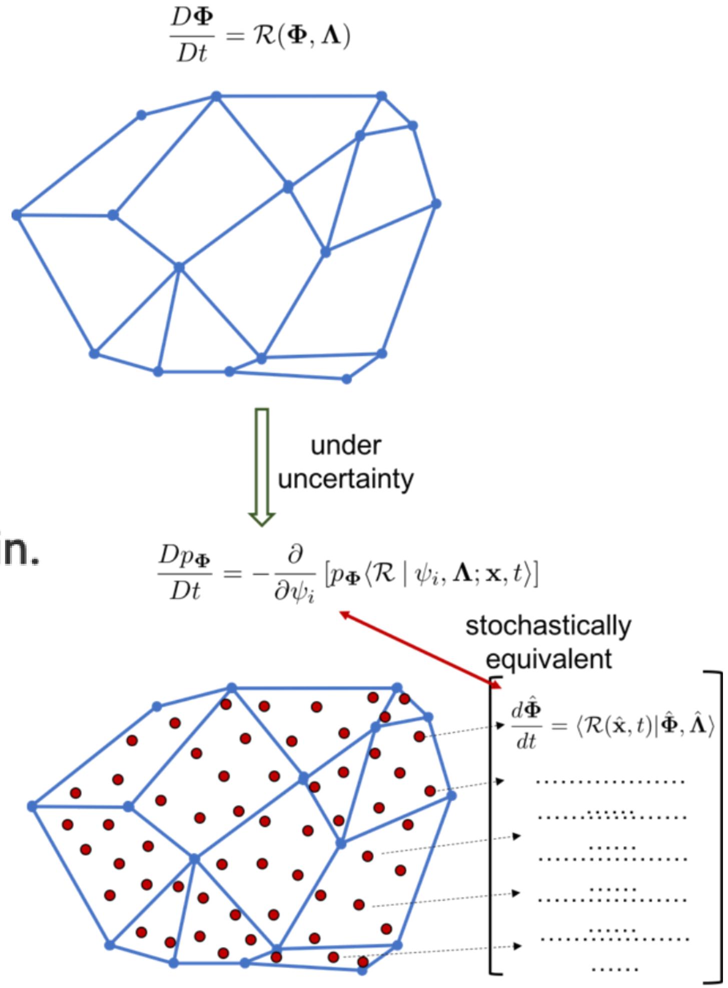
<u>Advantages:</u>

- The PDF, $\boldsymbol{p}_{\phi}(\boldsymbol{\Phi};\mathbf{x},t)$, has full field information of uncertainty statistics.
- QoIs for UQ are derivable from the joint PDF.
- More informative than moments of $\boldsymbol{\phi}$.
- Applications with non-Gaussian statistics are better characterized.

[1] S.B.Pope, *Prog. Energy. Comb. Sci.* , vol.11, pp:119, 1985 .
[2] D.M.Tartakovsky, P.A.Gremaud, In: *Handbook of Uncertainty Quantification*, pp:763, 2017.
[3] R.E.Jones, *et al.*, *Int. J. Num. Meth. Engg.* , vol.122, pp:6955, 2021.

Solving PDF Equation: Challenges & Proposed Solution

$$\frac{D\boldsymbol{p}_{\phi}}{Dt} = -\frac{\partial}{\partial \psi_i}\left[\boldsymbol{p}_{\phi}\langle \mathcal{R} | \phi_i, \Lambda; \boldsymbol{x}, t\rangle\right]$$



<u>Challenge:</u>

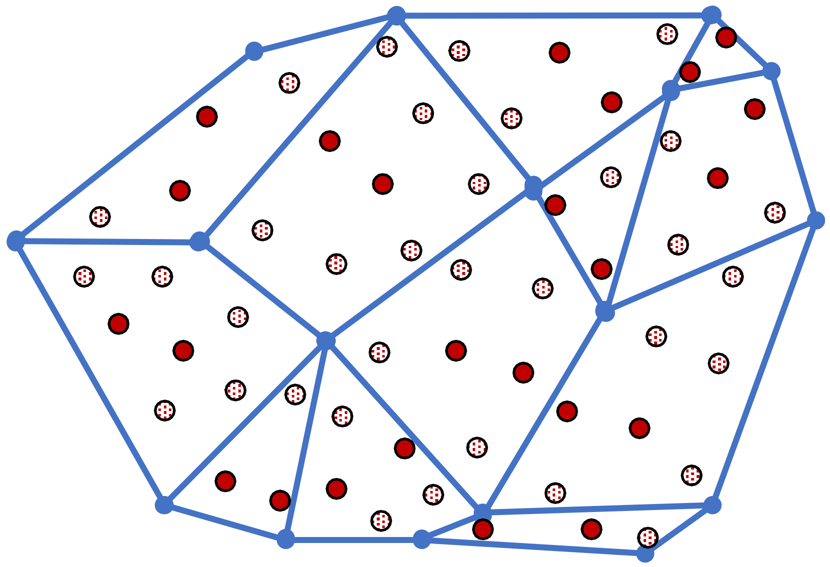
- Very high dimensional PDE, conventional discretizations will be unsuitable.

<u>Solution:</u> Hybrid Eulerian-Lagrangian approach[1]

- Sample the parameter distribution; solve each sample ODE over desired domain.
- "Stochastically equivalent"; PDF constructed from ensemble at any $(\boldsymbol{x}, \boldsymbol{t})$ is equivalent to that obtained from solving the PDF equation.
- Computational cost: solve only few samples exactly, rest approximately
  - Boils down to approximating $\mathcal{R} \approx f(\boldsymbol{\lambda})$
  - Existing UQ approaches seek the approximation $\boldsymbol{\phi} \approx f(\boldsymbol{\lambda})$

[1] S.B.Pope, *Prog. Energy. Comb. Sci.* , vol.11, pp:119, 1985 .

Solution Methodology & Closure

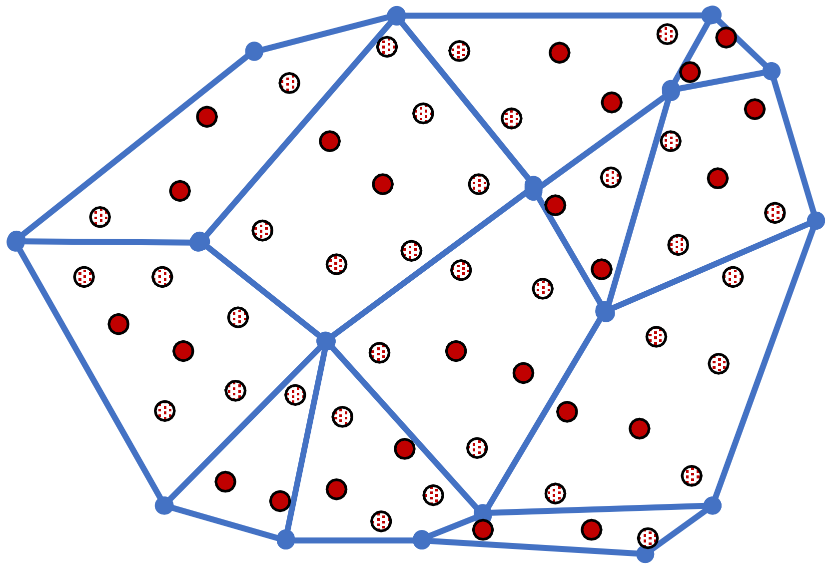


$\frac{d}{dt}\hat{\phi} = \mathcal{R}(\hat{\phi}, \hat{\Lambda}, x, t)$ solved for each Lagrangian sample

- "exact" samples, $\mathcal{R}_e = \mathcal{R}(\hat{\Lambda}_e)$
- "approximate" samples, $\mathcal{R}_a \approx f(\hat{\Lambda}_a, \mathcal{R}_e)$

collocation in the Λ space

Solution Methodology & Closure



$\frac{d\hat{\phi}}{dt} = \mathcal{R}(\hat{\phi}, \hat{\Lambda}, x, t)$ solved for each Lagrangian sample

- "exact" samples, $\mathcal{R}_e = \mathcal{R}(\hat{\Lambda}_e)$
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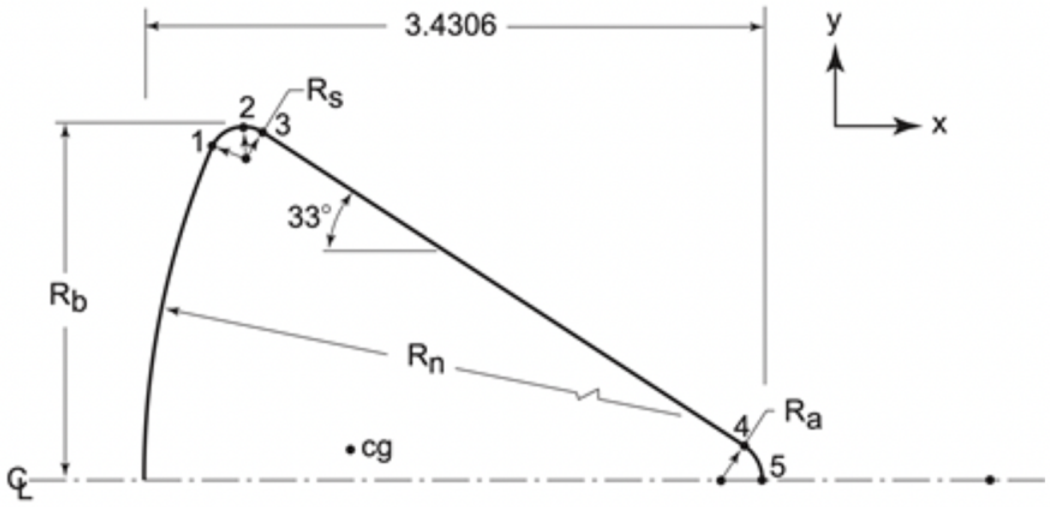
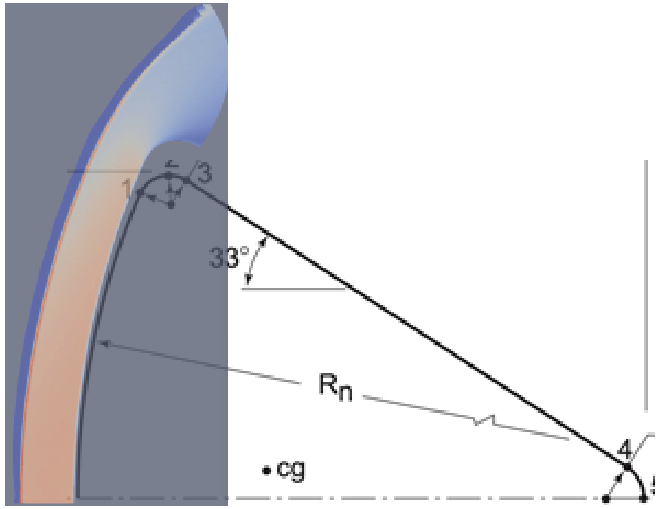
collocation in the Λ space

- For reacting flow CFD, further split $\mathcal{R}_a$:
  - non-local part, involving spatial derivatives (e.g. diffusion); requires approximation.
  - local part (e.g. chemical reactions); treated exactly.
- Further details in the paper.

Target Problem: Apollo Re-entry at Mach 30



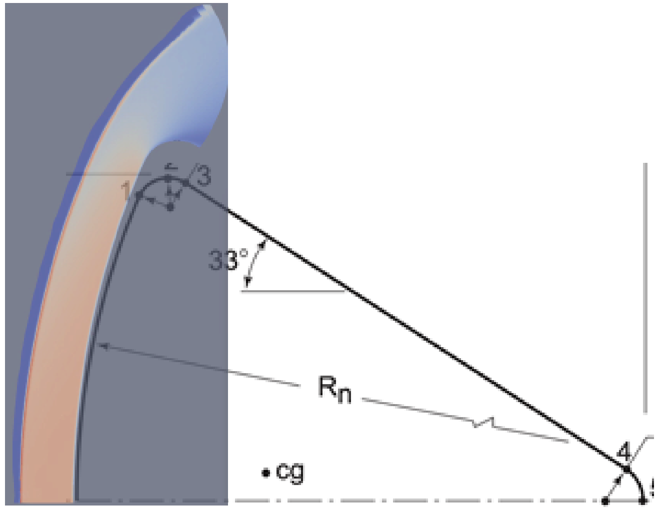


- UQ for hypersonic flow with thermochemical non-equilibrium
- Sandia Parallel Aerodynamics Reentry Code (SPARC[1])
- 2-temperature (T_{tr}, T_{vib}) formulation; 5-species chemistry of Park 1990.
- For steady problems, Lagrangian sample ≡ streamline tracing.

[1] B.A.Freno, B.R.Carnes, V.G.Weirs, *J. Comp. Physics*, vol.425, p.109752, 2021.

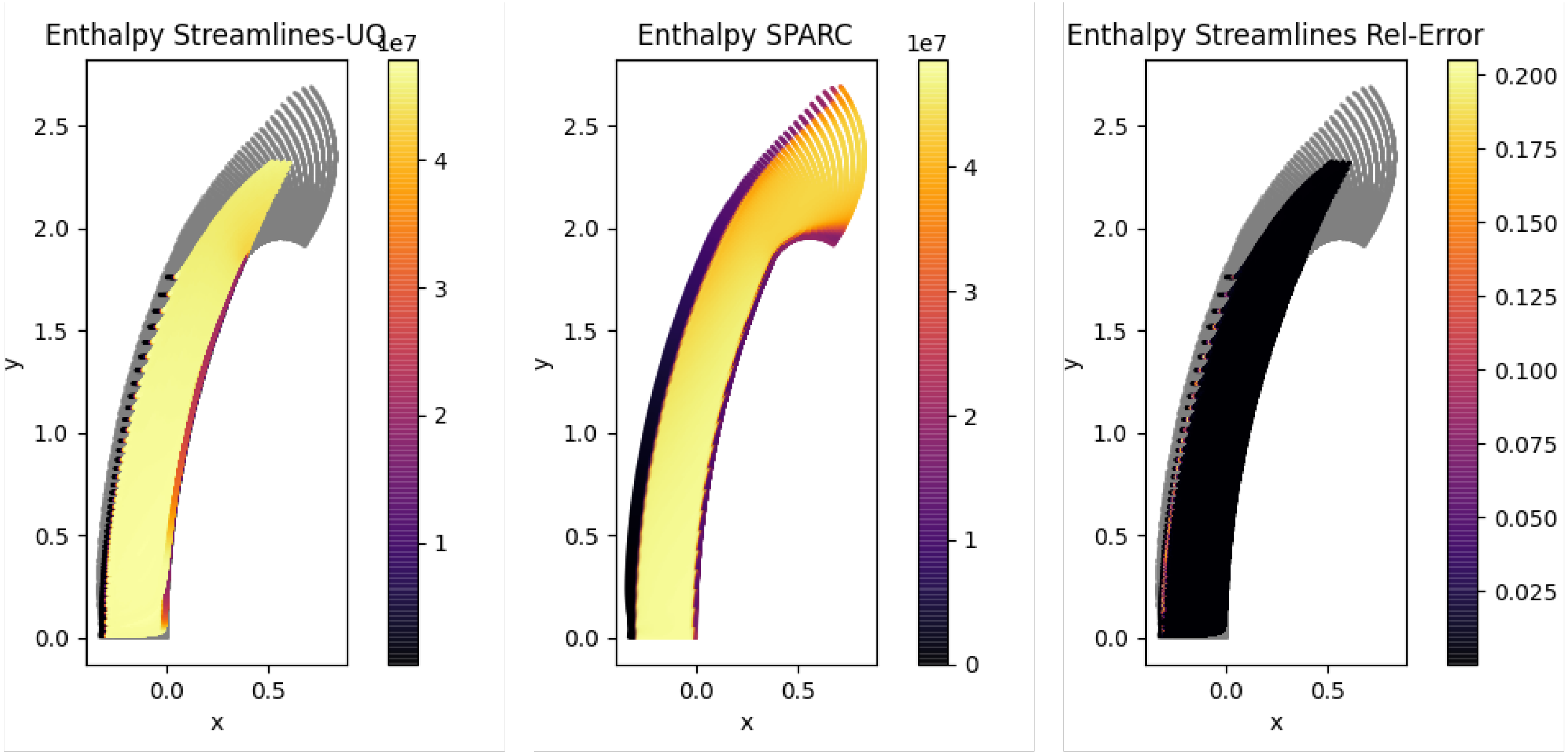
Target Problem: Apollo Re-entry at Mach 30

- Two cases with a chemistry parameter treated as uncertain.
- For each case:
  - 2 exact samples (exact SPARC solutions): $\lambda_{min}, \lambda_{max}$
  - Compute approximate streamline for $\lambda_a = 0.5(\lambda_{min} + \lambda_{max})$
- Assess accuracy of the approximate streamlines by a posteriori comparison with SPARC.



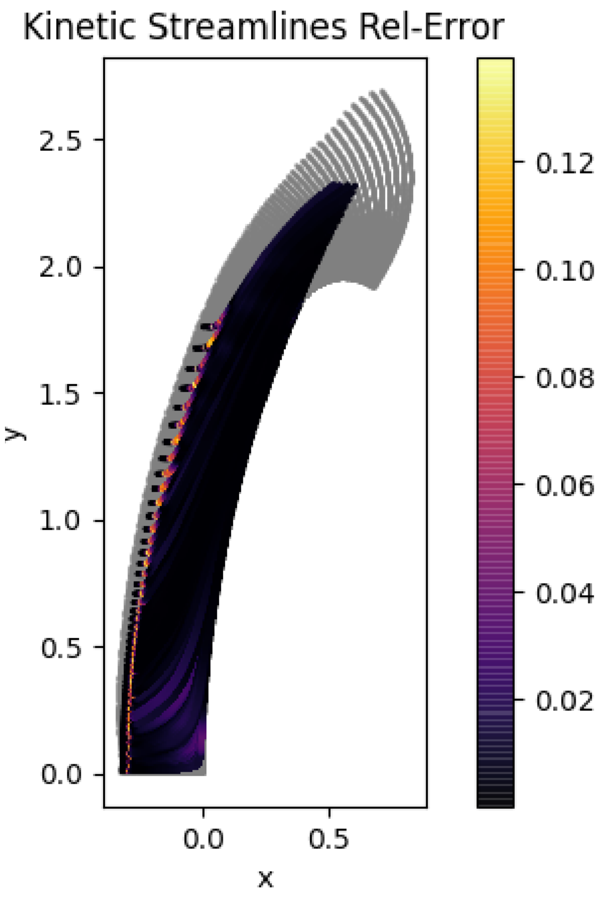
_	Description	Reaction	_min	_max
$\log_{10}($ $)$	: collision coefficients factor	$\#_2$ + " , # + # + "	-3.0	1.0
$\log_{10}($⇠$)$	⇠: pre-exp factor	$\#_2$ + $, #$ + #	14.80618	15.80618

Results: Accuracy of Streamlines Enthalpy

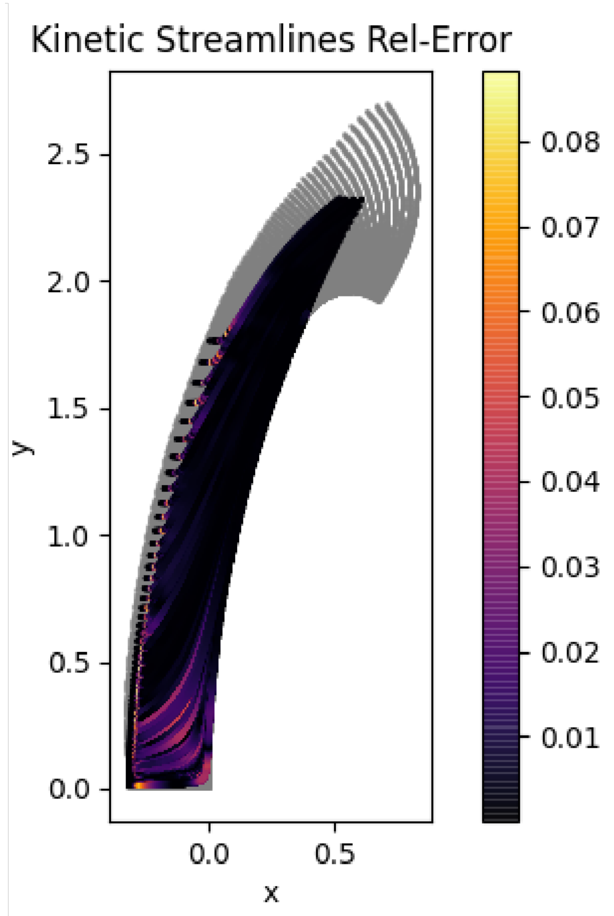


Results: Accuracy of Streamlines Kinetic Energy

Case-1

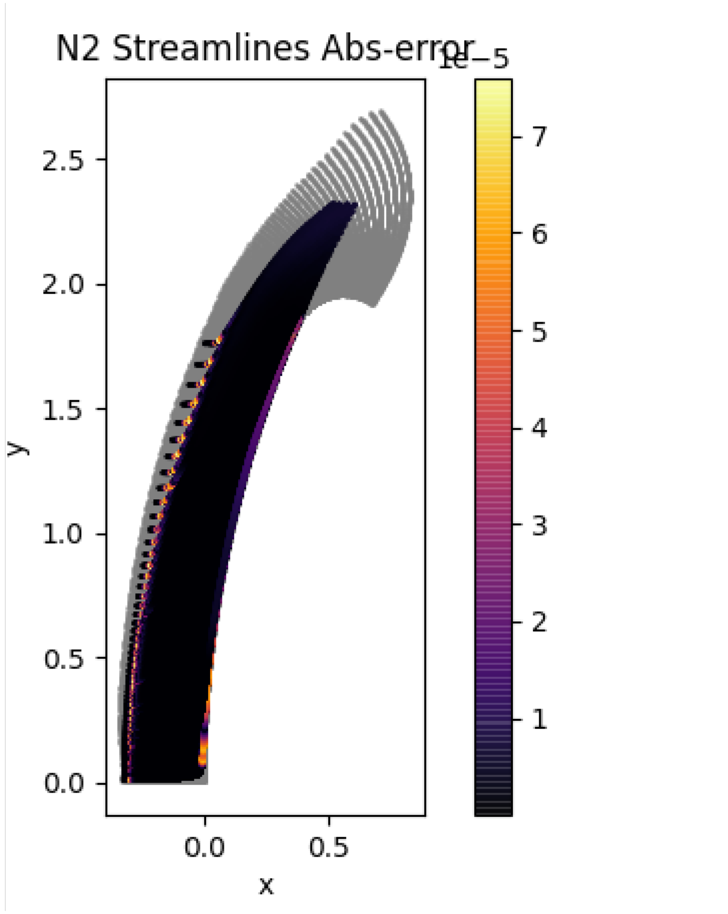


Case-2

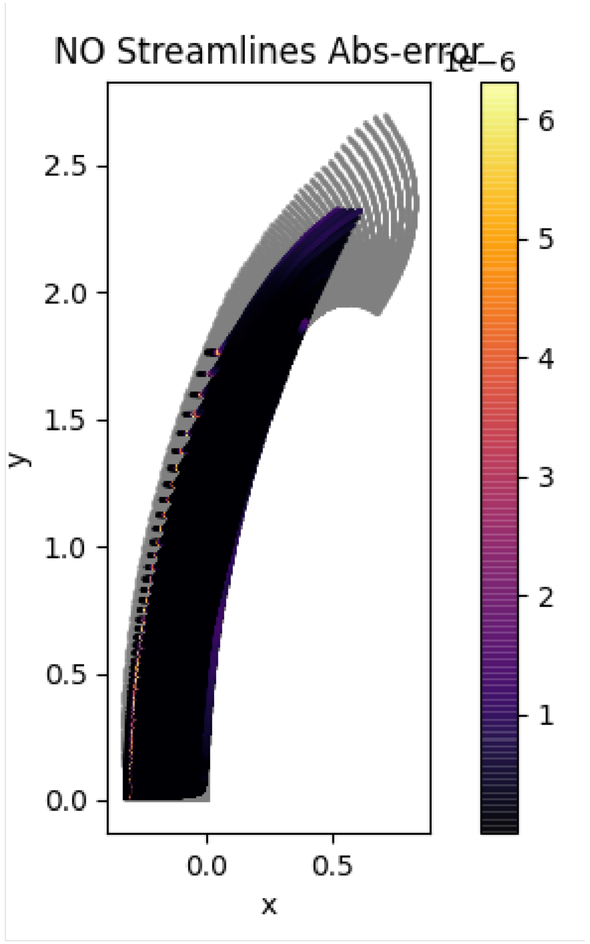


Results: Accuracy of Streamlines Species Mass Fractions

Case-1



Case-2



Conclusions & Future Work

- We propose a PDF equation approach for propagating parameter uncertainty.
- Equation is exact, but challenging to solve due to high-dimensionality.
- We adopt a hybrid Eulerian-Lagrangian approach, motivated by turbulence modelling.
- We apply the method to a hypersonic re-entry problem: Apollo capsule at Mach 30.
- We propagate uncertainty of chemistry parameters.
- Closure approach for approximate streamline integration gives good accuracy for both primitive (species mass fractions), and derived variables (enthalpy, kinetic energy).
- An ensemble of approximate streamlines, sampling the range of parameter uncertainty, provide the PDFs anywhere in the computational domain.
- Future work will extend to multiple parameters (collocation in higher dimensions), ensuring stability for approximate solutions, unsteady problems.

Thank You!

hnkolla@sandia.gov