Direct Numerical Simulation of Supersonic Reacting Mixing Layers

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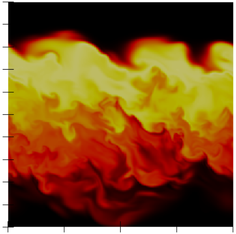
About Me

- Postdoctoral Research Fellow @ The Centre for Hypersonics, The University of Queensland, Australia
- Finished PhD in 2019 with Prof. Vince Wheatley

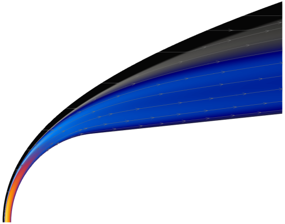
Things I do:

- The Gasdynamic Toolkit (`github.com/gdtk-uq/gdtk`)
- equilibrium-c: Calculator for eq chemistry (`github.com/uqngibbo/equilibrium-c`)
- Simulations:

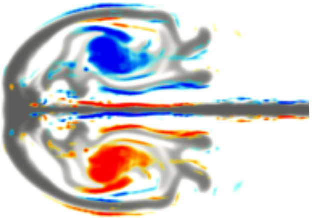
Supersonic Combustion



High Temperature Flows

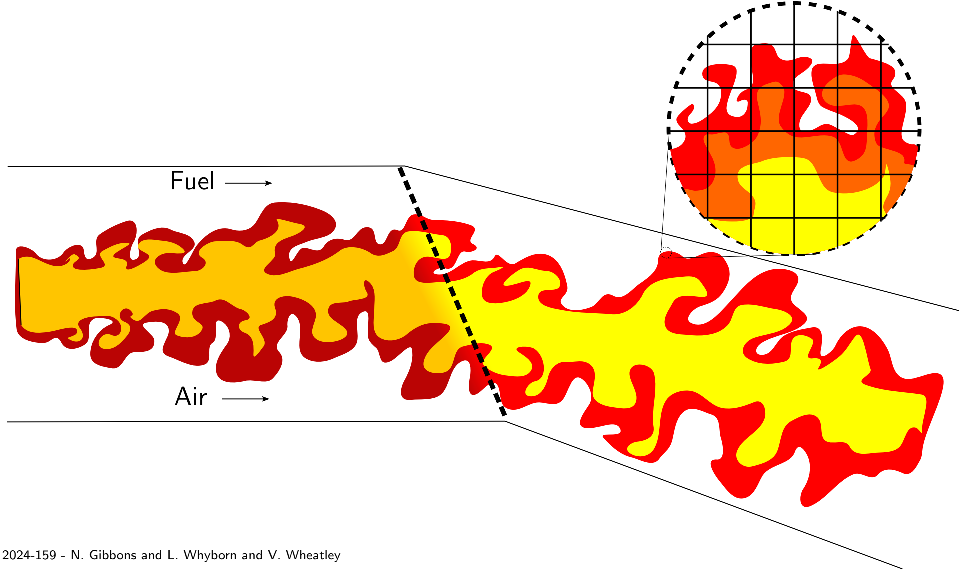


Compressible Turbulence



Today's Talk: Combustion Models for Compressible Flow

Models are needed to approximate turbulence on (typically) too-coarse CFD grids:



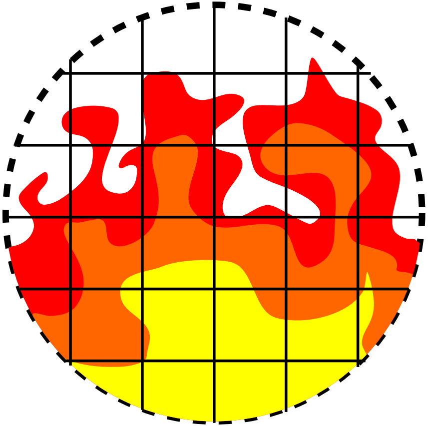
Today's Talk: Combustion Models for Compressible Flow

$\dot{\omega}$ are the reaction rates:

$$\dot{\omega} = M \sum_r (\nu^-_{rs} - \nu^+_{rs}) \left(k^+_r \Pi_n [X_n]^{\nu^+_{rn}} - k^-_r \Pi_n [X_n]^{\nu^-_{rn}} \right)$$

Integrate them over the PDF of the species and temperature:

$$\bar{\dot{\omega}} = \int P(Y'_s, T') \; \dot{\omega}(Y'_s, T') \; dY'_s dT'$$

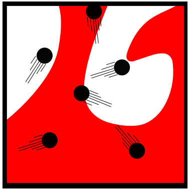


Today's Talk: Combustion Models for Compressible Flow

$$\bar{\dot{\omega}} = \int P(Y_s', T')\ \dot{\omega}(Y_s', T')\ dY_s' dT'$$

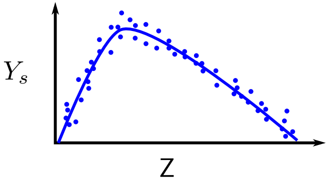
Multiple Mapping Closure:

- Lagrangian Monte-Carlo method
- Sparse stochastic particles
- Cleary and Klimenko, 2009



Conditional Moment Closure:

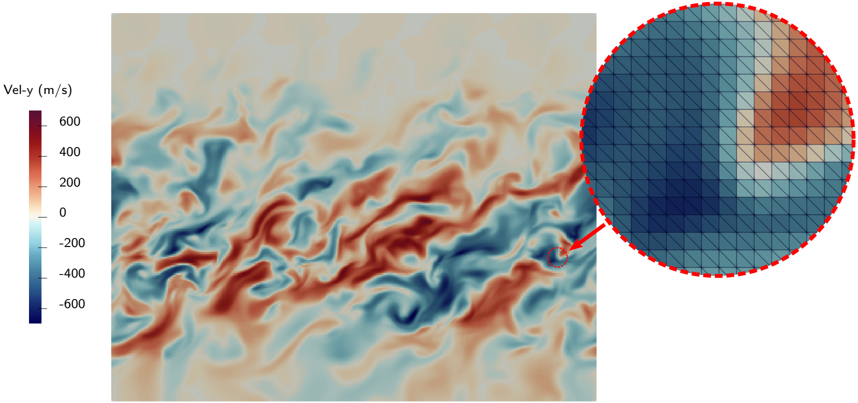
- Use correlations of Z and Y_s
- Model mixture fraction (Z) only
- Klimenko and Bilger, 1999



Methodology: Direct Numerical Simulations

It is possible to resolve turbulence at low enough Reynolds numbers:

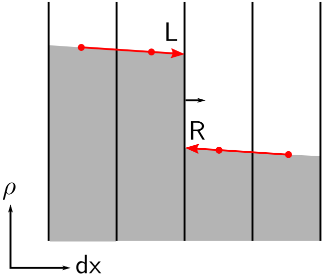
- In this work: time developing supersonic mixing layer from Gibbons, 2019
- Simulations using Eilmer, part of UQ's open-source GDTk
- Needs specialised numerics and high parallel performance



Methodology: Numerical Method

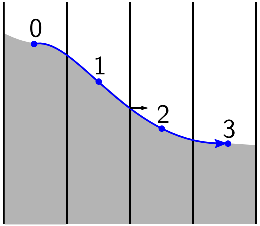
- Inviscid fluxes are computed using two very different kinds of numerical method:

AUSMDV: Wada and Liou, 1994



$$F^c = \frac{1}{2}(\rho u)_f \begin{bmatrix} 1 \\ u \\ H \end{bmatrix}_{L/R} + p_f$$

SPB-ASF: Fisher et al., 2012



$$\mathbf{F}^c_{div} = \frac{1}{12}\left[-\rho_0 u_0 + 7\rho_1 u_1 + 7\rho_2 u_2 - \rho_3 u_3\right]$$

$$\mathbf{F}^c_{prod} = \frac{1}{12}\left[-\rho_0 u_2 - \rho_2 u_0 + 8\rho_1 u_2 + 8\rho_2 u_1 - \rho_1 u_3 - \rho_3 u_1\right]$$

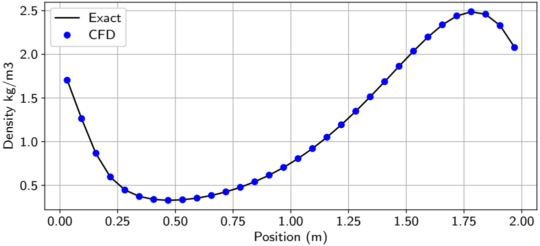
$$F^c = \alpha F^c_{div} + (1-\alpha) F^c_{prod}$$

Results: Steepening Wave Problem

- Analytic compressible flow solution from Landau and Lifshitz (1987)

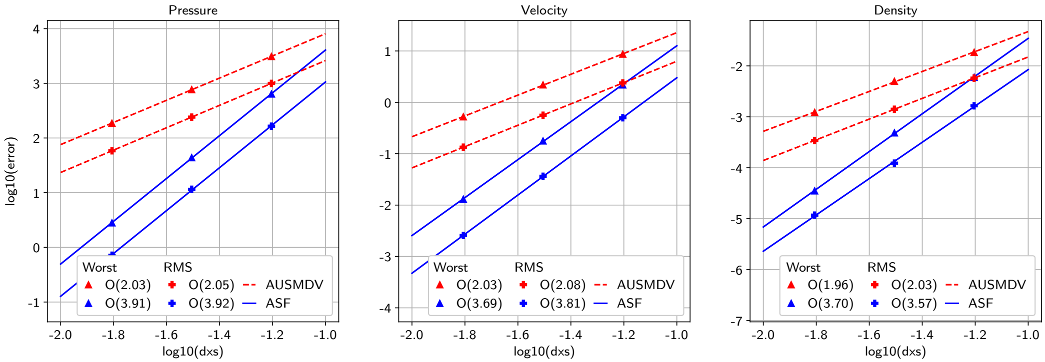
$$u(x) = u_0(x)\ sin\left(\pi(x - t(c_0 + \frac{1}{2}(\gamma+1)u(x)))\right)$$

$$p(x) = p_0\left(\frac{1+(\gamma-1)u(x)}{2c_0}\right)^{\frac{2\gamma}{\gamma-1}} \quad \rho(x) = \rho_0\left(\frac{1+(\gamma-1)u(x)}{2c_0}\right)^{\frac{2}{\gamma-1}} \quad T(x) = \frac{p(x)}{R\rho(x)}$$



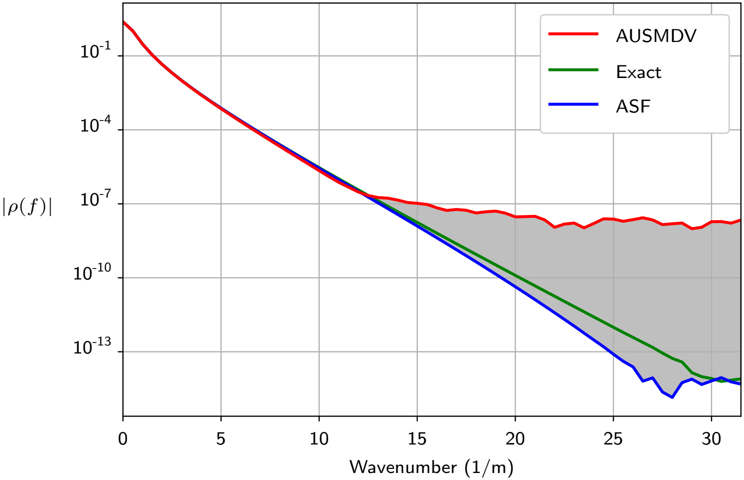
Results: Steepening Wave Problem

- Error should decrease with dx, slope in log-log space gives the order:



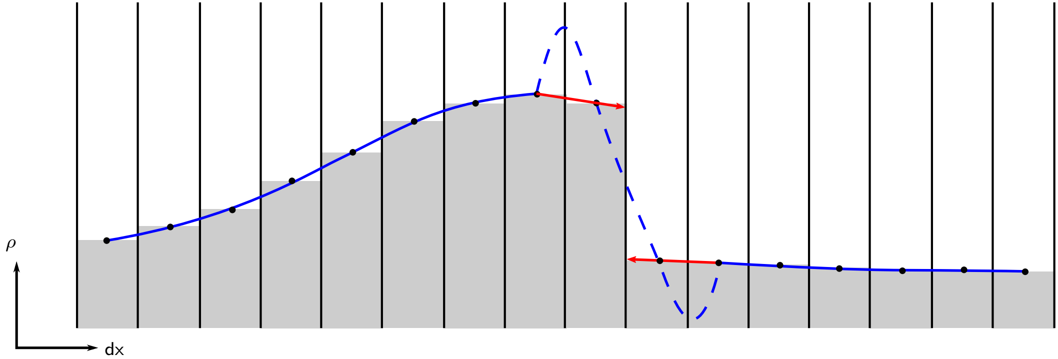
Results: Steepening Wave Problem

- Since the solution is periodic, we can analysis error by wavenumber:



Methodology: Numerical Method

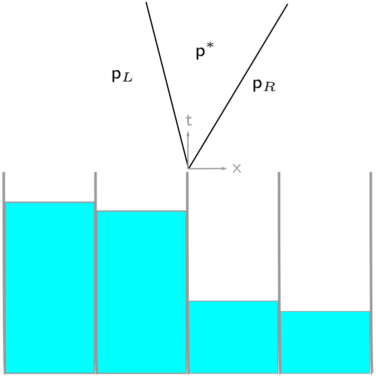
Hybridise the two approaches by detecting discontinuities:



Methodology: Discontinuity Detection

How do we actually detect discontinuities?

- Shockwave sensor uses the HLLC "hybrid" wavespeeds: Toro, Spruce, and Speares, 1994



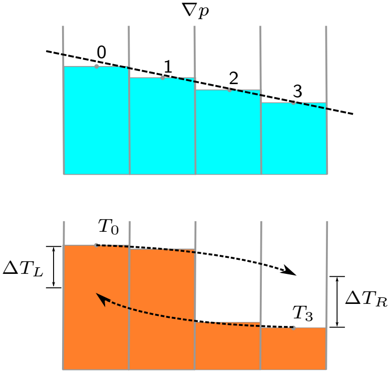
$$p^* = \frac{p_L + p_R}{2} - \frac{(u_R - u_L)}{2}\frac{(\rho_L + \rho_R)}{2}\frac{(a_L + a_R)}{2}$$

$$q_{L/R} = \begin{cases} 1 & p^*/p_{L/R} \leq 1 \\ \sqrt{1 + \frac{\gamma+1}{2\gamma}\left(\frac{p^*}{p_{L/R}} - 1\right)} & \text{otherwise} \end{cases}$$

$$S_{shock} = min\left(\frac{q-1}{\mathcal{M}}, 1.0\right) \quad : \quad q = max(q_R, q_L)$$

Methodology: Discontinuity Detection

- Thermal/interface discontinuity detection by isentropic extrapolation:



$$p_R/p_L = \frac{p_0 + p_1 + p_2 + p_3}{4} \pm \frac{3}{2}\frac{-3p_0 - p_1 + p_2 + 3p_3}{10}$$

$$T_R = T_0 \left(\frac{p_R}{p_0}\right)^{(\gamma-1)/\gamma} \quad T_L = T_3 \left(\frac{p_L}{p_3}\right)^{(\gamma-1)/\gamma}$$

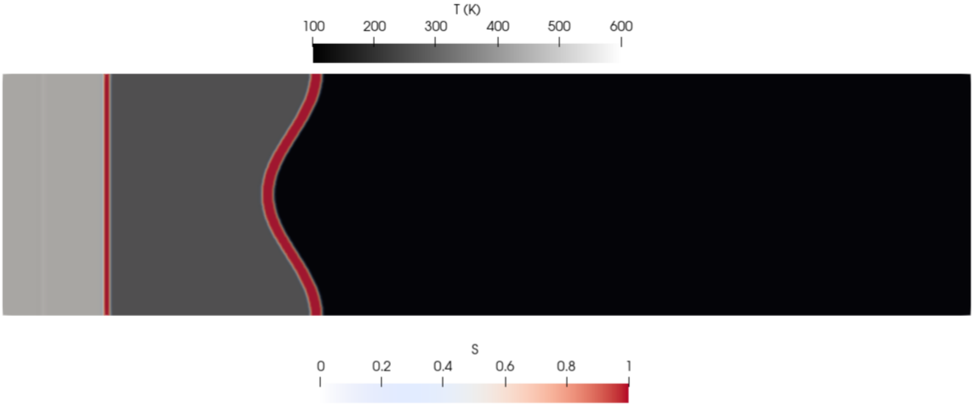
$$\Delta T = \frac{|T_L - T_0|}{T_0} + \frac{|T_R - T_3|}{T_3}$$

$$S^T_{contact} = \frac{1}{2}\tanh(6\Delta T - 2) + \frac{1}{2}$$

Methodology: Discontinuity Detection

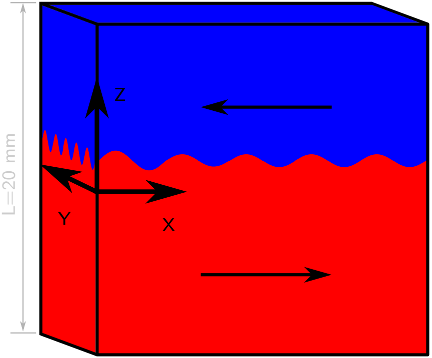
The final value of the shock detector is then the maximum of all three sensors:

$$S = max(S_{shock}, S^{\rho}_{contact}, S^{T}_{contact}) \quad (1)$$



Flow Description: Supersonic Mixing Layer

- Hydrogen conditions taken from Gibbons (2019)
- Hydrocarbon velocities reduced to match $M_c = 0.76$



Air:			
Hydrogen:		Hydrocarbon:	
p	101,000 (Pa)	p	101,000 (Pa)
T	1,400 (K)	T	1,400 (K)
u	-1,168.89 (m/s)	u	-500 (m/s)
Y$_{N_2}$	0.767	Y$_{N_2}$	0.767
Y$_{O_2}$	0.233	Y$_{O_2}$	0.233
Fuel:			
p	101,000 (Pa)	p	101,000 (Pa)
T	1,500 (K)	T	1,500 (K)
u	1,665.89 (m/s)	u	634.3 (m/s)
Y$_{H_2}$	1.0	Y$_{C_2H_4}$	1.0

Figure 1: Supersonic Mixing Layer Initial Conditions. (Interface perturbations are exaggerated.)

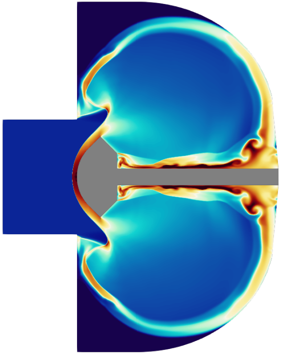
Methodology: Eilmer

Eilmer is our high-speed flow research simulation code:

- Developed at UQ by Rowan Gollan, Peter Jacobs, Kyle Damm, and me!
- Used for studies of re-entry flows, combustion, compressible flow and more
- Part of the Gasdynamic Toolkit (GDTk)

Features:

- Free and open-source
- Parallel scaling to thousands of cores
- Build structured/unstructured grids or read them in
- Extensively validated against hypersonic experiments
- Very capable turbulence, chemical and thermal nonequilibrium models



Website: `gdtk.uqcloud.net`
Paper: `doi.org/10.1016/j.cpc.2022.108551`

Numerical Details and Initial Condition

Slide of technical details for posterity:

- This talk will be on `gdtk.uqcloud.net/docs/pub-n-pres/presentations`

Initial Condition		
L	20 (mm)	Domain Size
A	1/100 L	Perturbation Amplitude
k	6	Perturbation Wave Number
D	1/6 L	Vertical Offset
ζ	3/100 L	Smearing Factor

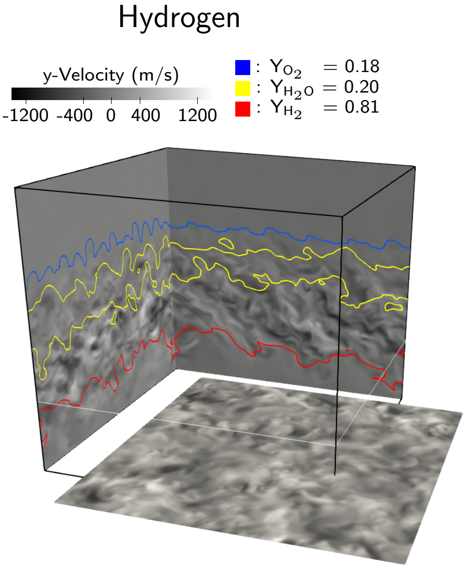
$$\psi = f\psi_{air} + (1-f)\psi_{fuel}$$

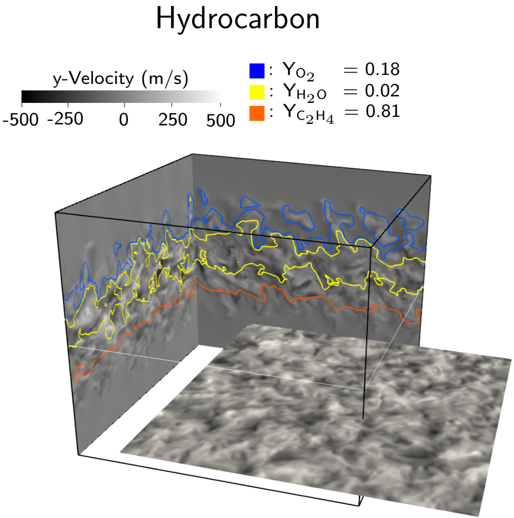
$$f = \frac{1}{2}tanh(\frac{6z'}{\zeta}) + \frac{1}{2}$$

$$z' = z - A(sin(\frac{2\pi kx}{L}) + sin(\frac{2\pi ky}{L})) + D$$

Solver Settings	
Eilmer Rev-id:	71d0040e
Fluid Time-Adv:	RK3 Explicit @ CFL=0.5
Chem Time-Adv:	RK45 Adaptive
Fluxes:	AUSMDV/SBP-ASF
n Smooth:	4
$\mathcal{M}$:	0.1
Cell Count:	299^3
Hydrogen Reactions:	Jachimowski, 1992
Ethylene Reactions:	Baurle and Eklund, 2002
Max Time:	100 μ s
RKF errTol	$1e-5$

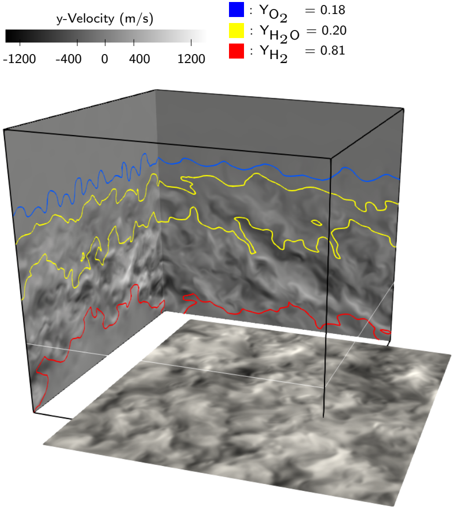
Results: Flow overview @ 40 μ s



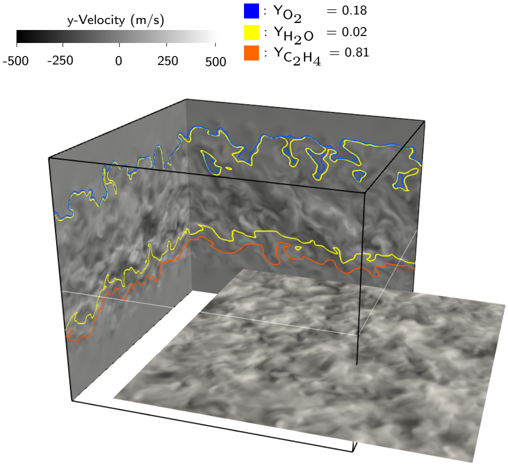


Results: Flow overview @ 60 μ s

Hydrogen

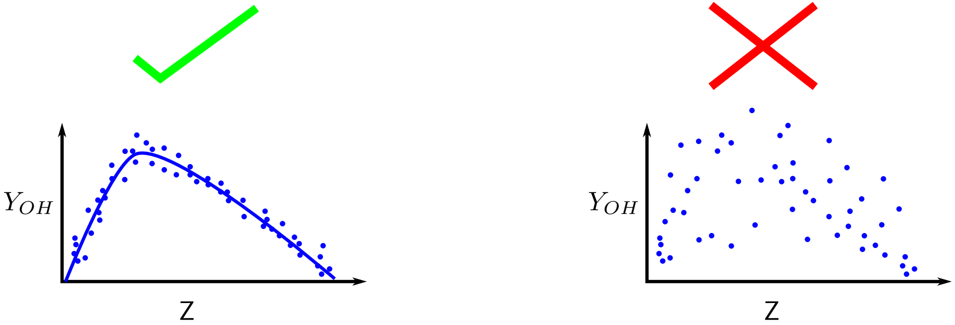


Hydrocarbon



Results: Conditional Statistics

Our goal is to develop extend Conditional Moment Closure for highly compressible flow:



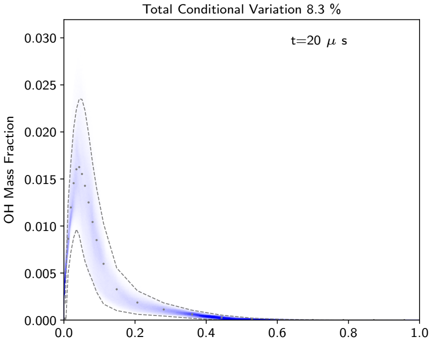
- The mixture fraction Z is the mass fraction of gas from the fuel stream:

$$Z = \sum_s Y_s \left(a_s^H \frac{M_H}{M_s} + a_s^C \frac{M_C}{M_s} \right) \tag{2}$$

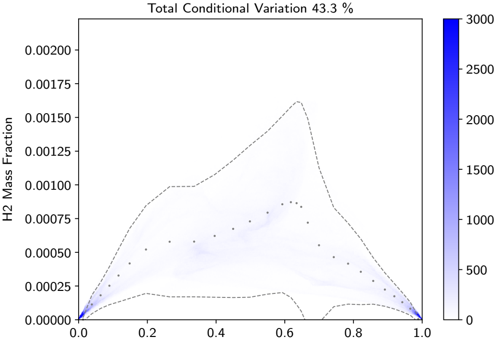
Results: Conditional Statistics

- Intermediate species OH and H_2 follow the Z curve at late times:

Hydrogen



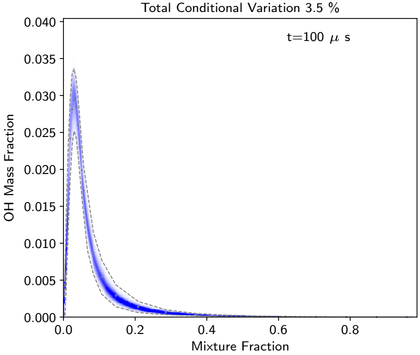
Hydrocarbon



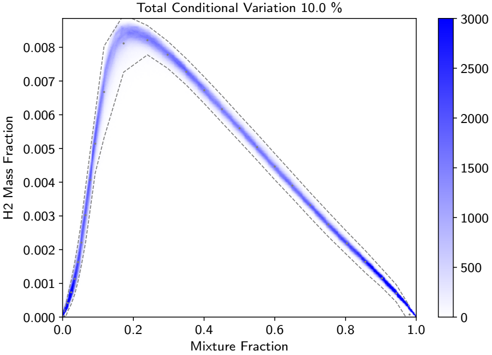
Results: Conditional Statistics

- Intermediate species OH and H_2 follow the Z curve at late times:

Hydrogen



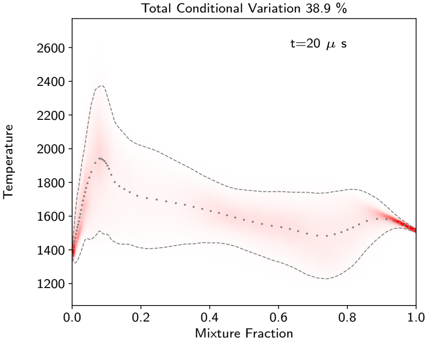
Hydrocarbon



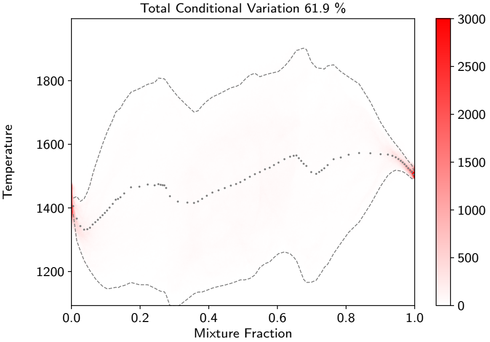
Results: Conditional Statistics

- Temperature is pretty bad initially:

Hydrogen



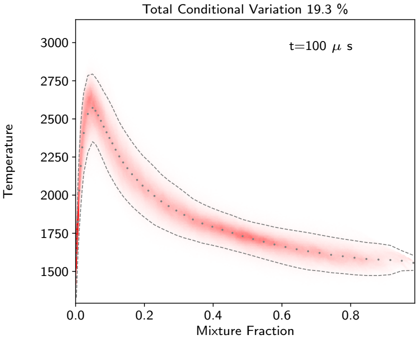
Hydrocarbon



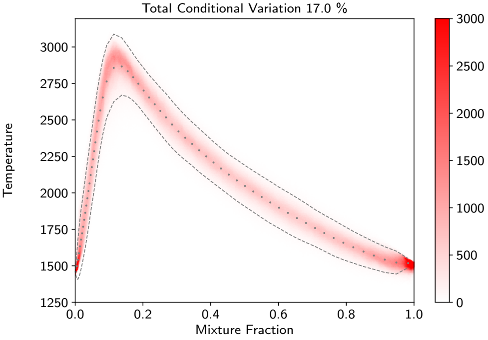
Results: Conditional Statistics

- Even at late times it has a fair bit of variation:

Hydrogen



Hydrocarbon



Conclusions and What's Next?

- Numerical method is holding water for reacting DNS calculations
- Have plans for a larger simulation with shocks in it
- Can then do statistical analysis of the whole flowfield for CMC

References I

R. A. Baurle and D. R. Eklund. "Analysis of Dual-Mode Hydrocarbon Scramjet Operation at Mach 4-6.5". In: Journal of Propulsion and Power 18.5 (2002), pp. 990–1002. DOI: 10.2514/2.6047.

M. J. Cleary and A. Y. Klimenko. "A Generalised Multiple Mapping Comditioning Approach for Turbulent COmbustion". In: Flow Turbulence Combustion 82 (2009), pp. 477–491. DOI: 10.1007/s10494-008-9161-3.

T. C. Fisher et al. "Discrete conservative finite-difference formulations for nonlinear conservation laws in split form: Theory and boundary conditions". In: Journal of Computational Physics 234 (2012).

N. N. Gibbons et al. "Eilmer: An open-source multi-physics hypersonic flow solver". In: Computer Physics Communications 282.108551 (2023). DOI: doi.org/10.1016/j.cpc.2022.108551.

Nicholas N. Gibbons. "Simulation and Dynamics of Hypersonic Combustion". PhD thesis. St Lucia, QLD 4072: The University of Queensland, School of Mechanical and Mining Engineering, 2019.

Rowan J. Gollan. "The Computational Modelling of High-Temperature Gas Effects with Application to Hypersonic Flows". PhD thesis. St Lucia, QLD 4072: The University of Queensland, School of Mechanical and Mining Engineering, 2008.

A. Honein and P. Moin. "Higher entropy conservation and numerical stability of compressible turbulence simulations". In: Journal of Computational Physics 201.2 (2004).

Casimir J. Jachimowski. An analysis of Combustion Studies in Shock Expansion Tunnels. Tech. rep. NASA TP-3224. Hampton, Virginia: National Aeronautics and Space Administration, 1992.

A. Y. Klimenko and R. W. Bilger. "Conditional moment closure for turbulent combustion". In: Progress in Energy and Combustion Sciences 25 (1999), pp. 595–687.

L. D. Landau and E. M. Lifshitz. Fluid Mechanics. 2nd. Butterworth-Heinemann, 1987. Chap. 10.

N. D. Sandham and W. C. Reynolds. "Compressible Mixing Layer: Linear Theory and Direct Simulation". In: AIAA Journal 28.4 (1990), pp. 618–624. DOI: 10.2514/3.10437.

H. Tamashita, M. Shimada, and T. Takeno. "A Numerical Study on Flame Stability at the Transition Point of Jet Diffusion Flames". In: Symposium (International) on Combustion 26.1 (1996), pp. 27–34. DOI: 10.1016/S0082-0784(96)80196-2.

E.F. Toro, M. Spruce, and W. Speares. "Restoration of the contact surface in the HLL-Riemann solver". In: Shock Waves 4 (1994), pp. 25–34.

Yasuhiro Wada and Meng-Sing Liou. "A Flux Splitting Scheme With High-Resolution and Robustness for Discontinuities". In: 32nd AIAA Aerospace Sciences Meeting and Exhibit. AIAA-94-0083. Reno, Nevada, 1994. DOI: 10.2514/6.1994-83.

J. A. White et al. "Low-dissipation advection schemes designed for large eddy simulations of hypersonic propulsion systems". In: 48th AIAA/ASME/SAE/ASEE Joint Propulsion Conference and Exhibit. 2012.

Lachlan Whyborn. "Direct numerical simulations of instabilities in the entropy layer of a hypersonic blunted slender cone". PhD thesis. St Lucia, QLD 4072: The University of Queensland, School of Mechanical and Mining Engineering, 2023.