A new computational fluid dynamics framework for multi-physics simulations*

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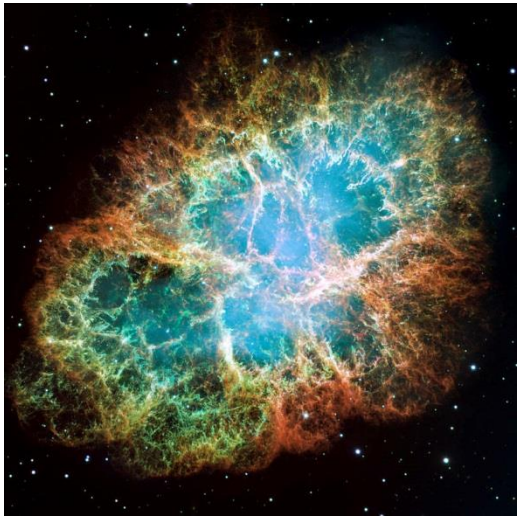
Stewardship Science Academic Program (SSAP) symposium
17-18 February 2016, Bethesda, MD
DOE/NNSA Award DE-NA0002382

* Parts of this research co-sponsored by AFOSR, NSF, Caltech, UIUC, UMN, UM, and other sources

What is this effort about and why is it important?

- Many variable-density flows and their applications are important to the DOE and DOE/NNSA, to DoD, NASA, geophysics, astrophysics, etc.
  - *ICF, Rayleigh-Taylor flows, baroclinically generated flows, local stabilization, combustion, flames in the presence of pressure gradients or shear, variable-density compressible flows, …*
- Predictive simulations of variable-density turbulent flows remain a challenge in many situations
  - *Predictive simulations are important if predictions are required when testing is difficult*
- Predictive simulations require modeling that can be
  - *<u>verified</u>, i.e., that the equations are solved correctly, and*
  - *<u>validated</u> against experiment or exact solutions, i.e., that the right equations are being solved.*
- The present effort targets flows with important small-scale variable-density dynamics

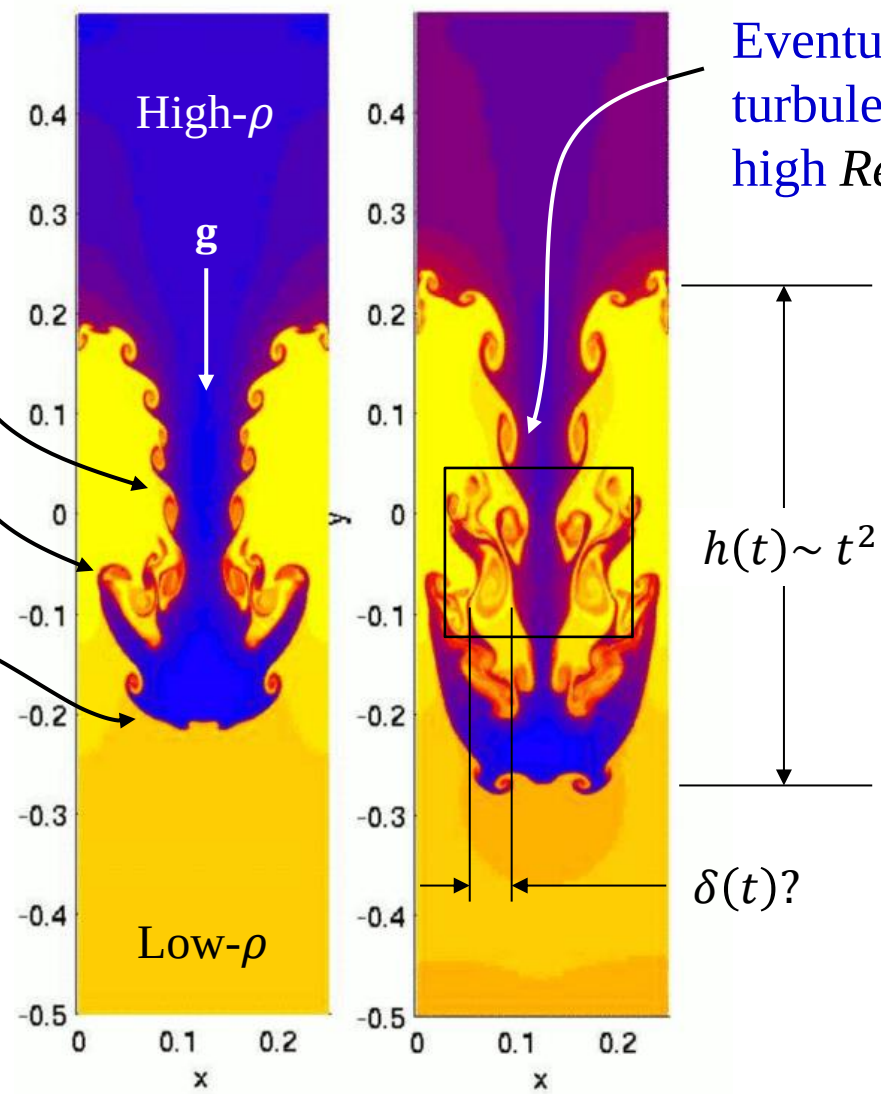


RT fingering in the Crab nebula

Project goal — *Flow environment and relevant SGS dynamics*

- SGS baroclinic torques $\nabla p \times \nabla \rho \neq 0$
- SGS local stabilization and stratification
  $$\nabla p \cdot \nabla \rho > 0$$
  – *10s to 100s of kilo-g local Lagrangian acceleration at high Re*
- SGS Rayleigh-Taylor instability $\nabla p \cdot \nabla \rho < 0$

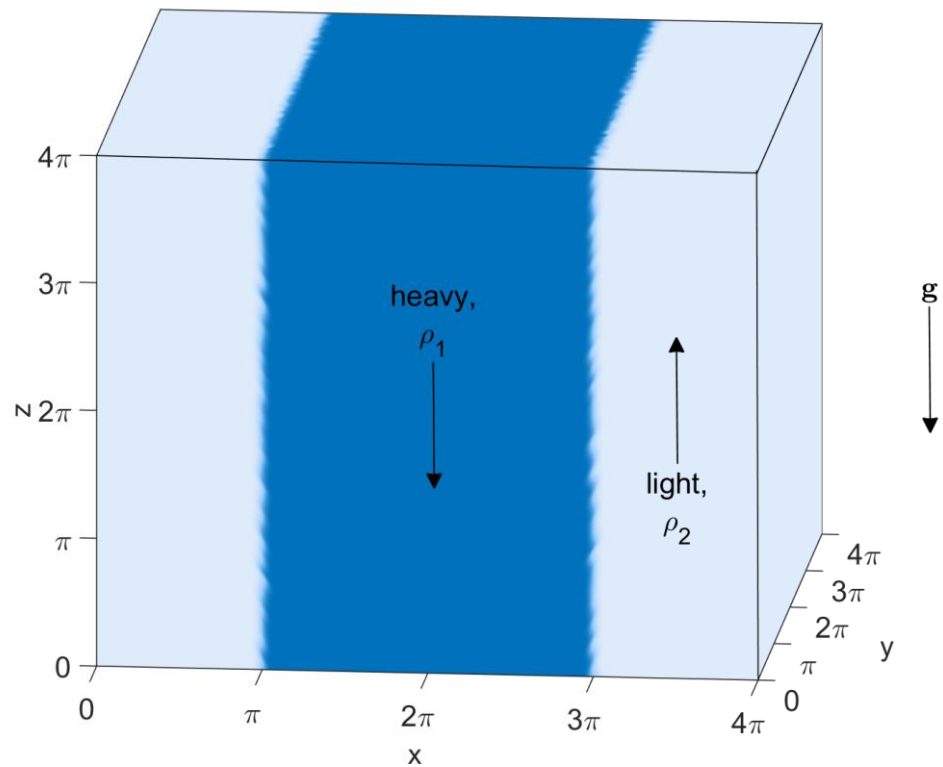
★ Project aims to develop a unified predictive framework for variable-ρ flows with no adjustable parameters.



Graphic: S. Li & H. Li: RTI simulation (Wikipedia)

Acceleration-driven variable-density flow

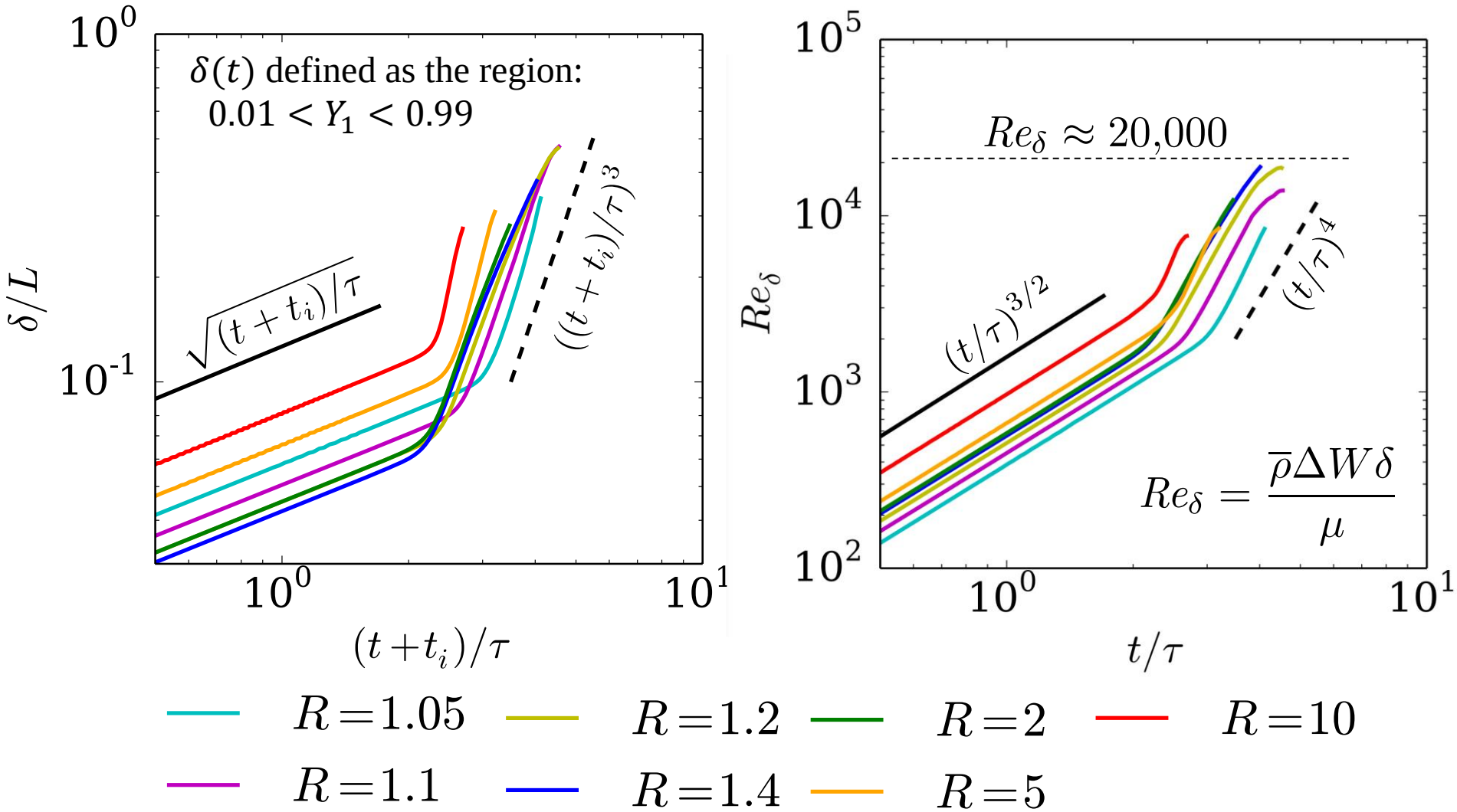
- High-density fluid between low-density fluid regions
  - *Vertical acceleration field, e.g., gravity, and pressure gradient*
  - *Initial horizontal density gradients*
- Flow initialized and driven by baroclinic torques: $\nabla\rho \times \nabla p$
- Triply-periodic domain



- Solve flow using (pseudo-)spectral direct numerical simulations (DNS)
  - *Grids of* 512^3 *and* 1024^3 *to date*
  - *Remains well-resolved,* $\min\{k_{\max}\eta\} > 1.5$*, by setting viscosity in accord with grid resolution and density ratio:* $1.05 < R = \rho_1/\rho_2 < 10$.
  - *Code verified by Chung & Pullin (2010) and further as part of this work*

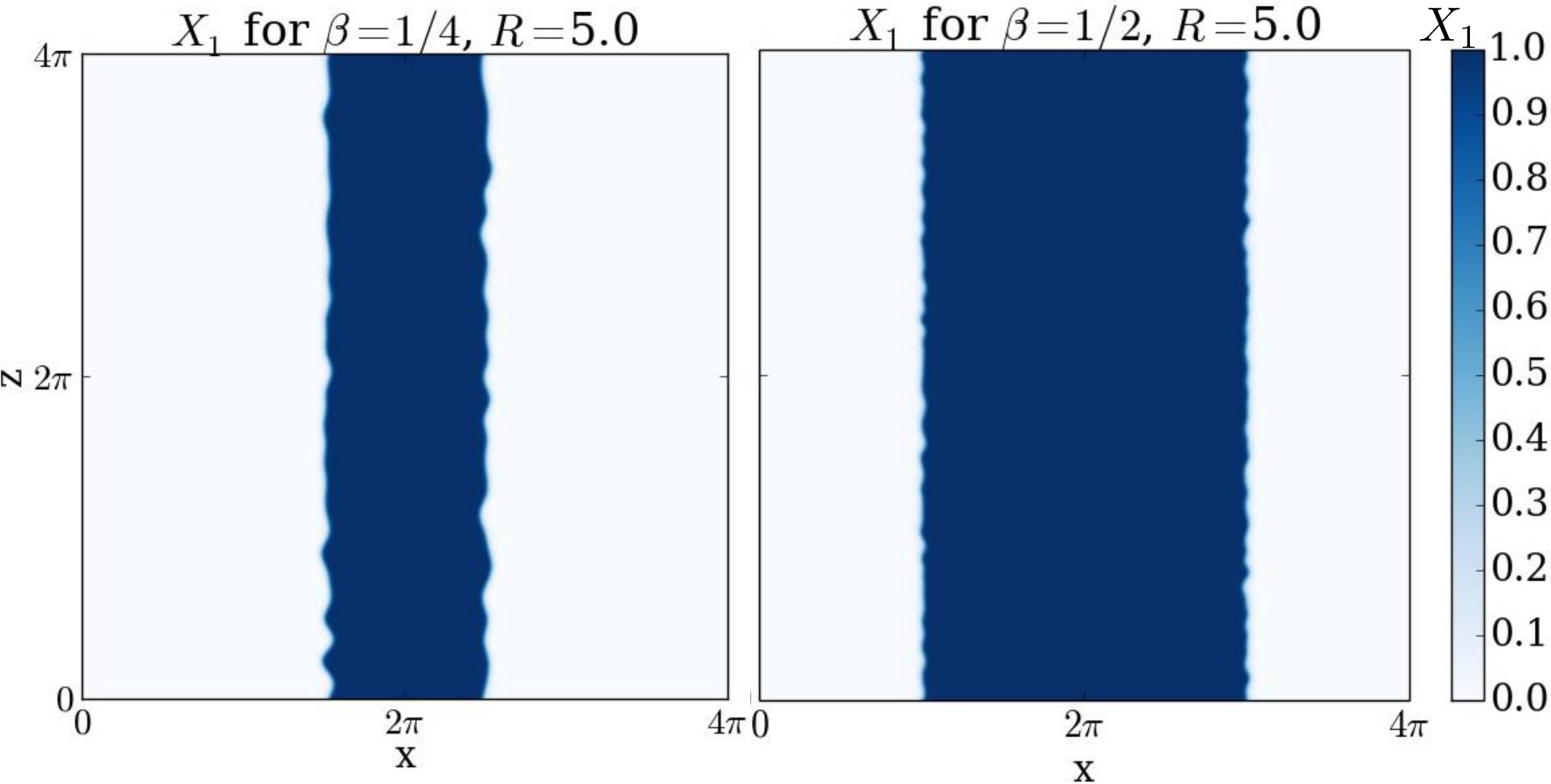
Gat, Matheou, Chung, & PD (2015, 2016)

Shear-layer width, $\delta(t)$, and Reynolds number, $Re_\delta(t)$



Gat, Matheou, Chung, & PD (2015, 2016)

Flow evolution — *2D slice*



- Convection velocity (empirical relation): $$\frac{W_c}{\Delta W} = \frac{\left\{(1-\beta)^2 W_1 + \beta^2 W_2\right\}/\Delta W}{\beta R^\beta + \frac{3}{2}(1-\beta)}$$

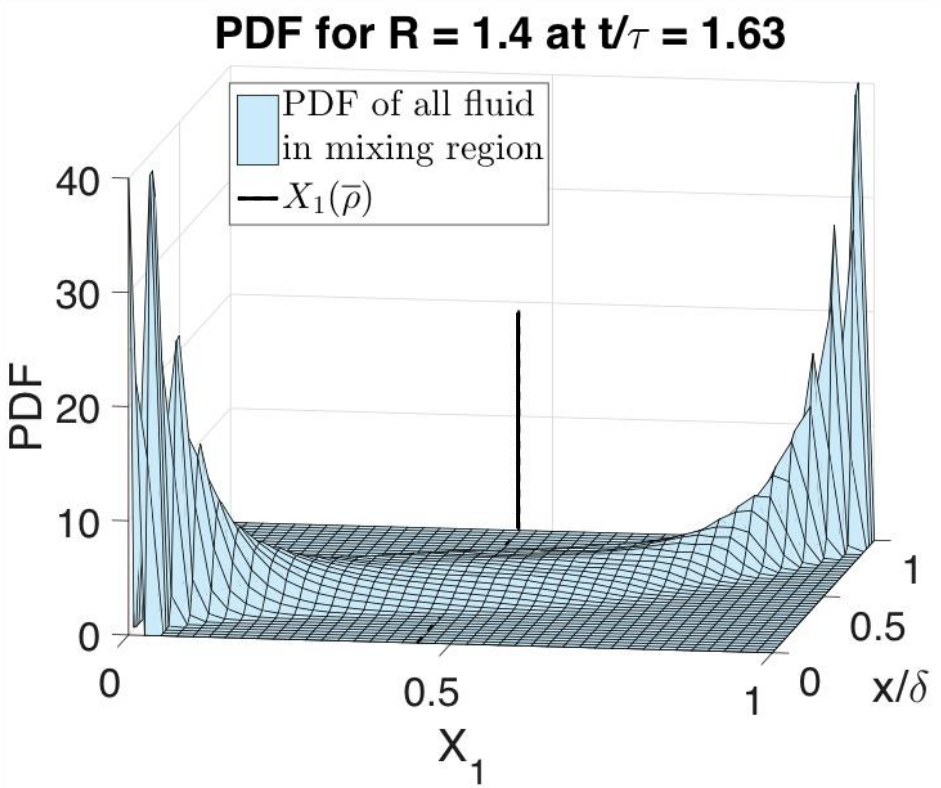
Gat, Matheou, Chung, & PD (2015, 2016)

Shear-layer mixed-fluid composition

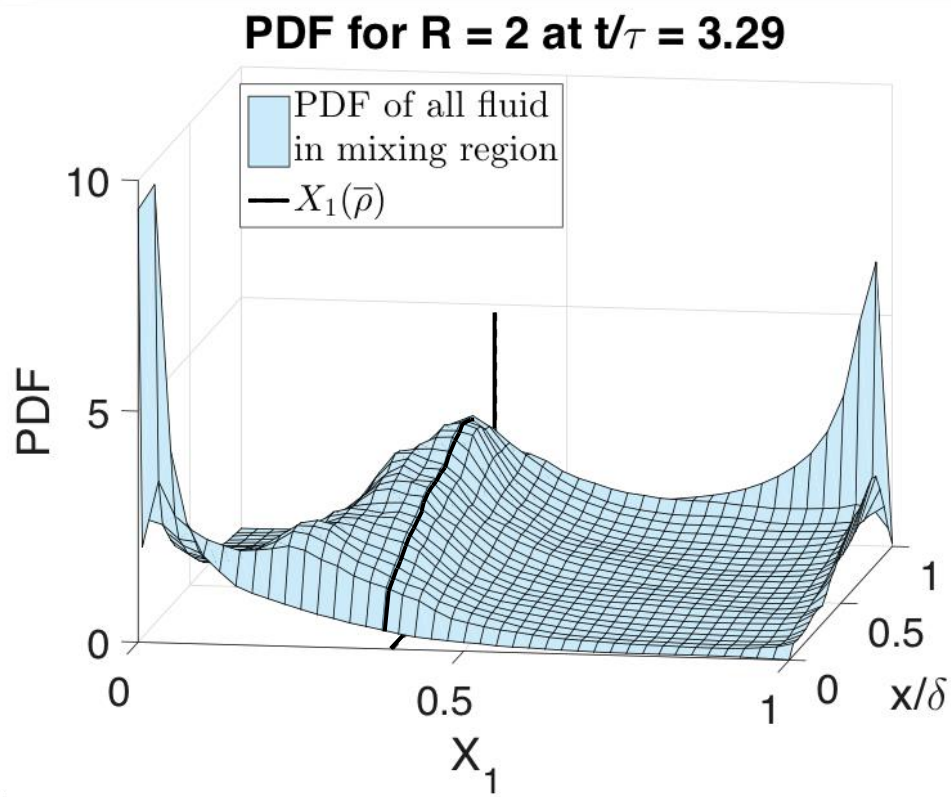
- Convection-frame apparent velocities dictate entrainment ratio (Dimotakis 1986)

$$E_v = \frac{X_2(\overline{\rho})}{X_1(\overline{\rho})} = \frac{W_2 - W_c}{W_c - W_1} \longrightarrow X_1(\overline{\rho}) = \frac{1}{E_v + 1} = \frac{\overline{\rho} - \rho_2}{\rho_1 - \rho_2}$$

- In accord with dominant measured shear-layer mixed-fluid mole fraction



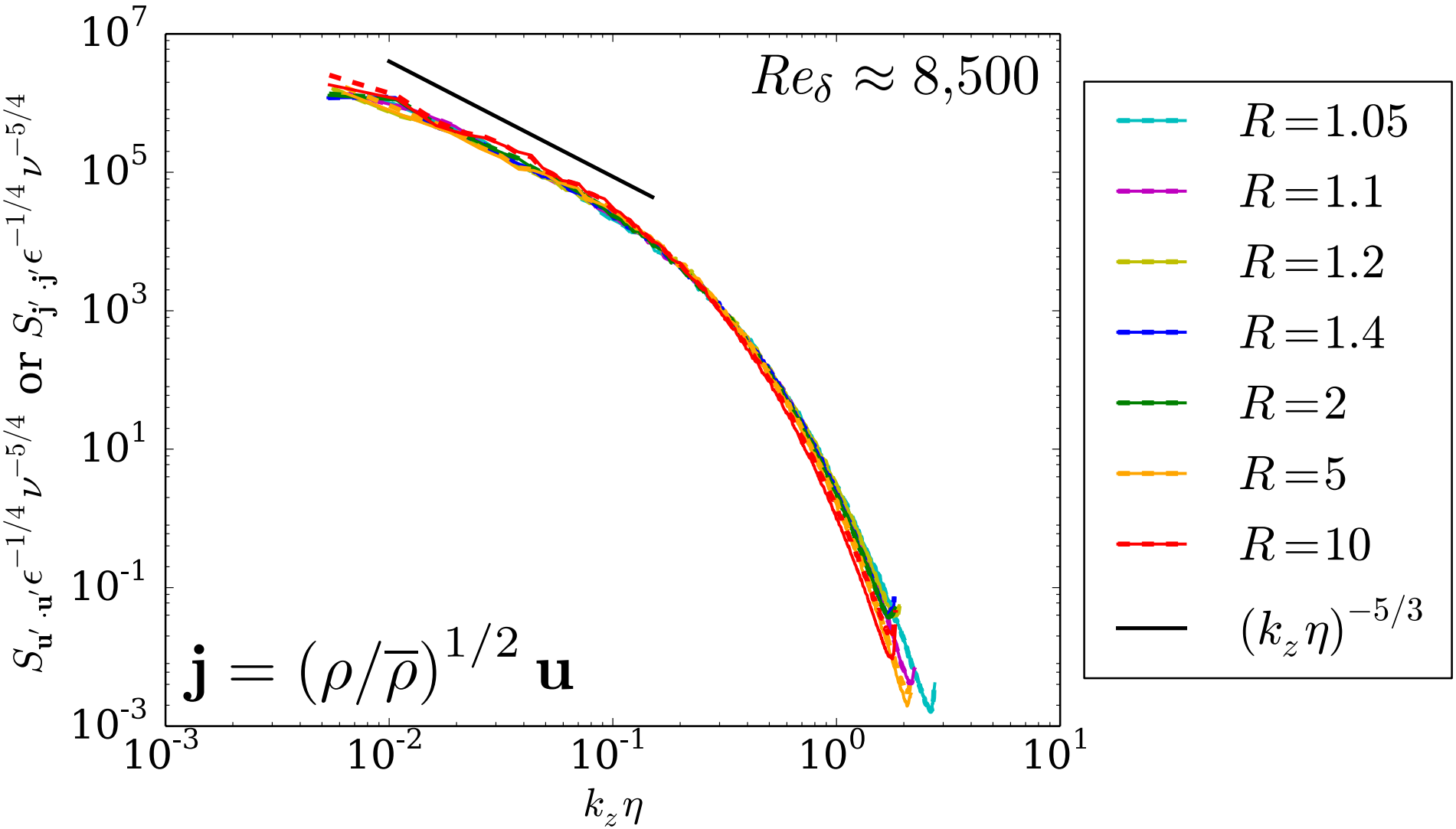
Diffusive regime



Turbulent regime

Gat, Matheou, Chung, & PD (2015, 2016)

Spectra: specific kinetic-energy (u^2) and kinetic-energy (ρu^2)

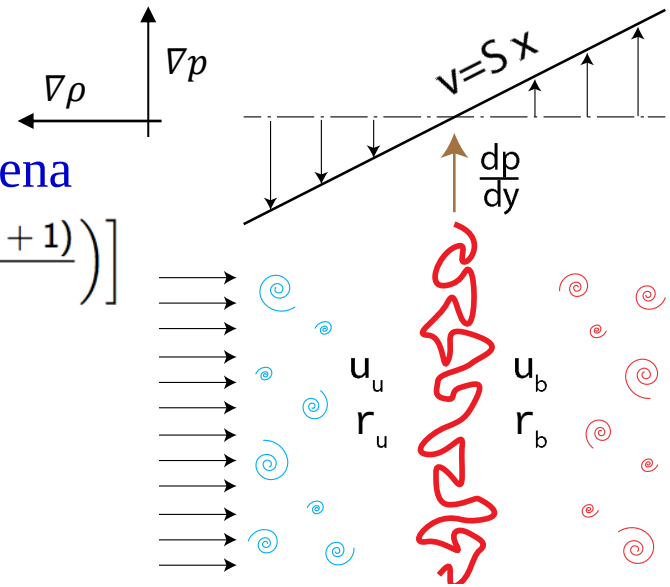


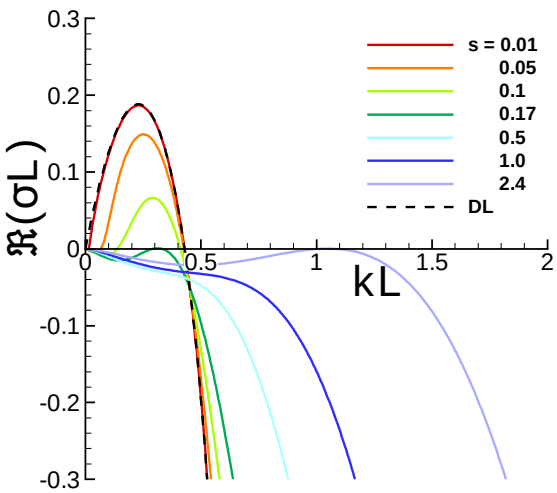
Gat, Matheou, Chung, & PD (2015, 2016)

Flames with lateral shear

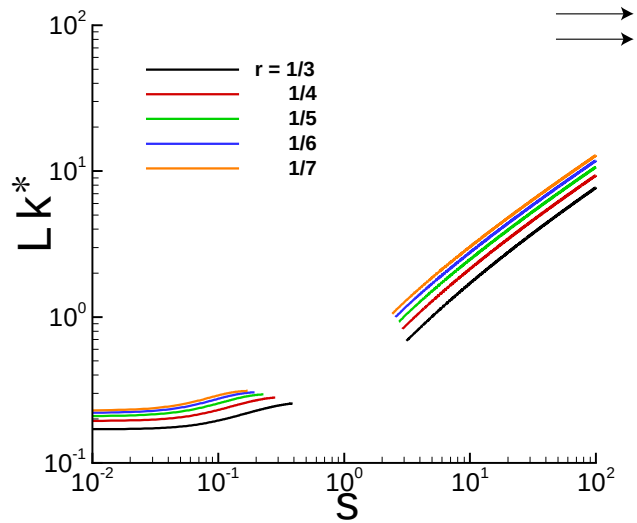
- Configuration with "active" baroclinic torque
- Linear stability analysis predicts new phenomena

$$\left[2is\phi+\zeta^2(r\phi+1)+\zeta r\phi(\phi+1)\right]e^{\frac{i\zeta(r\phi+1)^2}{2s}}\left[1-\mathrm{erf}\left(\frac{(1+i)\sqrt{\zeta}(r\phi+1)}{2\sqrt{s}}\right)\right]$$
$$+\frac{(-1+i)}{\sqrt{\pi}(r-1)}\sqrt{s\zeta}(\zeta+r(\zeta+2\phi+1)-1)=0$$
$$(\zeta=k\mathcal{L},\ \phi=\sigma/k,\ \text{and}\ s=rS\mathcal{L})$$





Amplification factor



Maximum wavenumber

r : density ratio
S : shear
$\mathcal{L}$: Markstein length

Lu & CP (2014 *JFM*, and in progress)

New DNS zero-Mach code — *Inflow/outflow BCs*

- High-order finite-difference DNS code for zero-Mach variable-ρ flow
- Inflow/outflow control using weak (penalty-type) boundary conditions (Nordstrom et al. 2007)

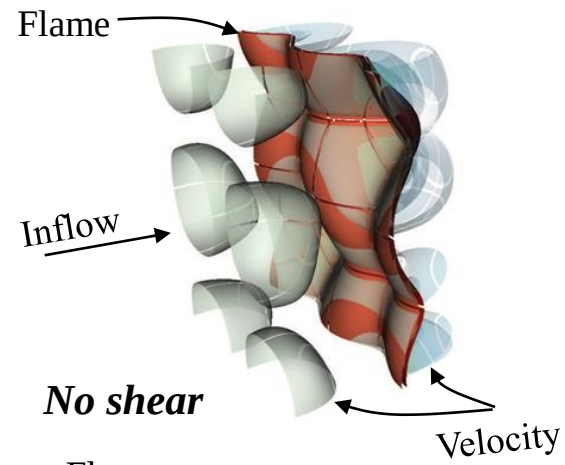
$$\mathrm{D}_t\mathbf{u} = \frac{1}{\rho}[-\partial_{\mathbf{x}}p + Pr\partial_{\mathbf{x}}\cdot\tau] - \boxed{\mathbf{H}^{-1}(\mathbf{L}-\mathbf{g})\otimes\mathbf{e}_0}$$

which have the bounded norm

$$2\mathbf{u}\cdot\mathbf{H}\mathrm{D}_t\mathbf{u} = \mathrm{D}_t\|u^2\|_{\mathbf{H}} = \mathbf{x}\cdot\mathbf{A}\mathbf{x} + \mathcal{O}(\partial_{\mathbf{x}}\cdot\mathbf{u})$$

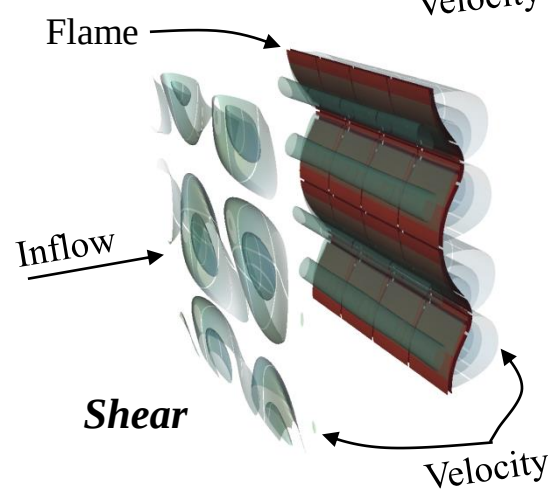
with

$$\mathbf{x} = (u_n, u_t, p, Pr\,\partial_n u_n, Pr\,\partial_t u_t)$$



- Simulations under way

Grid: $128 \times 256 \times 128$
128 processors
1-step combustion
$\beta = 8$
$\alpha_h = 0.75$
$q = 10$



Unphysical scalar excursions in large-eddy simulation (LES)

- For passive scalars, the range of values of scalar fields in turbulent flows is bounded by their boundary values
  - *Maximum Principle of the Laplace operator of the RHS of the scalar-transport equation*

$$\frac{\mathrm{D}Z}{\mathrm{D}t} = \mathcal{D}\,\nabla^2 Z$$

- Boundedness of passive-scalar values extends to filtered scalar fields in large-eddy simulation

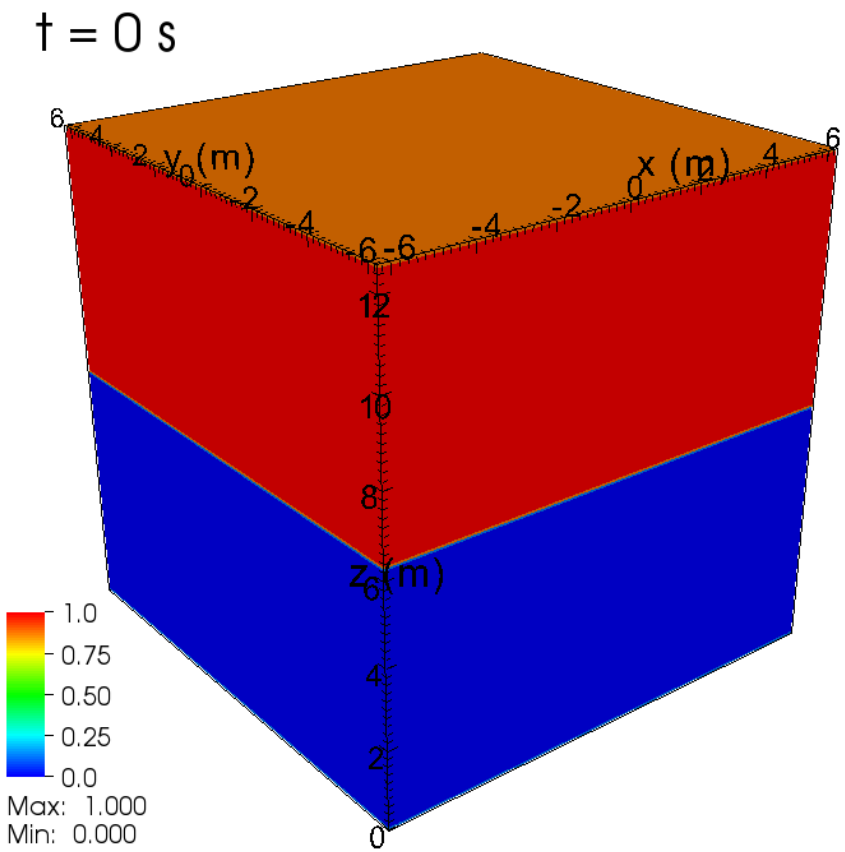
$$\partial_t \bar{Z} + \partial_{\mathbf{x}} \cdot (\bar{\mathbf{u}}\bar{Z}) = \partial_{\mathbf{x}} \cdot \boldsymbol{\sigma}_{\mathrm{sgs}} + \mathcal{D}\nabla^2 \bar{Z}$$

  - *Subgrid-scale (SGS) model should ensure that flow scales remain sufficiently resolved and bounded on the computational grid*
  - *Presently, assume that the SGS model is purely dissipative, SGS model with no backscatter for simplicity, however the presence of backscatters would not change the arguments*

– Scalar boundedness is both a global constraint (violations easy to diagnose) but also for excursions within global bounds (more-difficult to diagnose)

Test flow configuration

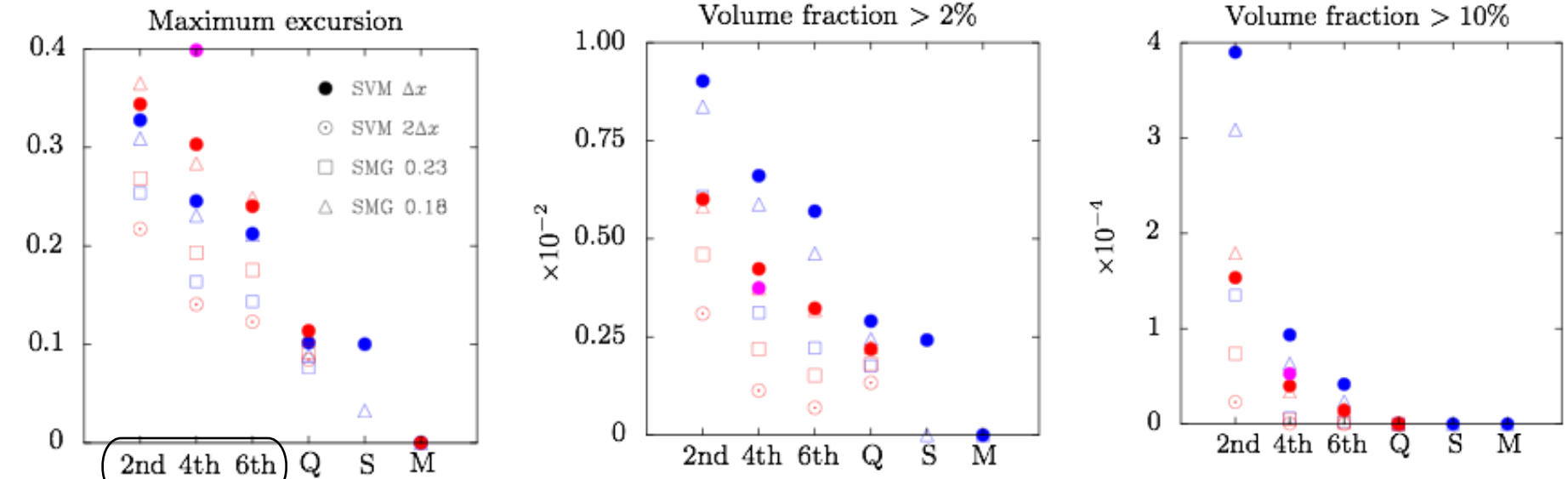
- Temporally evolving shear layer
  - *Simple enough for fundamental study*
  - *Infinite stack of vertical layers* $L = 4\pi$ m
  - *Alternating initial* $U = \pm 1$ m/s
  - *Initial freestream passive scalar values of* $Z = 0{,}1$
  - *Initial perturbations designed to excite 3D flow*
- Test flow exhibits characteristics of more-complex flows
- LES with final $Re \approx 5 \times 10^5$
  - *Well within fully-developed turbulence regime*



Matheou & PD (in progress)

Global scalar excursion statistics — *Overview*

- Numerics, SGS model, and grid significantly influence excursions
- Numerical-convection scheme ranking
  - *Spectral LES for reference*
  - *Flux-limited scheme produces no excursions (as expected), but at the expense of numerical dissipation (overestimates mixing)*



Fully conservative

QUICK

Monotone

Spectral

Magenta : 1024^3

Red : 512^3 grid

Blue : 256^3 grid

SVM: stretched-vortex model $\Delta = \Delta x,\ 2\Delta x$

SMG 0.23: Smagorinsky $C_s = 0.23$

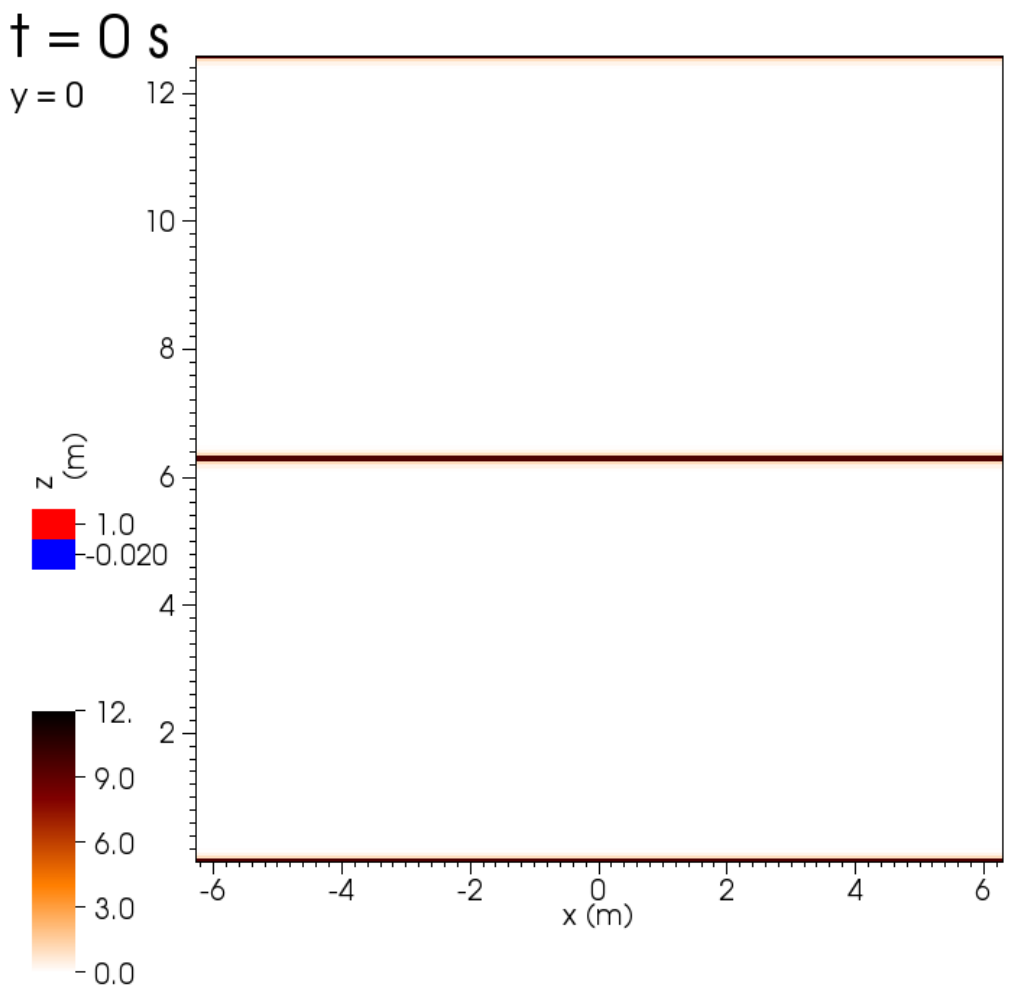
SMG 0.18: Smagorinsky $C_s = 0.18$

Matheou & PD (in progress)

Scalar excursions — *Not well-correlated with scalar gradients*

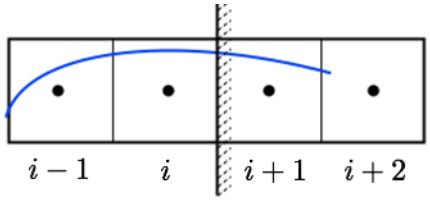
- Unphysical global excursions from dispersive errors of the numerical convection scheme
  - *Different behavior from continuous derivatives*
  - *(Smaller) errors from spectral schemes because of some aliasing (Gibbs oscillations)*
  - *Easy to diagnose*
- Unphysical scalar excursions can also be local/internal
  - *Do not cross global bounds*
  - *Occur throughout the domain (not shown)*
  - *More-difficult to diagnose*

★ Both types must be mitigated if LES is to inform/drive physics-based SGS models



Matheou & PD (in progress)

Flux limiters — *Scalars (passive) in non-reacting flow*



$$Y_s^L(x) = \theta_{i,s}(p_{i,s}(x_{i+1/2}) - \overline{Y}_{i,s}) + \overline{Y}_{i,s}$$

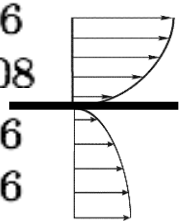
Linear scaling limiter

$$\theta_{j,s} = \min\left\{ \left|\frac{M - \overline{Y}^n_{j,s}}{M_j - \overline{Y}^n_{j,s}}\right|, \left|\frac{m - \overline{Y}^n_{j,s}}{m_j - \overline{Y}^n_{j,s}}\right|, 1 \right\}$$

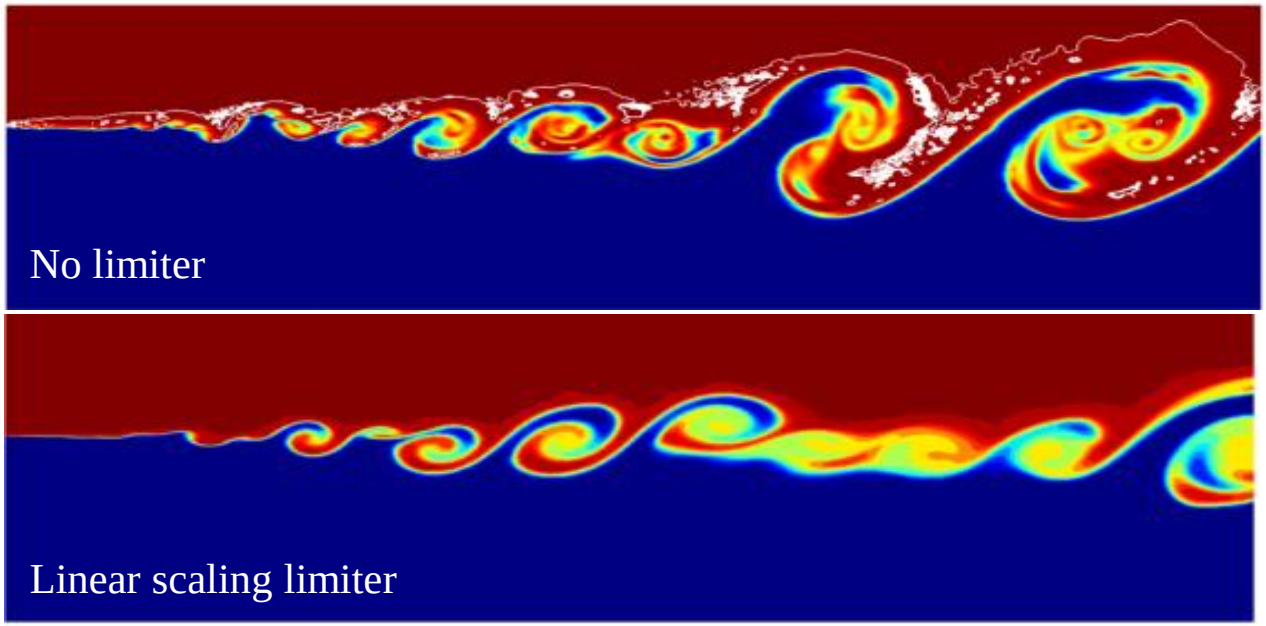
Zhang & Shu (2010, 2011,2013; *JCP*)
Subbareddy *et al.* (2014, *AIAA Paper*)

Experiments: Slessor, Bond, & Dimotakis (1998, *JFM*)

$$\begin{aligned} N_2 &= 0.76 \\ He &= 0.16 \\ Ar^A &= 0.08 \\ N_2 &= 0.76 \\ He &= 0.16 \\ Ar^B &= 0.08 \end{aligned}$$



4th-order KEC fluxes



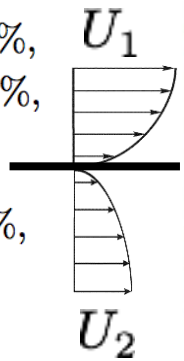
Contours of Ar^A Mass Fraction

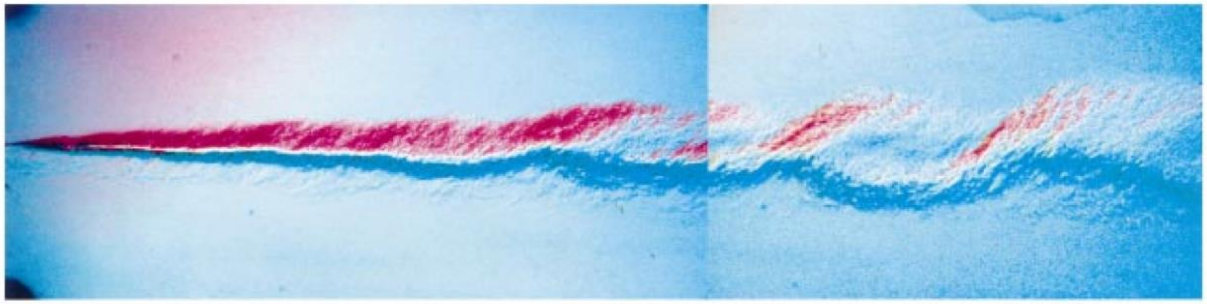
Kartha, Subbarreddy, GC, & PD (in progress)

Flux limiters — *Scalars (active) in reacting flow*

$H_2 = 0.93\%$, $NO = 0.14\%$,
$Ar = 8.00\%$, $He = 15.07\%$,
$N_2 = 75.86\%$.

$F_2 = 8.00\%$, $N_2 = 76.0\%$,
$He = 16.0\%$.





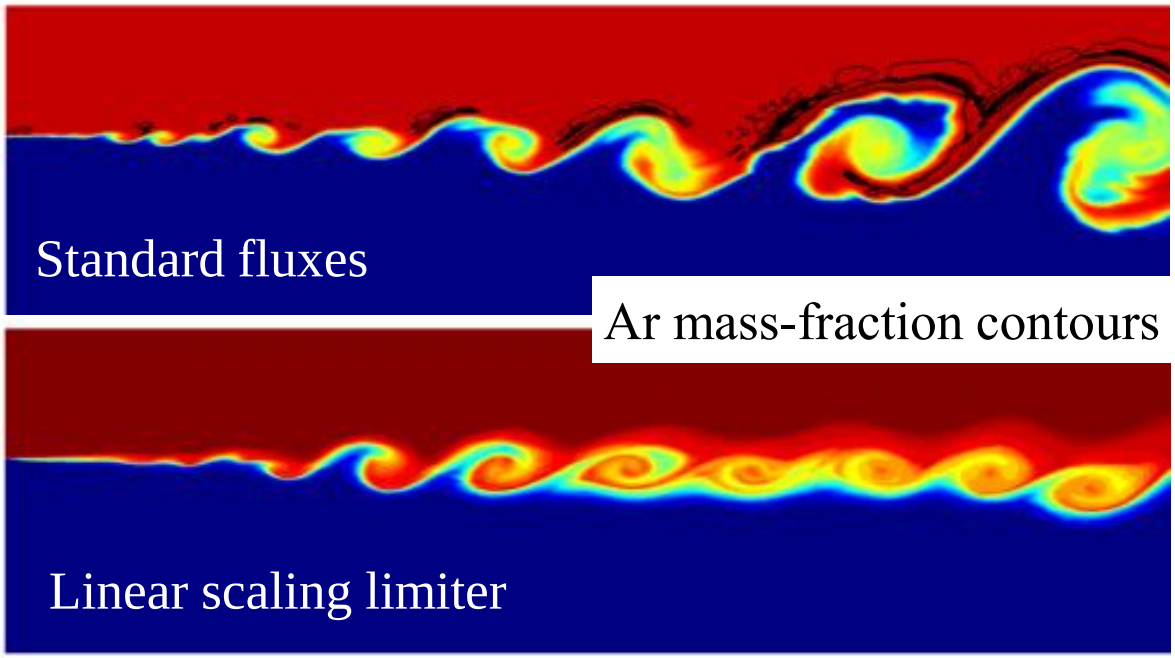
Experiments: Slessor, Bond, and Dimotakis (1998, *JFM*)

10 species: N_2, H_2, F_2, HF, NO, H, F, NOF, Ar, He

Hypergolic reaction system:

$$NO + F_2 \rightleftarrows NOF + F$$
$$H_2 + F \rightleftarrows HF + H$$
$$F_2 + H \rightleftarrows HF + F$$

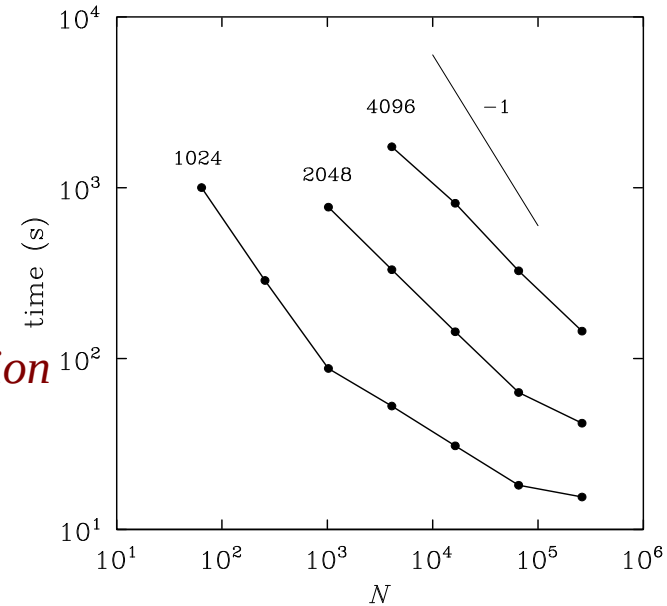
Limiter adds dissipation where flow is reacting



Kartha, Subbarreddy, GC, & PD (in progress)

Other and related work — *Not shown*

- Exploring extension to stretched-vortex model (SVM) for variable-ρ
- Variable-ρ turbulence spectral closure schemes for SGS modeling
- Improvement in time-stepping accuracy for variable-ρ flow simulations
- Shocks in complex-EOS fluids
  - *Extension to non-conservative systems and Riemann problems*
  - *Example: Shocks in van der Waals gas*
- Simulations of jet-injection to supersonic cross-flow
  - *Geometrical-optics simulations of correlation-image velocimetry for code validation by comparison with experiment*
- Spectral code for (hoped-for) 4096^3 runs
  - *Good scaling on Mira (ALCF, Argonne)*
  - *One MPI rank per core, single-thread runs*
  - *Proving ground with good scale separation for SGS model guidance, development, validation*
- Data-storage server development
  - *Computing and data storage pacing items*



Summary & conclusions

- New results/physics from spectral DNS of zero-Mach variable-ρ flow
  - *Larger data sets (future) to (first) inform and (then) test SGS models*
- Numerical-model (dispersion) errors in scalar transport
  - *Must be addressed for finite-difference LES to drive SGS models correctly*
  - *Active scalars pose considerably greater challenges*
  - *Preliminary mitigation measures*
- Variable-ρ flows in premixed flames
  - *Lateral shear and pressure gradients*
  - *New linear stability analysis reveals rich behavior*
  - *New code to extend study to non-linear regime*
- Shocks in complex-EOS fluids(not shown)
- Variable-ρ modeling (not shown)
  - *Turbulence closure, extending direct-interaction approximation*
- New codes in support of this effort:
  - *Spectral: good scaling demonstrated on* $1/3$ *of Mira for future runs*
  - *Finite-difference:* $M = 0$ *with inflow/outflow BCs*

Thank you