Simuation of Lean Premixed Turbulent Combustion

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Lean Premixed Turbulent Combustion

Rod-stabilized V-flame

4-jet Low-swirl burner (LSB)

Slot burner

- Potential for efficient, low-emission power systems
- Design issues because of flame instabilities
- Limitations of theory and experiment
- Can we safely and reliably burn hydrogen for power generation?

Basic Physics of Combustion

Focus on gas phase combustion

Fluid mechanics

- Conservation of mass
- Conservation of momentum
- Conservation of energy

Thermodynamics

- Pressure, density, temperature relationships for multicomponent mixtures

Chemistry

- Reaction kinetics

Species transport

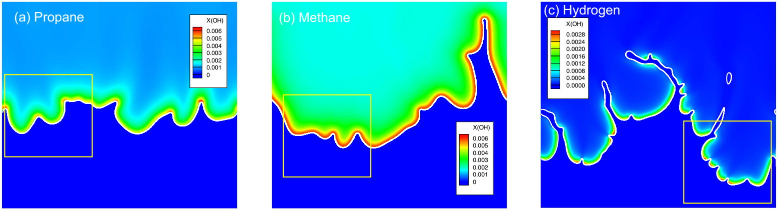
- Diffusive transport of different chemical species within the flame

Radiation

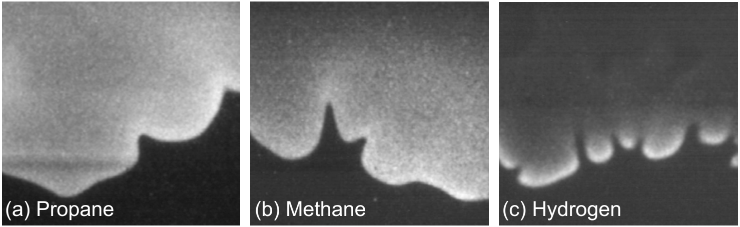
- Energy emission by hot gases

Low-swirl burner

Fuel dependence of flame structure



OH Mole fraction



OH PLIF

Compressible Navier Stokes

Gas phase combustion – mixture model for diffusion

Mass $\rho_t + \nabla \cdot \rho U = 0$

Momentum $(\rho U)_t + \nabla \cdot (\rho UU + p) = \rho \vec{g} + \nabla \cdot \tau$

Energy $(\rho E)_t + \nabla \cdot (\rho UE + pU) = \nabla \cdot \kappa \nabla T + \nabla \cdot \tau U + \sum_m \nabla \cdot (\rho h_m D_m \nabla Y_m)$

Species $(\rho Y_m)_t + \nabla \cdot (\rho U Y_m) = \nabla \cdot (\rho D_m \nabla Y_m) + \dot{\omega}_m$

Augmented with

- Thermodynamics
- Reaction kinetics
- Transport coefficients

Need to preserve chemical and transport fidelity

Relevant Scales

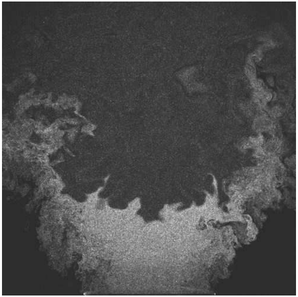
Spatial Scales

- Domain: ≈ 10 cm
- Flame thickness: $\delta_T \approx 1$ mm
- Integral scale: $\ell_t \approx 2 - 6$ mm

Temporal Scales

- Flame speed $O(10^2)$ cm/s
- Mean Flow: $O(10^3)$ cm/s
- Acoustic Speed: $O(10^5)$ cm/s

Wide range of length and time scales will make this computationally demanding



Mie Scattering Image

Issues

Simulation requirements

- No explicit model for turbulence, or turbulence/chemistry interactions
- Detailed chemistry based on fundamental reactions, detailed diffusion
- “Sufficient” range of scales to represent realistic flames

Simulation issues

- Wide range of length and time scale
- Multiple physical processes
- Complex state description
- Exploit high-performance architectures

Consider different approaches to attacking this problem

Computational strategies

Scaling is paramount: Low communication, explicit discretizations, balanced work load – let the machine do the work

- Generic mathematical model
- Define spatial discretization – structured, unstructured, adaptive
- Identify time step based on stability requirements
- Integrate with explicit ODE algorithm
- Range of time scales determines performance

Coupling is paramount: Fully implicit, method of lines, iterative algorithms – preconditioners do the work

- Generic mathematical model
- Define spatial discretization – structured, unstructured, adaptive
- Identify time step based on accuracy requirements
- Integrate with implicit ODE algorithm
- Efficiency of solver/preconditioner determines performance

Computational strategies, cont'd

Mathematical structure is paramount: Develop customized algorithms for specific problem classes. Exploit mathematical structure to compute more efficiently

Components of a computational model

- Mathematical model: describe the problem in a way that is amenable to representation in a computer simulation
- Approximation / discretization: approximate the mathematical model with a finite number of degrees of freedom
- Solvers and software: develop algorithms for solving the discrete approximation efficiently on high-end architecture

To fundamentally change the way we solve these types of problems, we need to consider each of these components and how they fit together

Mathematical formulation

Exploit natural separation of scales between fluid motion and acoustic wave propagation

Low Mach number model, $M = U/c \ll 1$ (Rehm & Baum 1978, Majda & Sethian 1985)

Start with the compressible Navier-Stokes equations for multicomponent reacting flow, and expand in the Mach number, $M = U/c$.

Asymptotic analysis shows that:

$$p(\vec{x}, t) = p_0(t) + \pi(\vec{x}, t) \quad \text{where} \quad \pi / p_0 \sim \mathcal{O}(M^2)$$

- p_0 does not affect local dynamics, π does not affect thermodynamics
- For open containers p_0 is constant
- Pressure field is instanteously equilibrated – removed acoustic wave propagation

Low Mach number equations

Momentum $$\rho \frac{DU}{Dt} = -\nabla \pi + \nabla \cdot \left[\mu \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \nabla \cdot U \right) \right]$$

Species $$\frac{\partial (\rho Y_m)}{\partial t} + \nabla \cdot (\rho U Y_m) = \nabla \cdot (\rho D_m \nabla Y_m) + \dot{\omega}_m$$

Mass $$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho U) = 0$$

Energy $$\frac{\partial \rho h}{\partial t} + \nabla \cdot \left(\rho h \vec{U} \right) = \nabla \cdot (\lambda \nabla T) + \sum_m \nabla \cdot (\rho h_m D_m \nabla Y_m)$$

Equation of state $p_0 = \rho \mathcal{R} T \sum_m \frac{Y_m}{W_m}$ constrains the evolution

System contains evolution equations for U, Y_m, ρ, h, with a constraint.

Low Mach number system can be advanced at fluid time scale instead of acoustic time scale but . . .

We need effective integration techniques for this more complex formulation

Constraint for reacting flows

Low Mach number system is a system of PDE's evolving subject to a constraint; differential algebraic equation (DAE) with index 3

Differentiate constraint to reduce index

Here, we differentiate the EOS along particle paths and use the evolution equations for ρ and T to define a constraint on the velocity:

$$
\begin{aligned}
\nabla \cdot U = \frac{1}{\rho}\frac{D\rho}{Dt} &= -\frac{1}{T}\frac{DT}{Dt} - \frac{\mathcal{R}}{R}\sum_m \frac{1}{W_m}\frac{DY_m}{Dt} \\
&= \frac{1}{\rho c_p T}\left(\nabla \cdot (\lambda \nabla T) + \sum_m \rho D_m \nabla Y_m \cdot \nabla h_m\right) + \\
&\quad \frac{1}{\rho}\sum_m \frac{W}{W_m}\nabla(D_m \rho \nabla Y_m) + \frac{1}{\rho}\sum_m \left(\frac{W}{W_m} - \frac{h_m(T)}{c_p T}\right)\dot{\omega}_m \\
&\equiv S
\end{aligned}
$$

Incompressible Navier Stokes Equations

For iso-thermal, single fluid systems this analysis leads to the incompressible Navier Stokes equations

$$U_t + U \cdot \nabla U + \nabla \pi = \mu \Delta U$$

$$\nabla \cdot U = 0$$

How do we develop efficient integration schemes for this type of constrained evolution system?

Vector field decomposition

$$V = U_d + \nabla \phi$$

where $\nabla \cdot U_d = 0$

and

$$\int U \cdot \nabla \phi dx = 0$$

We can define a projection **P**

$$\mathbf{P} = I - \nabla(\Delta^{-1})\nabla \cdot$$

such that $U_d = \mathbf{P} V$

Solve $-\Delta \phi = \nabla \cdot V$

Then $U_t = \mathbf{P}(\mu \Delta U - U \cdot \nabla U)$

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Projection method

Incompressible Navier Stokes equations

$$U_t + U \cdot \nabla U + \nabla \pi = \mu \Delta U$$

$$\nabla \cdot U = 0$$

Advection step

$$\frac{U^* - U^n}{\Delta t} + U \cdot \nabla U = \frac{\mu}{2}\Delta(U^* + U_n) - \nabla \pi^{n-1/2}$$

Projection step

$$U^{n+1} = \mathbf{P} U^*$$

Can we use this for LMC model?

- Finite amplitude density variation
- inhomogenous constraint

Variable coefficient projection

Generalized vector field decomposition

$$V = U_d + \frac{1}{\rho}\nabla\phi$$

where $\nabla \cdot U_d = 0$ and $U_d \cdot n = 0$ on the boundary

Then U_d and $\frac{1}{\rho}\nabla\phi$ are orthogonal in a density weighted space.

$$\int \frac{1}{\rho}\nabla\phi \cdot U \; \rho \; dx = 0$$

Defines a projection $\mathbf{P}_\rho = I - \frac{1}{\rho}\nabla((\nabla \cdot \frac{1}{\rho}\nabla)^{-1})\nabla\cdot$ such that $\mathbf{P}_\rho V = U_d$.

$\mathbf{P}_\rho$ is idempotent and $||\mathbf{P}_\rho|| = 1$

Generalized vector field decomposition

Use variable-ρ projection to define a generalized vector field decomposition

$$V = U_d + \nabla\xi + \frac{1}{\rho}\nabla\phi$$

where

$$\nabla \cdot \nabla\xi = S$$

and

$$\nabla \cdot U_d = 0$$

We can then define

$$U = \mathbf{P}_\rho(V - \nabla\xi) + \nabla\xi$$

so that $\nabla \cdot U = S$ with $\mathbf{P}_\rho(\frac{1}{\rho}\nabla\phi) = 0$

- This construct allows us to define a projection algorithm for variable density flows with inhomogeneous constraints
- Requires solution of a variable coefficient elliptic PDE
- Allows us to write system as a pure initial value problem

Low Mach number algorithm

Numerical approach based on generalized vector field decomposition
Fractional step scheme

- Advance velocity and thermodynamic variables
  - Advection
  - Diffusion
  - Stiff reactions
- Project solution back onto constraint

Stiff kinetics relative to fluid dynamical time scales

$$\frac{\partial(\rho Y_m)}{\partial t} + \nabla \cdot (\rho U Y_m) = \nabla \cdot (\rho D_m \nabla Y_m) + \dot{\omega}_m$$

$$\frac{\partial(\rho h)}{\partial t} + \nabla \cdot (\rho U h) = \nabla \cdot (\lambda \nabla T) + \sum_m \nabla \cdot (\rho h_m D_m \nabla Y_m)$$

Operator split approach

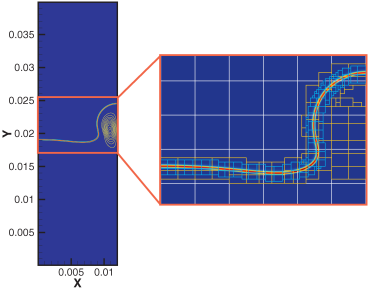
- Chemistry $\Rightarrow \Delta t/2$
- Advection – Diffusion $\Rightarrow \Delta t$
- Chemistry $\Rightarrow \Delta t/2$

AMR – exploit varying resolution requirements in space and time
Block-structured hierarchical grids

- Amortize irregular work

Each grid patch (2D or 3D)

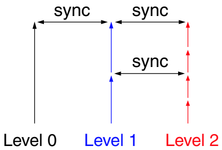
- Logically structured, rectangular
- Refined in space and time by evenly dividing coarse grid cells
- Dynamically created/destroyed



2D adaptive grid hierarchy

Subcycling:

- Advance level ℓ, then
  - Advance level $\ell + 1$
    level ℓ supplies boundary data
  - Synchronize levels ℓ and $\ell + 1$



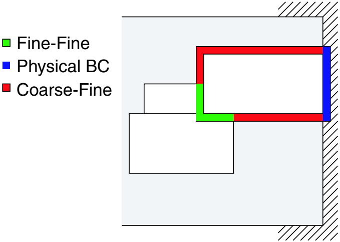
AMR Synchronization

Coarse grid supplies Dirichlet data as boundary conditions for the fine grids.

Errors take the form of flux mismatches at the coarse/fine interface.

Design Principles:

- Define what is meant by the solution on the grid hierarchy.
- Identify the errors that result from solving the equations on each level of the hierarchy "independently".
- Solve correction equation(s) to "fix" the solution.
- Correction equations match the structure of the process they are correcting.



Preserves properties of single-grid algorithm

Software Issues

Complex multiphysics application

- Advective transport – hyperbolic
- Diffusive transport – nonlinear parabolic systems
- Projections – variable coefficient elliptic equations
- Chemical kinetics – stiff ODE's

Dynamic adaptive refinement

Computation requires high-performance parallel architectures

Need to manage software complexity

- Develop data abstractions to support AMR algorithms
- Support parallelization strategy: Distribute grid patches to processors
- Encapsulate data / parallelization in reusable software framework

Software Infrastructure

BoxLib foundation library:

- Domain specific class library: supports solution of PDE's on hierarchical structured adaptive grid
- Functionality for serial, distributed memory & shared memory parallel architectures
    - MPI communication
    - Programming interface through loop iteration constructs

AMR framework library:

- Flow control, memory management, grid generation, checkpoint/restart and plotfile generation

Key issues in parallel implementation

- Dynamic load balancing
- Optimizing communication patterns
- Efficient manipulation of metadata
- Fast linear solvers

But . . .

Does all of this machinery buy us anything?

Folklore (urban legend) says “Since complicated AMR algorithms don’t scale, can’t I solve my problem faster with a scalable algorithm on a machine with a lot of processors?”

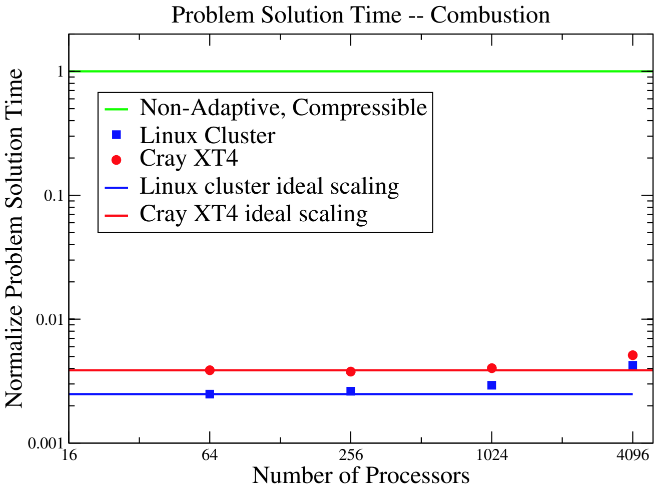
How well do these algorithms scale? What is the implication for solving hard problems?

Weak scaling

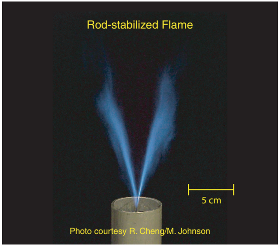
- Let problem get larger as we increase number of processors
- Constant work per processor
- Tests full algorithm
- AMR neutral – fraction of domain refined is invariant

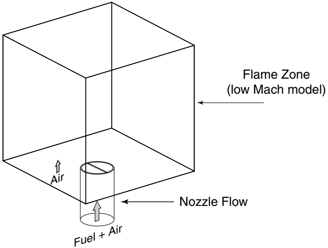
Compare to explicit non-adaptive CNS solver

LMC Performance – Methane Flame



V-flame Validation





Strategy - Treat nozzle exit as inflow boundary condition for combustion simulation

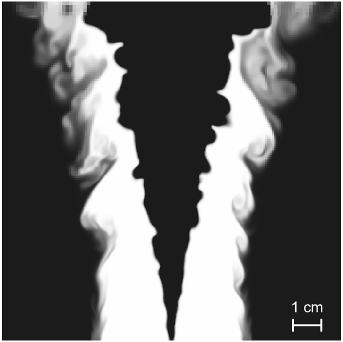
Problem specification

- 12cm x 12cm x 12cm domain
- DRM-19: 20 species, 84 reactions

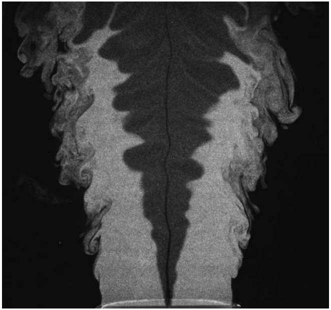
Inflow characteristics

- Mean flow
  - 3 m/s mean inflow
  - Boundary layer profile at edge
  - Noflow condition to model rod
  - Weak co-flow air
- Turbulent fluctuations
  - $\ell_t = 3.5mm$, $u' = 0.18m/sec$
  - Estimated $\eta = 220\mu m$

Results: Computation vs. Experiment

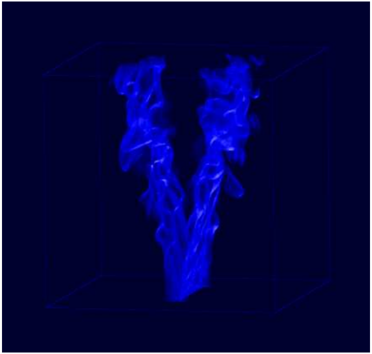


CH_4 from simulation

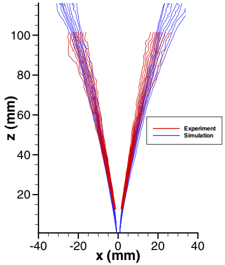


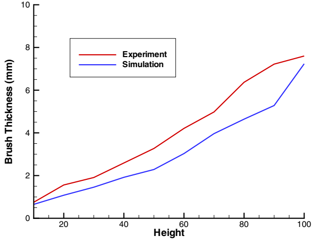
Single image from experimental PIV

Flame Surface

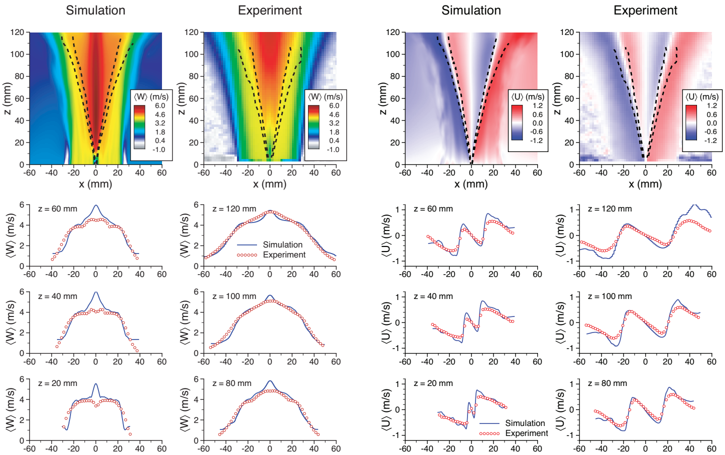


Instantaneous flame surface

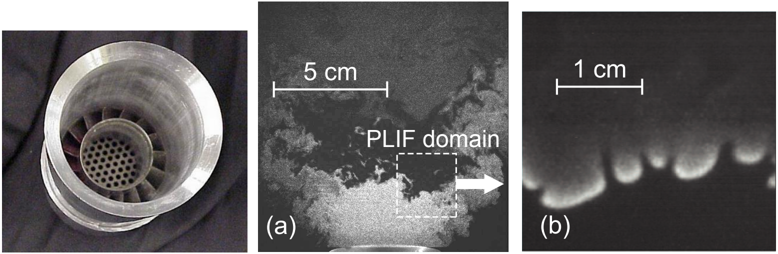




Velocity comparison



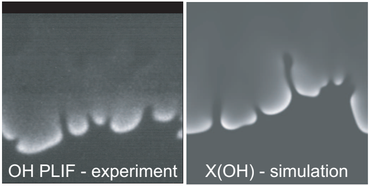
Hydrogen combustion



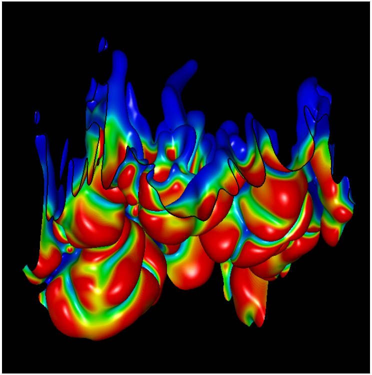
- OH PLIF shows gaps in the flame
- How do these flames burn?
- Are existing engineering models applicable?
- Can standard flame analysis techniques be used to analyze structure?

Hydrogen flame in 3D

3D control simulation of detailed hydrogen flame at laboratory scales ($3 \times 3 \times 9$ cm domain, $\Delta x_f = 58 \mu$m)



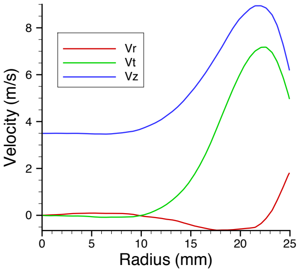
- Figure is “underside” (from fuel side of flame)
- Flame surface (isotherm) colored by local fuel consumption
- Cellular structures convex to fuel, robust extinction ridges



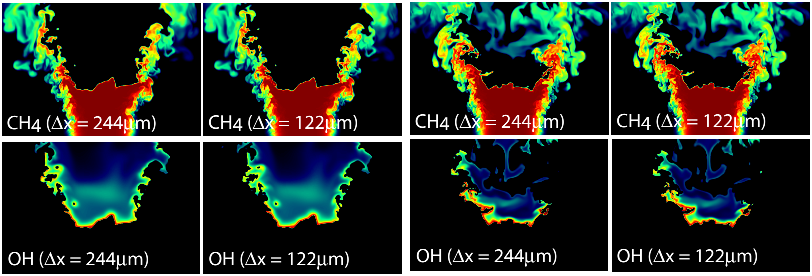
Low swirl burner simulations

Strategy:

- Treat outflow from the nozzle as an inflow boundary condition
  - Mean flow and turbulent intensities from measured data
  - Impose synthetic turbulence as a perturbation to mean inflow
- Simulate flow in a rectilinear domain sitting above the outflow
- Four cases
  - Hydrogen ($\phi = 0.37$) and methane ($\phi = 0.7$)
  - Laminar flame speed approximately 15 cm / sec
  - Two levels of mean flow and turbulence



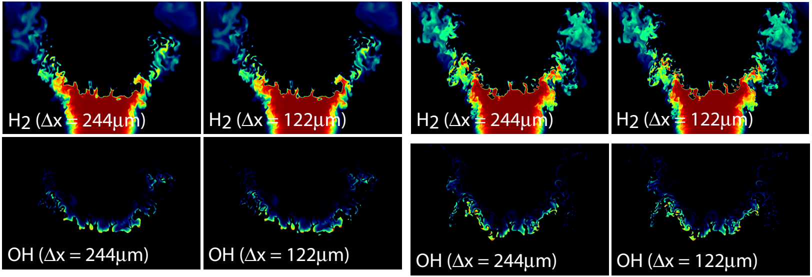
Methane swirl simulations



Weak Turbulence

Strong Turbulence

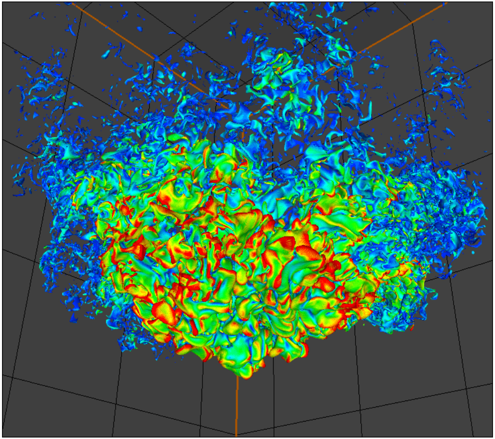
Hydrogen swirl simulations



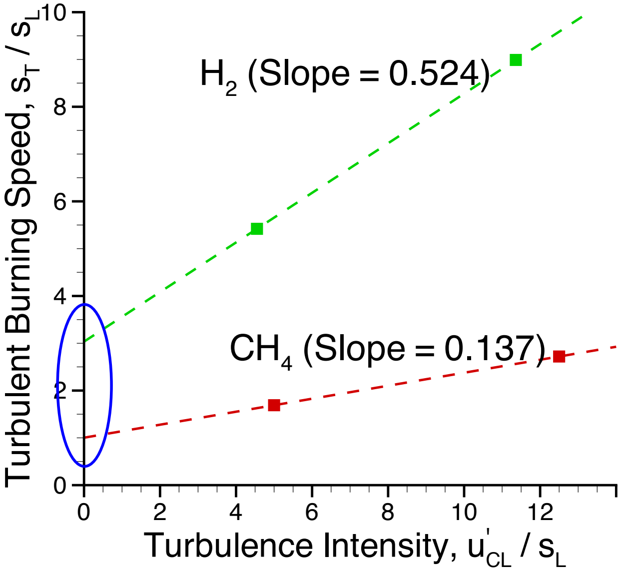
Weak Turbulence

Strong Turbulence

Hydrogen flame surface



Flame Speeds



Summary

Developed new methodology to simulate realistic turbulent flames based on exploiting mathematical structure of combustion problems

Consider all aspects of the problem

- Low Mach number formulation – models
- Projection-based integration methodology – algorithms
- Adaptive mesh refinement – algorithms
- Parallel software infrastructure – solvers and software

There is a tension between these different elements

Algorithms reflect mathematical properties of the problem: Analysis based discretization

Summary

Combining all of these elements resulted in several orders of magnitude improvement in performance, enabling simulations of laboratory-scale premixed turbulent flames with:

- Detailed chemistry and transport
- No explicit models for turbulence or turbulence / chemistry interaction

Future work

- Improved characterization of turbulence conditions
- Closed chamber simulations with long wavelength acoustics
- Include nitrogen chemistry for emissions
- High-pressure simulations