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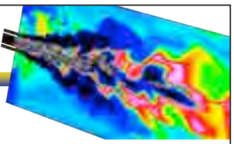

Modeling and Computational Challenges to Study Combustion Instability in Rocket Engine Model Simulations

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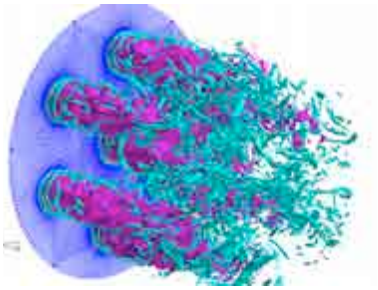

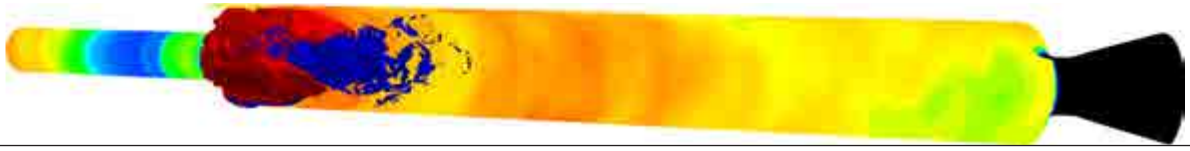

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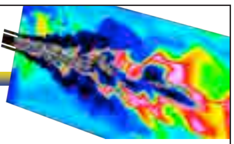
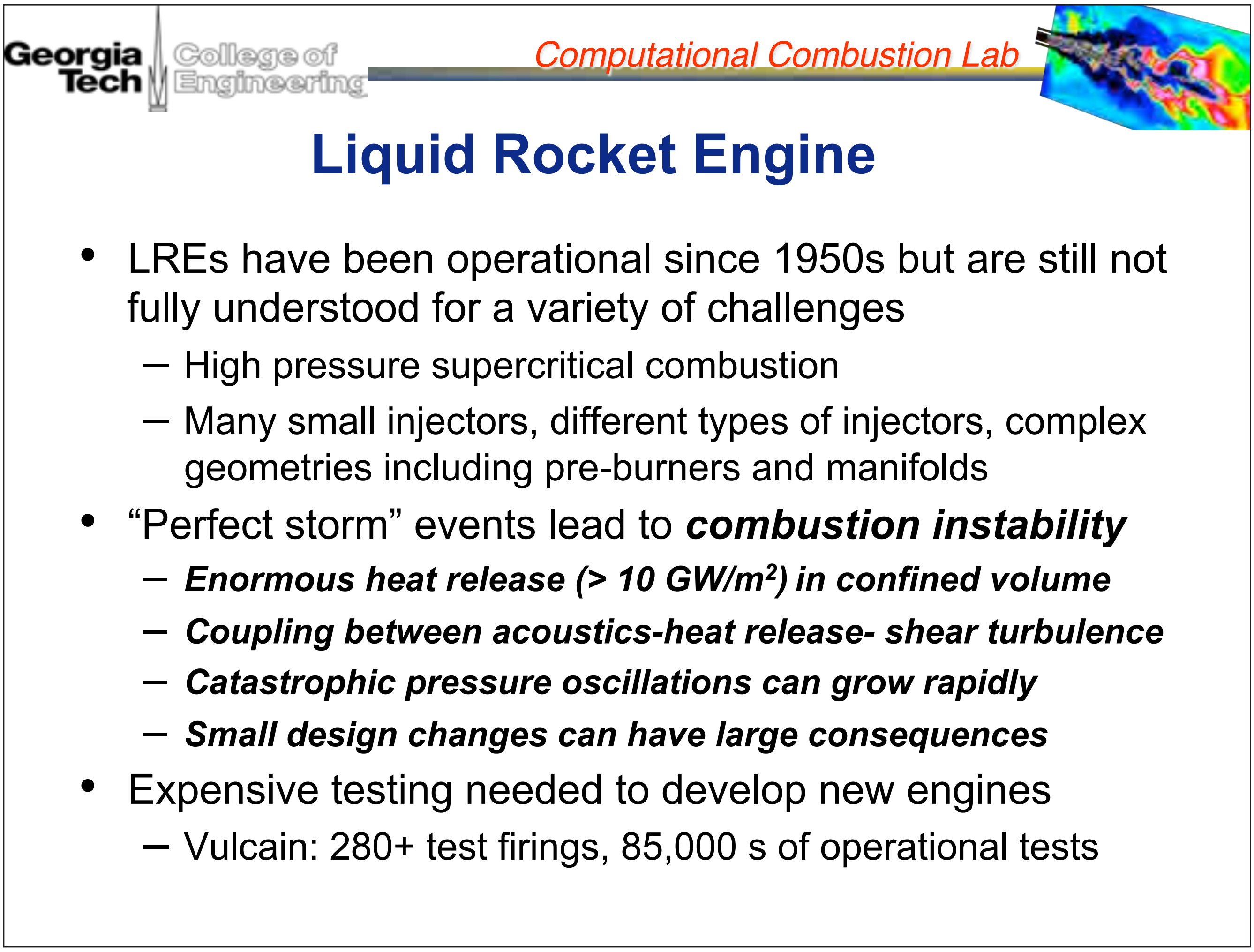


Outline

- Liquid Rocket Engines – Challenges
- Modeling Challenges
- Numerical Algorithm Challenges
- Implementation and Computational Challenges
- Results and Observations
  - Trans-critical mixing studies
  - Trans-critical reacting studies
  - Combustion Instability studies
- Conclusion and future outlook



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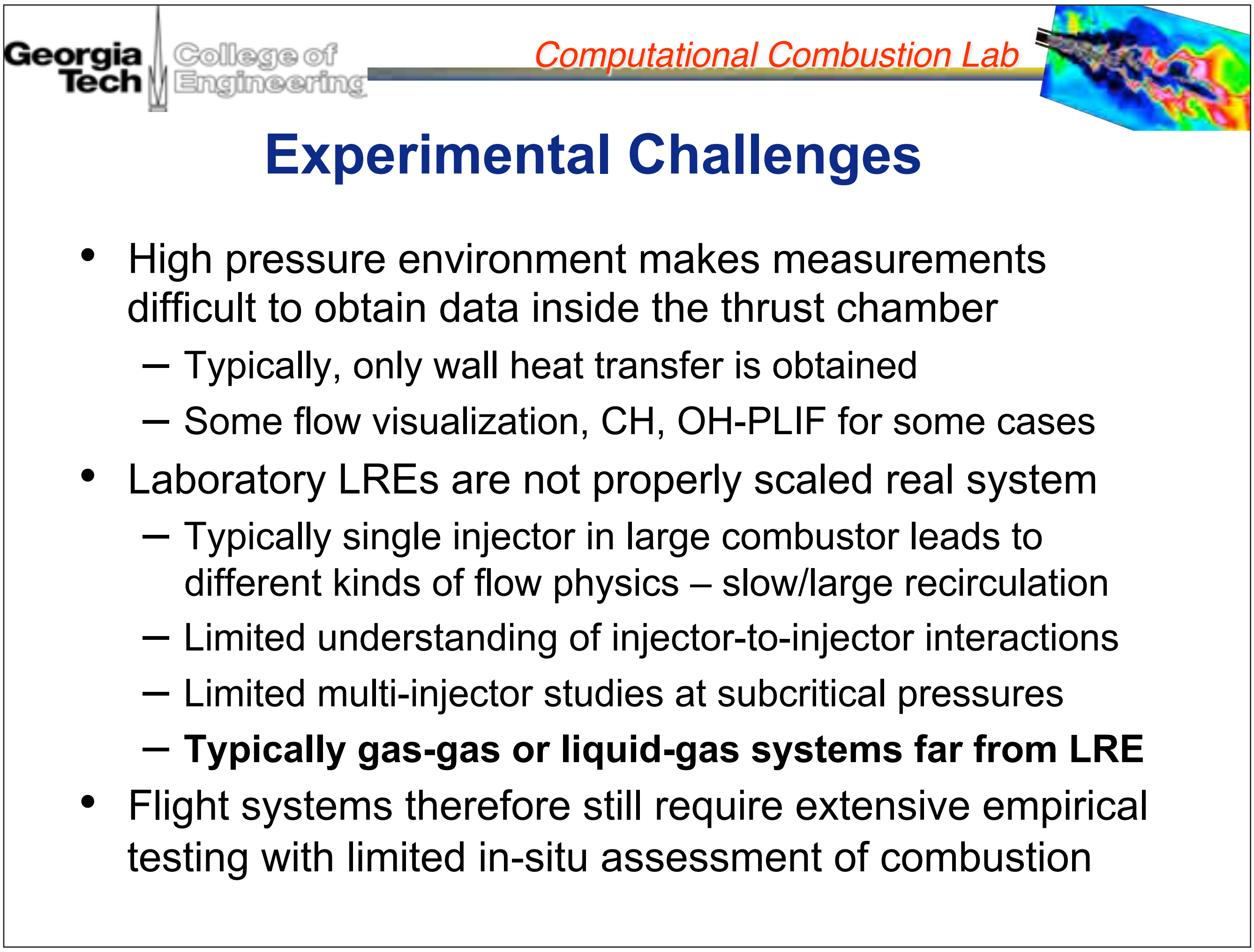
Liquid Rocket Engine

- LREs have been operational since 1950s but are still not fully understood for a variety of challenges
  - High pressure supercritical combustion
  - Many small injectors, different types of injectors, complex geometries including pre-burners and manifolds
- “Perfect storm” events lead to ***combustion instability***
  - ***Enormous heat release (> 10 GW/m^2) in confined volume***
  - ***Coupling between acoustics-heat release- shear turbulence***
  - ***Catastrophic pressure oscillations can grow rapidly***
  - ***Small design changes can have large consequences***
- Expensive testing needed to develop new engines
  - Vulcain: 280+ test firings, 85,000 s of operational tests



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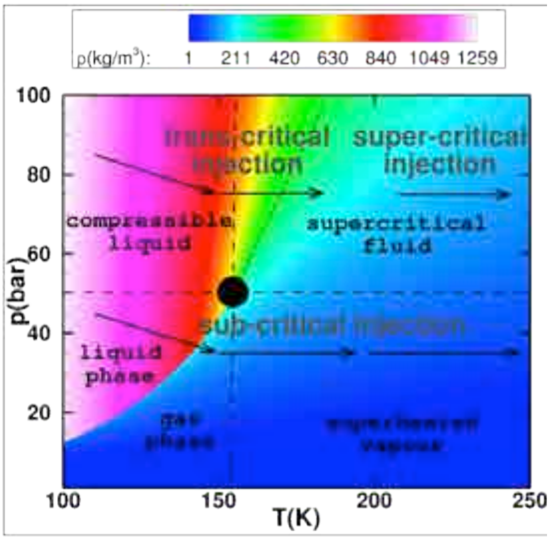
Experimental Challenges

- High pressure environment makes measurements difficult to obtain data inside the thrust chamber
  - Typically, only wall heat transfer is obtained
  - Some flow visualization, CH, OH-PLIF for some cases
- Laboratory LREs are not properly scaled real system
  - Typically single injector in large combustor leads to different kinds of flow physics – slow/large recirculation
  - Limited understanding of injector-to-injector interactions
  - Limited multi-injector studies at subcritical pressures
  - **Typically gas-gas or liquid-gas systems far from LRE**
- Flight systems therefore still require extensive empirical testing with limited in-situ assessment of combustion

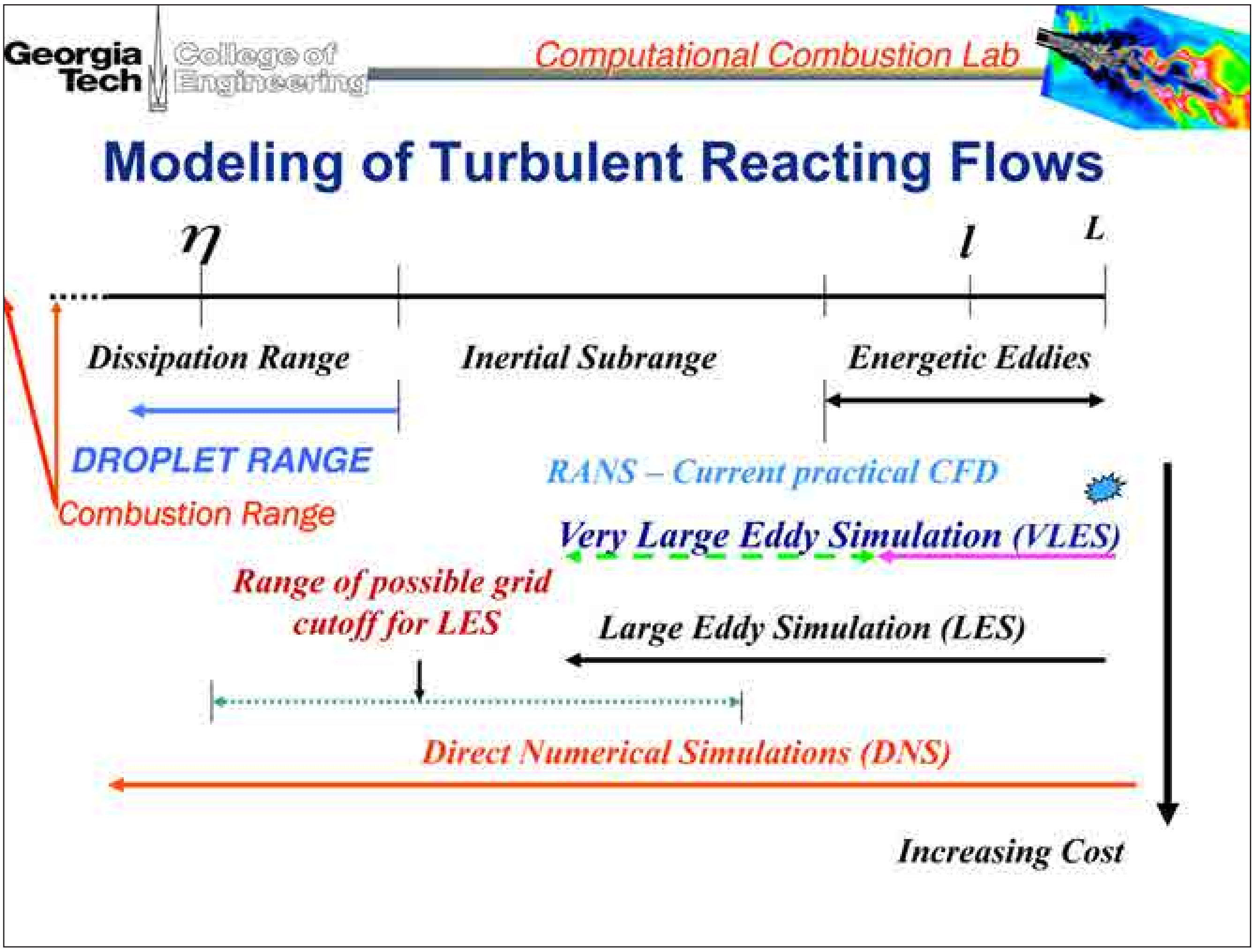
Modeling Challenges

- High pressure conditions
  - Supercritical conditions
  - Real Gas Equation of State
  - Trans-critical events
- 3D unsteady features
  - Simple geometry but complex physics in small narrow regions
- RANS cannot capture turbulent fluctuations and interactions
- DNS is too expensive
- Perhaps LES or something else?
- How to validate?



Turbulence Modeling Approaches

- Direct numerical simulation (DNS)
  - Transient, 3-D, resolve all fluctuations, no modeling
- Moment formulation (RANS/URANS-Models)
  - Mean, variances, co-variance predicted
  - Model the complete spectrum
- Large-Eddy-Simulation (LES or VLES)
  - Transient, 3-D, resolve large-scales, model ‘unresolved’ scale effect on the ‘resolved’ scale
  - Only ‘energy-containing’ scales resolved in VLES
  - Energy-containing and inertial scales resolved in LES
- Hybrid Schemes: Detached Eddy Simulation, RANS-LES
  - **New hybrid terms appear that require new closure**



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Modeling of Turbulent Reacting Flows

Dissipation Range

Inertial Subrange

Energetic Eddies

DROPLET RANGE

Combustion Range

RANS – Current practical CFD

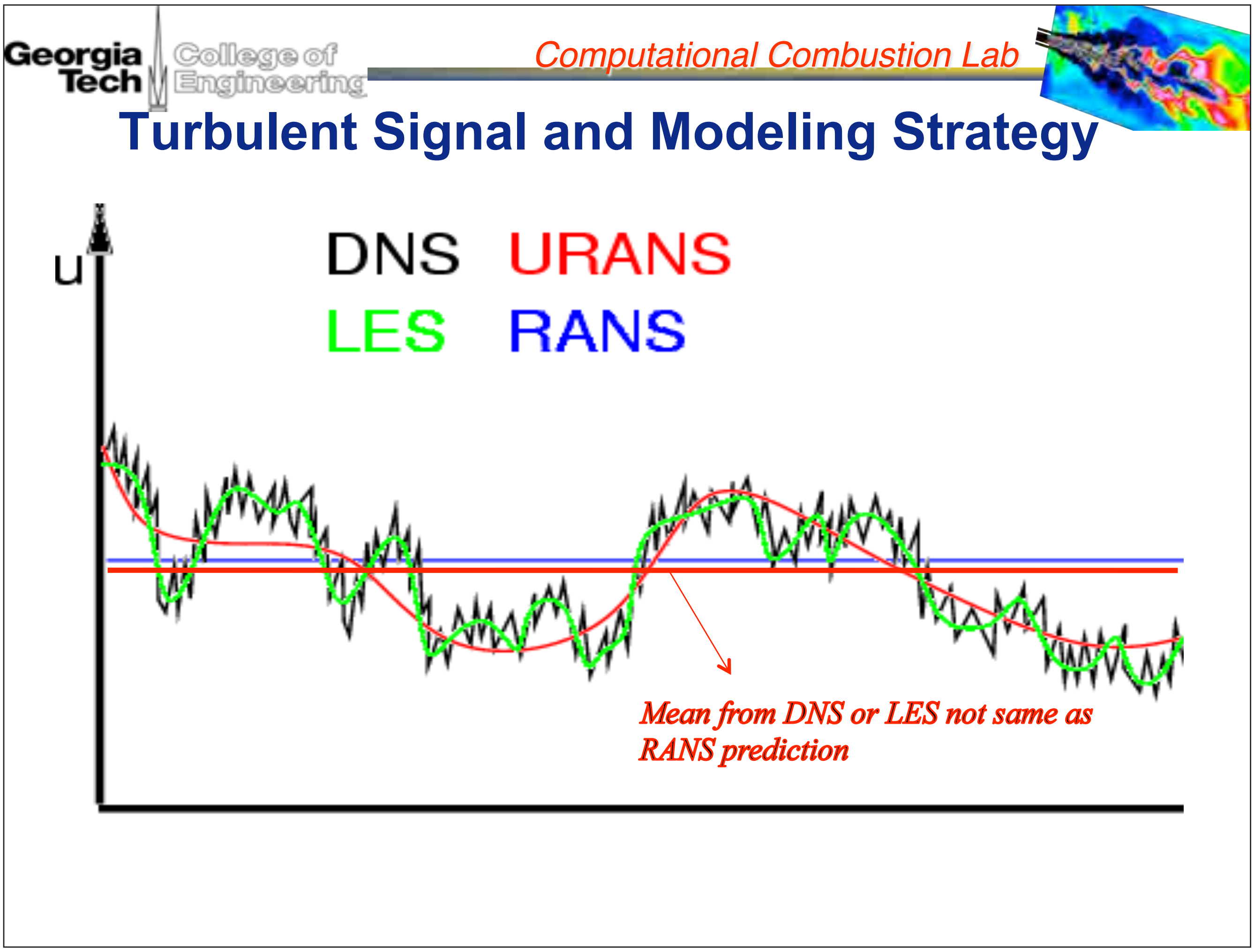
Very Large Eddy Simulation (VLES)

Range of possible grid cutoff for LES

Large Eddy Simulation (LES)

Direct Numerical Simulations (DNS)

Increasing Cost



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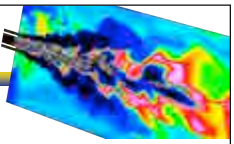
Turbulent Signal and Modeling Strategy

Mean from DNS or LES not same as RANS prediction



Modeling Strategy

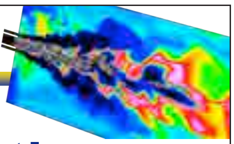
- Compressible conservative formulation needed to capture acoustic-vortex-flame interactions, shocks etc.
- Favre-filtered equations (with many assumptions)
  - Gradient – filter commute, top-hat filter, etc.

$$\frac{\partial\bar\rho}{\partial t}+\frac{\partial\bar\rho\tilde u_i}{\partial x_i}=0$$

$$\frac{\partial\bar\rho\tilde u_i}{\partial t}+\frac{\partial}{\partial x_j}\left(\bar\rho\tilde u_i\tilde u_j+p(\bar\phi)\delta_{ij}-\bar\tau_{ij}+\tau_{ij}^{sgs}+p^{sgs}\delta_{ij}\right)=0$$

$$\frac{\partial\bar\rho\tilde e_T}{\partial t}+\frac{\partial}{\partial x_i}\left(\bar\rho\tilde e_T\tilde u_i+p(\bar\phi)\tilde u_i+\bar Q_{i,IK}-\tilde u_j\bar\tau_{ji}+H_i^{sgs}+\sigma_i^{sgs}+p^{sgs}\tilde u_i\right)=0$$

$$\frac{\partial\bar\rho\tilde Y_k}{\partial t}+\frac{\partial}{\partial x_i}\left(\bar\rho\tilde Y_k\tilde u_i+\bar J_{i,k}+Y_{i,k}^{sgs}+\theta_i^{sgs}\right)=\dot{\bar\omega}_k \quad \text{for } k=1\ldots N_S$$



Compressible, conservative formulation

- Filtered Mass and Heat Flux (without cross-diffusion):
  - **Heat flux:**

$$\bar Q_{i,\mathrm{IK}} = -\bar\lambda\frac{\partial\tilde T}{\partial x_i}+\bar\rho\sum_{k=1}^{N_S}\tilde h_k\tilde Y_k\tilde{\mathcal{V}}_{i,k}+\sum_{k=1}^{N_S}Q_{i,k}^{\mathrm{sgs}}$$

  - **Mass flux:**

$$\bar J_{i,k} = \bar\rho\tilde Y_k\widetilde{\mathcal{V}_{i,k}} \qquad \tilde{\mathcal{V}}_{i,k} = -\frac{\bar{\mathcal{D}}_{k,m}}{\tilde Y_k}\frac{\partial\tilde Y_k}{\partial x_i}$$

- Filtered Real Gas Equation(s) of State (EOS)
  - Peng-Robinson (PR)
  - Soave-Redlich-Kwong (SRK)
  - Redlich-Kwong (RK)

$$p(\bar\phi)=\bar\rho\tilde Z\tilde R\tilde T+p^{sgs}$$

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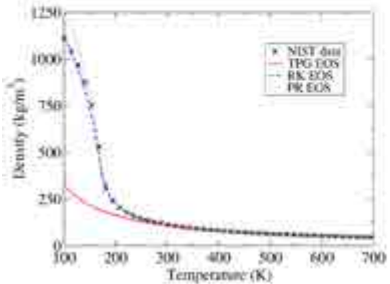
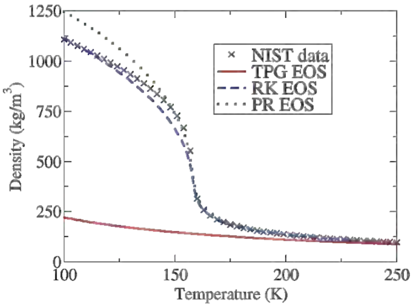
Thermodynamics and Transport properties for Real Gas Applications

- Corresponding state principles:
  - Peng-Robinson EOS
  - Chung's method for viscosity, thermal conductivity
  - Fuller's method for diffusion coefficient
- Proven good compromise cost/accuracy[1,2]
- Fully conservative formulation requires optimized non-linear solver
  - Use density and internal energy to obtain pressure and temperature



O2, P=60 bars



CH4, P=100 bars

[1] J. C. Oefelein. *Combustion Science and Technology, 178:229–252, 2006.*

[2] A. Congiunti, C. Bruno, and E. Giacomazzi. *AIAA 2003-478, 2003.*

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Subgrid Closure Terms

Reynolds Stress	$\tau_{ij}^{sgs} = \bar{\rho}\left(\widetilde{u_i u_j} - \tilde{u}_i \tilde{u}_j\right)$
Enthalpy Flux	$H_i^{sgs} = \bar{\rho}\left(\widetilde{E u_i} - \tilde{E}\tilde{u}_i\right) + \left(\overline{p u_i} - \bar{p}\tilde{u}_i\right)$
Viscous Work	$\sigma_i^{sgs} = \widetilde{u_j \tau_{ij}} - \tilde{u}_j \bar{\tau}_{ij}.$
Convective-Species	$Y_{i,k}^{sgs} = \bar{\rho}[\widetilde{u_i Y_k} - \tilde{u}_i \tilde{Y}_k]$
Heat Flux	$q_{i,k}^{sgs} = [\overline{h_k D_k \partial Y_k / \partial x_i} - \tilde{h}_k \tilde{D}_k \partial \tilde{Y}_k / \partial x_i]$
Species-Diffusive Flux	$\theta_{i,k}^{sgs} = \bar{\rho}[\widetilde{V_{i,k} Y_k} - \tilde{V}_{i,k} \tilde{Y}_k]$
Filtered EOS	$p^{sgs} = \bar{\rho}\left(\widetilde{ZRT} - \tilde{Z}\tilde{R}\tilde{T}\right) = \bar{\rho} R_u \sum \frac{1}{MW_k}\left(\widetilde{ZY_k T} - \tilde{Z}\tilde{Y}_k\tilde{T}\right)$

- Typically gradient transport for momentum and energy subgrid transport is used
  - Isotropic scalar eddy viscosity
  - Need length scale and velocity scale(s)

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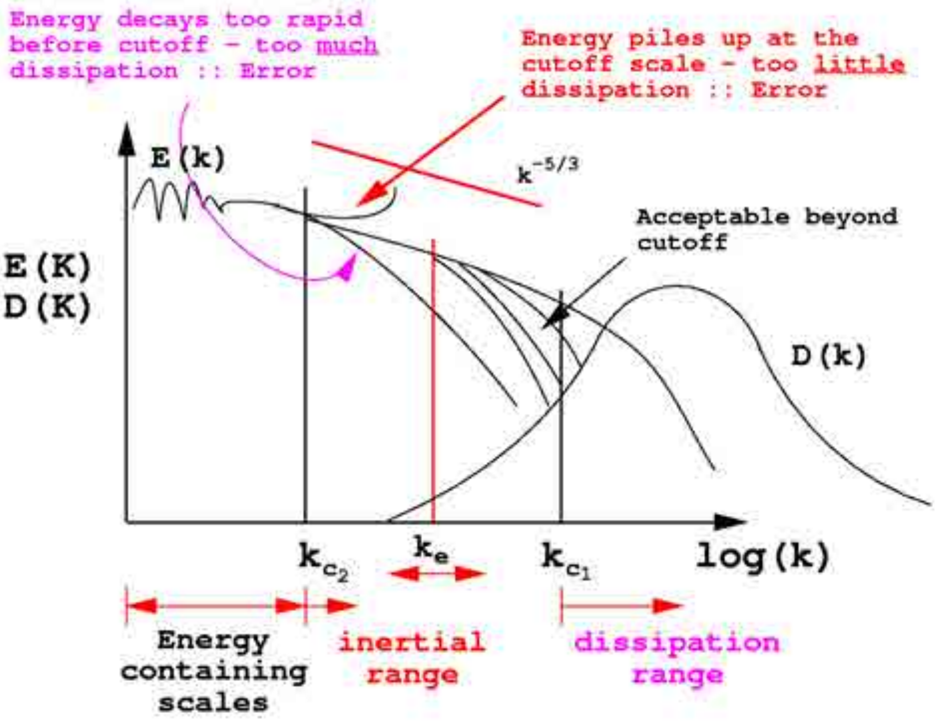
Impact of Filtering on Turbulence



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Localized Dynamic Kinetic Energy

- SGS Stress: $$\tau_{ij}^{sgs} = -2\bar{\rho}\nu_t\left(\widetilde{S_{ij}} - \tfrac{1}{3}\widetilde{S_{kk}}\right) + \tfrac{1}{3}\tau_{kk}\delta_{ij}$$
- Characteristic length provided by the local grid spacing
- Smagorinsky algebraic model for the subgrid stress

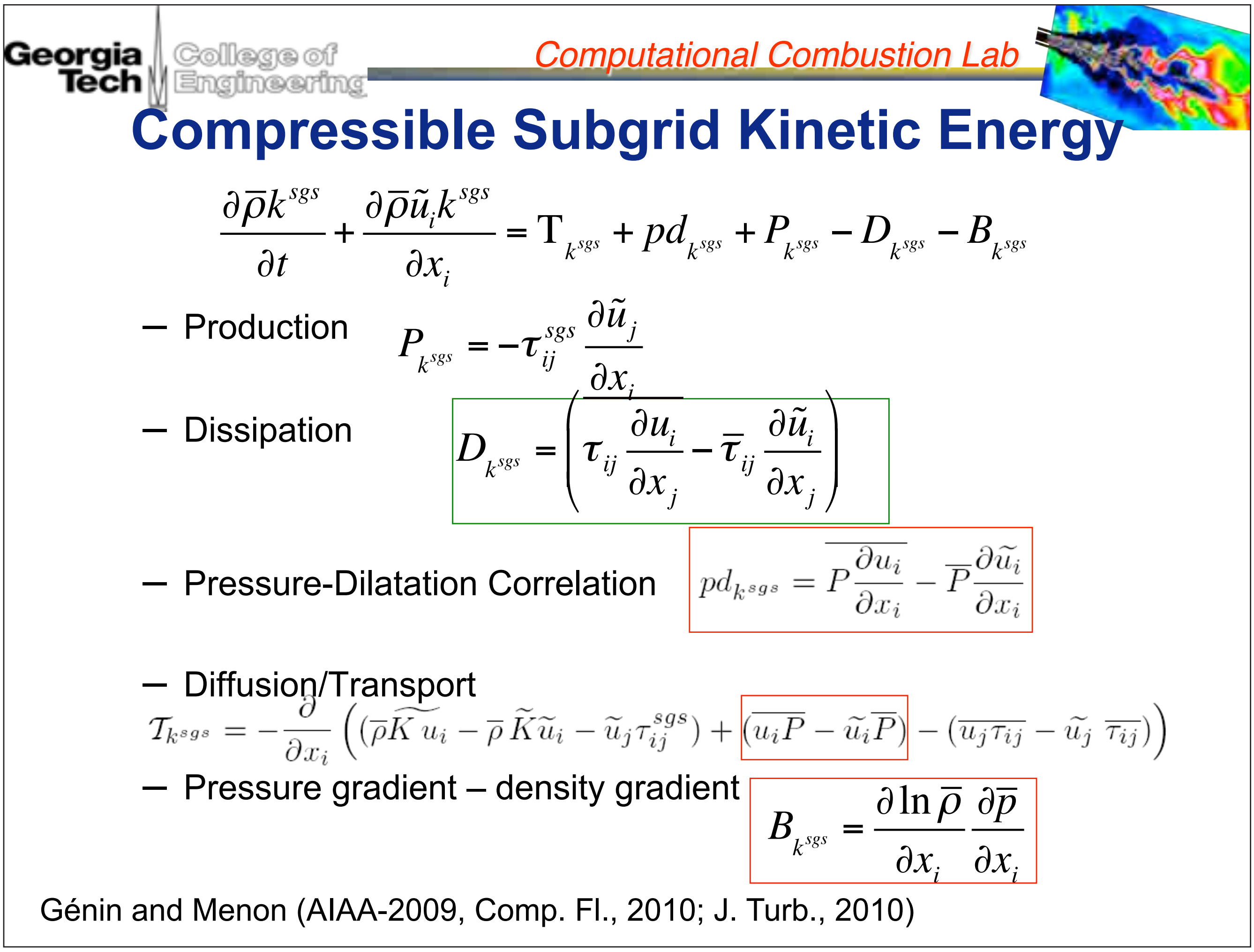
$$\nu_t = C\Delta^2|\widetilde{S}| \qquad |\widetilde{S}| = \sqrt{2S_{ij}S_{ij}}$$

- One-equation model for subgrid kinetic energy (Schumann)

$$\boxed{\nu_t \;=\; C_\nu\sqrt{k^{sgs}}\;\overline{\Delta}}$$

$$H_i^{\rm sgs} = \bar{\rho}\left[\widetilde{e_T u_i} - \tilde{e}_T\tilde{u}_i\right] + \left[\overline{pu_i} - \bar{p}\tilde{u}_i\right] \approx -\bar{\rho}\frac{\nu_t}{{\rm Pr}_t}\frac{\partial\tilde{h}}{\partial x_i}$$

$$Y_{i,k}^{\rm sgs} = \bar{\rho}\left[\widetilde{u_i Y_k} - \tilde{u}_i\tilde{Y}_k\right] \approx -\bar{\rho}\frac{\nu_t}{{\rm Sc}_t}\frac{\partial\tilde{Y}_k}{\partial x_i}$$



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Compressible Subgrid Kinetic Energy

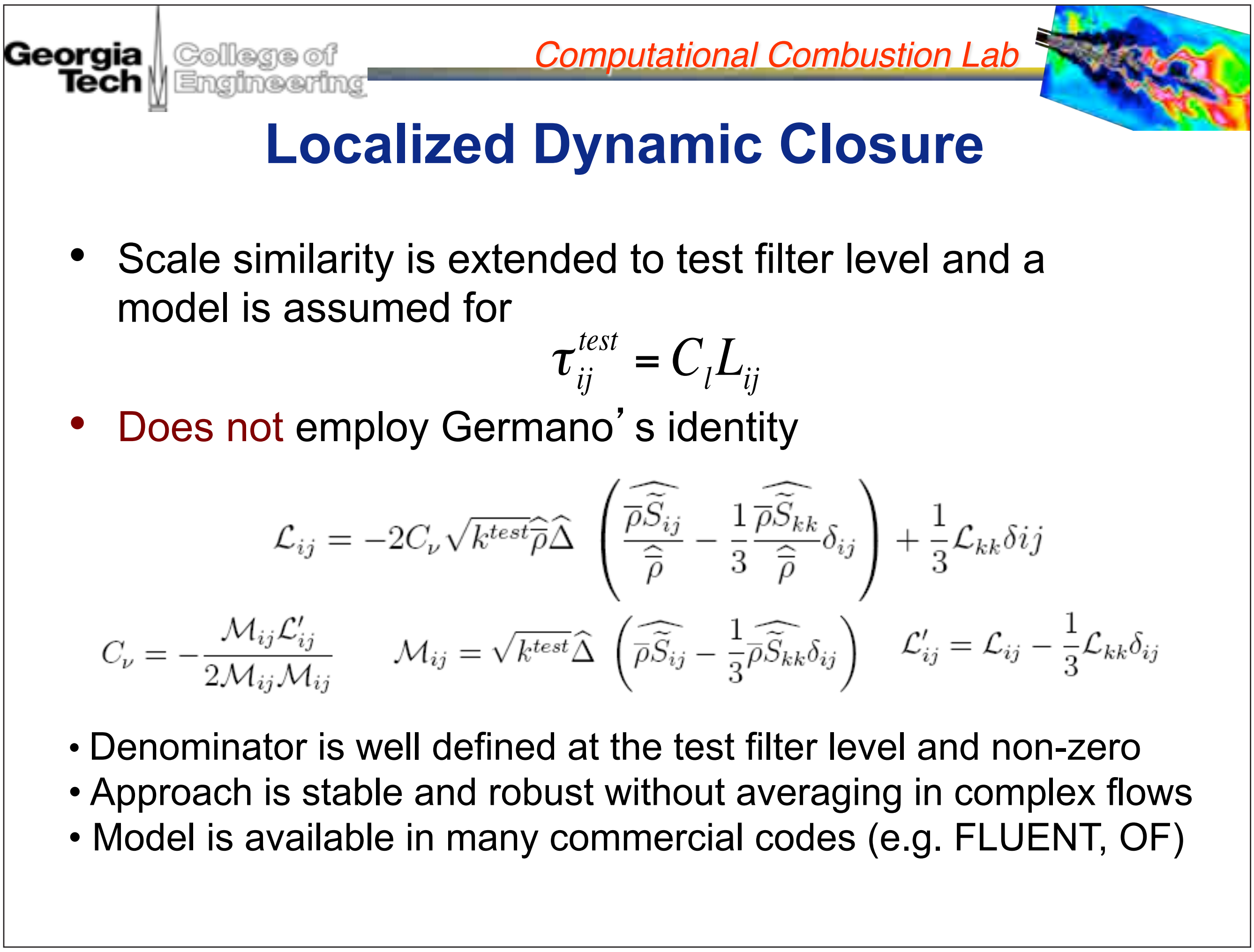
$$\frac{\partial\overline{\rho}k^{sgs}}{\partial t} + \frac{\partial\overline{\rho}\widetilde{u}_i k^{sgs}}{\partial x_i} = \mathrm{T}_{k^{sgs}} + pd_{k^{sgs}} + P_{k^{sgs}} - D_{k^{sgs}} - B_{k^{sgs}}$$

- Production $P_{k^{sgs}} = -\tau_{ij}^{sgs}\frac{\partial\widetilde{u}_j}{\partial x_i}$
- Dissipation $\boxed{D_{k^{sgs}} = \left(\overline{\tau_{ij}\frac{\partial u_i}{\partial x_j}} - \overline{\tau}_{ij}\frac{\partial\widetilde{u}_i}{\partial x_j}\right)}$
- Pressure-Dilatation Correlation $\boxed{pd_{k^{sgs}} = \overline{P\frac{\partial u_i}{\partial x_i}} - \overline{P}\frac{\partial\widetilde{u}_i}{\partial x_i}}$
- Diffusion/Transport

$$\mathcal{T}_{k^{sgs}} = -\frac{\partial}{\partial x_i}\left((\overline{\rho}\widetilde{K u_i} - \overline{\rho}\widetilde{K}\widetilde{u}_i - \widetilde{u}_j\tau_{ij}^{sgs}) + \boxed{(\overline{u_i P} - \widetilde{u}_i\overline{P})} - (\overline{u_j\tau_{ij}} - \widetilde{u}_j\,\overline{\tau_{ij}})\right)$$

- Pressure gradient – density gradient $\boxed{B_{k^{sgs}} = \frac{\partial\ln\overline{\rho}}{\partial x_i}\frac{\partial\overline{p}}{\partial x_i}}$

Génin and Menon (AIAA-2009, Comp. Fl., 2010; J. Turb., 2010)



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Localized Dynamic Closure

- Scale similarity is extended to test filter level and a model is assumed for

$$\tau_{ij}^{test} = C_l L_{ij}$$

- Does not employ Germano’s identity

$$\mathcal{L}_{ij} = -2C_\nu\sqrt{k^{test}}\widehat{\overline{\rho}}\widehat{\Delta}\left(\frac{\widehat{\overline{\rho}\widetilde{S}_{ij}}}{\widehat{\overline{\rho}}} - \frac{1}{3}\frac{\widehat{\overline{\rho}\widetilde{S}_{kk}}}{\widehat{\overline{\rho}}}\delta_{ij}\right) + \frac{1}{3}\mathcal{L}_{kk}\delta ij$$

$$C_\nu = -\frac{\mathcal{M}_{ij}\mathcal{L}'_{ij}}{2\mathcal{M}_{ij}\mathcal{M}_{ij}} \qquad \mathcal{M}_{ij} = \sqrt{k^{test}}\widehat{\Delta}\left(\widehat{\overline{\rho}\widetilde{S}_{ij}} - \frac{1}{3}\widehat{\overline{\rho}\widetilde{S}_{kk}}\delta_{ij}\right) \qquad \mathcal{L}'_{ij} = \mathcal{L}_{ij} - \frac{1}{3}\mathcal{L}_{kk}\delta_{ij}$$

- Denominator is well defined at the test filter level and non-zero
- Approach is stable and robust without averaging in complex flows
- Model is available in many commercial codes (e.g. FLUENT, OF)

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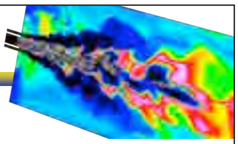

The Filtered Reaction Rate Closure

- Most difficult to close even without real gas effects
- Many alternate strategies developed to avoid the closure
- Critical to understand the application requirements
  - Assumptions valid in one flow may not work in another
- Mixed premixed-partially premixed-non-premixed regimes
- Scale Separation implicit or explicit in ALL closures
  - Turbulence and combustion scales separated in the inertial range
  - Mixing process in the inertial range independent of chemistry and simplify modeling considerable
  - Kolmogorov scaling laws are not modified by molecular mixing and heat release at the (even) smaller scales.
  - Reasonable but is this true at high Re or for Real Gas?

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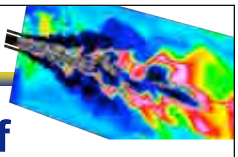

Turbulent Combustion Models in Terms of Chemistry and Mixing (Modified from Peters, pg 64)

	Premixed Combustion	**Nonpremixed Combustion**
Infinitely Fast Chemistry	**Bray-Moss-Libby** **Coherent Flame**	**Conserved Scalar Equilibrium Model**
Finite-rate w/o Molecular mixing	**PDF Transport**	**PDF Transport**
Finite-rate with filtered or modeled reaction rate	**Flamelet Model** **G-equation, G-Z, ATF** **EBU, FSD, PaSR…**	**Flamelet Model** **Z, ATF, CMC, PaSr…**
Finite-rate with Molecular mixing	**Linear-Eddy Model**	**Linear-Eddy Model**

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Flamelet or Finite-Rate?

- Flamelet concept is cost effective but may not be valid in LRE everywhere in the thrust chamber
- Non-premixed burning requires proper treatment of turbulent and Molecular (including differential) mixing
- Combustion instability can change flame structure
- Unsteady heat release coupling may require proper estimate of partially burned effects and radical chemistry
  - – Multi-component diffusion needed
  - – Finite-rate kinetics needed
- Flame structure may be much more complex

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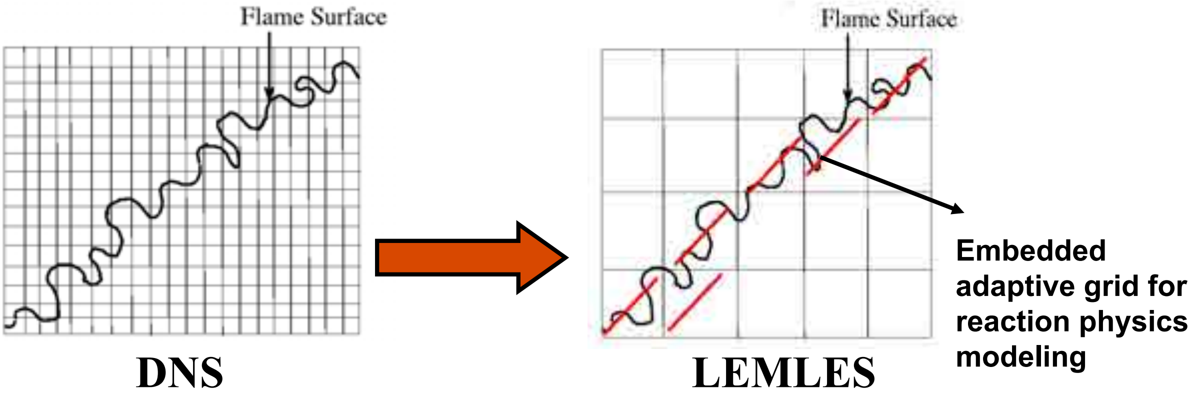
Turbulence-Flame Interactions



- Localized dynamic closure for subgrid kinetic energy
  - Scale similar closure that is stable in complex flows
- Grid-within-grid approach
  - Simulate large-scales on the LES grid
  - Simulate molecular processes: subgrid turbulent mixing, molecular diffusion and finite-rate at the SUBGRID level

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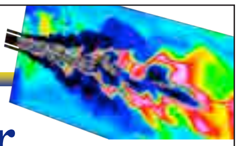

Species Equation: Two Scale Solver

- **Resolved Species Equation**

$$\frac{\partial(\rho Y_k)}{\partial t} + \underbrace{\frac{\partial(\rho u_i Y_k)}{\partial x_i}}_{\text{(Resolved+Unresolved) scale convection}} - \underbrace{\frac{\partial}{\partial x_i}\left(\rho D_k \frac{\partial Y_k}{\partial x_i}\right)}_{\text{Molecular diffusion}} = \underbrace{\dot{\omega}_k}_{\text{Chemical source term}} + \underbrace{\dot{S}_k}_{\text{Spray source term}}$$

- **Two scale procedure is used:** $u_i = \left(\tilde{u}_i + u'_{sgs}\right)_R + u'_{UR}$
  - **Unresolved Scale**

$$\frac{(\rho Y_k)^* - (\rho Y_k)^n}{\Delta t_{LES}} = -\underbrace{\frac{\partial\left(\rho^n u'_{UR} Y_k^n\right)}{\partial x_i}}_{\text{Convection}} + \underbrace{\frac{\partial}{\partial x_i}\left(\rho^n D_k \frac{\partial Y_k^n}{\partial x_i}\right)}_{\text{Molecular diffusion}} + \underbrace{\dot{\omega}_k^n}_{\text{Chemical source}} + \underbrace{\dot{S}_k^n}_{\text{Spray source}}$$

  - **Resolved Scale**

$$\frac{(\rho Y_k)^{n+1} - (\rho Y_k)^*}{\Delta t_{LES}} = -\underbrace{\frac{\partial}{\partial x_i}\left[\rho^* \left(\tilde{u}_i^* + u'_{sgs}\right)_R Y_k^*\right]}_{\text{Convection}}$$

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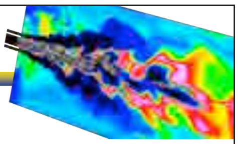
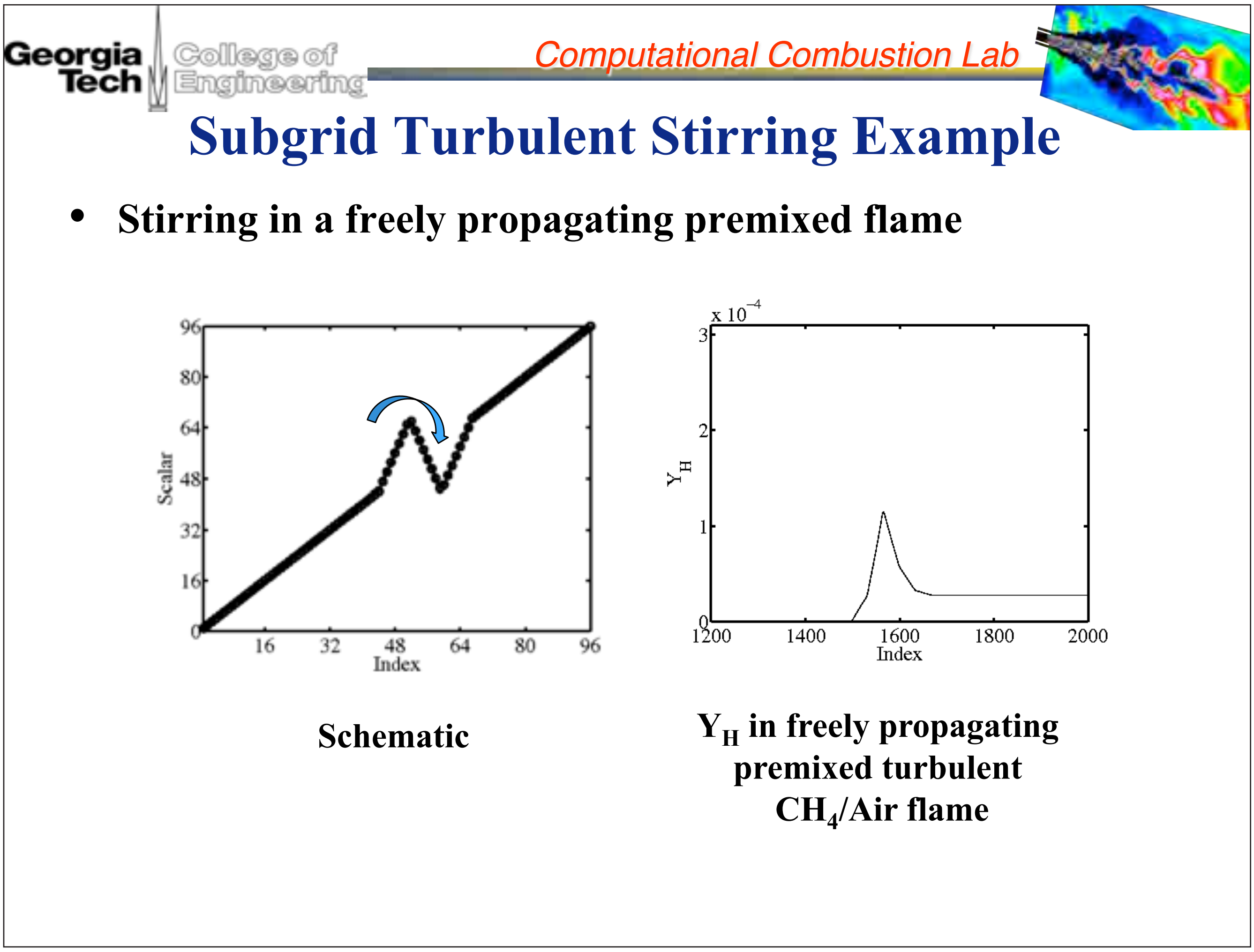


LEMLES Processes

- NO filtering of the species equations
  - Eulerian-Lagrangian solver for species equation
- Reaction-Diffusion processes
  - Evolves in a “grid” inside the LES grid
  - Full multi-component and differential diffusion included
  - Finite-rate kinetics included without needing closure
- Turbulent stirring by eddies smaller than LES grid
  - Stochastic process that is based on Kolmogorov scaling
- Volumetric expansion of subgrid field due to heat release
- Computational more expensive than flamelet but no need for a priori choice of flame type
  - Parallel optimization techniques can reduce cost



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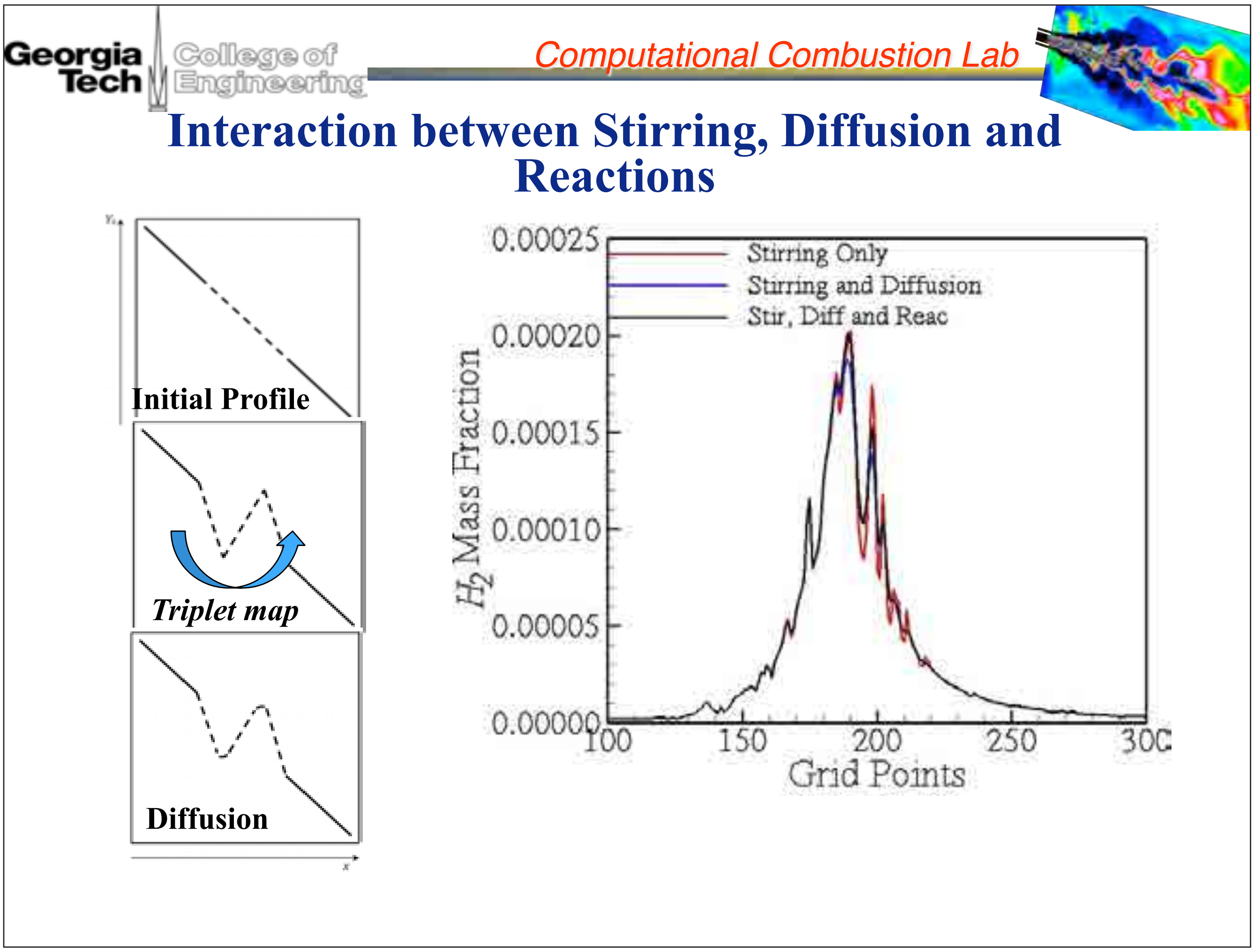
Subgrid Turbulent Stirring Example

- **Stirring in a freely propagating premixed flame**

Schematic

Y_H in freely propagating premixed turbulent CH_4/Air flame



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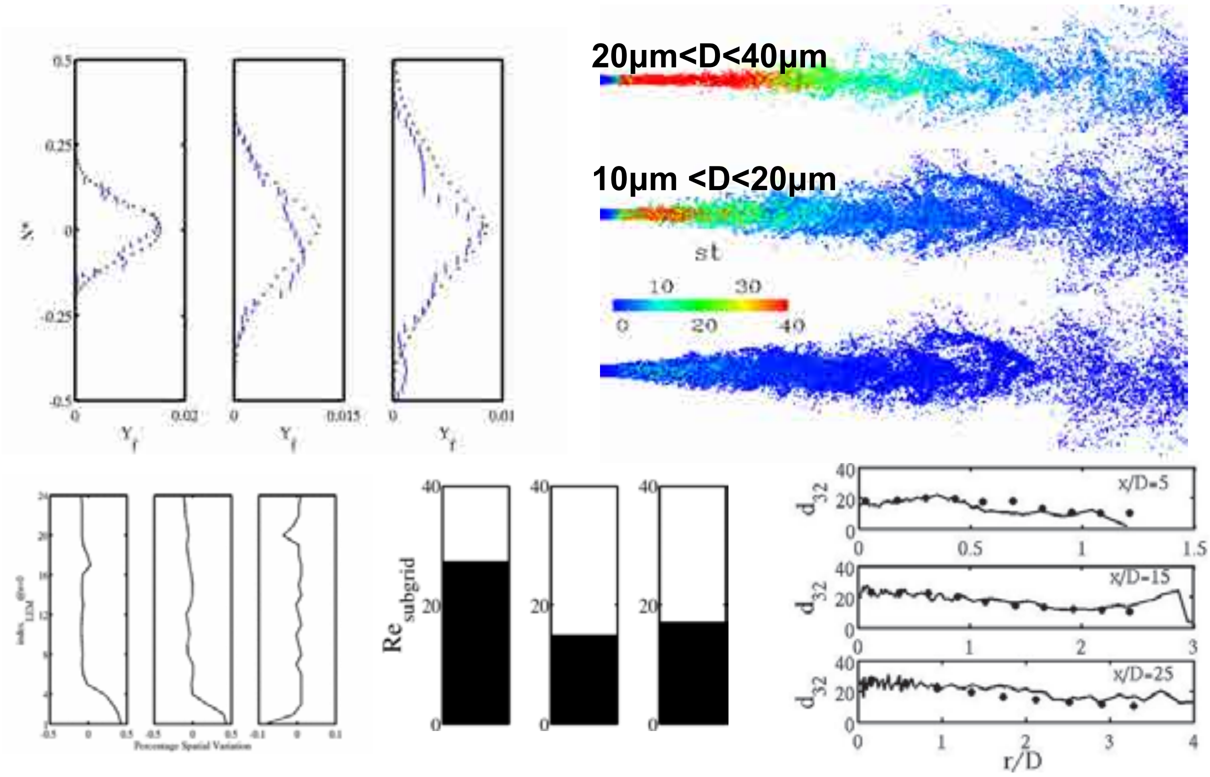
Interaction between Stirring, Diffusion and Reactions

LEMLES of Vapor & Droplet Distribution*



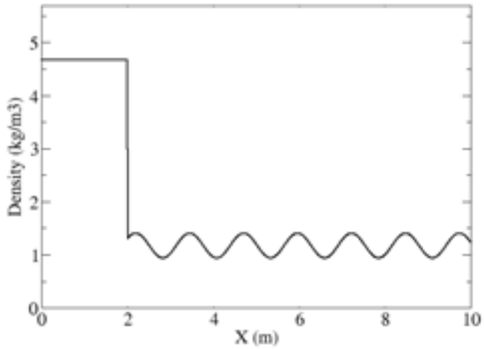
* Acetone spray Chen et al., 2006; Srinivasan et al. (DLES, 2010)

Numerical Challenges

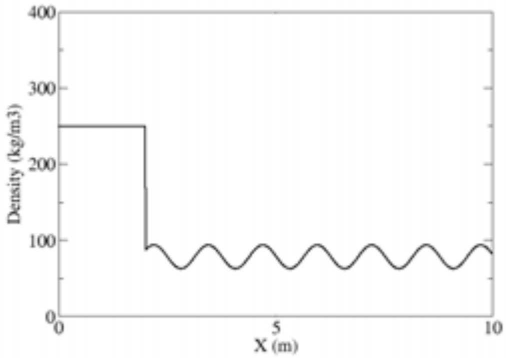
- Many solver strategies in existence but not all will work for Real gas and supercritical combustion
  - Very large density gradients and shear turbulence both need to be captured in a complex geometry
- Central and compact schemes require local or explicit artificial filtering or dissipation to stabilize
- DNS high order algorithms will not work in stretched and body conforming grid
- Hybrid solvers are being developed to capture both large-gradient interface and shear turbulence
  - Hybrid WENO – Central
  - Hybrid HLLC/E – Central/Predictor-Corrector

Hybrid central-HLLC scheme

- Locally adaptive sensor switches between schemes
- Shu-Osher test at Mach 3 with and without Real Gas



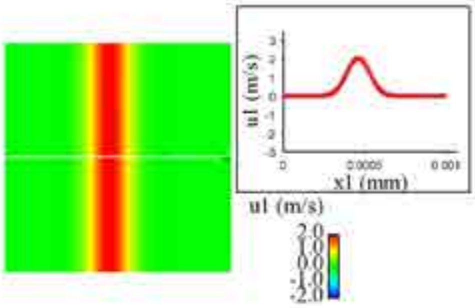
Standard air Z = 1



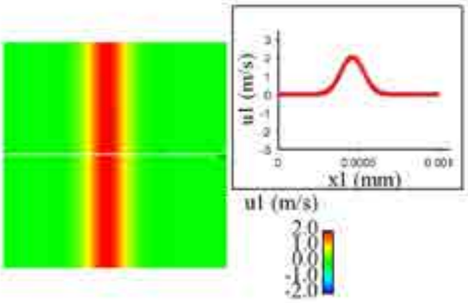
Compressed air,
Z = 0.85 pre-shock,
Z = 1.15 post-shock

Other Numerical Challenges

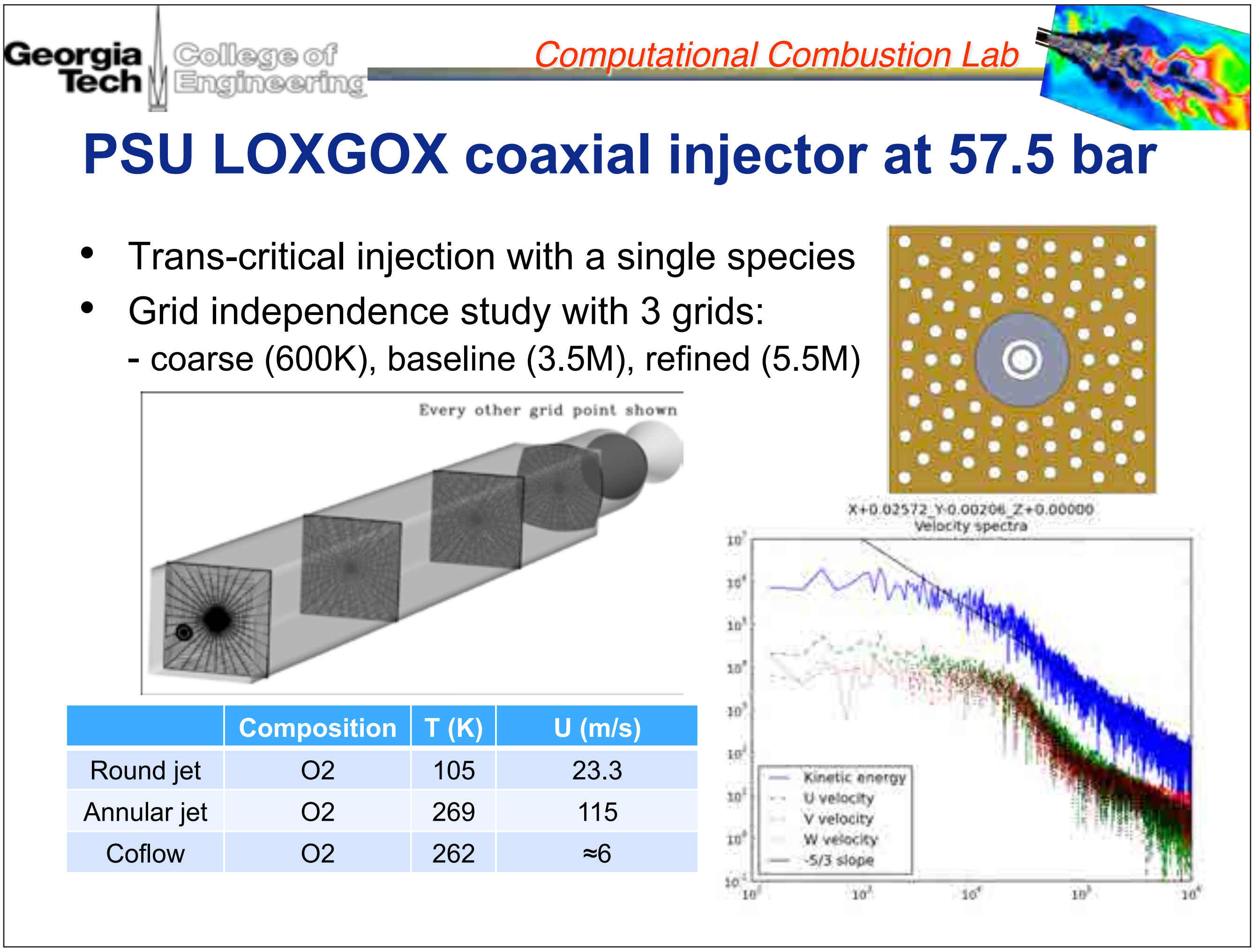
- Influence of boundary conditions very critical
  - Characteristic based inflow and inflow turbulence
    - Constant mass, reflected, semi-reflected?
  - Choked outflow or characteristic outflow?
  - Wall heat transfer – coupled fluid-structure interactions



Perfect Reflecting Inflow



Non-Reflecting Inflow



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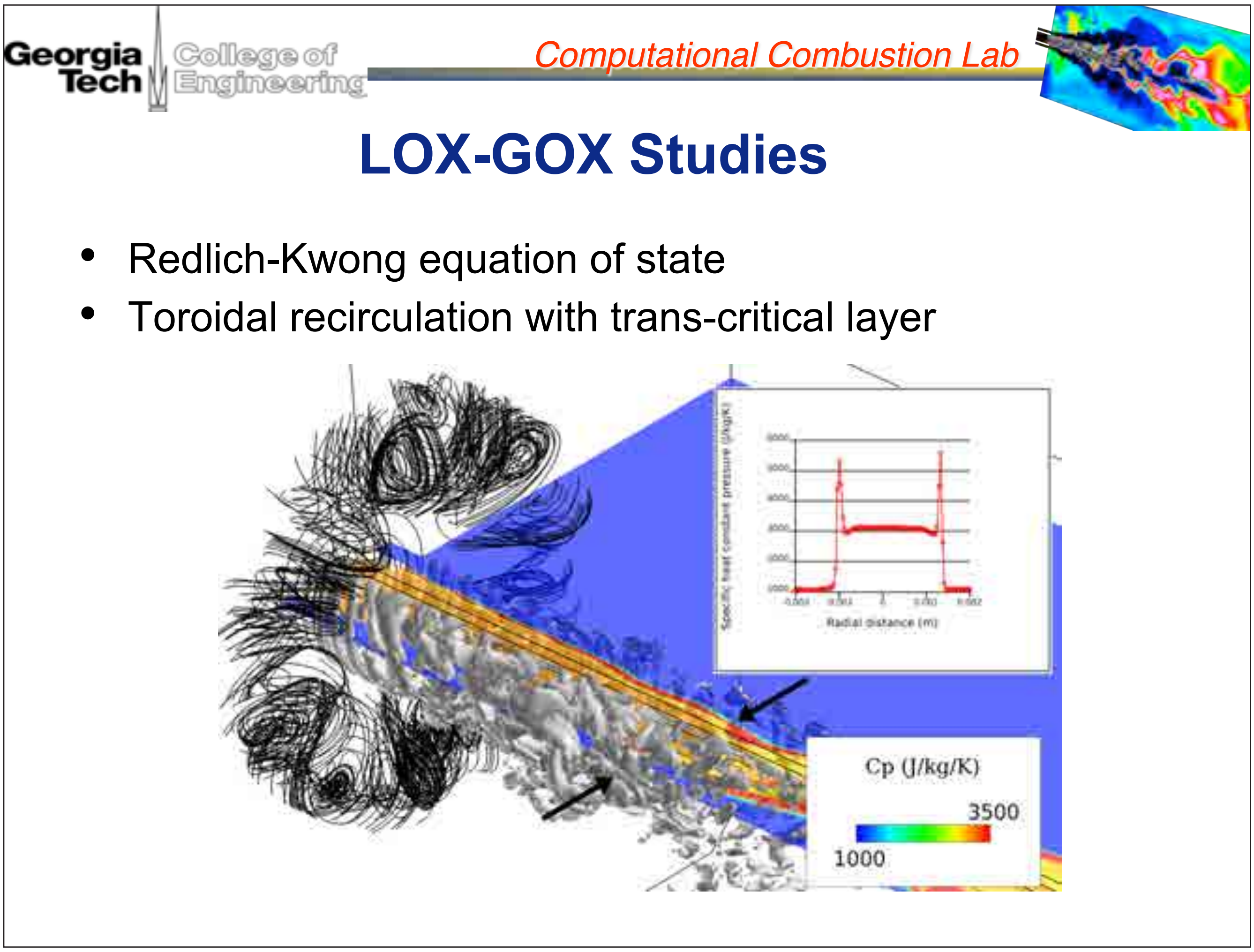
PSU LOXGOX coaxial injector at 57.5 bar

- Trans-critical injection with a single species
- Grid independence study with 3 grids:
  - coarse (600K), baseline (3.5M), refined (5.5M)

	Composition	T (K)	U (m/s)
Round jet	O2	105	23.3
Annular jet	O2	269	115
Coflow	O2	262	≈6



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LOX-GOX Studies

- Redlich-Kwong equation of state
- Toroidal recirculation with trans-critical layer

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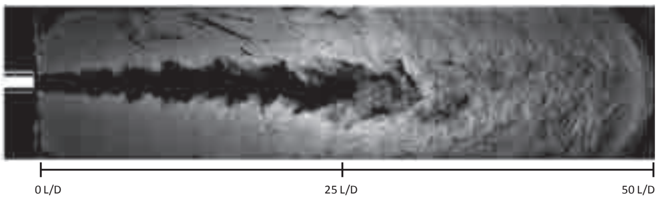
LOXGOX Jet Mixing

- Instantaneous comparison
  - Backlit image
  - Slice vs line-of-sight
- Time-averaged comparison
  - Processing raw data
  - Reaches stationary state in 10-15 ms



Time of averaging 1 ms

Time of averaging 10 ms

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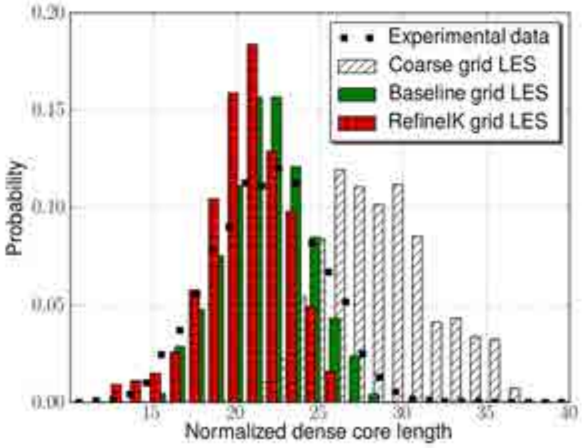
LOX-GOX Jet Mixing

- Main metric is dark core length $0.3 \le \rho^* = \dfrac{\rho - \rho^\infty}{\rho^0 - \rho^\infty} = \dfrac{\rho - 85}{1080 - 85} \le 0.6$
  - Similar to spray penetration
  - Important quantity for combustion instability [1]



[1] Chehroudi, B., "Physical Hypothesis for the Combustion Instability in Cryogenic Liquid Rocket Engines," Journal of Propulsion and Power, 2010.

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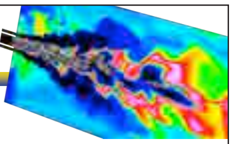
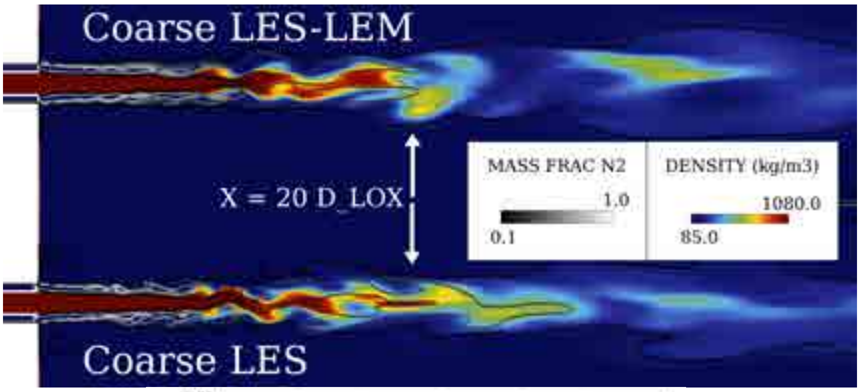
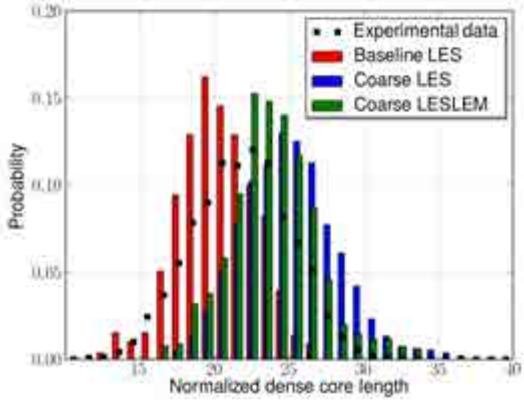


LEMLES and LES of LOX-GN2 Jet





- Similar flowfields but scalar mixing shows some differences at the small scales
- LEMLES predicts closer to gradient diffusion as expected for this non-reacting mixing case
- Reacting cases under study

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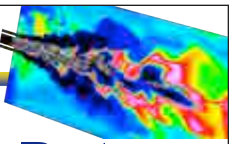
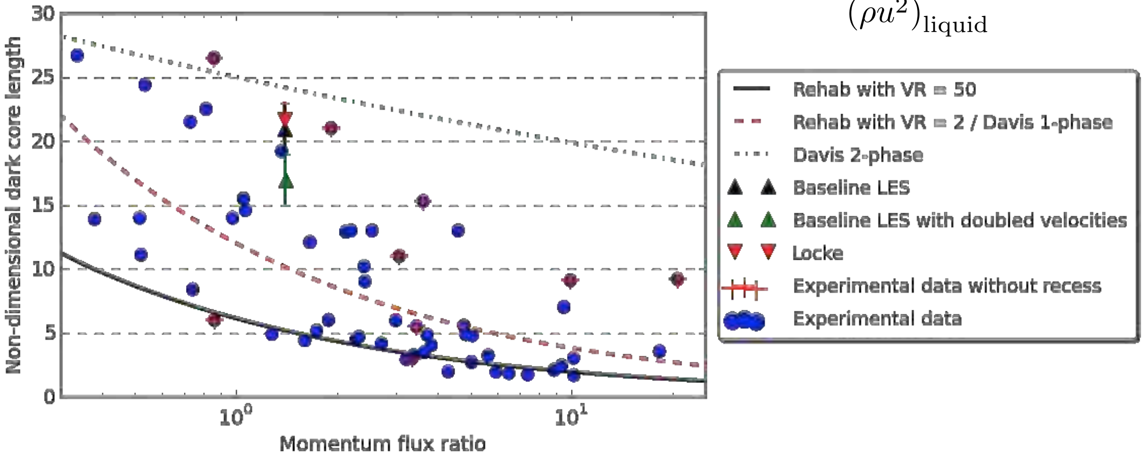
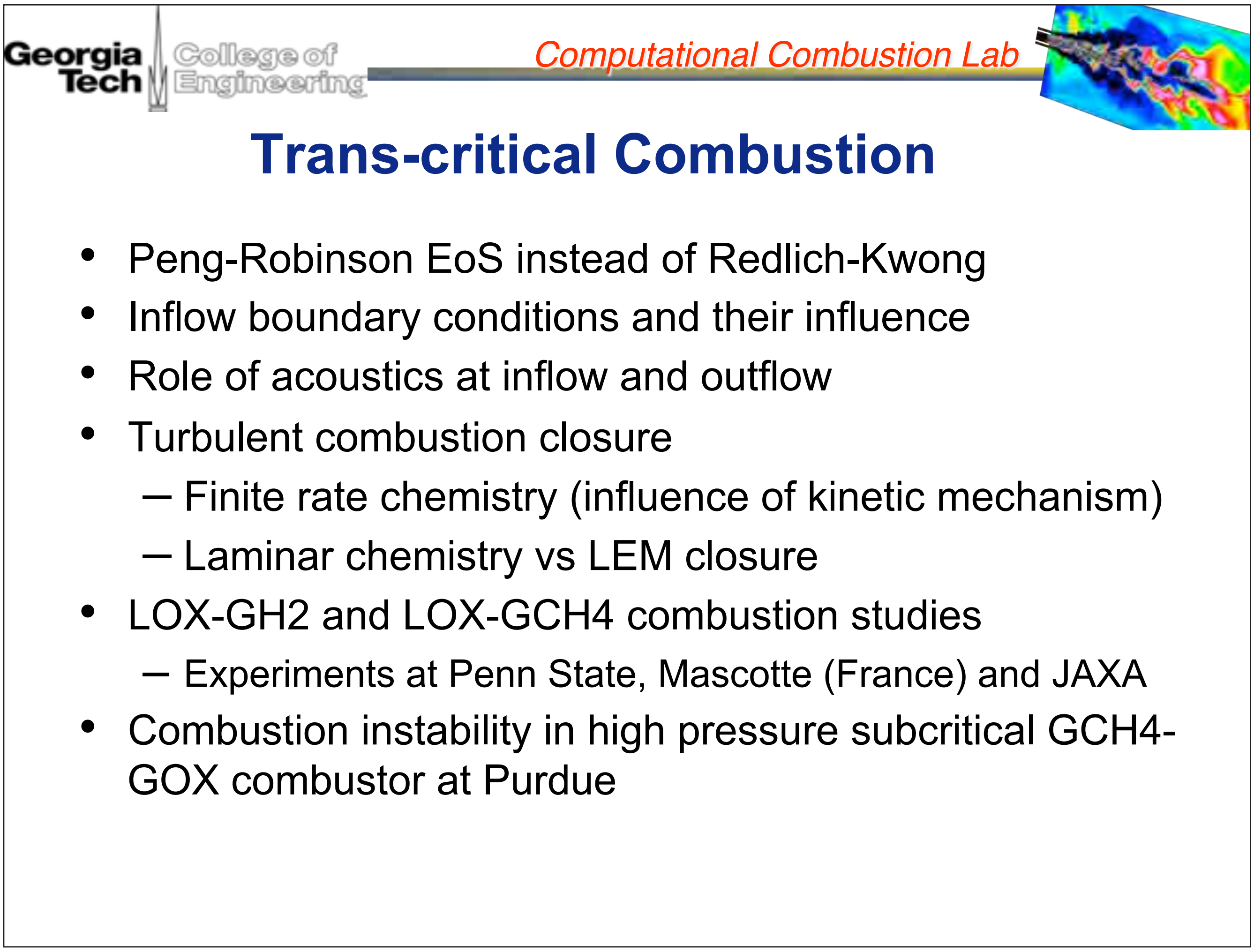


Wide Scatter in Trans-Critical Mixing Data

- LES can provide useful trends with correct physics
- LES can access flow conditions beyond sub-scale rigs
- Survey of coaxial, non-reacting supercritical flows
  - Main parameter: momentum flux ratio

$$J = \frac{(\rho u^2)_{\text{gas}}}{(\rho u^2)_{\text{liquid}}}$$





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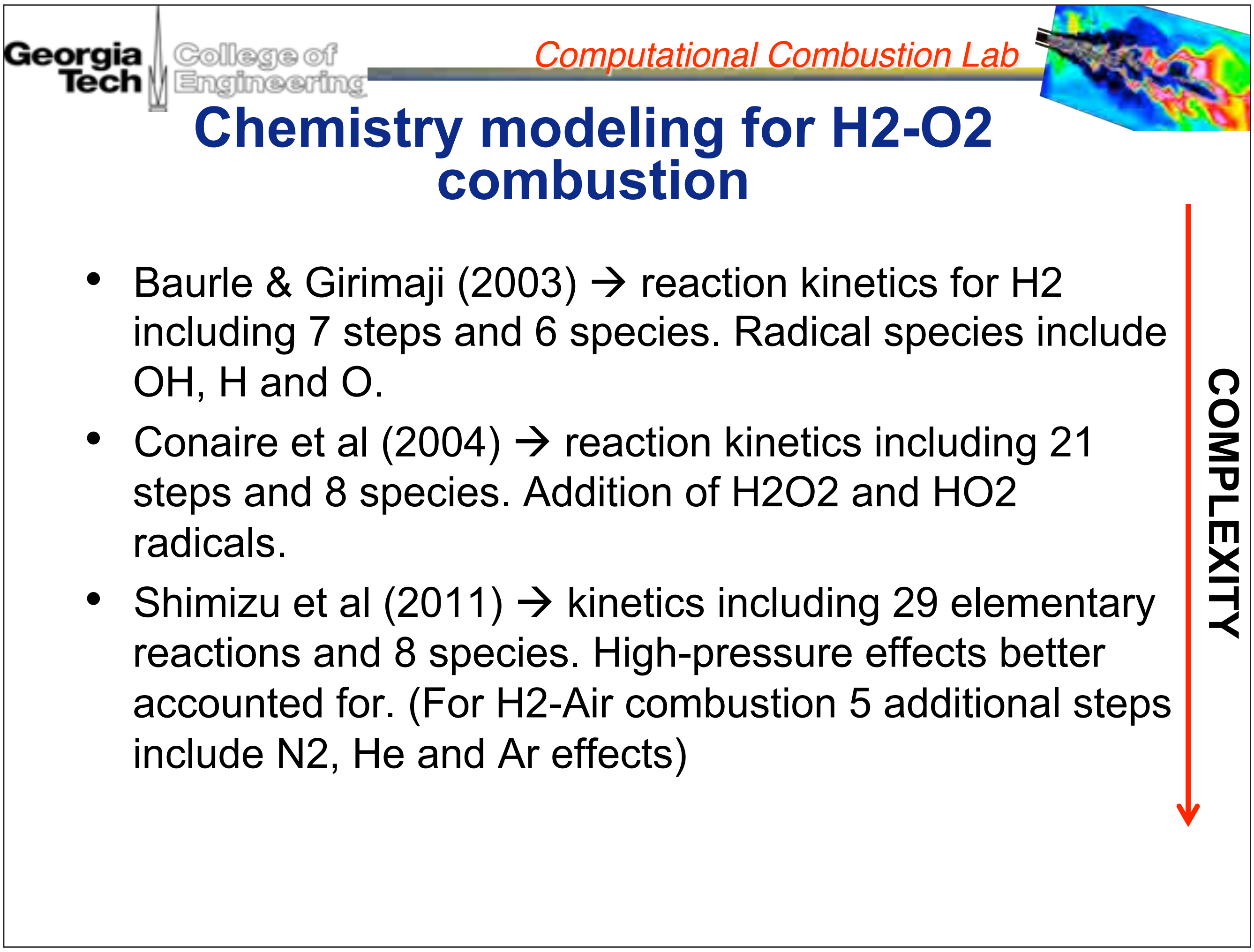
Trans-critical Combustion

- Peng-Robinson EoS instead of Redlich-Kwong
- Inflow boundary conditions and their influence
- Role of acoustics at inflow and outflow
- Turbulent combustion closure
  - Finite rate chemistry (influence of kinetic mechanism)
  - Laminar chemistry vs LEM closure
- LOX-GH2 and LOX-GCH4 combustion studies
  - Experiments at Penn State, Mascotte (France) and JAXA
- Combustion instability in high pressure subcritical GCH4-GOX combustor at Purdue



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Chemistry modeling for H2-O2 combustion

- Baurle & Girimaji (2003) → reaction kinetics for H2 including 7 steps and 6 species. Radical species include OH, H and O.
- Conaire et al (2004) → reaction kinetics including 21 steps and 8 species. Addition of H2O2 and HO2 radicals.
- Shimizu et al (2011) → kinetics including 29 elementary reactions and 8 species. High-pressure effects better accounted for. (For H2-Air combustion 5 additional steps include N2, He and Ar effects)

COMPLEXITY

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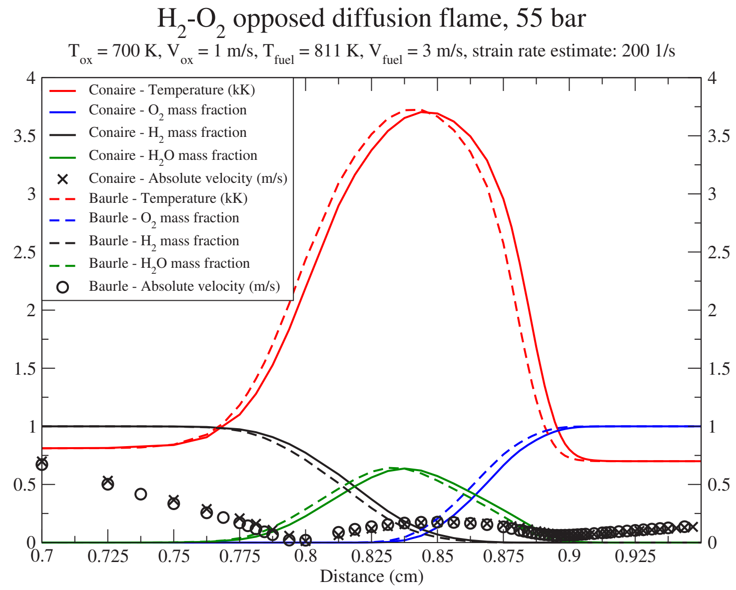
Chemistry modeling for H2-O2 System

- Opposed diffusion flame at high pressure
- Good agreement between 21-step and 7-step



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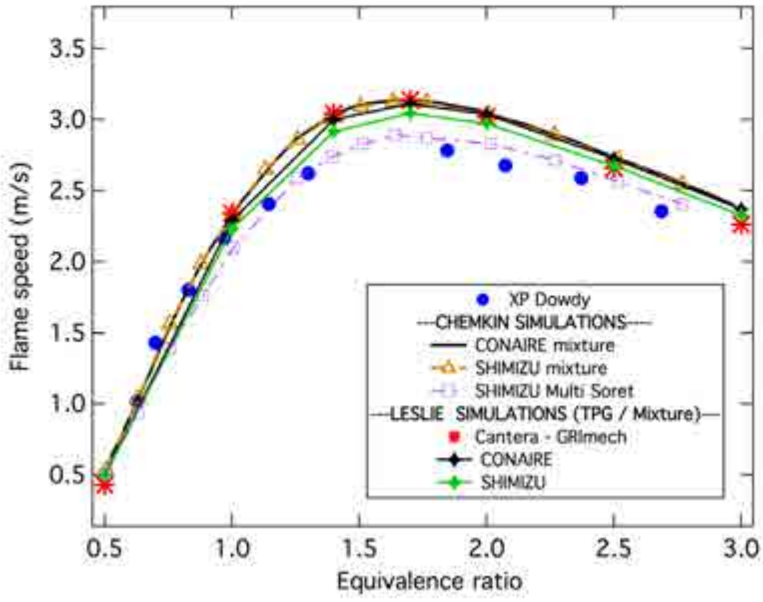
Chemistry modeling for H2-O2

- 1D-laminar flame at T=298K and p=1atm
- 21-step (Conaire et al.), 29-step (Shimizu et al.)



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Scaling from Lab to Sub-scale to Full-scale

	Sub-Scale LOX/GCH4 PWR	Lab Scale LOX/GH2 PSU	Lab Scale LOX/GCH4 CNRS
Re (LOX)	1.38E+06	5.53E+05	6.18E+04
Re (Fuel)	4.38E+05	1.83E+05	4.87E+05
Velocity Ratio	4.99	16.93	18.06
Momentum flux ratio	3.15	1.53	11.64
Equivalence ratio	1.28	1.36	13.09
Da	2.63	1.87	58.0

- Sub-scale multi-injector test case (83 injectors):
  - Chamber pressure: 138 bar, far from p_c (O2, CH4)
  - LOX: U = 20-40 m/s, T = 100-120 K
  - CH4: U = 130-250 m/s, T = 240-300 K, ϕ=1.1-2
  - Flow speeds much higher than lab-scale single injectors
- Can LES be used to study scaling issues?

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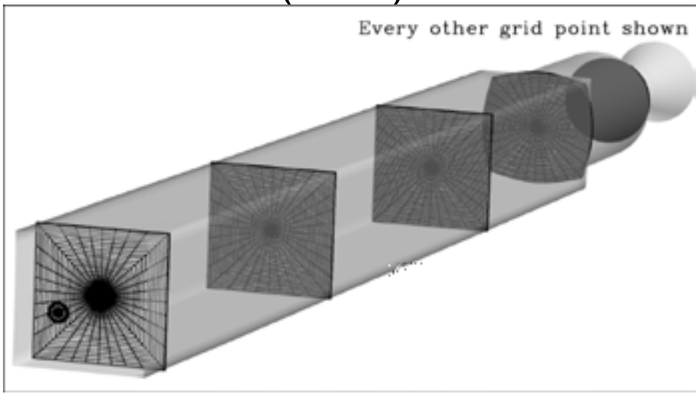
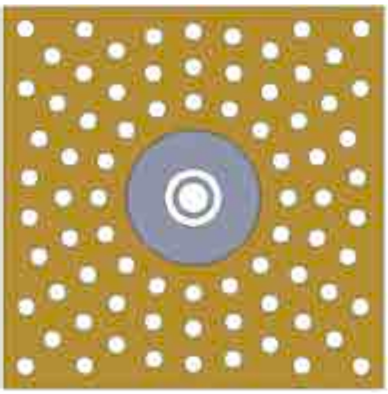
LOX coaxial injector rig

- Developed after NASA CUIP study [1]
- Square chamber for better optical access [2]
- Grid influence study with 4 grids:
- Coarse (600k), baseline (3.5M), I-refined (5M) and IK-refined (7.5M)



D_{LOX}=2.05 mm
L_{ch} = 0.35 m



[1] Tucker, Menon, Merkle, Oefelein, and Yang. In *44th JPC, AIAA 2008-522, 2008*
[2] J. M. Locke. *PhD thesis, The Pennsylvania State University, May 2011*

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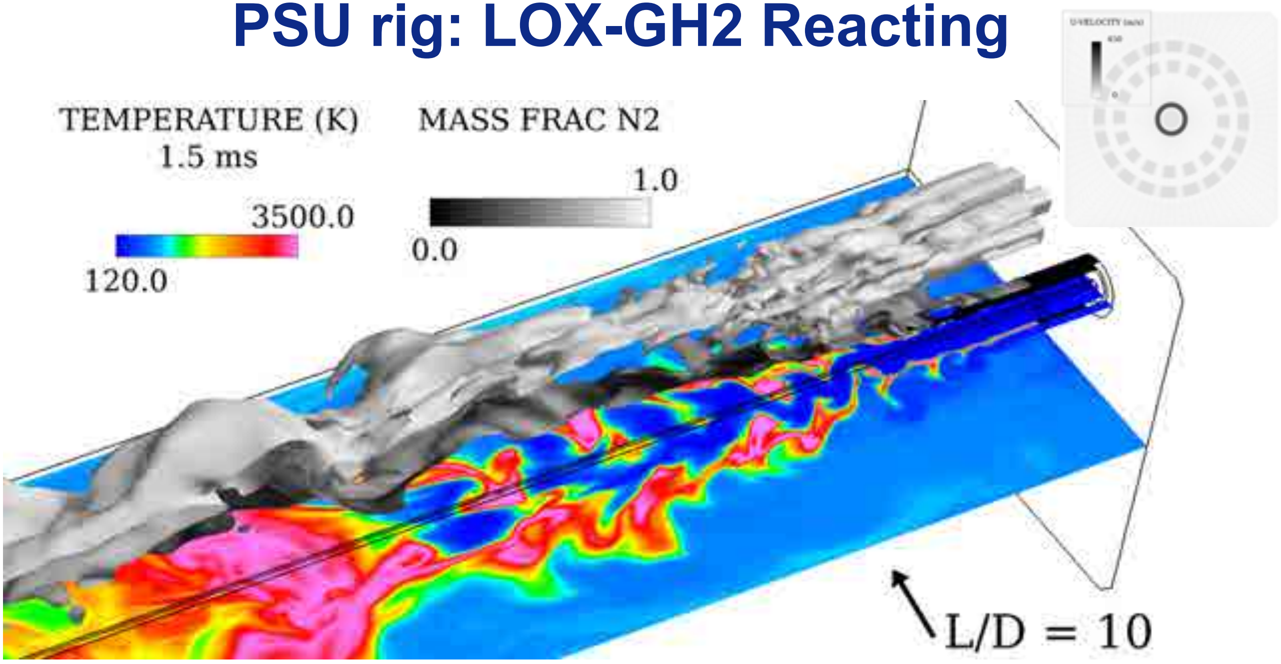
PSU rig: LOX-GH2 Reacting



- 21-step Conaire et al., 8.5 M grid points
- Strong sinuous and helicoidal modes

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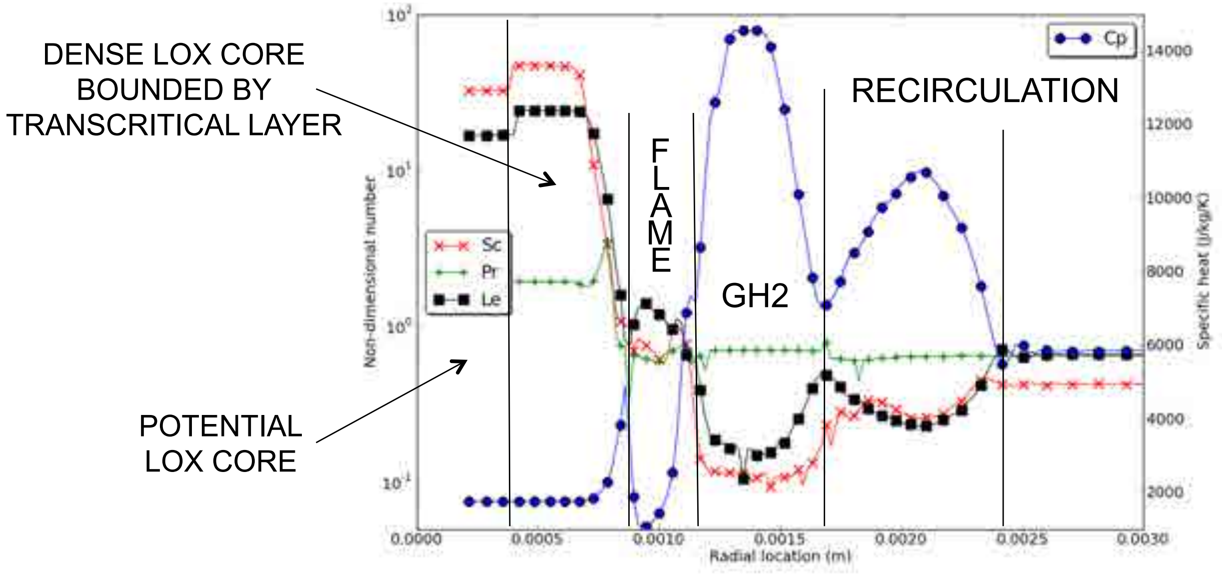
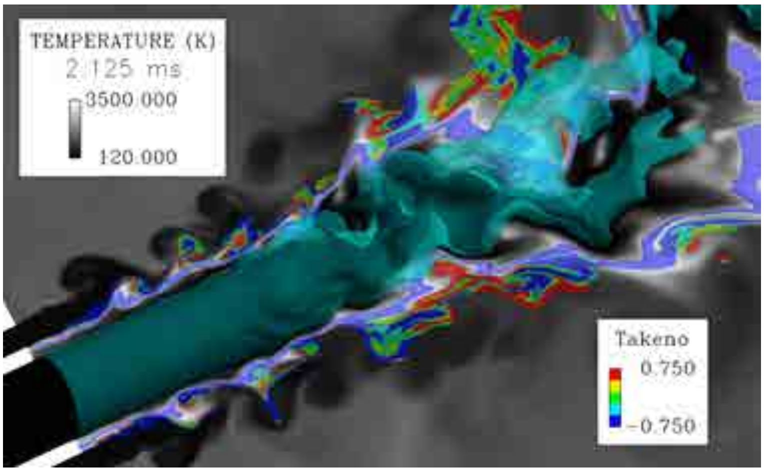
LOX-GH2 Flame Structure

- Pure diffusion flame in the near-field @ x/D = 1
- Radial profile @ x/D=1, flame structure clearly defined



LOX-GH2 Flame Structure

- Pure diffusion flame in the near-field
- Premixing present once dense core narrows
- Another reason to use Finite-Rate Kinetics



Why study CH4 combustion in LRE ?

- New interest in Liquid Rocket Engines (LRE) operating with methane as propellant.
- Important differences with hydrogen physics:
  - CH4 can be injected under both trans-critical and supercritical states[1].
  - $\rho_{CH_4} > \rho_{H2}$: large range of flux momentum ratio can be applied in LOX/CH4 injector, which allows different hydrodynamic and combustion regimes
  - Complex chemistry requires to revisit methods developed for H2/O2 combustion (mechanisms, LES closure of the reaction rate…)

[1] Singla et al. (Proceedings of the Combustion institute 2005)

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Reduced mechanism for O2/CH4 combustion

- Lack of reduced mechanism for oxy-combustion of CH4 at high pressure: at least 12 steps and 16 species[1]
  - Too expensive for real gas LES at this time!!
- Use global 1-step and 2-step kinetics with modified rates to match conditions at high pressure
- Computation of laminar premixed flames with Cantera:
  - Stoichiometric equivalence ratio
  - Pressure: 5.6 MPa
  - Real gas replaced by thermally perfect gas assumption.
  - Mechanisms: comparison of WD1[2] with GRIMECH.

[1] Sung et al. Int. Symp. Comb. (1998), [2] Westbrook & Dryer (CS&T 1982)

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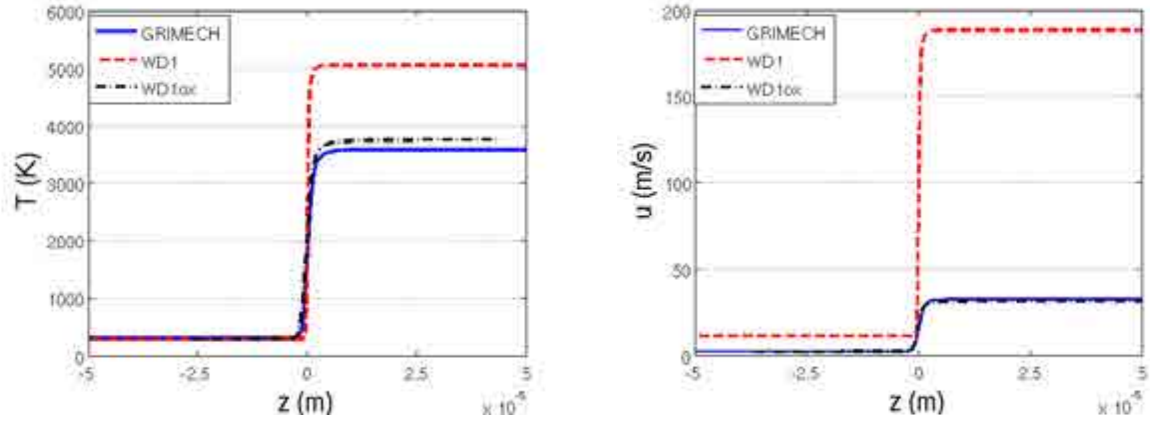
Comparison of WD1$_{ox}$ with GRIMECH



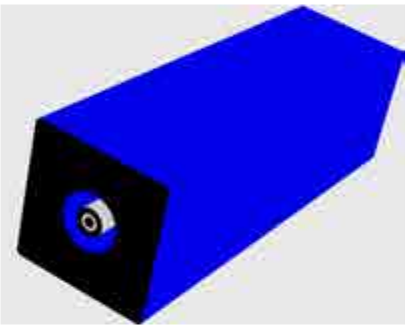
- Error on the adiabatic temperature < 5%
- Nearly perfect correction of the flame speed

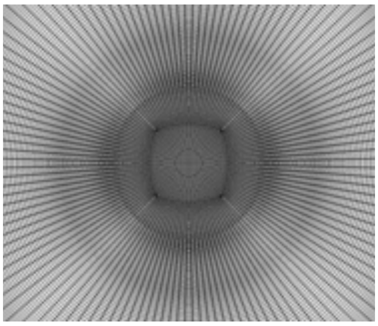
	T_{ad} (K)	s_L (m/s)
GRIMECH	3584	2.317
WD1	5051	11.11
WD1ox	3755	2.283

LES of Mascotte test case

- Coaxial LOX/CH4 injector (G2)[1]: P=5.6 MPa, $\phi_g = 13$
- 24 million grid points

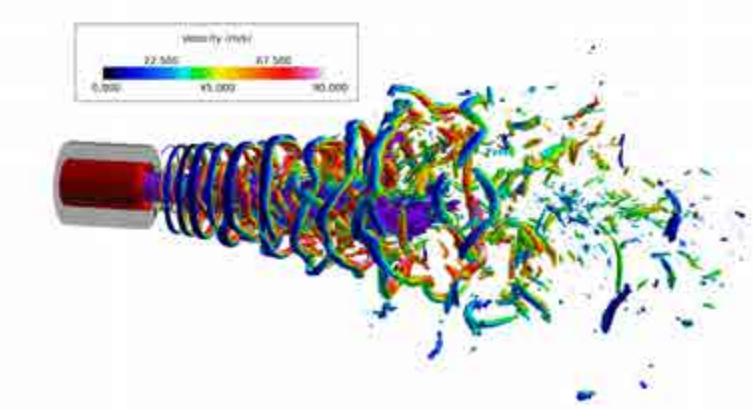
	Composition	T (K)	U (m/s)
Round jet	O2	85	3.70
Annular jet	CH4	288	63.2

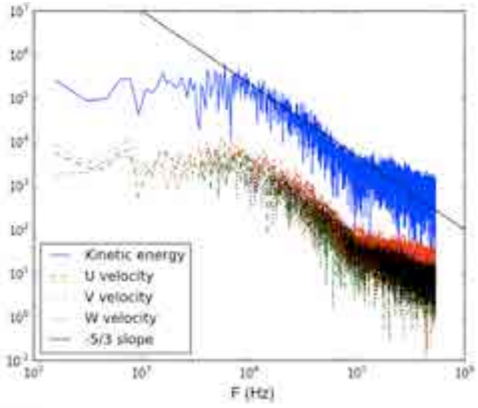




[1] Singla et al. (Proceeding of the Combustion institute 2005)

Turbulent Flow structure





- Strong coherent structures in the shear layers: entrainment of gas in coaxial jet and dense core wrinkling
- Good recovery of the Kolmogorov -5/3 spectrum

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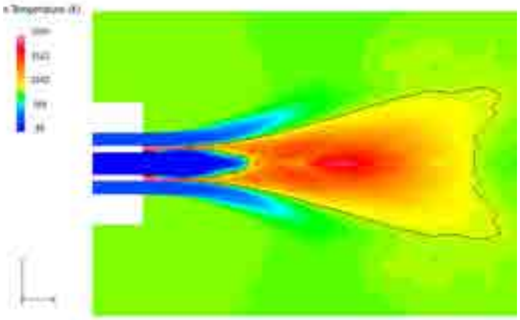
Flame structure

Experimental flame : Visualization

LES (MAX): iso surface T=1700K

- Good agreement
- Short flame: L~6 cm.
- Anchored on the LOX tip.
- Expansion angle:
  - Initial part : α<10°
  - Blooming angle : α~20°



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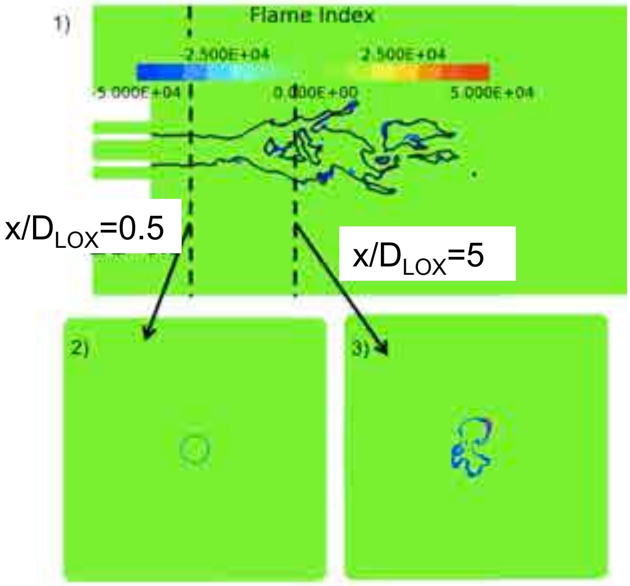
Combustion regime



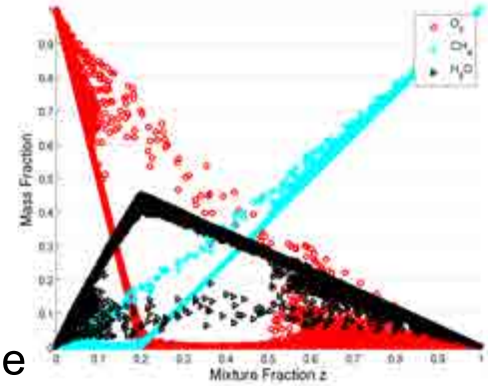
- Diffusion flame
- Combustion regime close to the laminar infinitely fast chemistry

- Flame index:

$$FI = \vec{\nabla} Y_{CH_4} \bullet \vec{\nabla} Y_{O_2}$$

$FI < 0$: Diffusion flame

$FI > 0$: Premixed flame



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3D v/s Axi v/s 2D LOX-GH2 Studies

- 3D is essentially the only proper way to do LES but is computationally very expensive
- Strategy needed for parametric study of unsteady flame-turbulence interactions that is cost effective
  - Axisymmetric, 2D or sector 3D
  - Pros and Cons for each approach
- Axisymmetric and 3D sector with centerline injector will always result in an artificially long LOX core
  - Off-center injector may avoid centerline effects but artificial
- 2D avoids centerline issues but no 3D relieving effect, choking is artificial and energy/volume may be too high
- LES closure is invalid for axisymmetric of 2D but unsteady effects can be captured

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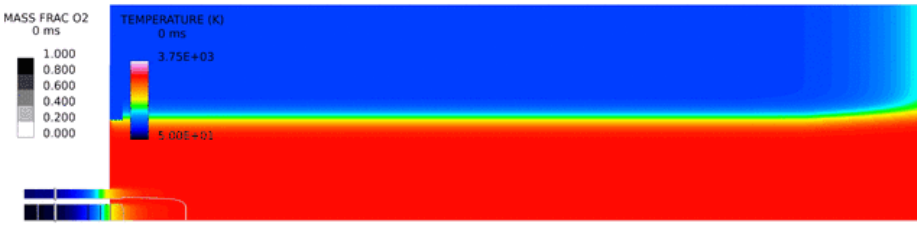
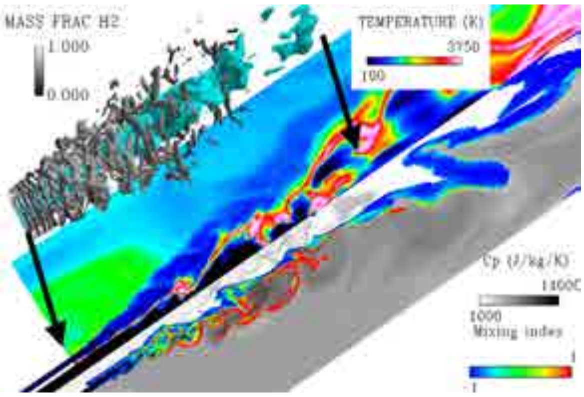
3D v/s Axisymmetric

- Liquid core length is too long in axisymmetric case



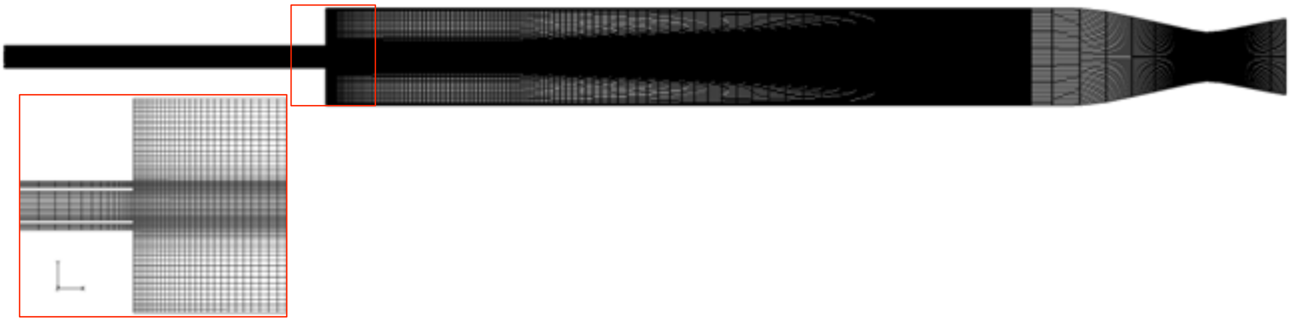
Axisymmetric



3D

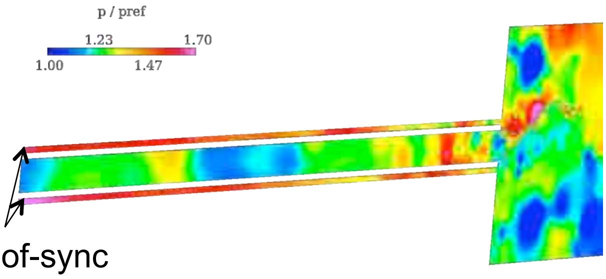
A 2D Evaluation Configuration

- 2D simplification of a shear coaxial injector including a convergent-divergent throat (injector studied by Nunome *et al.*, 2011 and Daimon *et al.*, 2011)
- Baseline mesh, total ~270,000 points, PR-EOS
- Effect of kinetics, Hydrogen temperature, recess all can be studied in a cost-effective manner
- Precursor simulations before doing full 3D

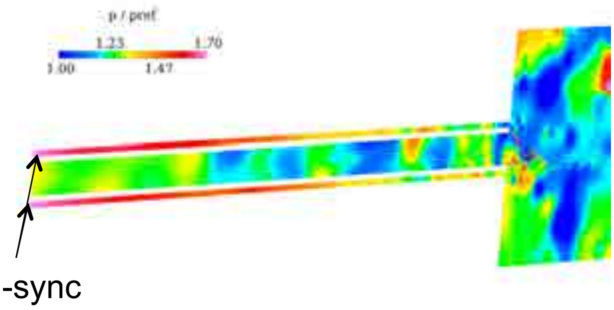


Boundary Conditions

- H_2 inlets are part of the same injector and would react identically to longitudinal pressure fluctuations
- In 2D pressure waves in inlet lines are not in phase
  - BC react differently in the two H_2 inlets
- H2 inlet BCs linked so that the same inflow conditions are applied at all times
  - The incoming waves are out-of-sync in the long inlets, the effect is limited



Out-of-sync



In-sync

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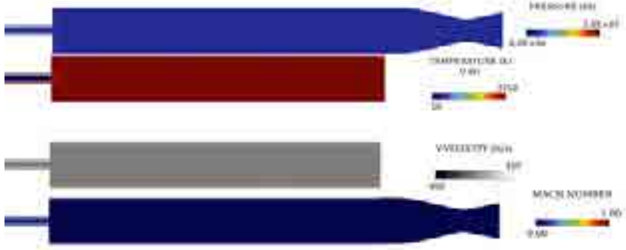
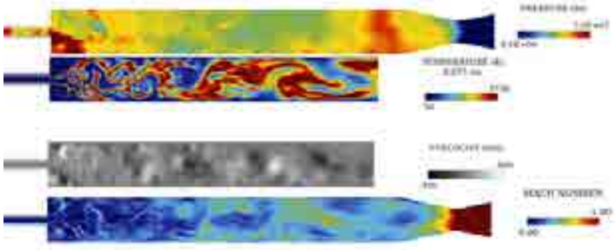
Effect of Kinetics for T_{H2} = 50 K

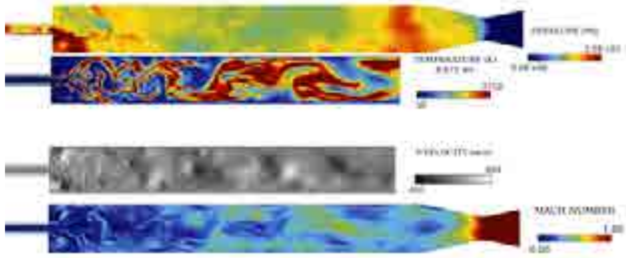
Baurle : 7-step 6-species



Conaire: 21-step 8-species



Shimizu: 29-step 8-species



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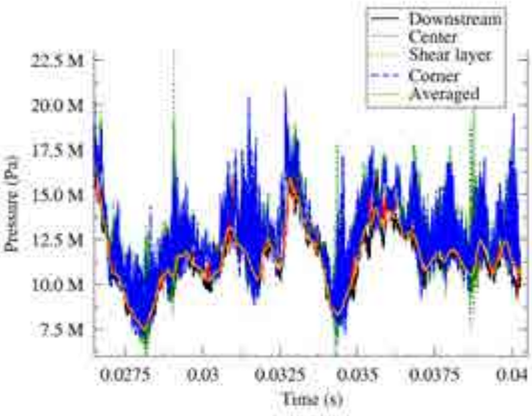
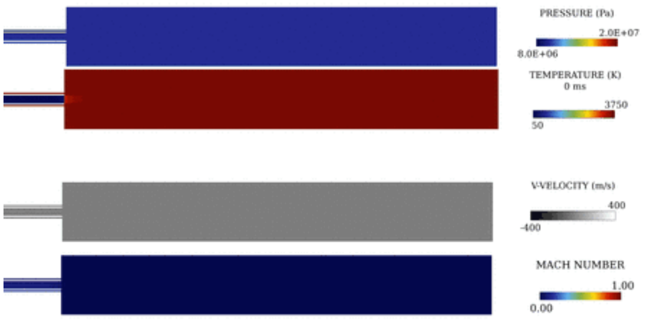
Implication of 2D Geometry

- High energy release to chamber volume ratio produces increase in mean pressure to 140 bar (design = 100 bar)
- Results similar with or without outflow choked conditions
- 2D simulations do not have the 3D relieving effect





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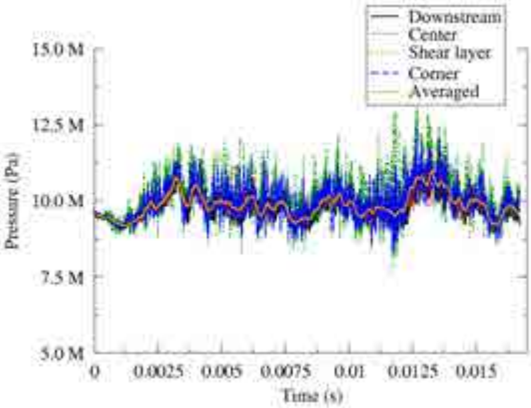
Energy/Volume ratio assessment

- Increase on chamber dimensions to reduce (energy/volume) ratio with same injector configuration
- Pressure now at design 100 bar but flow field has larger recirculation at the corner



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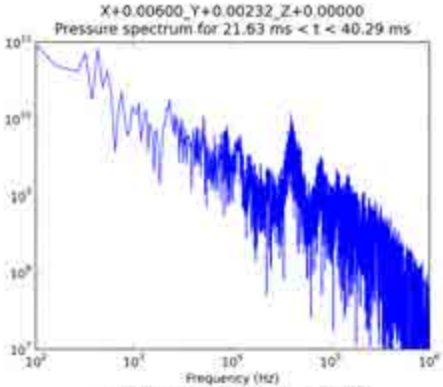
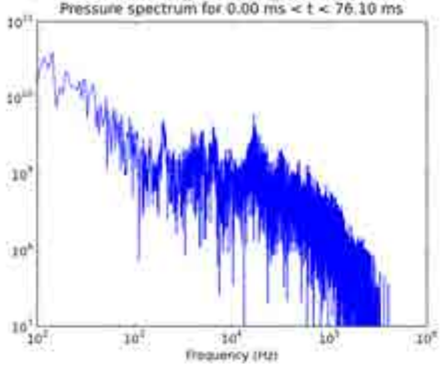
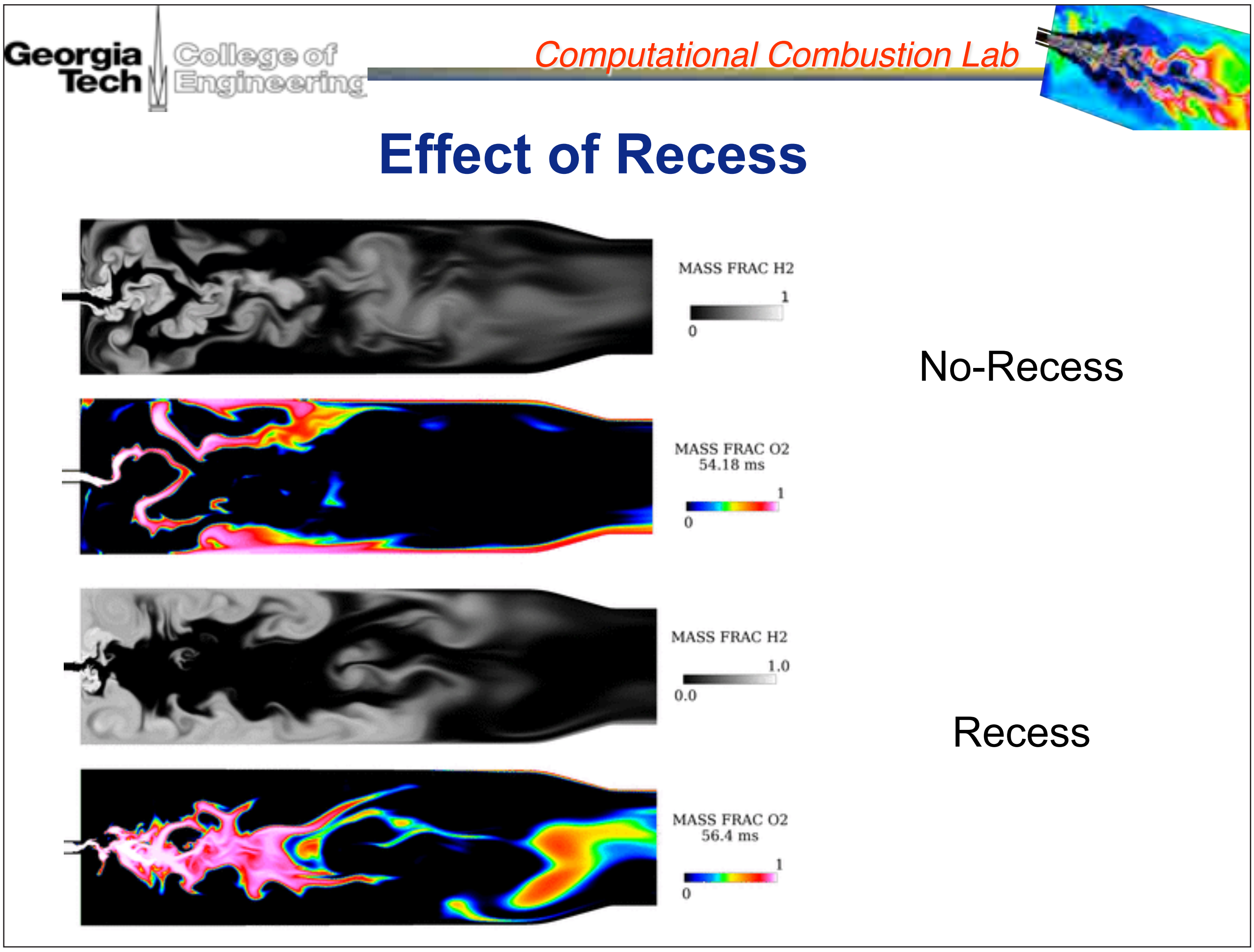
Pressure Spectra





- Both chambers show peak at the transverse mode frequency
  - Narrow case = 50 KHz
  - Wider case = 20 KHz
- Wider chamber has lower pressure amplitude



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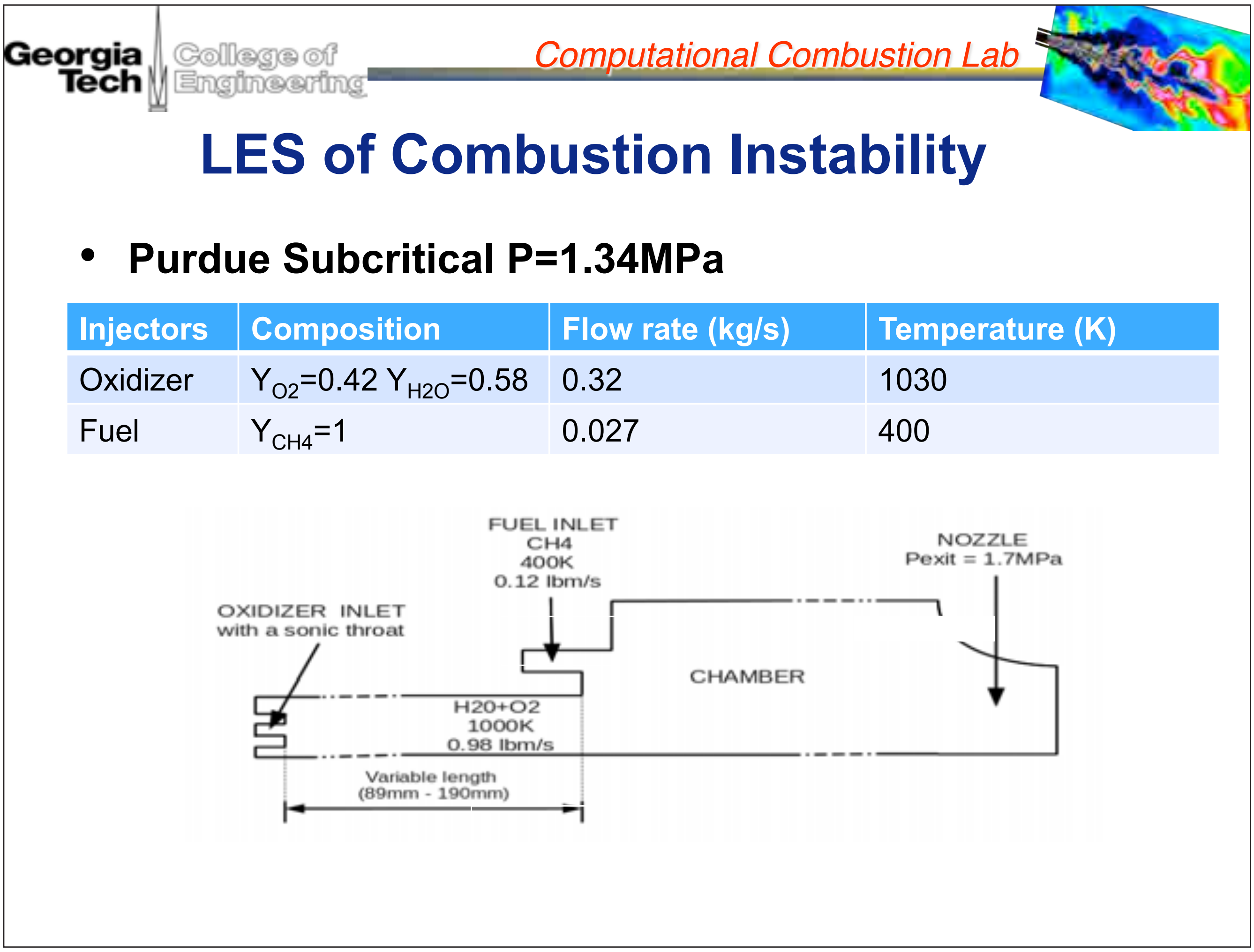
Effect of Recess

No-Recess

Recess



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LES of Combustion Instability

- **Purdue Subcritical P=1.34MPa**

Injectors	Composition	Flow rate (kg/s)	Temperature (K)
Oxidizer	Y_{O2}=0.42 Y_{H2O}=0.58	0.32	1030
Fuel	Y_{CH4}=1	0.027	400

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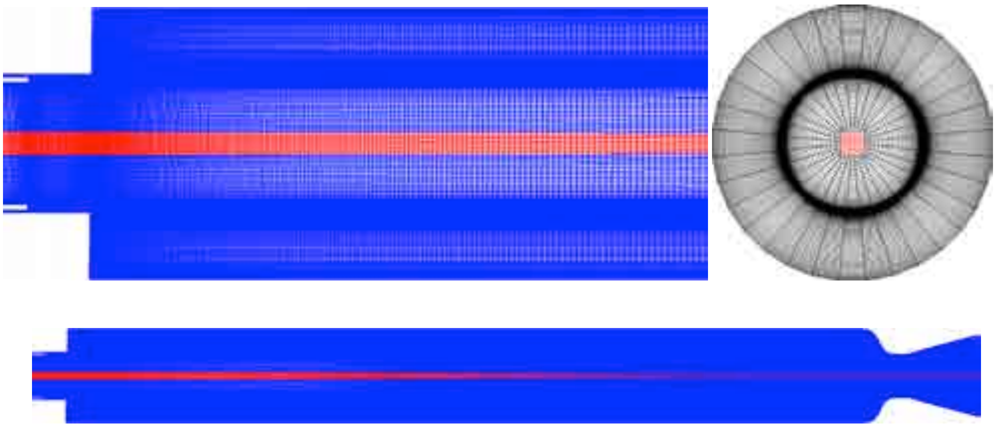
Computational Domain

- Axisymmetric and 3D studies
- Full combustor geometry with supersonic outflow nozzle
- LEMLES with two-step chemistry
  - flame speed correction for rich combustion regime.



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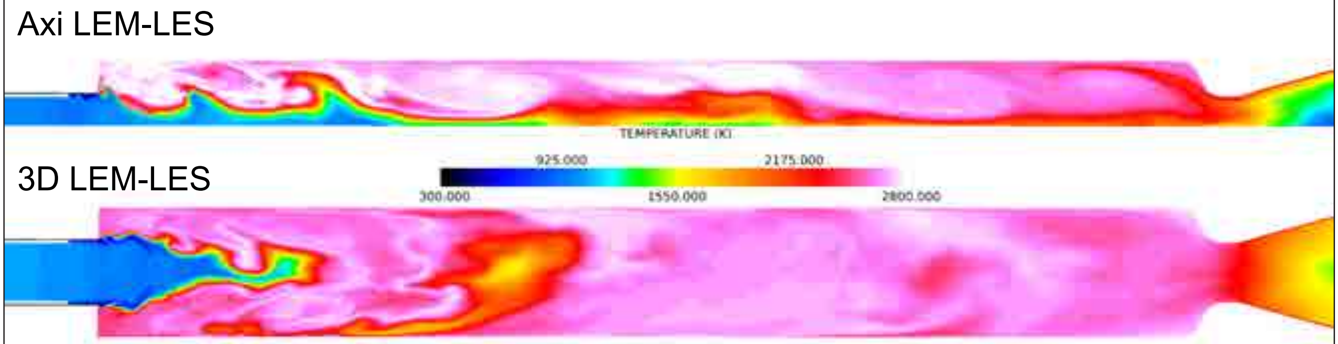
Axisymmetric v/s 3D

- Boundary condition on the axis center does not allow transverse jet flapping
- Flame anchoring identical but long oxidizer core even for gas-gas case



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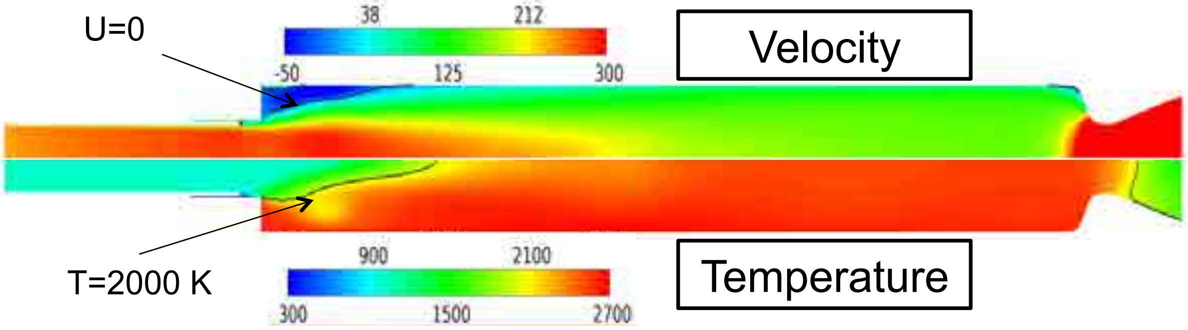
3D LES Mean Results



- Velocity field: long recirculation zone, supersonic flow in the nozzle and high velocity core along the center line
- Anchoring of the flame at the step corner.
- Stabilization of the flame in the mixing layer between the high velocity flow and the recirculation
- Distributed heat release: the flame is not compact (L_f ~8cm)

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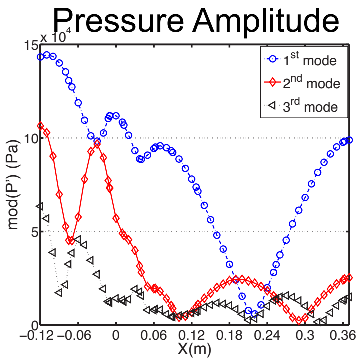
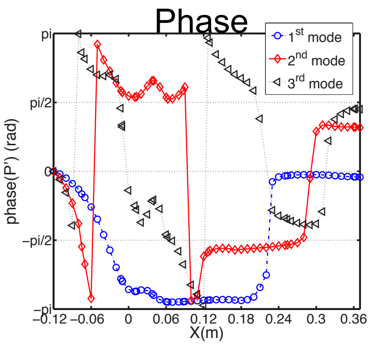
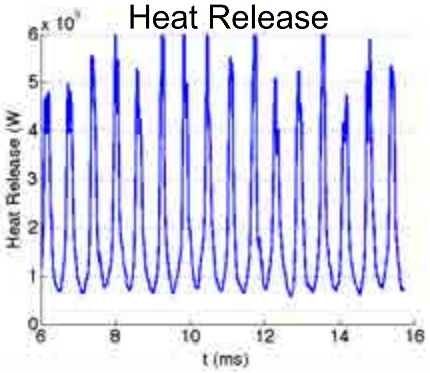
Computational Combustion Lab

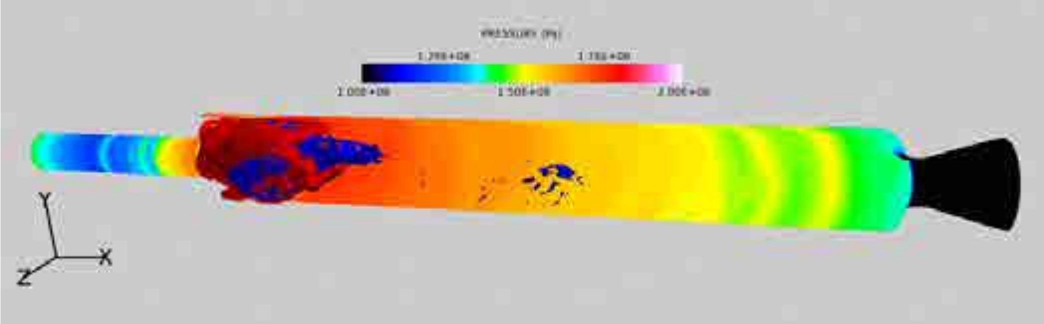
Resonant mode Structure

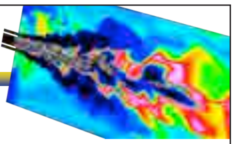




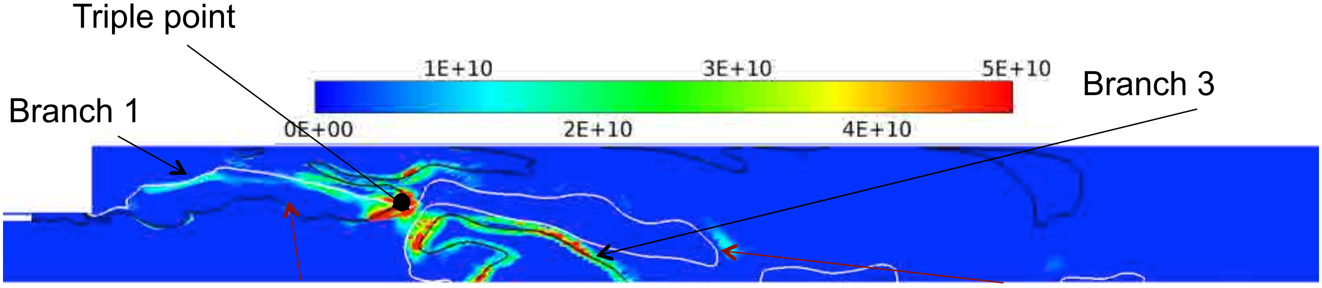


Two Standing Acoustic modes in the combustor





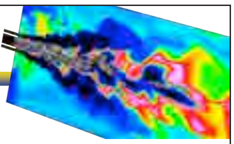
Flame Holding: A Complex Triple Flame



$z=z_{st}=0.095$ (black line)

T=2000 K (white line)

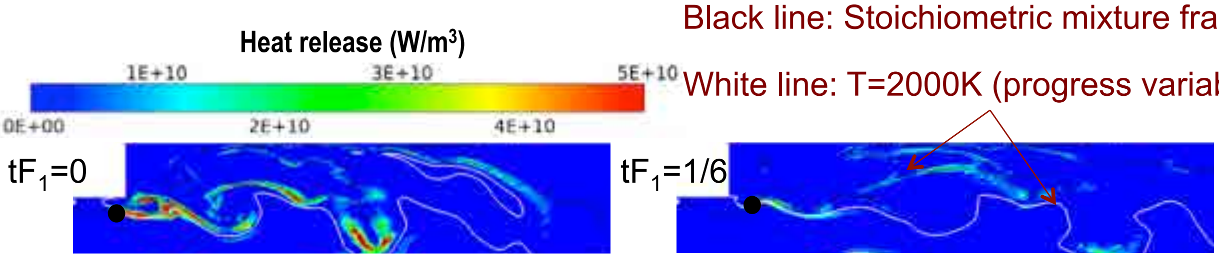
- Branch 1: rich premixed flame anchored at the step corner
- Branch 2: lean premixed flame
- Branch 3: diffusion flame (stoichiometric mixture fraction)
- Triple point : intersection of the three branches
  - Location of Maximum Heat Release



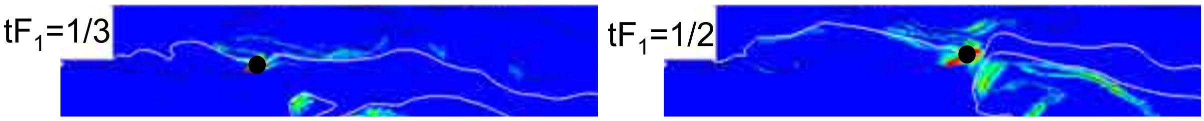
Triple Flame Structure

Black line: Stoichiometric mixture fraction

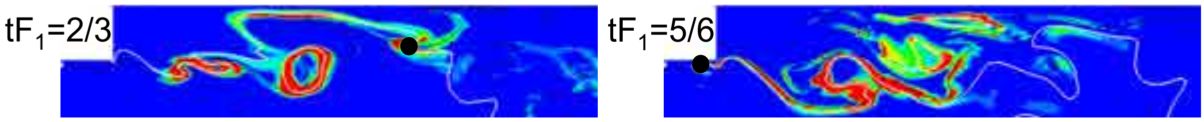
White line: T=2000K (progress variable)



1- Initiation of a triple point at the step corner: extinction of the downstream flame



2- Propagation of the triple point with the flow: weak combustion



3- Triple point is trapped in the recirculation zone: ignition of an intense rich flame. Start of a new cycle with the generation of a new triple point

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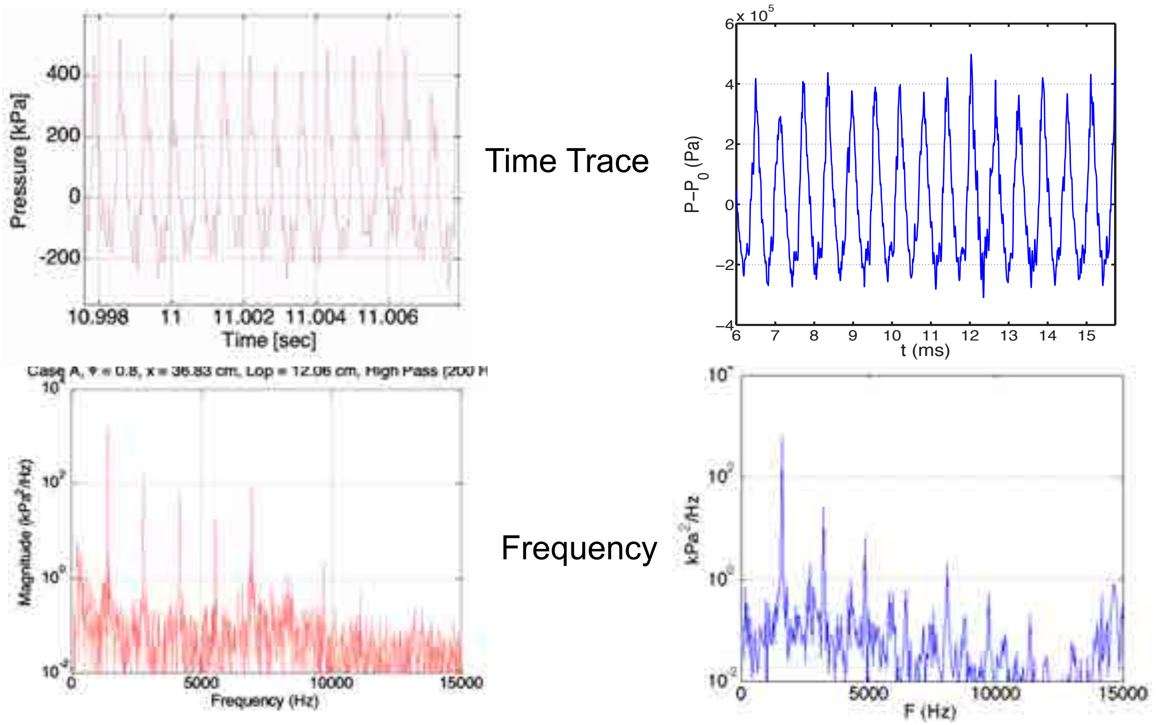
Pressure Signal and Spectra



Time Trace

Frequency

Experiment

LES

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Summary Comments

- LRE modeling and simulation are very challenging due to real gas effects, finite-rate kinetics, flame-turbulence-acoustic interactions and complexity of the geometry
- LES compressible solver with real gas and subgrid closures developed to address these challenges
- Application to trans-critical mixing experiments shows good agreement with data
- Application to trans-critical reacting experiments show much more is needed to reduce cost of kinetics
- Application to combustion instability in subcritical reacting cases shows ability of LES to capture dynamics
- Still a lot of studies needed to develop predictive capability for multi-injector applications