Lecture 8
CFD for Ramjets/Scramjets and Rockets

- High compressibility in the flow
  - Shock-vortex-turbulence-flame interactions
- Challenge
  - Shock capturing schemes are too dissipative and can overwhelm turbulent features
  - Turbulent features must show compressibility effects
- Some strategies
  - Hybrid solvers (WENO-central; MUSCL-central etc)
  - Artificial dissipation, high order PPM etc
- What will work for practical applications?
Challenges for Supersonic Combustion LES

- Algorithms for shock-turbulence-flame interactions
  - Shock capturing without dissipating turbulence or affecting combustion or flame within LES framework
- Subgrid closure for compressible turbulent flows
  - Shock interactions with (un)resolved turbulence
- Subgrid closure for compressible mixing and combustion
  - Interaction of compressible waves with flames
- Molecular mixing and chemical kinetics within subgrid
  - Detailed kinetics within LES framework
Compressible LES Governing Equations

- Favre-averaged filtered conservation equations

\[
\frac{\partial \rho}{\partial t} + \frac{\partial \rho \tilde{u}_i}{\partial x_i} = 0
\]

\[
\frac{\partial \rho \tilde{u}_i}{\partial t} + \frac{\partial}{\partial x_j} \left( \rho \tilde{u}_i \tilde{u}_j + \bar{p} \delta_{ij} - \tau_{ij} + \tau_{ij}^{\text{sgs}} \right) = 0
\]

\[
\frac{\partial \rho \tilde{E}}{\partial t} + \frac{\partial}{\partial x_i} \left[ \tilde{u}_i(\rho \tilde{E} + \bar{p}) - \tau_{ij} \tilde{u}_j + \bar{q}_i + [H_i^{\text{sgs}} + \sigma_i^{\text{sgs}}] \right] = 0
\]

\[
\tilde{q}_i = -K \frac{\partial \tilde{T}}{\partial x_i} + \rho \sum_{k=1}^{N_s} \tilde{h}_k \tilde{V}_{i,k} \tilde{Y}_k + \sum_{k=1}^{N_s} q_{i,k}^{\text{sgs}} \quad k = 1, N_s
\]

- Species solved using LEMLES

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Hybrid Algorithm for Shock-Turbulence-Flame

- Locally adaptive hybrid strategy switches from shock capturing solver to a smooth-flow (O(4)) solver dynamically in 3D
- Piecewise Parabolized Method (PPM – FLASH3D type)*
  - Extended to viscous flows, multi-domain, stretched grids
- MUSCL reconstruction with a Hybrid HLL Riemann Solver**
  - Non-contact preserving in shock transverse directions (Einfeldt, 1988, 1991)
  - Contact preserving Riemann solver (HLLC, Toro, 1997)
- Local shock detection using multiple sensors
- Algorithm validated for many canonical and complex test cases: Sod, Noh, Richtmyer-Meshkov, Shock-turbulence etc.**

VLES-LES $k-k\ell$ Model

- Hybrid RANS-LES for compressible flows using an additive filter (J. Comp. Phys. Vol. 228, 2009)
  - Hybrid terms need to be modeled – still under work
- Solve for the single point and two-point velocity correlations ($k$, $k\ell$) for near-wall treatment – model is still under development
  - $l_{sgs} > \Delta$, the grid size is the length scale
  - $l_{sgs} < \Delta$, the modeled length scale is used
- Distance from wall is used currently in the isolator (K-DES)

\[
\frac{\partial (\tilde{\rho}k_{sgs})}{\partial t} + \frac{\partial (\tilde{\rho}\tilde{u}_i k_{sgs})}{\partial x_j} = \tau_{ij} \frac{\partial \tilde{u}_i}{\partial x_j} - D_{sgs} + \frac{\partial}{\partial x_i} \left[ \tilde{\rho} \left( \frac{v}{Pr_t} + \frac{v_t}{\sigma_k} \right) \frac{\partial k_{sgs}}{\partial x_i} \right]
\]

\[
\frac{\partial (\tilde{\rho}(k\ell)_{sgs})}{\partial t} + \frac{\partial (\tilde{\rho}\tilde{u}_i (k\ell)_{sgs})}{\partial x_j} = C_{L1} \ell_{sgs} \tau_{ij} \frac{\partial \tilde{u}_i}{\partial x_j} - C_{L2} \tilde{\rho} k_{sgs}^{3/2} + \frac{\partial}{\partial x_i} \left[ \tilde{\rho} \left( \frac{v}{Pr_t} + \frac{v_t}{\sigma_{k\ell}} \right) \frac{\partial (k\ell)_{sgs}}{\partial x_i} \right]
\]


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General Realizability Constraints


\[
\begin{align*}
\tau_{aa}^{sgs} & \geq 0 \\
\left(\tau_{\alpha\beta}^{sgs}\right)^2 & \leq \tau_{aa}^{sgs} \tau_{\beta\beta}^{sgs} \quad \text{for} \quad \alpha \neq \beta \\
k^{sgs} & \geq \frac{\sqrt{3}}{C_\alpha} \nu_t \sqrt{2\tilde{S}_{ij}\tilde{S}_{ji} - \frac{2}{3}\tilde{S}_{kk}^2} \\
C_v &= \min(C_v, C_{v,\text{lim}}) \\
C_{v,\text{lim}} &= \frac{1}{\sqrt{6}s} \\
s &= \frac{l^{sgs}}{\sqrt{k^{sgs}}} \sqrt{\tilde{S}_{ij}\tilde{S}_{ji} - \frac{1}{3}\tilde{S}_{kk}^2} \\
l^{sgs} &= \min(l^{sgs}, l^{\text{lim}}) \\
l^{\text{lim}} &= \frac{1}{\sqrt{6}} \frac{\sqrt{k^{sgs}}}{C_v} \left(\tilde{S}_{ij}\tilde{S}_{ji} - \frac{1}{3}\tilde{S}_{kk}^2\right)^{-0.5}
\end{align*}
\]
K-KL Rearward Facing Step

$x/h = 4$

$x/h = 6$

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Scalar Fluctuation Modeling

- Used in typical RANS, URANS codes (e.g. CRAFTTech)
- Specify turbulent Prandtl and Schmidt numbers
  - First order effect impacts combustion efficiency
  - Use local estimates of turbulent Pr and Sc
    - Adjust to the flow rather than set a priori
    - Obtained from the turbulent closure
      - Used in URANS and in conventional LES
- Dynamic subgrid closures avoid this explicit relations but also capture variable and local turbulent Pr and Sc.
SCALAR FLUCTUATION MODEL (SFM)

Transport equations solved for scalar variance and its dissipation rate

\[
\frac{\partial (\bar{\rho} k_e)}{\partial t} + \frac{\partial (\bar{\rho} \tilde{u}_j k_e)}{\partial x_j} = \frac{\partial}{\partial x_j} \left[ \rho \left( \alpha + \frac{\alpha_t}{\sigma_{\varepsilon,e}} \right) \frac{\partial k_e}{\partial x_j} \right] + 2\overline{\rho \varepsilon} \left( \frac{\partial \tilde{\varepsilon}}{\partial x_j} \right)^2 - 2\overline{\rho \varepsilon}
\]

\[
\frac{\partial (\bar{\rho} \varepsilon_e)}{\partial t} + \frac{\partial (\bar{\rho} \tilde{u}_j \varepsilon_e)}{\partial x_j} = \frac{\partial}{\partial x_j} \left[ \rho \left( \alpha + \frac{\alpha_t}{\sigma_{\varepsilon,e}} \right) \frac{\partial \varepsilon_e}{\partial x_j} \right] + \overline{\rho \alpha_t} \left( C \frac{\varepsilon_e}{d_1 k_e} + C \frac{\varepsilon}{d_2 k} \right) \left( \frac{\partial \tilde{\varepsilon}}{\partial x_j} \right)^2 + C \frac{\hat{\varepsilon_e}}{d_3 k_e} - \left( C \frac{\varepsilon_e}{d_4 k_e} + C \frac{\varepsilon}{d_5 k} \right) \bar{\rho} \varepsilon + \xi_{\varepsilon T}
\]

Near-wall damping

Compressibility Correction

\[
\hat{P}_k = P_k - \alpha_1 \dot{M}_T^2 P_k - \alpha_2 \dot{M}_T^2 \bar{\rho} \varepsilon
\]

Turbulent Prandtl Number

\[
Pr_t = \frac{C_{\mu} f_\mu}{C_{\lambda} f_\lambda} \sqrt{\frac{k}{\varepsilon}} \frac{\varepsilon_e}{k_e}
\]

- Energy Variance \( k_e = \varepsilon_e'' \)
- Dissipation Rate \( \varepsilon_e \)

Turbulent Schmidt Number

\[
Sc_t = \frac{C_{\mu} f_\mu}{C_{\lambda} f_\lambda} \sqrt{\frac{k}{\varepsilon}} \frac{\varepsilon_f}{k_f}
\]

- Mixture Fraction Variance \( k_f = \tilde{f}'' \tilde{f}'' \)
- Dissipation Rate \( \varepsilon_f \)

\[C_{\alpha_1} = 2.0 \quad C_{\alpha_2} = 0.0 \quad C_{\alpha_3} = 0.72 \quad C_{\alpha_4} = 2.2 \quad C_{\alpha_5} = 0.8 \quad \sigma_{k_e} = 1.0 \quad \sigma_{k_e} = 1.0\]
Hot (800K) Supersonic Jet - SFM vs LES

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SCHOLAR COMBUSTION EXPERIMENT

Turbulent Prandtl Number

Turbulent Schmidt Number

AIAA CFD for Combustion Modeling

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Compressible Subgrid Kinetic Energy Closure

- Transport of the subgrid kinetic energy

\[
\frac{\partial}{\partial t} \bar{\rho} k_{\text{sgs}} + \frac{\partial}{\partial x_i} (\bar{\rho} \tilde{u}_i k_{\text{sgs}}) = T_{k_{\text{sgs}}} + pd_{k_{\text{sgs}}} + P_{k_{\text{sgs}}} - D_{k_{\text{sgs}}}
\]

- Production

\[P_{k_{\text{sgs}}} = -\tau_{ij}^{\text{sgs}} \frac{\partial \tilde{u}_i}{\partial x_i}\]

- Dissipation

\[\tau_{ij}^{\text{sgs}} = -2\bar{\rho} \nu_t \left( \tilde{S}_{ij} - \frac{1}{3} \tilde{S}_{kk} \delta_{ij} \right) + \frac{2}{3} \bar{\rho} k_{\text{sgs}} \delta_{ij}\]

- Diffusion/Transport

\[D_{k_{\text{sgs}}} = \left( \frac{\partial \tilde{u}_i}{\partial x_j} - \frac{\partial \tilde{u}_j}{\partial x_i} \right)\]

- Pressure-Dilatation Correlation

\[T_{k_{\text{sgs}}} = -\frac{\partial}{\partial x_i} \left( (\bar{\rho} \tilde{K} \tilde{u}_i - \bar{\rho} \tilde{K} \tilde{u}_i - \tilde{u}_j \tau_{ij}^{\text{sgs}}) + (u_i \bar{P} - \tilde{u}_i \bar{P}) - (u_j \tilde{\tau}_{ij} - \tilde{u}_j \tilde{\tau}_{ij}) \right)\]


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Closure for Compressible Flows

- Diffusion of $k^{sgs}$ due to pressure fluctuations transfers acoustic energy from shock front corrugation to subgrid kinetic energy

\[
\overline{w_i P} - \tilde{u}_i \overline{P} = \overline{\rho R (u_i T - \tilde{u}_i \tilde{T})} = -\frac{\overline{\rho v_t R}}{P_{rt}} \frac{\partial \tilde{T}}{\partial x_i}
\]

- Subgrid pressure – dilatation correlation

\[
p_d k^{sgs} = \alpha_p d M_t^{sgs} \overline{\rho S k^{sgs}}^2 \left( \frac{\overline{\rho S k^{sgs}}}{D_k^{sgs}} \right)^2 (P_{k^{sgs}} - D_{k^{sgs}})
\]

- Energy Equation closure (turbulent Prandtl number)

\[
H_i^{sgs} + \sigma_i^{sgs} = -\left( \overline{\rho v_t} + \mu \right) \frac{\partial k^{sgs}}{\partial x_i} - \frac{\overline{\rho v_t}}{Pr} \frac{\partial \tilde{T}}{\partial x_i} + \tilde{u}_j \tau_{ij}^{sgs}
\]

Genin and Menon (Comp. Fl., 2010; J. Turb., 2010)

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Localized Dynamic Evaluation

- Extension of LDKM (Kim and Menon, 1995, 1991) for low-speed flows to compressible flows
- SGS closure model constants obtained from shock-turbulence DNS/LES comparison (Comp. Fl., 2010)
- Dynamic closure using scale similarity at the test filter level
  - Numerically robust and stable in complex flows
- Localized dynamic evaluation of $Pr_t$ can be used to close
  - Subgrid energy diffusion in the energy equation
  - Diffusion of $k_{sgs}$ due to pressure fluctuations
- Localized dynamic evaluation of $Sc_t$ (if not using LEM)
- NO model parameters that are adjusted to match test case
AIAA CFD for Combustion Modeling

**LEMLES: Grid-Within-Grid Approach**

- Multi-scale (space and time) approach (LEMLES)
- Application to subsonic turbulent reacting flows since 2000
  - No ad hoc model constant adjustments
- Extension to shock-turbulence-flame interaction problems
  - LEM updated to allow for subgrid pressure variation
    - Subgrid compression and expansion
  - Explicit presence of shock in subgrid not yet included

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Hybrid Numerical Algorithm

- Locally adaptive hybrid strategy switches from shock capturing solver to a smooth-flow (O(4)) solver locally and dynamically
- Piecewise Parabolized Method (PPM – FLASH3D)
  - Extended to viscous flows, multi-domain, stretched grids
- MUSCL reconstruction with Hybrid HLL Riemann Solver
  - Non-contact preserving in shock transverse directions (HLLE, Einfeldt, 1988, 1991)
  - Contact preserving Riemann solver (HLLC, Toro, 1997)
- The current hybrid solver is identified as 4th/HLLC/E
  - Smoothness local sensors to switch between O(4) & HLL
  - Local shock detection to switch from HLLC to HLLE
Numerical scheme and accuracy

- Illustration for Scramjet flowfield: Supersonic airflow (M=2) over a 6 degrees wedge – vortex street and turbulence

1. Pure upwind is dissipative
2. Central with artificial dissipation is dispersive
3. Hybrid method to switch between numerical schemes
Riemann Solvers Instabilities and Remedy

- Odd-Even decoupling and Carbuncle phenomenon arise in numerical resolution of shock waves
  - neighboring mesh points along a shock front decouple
  - strongly deform shock fronts and creates parasitic oscillations in the post-shock region
- Design of a hybrid Riemann solver – Extension of Quirk’s cure to Riemann solvers: use of a non-contact preserving Riemann solver in the directions transverse to the shock normal
- Flattening (reduce reconstruction order close to strong shocks) to prevent post-shock oscillations
- M=10 air flow onto a cylindrical body
- Appearance of singular points for contact-preserving solvers
  - not seen for HLLE
- Even more reduced effect with HLLC/E
Normal Shock-Turbulence Interaction

- DNS (231x81x81) and LES (106x32x32)
- Isotropic turbulence (243x81x81) superposed on supersonic inflow:
  \[
  \begin{array}{ccc}
  M_{\text{inflow}} & 1.29 & 2 & 3 \\
  Re_\lambda & 19.1 & 19.0 & 19.7 \\
  M_t & 0.140 & 0.108 & 0.110 \\
  \end{array}
  \]

- Variations of local Mach number ➔ Shock corrugation
- Post-shock pressure fluctuations, acoustic wave
- Exchange between acoustic energy & turbulent kinetic energy

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Shock-Turbulence Interaction

- DNS (231x81x81) LES (106x32x32)
- Dynamic LES closure captures turbulence across shock

- Compressibility correction is important to account for transfer of acoustic energy from shock corrugations to sub-grid kinetic energy
Normal Shock / Turbulence Interaction

- LES captures most of the DNS features
- Dynamic model shows stable predictions for all simulated $M$
- Compressibility corrections appears to work well

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Numerical scheme and accuracy

- Proper capture of the flow discontinuities with upwind scheme and resolution of the instability and turbulence

1. Temperature field
2. Use of upwinding in the I-direction
3. Use of upwinding in the J-direction

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Numerical scheme and accuracy

- With reaction, more sharp fronts
- Sonic injection of $\text{H}_2$ at the base of the wedge

1. Temperature field
2. Use of upwinding in the $I$-direction
3. Use of upwinding in the $J$-direction
Non-Reacting and Reacting DLR Test Case

Time-averaged density gradient

Experimental Schlieren

COLD Instantaneous density HOT

Genin and Menon, AIAA (2010)
Comparisons with DLR Data

- Flame anchors by re-circulation of hot products with intermittent reverse flows
- Partially premixed ignition
- Diffusion flame along the shear layer

Sonic Jet in M=1.6 Cross-Flow

Current LES

Flow Vis (vanLarberghe, 2000)

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Comparison with Experiments

Expts. \((x/d=5)\) LES

Santiago and Dutton (JPP, 1997)

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Supersonic JICF
Adaptive Refined Level Set in LESLIE

- Application to moving shocks, flames and bodies
- ~ AMR for shocks and flames
- Interface tracking and cut-cell for moving bodies

- Osher and Fedkiw, Level Set Methods and Dynamic Implicit Surfaces, 2002
- Choi and Menon, AIAA-2010-414, 2011-417

Zaleski Disk    Deforming Ellipsoid in M = 6
Strategies in DIGGIT

- Compressible 5-equation two-fluid model included
- Time integration with TVD-RK O(3) or SDC (for higher order)
- AMR based on detecting inter-element discontinuity
- For smooth flows: Up to O(7) in space and O(5) in time
- Trouble cell detector to apply moment limiter for shocks

Gryngarten et al., 2011, Gryngarten and Menon, AIAA-2011-294
LDG: Shock – Gas Bubble in Air

- M=1.22 He-air 2D cylindrical bubble with 4-level AMR (right)
- M=1.7 Kr-air spherical bubble
- Layes and Le Metayer, (Phys. Fl., 2007)
LDG: Shock – Air 3D Bubble in Water

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Compressible Spatial Shear Layer

<table>
<thead>
<tr>
<th>Parameter</th>
<th>$M_c = 0.28$</th>
<th>$M_c = 0.62$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$M_1$</td>
<td>1.64</td>
<td>2.0</td>
</tr>
<tr>
<td>$M_2$</td>
<td>0.91</td>
<td>0.4</td>
</tr>
<tr>
<td>$U_1 (m/s)$</td>
<td>430</td>
<td>480</td>
</tr>
<tr>
<td>$U_2 (m/s)$</td>
<td>275</td>
<td>130</td>
</tr>
<tr>
<td>$T_1 (K)$</td>
<td>172</td>
<td>150</td>
</tr>
<tr>
<td>$T_2 (K)$</td>
<td>223</td>
<td>252</td>
</tr>
<tr>
<td>$P_{O_1} (Kpa)$</td>
<td>302</td>
<td>495</td>
</tr>
<tr>
<td>$P_{O_2} (Kpa)$</td>
<td>115</td>
<td>75</td>
</tr>
<tr>
<td>$\rho_2/\rho_1$</td>
<td>0.77</td>
<td>0.59</td>
</tr>
<tr>
<td>$U_2/U_1$</td>
<td>0.63</td>
<td>0.27</td>
</tr>
<tr>
<td>$\lambda_B$</td>
<td>1.7</td>
<td>0.8</td>
</tr>
<tr>
<td>Resolution</td>
<td>$2 - 7 \lambda_B$</td>
<td>$5 - 14 \lambda_B$</td>
</tr>
</tbody>
</table>

- LEMLES resolution same as experiment deliberately
- Passive scalar mixing

$182 \times 150 \times 5$ - Quasi-3D
$182 \times 150 \times 100$ - Full 3D
$y^+ = 15$ @ splitter plate
Uniform grid in Z direction

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Profiles of Axial Velocity, $Mc = 0.62$

- GRAD-DIFF and LEMLES employs same k-sgs closure
- Both methods agree well with the experiments

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RMS Axial Velocity, $Mc = 0.62$

- 3D captures the shear layer spread correctly

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RMS Transverse Velocity, $Mc = 0.62$

- GRAD-DIFF and LEMLES over-predicts the peak by $< 6\%$
- Good agreement in the shear layer region

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Normalized Growth Rate

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Mean Mixture Fraction, $Mc = 0.62$

- Improvement in mean mixture fraction prediction for GRAD-DIFF
- LEMLES results are closer to the experiment near the edges

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RMS of the Mixture Fraction, $Mc = 0.62$

- GRAD-DIFF predicts a higher RMS compared to LEMLES

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LEMLES correctly predicts the shape and width of the PDF
Gradient diffusion LES fails to predict both these features
Note: given PDF all scalar moments can be predicted
Numerical Studies of WPAFB TC19

- Full test facility is numerically simulated
- Hybrid VLES-LES in the isolator
- Two configurations studied
  - Cavity with 11 injectors on aft ramp
  - Strut upstream of cavity with 6 injectors
- 8+ million cells, 12/18 LEM cells per LES cell
  - Smallest mesh size ~ 0.01 mm
  - 30+ points in wall boundary layer

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Mach 2 Flow Conditions

| Test Configuration | Stagnation Conditions | Isentropic Conditions at Isolator |  |  |  |  |  |  |
|--------------------|-----------------------|-----------------------------------|---|---|---|---|---|
|                    | P\(_0\) (kPa)         | T\(_0\) (K)                       |  |  |  |  |  |  |
| No-Strut           | 414                   | 589                               |  |  |  |  |  |  |
| Strut (Reacting)   | 207 (449)             | 564 (600)                         |  |  |  |  |  |  |

- CH\(_4\) – H\(_2\) blended fuel (70% - 30%)
- Reduced 4-step, 8 species mechanisms*
- Local Reynolds number, Re\(_x\) ~ 42e6 m\(^{-1}\)
- Stagnation conditions for strut reacting case are changed (shown in red)

\[
\begin{align*}
    CH_4 + 2H + H_2O & \rightarrow 4H_2 + CO \\
    H_2O + CO & \rightarrow H_2 + CO_2 \\
    2H + M & \rightarrow H_2 + M \\
    3H_2 + O_2 & \rightarrow 2H + 2H_2O
\end{align*}
\]

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* Klassen, Menon et al., 2009, AFRL-FA8650-06-C-2659, AFRL Final Report
Energy Spectrum

(a) No-Strut: $X = 53.8$ mm within the shear layer and (b) Strut: $X = 33.8$ mm in the strut wake

Recover $k^{-5/3}$ law in shear layer and strut wake
Non-reacting Flow: Cavity without Strut

- Large vortical flow inside cavity
- Good agreement with data

Time averaged mean velocity streamlines

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Wall Pressure

Grady, N.R., et al., 2010, AIAA-2010-1405
Velocity Comparisons: Non-Reacting, Strut

- Multiple shear layers in the wake of strut
- The overall spreading of wall-bounded cavity shear layer and velocity fluctuations are captured reasonably well

Grady, N.R., et.al., 2010, AIAA-2010-1405
Wall Pressure Strut

- Shock off strut LE (X = -30 mm)
- re-compression shock at aft ramp portion (X ~ 86 mm)
- Expansion at the cavity leading edge
- Expansion-compression around strut top edge

Wall Pressure

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Grady, N.R., et al., 2010, AIAA 2010-1405
Reacting Case: Temperature Field No-Strut

- Mean $<T>$ shows that the cavity is full of products
  - Lifts shear layer for oxidizer entrainment into the cavity
- Instantaneous Temperature shows more variation in the cavity
- $T$ at span-wise location ($X = 27$ mm) shows significant 3D structures
- High level of turbulence generated by aft wall fuelling

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Flame Structure and Reaction Rate: No-Strut

Reaction rate of CH4 at (a) Z = 0 plane and (b) X = 27 mm span-wise plane

Reaction rate of H2 at (c) Z = 0 plane and (d) X = 27 mm span-wise plane

Methane and Hydrogen flame structures

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Reacting Case: with and without Strut

- Pressure comparison shows some reasonable agreement
- Peaks observed at locations where there are no pressure data locations of secondary shocks

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Instantaneous Contours of Products: Strut

Contours of CO₂ at (a) Z = 0 plane and (b) X = 27 mm span-wise plane

Contours of H₂O at (a) Z = 0 plane and (b) X = 27 mm span-wise plane
Streamlines

No Strut, Reacting

Strut, Reacting

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Strut and No-Strut Comparison

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Flame Index = normalized $\nabla Y_F \cdot \nabla Y_O$

- Flame Index $> 0$ for premixed flame and $< 0$ for diffusion flame

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**Reacting Flow – Flame Regimes for LES**

- Strong variation of Ka from flamelet to broken reaction zone
- LEMLES captures all regimes without model change

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The description of the chemical kinetics is very important as its time-scales ($\tau_c$) are on the same order-of-magnitude as those of the flow ($\tau_I$, $\tau_\Delta$, $\tau_T$).
The Waidmann *et al* Combustor

**DLR experimental investigation**


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**Fureby *et al***

3 injectors, 5 Mcells
15 injectors, 25 Mcells

**Génin & Menon**

2 injectors, 2.5 Mcells

---


*Génin & Menon, 2009, AIAA 2009-0132*

*Fureby et al., 2011, 28th ISSSW, Manchester*
Sunami-Magré Combustor

Joint ONERA / JAXA experimental (scramjet) combustor study

Spontaneous flame images

ONH10 flameholder
\( t=10\text{mm} \)

ONH15 flameholder
\( t=15\text{mm} \)

Fuel injection

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Supersonic flame structure investigation (ONH10) and OH comparison

Berglund et al, 2009, AIAA J.
Sabelnikov & Fureby In Preparation 2011
Real Gas: Basic thermodynamics

- Under atmospheric conditions, most fluids require a phase change to go from liquid to gas
  - Multiphase field: breakup, atomization, evaporation…
- Not necessary if $T > T_c$ OR $p > p_c$:
  - Smooth interface
  - No surface tension
  - No latent heat of vaporization
- If $T > T_c$ AND $p > p_c$, fluid is supercritical
Basic thermodynamics

- A supercritical fluid may or may not follow the Ideal Gas Equation of State (IG EoS) \( pV = RT \).
- Departure from IG EoS caused by inter-molecular effects:
  - Molecules cannot be assumed to be points
  - Inter-molecular forces on top of simple collisions
- These real gas, i.e. non-ideal, effects occur when the density of the fluid is large enough
  - What is large enough?
Basic thermodynamics

- Introduce compressibility
  - $Z=1 \Rightarrow$ ideal gas
  - $Z\neq1 \Rightarrow$ real gas
- Hint at a universal behavior
  - $Z$ is equivalent for simple species when normalizing $T$ and $p$ by $T_c$ and $p_c$
- Mathematical translation into new EoS

$$Z = \frac{pV}{R_u T}$$

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Relevance to combustion

- Overall trend is to increase pressure (GT, ICE, rockets)
- Three flows where real gas effects are important:
  - Sub-critical flows
    - All species gaseous, mild departures from $Z = 1$
  - Super-critical flows
    - Some species supercritical, $Z = 0.3$ to 1
  - Trans-critical flows
    - Some species are compressed liquids, $Z$ can vary from 0.3 to 1 and pseudo-phase change phenomena
Relevance to combustion

- Concrete example: surrogate aircraft fuel
  - 82.6% n-decane and 17.4% trimethylbenzene (Pitsch_2008a)
- Corresponding states principle (CSP)
  - Mixture behaves like a pure pseudo-fluid with pseudo critical properties

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Issues for combustion modeling

- Large density gradients
- Computational cost
- Additional unclosed terms
- Pressure dependence in reaction mechanisms
- EoS validity for a wide range of flow conditions and species must be understood and established
  - Cubic EoS such as Peng-Robinson (PR), Soave-Redlich-Kwong (SRK)
  - Higher order empirical EoS such as Benedict-Webb-Rubin (BWR)
Dealing with density gradients

- Need to capture both large density gradients & turbulence at the same time
- Implement within the real gas EoS:
  - TVD MUSCL scheme using approximate Riemann solver for 3rd order accuracy
  - Dynamic switch based on local density gradients
- Pure central schemes cannot handle these gradients without huge resolution requirements
- Pure upwind schemes are too dissipative
Dealing with density gradients

- Shu-Osher test

Standard air $Z = 1$

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

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PSU RCM1

- Super-critical combustion without trans-critical event
  - Injection temperatures are high enough that real gas effects are negligible
  - Still large density gradients
  - Importance of pressure on reaction mechanism
- Simplest configuration relevant to staged combustion
  - Gas-gas $\text{H}_2$-$\text{O}_2$ shear coaxial injector
  - Cylindrical chamber instrumented for heat flux measurement
• Butterfly grid with 3.2M grid points
PSU RCM1 - Combustion modeling

- Characteristics of the PSU simulation
  - Good resolution in near-field and slow secondary combustion
  - Eddy Break-Up not adapted
- Detailed 21-step, 8-species mechanism (Conaire_2004)
  - Very stiff to integrate
- Simplest closure: sub-iteration scheme
- Future strategies
  - Reduced mechanism
  - LEM with ANN

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PSU RCM1 - Flowfield description

- Distinguishing 4 different zones:
  - A: oxygen jet core >>> primary diffusion flame
  - B: accelerating then decelerating flow >>> secondary combustion
  - C: recirculation zone >>> very little combustion
  - D: homogeneous flow >>> no more reaction
Oxygen jet break-up

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Wide range of CFD tools
- Similar heat flux
- Different flow structure
- Best prediction: wall-resolved LES?
- Many parameters influence heat flux
PSU RCM1 – Comparison CFD solvers

- LES
- LES
- AXI-LES
- AXI-URANS
- AXI-RANS

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PSU RCM1 - Comparison 3D - 2D-axi LES

Baseline grid (610x94)
Wall-refined grid (610x144)
Globally refined grid (916x273)
LOXGOX Experiment (PSU)

- Work on previous configuration has helped design new experimental facility
  - Square chamber for easy optical access
  - Coflow to eliminate recirculation zones
- Perforated plate approximated as uniform flow for now
LOXGOX – Operating conditions

- Focus on the case with trans-critical injection
  - \( P > P_c \) AND \( T_{\text{inj}} < T_c \) for pure oxygen
- Hybrid scheme can capture trans-critical layer

<table>
<thead>
<tr>
<th>Description</th>
<th>Units</th>
<th>Value</th>
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<tbody>
<tr>
<td><strong>Main chamber</strong></td>
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<td>Chamber pressure</td>
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<td>Inflow velocity</td>
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<td><strong>Injector inner post flow</strong></td>
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<td>Inflow velocity</td>
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<td><strong>Injector annular flow</strong></td>
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<td>Compressibility</td>
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<tr>
<td>Inflow velocity</td>
<td>m.s(^{-1})</td>
<td>101</td>
</tr>
</tbody>
</table>
LOXGOX – Qualitative validation

- Trying to reproduce backlit images
- Good qualitative agreement

**DENSITY (kg/m³)**

<table>
<thead>
<tr>
<th>Density (kg/m³)</th>
</tr>
</thead>
<tbody>
<tr>
<td>100.000</td>
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<tr>
<td>150.000</td>
</tr>
<tr>
<td>200.000</td>
</tr>
<tr>
<td>250.000</td>
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</tbody>
</table>

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LOXGOX – Quantitative validation

- Measuring dark-core length
- Flow physics is captured with reasonable accuracy
Observations from Rocket LES

- 3D simulations are required
  - Axisymmetric cannot capture flow physics
- Complex turbulent features require LES
  - But proper subgrid closures are still needed
- Validation of single-injector flow is still difficult
  - Good experimental data is rare
- Focus should move to multi-injector flows
  - More realistic configuration
Final Summary Comments

- CFD is a tool that can be exploited with various levels of confidence and reliability for a range of problems
- Sometimes asking too much of a simple and reliable model may not be the proper thing to do...
- Key areas to be aware of
  - Numerical scheme’s strengths and limitations
  - Choice of grid and boundary conditions
  - Turbulence closures (RANS, URANS, DES or LES)
  - Scalar mixing closure (turbulent and molecular)
  - Reaction kinetics closure (finite-rate, mixture fraction)
  - Parallel optimization and scalability is essential
Further Reading

• All models and results discussed are in published papers
  – Cited work papers are available upon request

• Many excellent reviews and books are also available
  – Poinsot & Veynante: Theoretical and Numerical Combustion, Edwards, 2nd
  – Reviews by Pitsch (Ann. Rev. 2006), Janicka (Symp 2006), Peters (2008), Candel etc…

• Other papers are available

• LEM stand-alone codes can be used to learn and in needed implemented into in-house codes