Advanced Modeling and Simulations

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National Center for Hypersonic Combined Cycle Propulsion
Two Main Components of Advanced Modeling

- Turbulence & Turbulence-Chemistry Interactions
  Farhad JaberI Presents

- Chemistry & Kinetics
  Steve Pope Presents
Modeling and Simulations

**Generation I:** RANS

**Generation II:** Hybrid LES-RANS and LES via Scalar-FMDF

**Generation III:** LES via stand alone Energy-Pressure-Velocity-Scalar (EPVS)-FMDF

**DNS:** For *a priori* appraisal of sub-closures and *a posteriori* assessments of final predictions

**Experiments:** For *a posteriori* assessments

**Main Objectives:** Development, testing & Application of Gen II
Development & Testing of Gen III
Modeling and Simulation Roadmap

2009

- RANS Application to TBCC, Turbulence Model, Grid Generation, ...........

2010

- RANS and Hybrid LES-RANS Application to UVa Rig, wall and turbulence models, ....

2011

- Compressible Turbulence Models For RANS and LES

VULCAN
- Implement SFMDF in VULCAN
- Simple Flow/Grid

Scalor FMDF
- Improve SFMDF Submodels and Numerical Solver

DNS
- Temporal and Spatial Mixing Layer

Chemistry
- New Reduced Kinetics Mechanisms for Hydrocarbons

Efficient Chemistry Solver
- ISAT+Message Passing, Parallel Methods,....

2012

VULCAN
- Implement SFMDF in VULCAN
- Complex Structured Grid

Scalar FMDF
- LES-SFMD of Mixing Layer, jet,.....

DNS
- Shock-homogeneous turbulence Mixing Layer, \( H_2 \) Reactions

2013

VULCAN
- Simulations of UVa Experiment

Scalar FMDF
- LES-SMFDF of UVa Combustor

DNS
- A priori and A Posteriori Testing of LES/FMDF Submodels

2014

EPFVS-FMDF
- Formulate

EPFVFS-FMDF
- Evaluate/Improve submodels

EPFVS-FMDF
- Mixing and Reaction

EPFVS-FMDF
- Applications
Progress in Generation II and III

- Gen II Scalar-FMDF model has been/is being employed for LES of several high speed flows (we used our In-house Structured Code).
- Scalar-FMDF model is being transported into VULCAN (Structured Code).
- Scalar-FMDF model is being transported to US3D (Unstructured Code).
- Gen III Energy-Pressure-Velocity-Scalar FMDF formulation is completed.
- A consistent solver is developed for the numerical solution of Energy-Pressure-Velocity-Scalar FMDF.
- DNS has been/is being conducted of several flows.
Filtered (Mass) Density Function: FDF/FMDF
Background and Terminology

**FDF, FMDF: A SGS PDF model for LES of Turbulent Reacting Flows**

- The main benefit of FDF/FMDF is that the filtered reaction source term in the FDF transport equation appears in a closed form and does not require further modeling.
- FDF models are readily adaptable to systematically including models for increasing details of subgrid physical phenomena.
- Various versions of FDF/FMDF models are in use today:
  - Scalar (Energy & Species Mass Fraction) FMDF (S-FMDF)
  - Velocity-Scalar FMDF (VS-FMDF)
  - Velocity-Scalar-Frequency FMDF (VSF-FMDF)
  - Two-Phase Scalar FMDF for Spray Combustion
  - Compressible Scalar FMDF for High Speed Reacting Flows
  - Energy-Pressure-Velocity-Scalar FMDF (EPVS-FMDF)
Scalar-FMDF Model for LES of Turbulent Reacting Flows

A Hybrid Eulerian-Lagrangian Mathematical/Computational Methodology

- Eulerian: Transport equations for the SGS moments
  - Deterministic simulations

- Lagrangian: Transport equation for the FMDF
  - Monte Carlo simulations

- Coupling of Eulerian & Lagrangian fields and a certain degree of "redundancy"

Filtered continuity and momentum equations via a generalized multi-block high-order finite difference Eulerian scheme for high Reynolds number turbulent flows in complex geometries

Various closures for subgrid stresses

Filtered Mass Density Function (FMDF) equation via Lagrangian Monte Carlo method - Ito Eq. for convection, diffusion & reaction

Kinetics: (I) reduced kinetics schemes with direct ODE or ISAT solvers, and (II) flamelet library with detailed mechanisms or complex reduced schemes.

Fuels: methane, propane, decane, kerosene, heptane, JP-10 Hydrogen & Ethylene

Chemistry

Gasdynamic Field

Scalar Field (mass fractions and temperature)

Monte Carlo Particles

Vorticity Contours & Monte Carlo Particles

Pressure Isolevels

Nozzle

Wall

CO\(_2\) and C\(_7\)H\(_{16}\) Mass Fractions

Conventional LES Solver (LES-FD)

Overlap

FMDF Solver

\[ \langle \rho \rangle_L \]
\[ \langle u_i \rangle_L \]
\[ \langle \phi_\alpha \rangle_L \] (conserved scalar)

\[ \langle \rho \rangle_L \]
\[ \langle T \rangle_L \]
\[ \langle \rho S_\alpha \rangle_L \]
\[ \langle \phi_\alpha \rangle_L \]
**Filtered LES Equations - Eulerian**

\[
\langle f(x,t) \rangle = \int_{-\infty}^{+\infty} f(x',t)G(x',x)dx' \quad \hat{f} = \frac{\rho f}{\bar{\rho}} = \langle f(x,t) \rangle_L = \frac{\langle \rho f \rangle}{\langle \rho \rangle}
\]

\[
J \frac{\partial \bar{p}}{\partial t} + \bar{p} \frac{\partial \bar{J}}{\partial t} + \frac{\partial \bar{p} \hat{u}_i}{\partial t} = 0
\]

\[
J \frac{\partial \hat{u}_i}{\partial t} + \bar{p} \frac{\partial \hat{u}_i}{\partial t} + \frac{\partial \bar{p} \hat{u}_j}{\partial \xi_j} = - \frac{\partial \bar{p}}{\partial \xi_i} + \frac{\partial}{\partial \xi_i} \left( \mu_e \frac{\partial \hat{u}_j}{\partial \xi_j} \right) + \frac{\partial}{\partial \xi_j} \left( \mu_e \frac{\partial \hat{u}_i}{\partial \xi_j} \right)
\]

\[
J \frac{\partial \hat{E}}{\partial t} + \bar{p} \frac{\partial \hat{E}}{\partial t} + \frac{\partial \bar{p} \hat{E} \hat{u}_i}{\partial \xi_i} = - \frac{\partial \bar{P} \hat{u}_i}{\partial \xi_i} - \left( \frac{\partial \hat{u}_i}{\partial \xi_j} \right) \frac{\partial \bar{q}}{\partial \xi_j} + J \rho S_{\alpha}
\]

\[
J \frac{\partial \hat{\phi}_\alpha}{\partial t} + \hat{\phi}_\alpha \frac{\partial \hat{J}^\alpha}{\partial t} + \frac{\partial \hat{\phi}_\alpha \hat{u}_i}{\partial \xi_i} = - \frac{\partial \hat{J}^\alpha}{\partial \xi_i} - \frac{\partial M^\alpha}{\partial x_i} + J \rho S_{\alpha}
\]

\[
\bar{P} = \bar{\rho} (RT) \approx \bar{\rho} TR^0 \sum_{\alpha=1}^{NS} \left\langle \phi_{\alpha} \right\rangle \frac{MW_\alpha}{1}
\]

**Numerical Solution of FMDF - Lagrangian**

**Stochastic Differential Equations**

**Lagrangian Monte Carlo Method**

\[
dX^+_i = \left[ \langle U_i \rangle_L + \frac{1}{\langle \rho \rangle_L} \frac{\partial (\Gamma + \Gamma_r)}{\partial x_i} \right] dt + \sqrt{\frac{2(\Gamma + \Gamma_r)}{\langle \rho \rangle_L}} dW_i(t),
\]

\[
d\phi^+_\alpha = -\Omega_m (\phi^+_\alpha < \langle \phi_{\alpha} \rangle_L) dt + (S^R_{\alpha}(\phi^+) + S^{cmp}_{\alpha}) dt
\]

**FMDF Equation**

\[
P_L(\Psi; x, t) = \int_{-\infty}^{+\infty} \rho(x', t) \xi(\Psi, \Phi(x', t))G(x' - x)dx'
\]

\[
\xi(\Psi, \Phi(x, t)) = \prod_{\alpha=1}^{NS} \delta(\Psi, \Phi(x, t))
\]

\[
\frac{\partial P_L}{\partial t} + \frac{\partial}{\partial x_i} \left[ \langle u_i \rangle_L P_L \right] = \frac{\partial}{\partial x_i} \left[ (\hat{\gamma} + \hat{\gamma}_t) \frac{\partial \langle P_L / \rho \rangle_L}{\partial x_i} \right] + \frac{\partial}{\partial \Psi} \left[ \Omega_m \left( \Psi - \langle \phi_{\alpha} \rangle_L \right) P_L \right] - \frac{\partial}{\partial \Psi} \left[ S^R_{\alpha}(\Psi) P_L \right]
\]

\[
+ \left[ S^{cmp}_{\alpha} \Psi \langle P_L / \rho(\Psi) \rangle \right]
\]

**Reaction terms**

**Reaction term**

*Added to FMDF equation as a source/sink term*
Energy-Pressure-Velocity-Scalar FMDF

**EPVS-FMDF**: 
\[ F_L(v, \psi, \theta, \eta, x; t) \equiv \int_{-\infty}^{+\infty} \rho(x', t) \zeta[v, \psi, \theta, \eta; u(x', t), \phi(x', t), e(x', t), p(x', t)] G(x' - x) \, dx' \]

**Fine Grained Density**: 
\[ \zeta[v, \psi, \theta, \eta; u(x, t), \phi(x, t), e(x, t), p(x, t)] = \left( \prod_{k=1}^{3} \delta[v_k - u_k(x, t)] \right) \times \left( \prod_{\alpha=1}^{N_s} \delta[\psi_\alpha - \phi_\alpha(x, t)] \right) \times \delta[\theta - e(x, t)] \times \delta[\eta - p(x, t)] \]

By Integrating EPVS Fine Grained Density Equation:

\[
\frac{\partial P_L}{\partial t} + \frac{\partial V_j P_L}{\partial x_j} = \frac{\partial}{\partial V_i} \left( \frac{1}{\rho} \frac{\partial p}{\partial x_i} \right)_l P_L - \frac{\partial}{\partial V_i} \left( \frac{1}{\rho} \frac{\partial \tau_{ij}}{\partial x_j} \right)_l P_L \\
+ \frac{\partial}{\partial \psi_\alpha} \left( \frac{1}{\rho} \frac{\partial J_{\alpha,j}}{\partial x_j} \right)_l P_L + \frac{\partial}{\partial \theta} \left( \frac{1}{\rho} \frac{\partial q_i}{\partial x_i} \right)_l P_L \\
- \frac{\partial}{\partial \theta} \left( \frac{1}{\rho} \frac{\partial u_{ij}}{\partial x_j} \right)_l P_L + \frac{\partial}{\partial \theta} \left( \frac{1}{\rho} p \frac{\partial u_j}{\partial x_j} \right)_l P_L \\
+ (\gamma - 1) \frac{\partial}{\partial \eta} \left( \frac{\partial q_i}{\partial x_i} \right)_l P_L - (\gamma - 1) \frac{\partial}{\partial \eta} \left( \tau_{ij} \frac{\partial u_i}{\partial x_j} \right)_l P_L \\
+ \gamma \frac{\partial}{\partial \eta} \left( p \frac{\partial u_j}{\partial x_j} \right)_l P_L
\]
Stochastic Modeling of $V$, $S$, $E$ and $P$

**Velocity and Scalar (LMSE+GLM) Models:**

\[
\begin{align*}
\frac{dX_i^+}{i} &= U_i^+ \, dt + \sqrt{2\mu \langle \rho \rangle_i} \, dW_i \\
\frac{dU_i^+}{i} &= \left[ -\frac{1}{\langle \rho \rangle_i} \frac{\partial \langle p \rangle_i}{\partial x_i} + \frac{2}{\langle \rho \rangle_i} \frac{\partial}{\partial x_j} \left( \mu \frac{\langle u_i \rangle_L}{\partial x_j} \right) + \frac{1}{\langle \rho \rangle_i} \frac{\partial}{\partial x_i} \left( \mu \frac{\langle u_i \rangle_L}{\partial x_i} \right) \right] \, dt + G_{ij} \left( U_j^+ - \langle u_j \rangle_L \right) \, dt + \sqrt{C_0 \frac{\varepsilon}{\langle \rho \rangle_i}} \, dW'_j \\
\frac{d\phi^+}{\alpha} &= -C_\phi \omega \left( \phi^+ - \langle \phi \rangle_L \right) \, dt \\
\end{align*}
\]

**Where:**

\[
\omega = \frac{1}{\langle \rho \rangle_i} \varepsilon \quad ; \quad \varepsilon = C_\varepsilon \langle \rho \rangle_i \frac{k^{3/2}}{\Delta_L} ; \quad k = \frac{1}{2} \tau_L (u_i, u_i)
\]

**Energy and Pressure Models:**

\[
\begin{align*}
\frac{dE^+}{i} &= \left[ \frac{1}{\gamma} \left( -\frac{1}{\langle \rho \rangle_i} \frac{\partial \tilde{q}_i}{\partial x_i} + \frac{\varepsilon}{\langle \rho \rangle_i} + \frac{1}{\langle \rho \rangle_i} \tilde{\tau}_{ij} \frac{\partial \langle u_i \rangle_L}{\partial x_j} \right) + \frac{\gamma-1}{\gamma} E^+ \left( A - \frac{B^2}{\gamma} \right) \right] \, dt + \frac{\gamma-1}{\gamma} E^+ B dW_p \\
\frac{dP^+}{i} &= P^+ \left( Adt + BdW_p \right)
\end{align*}
\]
Fokker-Planck Eq. from Stochastic Eqs.

\[
\frac{\partial F_L}{\partial t} + \frac{\partial [V_i F_L]}{\partial x_i} = \frac{1}{\langle \rho \rangle_L} \frac{\partial \langle p \rangle_i}{\partial x_i} \frac{\partial F_L}{\partial V_i} - \frac{2}{\langle \rho \rangle_L} \frac{\partial}{\partial x_j} \left( \mu \frac{\partial \langle u_i \rangle_L}{\partial x_j} \right) \frac{\partial F_L}{\partial V_i}
\]

\[
- \frac{1}{\langle \rho \rangle_L} \frac{\partial}{\partial x_j} \left( \mu \frac{\partial \langle u_j \rangle_L}{\partial x_i} \right) \frac{\partial F_L}{\partial V_i} + \frac{2}{3} \frac{1}{\langle \rho \rangle_L} \frac{\partial}{\partial x_i} \left( \mu \frac{\partial \langle u_i \rangle_L}{\partial x_j} \right) \frac{\partial F_L}{\partial V_i}
\]

\[
- \frac{\partial}{\partial V_i} \left[ G_{ij} \left( V_{ij} - \langle u_j \rangle_L \right) F_L \right] + \frac{\partial^2}{\partial x_i \partial x_i} \left[ \frac{\mu}{\langle \rho \rangle_L} F_L \right]
\]

\[
+ \frac{\partial}{\partial x_i} \left[ \frac{2\mu}{\langle \rho \rangle_L} \frac{\partial \langle u_j \rangle_L}{\partial x_i} \frac{\partial F_L}{\partial V_j} \right] + \frac{\mu}{\langle \rho \rangle_L} \frac{\partial \langle u_k \rangle_L}{\partial x_j} \frac{\partial \langle u_i \rangle_L}{\partial x_j} \frac{\partial^2 F_L}{\partial V_k \partial V_i} + \frac{\partial^2}{\partial V_i \partial V_i} \left[ \frac{C_0 \epsilon}{2} F_L \right]
\]

\[
+ C_{\phi} \omega \frac{\partial \left[ \left( \psi_a - \langle \phi_a \rangle_L \right) F_L \right]}{\partial \psi_a} + \frac{1}{\gamma} \left( \frac{1}{\langle \rho \rangle_L} \frac{\partial q_i}{\partial x_i} - \epsilon \frac{\langle q \rangle_L}{\langle \rho \rangle_L} - \frac{\partial \langle u \rangle_L}{\partial x_i} \right) \frac{\partial F_L}{\partial \theta}
\]

\[
- \frac{\gamma - 1}{\gamma} \frac{\partial \left[ \theta A F_L \right]}{\partial \theta} + \frac{\gamma - 1}{\gamma^2} \frac{\partial \left[ \theta B^2 F_L \right]}{\partial \theta} - \frac{\partial \left[ \eta A F_L \right]}{\partial \eta}
\]

\[
+ \frac{1}{2} \frac{\partial^2}{\partial \varphi \partial \theta} \left[ \left( \frac{\gamma - 1}{\gamma} \right)^2 \theta^2 B^2 F_L \right] + \frac{\partial^2}{\partial \varphi \partial \eta} \left[ \frac{\gamma - 1}{\gamma} \eta \theta B^2 F_L \right] + \frac{1}{2} \frac{\partial^2}{\partial \eta \partial \eta} \left[ \eta^2 B^2 F_L \right]
\]

Closures Needed for: $G_{ij}$, $A$, $B$, .....
### Exact SGS Kinetic Energy Equation:

\[
\frac{\partial \langle \rho \rangle_i}{\partial t} + \frac{\partial \langle \rho \rangle_i \langle u_k \rangle_L}{\partial x_k} = \langle \rho \rangle_i P + \Pi_d - \varepsilon
\]

\[
- \frac{\partial}{\partial x_k} \left( \frac{\langle \rho \rangle_i \tau_L(u_i,u_i,u_k)}{2} + \tau_i(p,u_i) \delta_{ik} - \tau_L(u_i, \bar{u}_i) \right)
\]

**Modeled SGS Kinetic Energy Equation:**

\[
\frac{\partial \langle \rho \rangle_i}{\partial t} + \frac{\partial \langle \rho \rangle_i \langle u_k \rangle_L}{\partial x_k} = \left[ -\langle \rho \rangle_i \tau_L(u_i,u_i) \frac{\partial \langle u_i \rangle_L}{\partial x_k} + G_{ik} \langle \rho \rangle_i \tau_L(u_k,u_i) + \frac{3C_0}{2} \varepsilon \right]
\]

\[
- \frac{1}{2} \frac{\partial \langle \rho \rangle_i}{\partial x_k} \tau_L(u_k,u_i,u_i) + \frac{\partial}{\partial x_k} \left( \mu \frac{\partial k}{\partial x_k} \right)
\]

### Exact Energy Transport Equation:

\[
\frac{\partial \langle \rho \rangle_i \langle e \rangle_L}{\partial t} + \frac{\partial \langle \rho \rangle_i \langle u_i \rangle_L \langle e \rangle_L}{\partial x_i} = -\frac{\partial q_i}{\partial x_i} - \frac{\partial \langle \rho \rangle_i \tau_L(e,u_j)}{\partial x_j} + \varepsilon + \bar{\tau}_{ij} \frac{\partial \langle u_i \rangle_L}{\partial x_j} - \Pi_d - \langle p \rangle_i \frac{\partial \langle u_i \rangle_L}{\partial x_i}
\]

**Modeled Energy Transport Equation:**

\[
\frac{\partial \langle \rho \rangle_i \langle e \rangle_L}{\partial t} + \frac{\partial \langle \rho \rangle_i \langle u_i \rangle_L \langle e \rangle_L}{\partial x_i} = -\frac{1}{\gamma} \frac{\partial q_i}{\partial x_i} - \frac{\partial \langle \rho \rangle_i \tau_L(u_i,e)}{\partial x_i} + \frac{1}{\gamma} \varepsilon + \frac{1}{\gamma} \bar{\tau}_{ij} \frac{\partial \langle u_i \rangle_L}{\partial x_j} + \frac{1}{\gamma} \langle \rho eA' \rangle_i - \frac{1}{\gamma^2} \langle \rho eB'^2 \rangle_i + \frac{\partial}{\partial x_j} \left( \mu \frac{\partial \langle e \rangle_L}{\partial x_j} \right)
\]

\[
A = \frac{1}{E^+} \left[ -\frac{1}{\langle \rho \rangle_i} \frac{\partial q_i}{\partial x_i} + \frac{\varepsilon}{\langle \rho \rangle_i} + \frac{1}{\langle \rho \rangle_i} \bar{\tau}_{ij} \frac{\partial \langle u_i \rangle_L}{\partial x_j} \right] - \gamma \left( \frac{\Pi_d}{\tau_i(p,p)} (P^+ - \langle p \rangle_i) - \gamma \frac{\partial \langle u_i \rangle_L}{\partial x_i} \right)
\]

\[
B = 0
\]

**Dissipation & Pressure-Dilatation are modeled with Dynamic Models**
• Compressibility effects are included in FMDF-MC; without compressible term FMDF-MC results are very erroneous.
• By varying the initial number of MC particles per cell, the filtered temperature does not noticeably change.
• By increasing the initial particle/cell number, MC particle number density becomes smoother and nearly the same as filtered fluid density.
LES via Scalar-FMDF: NASA Co-Annular Jet

3D LES Calculations with Compact Scheme

Grid System for LES

Iso-Levels of Mach Number

Reacting Case

Cutler et al. 2007

10 mm diameter jet

Instantaneous Scalar

Iso-Levels of Mach Number

Grid System for LES
Comparison with Experiment

- Experiment
- Smagorinsky
- MKEV 0.02
- MKEV 0.03
LES/FMDF of Supersonic Co-Annular Jet - Mixing Case

Consistency of LES-FD and FMDF-MC data

(a) Temperature

- With Pressure Term
  - \( R = 0.97 \)
- Without Pressure Term
  - \( R = 0.74 \)

(b) Temperature

- LES-FD
- FMDF-MC

(c) Mean He Mass Fraction

- LES - FD
- FMDF - MC
LES/FMDF of Supersonic Co-Annular Jet - Reacting Case

Consistency of LES-FD and FMDF-MC data

H₂+Air Combustion

H₂ Mass fraction

LES-FD

FMDF-MC

Temperature (K)

LES-FD

FMDF-MC

Air

\( P_t = 580 \text{ kPa} \)

\( \rho_t = 6.735 \text{ kg/m}^3 \)

\( Y_{H2} = 0.3 \)

\( Y_{N2} = 0.7 \)

\( P_t' = 628.3 \text{ kPa} \)

\( \rho_t' = 1.334 \text{ kg/m}^3 \)
Toward Simulations of UVa Combustor via LES/FMDF

Hybrid LES-RANS or LES

LES/RANS or LES of Supersonic BL Inlet Flow with and without Isolator

LES/FMDF of Supersonic BL flow over the Ramp

Hybrid LES-RANS or LES
LES of Fuel-Air Mixing in UVa Set Up

Simple Fuel Jet in Supersonic Cross Flow

Jet Mixing in Ramp Stabilizer

Jet Mixing in Cavity Stabilizer

Sonic Fuel Jet
Implement SFMDF in VULCAN
Simple Flow/Grid

2009-2011

✓ Improve SFMDF submodels and numerical solver
✓ Set up LES Flow solver for simple planar mixing layer flow (Cartesian single-block grid) No Reaction, No FMDF
✓ Develop a simple version of SFMDF subroutine for VULCAN (single-scalar, Cartesian mesh) Isothermal, No Reaction
✓ Implement simple SFMDF subroutine in VULCAN by Drozda & Baurle, - Jaberi & Givi helping
✓ 2D Simulations of Planar Mixing Layer No Reaction, No FMDF
✓ 3D Simulations of Planar Mixing Layer No Reaction, 1-scalar with FMDF

Comparison of NASA’s VULCAN results with MSU’s SFMDF results for planar mixing layer

Complex Structured Grid

2013-2014

✓ Transfer Flow/Velocity Solver Information (flow configuration, grid, inflow/BC, SGS models) to NASA
✓ Transfer SFMDF Subroutine, data, and scalar solution Conditions to NASA

Implement SFMDF in VULCAN

Simulations of UVa Experiment with VULCAN
Development focuses on three reusable software modules:

• **Eulerian-Lagrangian Geometry and BC Module**
  - Define geometric data for tracking Lagrangian particles
  - “Move” data from cell centers to vertices (interpolation) and vice versa (weighted ensemble averaging)
  - **Benefit:** Any mesh type can be “cast” into new geometric structures thereby facilitating easy integration into existing Eulerian solvers

• **Lagrangian Particle Tracking Module**
  - Continually track particle location with respect to Eulerian cell (no costly near-neighbor search required)
  - Second order tracking (particle properties may be updated when crossing cell interfaces)
  - Dual use with multiphase flows (via pointers)
  - **Benefit:** Efficient and robust particle tracking on arbitrary Eulerian structured/unstructured meshes

• **Transport PDF/FDF Solver**
  - Applicable to both RAS and LES
  - Temporal integration of transport, mixing, and reaction performed in a split form (eliminates issues related to prediction of incorrect shock propagation speed due to stiff chemistry on finite mesh)
  - Flexible framework to solve various flavors of PDF/FDF methods
  - **Benefit:** Provides high-fidelity physics-based model for turbulence-chemistry interactions
**S-FMDF in US3D: Unstructured Grids**

3D unstructured finite volume code
- Hybrid grids: hex, prism, pyramid, or tetrahedral
- Scalable to 1000’s of processors and 100M’s of cells

Lagrangian Monte Carlo particles on unstructured mesh of tetrahedral cells
DNS of High Speed Turbulent Flows

Isotropic Turbulence Interacting with a Normal Shock

Spatially Developing Mixing Layer plus Shock

Temporally Developing Mixing Layer

Shock-Boundary Layer Interactions

Oblique Shock Wave

Normal Shock Wave

Incident shock $\beta = 30^\circ$

$M_1=6.0$

Temperature

Pressure

National Center for Hypersonic Combined Cycle Propulsion
DNS of Shock-Isotropic Turbulence Interaction

M1=2.0

M1=2.0

M1=5.0

Normal Shock Wave

Vorticity

Normal Shock Wave

Reactive
Non-reactive

k \times (x-x_s)

w'w'/u'u'
Mixing in Shock-Isotropc Turbulence Configuration

Abbreviation:  WS------- With Shock  
NS-------- No Shock  
Ks0--------Wavenumber for peak of initial scalar spectrum
Reaction in Shock-Isotropic Turbulence Configuration

M1=2.0, Ks0=2.0

M1=2.0, Ks0=8.0
DNS of Supersonic Turbulent Mixing-Layer with Shock

With Different Incident Shock Angles
DNS and LES of Supersonic Turbulent Mixing-Layer

Mean Axial Velocity

Mean Scalar

Vorticity

Mean Axial Velocity

Mean Scalar

Vorticity

Pre-Contour

With Incident Shock

Imposed Shock

Pressure

Scalar

$X=347$

$X=347$

$X=275$

$X=222$

$X=347$

$M_1=4.2$

$M_2=1.8$

$\Re_\delta=300$ $\Ma=1.2$

$\phi$

$\alpha=18^\circ$

$\phi$

$X=340$

$X=380$

$\Re_\delta=300$ $\Ma=1.2$

$\phi$

$X=380$

$\alpha=18^\circ$

$\phi$

$X=380$
DNS of Supersonic Turbulent Mixing Layer with Combustion

Re=400  \( \phi=0.50 \)  \( CP_x = CP_{x}(T) \)
T1=430k  M1=3.16
T2=293k  M2=1.36  \( t=900 \)

Air

\( H_{2}+Air \)

Re=400  \( \phi=0.35 \)  \( CP_x = \text{CONST} \)
T1=396k  M1=3.32
T2=293k  M2=1.42  \( t=1100 \)

\( t=1300 \)

Re=400  \( \phi=0.30 \)  \( CP_x = \text{CONST} \)
T1=T2=293k
M2=1.40  \( t=1100 \)

\( t=1300 \)
Validation of EPVS-FMDF

- **DNS**: $256 \times 256 \times 256$
- **LES**: $33 \times 33 \times 33$ with 320 particles per cell
- **Ma**: 0.2-2.0
Validation of EPVS-FMDF via DNS

**Mean Values**

**RMS Values**
Consistency Assessments of EPVS-FMDF

- x-velocity
- y-velocity
- z-velocity

Density
Temperature
Energy
Pressure
Collaborations with Center PIs and NASA & AFRL Scientists

- Rob Baurle (NASA LaRC)
- Tom Drozda (NASA LaRC)
- Barry Kiel (AFRL)

- LES-RANS for UVa Dual-Mode Experiment
  Edwards and Jaberi

- Improved Turbulence Models for High Speed Non-Reacting and Reacting Flows
  Ristorcelli, Edwards, Givi

- Formulations of EPFVS-FDF for High Speed Reacting Flows
  Givi, Pope, Jaberi

- Experimental Data for Model Validation – NASA Coannular Jet, AFRL Jet in Cross Flow, UVa Dual Mode, HYPULSE etc.
  Goyne, MacDaniel, Cutler, Hanson, Carter

- Improved Subgrid Models and Numerical Methods for Scalar FMDF
  Jaberi, Givi

- Implementation of scalar FMDF in VULCAN
  Drozda, Baurle, Jaberi

- DNS Data for Model Development and Testing – Supersonic Mixing Layer, Shock-Isotropic Turbulence
  Madnia, Jaberi

- Reliable and Efficient Chemical Kinetics Models for RANS, LES and FDF
  Pope, Chelliah, Tsang
The most challenging modeling aspect, namely modeling of turbulence-chemistry interaction, appears in a closed form in FMDF.

FMDF is readily adaptable to systematically including models for increasing detail of subgrid physical phenomena (in contrast to most other models that represent the subgrid as a function of large scale quantities only).

Well characterized and relevant DNS data have been/are being developed for systematic validation of FMDF models.

Primary barriers to utilizing LES/FMDF in production codes are related to computational implementation and algorithmic implementations with plenty of room for improvements.