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Outline

• Update on US3D CFD code
  – Decoupled implicit method
  – Low-dissipation kinetic energy consistent fluxes
  – Recent simulations

• STABL / STABL-3D

• Advanced DSCM code / Molecular Dynamics

• Emerging capabilities
US3D Code

- US3D = unstructured grid implementation of NASA DPLR code
- Extensions for unsteady simulations (Hybrid RANS-LES, DNS)
- Numerics:
  - Upwind 2nd, 3rd order MUSCL fluxes
  - 2nd, 4th, 6th order kinetic energy consistent fluxes with LS gradients
  - Variety of forms of dissipation / limiters / shock sensors
  - DPLR, 1st, 2nd order FM point implicit, RK3, explicit/implicit RK3
  - Decoupled implicit method
- Thermo-chemical nonequilibrium, non-trivial boundary conditions
- RANS (S-A & SST), Hybrid RANS/LES, DNS
- Fluid-structure interactions, moving grids
- Lagrangian particle tracking and FMDF
- Designed for scaling to large grids / processor count
- Post-processing / data analysis tools
US3D Simulations
Decoupled Implicit Method

DPLR block tridiagonal solve (2D example):

\[
\begin{pmatrix}
\vdots & \ddots & \ddots & \ddots & \ddots \\
& \ddots & \ddots & \ddots & \ddots \\
& & \ddots & \ddots & \ddots \\
& & & \ddots & \ddots \\
& & & & \ddots
\end{pmatrix}
\begin{pmatrix}
\delta U_{i,j-1}^{(k)} \\
\delta U_{i,j}^{(k)} \\
\delta U_{i,j+1}^{(k)} \\
\vdots \\
\vdots
\end{pmatrix}
= 
\begin{pmatrix}
\vdots \\
\text{RHS}_{i,j} \\
\vdots \\
\vdots
\end{pmatrix}
- \nabla \delta U_{i+1,j}^{(k-1)} - \nabla \delta U_{i-1,j}^{(k-1)}
\]

Decoupled scalar tridiagonal solve:

\[
\begin{pmatrix}
\vdots & \ddots & \ddots & \ddots \\
& \ddots & \ddots & \ddots \\
& & \ddots & \ddots \\
& & & \ddots \\
& & & & \ddots
\end{pmatrix}
\begin{pmatrix}
\delta \tilde{V}_{i,j-1}^{(k)} \\
\delta \tilde{V}_{i,j}^{(k)} \\
\delta \tilde{V}_{i,j+1}^{(k)} \\
\vdots \\
\vdots
\end{pmatrix}
= 
\begin{pmatrix}
\vdots \\
\text{RHS}_{i,j} \\
\vdots \\
\vdots
\end{pmatrix}
- \nabla \delta \tilde{V}_{i+1,j}^{(k-1)} - \nabla \delta \tilde{V}_{i-1,j}^{(k-1)} + \nabla \delta \tilde{V}_{i,j}^{(k-1)}
\]
Comparison of Computational Cost

Mach 15, 21-species, 32-reaction air-CO$_2$ kinetics model on a resolved grid
Low-Dissipation Numerical Methods

- Most CFD methods for high-speed flows use upwind methods:
  - Works well for steady laminar flows and RANS
  - For LES/DES, dissipation overwhelms the flow physics
- Develop a new numerical flux function:
  - Conserve a secondary quantity
  - Make discrete kinetic energy flux consistent with KE equation
  - 2nd, 4th and 6th order accurate formulations
  - Add dissipation using shock sensor

\[
\begin{pmatrix}
-k^* \\
u^* \\
v^* \\
w^*
\end{pmatrix}
= \begin{pmatrix}
\frac{-u^{*2} + v^{*2} + w^{*2}}{2} \\
\frac{\rho^{n+1}u^{n+1} + \sqrt{\rho^n u^n}}{\sqrt{\rho^{n+1} + \sqrt{\rho^n}}} \\
\frac{\rho^{n+1}v^{n+1} + \sqrt{\rho^n v^n}}{\sqrt{\rho^{n+1} + \sqrt{\rho^n}}} \\
\frac{\rho^{n+1}w^{n+1} + \sqrt{\rho^n w^n}}{\sqrt{\rho^{n+1} + \sqrt{\rho^n}}}
\end{pmatrix}
\]

\[
\begin{pmatrix}
\rho u' \\
\rho u' u \\
\rho u' v \\
\rho u' w \\
\rho u' k
\end{pmatrix}_f = \rho_f u'_f
\]

\[
p_f = \frac{(1 - \epsilon)p^n + (1 + \epsilon)p^{n+1}}{2}
\]

\[
\rho_f = \frac{\rho^n + \rho^{n+1}}{2}
\]

Subbareddy & Candler (2009)
Low-Dissipation Numerical Method

Propagation of a Gaussian density pulse

Upwind methods rapidly damp solution
Low-order methods are dispersive

Enables a new class of simulations

Subbareddy & Bartkowicz
Low-Dissipation Numerical Methods

Compressible Mixing Layer

2nd order KE consistent method

3rd order upwind method

Propagation of a 2D density pulse

6th-order accuracy on practical grids
Discrete Roughness Wake

Cylinder mounted in wall of Purdue Mach 6 Quiet Tunnel

270M element simulation:
100D = 0.6 meters length

Bartkowicz & Subbareddy

Wheaton & Schneider
Discrete Roughness Wake

Comparison with experiment: Pressure fluctuations at $x/D = -1.5$

Simulation
Experiment

6th order KEC
4th order KEC
3rd order upwind
2nd order KEC

Impossible with upwind methods
Dynamic Mode Decomposition

• What is the source of the unsteadiness?
  – “Breathing” of separation zone
  – Coupling between mass ingestion and shocks…
• Use dynamic mode decomposition – solve for eigenmodes

Shows that acoustic waves are amplified by normal shock and feed back into primary vortex.
Crossflow Instability on a Cone

Purdue M6 Quiet Tunnel experiments:
- 7° cone, 41 cm long
- 0.002” (51 μm) nose radius
- Random roughness on windside:
  - 10, 20 μm height (~ paint finish)

Simulation (shear stress)

Purdue Oil Flow Experiment

Surface and BL Edge Streamlines

Grid Topology

Gronvall AIAA-2012-2822
Simulations of Capsule Dynamic Stability

6-DOF moving grid simulation
Capture wake unsteadiness

2nd Order Upwind

6th Order Central

Stern (AIAA-2012-3225)

DES Improves Aero Prediction

Pitch-Yaw Coupling: Divergence
Example: Simulation of Scramjet Flows

Fuel Injection into Supersonic Crossflow

Mean injectant mole fraction (AFRL)

$x/d = 5$

CUBRC Combustion Duct

Isolator
Material Response, Ablation, Shape-Change

- Re-Entry F Flight Experiment
- Simulations:
  - Finite-rate gas kinetics and surface model
  - Thermal response, shape change
  - Fly the trajectory

Comparison with Thermocouple on Frustum
Advanced DSMC Code

- New Direct Simulation Monte Carlo code for low-density flows:
  - Written by Tom Schwartzentruber and Ioannis Nompelis
  - Parallel and scalable; unprecedented problem size
  - Cartesian grid with cut cells and automatic mesh refinement

242M particles; Overnight on 960 cores
Emerging Capabilities

- Automatic Mesh Refinement (AMR)
- Eulerian / Lagrangian methods
- Subgrid-scale turbulence models
- Direct solution of PSE
- Advanced numerical methods
- Improved thermochemical models
- DNS for flow physics / modeling
- Flight dynamics with control
- Hybrid CFD / DSMC