SIERRA Thermal/Fluid/Aero Code Development Activities

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Outline

– Thermal/Fluid Capabilities
  • Current capabilities
  • Consolidation Effort

– Code Verification and Software Quality

– Support for NW Applications
  • Bombs (ie B61)
  • RB/RVs

– Future Work
Computational Thermal & Fluid Mechanics

– Capabilities
  • Thermal Response
  • Compressible Flow / Aerodynamics
  • Turbulent, Reacting Flow
  • Multi-phase, Non-newtonian Flow

– Nuclear Weapons Application Areas
  • Normal, Abnormal, and Hostile Environments
    – Bomb and RV/RB Aero
    – Bomb and RV/RB Component Thermal Response
    – Weapon Component Manufacturing Processes
    – Fire Safety

– Dual use -- Industrial Partners and Other Gov’t Agencies
  • Goodyear, Proctor & Gamble, DoD, NASA, AWE
Computational Thermal & Fluid Mechanics

- **Thermal** – Heat Transfer, Enclosure Radiation and Chemistry
  - Dynamic enclosures
  - Element birth death
  - Contact
- **Aero** – Compressible Fluid Mechanics
  - Subsonic through hypersonic
  - Laminar and turbulent
  - Unstructured mesh
- **Multiphase** – Non-Newtonian, Multi-physics, and Free Surface Flows
  - Complex material response
  - Level sets for surface tracking
  - Flexible coupling schemes
- **Fire/Combustion** – Low Speed, Variable Density, Chemically Reacting Flows
  - Eddy dissipation and mixture fraction reaction models
  - RANS and LES based turbulence models
  - Unstructured Mesh
  - Pressurization models
Thermal/Fluids Code Consolidation

• User Benefits:
  – Tightly-coupled thermal/fluid capability in one code (instead of previous four)
    • “One” syntax
    • Potential for added robustness and faster convergence due to tight coupling
  – Faster response to user needs
    • Agile programming teams, simplified distribution

• Development Benefits:
  – Capabilities need not be duplicated
    • Though under one Framework, implementation details of adaptivity, error estimation, load balancing, solution control, etc., are duplicated in each code
  – Agile programming teams.
    • Previously: 1 or 2 developers per code
    • Now: core team contributing to all application areas
    • Core team is growing as more developers gain experience
  – Simplified distribution
    • Reduced inter-code dependence make releasing and shipping code easier
  – Increased collaboration between different groups
Code Consolidation Status
Thermal Capability

• Governing Equations
  – 3D unsteady, energy equation
  – Volumetric heat sources
    • Chemistry - heat of reaction
    • Arbitrary Q(x,t)
    • Arbitrary Q(T)
    • Q(ϕ), ϕ = solution field

• Solution Algorithm
  – 2nd order GFEM scheme
  – Weighted residual form
  – Integration by parts
  – Stabilization for advection
  – 1st order: Forward Euler/Backward Euler
  – 2nd order: Adams-Bashforth/Crank-Nicolson
  – Automatic time stepping

• Spatial Discretization
  – Isoparametric elements
  – Super-parametric elements

• Thermal Capabilities
  – Enclosure radiation
  – Banded wavelength enclosure radiation
  – Generalized contact
  – ChemEQ chemistry model (w/ activation & deactivation controls)
  – Local coordinate systems for anisotropic materials
  – Standard and gradient shells
  – Block toggling/skinning capabilities
  – Thermoelectric coupling
  – Bulk fluid element capability is nearly complete
  – Element death capability is underway (CDFEM approach)

• Boundary Conditions
  – Temperature, Specified Flux, Convective Flux, Radiative
  – Flux, code specified or from transfers
• **Governing Equations**
  - 2D/3D compressible RANS
  - Ideal gas and non-equilibrium chemistry

• **Solution Algorithm**
  - Fully-implicit, fully-coupled, stabilized finite element formulation (SUPG)
  - Linear Lagrange basis: second order
  - First and second order time integration
  - Fixed or auto time step size selection
  - H-adaptivity

• **Viscosity Models**
  - Sutherland’s viscosity law
  - Keyes’ viscosity law

• **Turbulence**
  - Spalart-Allmaras turbulence model
  - k-ω turbulence model
  - Menter’s k-ω turbulence model

• **Boundary conditions:**
  - Supersonic inflow
  - Supersonic outflow
  - Subsonic inflow (reservoir)
  - Subsonic outflow (pressure)
  - Slip/symmetry
  - No slip isothermal wall
  - No slip adiabatic wall
  - Blowing wall, Coupled aerothermal heating
Code Consolidation Status
Fire Capabilities

• **Solution Algorithm**
  – 2nd order CVFEM Scheme
  – Backward Euler and Steady solver; variety of predictors

• **Pressure Stabilization**
  – Second order and fourth order pressure stabilization
  – Time step and characteristic scaling

• **Coupling Strategy**
  – Fully-coupled scheme
  – Fully-segregated scheme

• **Property Evaluations**
  – Cantera along with standard Aria properties

• **Convection Operators**
  – Upwind, Geometric upwind and Central with automatic blending

• **Energy/Species**
  – Temperature form (heat conduction) and static Enthalpy
  – Arbitrary subindex-ed mass fraction (EDC combustion) and mixture fraction transport
  – Non-unity laminar transport with energy due to mass transport and correctional terms for appropriate behavior for $j_{jk}$

• **Turbulence**
  – LES Ksgs, TFNS, $k-\omega$ and $k-\varepsilon$
  – Iso-tropic eddy viscosity closure
  – Gradient diffusion closure for scalars ($h, Y_k, Z_k$)

• **Boundary Conditions**
  – Inflow, Open (dynP), Symmetry, Wall Function
New Capability Additions

- Investigation of unified FEM algorithms for extension to high speed compressible flows and fire applications
- Improved Thermal Contact and Enclosure Radiation
- Shallow Water Equations (flowing liquids)
- Aluminum propellant fire support (reacting, evaporating particles with participating media radiation and Eulerian gas phase coupling)
- Strained laminar flamelet model with heat loss due to radiation in combustion applications
- Finite rate chemistry and ablation for re-entry