SIERRA Thermal/Fluid/Aero Code Development Activities

Basil Hassan

**Computational Thermal and Fluid Mechanics Dept.
Engineering Sciences Center**

April 6, 2010

Sandia National Laboratories is a multi-program laboratory operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

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 $Q(T)$
 - $Q(\phi)$, 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

Code Consolidation Status

Aero Capability

- **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 $k-\epsilon$
 - 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