ACE014

2010 DOE Merit Review

LA-UR-10-01879

KIVA-4 Development

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Los Alamos National Laboratory
T-3 Fluid Dynamics and Solid Mechanics

Project ID # ace014_carrington_2010_o

Overview

Timeline

- 10/01/08
- 09/30/12
- Percent complete 30%

Budget

- Total project funding
  - $580 K
  - Contractor share 21% (actual $)
- Funding received in FY09 &FY10

Barriers

- Barriers addressed
  - All new Characteristic-based Split finite element algorithm with h-adpatation for sub, trans and supersonic flow.
    - Many FEM operators & multi-species
  - Development of software for in-situ Cut-cell grid generation software
    - Generalizing algorithm – better method

Partners

- Iowa State University
  - Dr. Song-Charng Kong PI
- Univesity of Nevada, Las Vegas,
  - Dr. Darrell W. Pepper PI
- University of Purdue, Calumet,
  - Dr. Xiuling Wang PI

Collaborations

- Partners
  - David Torres at Los Alamos National Lab: *collaborating on KIVA-4mpi, making KIVA-4 changes, developing Cut-Cell method.*
  - Song-Charng Kong at *Iowa State University: collaborating / developing Conjugate Heat Transfer (CHT) in KIVA-4.*
  - Darrell W. Pepper at University of Nevada, Las Vegas: *collaborating on Characteristic-Based Split (CBS) finite element method (FEM) algorithm development and benchmarking the developments.*
  - Xiuling Wang at Purdue University, Calumet: *collaborating on Characteristic-Based Split (CBS) finite element method (FEM) algorithm development and benchmarking the developments.*
- Technology Transfer
  - KIVA-4 with CHT model to LANL
  - *h*-adaptive CBS FEM solver to:
    - University of Nevada, Las Vegas
    - Purdue University, Calumet

Objectives

- Robust and Accurate Algorithms
  - Developing more robust and accurate algorithms for helping to understand better combustion processes in internal engines
    - This to provide a better mainstay tool for improving engine efficiencies and help in reducing undesirable combustion products.
- Newer and mathematically rigorous algorithms will allow KIVA to meet the needs of future and current combustion modelers and engine designs.
  - Developing the Characteristic-Based Split *hp*-adaptive finite element method for combustion modeling and implement for internal combustion engines – KIVA-4 like engine grids.
- Verification and Validation (**V&V**) of KIVA-4mpi
  - Released to users LANL license # (LA-CC-09-0103) in Beta.
  - Users help to provide valuable information about performance.

Objectives

- Conjugate Heat Transfer
  - More accurate prediction in wall-film and its effects on combustion and emissions under PCCI conditions with strong wall impingement.
- Cut-Cell grid implementation
  - To allow for easier and quicker grid generation.
- KIVA-4 Support for LLNL HCCI simulation (completed)
  - Modeling of Piston crevice to ring gap was causing difficulty with solution
    - Modeling the crevice helps to understand the physical processes and amounts of residual components in the crevice.
- Grid interface (completed)
  - Increase the accessibility of KIVA-4 by allowing use of grids generated by the Cubit software.

Milestones for FY - 10

10/09 - 2D and 3D Characteristic-based Split Finite Element Algorithm Developed. (Carrington, 2009)

- Cubit (Exodus II) grid extraction and output for KIVA-4, running in KIVA-4.

- Piston crevice simulations running in KIVA-4 and KIVA-4mpi.

11/09 - *h*-adaptive grid technique/algorithm implement in CBS-FEM method for 2D

12/09 - *h*-adaptive grid technique/algorithm implement in CBS-FEM method for 3D

- Maintenance (refactor&debugging) KIVA-4 and development of KIVA-4mpi

- KIVA-4mpi beta version released with LANL license LA-CC-09-0103

01/09- PCG solver package implemented in CBS-FEM method (Carrington 2008).

- New Makefile System.

- Preconditioning methods implemented (Carrington, 2008).

- New algorithm sent to contracted partners, UNLV and Purdue.

03/10 - Multi-Species Transport implemented in CBS-FEM algorithm

- Simpler algorithm and logic for determining intersections of facets with overlaying grid.

- New algorithm for Cut-Cell grid generation being developed – more robust.

Approach – General Guidelines

- Computational Physics & Engineering generally requires the following:
  - Understanding of the physical processes to be modeled and the assumptions inherent in any particular model.
  - The ability of the chosen method, the mathematical formulation, and its discretization to model the physical system to within a desired accuracy.
  - The ability of the models to meet and or adjust to users' requirements.
  - The ability of the discretization to meet and or adjust to the changing needs of the users.
  - Validation and Verification (V&V) – meeting requirements and data.
  - Also, a critical component of effective modeling is related to employing good software engineering practices.
  - **We are using the above general approaches in our efforts to meet the objectives and provide a robust numerical platform/solver for internal combustion engine modeling.**

FY-10 Technical Accomplishments

- **Progress and Results**
  - *hp*-adaptive CBS FE method.
    - CBS FEM method developed for both 2d and 3d.
    - *h*-adaptive grid developed and working in both 2d and 3d.
    - *Multi-species* transport implemented in both 2d and 3d.
    - **V&V** and algorithm adjustment – started in January.
    - *hp*-adaptive with hierarchical basis function ongoing – started in February.
  - KIVA-4mpi
    - Parallel version of KIVA-4 released as a Beta
  - Cut-cell technique for grid generation
    - Changing algorithm to more general form applicable to general complex domains.
  - HCCI support for KIVA-4 modeling - Completed
    - Modeling of Piston crevice to ring gap was causing difficulty with solution. Modeling the crevice helps to understand the physical processes and amounts of residual components in the crevice.

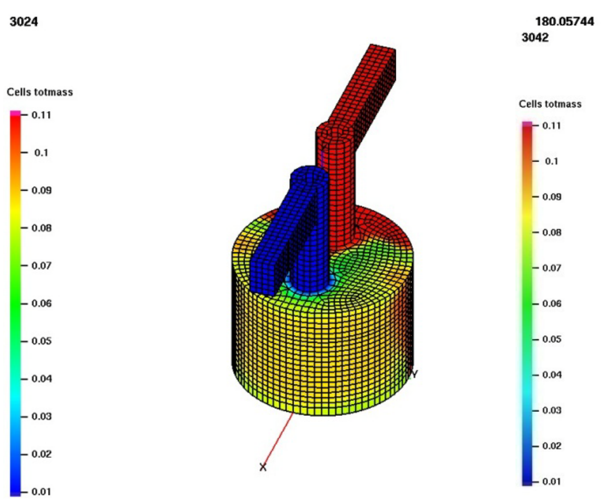
FY-10 Technical Accomplishments –
Iowa State University

- **Progress and Results**
  - Conjugate heat transfer
    - Extended KIVA-4 capability to predict heat conduction in solids, that is, the combustion chamber, cylinder, valves, head, and piston, FY09.
    - Using KIVA-4 to perform simultaneous simulation of in-cylinder processes and heat conduction in mechanical components.
    - Predicted combustion chamber wall temperature distributions – piston & cylinder (started January 2010).
    - Time-dependent in-cylinder surface temperatures affects wall film and near wall combustion. Implications on combustion and emissions are being investigated.
      - More accurate prediction in wall film and its effects on combustion and emissions under PCCI conditions with strong wall impingement.

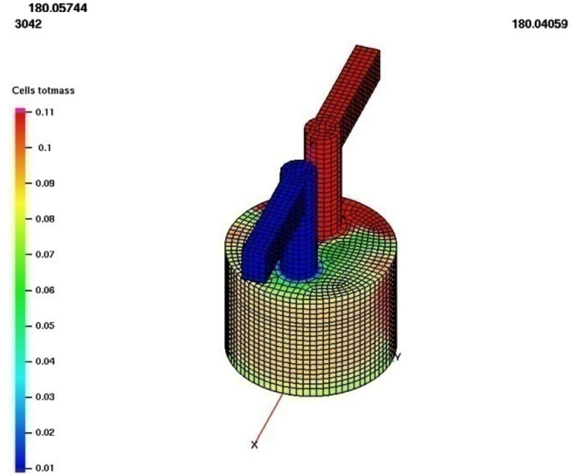
FY-10 Technical Accomplishments

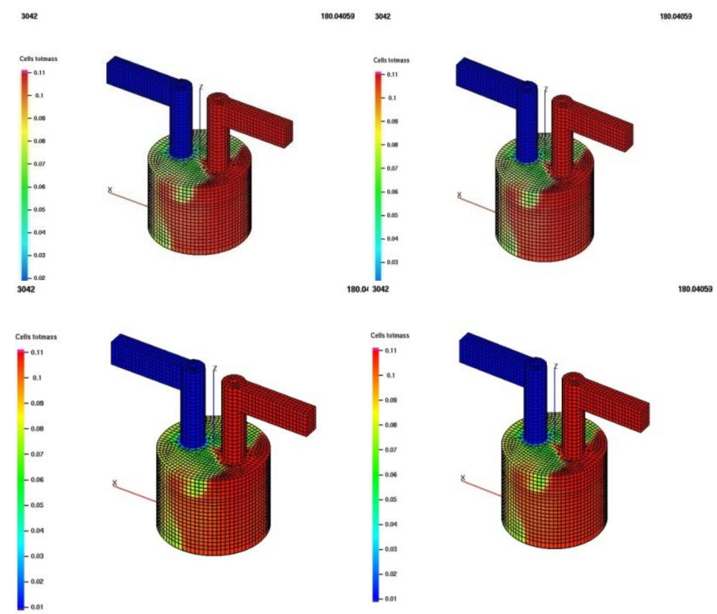
- Release KIVA-4mpi – LA-CC-09-0103
  - With **various test cases** – a beta release.
  - Demonstrating parallel solution on par with serial.
    - Vertical Valve Engine
      - view graph norm and **output differencing**

▪KIVA-4 Serial



▪KIVA-4 MPI

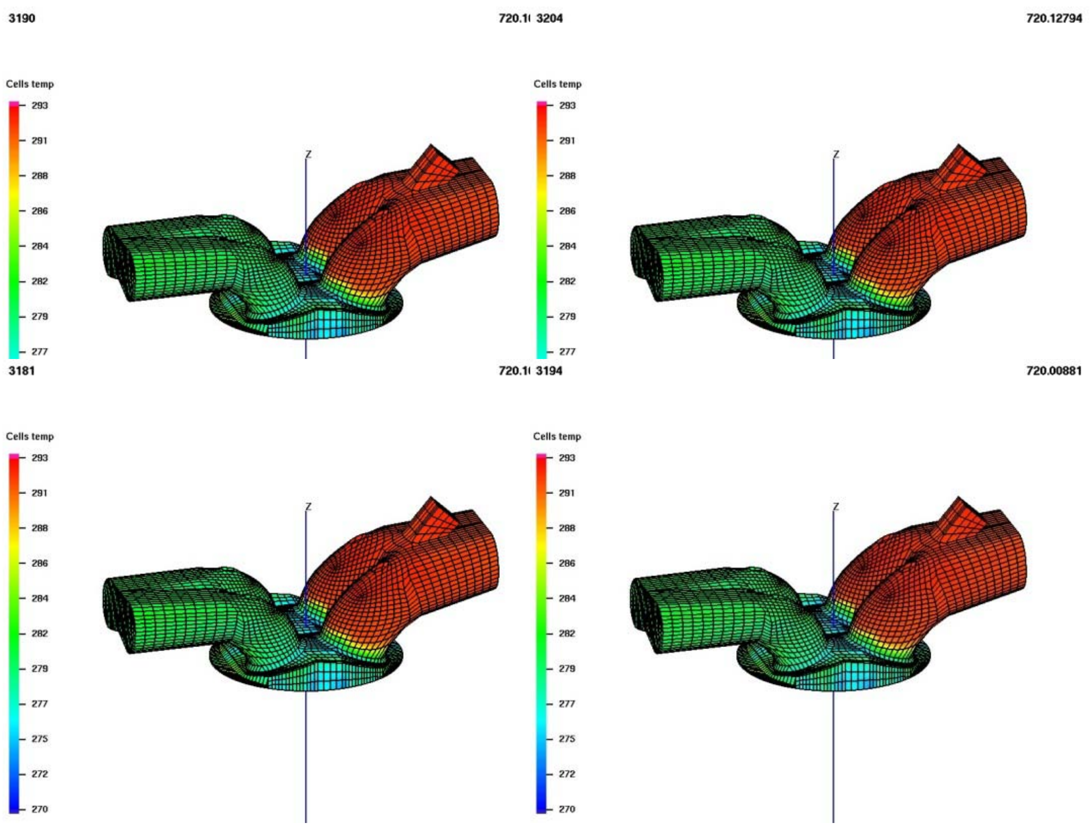




PEs
2 4
8 16

FY-10 Technical Accomplishments

- Release KIVA-4mpi – LA-CC-09-0103
  - With various test cases – a alpha/beta release
    - **V&V -** Demonstrating parallel solution on par with serial.

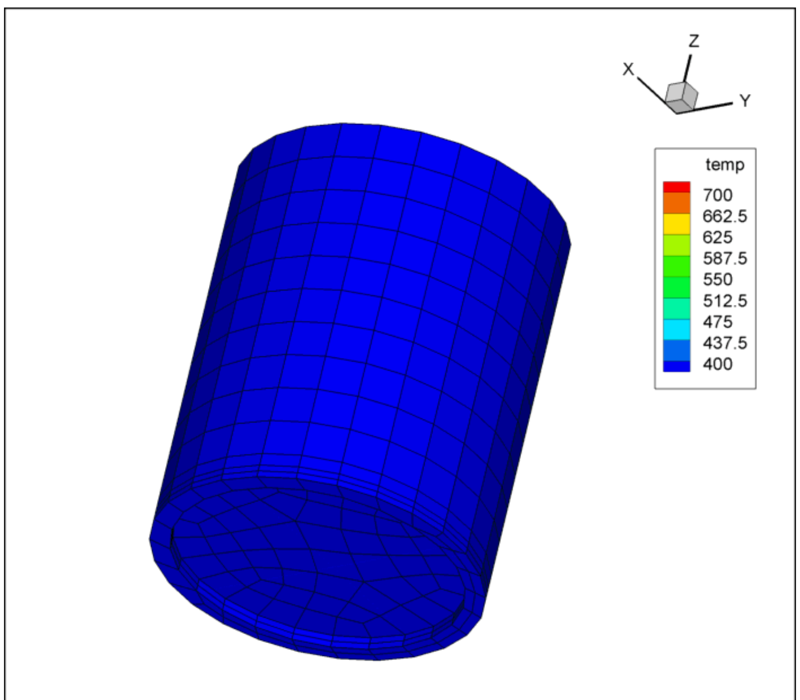


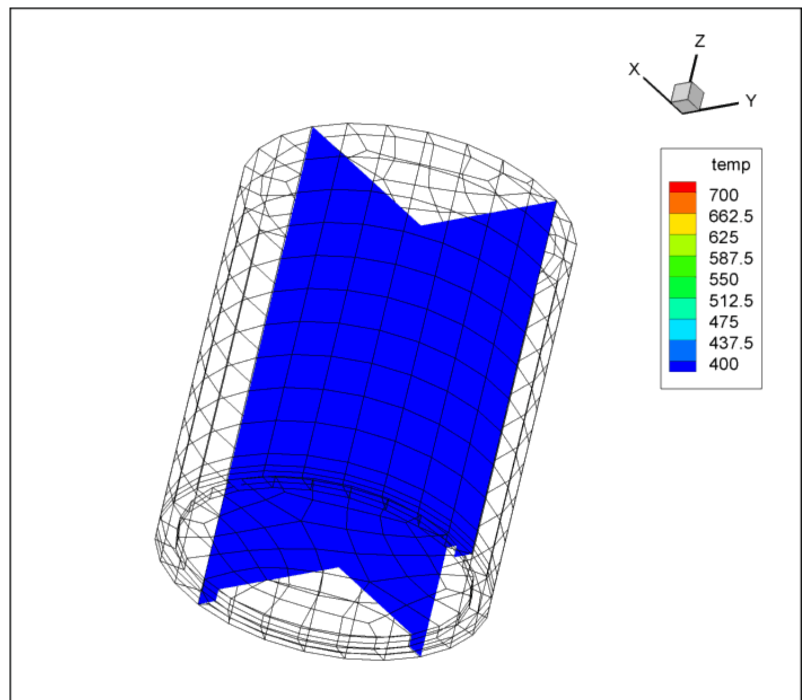
PEs

2 4
8 16

FY-10 Technical Accomplishments

- Cubit Grid
  - Simple 3-d Piston with large Ring Crevice
  - Demonstrating Cubit compatibility
    - Use in code development for unstructured grids with piston crevices and parallel implementation.
  - 4 PE solution showing Isotherms

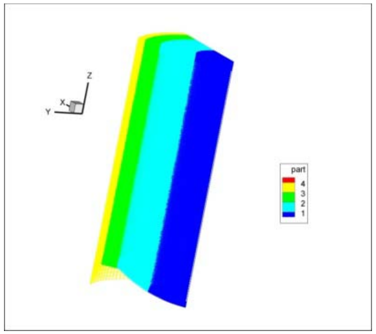




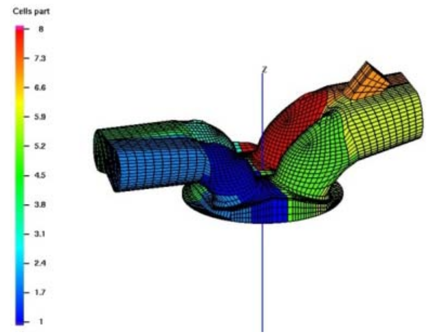
FY-10 Technical Accomplishments

- HCCI and 4-Valve Solution on Multiple Processors

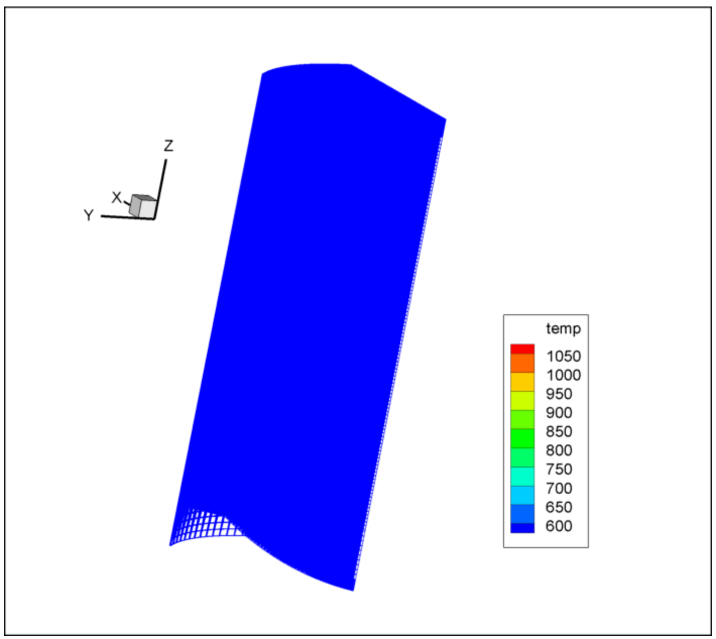
Domain decomposition in colors

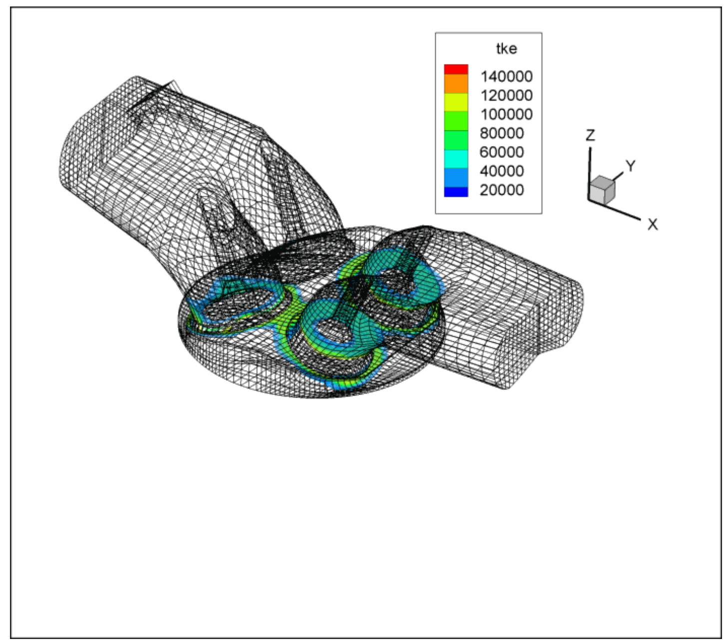


HCCI experimental engine
4 PEs



4 slanted valve
Pentroof engine
8 PEs





FY-10 Technical Accomplishments

- Developing *hp*-adaptive CBS FEM
  - Discretization for KIVA Reactive Flow Turbulence Modeling
  - 2-D and 3-D CBS *h*-adaptive FEM codes are **Developed**
    - Equal-order – same basis for pressure and momentum.
    - Petrov-Galerkin Stabilization (SUPG)
      - 3rd order accuracy, numerical dispersion precisely measured and removed prior to solution advancement.
    - 1 pressure solve per time step.
    - *h*-adaptive with Residual error & Gradient control.
    - *k-ω* turbulence model
      - (k-ε has also been developed in FEM – Wang, Carrington, Pepper (2009)).
    - New wall function system for both 2D and 3D.
    - PCG Solver & in-situ stationary preconditioning (SSOR, BJ, 2-level (Carrington, 2008).
    - New MAKE system.
    - Stochastic particle model - now porting KIVA-4 model to FEM method.

FY-10 Technical Accomplishments

- The *hp*-adaptive CBS FEM Discretization FEM:
  - **Spatially accurate**, to any degree required.
  - **Conservative** both method via Petrov-Galerkin (P-G) stabilizing.
  - **Pressure is C_o continuous** - not piecewise constant.
  - **Resolution when and where required!**
  - Easy to understand FEM coding.
  - **Hooks to models nearly the same**
    - We supply models which can be changed or enhanced to help further development. Gladly offering assistance in enhancements as requested.
  - More **computational tractable** injection/particle transport.
  - **Variable density boundary** layer – **compressible** boundary layer.
- The *hp*-FEM removes from current FVM discretization at each time step:
  - Virtual volume, flux creations for each element
  - Need for 6 of neighboring cell data and normal vectors.
  - Pressure iterations.
  - Cumbersome stencils associated with 2^{nd} or 3^{rd} order combined h-adaptive grid.

FY-10 Technical Accomplishments

- Discretization for CBS h-adaptive FEM
  - Derived from Taylor Expansion to produces the Characteristic-Based Split (see Zienkiewicz, et al.)
  - The weighted residual matrix equations are as follows (each dependent variable is approximated with shape functions:
    - Momentum, the split is solved for $\left\{\Delta \mathbf{V}_i^*\right\} = \left\{\mathbf{V}_i^*\right\} - \left\{\mathbf{V}_i^n\right\}$

$$\left\{\Delta \mathbf{V}_i^*\right\} = -\Delta t\left[\mathbf{M}_v^{-1}\right]\left[\ [\mathbf{A}_u]\{\mathbf{V}_i\} + [\mathbf{K}_\tau]\{\mathbf{V}_i\} - \left\{\mathbf{F}_{v_i}\right\} - \frac{\Delta t}{2}\left([\mathbf{K}_{char}]\{\mathbf{V}_i\} - \left\{\mathbf{F}_{char_i}\right\}\right)\right]^n$$

    - Change in Pressure or Density is then solved (derived from continuity)

$$\Delta \rho_i = \left(\frac{1}{c^2}\right)^n \Delta p_i = -\left[\mathbf{M}_\rho^{-1}\right]\Delta t\left((1-\theta_1)\frac{\partial U^n}{\partial x} + \theta_1\frac{\partial U^*}{\partial x} - \Delta t\theta_1\left(\frac{\partial^2 p^n}{\partial x \partial x} + \theta_2\frac{\partial^2 \Delta p}{\partial x \partial x}\right)\right)$$

    - Which is when formed into a weak or variational statement via Green's Theorem produces (with boundary integral)

$$\left(\left[\mathbf{M}_p\right] + \Delta t^2\theta_1\theta_2\mathbf{H}\right)\{\Delta p_i\} = \Delta t\left[\ \left\{\mathbf{V}_i^n\right\} + \theta_1[\mathbf{G}]\left\{\Delta \mathbf{V}_i^*\right\} - \Delta t\,\theta_1[\mathbf{H}]\left\{p_i^n\right\} - \left\{\mathbf{F}_{P_i}\right\}\right]$$

$$\mathrm{p}^{\mathrm{n+1}} = \mathrm{p}^{\mathrm{n}} + \Delta \mathrm{p} \qquad \rho^{\mathrm{n+1}} = \rho^{\mathrm{n}} + \Delta\rho$$

FY-10 Technical Accomplishments

- from nth to n+1 level is the Velocity corrector $\Delta \mathrm{V} = \mathrm{V}^{n+1} - \mathrm{V}^{n} \quad \Delta V^{*} = V^{*} - V^{n}$ with

$$\{\Delta \mathbf{V}_i\} = -\Delta t \left[\mathbf{M}_v^{-1}\right]\left[[\mathbf{G}]\left(\{p_i^{\,n}\} + \theta_2 \{\Delta p_i\}\right) - \frac{\Delta t}{2}\mathbf{P}\{p_i^{\,n}\}\right]$$

  - Producing time-advanced velocity $\mathrm{V}^{n+1} = \Delta \mathrm{V} + \Delta \mathrm{V}^{*} + \mathrm{V}^{n}$

- Energy (internal)

$$\Delta E_{\mathbf{i}} = -\Delta t\left[\mathbf{M}_e^{\mathbf{-1}}\right]\begin{bmatrix} [\mathbf{A}_e]\{\mathbf{E}_{\mathbf{i}}\} + [\mathbf{C}_P]\{p_{\mathbf{i}}\} + [\mathbf{K}_{\mathbf{T}}]\{\mathbf{T}_{\mathbf{i}}\} + \{\mathbf{F}_{e_{\mathbf{i}}}\} - \\ \Delta t\left([\mathbf{K}_{uE}]\{\mathbf{E}_{\mathbf{i}}\} + [\mathbf{K}_{up}]\{p_{\mathbf{i}}\} + \{\mathbf{F}_{es_i}\}\right) \end{bmatrix}^{n}$$

- Turbulence Closure – *k-ω*

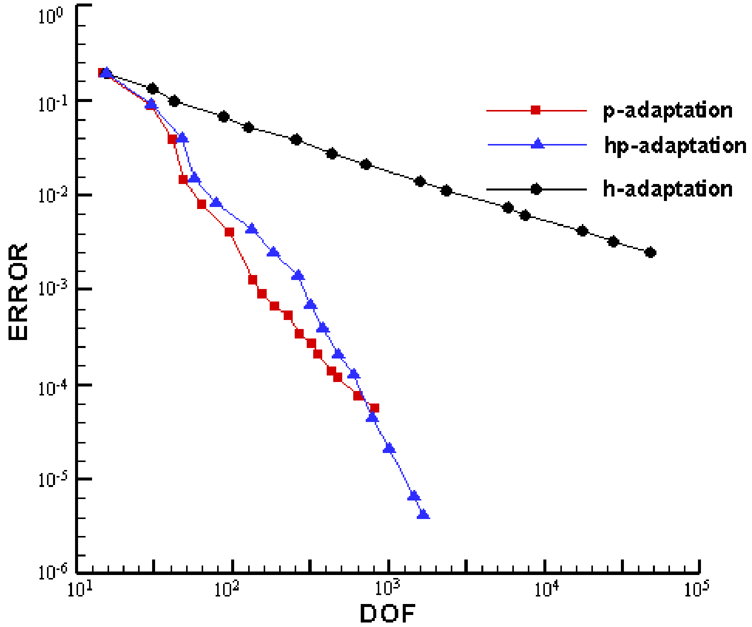
$$\Delta k_{\mathbf{i}} = +\Delta \mathbf{t}\left[\mathbf{M}^{\mathbf{-1}}\right]\begin{bmatrix} \{\mathbf{F}_k\} + \{\mathbf{P}_k\} + \{\beta^{*}\mathbf{k}\,\mathbf{w}\} - \\ [\mathbf{K}_k]\{k\} - [\mathbf{A}_v]\{k\} \end{bmatrix}^{n} \quad \Delta \boldsymbol{\omega}_{\mathbf{i}} = -\Delta \mathbf{t}\left[\mathbf{M}^{\mathbf{-1}}\right]\begin{bmatrix} \{\mathbf{F}_{\varpi}\} + \{\alpha\, \mathbf{k}/\boldsymbol{\omega}\}\{\mathbf{P}_k\} + \{\beta\,\mathbf{w}^2\} - \\ [\mathbf{K}_{\varpi}]\{\omega\} - [\mathbf{A}_v]\{\varpi\} \end{bmatrix}^{n}$$

FY-10 Technical Accomplishments

- Why hp-adaptive method
  - The use of *h*-adaptation can yield accurate solutions and rapid convergence rates.
  - Exponential convergence when higher-order, hp-adaptation
  - Error bounded by the following well known relation

$$\left\| u - u_h \right\|_m \leq c h^{k+1-m} \left\| u \right\|_r$$

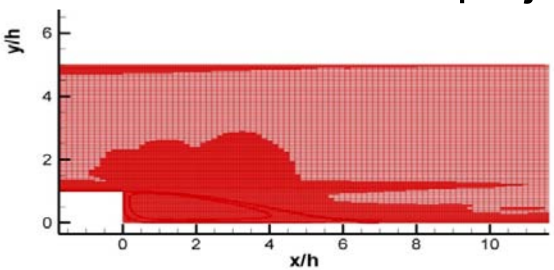
'*u*' is assumed smooth in an H^{k+1} Sobolev norm, *m* is norm space, *r=k+1*, degree of integrable derivates in *H.*

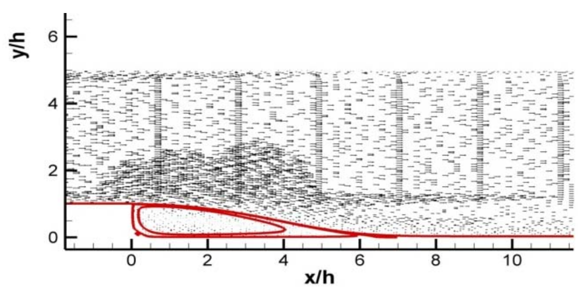


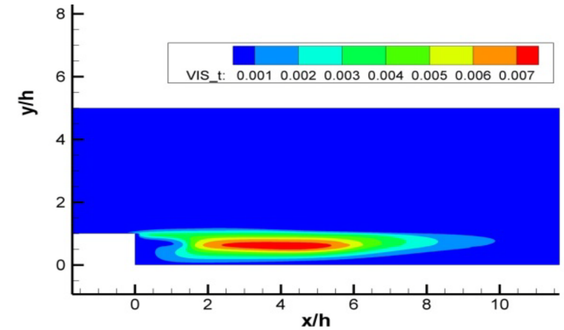
Convergence of *hp* about same as *p*. Speed of solution is better for *hp,* since the higher-order polynomials are used judiciously.

FY-10 Technical Accomplishments

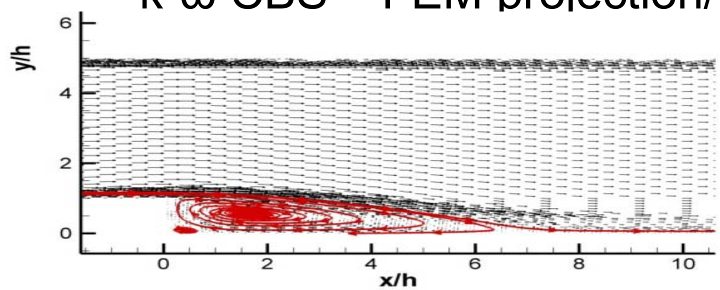
- **Unsteady Turbulence Modeling:** k-w closure and h-adaptive unstructured grid is error driven, not just for boundary layer (can be y+ constrained for wall function).
  - k-ω (FEMFP 2007 and ICESS/CMES ’10) & k-ε (CTS ’09) for benchmark problem. Re=28,000, inflow is 17m/s (Mach number ~0.05) matches data. This is around the lower velocity in a typical internal combustion engine.
  - k-ω FEM projection/fractional step model

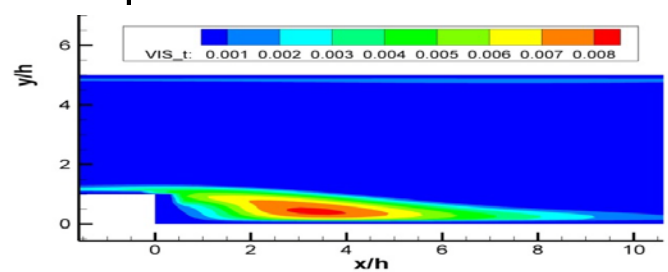






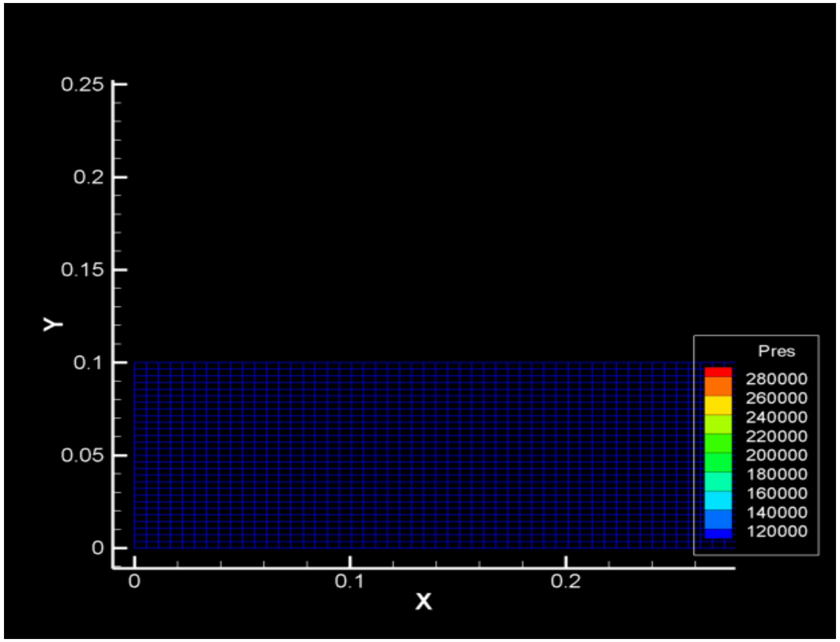
  - k-ω CBS – FEM projection/fraction step

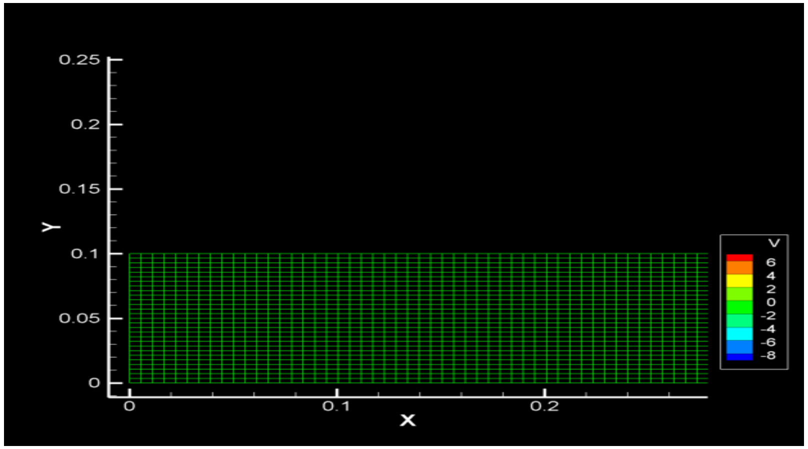


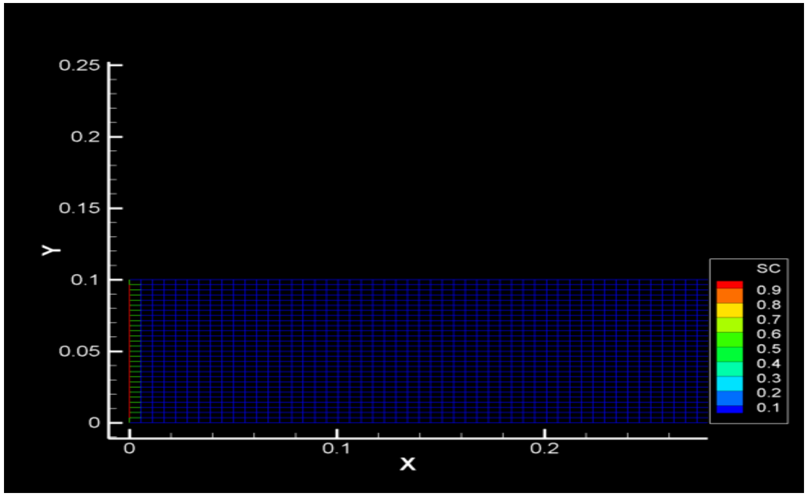


FY-10 Technical Accomplishments

- **2-D Unsteady Turbulence Modeling**
  - Characteristic-Based Split – FEM
  - Two-equation *k-ω* closure and *h*-adaptive unstructured grid





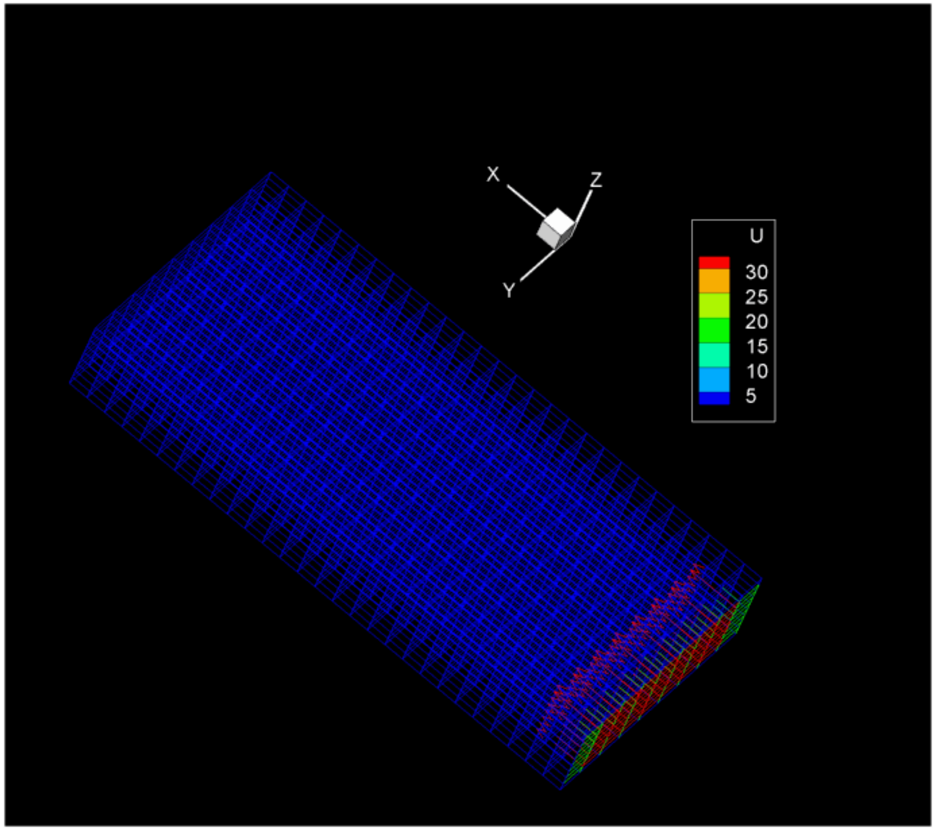


Subsonic Compressible Flow
Mach = 0.5

FY-10 Technical Accomplishments

- **3-D Unsteady Turbulence Modeling**
  - h-adaptive *k-ω* Characteristic-Based Split
  - Two-equation k-w closure and h-adaptive unstructured grid

Incompressible Flow
Mach = 0.1

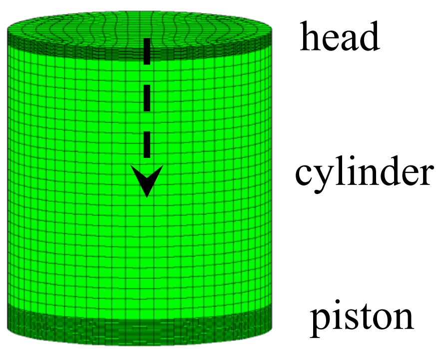


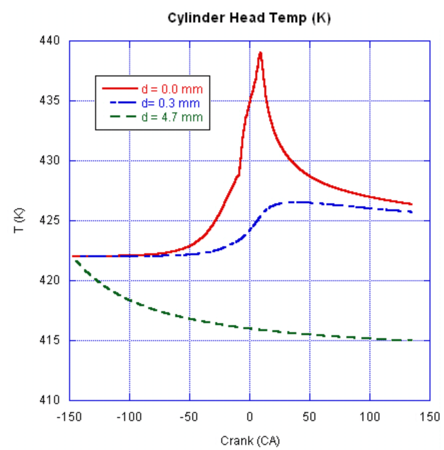
FY-10 Technical Accomplishments

- Conjugate Heat Transfer (CHT)
  - Motivation
    - Extend KIVA-4 capability to predict heat conduction in solids.
    - Use KIVA-4 to perform simultaneous simulation of in-cylinder processes and heat conduction in mechanical components.
  - Expected outcome
    - Prediction of combustion chamber wall temperature distribution.
    - More accurate prediction of wall film and its effects on combustion and emissions under PCCI conditions with strong wall impingement.
  - Approach
    - Modify KIVA-4 for heat conduction calculation in solid.
    - Extend the computational domain to include both fluid and solid domains.
    - Perform integrated thermo-fluids modeling in one simulation using the same code.
    - Applicable energy equation is solved for temperature distribution in solids

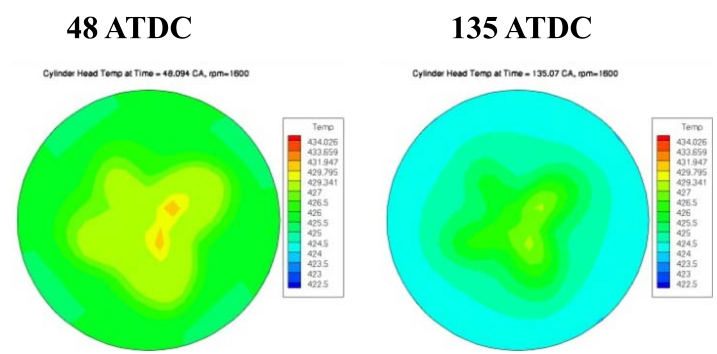
FY-10 Technical Accomplishments

- CHT & Diesel spray combustion (SOI= –9 ATDC)

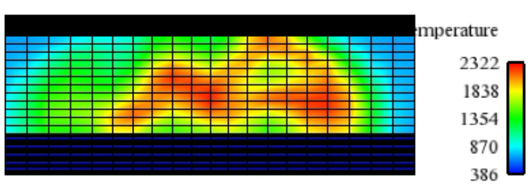


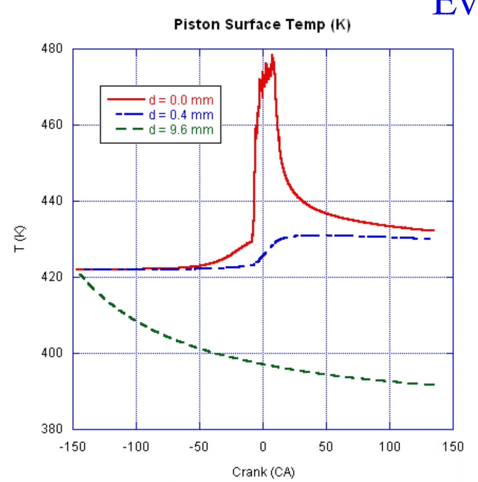


Evolution of the head T at different depths

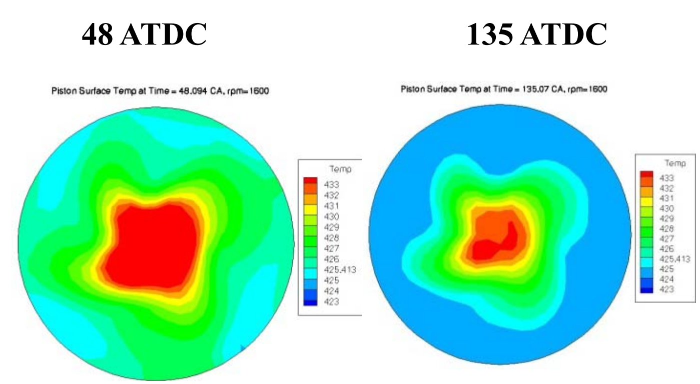


In-cyl T @ 48 ATDC



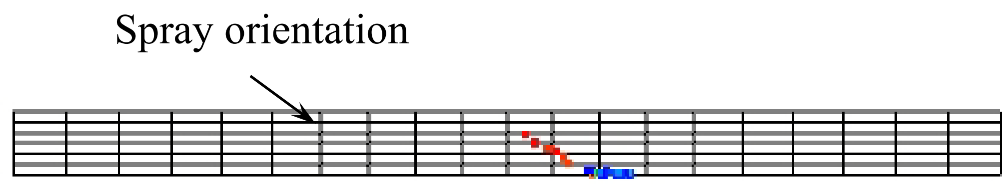


Evolution of the piston T at different depths

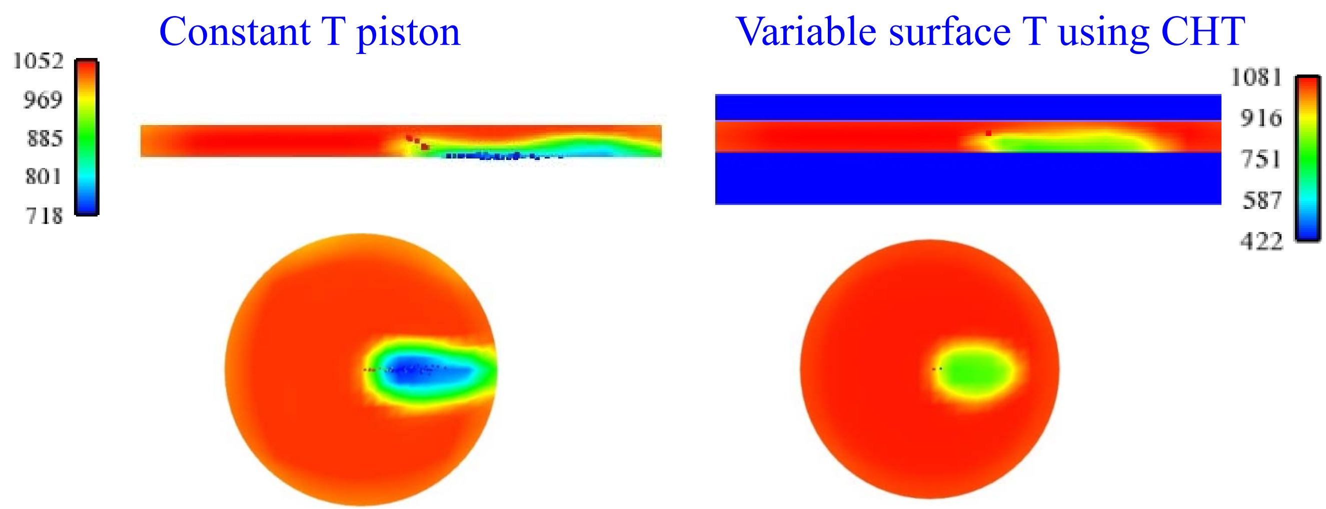


FY-10 Technical Accomplishments

- CHT and Effects on the spray/wall interaction, wall film, and near-wall combustion



<u>Gas</u> temperature contour with spray drops @ –2 ATDC



Conjugate H.T. modeling affects wall film and near wall combustion; Implications on combustion and emissions to be investigated.

FY-10 Technical Accomplishments

- Cut Cell Strategy
  - 3D grid can be formed in hours
    - In contrast to days for complex geometries.
    - CAD Surface is described by a stereo lithographic (STL) format
      - Format tessellates the surface of the geometry with a triangles.
      - Vertices and the normal of each triangle are provided.
    - The boundary cells are cut by the surface.
  - Begin with an orthogonal Cartesian grid.
  - The surface stereolithographic (STL) file is used to cut the Cartesian grid.
    - Interior cells are left intact.
    - The boundary cells are cut by the surface.
    - The resultant boundary cells can have many facets (polyhedral) which are converted to KIVA type elements (tet, prism, hex).

FY-10 Technical Accomplishments

- Creation of the cut-cells
  - Uses the divergence theorem to compute volumes

$$V_{cell} = \int_V \frac{1}{3} \nabla \bullet \vec{x}\, dV = \frac{1}{3} \int_S \vec{x} \cdot \hat{n}\, dS = \frac{1}{3} \sum_{faces} (\vec{x}_{cen})_{face} \cdot \hat{n}_{face} A_{face}$$

  - Area of faces that are fluid are computed using Stokes theorem.

$$A_{face} = \int_s (\nabla \times \vec{F}) \cdot \hat{n}\, dS = \int_L \vec{F} \cdot d\vec{R}$$

  - Chose F such that n is the unit normal of the face (e.g. n = i,-i,j,-j,k,-k).

$$\nabla \times \vec{F} = \hat{n}$$

    - Then the line integral is easier to compute.
    - The need to account for the many different permutations which arise when a solid surfaces intersect a face is mitigated.

Continuing Work for FY 10

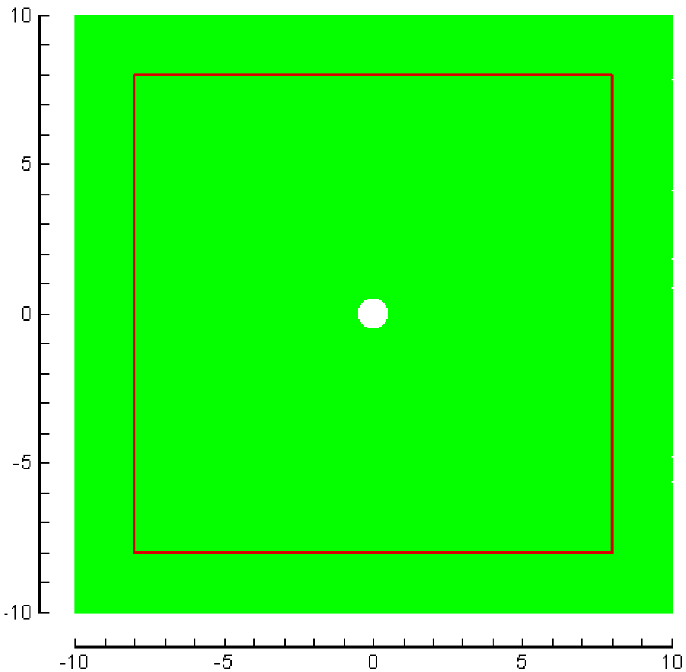
- *hp*-adaptive grid CBS-FEM
  - Packages/Models to Implement
    - Injection Spray Model
    - Chemical Kinetics
  - Algorithm Testing, adjustments for combustion modeling , and **V&V**
  - *p*-adaptive method married to existing *h*-adaptive method to form *hp*-adaptive method
    - Hierarchical basis functions
- KIVA-4mpi – more **V&V** and some more code refactoring.
- Cut-cell grid generation method.
  - Reformulating and simplifying the algorithm.
  - Benchmarks solutions on simple geometries.
- CHT transfer to/from combustion chamber.

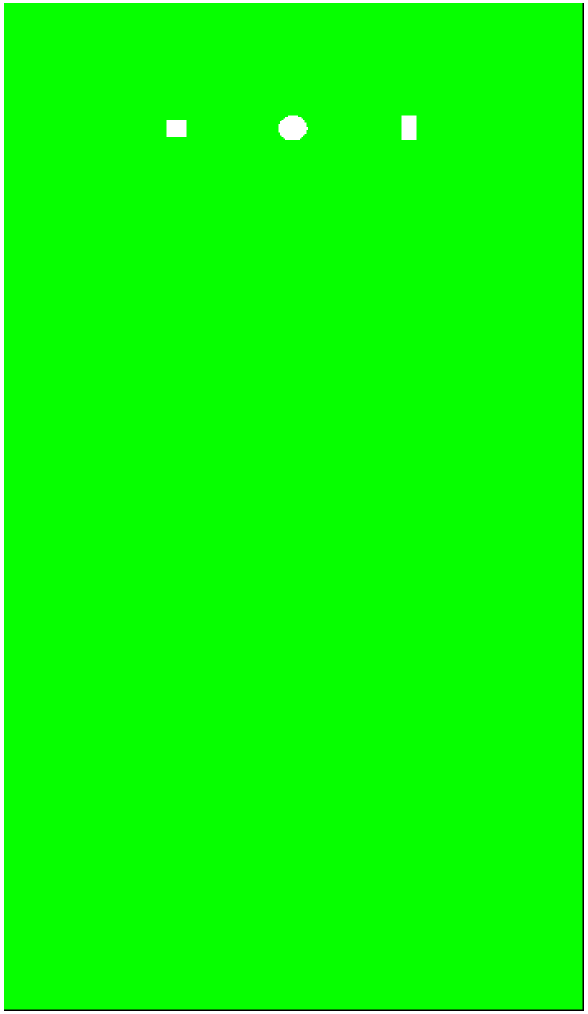
Future work for FY 2011

- **Continue Implementing the Characteristic-Based Split (CBS) FEM:**
  - General **V&V** and for Multi-species in the CBS-FEM.
    - Altering method as needed - Petrov-Galerkin upwinding conservative form.
  - To include both grid and polynomial adaptive methods with hierarchical basis
    - *hp*-FEM -- Is well founded in mathematics of functional analysis and allows for determination of the discretization error.
    - Investigate Arbitrary Eulerian-Lagrangian (ALE) implementations.
    - Mixed elements of: tetrahedral, hexahedral & prisms.
    - Allows minimizing discretization errors to any desired level of accuracy.
  - Use of the following existing methods and constructions in KIVA-4:
    - Chemistry and Injection models.
    - Unstructured format including movement of piston (snappers) and values
    - MPI parallel constructions
    - Support for existing and new models – easy hooks into the discretization
    - I/0, etc…
- **Perfecting the Cut-Cell Grid Generation method**
  - New algorithm implementation and testing on actual STL files of an engine.
- **Develop Immersed and Moving Body Algorithms**
  - Removal of mesh problems associated with valve movements (tangling/skewing) even on fine resolutions.

Future work for FY 2011

- Immersed/Moving Body Algorithm
  - Working to improve the current algorithms
    - Increase robustness - generic method.
    - Needed for simulations with
      higher resolution.





Movies of immersed moving objects from Juan Heinrich (University of New Mexico).

Summary

- **More Accurate and Robust algorithms for FY10 and beyond**
  - Developing and implementing more robust and extremely accurate algorithms in KIVA-4 architecture – CBS *hp-adaptive* FEM. Reducing model's physical assumptions.
- **KIVA-4mpi**
  - Beta release providing faster turnaround – LANL license #LA-CC-09-0103.
- **Conjugate Heat Transfer**
  - More accurate prediction in wall film and its effects on combustion and emissions under PCCI conditions with strong wall impingement.
- **Cut-Cell grid Generation and Implementation**
  - Quickly generate grids from CAD surfaces of complex domains. New algorithm being developed, more generic.
- **KIVA-4 Support for LLNL HCCI simulation**
  - Supported KIVA-4 solver for grids using piston ring crevices.
- **Cubit Grid interface**
  - Increased flexibility of KIVA-4 with use of more grid generators.