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Merit Review
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KIVA Modeling to Support Diesel Combustion Research

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Project ID #
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Overview

Timeline

- 10/01/08
- 09/30/10
- Percent complete 40%

Budget

- Total project funding
  - $325 K
  - Contractor share 12%
- Funding received in FY08 and FY09

Barriers

- Barriers addressed
  - Development of software from in-situ Cut-cell grid generation software
    - From reading and interpretation of stereolithographic CAD surface to 3d grid
    - Generalizing KIVA to accommodate cut-cell grids – discretization changes

Partners

- Iowa State University
- Dr. Song-Charng Kong is the PI

Objectives

- **Cut-Cell grid implementation**
  - To allow for easier and quicker grid generation.
  - To develop grids for simulations that are mostly Cartesian.
- **KIVA-4 Support for LLNL HCCI simulation**
  - **Modeling of piston crevice to ring gap was causing difficulty with solution**
    - Partially or unburned fuel in the piston-ring crevice results in higher levels of pollutants.
    - Modeling the crevice helps to understand the physical processes and amounts of residual components in the crevice.
- **Cubit Grid interface**
  - Increase the accessibility of KIVA-4 by allowing use of grids generated by the Cubit software

Objectives

- **Developmental R&D engineering – groundwork**
  - Newer and mathematically rigorous algorithms will allow KIVA to meet the needs of future and current combustion modelers.
  - Study how to effectively and efficiently bring to bear our research in h-p adaptive finite element methods.
- **Wall-Film Wetting**
  - More realistic modeling of wetted surfaces for better modeling of evaporation at wetted surfaces.
- **Conjugate Heat Transfer**
  - Extend KIVA-4 capability to predict heat conduction in solids, that is, the combustion chamber.
  - More accurate prediction of wall-film and its effects on combustion and emissions under PCCI conditions with strong wall impingement.

Milestones for FY - 09

11/08

- **Concept of using extra side(s) in divergence calculation.**

12/08

- **Concept of adjusting nodal locations to create gradients in geometric coefficient type discretization representation for seamless integration into the KIVA-4 code.**

01/09

- **Representative geometries using cut-cell at various levels of resolution.**

02/09

- **Cubit (Exodus II) grid extraction and output for KIVA-4**
- **HCCI grid construction recommendation**
  - **Work with LLNL to experiment with various grid resolutions.**

Approach - General

- Computational Physics & Engineering
  - Generally requires the following:
    - Understanding of the physical processes to be modeled.
    - 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.
    - Also, a critical component of effective modeling is related to employing good software engineering practices. This reduces costs associated with production, support, and increases overall flexibility of the software.

Technical Accomplishments FY-08

- Implemented parallel KIVA-4 LES capability.
- Implemented KIVA-4 multi-zone capability in collaboration with Lawrence Livermore.
- Iowa State has tested KIVA-4's UW-ERC models against experimental results (using LANL's initial implementation of UW-ERC models into KIVA-4).
- Simulated spray using overset method in KIVA-4.

FY-09 Technical Accomplishments

- **Progress and Results**
  - Cut-cell technique for grid generation
    - Simple geometric shape representative of parts in an internal combustion engine.
    - Various levels of grid resolution.
  - HCCI support for KIVA-4 modeling
    - Grid recommendations for LLNL HCCI engine simulation.
  - Cubit grid (Exodus II format) output to KIVA-4
    - Use of extensive C++ constructions to extract grid structure from Exodus format and make compatible with KIVA-4 input requirements.
  - Developmental R&D engineering – groundwork
    - Engineering for a change in the discretization in KIVA-4.
    - Planning/engineering the path forward to change discretization to an h-p adaptive finite element method.

FY-09 Technical Accomplishments – Iowa State University

- **Progress and Results**
  - Wall-film model -- an improved wetting mechanism
    - Implement wetted surface model, a new smoothing model for KIVA-4.
    - More realistic modeling of wetted surfaces for better modeling of evaporation at wetted surfaces.
  - Conjugate heat transfer
    - Extend KIVA-4 capability to predict heat conduction in solids, that is, the combustion chamber.
    - Use KIVA-4 to perform simultaneous simulation of in-cylinder processes and heat conduction in mechanical components.
    - Prediction of combustion chamber wall temperature distribution.
    - More accurate prediction in wall film and its effects on combustion and emissions under PCCI conditions with strong wall impingement.

Cut-Cell Technique

- 3D grid can be formed in hours
  - In contrast to days for complex geometries.
  - CAD Surface is described by a stereolithographic (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. The resultant boundary cells can have many facets (polyhedral).

Cut Cell Strategy

- 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).

Accuracy Issues

- The cut cell technique constructs an orthogonal grid in the interior.
- The orthogonal grid allows the Navier-Stokes equations to be solved which much greater accuracy in the region given the current equation discretization.
- The boundary cells of a cut-mesh can generate less accurate solutions than grids constructed to initially conform to the boundaries of the geometry.

Phases I and II

- Phase I: Implement software to cut a Cartesian grid. The software will determine the areas of faces and volumes of all cells (interior and boundary).

- Phase II: Make the appropriate modifications to collocated KIVA-4 code to accommodate a cut cell mesh.

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.

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

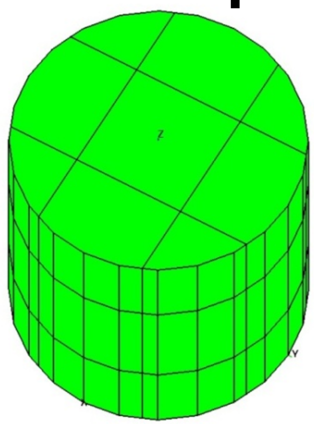
- Chose F such that n is the unit normal of the face (e.g. n = i,-i,j,-j,k,-k).

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

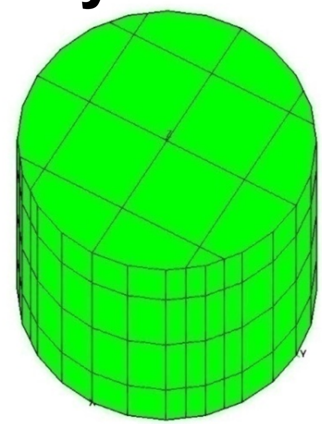
  - Then the line integral is easier to compute.
  - The need to account for the many different permutations which arise when a solid surfaces intersect a face is mitigated.

Cut-cells grids on a cylinder

Various grid sectioning levels for resolving piston cylinder geometry.



1st level



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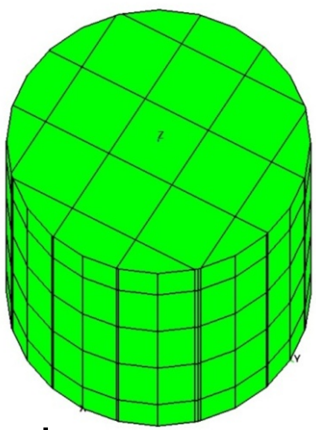

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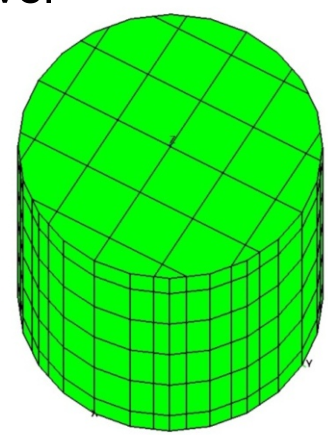


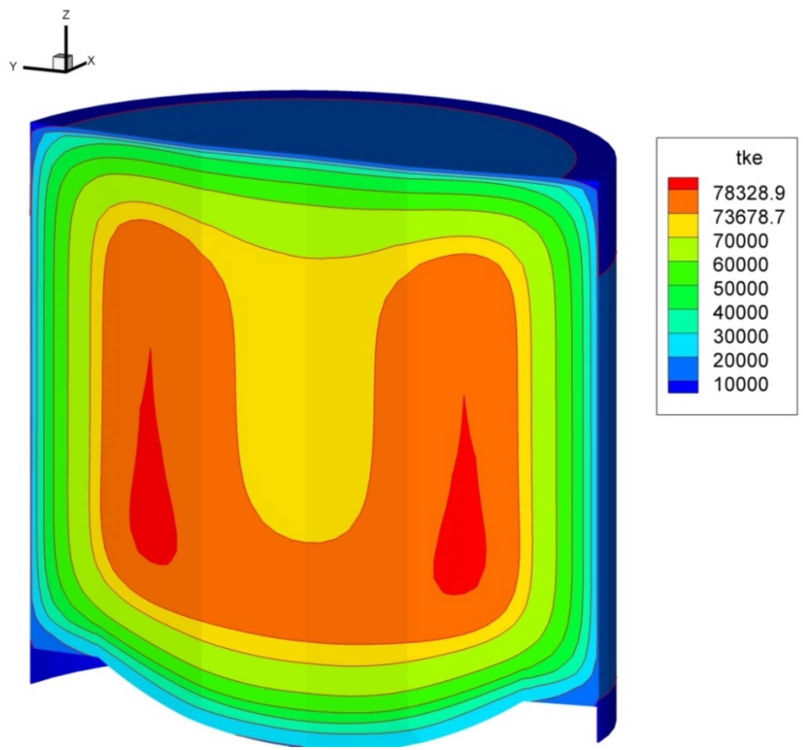
4th level

HCCI Model with Piston Crevice

- Kiva-4 Support
  - Piston-ring crevice modeling causing solution failure in KIVA-4 for LLNL grids.
    - Considered various grids and determined problems in collaboration with Tom Piggot at LLNL.
  - Tested various grids
    - Finding grids to fit model’s physical assumptions and numerical discretization at the boundary.
  - Assigned bowl regions to crevice..

HCCI Piston Crevice

- Tested full cycle functioning
  - Simulations shows turbulent kinetic energy from *k-ε* RNG model for piston with ring crevice.



Grids Generated by Cubit

- Cubit grid (Exodus II format) output to KIVA-4 input
  - Develop C++ coding for:
    - Interfacing with extensive C++ constructions that are available in a LANL in-house code package to extract the grid structure from Exodus II format.
    - Write out input file that is compatible with KIVA-4.
  - Input file being read in by KIVA-4
    - Adjusting setup and connectivity subroutines to accept the Cubit file input.

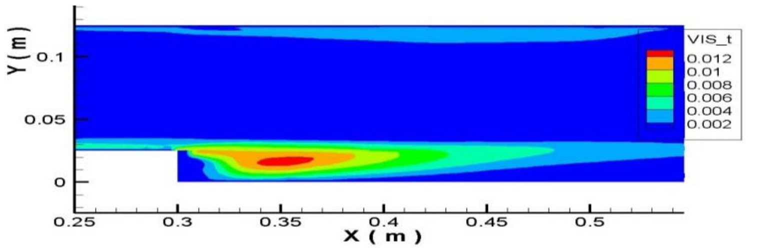
Developmental R&D Engineering

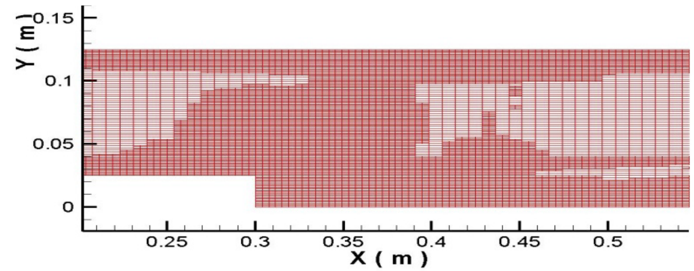
- Engineering for a change in the discretization for KIVA-4
  - Development of an h-p adaptive finite element method (h-p FEM) for turbulent flow is nearly complete.
  - Altering current FEM formulation to a Characteristic-Based Split (CBS) FEM (O.C. Zienkiewicz and R. Codina, 1995).
    - Flow regimes from incompressible to supersonic in one algorithm.
    - Highly accurate and flexible discretization.
    - Relatively seamless integration into current KIVA-4 structure.
    - Similar to current KIVA-4 solver algorithm.

Unsteady Turbulence Modeling with h-adaptive FEM

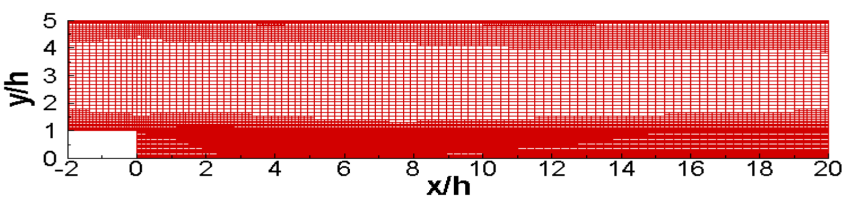
- Two-equation k-w closure and h-adaptive unstructured grid
  - Octree storage with adjacency
  - Plug into KIVA-4 unstructured grid with some augmentation of structure (FEM projection model similar to KIVA SIMPLE algorithm and CBS (both 2d and 3d versions – Carrington and Pepper, NHT 2002, CNMF 2002, INJNMF 1999).

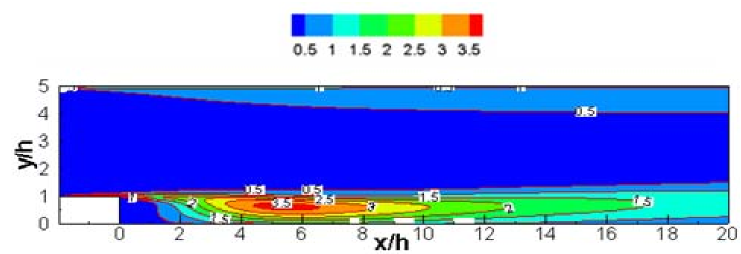
    - Solution using residual error measure (exact error) for driving the grid resolution.





- Stress error measure to drive grid resolution via Zienkiewicz - Zhu
  - Wang, Carrington and Pepper, 2008 (CHT-08 & CTS- 2009).





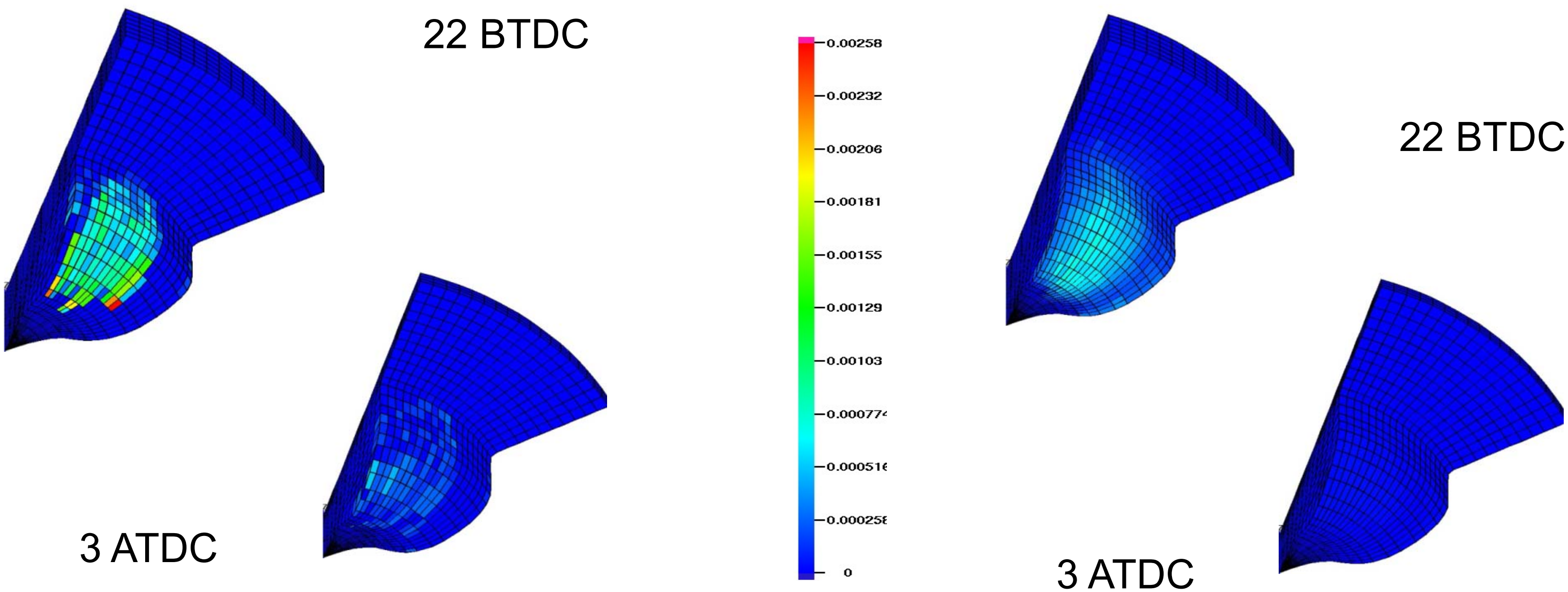
Wall-Film - improved wetting mechanism

Employing "smoothing subroutine" by LANL

Wall-Film Height – Old vs. New

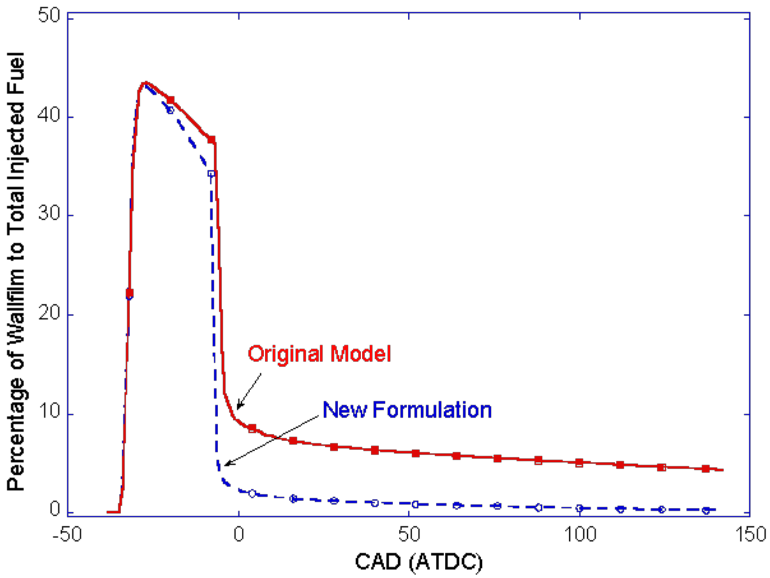
Original Model

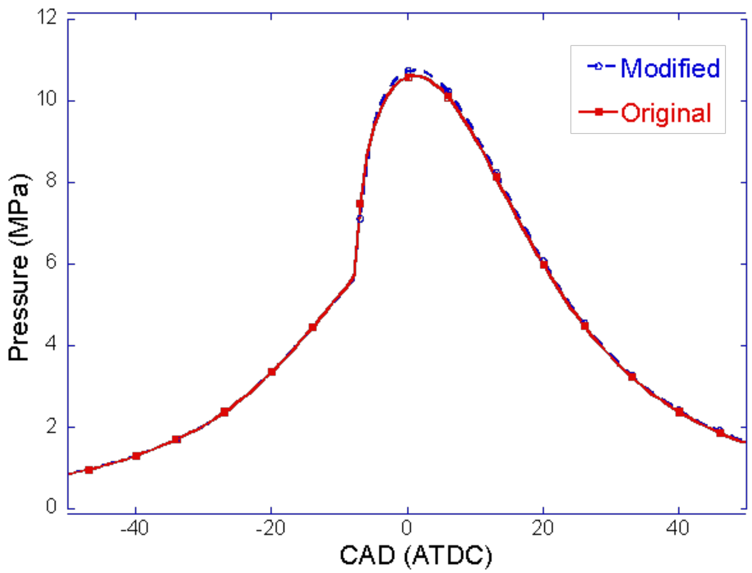
New Formulation



Results of Wall-film Vaporization

- Complete vaporization of wall-film.
- Cylinder pressure changes slightly.
  - Soot emissions prediction reduced by 12%.
- Results are consistent for other injection timing.

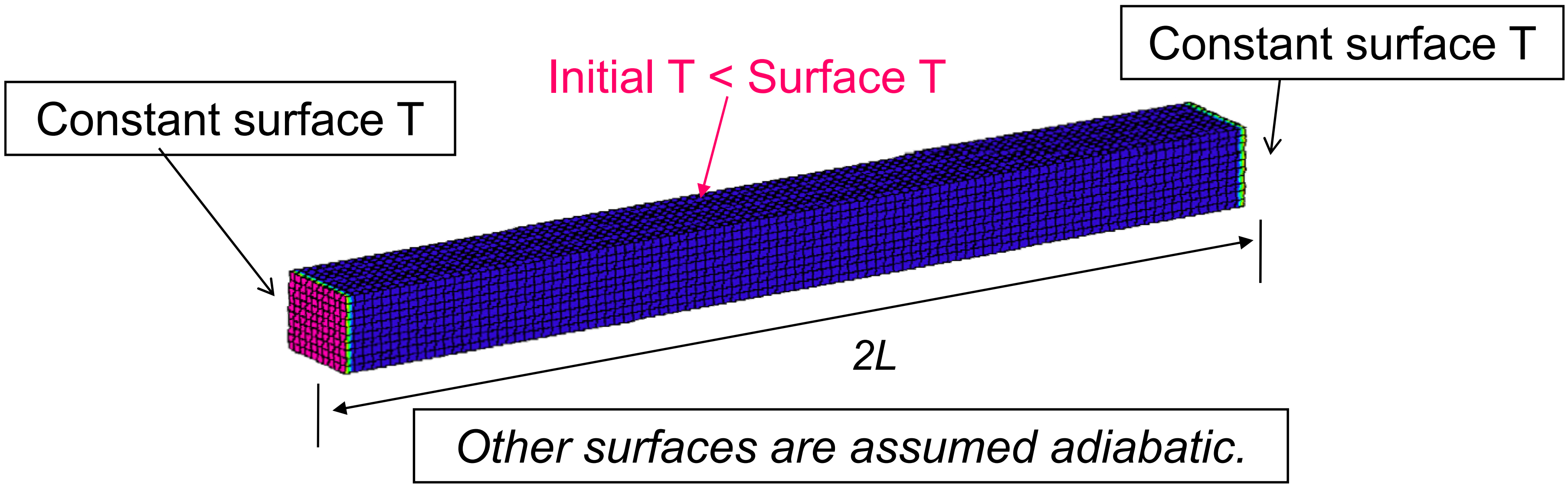




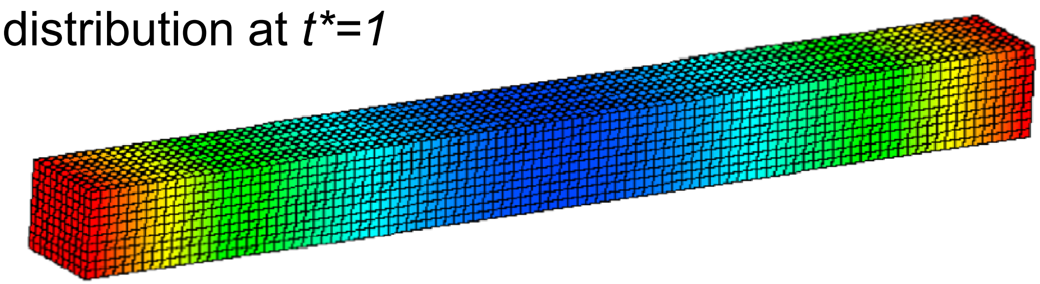
Conjugate Heat Transfer

- **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.
    - Continuity equation is solved based on a constant density.
    - Momentum equations are solved based on zero velocities.

Validation for heat conduction in a slab



Temperature distribution at $t^*=1$



ρ = 7870 kg/m^3
K= 53.1 w/(m*k)
c_p = 447 J/(kg*k)

Temperature History - Validation

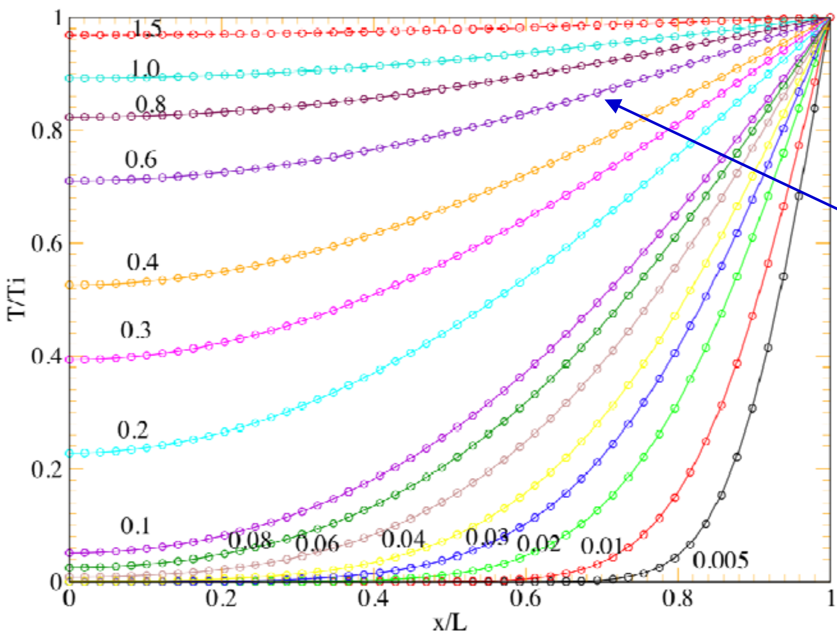
KIVA-4 vs. Analytically derived

- Non-dimensional parameters: T/T_s, x/L, and $t^*=\alpha t/L^2$

______ KIVA-4 results

<> Analytical solutions

Mid-plane of slab



Increasing t^*

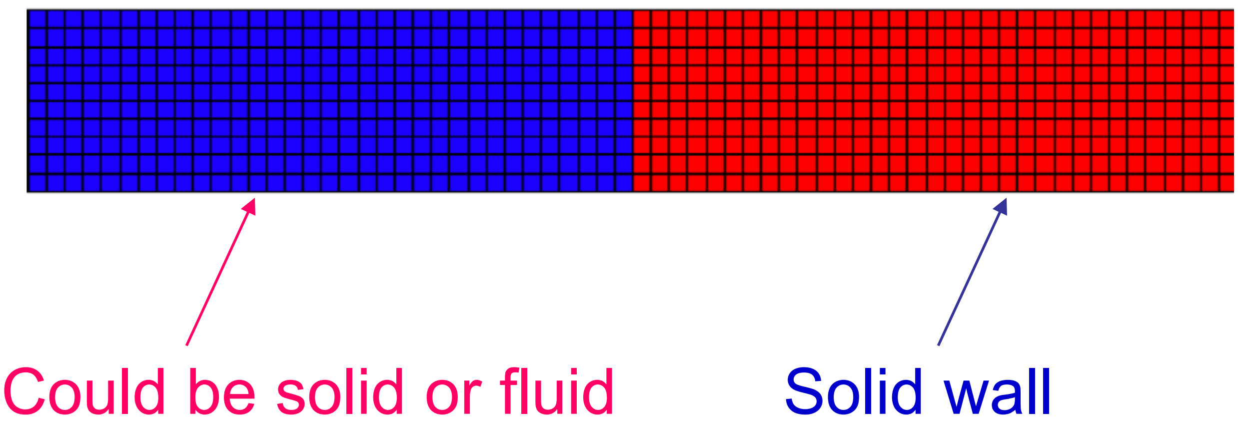
End of slab

Continuing Work for FY 09

- **Developing cut-cell grid generation method.**
  - Benchmarks solutions on simple geometries, e.g.,
    - Cylinder/Duct flow, driven cavity flow, shock tube problem
- **Implementing conjugate heat transfer to/from combustion chamber.**
- **Implementing capability to use grids from Cubit.**
- **Engineering and research for FY10.**
  - Finish detailed plan and method to implement new discretization in KIVA-4
    - Use of existing research codes to investigate and “iron-out” details of new discretization.
    - Evaluating existing KIVA-4 code to best accept a discretization change.

Conjugate Heat Transfer

- Modeling heat conduction of a slab composed of two solids with different properties.
- Modeling heat convection in fluids and heat conduction in solid simultaneously.



- Performing simulation in diesel combustion chamber.
- Considering in-cylinder spray combustion processes.

Future work for FY 2010

- **Perfecting the cut-cell grid generation method**
  - Interfacing with the KIVA-4 solver/software.
  - *a-priori* grid refinement around complex structural features.

- **Implementing a Characteristic-Based Split (CBS):**
  - A conservative form of the Generalized Petrov-Galerkin Finite Element Method (GPG-FEM). With FEM, the flux i.e, the gradients are inherently considered in the variational form. The P-G weighting allows for 3rd order accuracy of the advection or fluxing.
  - To include both grid and polynomial adaptive methods
    - h-p FEM -- a gold standard fir accurately predicting fluid-thermal dynamics. Is well founded in mathematics of functional analysis and allows for exact determination of the discretization error.
    - Allows minimizing discretization errors to any desired level of accuracy.
  - Use of the following existing methods and constructions in KIVA-4:
    - Conservative Arbitrary Lagrange-Eulerian (ALE) method
    - Chemistry
    - Injection
    - Equation solvers
    - 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…

Summary

- **Cut-Cell grid Generation and Implementation**
  - Reducing total simulation time by creating cut-cell grid capability.
  - Quickly generate grids from CAD surfaces of complex domains.
- **KIVA-4 Support for LLNL HCCI simulation**
  - Support KIVA-4 solver for grids using piston ring crevices.
- **Cubit Grid interface**
  - Increase flexibility of KIVA-4 with use of more grid generators.
- **R&D engineering research for FY10 and beyond**
  - Begin designing the implementation of a faster, extremely accurate, and robust algorithm in KIVA-4.
- **Wall-Film Wetting**
  - More realistic modeling of wetted surfaces for better modeling of evaporation at wetted surfaces.
- **Conjugate Heat Transfer**
  - More accurate prediction in wall film and its effects on combustion and emissions under PCCI conditions with strong wall impingement.