KIVA Modeling to Support Diesel Combustion Research

David B. Carrington
David Torres
Los Alamos National Laboratory
Song-Charng Kong
Iowa State University
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ace_14_carrington

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

- Area of faces that are fluid are computed using Stokes theorem.
  \[
  A_{\text{face}} = \int_S (\nabla \times \vec{F}) \cdot \hat{n} \, dS = \int_L \vec{F} \cdot d\vec{R}
  \]

- 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

2nd level

3rd level

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 show turbulent kinetic energy from $k-\varepsilon$ 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

2009 DOE Merit Review
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

2009 DOE
Merit Review

Constant surface T

Initial T < Surface T

Other surfaces are assumed adiabatic.

Temperature distribution at $t^*=1$

$\rho = 7870 \text{ kg/m}^3$

$K = 53.1 \text{ w/(m*k)}$

$c_p = 447 \text{ J/(kg*k)}$
Temperature History - Validation

KIVA-4 vs. Analytically derived

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

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Mid-plane of slab

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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.
  – \textit{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 3\textsuperscript{rd} order accuracy of the advection or fluxing.
  – To include both grid and polynomial adaptive methods
    • h-p FEM -- a gold standard for 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/O, 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.