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Title: 2016 KIVA-hpFE Development: A Robust and Accurate Engine Modeling Software

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2016 KIVA-hpFE Development: A Robust and Accurate Engine Modeling Software

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Objectives

- Develop algorithms and software for the advancement of speed, accuracy, robustness, and range of applicability of the KIVA internal engine combustion modeling – to be more predictive. This to be accomplished by employing higher-order spatially accurate methods for reactive turbulent flow, and spray injection, combined with robust and accurate actuated parts simulation and more appropriate turbulence modeling.
- To provide engine modeling software that is easier to maintain and is easier to add models to than the current KIVA. To reduce code development costs into the future via more modern code architecture.

Fiscal Year (FY) 2016 Objectives

- Continue developing code and algorithms for the advancement of speed, accuracy, robustness, and range of applicability of combustion modeling software to higher-order spatial accuracy with a minimal computational effort.
- Finish developing a Large Eddy Simulation turbulence model that is capable of spanning transition to turbulence and hence fluid boundary layers without the law-of-the-wall.
- Finish developing the KIVA-hpFE to be parallel using Message Passage Interface (MPI) to facilitate speed of solution of more fully resolved domains including moving parts, chemistry and sprays.
- Continue developing the 3-D overset grid system; to quickly utilized ‘stl’ file type from grid generator for quick/automatic overset parts surface generation.
- Start developing parallel implementation of 3-D *hp*-adaptive FEM system.
- Start developing a predictive initial spray break-up model that transitions to atomized droplets by directly modeling and evaluating the forces involved of any given fluid properties.
- Start implementing higher fidelity reactive chemistry packages, such as ChemKin-Pro and LLNL’s zeroRK2.

Accomplishments

- Finished developing a Large Eddy Simulation (LES) turbulence model that is capable of spanning transition to turbulence and hence fluid boundary layers.
- Finished developing the KIVA-hpFE to be parallel using Message Passage Interface (MPI) to facilitate speed of solution of more fully resolved domains and parallel solution method for the moving parts, reactive chemistry and sprays, showing ~30x speed-up over serial version.
- Developed implicit solution system for diffusive and stress forces for an extra 10x speed-up per processor in some cases, giving a 300x speed-up over our original serial version.

- Started parallelization the *hp*-adaptive FEM methods; serial version completed.
- Continued development of the 3-D overset grid system; to quickly utilize 'stl' file type from grid generator for quick/automatic overset parts surface generation.
- Developing a Volume of Fluid (VOF) method for use in spray modeling to be more predictive modeling capability on initial break-up. System includes fluid surface curvatures, and interacting stress on the fluid/gas interface.
- Implementing higher fidelity reactive chemistry packages, such as ChemKin-Pro and LLNL's ZeroRK.
- Continued Validation & Verification adding capabilities for many benchmark problems.

Future Directions

- Continue developing the parallel system in the *hp*-adaptive FEM. Continue implementing this method to perform modeling of internal combustion engines, other engines, and general combustion. Parallel structure is MPI (MPICH2) with nested OpenMP system that has a maximum efficiency on clusters with multi-core processors
- Complete a development of Conjugate Heat Transfer between the engine block
- Continue developing comprehensive comparative results to benchmark problems for V&V, and spray experimental data available from the Engine Combustion Network (ECN) as part of the verification and validation system. Collaborations with John Deere (Dr. Ge) and Oakland University (Dr. Zhoa).
- Develop the hierarchical basis or shape functions for prisms and tetrahedral to be used with the 3-D overset moving surface/volume system.
- Incorporate the Kelvin-Helmholtz to Rayleigh-Taylor (KHRT) spray model in the KIVA multicomponent spray system.

Introduction

Los Alamos National Laboratory and its collaborators are facilitating engine modeling by improving accuracy and robustness of the modeling, and improving the robustness of software. We also continue to improve the physical modeling methods. We are developing and implementing new mathematical algorithms, those that represent the physics within an engine. We provide software that others may use directly or that they may alter with various models e.g., sophisticated chemical kinetics, different turbulent closure methods or other fuel injection and spray systems.

Approach

Our approach is founded in design and invent new modeling methods and code. The new design is change of discretization to FEM, essentially every other beneficial and salient attribute of the software stems from this foundation. We invented and developed the following systems to date

1) Invented the FEM PCS projection method,
2) Developed the *hp*-adaptive system,
3) Invented the local-ALE method more moving bodies,
4) Developed new dynamic LES,
5) Invented a method for implementing MPI for today's & future platforms.

We are building models and code in order to meet all the objectives in a clean, easy to maintain software which easily handles addition of submodels. Careful verification and validation is required. The development of this technology utilizes many areas of expertise in the areas of multi-species turbulent reactive flow modeling with liquid sprays, modeling of immersed moving bodies, and numerical methods for the solution of the model and governing equations.

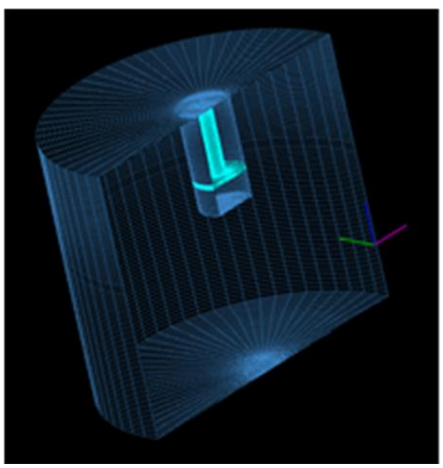
Results

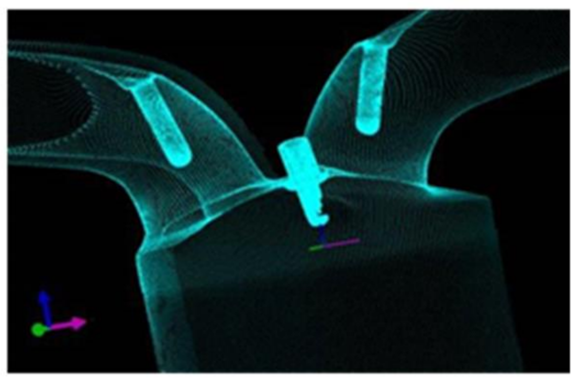
When considering the development of algorithms and the significant effort involved producing reliable software, it is often best to create algorithms that are more accurate at a given resolution and then resolve the system more accurately only where and when it is required. We began developing a new KIVA engine/combustion code with this idea in mind [1]. This new construction is a Galerkin FEM approach that utilizes conservative momentum, species, and energy transport. The FEM system is Petrov-Galerkin (P-G) and pressure stabilized [2].

A projection method is combined with higher order polynomial approximation for model dependent physical variables (*p*-adaptive) along with grid enrichment (locally higher grid resolution – *h*-adaptive). Overset grids are used for actuated and immersed moving parts to provide more accurate and robust solutions in the next generation of KIVA. The scheme is particularly effective for complex domains, such as engines.

The *hp*-adaptive FEM becomes higher order, more accurate, where required as prescribed by the adaptive procedures that is determined by the mathematical analysis of solution's error as the solution proceeds [2]. The *hp*-adaptive method employs hierarchical basis functions, constructed on the fly as determined by a stress-error measure [3]. In the following we discuss the progress made during the last year on Grid Generation, dynamics LES, Parallelization, Comparison to older KIVA system, and Spray Modeling.

Grid Generation and LANL's local-ALE FEM





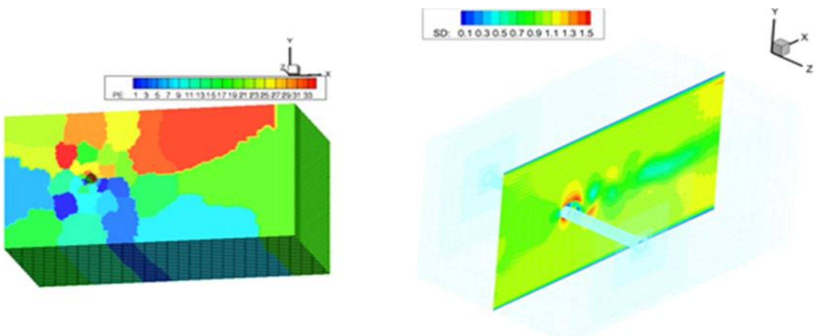
a) b)

Figure 1. Engine parts to be overlaid onto the grid a) valve overlaying the grid as constructed in GridPro b) Sandia's DISI 4-valve engine with spark and injection ports ready for overlaid parts.

The overset parts of the ALE system adjust the grid locally as the parts move through the fluid grid. The fluid grid is formed as continuous grid without having to form the grid around the complex parts. This system maintains 2nd order spatial accuracy while never allowing the grid to tangle [4]. Since the fluid is represented continuously, fluxing of material through the grid, as it is moves is not required. This need to flux through the grid is just one portion of the error when the usual ALE method is employed with finite volumes. Here the fluid solver remains Eulerian and the moving grid portions are no longer entwined with fluid solution. The local-ALE method is robust, the grid will never tangle and the parts can move in any way desired through the cylinder's grid. We are using GridPro tools for robust and automatic grid generation and collaborating with the GridPro team on use for engine modeling for all KIVA versions. Figure 1 shows use of GridPro for the FEM code using LANL's local-ALE method, the overset parts system. Figure 1a) shows a simple cylinder with 1 port and the valve overlaid and b) the grid for Sandia's DISI engine with spark plug, injection ports, and valve guides, waiting for the valves to be overlaid.

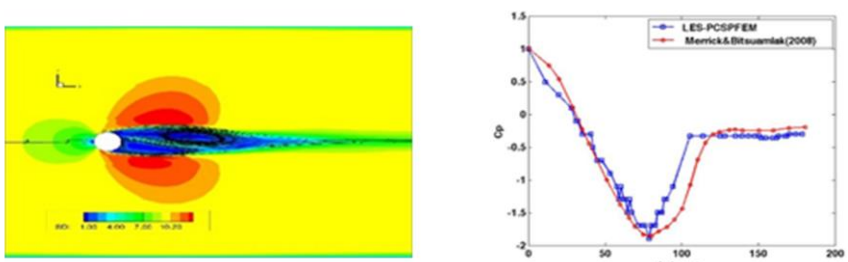
Dynamic LES

A dynamic LES method has been completed for the PCS FEM system that spans flow regimes from the laminar to highly turbulent flow without needed special damping such wall functions. This dynamic LES is based on a scheme developed by Vreman [5]. The model removes assumptions about the laminar sublayer and allows modeling non-equilibrium turbulent flows. The method allows backscatter, a natural process that is inherent turbulent flow. The results for flow over a 3-D cylinder is shown in Fig. 2 at Reynolds numbers of 1.2e+5 solved in parallel with KIVA-hpFE. Figure 2a shows the domain decomposition (#PE's) and Fig. 2b the flow streamlines and 2c demonstrates the simulation results compared to experimental data along the centerline on average. In figure 3 a snapshot in time of the unsteady solution is shown for Re=1.2e+5 and the resulting average coefficient of pressure as compared data from Merrick and Bitsuamlak [6].



a) b)

Figure 2. Subsonic flow over a cylinder at Re = 1000 a) 450K cells decomposed onto 36 processors b) vortex street of the fully developed flow.

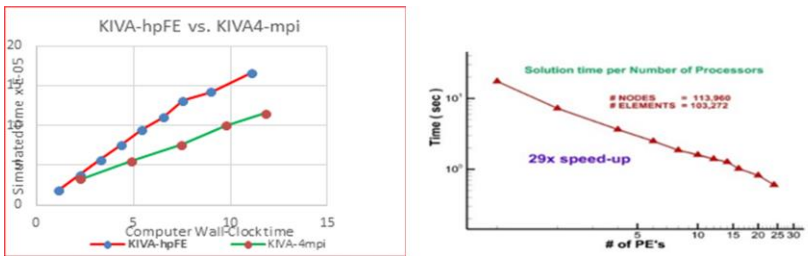


a) b)

Figure 3. Subsonic flow over a cylinder at Re = 1.2e+5 a) vortex street developing at t= b) average coefficient of pressure compared to data.

Parallelization and new KIVA-hpFE versus older KIVA-4mpi

Determining how much headway we've made to date over our previous software called KIVA-4mpi we investigate a problem of flow over cylinder. This test case uses the same grid resolution (the same grid), the same size time step, and solving in the same manner. Shown in Fig. 4 a) is the simulation fluid motion elapsed time versus wall-clock. KIVA-hpFE is speed is faster at every time step, shown by the diverging curves. For example, at 10 minutes of computational time, the new code is 1.5x faster than the old KIVA-4mpi code. KIVA-hpFE is not only faster, but is more accurate given the same number of cells, and often requires far fewer cells for the same accuracy as older KIVA codes (shown this behavior on numerous benchmark cases), without using the higher order approximations. Second-order accuracy states little about the actual accuracy of a method, just revealing the convergence is with a slope of 2. A method can have error and be 2nd order accurate; our new system is more accurate than previous versions when using the same number of cells.



a) b)

Figure 4. Solution speed for flow over cylinder benchmark problem, KIVA-hpFE vs. KIVA-4mpi

We have finished developing KIVA-hpFE parallel version using Message Passage Interface (MPI) to facilitate speed of solution of more fully resolved domains showing a 30x speed-up over serial system, as shown in Fig. 4 b). The speed-up is super-linear, meaning; the speed-up for any particular problem will continue to increase linearly provided the problem size (number degrees of freedom) increases! In addition, we developed and implicit solution system for diffusive and stress forces for an extra 10x speed-up per processor for an overall 300x speed-up over serial version on some problems.

Spray Modeling

Sprays can be described by a cloud of diffuse particles; 10's of thousands of droplets of various sizes streaming through what is usually a gaseous media. These particle clouds proceed through numerous processes of agglomeration and break-up as they move through the conveying fluid (often air). The droplets experience interactions with this conveying media where stresses on the droplets force breakup and agglomeration Droplet sizes changes occur when they breakup, agglomerate and evaporate. Newton's 3rd Law allows for the evaluation of opposing forces acting on the conveying fluid.

Solution of the dispersed spray equation, requires initial conditions for the droplets after it transforms from a continuously connected fluid. In jet atomization, liquid fuel is injected through a nozzle and forms a jet which breaks into very fine droplets. Understanding the effect of the geometry of the injector nozzle, the initial jet conditions, the fluid properties in the liquid film the break-up and the resulting droplet sizes and distribution are of primary importance to improve fuel efficiency and lower gas emissions.

Supplying predictive initial conditions for the phase-space represented in the spray equation at the time the model spray equation is applicable would go a long way to having a predictive capability for sprays in combustion modeling. In addition, properly applying any dispersed droplet solution method requires determining the point in time where the jet breakup occurs. Phase-space information that is vital to solving the spray equation needs to include spatial position, velocities, sizes and temperatures. To accomplish the task of predictively initiating the Lagrangian particle transport method we are developing a VOF method to track the evolving interface of fluid stream immerges from the injector, providing needed initial phase-space information and time of applicability for the spray equation to be employed. In the VOF method a single-velocity field with a single pressure field formulation is used for solving the mass and momentum conservation equations on a fixed computational mesh. The interface is capture through a “color” function, C, and its kinematics is represented by the following evolution equation:

$$\frac{\partial C}{\partial t} + \nabla \cdot \left(C\vec{u} \right) = 0$$

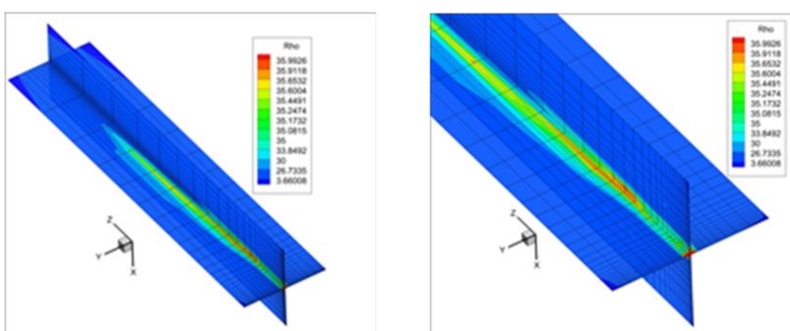
The color function is the volume fraction (amount) of each fluid in a computational cell, and is intrinsically mass conserving and can automatically handle change in topology (break-up and coalescence) because of the nature of the evolution equation at the interface.

Coupling of a Lagrangian particle transport (LPT) method with a volume tracking method or VOF concurrently in a single domain is not straightforward and requires new research. The first task is to derive transition criteria to identify if the fluids are “separated” or “dispersed”. An obvious criterion is based on the interface length scale relative to the mesh resolution. Can the mesh spacing resolve the interface structure? Is the interface characteristic length scale, such as droplet diameter, greater or smaller than the mesh spacing? To answer these questions, we propose to use interface curvature, κ,

$$\kappa = -\nabla \cdot \vec{n} = -\nabla \cdot \left(\frac{\nabla C}{\left\| \nabla C \right\|} \right)$$

which is an interface characteristic length scale as our first criterion

In Figure 5, we show the current progress of our initial break-up model of an injected jet of gasoline at 100 m/s. The liquid core is showing ligaments more clearly seen in Fig. 5 b) by the density variations. Both curvature and stresses between the liquid and gas fluids are incorporated into the solution of the governing equations. The solution currently is being performed on a very coarse grid to expedite development purposes, reducing the accuracy of the VOF method. The h-adaptive mesh refinement scheme will be used in conjunction with VOF to precisely capture the liquid/air interface without requiring a priori information about the jet’s behavior. Thereby reducing the need for a highly refined grid everywhere to precisely capture the interface. Simulations of an engine injector are now being developed using this method. Once the initial break-up shows the liquid ligaments smaller than the cell size, we intend to transfer those small ligaments (large droplets), to the secondary break-up model and transport the drops with our standard LPT model.



a) b)

Figure 5. Multi-phase flow modeling of initial jet break-up.
VOF system with stresses and curvature of liquid interface calculated on a jet of density 35 g/cm^3 into air at 1 atm. Inlet velocity is 100 m/s.

Conclusions

In FY 2016, we continued advancing the accuracy, robustness, and range of applicability internal combustion engine modeling algorithms and coding for engine simulation. We have performed the following to advance the state-of-the art:

1) Finished developing a Large Eddy Simulation (LES) turbulence model that is capable of spanning transition to turbulence and hence fluid boundary layers.
2) Finished developing the KIVA-hpFE to be parallel using Message Passage Interface (MPI) to facilitate speed of solution of more fully resolved domains and parallel solution method for the moving parts, reactive chemistry and sprays, showing a 30x speed-up over serial system.
3) Developed implicit solution system for diffusive and stress forces for an extra 10x speed-up per processor for an overall 300x speed-up over serial version.
4) Continued development of the 3-D overset grid system to quickly utilize 'stl' file type from grid generator for quick/automatic overset parts surface generation.
5) Incorporating the Volume of Fluid (VOF) method in spray modeling for more predictive modeling capability on initial break-up.
6) Continued Validation & Verification adding capabilities for many benchmark problems.

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6) Merrick, R., and Bitsuamlak, G., (2008), "Control of flow around a circular cylinder by the use of surface roughness: A computational and experimental approach." *Internet publication at http://www.ihrc.fiu.edu/wpcontent/uploads/2014/03/MerrickandBitsuamlak_FlowAroundCircularCylinders.pdf*

FY 2016 Publications/Presentations

1) Waters J., Carrington, D. B., Pepper, D.W. (2016), "An Adaptive Finite Element Method with Dynamic LES for Turbulent Reactive Flows," Journal of Computational Thermal Sciences, Begell House Inc., vol. 8, no. 1, pp. 57-71
2) V. D. Hatamipour, David B. Carrington, Juan C. Heinrich (to appear), "Accuracy and Convergence of Arbitrary Lagrangian-Eulerian Finite Element Simulations based on a Fixed Mesh," Progress in Computational Fluid Dynamics, An International Journal
3) Carrington. D. B., Mazumder, M., Heinrich, J.C., (to appear), "Three-Dimensional Local ALE-FEM Method for Fluid Flow in Domains Containing Moving Boundaries/Objects Interfaces", Progress in Computational Fluid Dynamics, An International Journal.
4) Waters, J ; Carrington, D. B., (2016), "A parallel Large Eddy Simulation in a finite element projection method for all flow regimes," Numerical Heat Transfer Part A-Applications, vol.70 (2), pp.117-131
5) J. Waters, D.B. Carrington (2016), "Modeling Turbulent Reactive Flow in Internal Combustion Engines with an LES in a semi-implicit/explicit Finite Element Projection Method," *Procs. of the ASME 2016 Internal Combustion Engine Fall Tech. Conf.*, ICEF2016, Oct. 9-12, 2016, Greenville, SC, USA

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Special Recognitions & Awards/Patents Issued

- Outstanding Innovation Award – 2011 Distinguished Licensing Award. Awarded by Los Alamos National Laboratory Technology Transfer Division, August 9th, 2012.
- Outstanding Innovation Award – 2010 Distinguished Copyright Award. Awarded by Los Alamos National Laboratory Technology Transfer Division, August 11th, 2011

Acronyms

FEM - Finite Element Method
CHT – Conjugate Heat Transfer
LES - Large Eddy Simulation
MPI - Message Passing Interface
LPT – Lagrangian Particle Transport method or model
Re – Reynolds number

Figure Captions (Six Figures Max., submit figures separately)

Figure 1. Engine parts to be overlaid onto the grid a) valve overlaying the grid as constructed in GridPro b) Sandia's DISI 4-valve engine with spark and injection ports ready for overlaid parts.
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