Title: KIVA Development 2014

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# II.13 KIVA Development 2014

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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 KIVA 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. The new code is KIVA-hpFE, an *hp*-adaptive finite-element method (FEM).

## Fiscal Year (FY) 2014 Objectives

- Continue developing code and algorithms for the advancement of speed, accuracy, robustness, and range of applicability of the KIVA combustion modeling software to higher-order spatial accuracy with a minimal computational effort.
- Finish developing underlying discretization to an *hp*-adaptive predictor-corrector split (PCS) using a Petrov-Galerkin (P-G) FEM for multi-species flow, fluids with multiple components.
- Develop a plasma kernel spark model to supply heat at a single node based on engine manufacturer-specified spark current.
- Validate KIVA chemistry in the KIVA-hpFE solver to lower heating values (LHV) of fuel based on exact amount of fuel burned.
- Continue developing the three-dimensional (3-D) overset grid system to quickly utilized ‘stl’ file type from grid generator for quick/automatic overset parts surface generation.
  - Simulate 3-D flow with immersed actuated parts of valves and scalloped bowled piston.
- Finish developing dynamic large-eddy simulation (LES) for the PCS FEM system
- Continue developing the Message Passing Interface (MPI) parallel solution methods for the domain-decomposed geometry that has nest OpenMP threaded for maximal use of multi-core processors.

## FY 2014 Accomplishments

- Finished developing underlying discretization to an *hp*-adaptive PCS using a P-G FEM for multi-species flow inclusive the chemistry input system and setup.
- Validated 3-D local-Arbitrary Lagrangian-Eulerian (ALE) moving parts algorithm/code with extensive error and convergence analysis. The method demonstrates near-zero error as determined by comparison to a moving surface problem that has a closed form or analytic solution.
  - Simulated 3-D flow with immersed actuated parts, a scalloped bowled piston.
- Developed a plasma kernel spark model, to supply heat at a single node based on engine manufacturer-specified spark current.
- Installed and validated KIVA chemistry package into the PCS FEM solver. Chemistry and burn model validated in the FEM system showing less than 1% error in LHV. The spark model does not supply significant heat to the energy in the domain.
- Developed a dynamic LES turbulence modeling for wall-bounded flows, and will be especially applicable to internal combustion engine modeling.
- Merged the grid formats, KIVA chemistry and spray along with multi-species component fluids into *hp*-adaptive FEM framework. Validation continues on this effort.
- Parallel global pressure solver system completed, wrappers for MPI installed with algorithms and coding for the solution of the primitive variables being completed and testing debugging continuing.

## 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, portable implementation of MPI) with nested OpenMP system that has a maximum efficiency on clusters with multi-core processors.
- Continue developing comprehensive comparative results to benchmark problems and to commercial software as part of the verification and validation of the algorithms.
- Continue developing the implicit solver system for the PCS FEM system, for no error 3-D moving parts method.
- Validate the KIVA chemistry and spray with *hp*-adaptive scheme.
- Continue developing the parallel solution method for the *hp*-adaptive PCS algorithm. Continue developing more appropriate turbulence models for more predictive modeling.
- Continue to verify and validate combustion and spray models, and the local ALE in 3-D.
- Incorporate volume of fluid method in spray modeling for more predictive modeling capability. Incorporate the Kelvin-Helmholtz Rayleigh-Taylor, spray in the KIVA multicomponent spray model.

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## 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

Development of computational fluid dynamics models and algorithms relies on basic conservation laws and various mathematical and thermodynamic concepts and statements. The process encompasses a great many requirements including:

- Expertise in turbulence and turbulent modeling for multiphase/multispecies fluid dynamics.
- Expertise in combustion dynamics, modeling, and spray dynamics modeling.
- Skill at developing and implementing numerical methods for multi-physics computational fluid dynamics on complex domains with moving parts using variational methods.
- Careful validation and error analysis of the developed code and algorithms.

## 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 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 is at a minimum second-order accurate in space and third-order for advection terms, but becomes higher-order where required as prescribed by the adaptive procedures that is determined by the mathematical analysis of solution's error as the solution proceeds or error measures [2]. The *hp*-adaptive method employs hierarchical basis functions, constructed on the fly as determined by a stress-error measure [3].

A dynamic LES method was developed for the PCS FEM system that spans from laminar to highly turbulent flow without needed special damping such wall functions. This dynamic LES is based on a scheme developed by Vreman [4]. 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 Mach 2.25 flow over an 18 degree inclined ramp are shown in Figure 1. Figure 2 demonstrates reasonable accuracy compared to experimental data [5]. Note though, the experimental data is the magnitude of the mean velocity, so we show the absolute value of the velocity from the simulation for comparison. The recirculation zones caused by the adverse pressure gradients create the detached shocks are the correct size and location compared to experiment.

Using the FEM method with the spray models provides a more accurate representation of the droplets interaction with the conveying fluid and with walls than the original finite volume method of KIVA. Because the FEM method allows for a continuous representation of phase-space, grid-scale accuracy can be applied everywhere. Problems with coarse grids influencing the spray are only related to the solution accuracy—the spatial representation of the spray model is therefore grid convergent, something that has not been true in the past. This nodal valued primitive variables system, allows for better accuracy of the species and heat distribution within a cell/element. The new plasma kernel model takes advantage of those nodal values, allowing the spark heat to be supplied at a single node, and mimics the solution to the plasma kernel equation. The spark model is based on the solution of the plasma kernel equations. These equations are solved as shown in a paper by K. Eisazadeh-Far et al. [6] and J. Song and M. Sunwoo solve the radius and temperature of the kernel [7]. The plasma kernel equation terms are as follows, *Tk* is the spark kernel's temperature, *dWspark/dt* is the change in spark current over time, *h* is enthalpy of the kernel *Vk* is the kernel's volume, *Ak* kernel's surface area, *Seff* is the effective flame speed, *P* is the pressure, *rk* the radius of the spark kernel and *dQloss/dt* is the change in heat loss in the kernel over time.

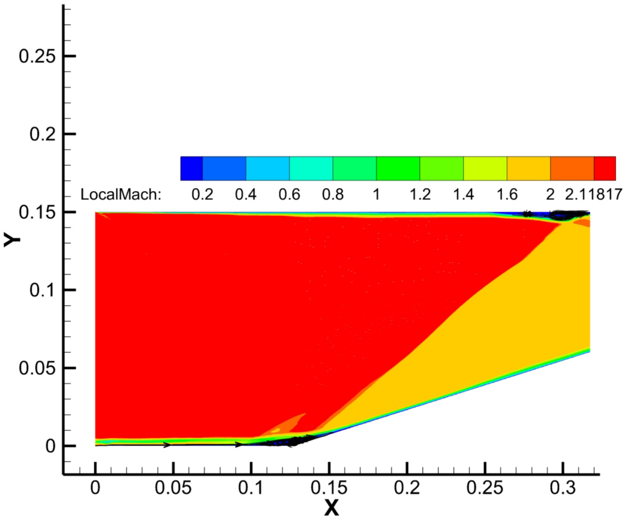

**FIGURE 1.** Supersonic Compression Ramp, Mach 2.25 Inlet Flow over 18 Degree Incline

$$\frac{dT_k}{dt} = \frac{1}{m_k c_{p,k}} \left( \frac{dW_{spark}}{dt} + \left(h_{chem} - h_k\right) \rho \; A_k S_{eff} - \frac{dQ_{loss}}{dt} + V_k \frac{dP}{dt} \right)$$

$$\frac{dV_k}{dt} = \frac{\rho_f}{\rho_k} A_k S_{eff} + V_k \left( \frac{1}{T_k} \frac{dT_k}{dt} - \frac{1}{P} \frac{dP}{dt} \right)$$

$$\frac{dr_k}{dt} = \frac{\rho_f}{\rho_k} S_{eff} + \frac{V_k}{A_k} \left( \frac{1}{T_k} \frac{dT_k}{dt} - \frac{1}{P} \frac{dP}{dt} \right)$$

A collimator test shown in Figure 3 is for near-engine operating temperatures and pressure. Gasoline is injected at 325 K at 15.8 atm and 525 K$^o$. The results show less than 1% error in the LHV for the mass of gasoline burned in the collimator.

In 2014, we completed the 3-D local ALE method as shown in Figure 4 for a bowled piston moving in a cylinder. The local ALE scheme uses overset grids for immersed parts described by points on their boundaries which overlays the fluid grid. The moving parts within the fluid are not taken into account during the grid generation process. Hence, ports and cylinder portions of the grid are continuously represented. The overset grid method allows for computer aided design-to-grid in nearly a single step, providing nearly automatic grid generation.

The ALE system adjusts the grid locally as the parts move through the fluid, and maintains second-

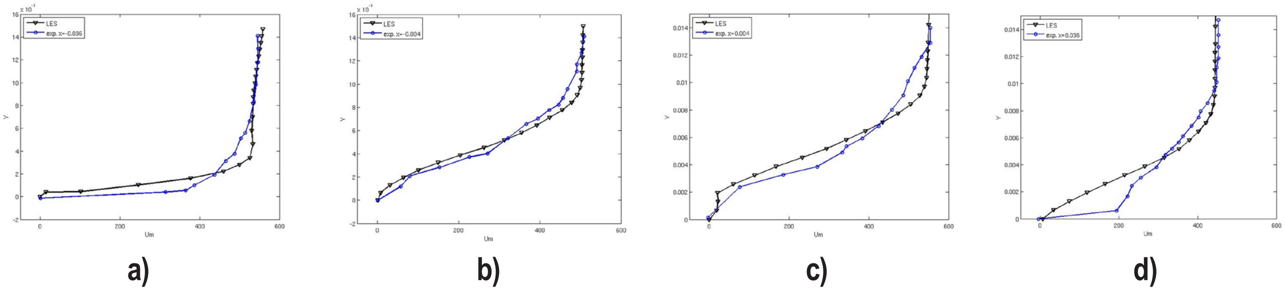

**FIGURE 2.** U (Mean Velocity) in Bottom Boundary Layer Using a Dynamic LES Model
Comparison to data at various locations: u upstream(-) and downstream(+) of the ramp a) -0.036 m , b) -0.004 m, c) +0.004 m, and d) +0.036 m.

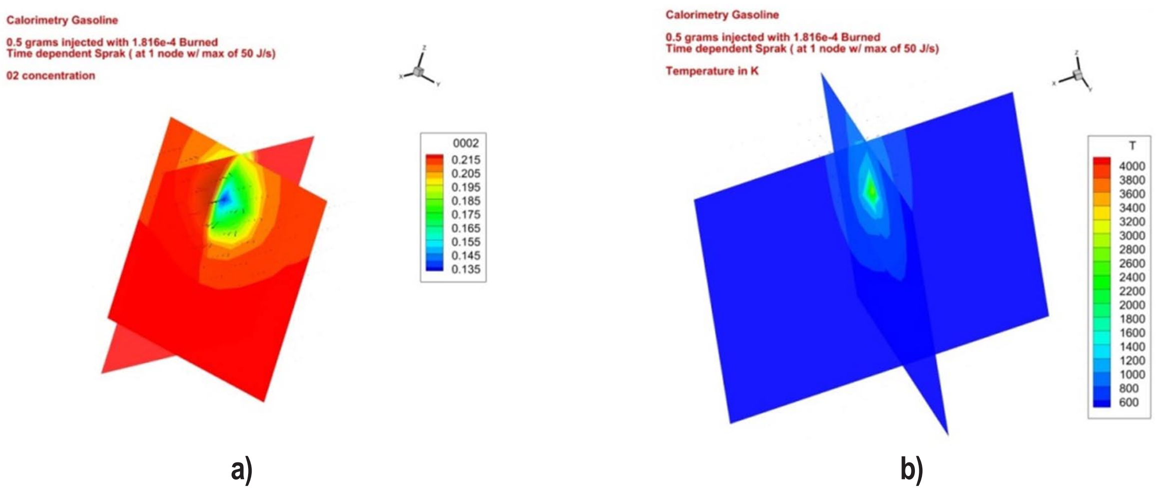

**FIGURE 3.** Gasoline being ignited by the plasma kernel model: a) oxygen concentration during burn and b) temperature of the fluid and also showing the temperature in the plasma kernel a short time after ignition.

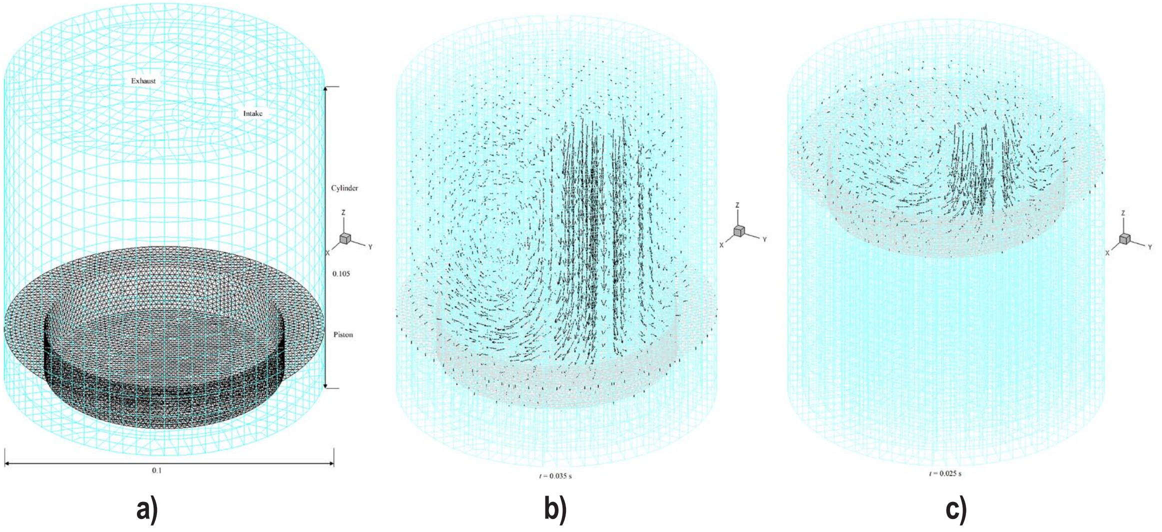

**FIGURE 4.** Cylinder with moving piston showing: a) piston surface of markers and triangles, b) and c) velocity vectors, piston location, and cylinder grid as piston moves.

order spatial accuracy while never allowing the grid to tangle or producing an element that cannot be integrated accurately [8]. 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. Figure 5 shows error and convergence compared to an analytic solution for the moving parts algorithm. The method demonstrates second-order spatial accuracy in Figure 5a and near zero error in Figure 5b. The method is robust, the grid will never tangle and the parts can move in any way desired through the cylinder's grid.

## CONCLUSIONS

In FY 2014, 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:

- Development of an *hp*-adaptive PCS FEM for all for multi-component fluids

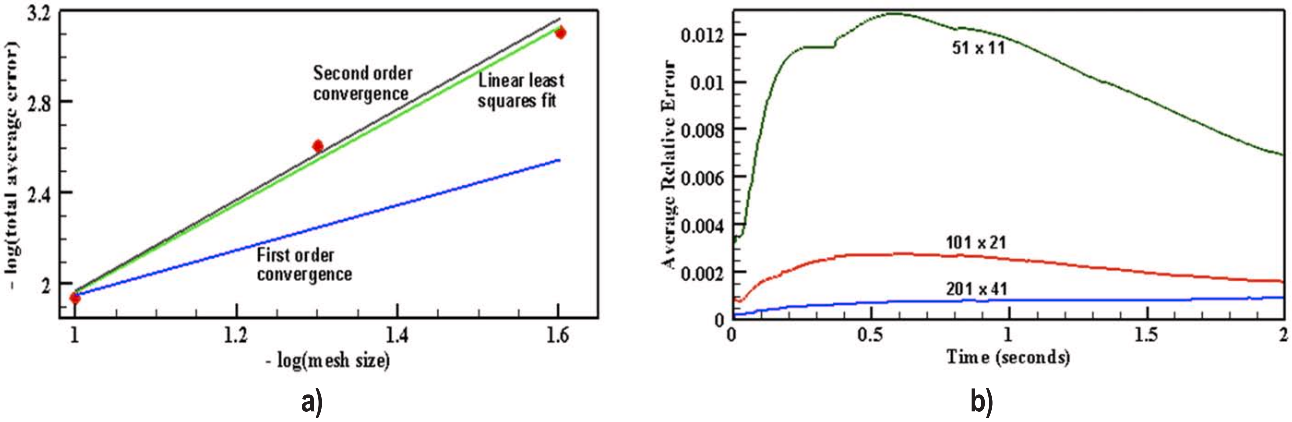

**FIGURE 5.** Convergence rates a) and solution error b) compared to the analytic solution for flow between moving parallel plates with inlet on one open side.

- Validated the immersed moving parts method in 3-D with extensive error analysis and comparisons to analytic solution.
- Developed a plasma kernel spark model for spark ignition that mimics the energy transport and timing of true spark, is applied as a single nodal source, and is a function of engine manufacturer-specified spark current.
- Validated the KIVA reactive chemistry model into PCS FEM solver.
- Developing the rest of MPI parallel system that will contain OpenMP threading to in the *hp*-adaptive FEM.
- Developed LES turbulence modeling for wall-bounded flows.

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## FY 2014 PUBLICATIONS/PRESENTATIONS

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