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

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3:15 p.m.

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Project ID # ACE014

Overview

Timeline

- 10/01/09
- 9/31/18
- 85% complete (the last 10% in CFD development takes the most effort)

Barriers

- Improve understanding of the fundamentals of fuel injection, fuel-air mixing, thermodynamic combustion losses, and in-cylinder combustion/ emission formation processes over a range of combustion temperature for regimes of interest by adequate capability to accurately simulate these processes
- Engine efficiency improvement and engine-out emissions reduction
- Minimization of time and labor to develop engine technology
  - User friendly (industry friendly) software, robust, accurate, more predictive, & quick meshing

Budget

- Total project funding to date:
  - 4000K
  - 705K in FY 16
  - Contractor (Universities) share ~15%

Partners

- Dr. Jiajia Waters, LANL
- University of New Mexico- Dr. Juan Heinrich
- University of Purdue, Calumet - Dr. Xiuling Wang
- Informal collaboration Reactive-Design/ANSYS
- Informal collaboration GridPro Inc.

Objectives FY 10 to FY 15 KIVA-Development

- **Everything we are doing in R&D is to develop methods and a code for:**
  - **Robust, Accurate and Efficient Algorithms in a Parallel (MPI) Modular Object-Oriented code for Industry and Researchers to meet:**
    - **Relevant** to accurately predicting engine processes to enable better understanding of: fuel injection, fuel-air mixing, thermodynamic combustion losses, and in-cylinder combustion/ emission formation processes over a range of combustion temperature for regimes of interest by adequate capability to accurately simulate these processes
      - **More accurate modeling requires new algorithms and their correct implementation.**
        - Developing more robust and accurate algorithms with appropriate/better submodeling
          - Relevant to understand better combustion processes in internal engines
        - Providing a better mainstay tool
          - Relevant to improving engine efficiencies and
          - Relevant to help in reducing undesirable combustion products.
        - Newer and mathematically rigorous algorithms will allow KIVA to meet the future and current needs for combustion modeling and engine design.
  - **Easier and quicker grid generation**
    - **Relevant to minimizing time and labor for development of engine technology**
      - CAD to CFD via Cubit Grid Generation Software – still in development
      - KIVA-4 engine grid generation (pretty much automatic but some snapper moving parts still difficult).
      - Easy CAD to CFD using Cubit grid generator - *hp*-FEM CFD solver with overset actuated parts and new local ALE in CFD, removes problems with gridding around valves and stems.

- **Objective**

More Predictive Turbulent Reactive Flow Modeling in Engines

(most of the following attributes are those heralded by industry as necessities)

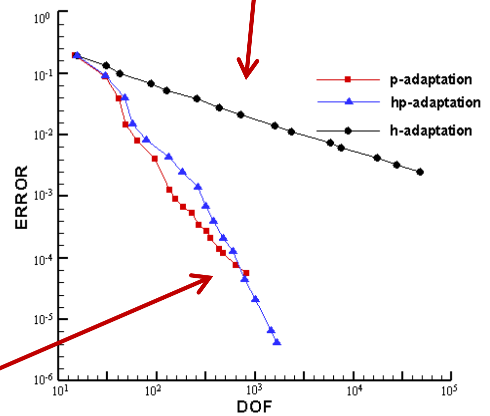
1) ***Fast grid generation*** **- CAD to CFD** grid in nearly a single step
2) ***Robust Moving parts newly invented 2nd order accurate Local ALE***
3) ***Higher order accurate*** - **higher spatial accuracy**
4) **Computational Speed with MPI** for parallel processing
5) ***Minimal communication*** for faster parallel processing
    1) **Exascale possibilities** because most operations are local to elements, GPU friendly CFD
6) Surfaces are represented exactly
7) ***Evolving solution error drives grid***
8) ***Accurate Spray modeling***
9) **Eulerian Solve throughout**
10) Great **LES designed for engine flows**
11) **Good RANS** ***k-ϖ*** **turbulence modeling**
12) ***Conjugate Heat Transfer (CHT)***
13) **Plasma Spark Model applied at the element node**
14) ***hp-***adaptive FEM – **exponentially grid convergent**
15) **Multiphase flow is more easily accomplished with this solver**
16) **A software for industry via commercialization and collaboration**

Many win-win-win combinations?

The choices we have made upfront in the discretization:

***hp*-Adaptive FEM with local -ALE allows all of new advantages of traditional CFD methods!**

Error as function(*grid size*)
Typical CFD method



hp-adaptive **FEM**
– exponential grid convergent !

Milestones for FY 10- FY15

01/12 – 2-D hp-adaptive PCS FEM validated subsonic flow
02/12 – Injection Spray model into the PCS FEM formulation
08/12 – 2&3-D hp-adaptive PCS FEM completed – validated subsonic & transonic flow
09/12 – Droplet Evaporation implemented
10/12 – 2-D supersonic turbulent flow Validated
10/12 – Analytic (similarity solution process) Pressure for 2-D ALE Validated
11/12 – Break-up, Collision, Wall-film, Spread and Splash, rewritten and integrated into FEM
01/13 – Chemistry fully implemented in FEM, reformatting and calometric testing
01/13 – OpenMP parallel system in PCS FEM formulation with testing
02/13 – 3-D Local ALE method for immersed moving parts on rectangular domains
07/13 – 2-D Local ALE rewritten to 3-D local ALE form, for easier testing CFD implementations
07/13 – Spray with evaporation, break-up, new particle tracking, new two-way coupling developed & Validated.
08/13 – Wall film model change, bug discovered, removed and tested.
09/13 – Reactive chemistry installed and Validated
01/14 – Domain decomposition with Scotch and Metis domain decomposition packages
03/14 – PCG solver (LANL parallel linear algebra) integrated with KIVA's new in-situ parallel preconditioning methods.
03/14 – Software Released: ReacTCFD (subset of KIVA-hpFE) & PCG linear equation system solver
07/14 – Error Analysis of new local-ALE method
08/14 – 3-D LANL local-ALE on piston with bowl
09/14 – 3-D LANL LES
12/14 – *hp*-Adaptive module in 3-D KIVA PCS routines formerly making KIVA-hpFE!
02/15 – Conjugate Heat Transfer proof of concept implement in KiVA-hpFE, simple test
01/15 – MPI parallel working in KIVA-FE with RANS and dynamic LES
02/15 – ALE with piston and curved bowled, scalloped bowl
03/15 – ALE implemented in the KIVA-hpFE solver system
04/15 – Methane benchmark test started, completion of 3D backward-facing step & 3-D flow over cylinder benchmarks with dynamic LES and RANS
10/15 – Parallel Spray Model complete and partial validation with dynamic LES turbulence modeling
01/16 – Parallel Moving Parts complete with compressible flow KIVA-hpFE
02/16 – Implicit Solution Algorithm completed
03/16 – Engine system modeling burning gasoline tested with plasma kernel spark model
02/16 – Starting incorporating ChemKin-Pro and ChemKin
02/16 – Issued and Received replies on RFI for commercialization of the software, processing replies to RFI
03/12 to 03/16 – Presentations AEC, ASME, ICHT, IHTC, V&V with Papers to ICHT, IHTC, NHT, and CTS

Approach to achieve Objectives

- **Design** and **Invent new** **modeling** **methods** and software
  - The **new** **Design** is change of discretization to FEM method
    - The FEM allows for many improvements:
      - Invent the FEM PCS projection method
      - Develop the *hp*-adaptive system
      - Invent the local-ALE method more moving bodies
      - Develop new Dynamic LES,
      - Invent Method for implementing MPI for today's & future platforms.
      - Develop
        - *Design, Invent, Develop, Validate, Verify…*
  - **Build** the model/code so that it meets all the objectives
    - Build the model in new Fortran, objective, clean, easy to maintain and add submodels
    - Careful Verification and Validation on pertinent problems

Technical Accomplishments***

New Methods and Models for more Predictive Modeling

FEM Flow modeling

- More Accuracy in KIVA multi-component Spray model: evaporation, break-up, wall film
- More Accurate (new) droplet transport modeling
- Eulerian, with better RANS with k-ϖ turbulence modeling
- Dynamic LES capable of transitioning from laminar to fully turbulent flow
- Spark Plasma Kernel Approximation, a nodal valued Model
- Chemistry and Fuels incorporated (KIVA 30+ fuels - ChemKin-Pro being added)
- Conjugate Heat Transfer method being developed
- Implicit Solution Algorithm and linear equation solvers fully implemented

hp-adaptive FEM

- Higher order accurate - 2^{nd} and better spatial accuracy everywhere & always
  - Minimum 3^{rd} order accuracy for advection terms
- Minimal communication for faster processing – Super linear speed-up
- Evolving solution error drives grid
  - Resolution and higher-order approximation
- *hp*-adaptive FEM – exponentially grid convergent

*** Some of the accomplishments are demonstrated in reviewer-only slides or in previous presentations and papers

Local ALE in FEM

- Quick, accurate, robust moving parts (Mesh can never tangle)
  - Robust and 2^{nd} order accurate Local ALE for moving parts!
- Faster grid generation - CAD to CFD grid in nearly a single step

Parallel Solution

- Efficient MPI and OpenMP processing on moderate computer platforms.
- Beam-Warming Method with Parallel Additive Schwartz preconditioning developed for LANL PCG (Joubert & Carey) solver package.

Technical Accomplishments in 2016

KIVA-hpFE for *achieving robust, efficient, & accurate Engine Modeling*

- ***Implicit Solution*** Algorithms completed and tested
  - **Allows for larger time step size – up to 1000x larger than explicit method and is faster than explicit**
  - **Implicit Viscous and other diffusive terms with explicit advection for CFL limit**
- ***LES turbulence modeling***
  - ***LANL's LES has the following attributes (must have for appropriate engine modeling)***
    - *Spans laminar to fully turbulent flows*
    - *Wall bounded flows without need for wall-law functions*
    - ***Testing benchmark problems and running in engine type configurations***
- ***Parallel Solution (MPI with KIVA-hpFE)***
  - ***Efficient MPI processing for moderate to LANL type computer platforms.***
    - By design - **Minimal communication for faster processing – Super linear speed-up**
    - *New linear equation solver system fully utilized with implicit solution algorithm*
    - *No flux calculations required, the mathematical statement automatically conserves flux*
    - ***Parallel moving parts and spray modeling with LES completed***
      - ***Tested against 1 experiment so far – ECN testing to start***
- ***hp-adaptive FEM exponentially convergent > p > 2***
  - ***Testing the KIVA-hpFE compressible / all-flow solver***
- ***Local-ALE in FEM methods***
  - ***Tested in 3D on curved domains***
  - ***Testing and finish implementing in KIVA-hpFE engine solver***
  - ***Testing engine configurations with Combustion and Spark Kernel Model***
- ***Spray modeling enhancement with VOF system***

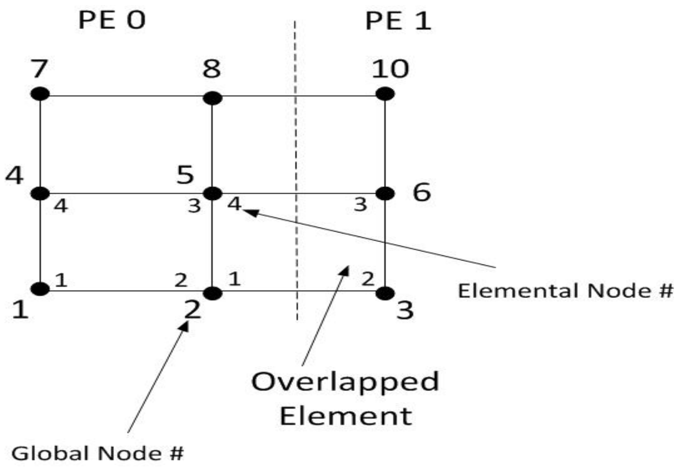
Source code completed, testing solutions and debugging

Dynamic LES for wall-bounded and transitional flow

- **LANL's KIVA-hpFE LES**
  - Laminar to turbulent, method handles transitional flow
    - **Required for engines, not always turbulent, and is certainly wall-bounded flow**
  - Self-damping at wall, no law-of-the-wall (required for accurate modeling)
- **Dynamic LES**
  - Backscatter (upscaling of small eddy energy)
  - Results comparable to k-ϖ RANS and matches experiments
  - The DSGS model calculates the model coefficient from the energy of the smallest resolved scale
  - Governing Navier-Stokes and transport equations become filtered equations

Parallel Solution of the Implicit Diffusion/Viscous Predictor-Corrector Scheme

- Two sets of decomposition: one for the elements and one for the nodes
  - Read an element and processor file (par-metis to decompose the mesh)
  - Use the element and processor file to generate a node and processor file.
- The integration over an **overlapped element** requires gathering values whenever a node value is off processor.

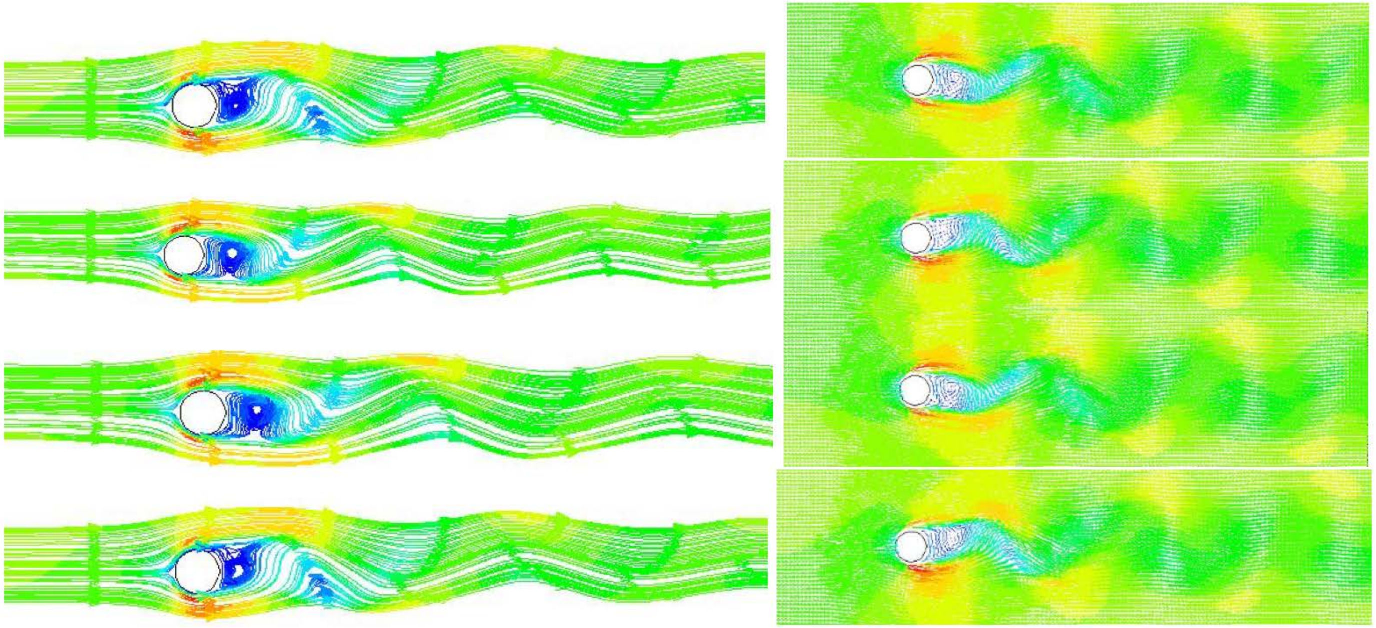


Non-overlapped grid portion and an overlapping grid portion of the domain

Dynamic LES Turbulence Modeling:

Incompressible flow over a cylinder

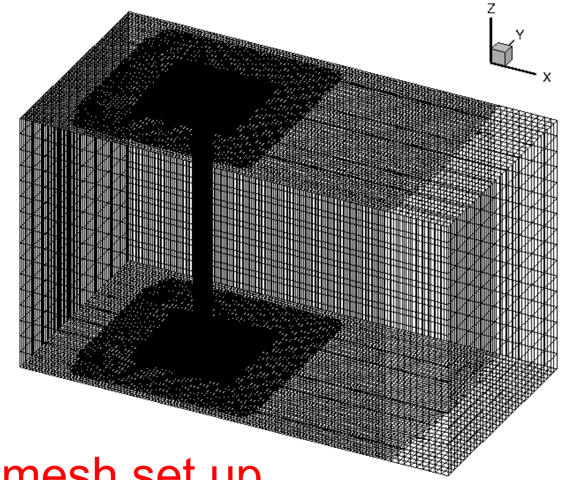
- Incompressible flow over a cylinder with $\mathrm{Re} = 1000$
- The simulation setup is for flow having an inlet velocity of U=0.9m/s. The walls are no slip boundaries.
- we can see the flow starts to separate from *θ=80°* which agrees with the analytic theory.



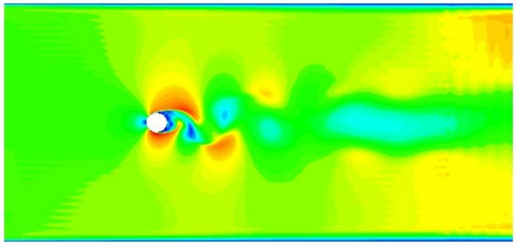
Streamlines (left) and velocity (right) at time 4.3s, 4.4s, 4.5s and 4.6s (from top to bottom)

Dynamic LES Turbulence Modeling

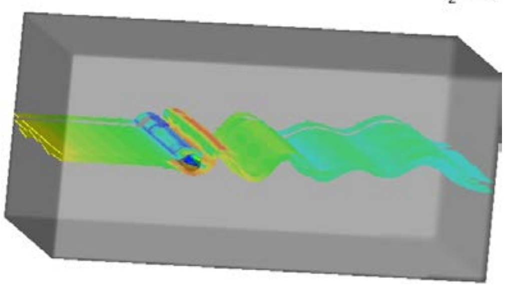
Compressible flow solver over a cylinder with Re= 1000



mesh set up
~450K cells

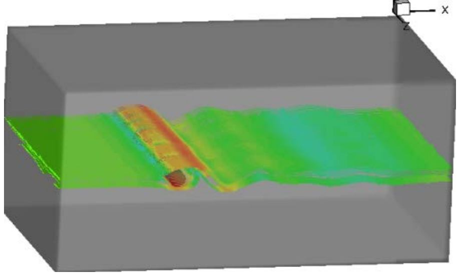


Velocity contour at meridian
1.0 second.

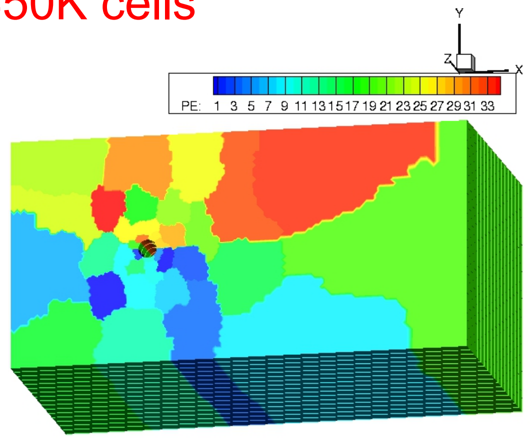


0.7 seconds

Streamlines

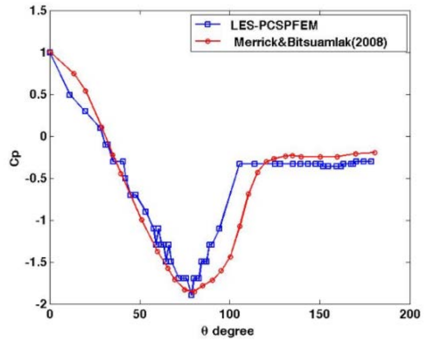


1.0 seconds.

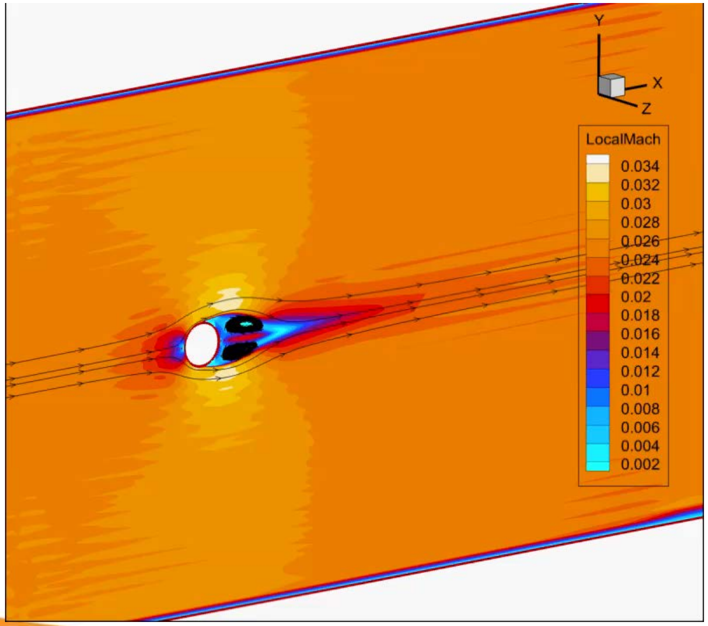


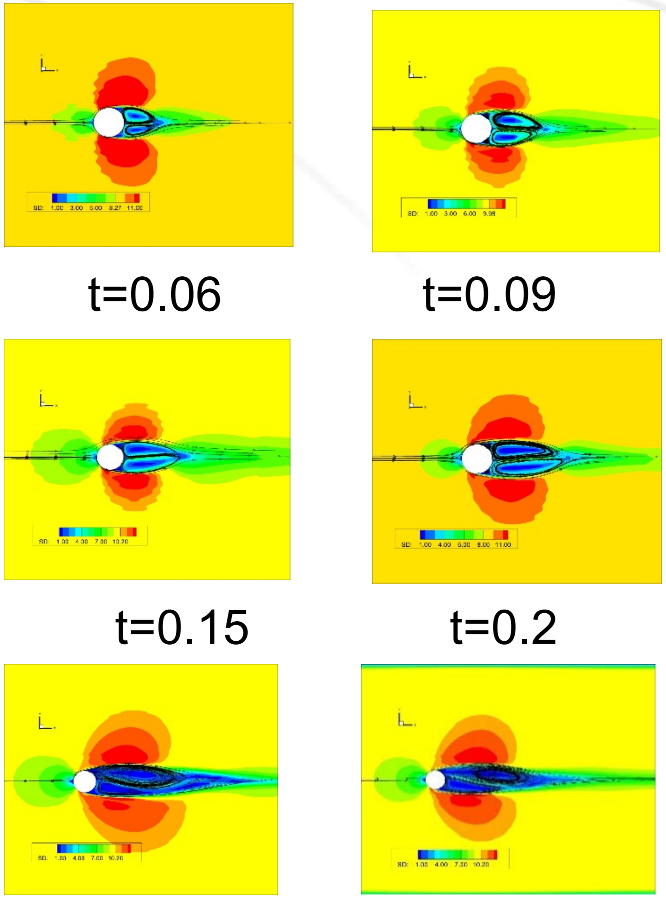
Simulation domain decomposition
onto 36 processors

Dynamic LES Turbulence Modeling
Compressible flow over a cylinder with Re= 1.2e+05



Coefficient of Pressure
(Re= 1.2×10^5)





t=0.06 t=0.09

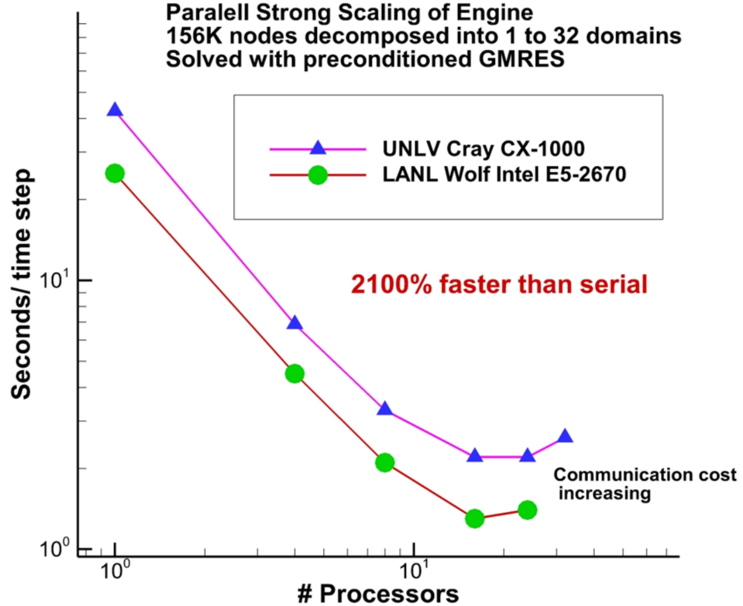
t=0.15 t=0.2

t=0.5 t=1.0

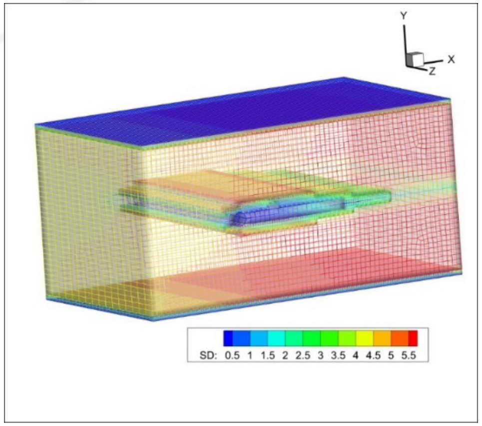
Instantaneous velocity streamlines for Re=1.2×10^5

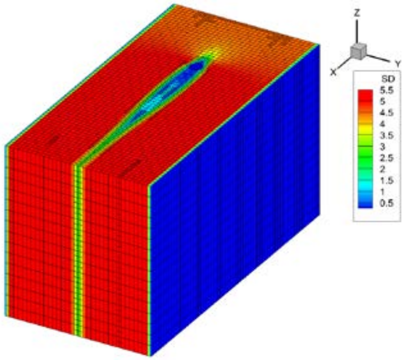
Parallel Solution of the PCS Scheme

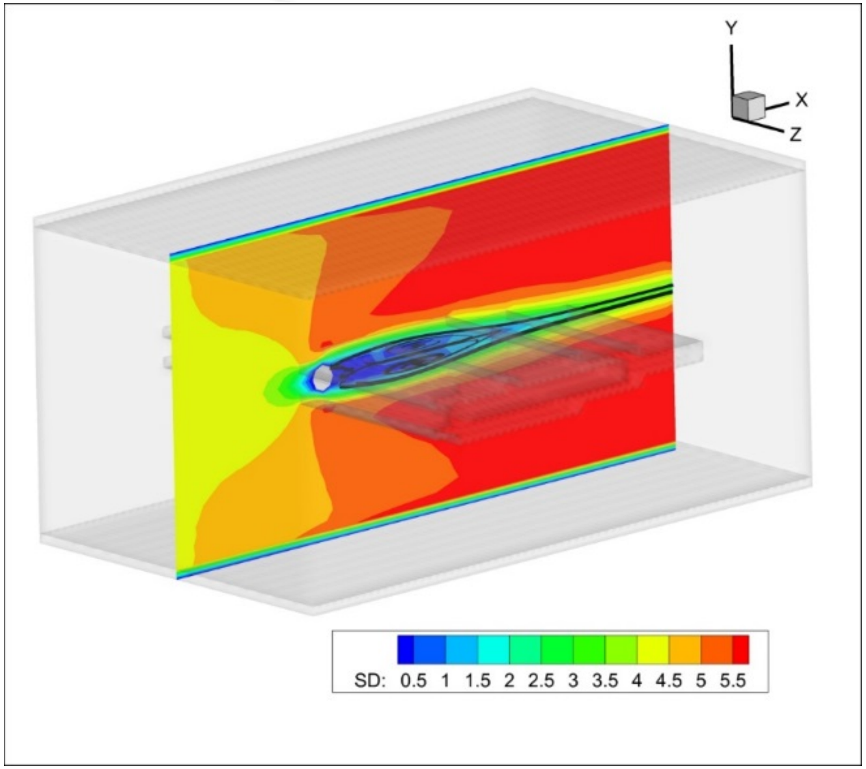
- Parallel Strong Scaling - **Super-Linear** speed-up 29x speed-up.
  - Minimal communication requirements and easy vectorization
  - Exascale compatabile algorithm – vectorizable algorithm
    - no flux calculations requiring communication
    - no ghost cells needing filled - no material properties or flux calculations collected



Flow over cylinder benchmark with RANS and h-adaptation in KIVA-hpFE





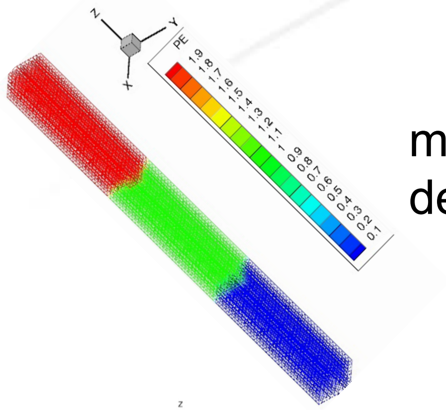


KIVA-hpFE with RANS showing vortex shedding
Re = 1e+05 using h-adaptive system.

Parallel LES and Multicomponent Lagrangian Particle Liquid Spray Modeling

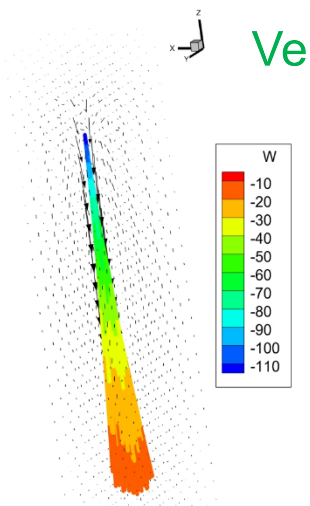
2016 DOE Merit Review

Validation of spray penetration

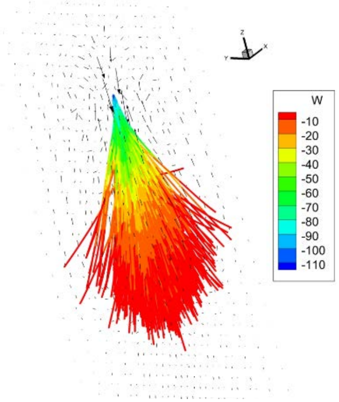


mesh decomposition

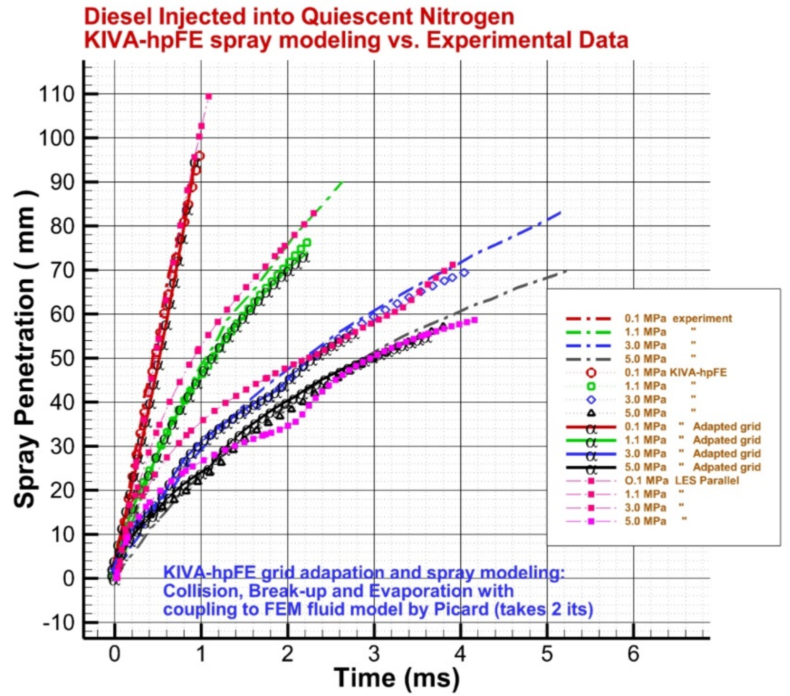
Velocity of injected spray



1.1 MPa



5.0 MPa

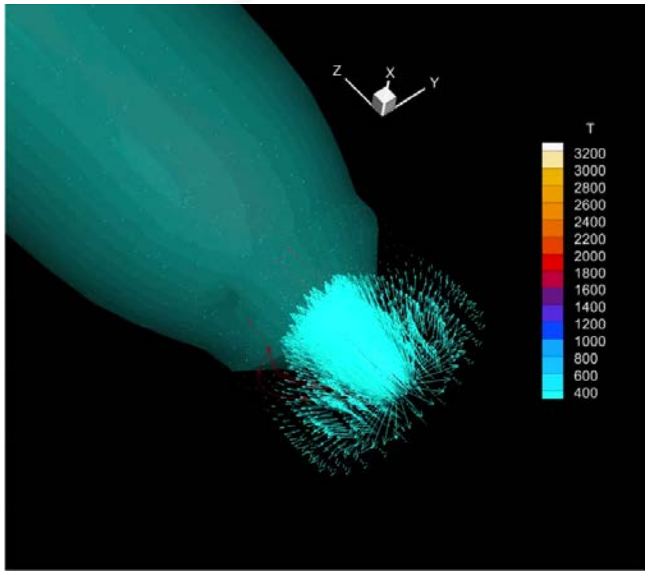


Parallel LES and particle spray
Penetration vs. time
compared to experiment and grid resolution

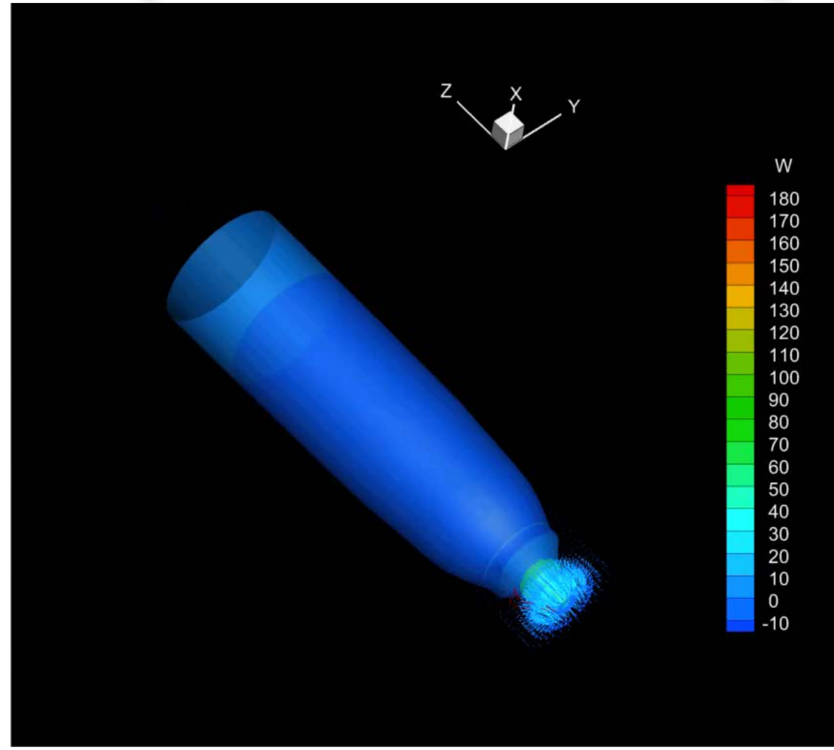
Experimental data from Hiroyasu and Kadota [20] and KIVA-hpFE serial code and adapted grid by Carrington et. al.

Coaxial Jet Methane Burner Methane

Benchmark in Progress



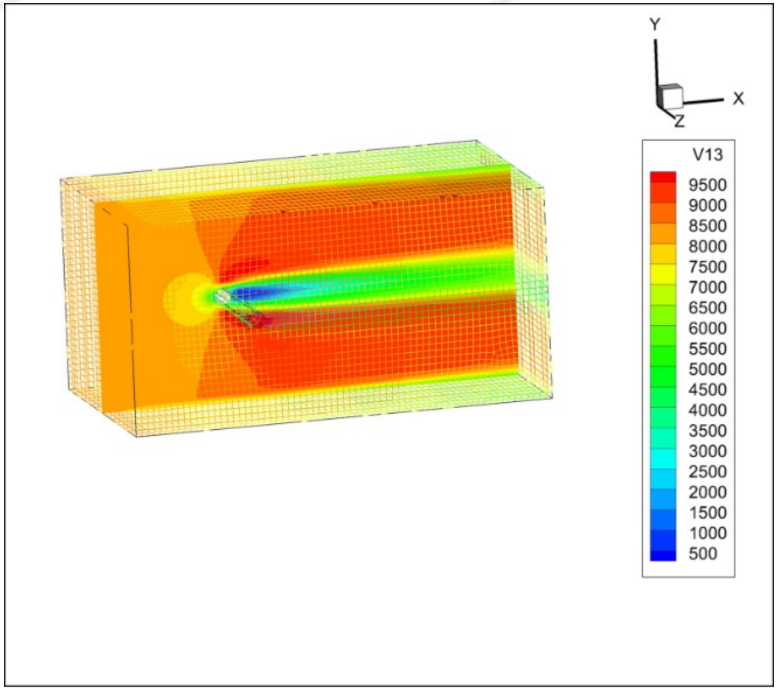
Temperature in time



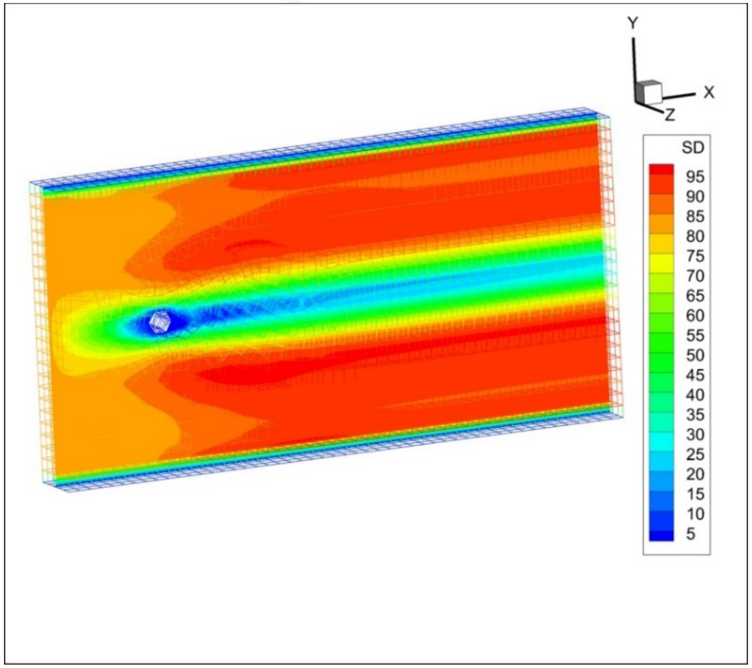
W component Velocity in time

- Coarse grid of ~8K cells
- Preliminary results with k-ω RANS and Plasma Spark Kernel Model
- Developing test case for KIVA-hpFE(vs. simulations* & experimental data**)
  - * Kim, Y.M., Chung, T.J. (1989)
  - ** Lockwood , F.C, El Mahallawy, F.M., and Spalding, D.B.(1974)

Comparison of KIVA-4mpi to KIVA-hpFE

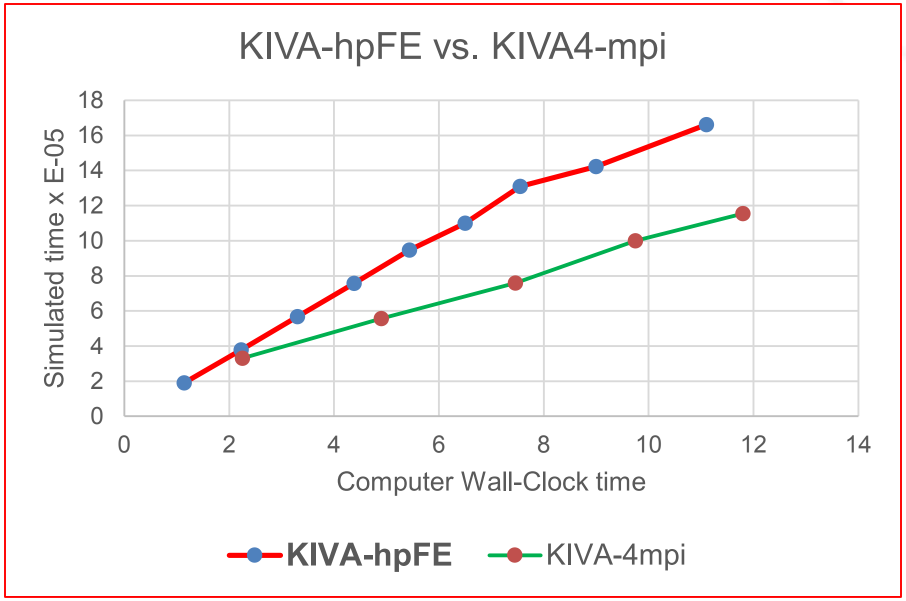


KIVA-4 with 34K cells
tests shows no vortex shedding



KIVA-hpFE shows vortex shedding at somewhat lower resolution than the KIVA-4 at 34K

Side by Side comparison of KIVA-4mpi to KIVA-hpFE



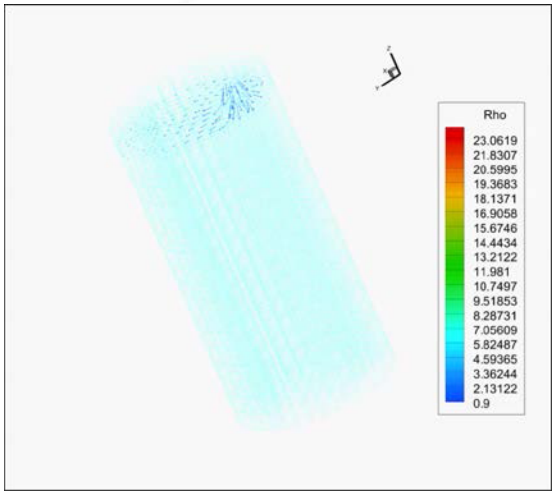
- KIVA-hpFE explicit is at least 1.5x faster (Wall clock 10 minutes) than KIVA-4 explicit on the same computer using the same grid and settings (34K cells domain)
- Since the curves continue to diverge => KIVA-hpFE speed >> older KIVA's speed

The way we've coded this, **could be the a 1st for FEM faster than FV.** The FEM is a more accurate (essentially any order desired), with concise coding and error measure.

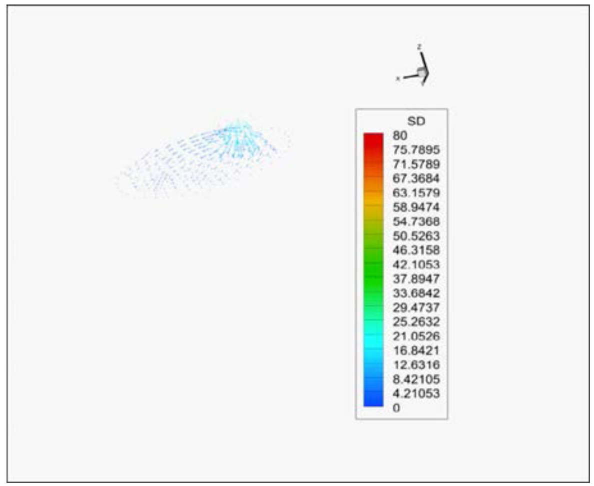
KIVA-hpFE Parallel Implicit Viscous PCS solve with reduced matrices

Local 3-D ALE for moving parts on unstructured grids

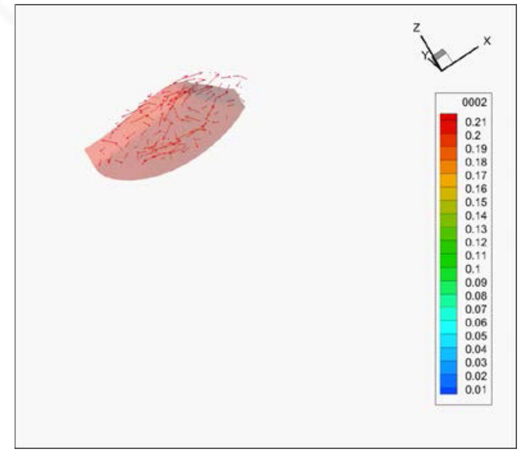
Operating Engine System



Density f(CA)



Speed of gases f(CA)

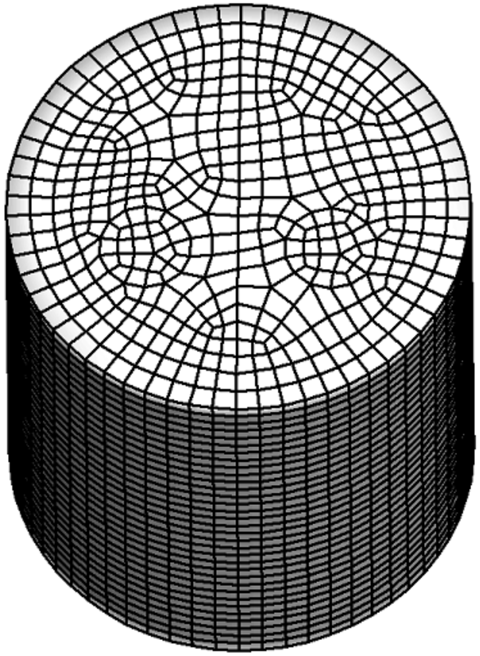


Gasoline combustion TDC
Spark Plasma Kernel ~25 W
O_2 Iso-surfaces

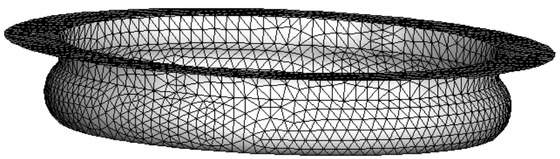
Flat Piston Engine Geometry at 1000 rpm

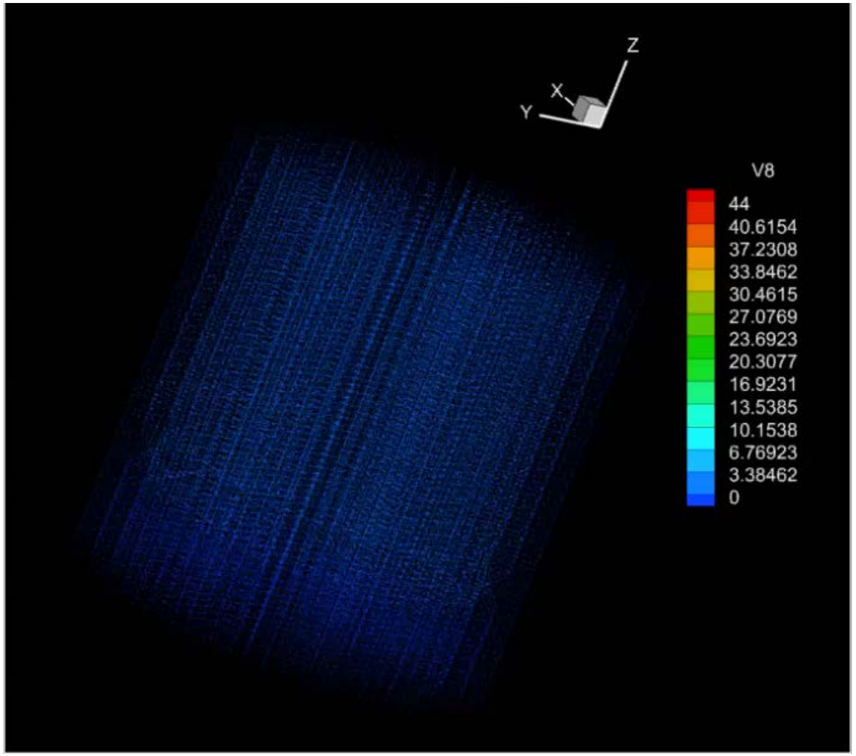
- Dynamic LES is implemented
- Similar results with RANS k-ω
- Comparing to KIVA-4 results as first cut
- **Only 1% of CPU time for grid movement**

Local 3-D ALE for moving parts on unstructured grids in KIVA-hpFE

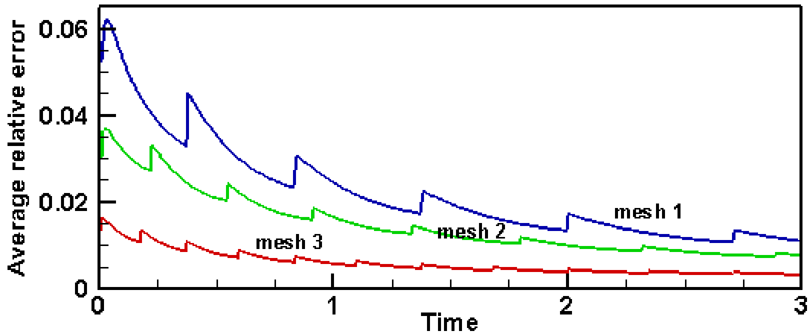


Piston with curved bowl

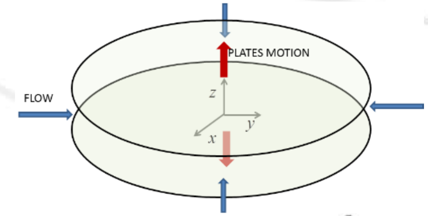


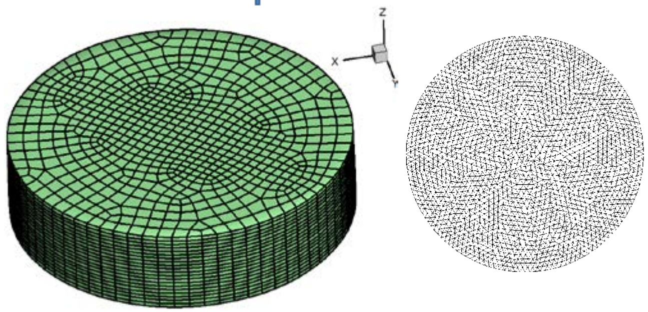


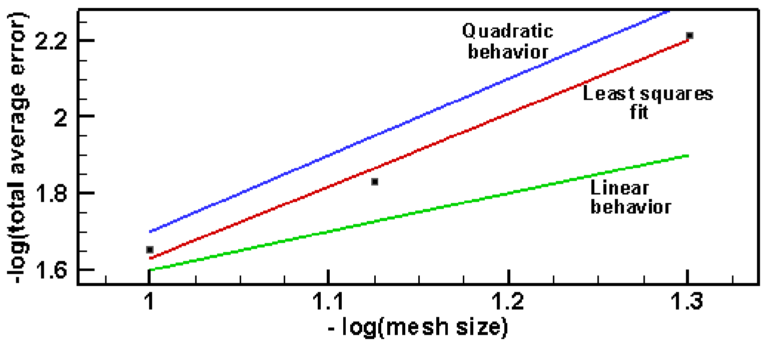
Error of the Local-ALE system in 3-D



Relative error in the velocity magnitude for Meshes 1, 2 and 3.







Convergence rate for the velocity magnitude in flow between parallel plates separating with prescribed velocity. The calculated convergence rate is 1.901.

$j^{th}\, grid$	h_j	$\left(\bar{E}\right)_j$
1	0.1	0.02235
2	0.075	0.01475
3	0.05	0.00607

Total averaged spatial relative error for the separating disks problem.

1. Hatamipour, V.D., Carrington, D.B., Heinrich, J.C., “Accuracy and Convergence of Arbitrary Lagrangian-Eulerian Finite Element Simulations based on a Fixed Mesh,” Progress in Computational Fluid Dynamics, an Int. Jour (submitted December 2015).

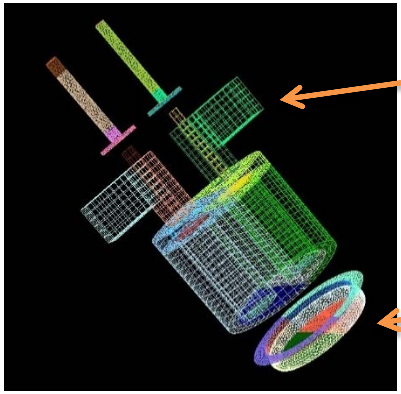
Grid Generation

2016 DOE Merit Review

- Overlaying parts for easy/automatic grid generation.

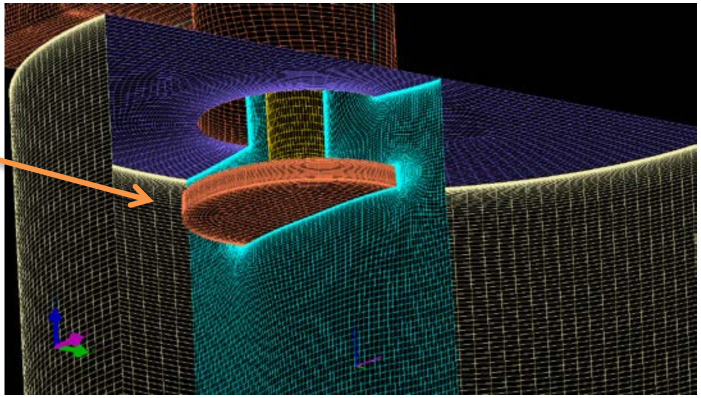
New Local ALE method allows for:

- Overset grid generation – fast CAD to CFD grid
  - Labor not nearly as significant as traditionally done
- Robust and Accurate moving parts representation
- Collaborating with Peter Eissmen at GridPro Inc. to incorporate KIVA-hpFE format



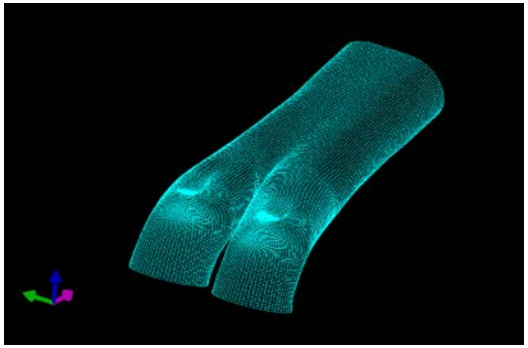
Overlaid valves

Overlaid piston



Grid Pro

Cubit Meshing Tool



Intake Manifold of Sandia DISI engine taken from X-ray generated faceted surface

GridPro is the better option versus Cubit Grids

Test Engine with 3D ALE beginning

Challenges and Barriers

- Challenges include:
  - Turbulence modeling
    - HPC with LES and combustion/spray modeling
    - LES with combustion modeling
  - Better spray modeling, primary break-up and interface capture
    - Two-phase turbulent flow for wall film and primary break-up
      - VOF Interface tracking with solution of interface stress
    - Better Dispersed Spray modeling
  - Full up engine modeling with KIVA-hpFE
  - Conjugate Heat Transfer seamlessly with parts and engine block
    - Meshless Method Condition model combined with FEM CFD
- Barriers include:
  - Proper sub-modeling of the primary break-up and turbulence along with interface tracking system for two-phase flow.
  - Combustion modeling with LES – interface tracking
  - Heat Transfer to the engine block and parts
    - Methods to develop is FEM for moving parts, and also research Meshless method for engine block/parts coupled to FEM

Reviewers' Comments

- **A reviewer felt that improved computational modeling for KIVA is very important: to have it more robust, and accurate**. We concur, and is exactly what out pursuit:
- **A few reviewers felt technical accomplishments demonstrated in the new KIVA code are excellent. They also felt it was important to have ICE & CFD examples versus another code so others can appreciate the differences.**
  - *We greatly appreciate the acknowledgement of good technical accomplishments. This effort is a complex process; developing a new system for engine modeling that makes a great deal fewer assumptions and provides much higher accuracy, while at the same time is faster than older methods or even Finite Volume methods. The current codes in use are the product of > decade of development (e.g. Convergent 2002 and is not state-of-the-art)*
  - ***Our accomplishments so far done in ~5 years with limited budgets a couple of people**.*
  - ***We are nearing that engine modeling capability to do side-by-side comparisons with other codes and validate with experimental engine data and engine standard cases***
    - ***The issue is more than just submodels**. Good submodels on an inherently inaccurate solver doesn't address the problem. Properly representing flow including its boundaries and moving parts are critical to proper submodel performance as demonstrated by our new spray modeling system, with greater accuracy and coupling. More accurate modeling with new algorithms is being developed. We have proceeded with great emphasis and promise by using newest algorithms and leveraging our recent research in state-of-the-art methods.*
    - ***Careful validation is critical** to having a software capable of predictability. We insure each portion the solver works as expected, requiring careful testing and analysis on the proper problems.*
    - ***Comparisons are made of current KIVA versus the PCS FEM.** Tests conducted to date, the older KIVA does not do nearly as well as the FEM method and typically needs an **order of magnitude more cells** than the method being developed. Often older KIVA does not produce exact answers. In this report we show comparison to KIVA on a benchmark problem where KIVA-4 fails (shown in the past too).*
    - *We've been comparing with Convergent in an informal collaboration to understand issues with Convergent.*
- ***A reviewer suggested we do more spray modeling comparison work in the ECN Network.***
  - *We are starting work on the spray modeling in greater detail to be predictive, and have begun to participate in the ECN now. We are hoping also to collaborate with a University to help us perform the ECN experiments with the new KIVA-hpFE.*
- ***Many reviewers wondered how this might benefit more than just university researchers, how would it be supporting industry's needs, and in the hands of industrial users.***
  - *We greatly appreciate this comment and have taken many things in the development process to meet many different requirements of the code. One requirement is open source, another is the ability to support industrial users.*
  - *The design of the code allows for just this, university and industry access to the source code, yet because the code is levelized, much of the inner workings should never be adjusted are underneath, allowing for commercialization of the software.*
  - ***We are now considering the replies to our RFI for commercialization of the software and which one (or all) will best suit industries needs and fit all goals. ANSYS also has expressed interest in putting KIVA-hpFE into their suite of software. We are starting to develop in collaboration with ANSYS, ChemKin-Pro links too.***

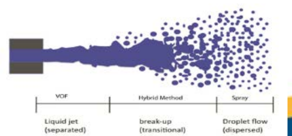
LANL & collaborations, KIVA-hpFE Development Team

Breakdown of efforts for the code and model components

1) ***Fast grid generation*** **- CAD to CFD** grid in nearly a single step
   Dr. Carrington and Brad Philipbar (GRA)
2) ***New FEM Solver algorithm and code for turbulent multi-species for all-speed flows***
   Dr. Carrington
3) ***Conjugate Heat Transfer*** **is free and seamless**
   Dr. Carrington and Waters
4) ***Local ALE - Mesh never tangles, robust 2nd order accurate*** **moving parts**
   Drs. Heinrich, Mazumder, Carrington and Mr. Dominic Munoz
5) ***hp*-adaptive FEM – exponentially grid convergent & evolving error drives the approximation**
   Drs. Wang, Waters and Carrington
6) **MPI with for massively parallel processing, from small clusters to LANL sized supercomputers**
   Drs. Waters and Carrington
7) **Dynamic LES turbulence modeling for all flow speeds (transition to turbulence)**
   Dr. Waters and Carrington
8) ***2nd Order accurate multi-component Spray model***
   1) ***Accurate even on coarser grids***
   2) ***Volume of Fluid (VOF) for initial spray break-up and wall films***
   Drs. Water, Francois, and Carrington
9) **Better RANS *k-ϖ* turbulence modeling**
   Dr. Carrington
10) **Plasma Spark Model applied at an element node**
   Dr. Carrington

Future or Ongoing effort in FY17 to FY 19

- V&V of Spray and Combustion Systems (ongoing)
  - *Incorporate LLNL* fast chemistry system for ChemKin
  - Incorporate ChemKin and ChemKin-Pro
  - Combustion and Engine V&V (desire to work with other lab/university collaborators
  - Investigate and implement burn/flame models
- Conjugate heat transfer between combustion chamber rest of engine
  - FEM system development for solid and moving parts (ongoing)
  - FEM coupled to Meshless method for solid and moving parts (proposed)
- Parallel *hp*-adaptive PCS FEM in 3-D (ongoing)
  - MPI on the *hp*-adaptive modules
  - OpenMP embedded in MPI Parallel constructions (MPI, enhanced by OpenMP)
- LANL Local-ALE in 3-D (ongoing)
  - ***Full engine system, port, valves and piston***
  - Adding hierarchical prisms & tetrahedral elements for *hp*-adaptation and moving parts
- LANL LES Turbulence modeling development (ongoing)
  - **Dynamic LES tested with the *hp*-adaptive module in the PCS FEM.**
  - **Validating**
  - Other turbulence closure (future Reynolds Stress Modeling – 2nd moment methods)
- Spray model development in FEM (ongoing)
  - Two-phase turbulence modeling with interface tracking
  - VOF allows ligaments in flow by true stress modeling



Summary

New Methods and Models – *achieving robust, effective, efficient, & accurate Engine Modeling*

FEM **for with Turbulence Reactive Flow with sprays**

- ***Accurate KIVA multi-component Spray model: evaporation, break-up, wall film***
- ***Accurate (new) droplet transport modeling***
- ***Eulerian, with better/okay k-ϖ turbulence and Dynamic LES model***
- ***Conjugate Heat Transfer proven and partially implemented***
- ***Mixed elements to support Local ALE module***
- ***Matrix Reduction for active elements***
- ***Implicit Solver system for viscous and diffusion terms in all physics equations ~ 1000x larger dt***
- ***KIVA-hpFE is at least 1.5x faster than KIVA-4 and far more accurate***
- ***Fast Grid Generation, in collaboration with GridPro Inc.***
- ***ChemKin-Pro links being developed in collaboration with ANSYS Inc.***

hp-adaptive FEM

- Higher order accurate - greater spatial accuracy everywhere & always
- ***Evolving solution error drives grid***
- ***hp-adaptive FEM incorporated in the 3D PCS FEM all flow solver with some benchmarking (V&V)***

Local ALE in FEM

- ***2nd order accurate and the Mesh never tangles***
- ***Only 1% of solution time is spent on grid movement***
- ***Faster grid generation*** - CAD to CFD grid in nearly a single step

Parallel Solution

- ***MPI processing on moderate computer platforms.***
- ***Good Domain Decomposition and linear equation solver system***
- ***Beam-Warming Method with Parallel Additive Schwartz preconditioning***
- ***Parallel Spray and Moving Parts system demonstrated and partially validated***

Technical Back-Up Slides

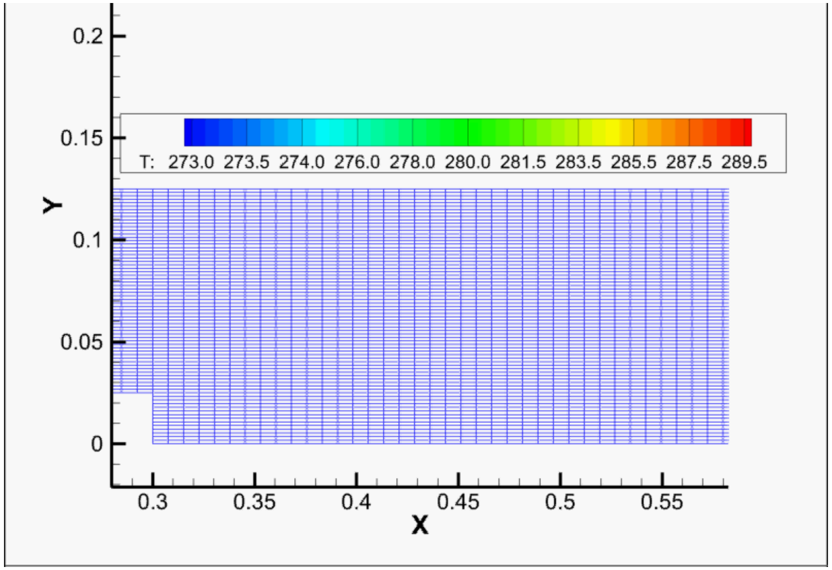
Dynamic LES for Wall Bounded Flows

Backward-facing step Re=27,000
Pr = 0.71, Air at 273 deg K
Incompressible flow

Convective flow: heat flux determines wall temperature.

- This is similar to the Conjugate Heat Transfer. Here heat flux is prescribed at the wall, rather than solving for it too.

Compares well to experimental data of Vogel and Eaton as shown in the previous slide.

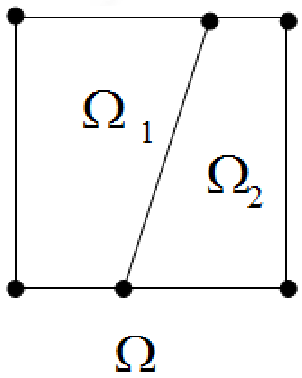


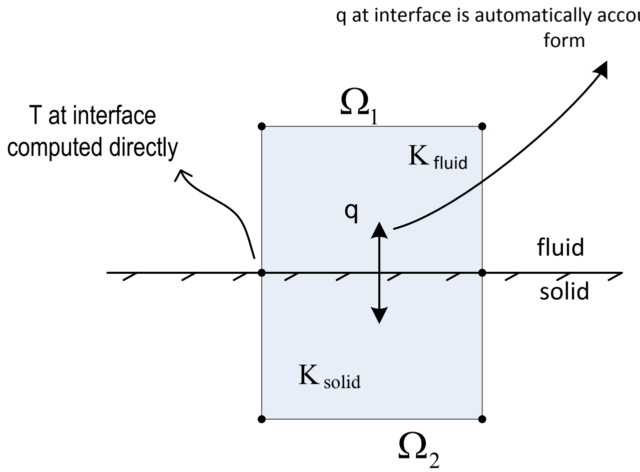
View is only around the step's vicinity

UNCLASSIFIED

Internal Energy Transport with Conjugate Heat Transfer

- **Eliminates need for heat transfer coefficient**
- **All the temperatures to be computed directly, heat flux automatically preserved.**
- Simple process when nodes are shared and easy for an interface element of moving solid and fluid.
  - Ω the interface element, Ω_1 **fluid**, Ω_2 **solid**
  - Energy and T at all nodes of solid, liquid and interface are calculated
  - Energy is advected at fluid nodes, convective heat transfer
  - Accurately establishes the temperatures and heat flux

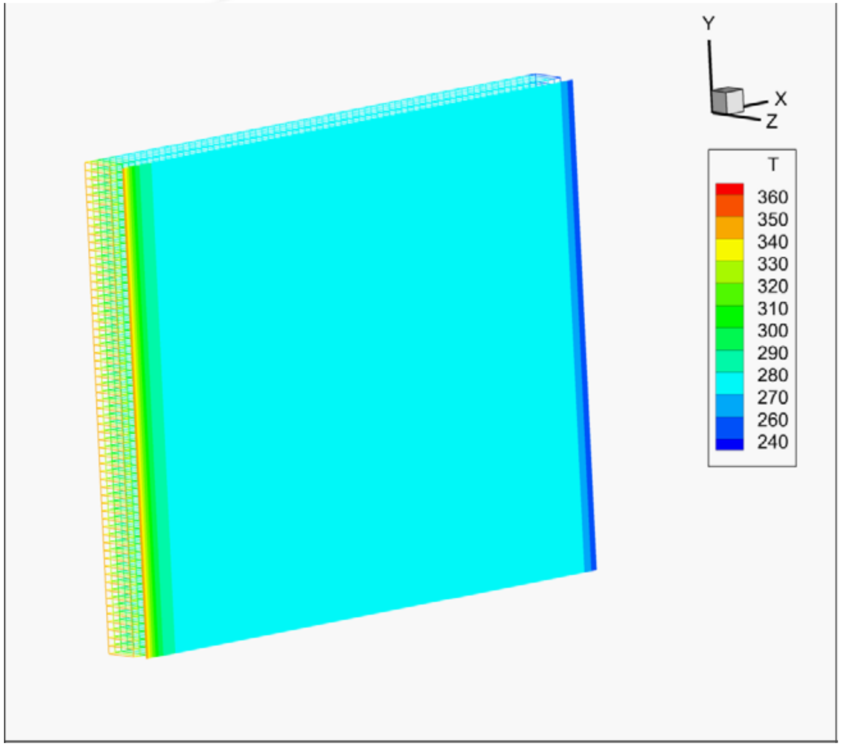




$$\int_{\Omega} N_i R(T_i)\, d\Omega = \int_{\Omega_1} N_i R(T_{1_i})\, d\Omega_1 + \int_{\Omega_2} N_i R(T_{2_i})\, d\Omega_2$$

Conjugate Heat Transfer

Differentially Heat Cavity filled with Air 279 K°



Steel case:

- 2 sides with fixed temperature
- Code identifies Solid and Fluid type Cells
- Standard boundary condition types:
  - Fixed temp walls outer walls
  - Fixed no-slip inner walls

Heat/Energy Conduction is solved in solids
Momentum, Energy, Species, Chemistry solved in fluids

Spark Kernel Model

- Heat from spark as function of time to *mimic* solution of Spark Kernel
  - Spark wattage as function of time (from ignition specification)
    - Discrete empirical model applied
    - 5 averaged pieces from the experimental values in J/s
  - Kernel heat loss as function of time from heat transfer mechanisms
  - Spark energy applied at single point (node) and processed through the momentum and energy equations before chemistry solve

Governing Eq. Spark Plasma Kernel

$$\frac{dU}{dt} = \frac{dW}{dt} + \frac{dQ_{chem}}{dt} - \frac{dQ_{loss}}{dt} - p\frac{dV_k}{dt}$$

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

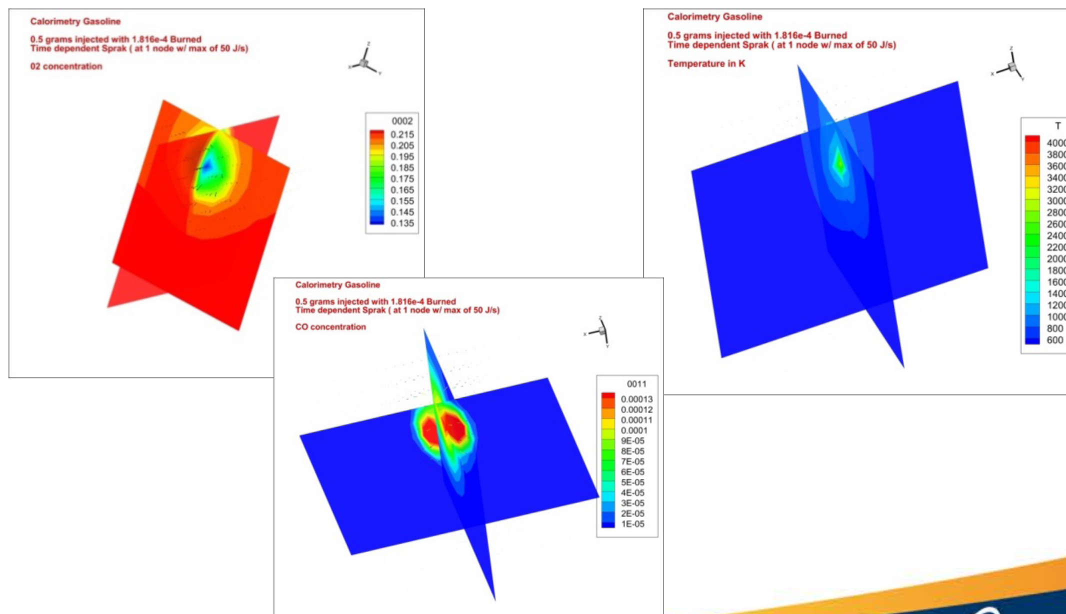
$$\frac{dV_k}{dt} = \frac{\rho_f}{\rho_k} A_k S_{eff} + V_k\left(\frac{1}{T_k}\frac{dT_k}{dt} - \frac{1}{P}\frac{dP}{dt}\right)$$

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

$$\frac{dh_k}{dt} = c_{p,k}\frac{dT_k}{dt} \qquad S_{eff} = S_{flame} + S_{heat\_diff}$$

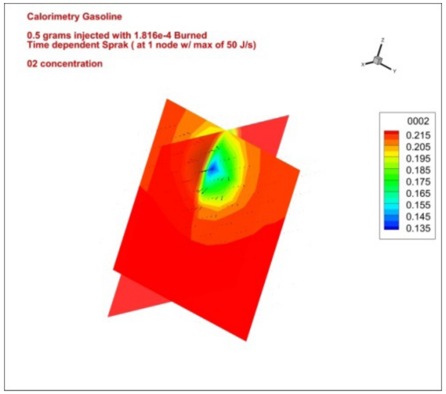
Velocity of Flame + Heat diffusion

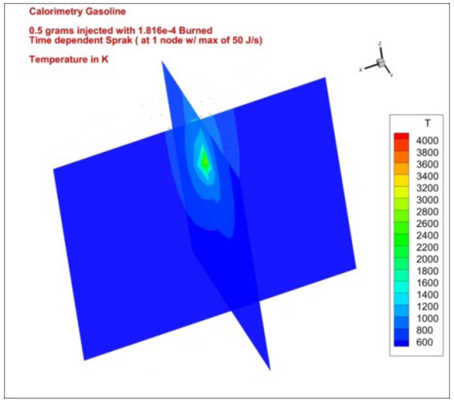
- Calorimetric validation to LHV
  - 0.5 grams Gasoline (KIVA) at 325K injected into Air at 1atm & 296 K
  - Spark at node at max of 50 J/s

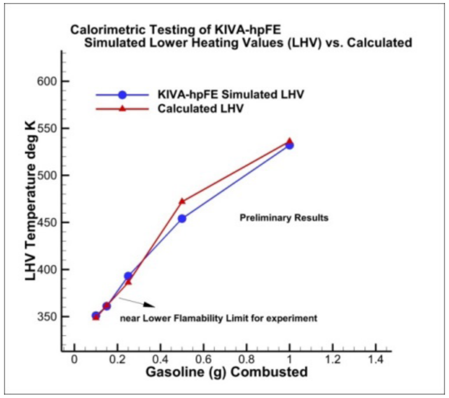


Spark/Flame Kernel Approximation Model

- Spark Heat Transfer - *f*(Δt)
  - Spark wattage as function of time (from ignition specification)
    - Discrete empirical model applied $\Delta t >> dt$
    - 5 averaged pieces from the experimental values in J/s
  - Kernel heat loss as function of time
    - Discrete model based on reported solution to equations $\Delta t >> dt$
    - 5 averaged pieces from the Plasma kernel model equation results in J/s
  - Spark energy applied at single point (node)
    Then solve momentum and energy equations before chemistry solve







- Calorimetric validation to LHV
  - Gasoline (KIVA) at 325K injected into Air at 1atm & 296 K
  - Spark at node at max of 50 J/s