

2015 **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
- 9/31/16
- 80% complete (the last 10% in CFD development takes the most effort)

Budget

- Total project funding to date:
 - 3400K
 - 705K in FY 14
 - Contractor (Universities) share ~40%

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

Partners

- University of New Mexico- Dr. Juan Heinrich
- University of Purdue, Calumet - Dr. Xiuling Wang
- University of Nevada, Las Vegas - Drs. Jiajia Waters and Darrell W. Pepper

- **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 – some issues
 - KIVA-4 engine grid generation (pretty much automatic but some snapper work around 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.

Milestones for FY 10- FY15

2015 DOE
Merit Review

09/09 – 2D and 3D P-G Fractional Step (PCS/CBS) Finite Element Algorithm Mathematical formulated.
02/10 – h-adaptive grid technique/algorithm implement in PCS-FEM method for 3D
02/10 – hp-adaptive FEM Algorithm & Framework: continued development and changes.
02/10 thru 09/10 – Successful at meeting standard incompressible benchmark problems.
05/10 – Multi-Species Transport testing in PCS-FEM algorithm.
10/10 – P-G found to be more flexible than CBS stabilization via benchmark comparisons.
12/10 to 03/12 – Developing PCS algorithm/coding into hp-adaptive Framework.
01/11 – FY11 Engineering documentation and precise algorithm details published (available publicly from library reference).
05/11 – Compressible flow solver completed, benchmarked inviscid supersonic
09/11 – Completed incorporating Cubit Grids for KIVA-4 and the FEM method too Cubit2KIVA4 & Cubit2FEM
10/11 – 2-D subsonic and supersonic viscous Flow benchmarks with turbulence
10/11 – Local ALE for immersed moving parts with overset grid system 2-D
12/11 – Benchmarked 2-D Local ALE for velocity
12/11 – Parallel Conjugate Heat Transfer KIVA-4mpi
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 calorimetric 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!

12/15 – Conjugate Heat Transfer installed, tested but not validated

01/15 – MPI parallel working in KIVA-FE

02/15 – ALE with piston and curved bowled, scalloped bowl

03/15 – ALE implemented in the KIVA-hpFE solver system

03/12 to 02/15 – Presentations AEC, ASME, ICHT, IHTC, V&V with Papers to ICHT, IHTC, IJNMF and CTS

Slide 4

• Objective

To have a more Predictive Turbulent Reactive Flow Modeling software for engines with the following attributes
(most of the following attributes are those heralded by industry as necessities)

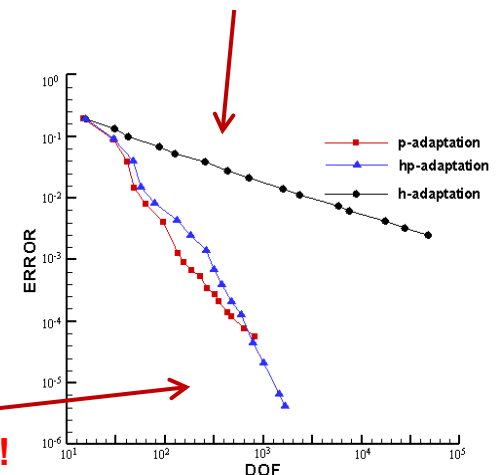
- 1) **Fast grid generation** - CAD to CFD grid in nearly a single step
- 2) **Mesh never tangles** – Robust and 2nd order accurate Local ALE for moving parts
- 3) **Higher order accurate** - higher spatial accuracy - everywhere & always with minimum 3rd order accuracy for advection terms
- 4) **Computational Speed with MPI** for parallel processing, from small clusters to LANL sized supers
- 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:**
 - i. Resolution and higher-order approximation
- 8) **Accurate Spray modeling**
 - 1) **2nd order accurate spray modeling even on coarser grids**
- 9) Eulerian Solve throughout
- 10) **Great LES** with attributes designed for engine flows
- 11) **Good RANS $k-\epsilon$ turbulence modeling**
- 12) **Conjugate Heat Transfer (CHT)**
- 13) **Plasma Spark Model applied at the element node**
 - 1) **More accurate and local heating from the plasma spark model**
- 14) **hp-adaptive FEM – exponentially grid convergent**

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 !

Slide 5

Approach to achieve Objectives

- **Design** and **Invent new modeling methods** and code
 - The **new Design** is change of discretization to FEM
 - Everything else just falls into place
 - 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.
 - *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

Breakdown of efforts for the code and model components

- 1) **Fast grid generation - CAD to CFD** grid in nearly a single step
Dr. Carrington
- 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
- 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 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, Carrington and Pepper
- 8) **2nd Order accurate multi-component Spray model, accurate even on coarser grids**
Dr. Carrington
- 9) **Better RANS $k-\omega$ turbulence modeling**
Dr. Carrington
- 10) **Plasma Spark Model applied at an element node**
Dr. Carrington

Technical Accomplishments

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Merit Review

New Methods and Models for more Predictive Modeling – *achieving robust & accurate Engine 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 $k-\omega$ 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 or ChemKin)*
- *Conjugate Heat Transfer method developed*

hp-adaptive FEM

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

Local ALE in FEM

- **Mesh never tangles**
 - *Robust and 2nd order accurate Local ALE for moving parts*
- **Faster grid generation** - CAD to CFD grid in nearly a single step

Parallel Solution

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

Slide 8

Technical Accomplishments in 2015

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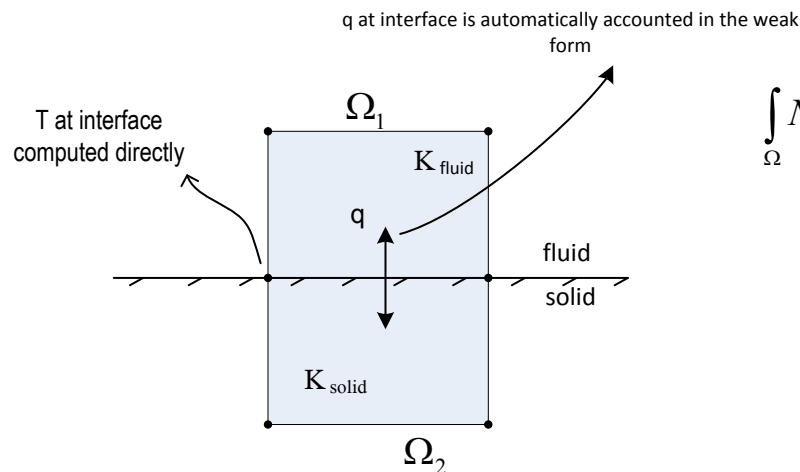
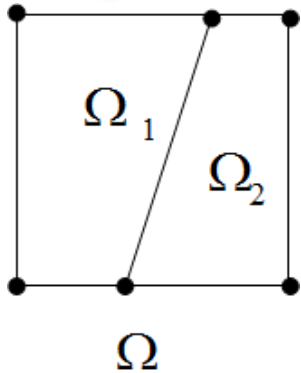
KIVA-hpFE for achieving robust, efficient, & accurate Engine Modeling

- **Conjugate Heat Transfer** (is essentially free)
 - More accurate prediction in wall-film and its effects on combustion and emissions
 - Providing accurate boundary conditions.
- **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**
- **Parallel Solution (MPI with KIVA-hpFE)**
 - **Efficient MPI processing for moderate to LANL type computer platforms.**
 - By design -- minimal communication for faster processing
 - **New linear equation solver system**
 - **Effective parallel solution scheme, clean and easier to implement than ghost cell systems**
 - **No flux calculations required, the mathematical statement automatically conserves flux**
- **hp-adaptive FEM exponentially convergent $> p > 2$**
 - **Finished Installation into the KIVA-hpFE compressible / all-flow solver**
- **Local-ALE in FEM methods**
 - **Tested in 3D on curved domains**
 - **Implemented in KIVA-hpFE engine solver**

Internal Energy Transport with Conjugate Heat Transfer

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Merit Review

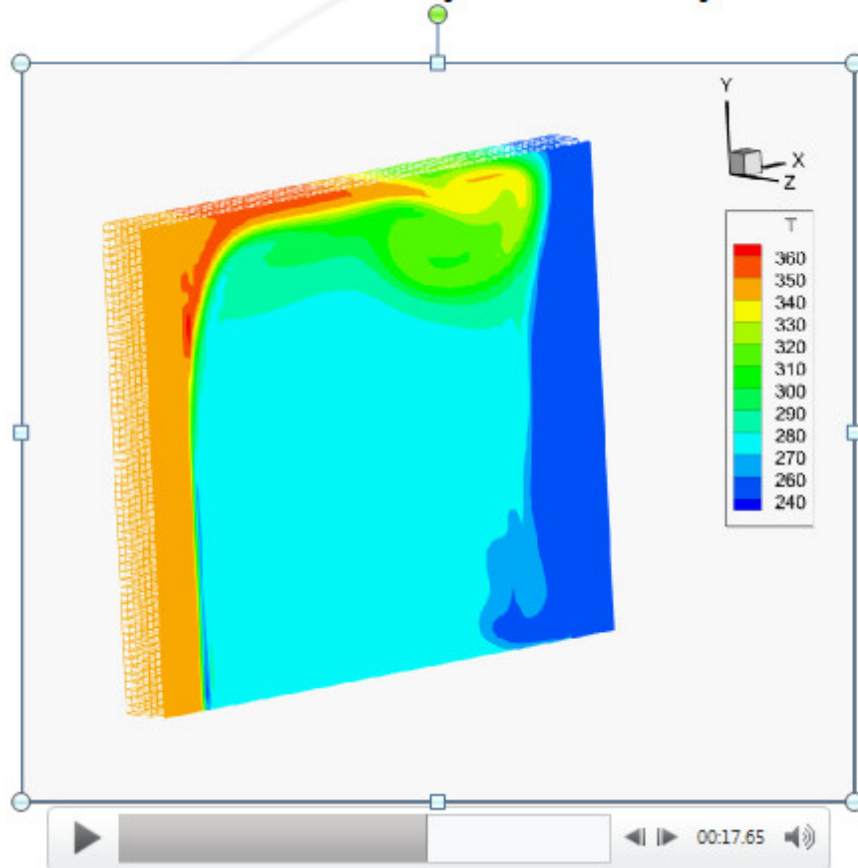
- **Eliminates need for heat transfer coefficient**
- **All the temperatures to be computed directly, heat flux automatically preserved.**
- Simple process when nodes are shared and easy for an interface element of moving solid and fluid.
 - Ω the interface element, Ω_1 **fluid**, Ω_2 **solid**
 - Energy 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



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

Conjugate Heat Transfer

Differentially Heat Cavity filled with Air 279 K_o



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

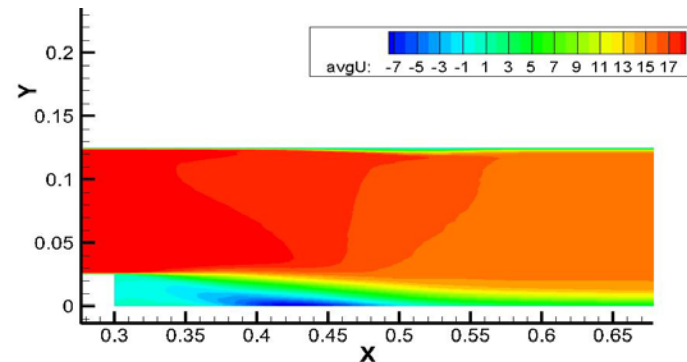
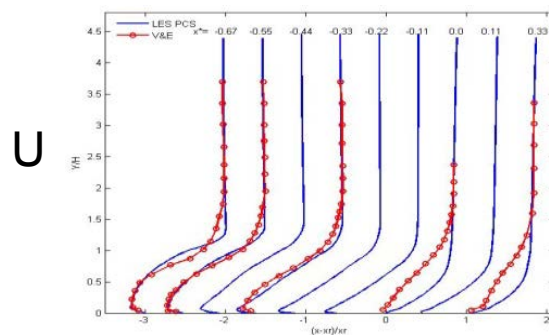
Dynamic LES wall-bounded and transitional flow

- **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 $k-\omega$ 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

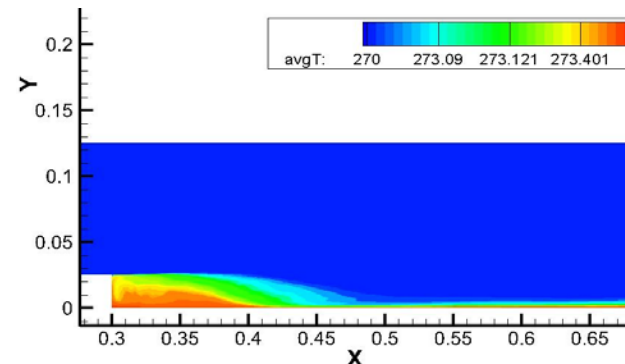
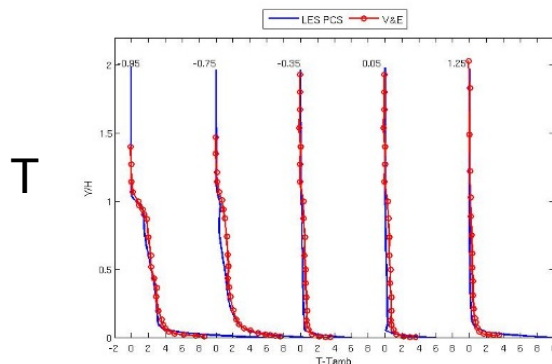
Dynamic LES method

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- 2-D Unsteady Turbulence Modeling
- h-adaptive Dynamic LES Predictor-Corrector Split FEM
- Backward facing step at $Re=27,000$ (incompressible) domain same as experiment
- Transitions through laminar flow; doesn't require wall-law or functions
- Dynamic model provides backscattering (upscaling)



View is only around
the step's vicinity



Truncated graphics
Inlet section is 30 cm
Outlet 30x step height

Exp. Data from Vogel and Eaton

Dynamic LES for Wall Bounded Flows

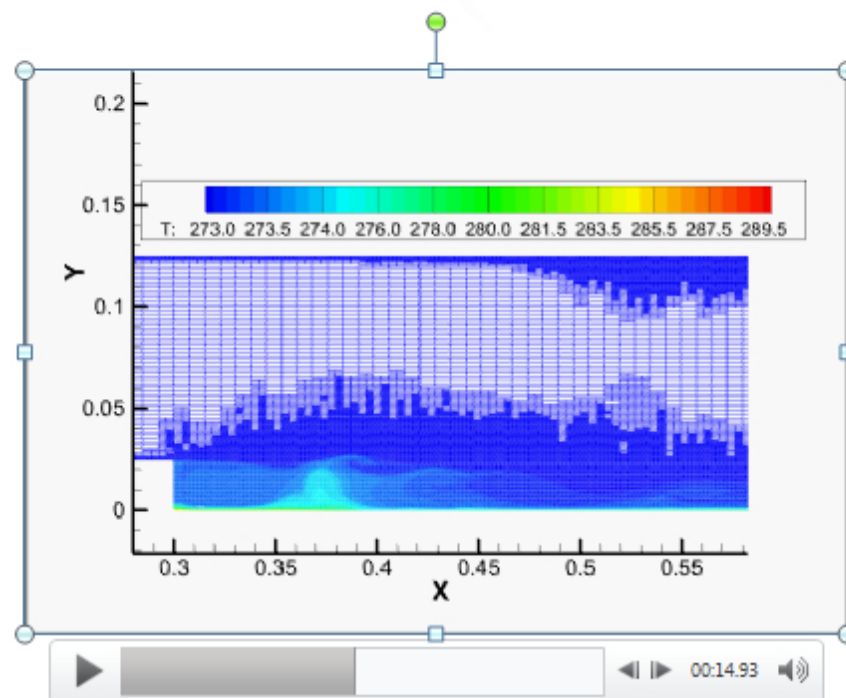
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Backward-facing step $Re=27,000$
 $Pr = 0.71$, Air at 273 deg K
Incompressible flow

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.

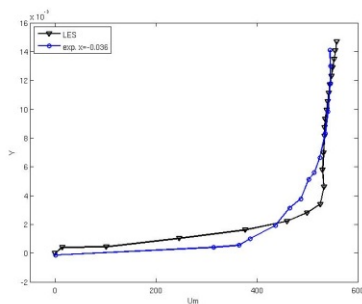
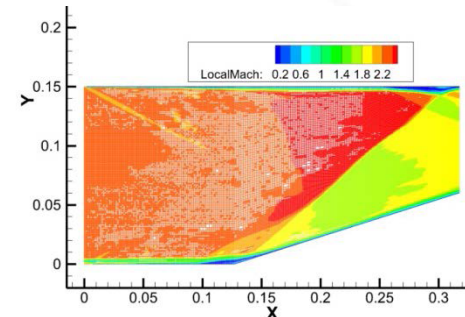
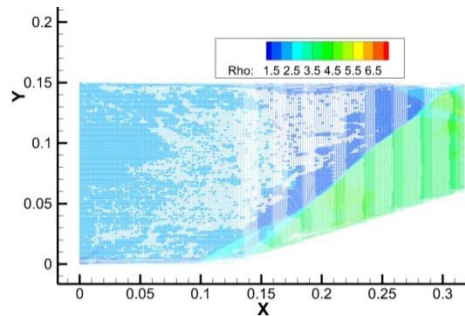
Compares well to experimental data of Vogel and Eaton as shown in the previous slide.



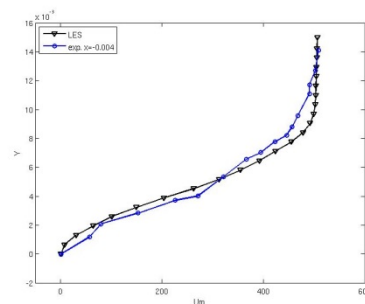
View is only around
the step's vicinity

Dynamic method LES

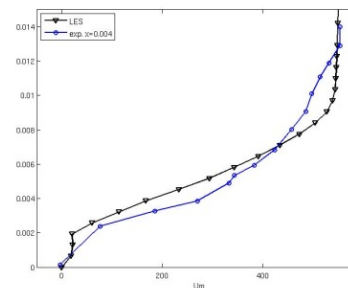
- 2-D Mach=2.25 Supersonic Flow over Compression Ramp
- **h-adaptive Dynamic LES** in the Predictor-Corrector Split scheme of **KIVA-hpFE**
- 18° compression ramp inlet speed Mach = 2.25



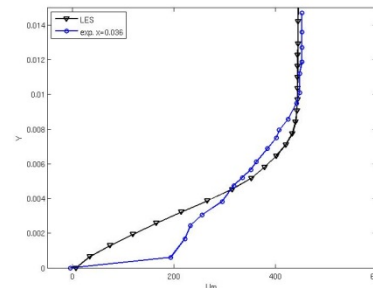
a)



b)



c)



d)

U (mean velocity) in bottom boundary layer using $k-\omega$ 2-equation model.

Comparison to data at various locations:

u upstream(-) and downstream(+) of the ramp a) -0.032m , b) -0.004m, c) +0.004m, and d) +0.032m.

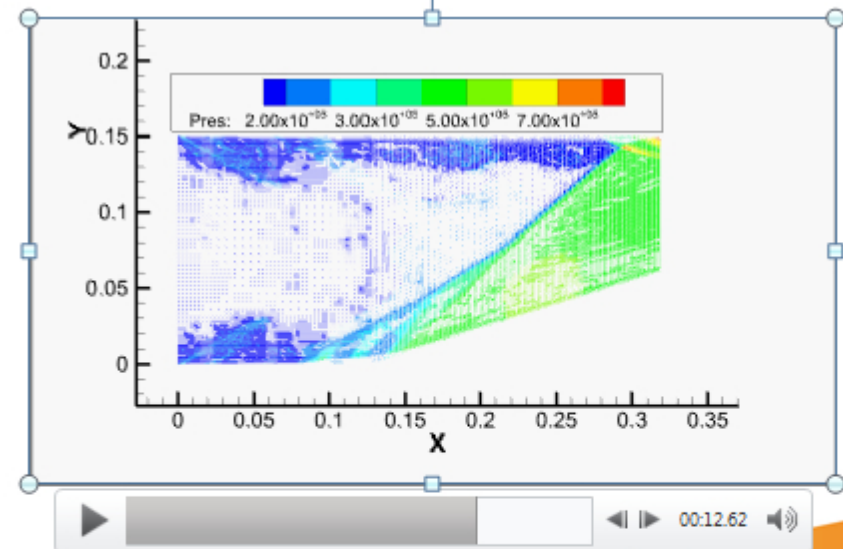
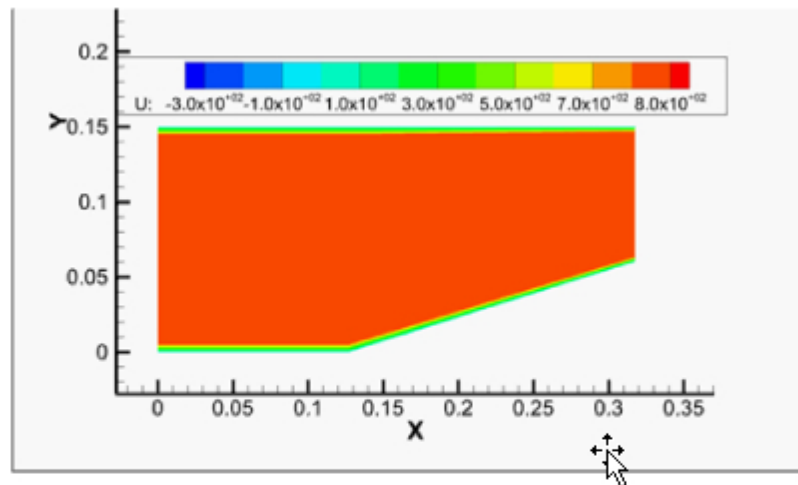
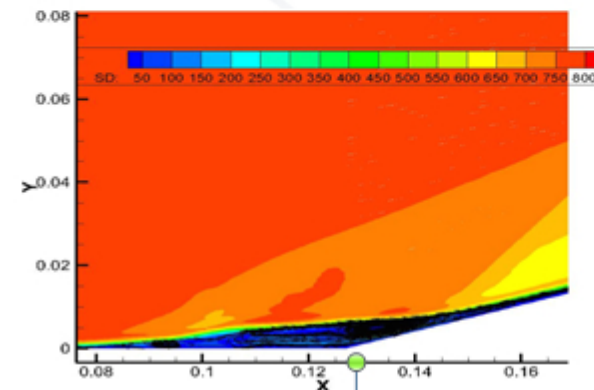
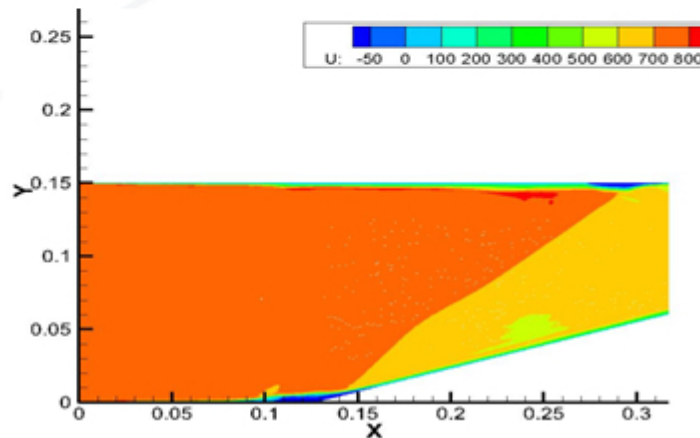
Dynamic LES Supersonic Compression Ramp

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2-D Mach 2.25 Supersonic Flow over Compression Ramp

h-adaptive method with **Dynamic LES** in the **KIVA-hpFE** code

18° compression ramp inlet speed Mach = 2.25



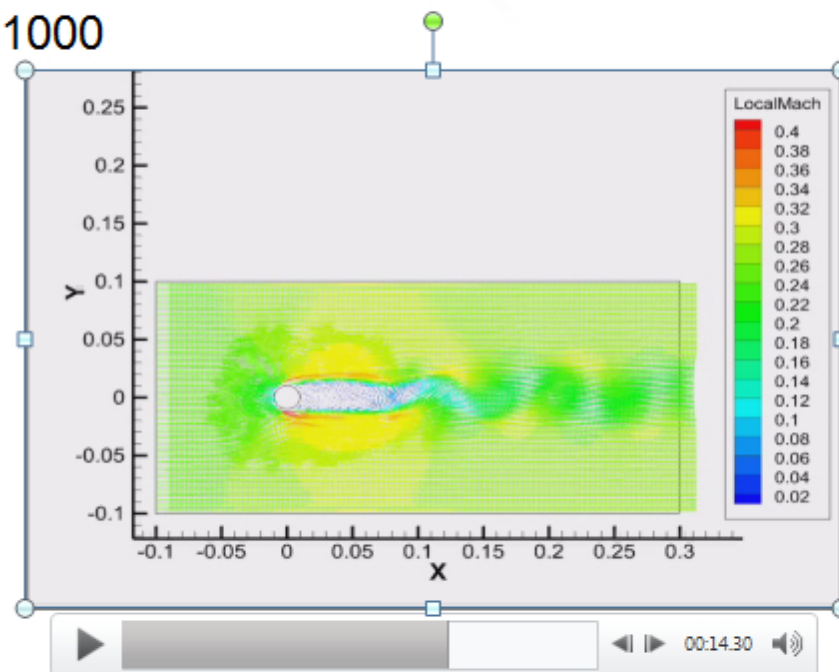
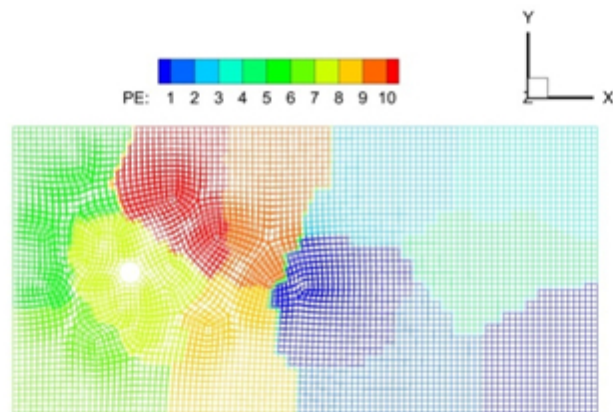
Slide 16

Dynamic LES Turbulence Modeling

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- Dynamic LES system
 - Model for self damping at the boundary, spanning the laminar sublayer through to the fully turbulent flow.

Subsonic Compressible Flow
 $Re \gg 1000$

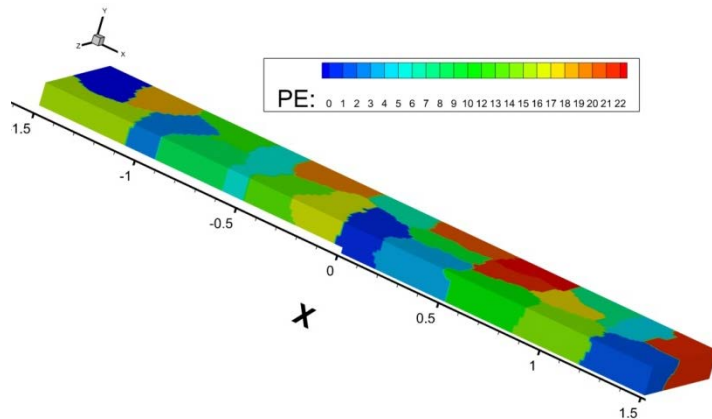


MPI in KIVA-hpFE using
Metis or Scotch for domain decomposition
Solution shown here on 12 Processors
LES Model

MPI system in 3-D KIVA-hpFE

- MPI in KIVA-hpFE using
 - Metis or Scotch for domain decomposition
 - Solution shown here on 22 Processors

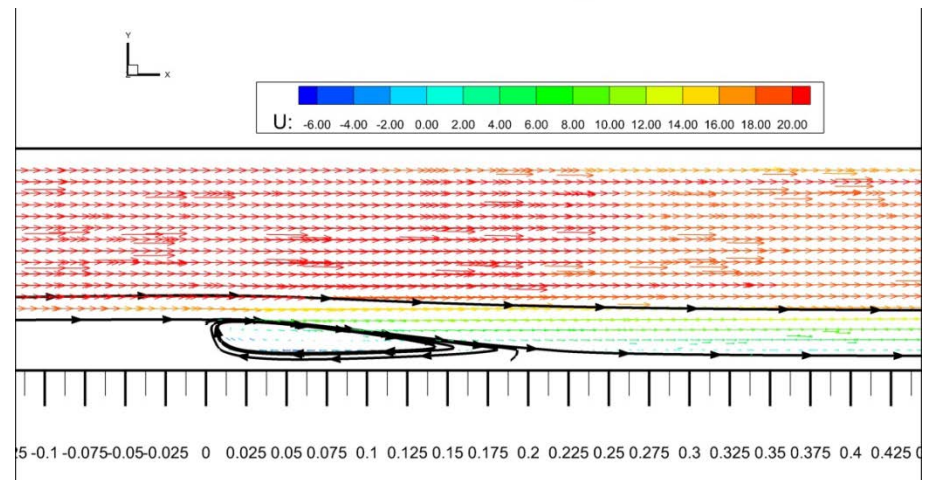
3-D Incompressible Flow
 $Re = 28K$ using $k-\omega$



Domain Decomposition

Nodes = 456,873

Elements = 422,400



Recirculation Length 7.8 step heights
on this coarse grid (grid refinement at step needed)
~ Vogel and Eaton experiment

Execution time for 125,000 time steps to Steady State is currently
36 hours on 22 PE's of a Cray CX-1000 cluster run in semi-implicit mode

Slide 18

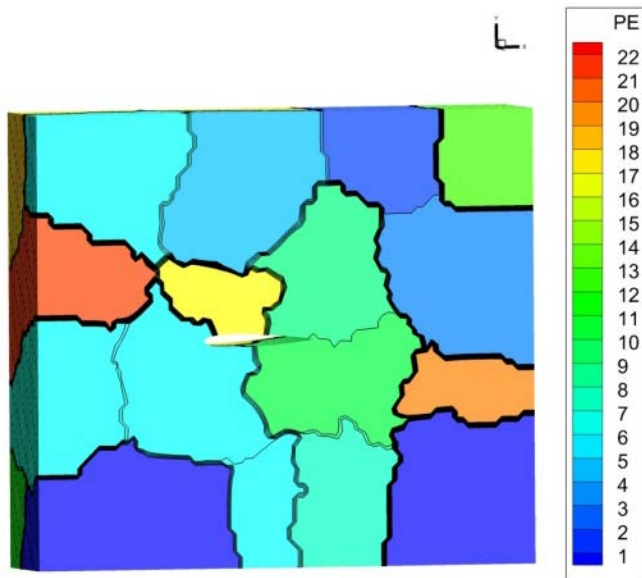
MPI & Parallel Speed-up of Solution in 3-D **KIVA-hpFE** (k- ω RANS)

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Merit Review

Solution of 3-D flow over of NACA0012 airfoil at Mach 0.5

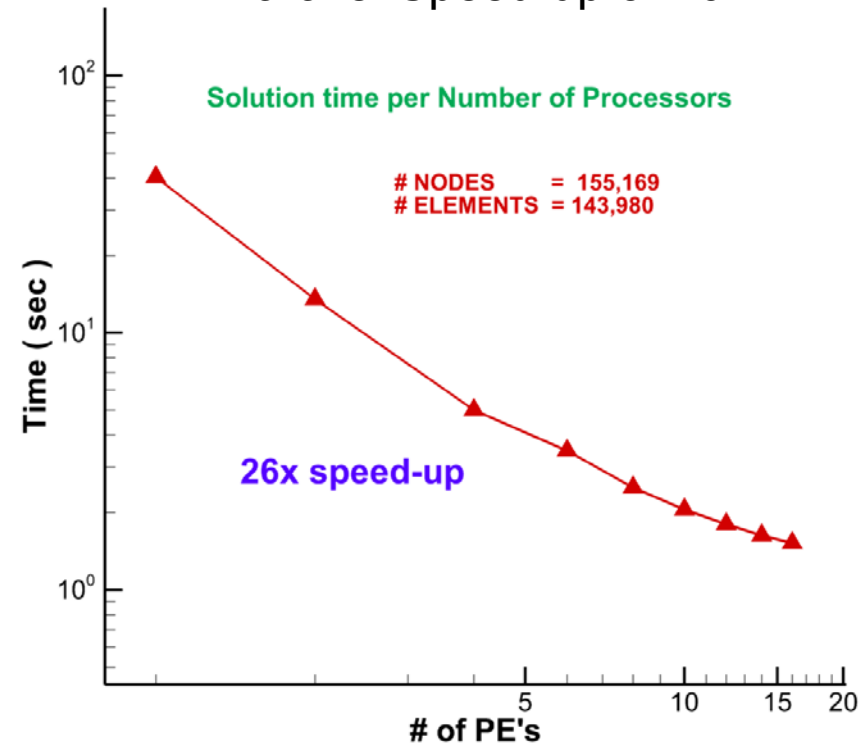
No. Nodes = 155,169

No. Elements = 143,980



Domain decomposition

Parallel Speed-up of 26x



We are expecting 30 to 40x speed-up so some solver optimization still required
Perhaps ~60x when MPI is nested with OpenMP threading

Slide 19

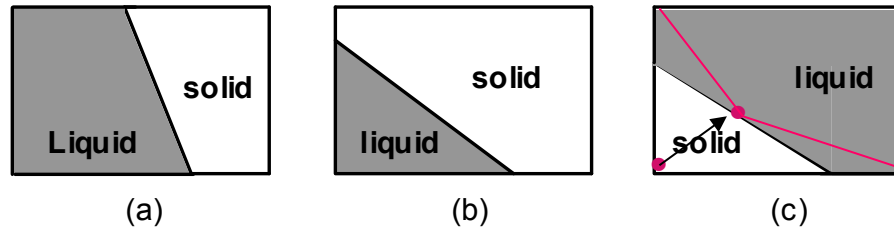
ARBITRARY LAGRANGIAN – EULERIAN (ALE) METHODS

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Based on the Reynolds Transport Theorem

$$\frac{d}{dt} \left\{ \iiint_{V(t)} \mathcal{F}(\mathbf{x}, t) dV \right\} = \iiint_{V(t)} \left\{ \frac{d\mathcal{F}}{dt} + \mathcal{F}(\nabla \cdot \mathbf{v}) \right\} dV = \iiint_{V(t)} \frac{d\mathcal{F}}{dt} dV + \iint_{S(t)} \mathcal{F}(\mathbf{v} \cdot \mathbf{n}) dS$$

- Fluid structure interactions
- Plastic deformations (impact, cracks)
- Solidification
- Engines



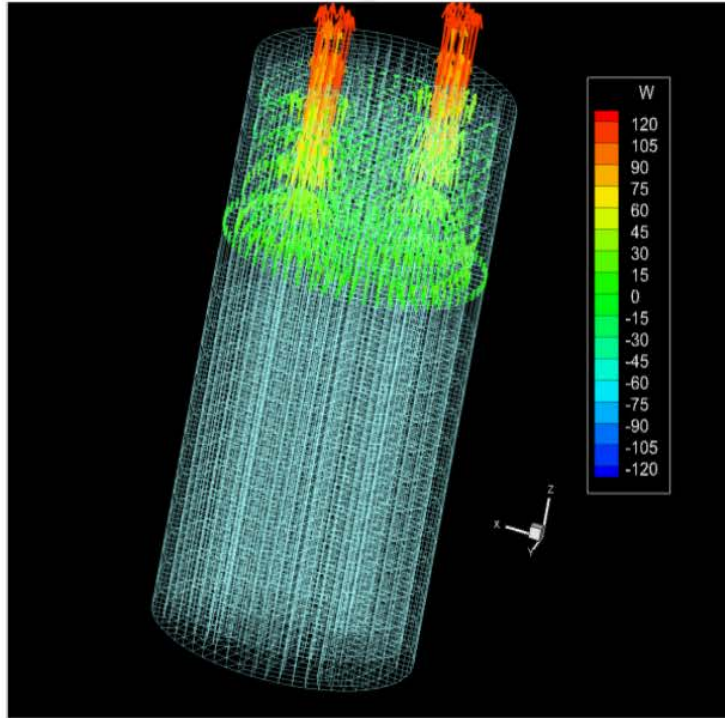
Local ALE:

The mesh is altered locally at each time step.

Mesh history is eliminated, therefore mesh entanglement is not possible.

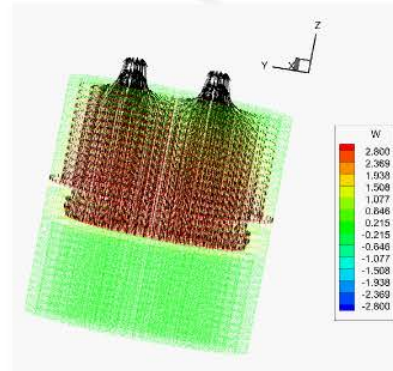
Local 3-D ALE for moving parts on unstructured grids in KIVA-hpFE

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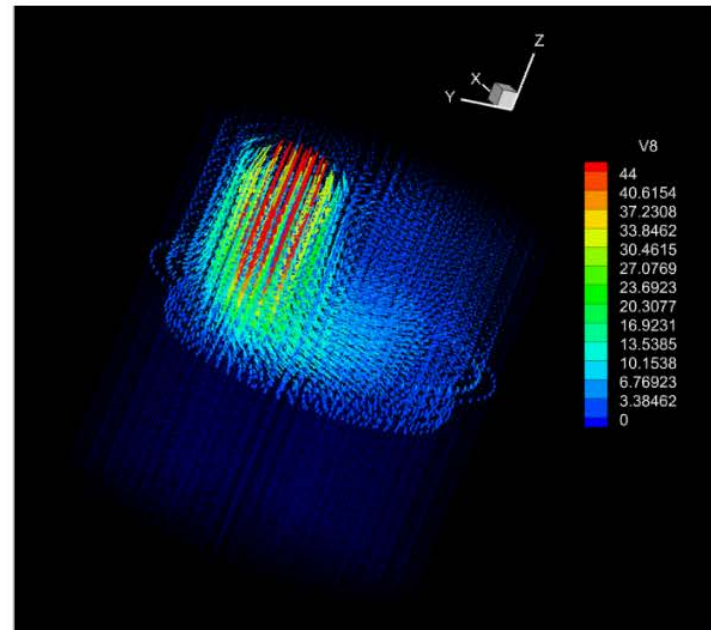


Piston with bowl

KIVA-hpFE compressible solver

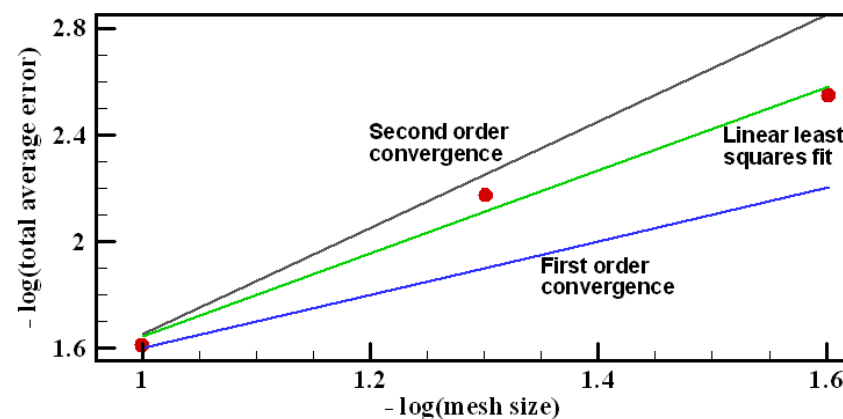
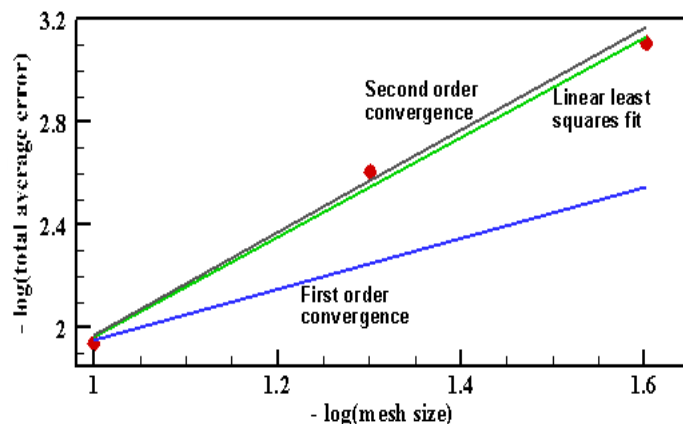


Piston with curved bowl



Convergence Rate for Local-ALE system

Convergence rate for the velocity and pressure



Slope of the least squares fit line is $p = 2.25$

Dashed blue line is linear convergence, $p = 1$

Dotted green line is second order convergence, $p = 2$

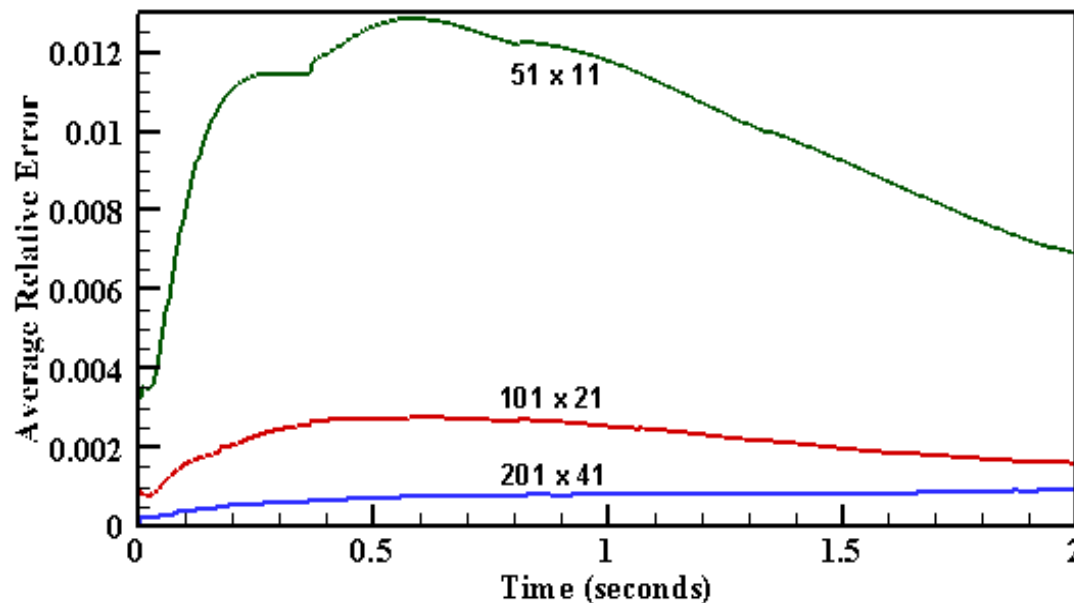
Slope of the least squares fit line is $p = 1.81$

Dashed purple line is second order convergence $p = 2$

Dotted green line is linear convergence $p = 1$

Error of the Local-ALE system

Average relative error in the velocity magnitude as a function of time.

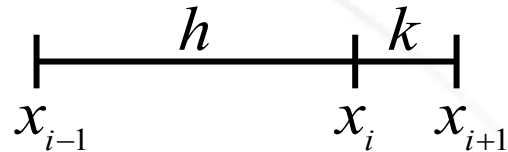


Average Relative Error at $x = 2.5$ as a function of time for 51x11, 101x21, and 201x41 nodes meshes.

It is not enough to show convergence rate, amount of error is required

Error Analysis of Pressure as the moving part interface closes in on a element face

$$\nabla^2 P = \nabla \bullet u$$



By using a difference equation for 3D element using linear basis the Truncation Error is

$$9 \frac{1}{3!} \frac{1}{36} (k_1 + k_2)(l_1 + l_2)(h_1 + h_2) \begin{pmatrix} + (h_1 - h_2) \left((p_{ijk})_{xxx} + (p_{ijk})_{xyy} + (p_{ijk})_{xzz} \right) \\ + (k_2 - k_1) \left((p_{ijk})_{yyy} + (p_{ijk})_{xxy} + (p_{ijk})_{yzz} \right) \\ + (l_1 - l_2) \left((p_{ijk})_{zzz} + (p_{ijk})_{xxz} + (p_{ijk})_{yyz} \right) \end{pmatrix}$$

Error is the derivative of the RHS

- This error is only significant when $h \gg k$ -- the moving face is very close to the element face and is now about 1%.
- We know the error!
- By appropriately evaluating the distance this error can be removed by a Petrov-Galerkin approach – headed to less than 1%.

Challenges and Barriers

- Challenges include:
 - Turbulence modeling,
 - try 2nd Moment
 - Better spray modeling, primary break-up and interface capture
 - Dispersed Spray modeling, perhaps Quadrature Moment Method Eulerian method
 - Two-phase turbulent flow
 - Interface tracking and solution of interface stress
 - Spark plasma kernel model development
 - LES with combustion modeling
 - Full up engine modeling with KIVA-hpFE & comparison to experiment
- Barriers include:
 - Proper sub-modeling of the primary break-up and turbulence along with interface tracking system for two-phase flow.
Dispersed spray model
 - Combustion modeling with LES – interface tracking

- A reviewer felt that improved computational modeling is required for both conventional and advanced engine combustion studies and design.
 - **We concur, and this is exactly what we are pursuing:** Developing new predictor-corrector based split (PCS) hp-adaptive FEM for state-of-the-art modeling capabilities providing any degree of spatial accuracy
- A reviewer felt that work would be more appreciated simulating an internal combustion engines.
 - **We are developing that engine modeling capability:**
 - CFD is far from being predictive for turbulent reactive flow with liquid sprays on complex geometries.
 - **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.
 - **We have a new underlying solver** that is robust and accurate, we are incorporating new submodels such as turbulence closures and LES which are more appropriate for the flow in engines.
 - **Very careful validation is critical** to having a software capable of predictability. We need to be sure each portion of a solver works as expected, and also works together with the other portions as expected. This requires careful testing on the proper problems.
 - **We have a new moving parts** algorithm which is demonstrated by careful analysis to be accurate.
 - 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 requires typical an **order of magnitude more cells** than the method being developed.
 - We feel it is much **better to have an accurate algorithm for modeling** that is also robust (high resolutions for good turbulence modeling and better spray modeling require robust and accurate algorithms) and also is extensible to many computer architectures and any conceivable engine design.
- A reviewer strongly suggested we do more spray modeling comparison work in the ECN Network.
 - We certainly like to see the work being performed in the ECN group. However, R&D on many new methods are being completed by us at this time for predictive modeling. We've already shown 2nd order spatial convergence on spray models with our new system, even for coarse grids, something no one else has shown. We don't have the funding nor the personnel to perform much in the way of spray modeling at this time because of all the work described in this review, but it certainly is on our radar and existing submodels will work better in our newly created system.
- A reviewer asked how the present effort compared with the work being carried out in other institutions, work being done by SNL and with Convergent Science. **Our work is complementary to these bodies of work and are foundational in addition to providing new sub-modeling of the physics.**
 - Is either SNL's work have higher order accuracy? **No**, not presently, but at their resolutions that isn't necessary either.
 - Is Convergent 2nd order spatially? **Only on structured grids** and then probably not at the boundary.
 - Is Convergent easy to use and robust? **Yes**, but by sacrificing accuracy on unstructured grids and at the boundary.
 - Can Convergent or SNL's work do Conjugate Heat Transfer (CHT)? **No**, Convergent probably never will be able to do CHT in its present form, and SNL's method could with an assumed heat transfer coefficient.
 - **We can evaluate the error** in the solution to drive the solution to convergence, nobody else can do this
 - **We know the error in the our new local-ALE** method, nobody else can measures error as the solution proceeds.

Future or Ongoing effort in FY15 to FY 16

Parallel hp-adaptive **KIVA-hpFE**

2015 DOE
Merit Review

- **V&V of Spray and Combustion Systems (ongoing)**
 - *Incorporate LLNL fast chemistry system*
 - Combustion V&V
 - Investigate *burn models for LES*
 - More R&D on flame kernel model for predictive ignition
- **Parallel hp-adaptive PCS FEM in 3-D (ongoing)**
 - OpenMP embedded in MPI Parallel constructions
 - MPI, enhanced by OpenMP
- **LANL Local-ALE in 3-D (ongoing)**
 - *Full engine system, port, valves and piston*
 - **Implicit Momentum Solve for highest pressure accuracy**
 - *Critical for reactive flows*
 - Module installation into KIVA-hpFE all flow speed solver
 - add hierarchical prisms & tetrahedral elements
- **LANL LES Turbulence modeling development (ongoing)**
 - **Dynamic LES incorporated with the hp-adaptive module in the PCS FEM.**
 - Other turbulence closure (future Reynolds Stress Modeling – 2nd moment methods)
- **Spray model development in FEM (future)**
 - Develop model to predict instabilities and waves in jet near nozzle
 - *Two-phase turbulence modeling with interface tracking*

Slide 27

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

FEM

- *Accurate KIVA multi-component Spray model: evaporation, break-up, wall film*
- *Accurate (new) droplet transport modeling*
- *Eulerian, with better/okay $k-\omega$ turbulence and*
- *LANL Dynamic LES (2015) model*
- *Conjugate Heat Transfer implemented (2015)*
- *Nodal valued Spark Kernel Model*
- *Chemistry implemented*
- *Conjugate Heat Transfer implemented (2015)*

hp-adaptive FEM

- *Higher order accurate - 2nd and greater spatial accuracy everywhere & always*
- *Evolving solution error drives grid*
 - *Resolution and higher-order approximation*
- *hp-adaptive FEM incorporated in the 3D PCS FEM all flow solver (2015)*

Local ALE in FEM

- *Mesh never tangles*
- *Piston with curved geometries (2015)*
- *System implemented in the 3D PCS FEM all flow solver (2015)*
 - *Robust and 2nd order accurate Local ALE for moving parts*
- *Faster grid generation - CAD to CFD grid in nearly a single step*

Parallel Solution

- *MPI processing on moderate computer platforms (2015).*
- *Good Domain Decomposition and linear equation solver system (2015)*
- *Beam-Warming Method with Parallel Additive Schwartz preconditioning integrated (2015).*

Technical Back-Up Slides

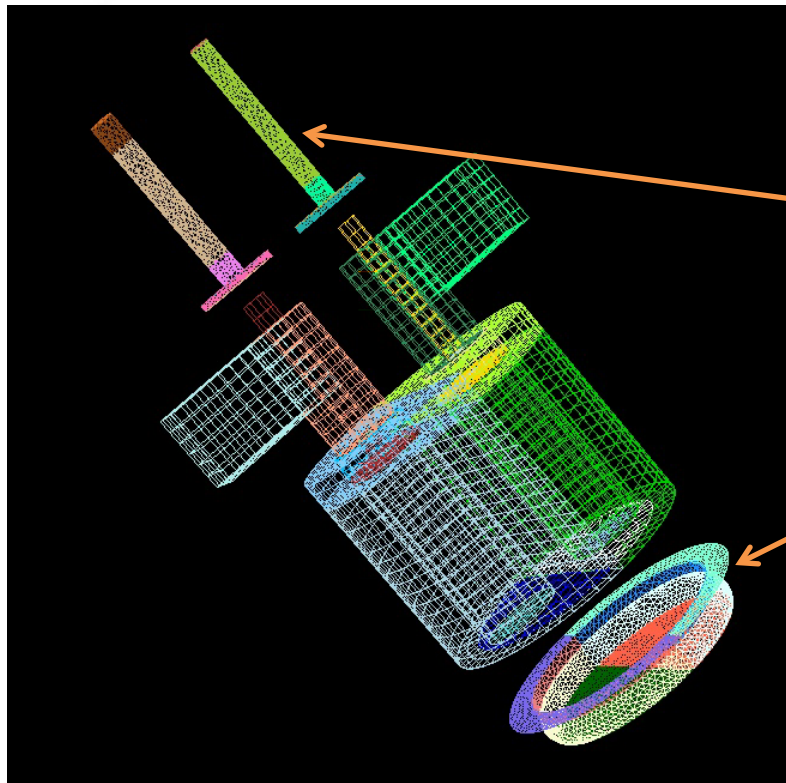
(Note: please include this “separator” slide if you are including back-up technical slides (maximum of five technical back-up slides). These back-up technical slides will be available for your presentation and will be included in the DVD and Web PDF files released to the public.)

Grid Generation

- 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

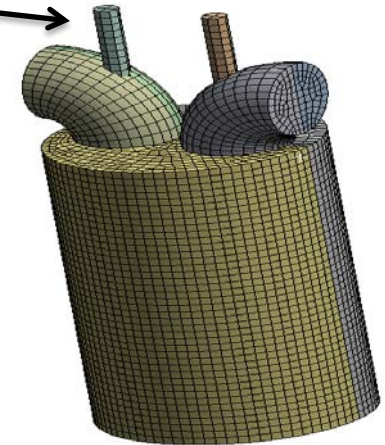


Overlaid valves

Overlaid piston

Cubit Meshing Tool

ANSYS MeshTool

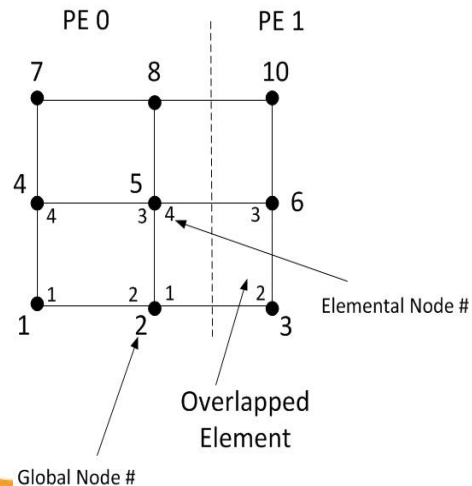


Test Engine with 3D ALE beginning

Parallel 2-D and 3-D KIVA-hpFE using MPI

2015 DOE
Merit Review

- Mixing MPI version of the code
 - Flow domain decomposed
 - Multiple MPI processes - each process computing one sub-domain.
 - Linear Solver system is a **Beam-Warming iterator** around the **in-situ preconditioning** and matrix multiples using **LANL Krylov Solver package (PCG)** (Carrington, 2008)
 - Solver system based on the MPI code for
LANL's spherical harmonics radiation transport solver
 - Our linear equation system uses PCG package
using GRMES solve and in-situ preconditioning
of Point Jacobi, SSOR and Block Jacobi
 - Data exchange across sub-domains with MPI
only needed at shared nodes
 - Integration information for shared nodes
additive from shared processor integration =>
can be processes simultaneously.



ao	ja	ia
[comm to evaluate 2]	[2]	
3	3	
6	6	
3	3	
[comm to evaluate 5]	5	[1]
6	6	4
9	9	8
6	6	11
[comm to evaluate 8]	8	
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ao	ja	ia
1	1	
2	2	
4	4	
1	1	
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[comm to evaluate 3]	3	
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4	4	16
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[comm to evaluate 6]	6	23
4	4	
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7	7	
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[comm to evaluate 9]	9	

Adaptation and Error – the driver for resolution

$$\|e_V\| = \left(\int_{\Omega} e_V^T e_V d\Omega \right)^{1/2} \quad \text{L}_2 \text{ norm of error measure}$$

$$\|e_V\|^2 = \sum_{i=1}^m \|e_V\|_i^2 \quad \text{Element error}$$

$$\eta_V = \left(\frac{\|e_V\|^2}{\|V^*\|^2 + \|e_V\|^2} \right)^{1/2} \times 100\% \quad \text{Error distribution}$$

$$\bar{e}_{avg} = \bar{\eta}_{max} \left[\frac{(\|V^*\|^2 + \|e_V\|^2)}{m} \right]^{1/2} \quad \text{Error average}$$

$$\xi_i = \frac{\|e\|_i}{\bar{e}_{avg}} \quad \text{Refinement criteria}$$

$$p_{new} = p_{old} \xi_i^{1/p} \quad \text{Level of polynomial for element}$$

- **Error measures:**
 - Residual, Stress Error, etc..
- **Typical error measures:**
 - Zienkiewicz and Zhu Stress
 - Simple Residual
 - Residual measure - How far the solution is from true solution.
 - “True” measure in the model being used to form the residual.
 - If model is correct, e.g., Navier-Stokes, then this is a measure how far solution is from the actual physics!