2014 DOE
Merit Review

2014 KIVA Development

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June 17, 2014

3:15 p.m.

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LA-UR-14-22477

Project ID # ACE014

Overview

Timeline

- 10/01/09
- 9/31/15
- 75% complete

Budget

- Total project funding to date:
  - 2700K
  - 695K in FY 13
  - 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 - Dr. Darrell W. Pepper
- Many users of KIVA are supported and collaborations exist.

Objectives

FY 09 to FY 14 KIVA-Development

- **Robust, Accurate Algorithms in a Modular Object-Oriented code**–
  - **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.
      - Developing Fractional Step (PCS) Petrov-Galerkin (P-G) and Predictor-Corrector Split (PCS) *hp*-adaptive finite element method
      - Conjugate Heat Transfer providing
        - More accurate prediction in wall-film and its effects on combustion and emissions
        - Providing accurate boundary conditions.
- **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- FY14

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09/09 – 2D and 3D P-G Fractional Step (PCS/CBS) Finite Element Algorithm Developed.
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 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 domain decomposition package
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
04/14 – P-G type term for diffusive stability in ALE system when rpm dt > stable Fourier Number dt
03/12 to 12/14 – Presentations AEC, ASME, ICHT, IHTC, V&V with Papers to ICHT, IHTC, and CTS

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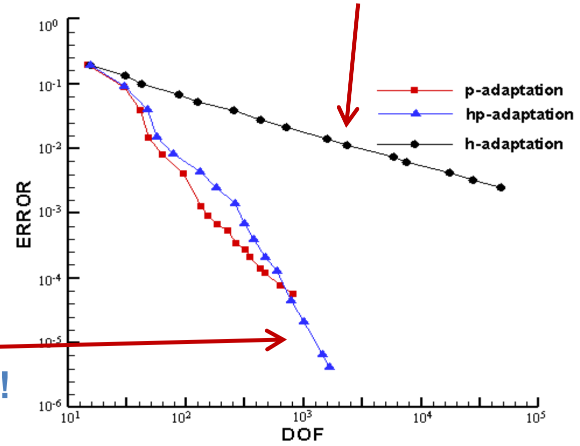
- **What if we had a turbulent reactive flow modeling software for Engines that could provide:**

1) ***Faster grid generation* - CAD to CFD** grid in nearly a single step
2) **1 pressure solve** per time step – no more than 1 matrix solver per time step
3) ***Mesh never tangles – Robust and 2nd order accurate Local ALE* for** moving parts
4) ***Higher order accurate*** - **2nd and better spatial accuracy - everywhere & always**
5) **3rd order accuracy** for advection terms
6) ***Minimal communication*** for faster parallel processing on all computer architectures.
7) Curved surfaces can be represented exactly.
8) ***Evolving solution error drives (measure of error in Hilbert/Banach vector space):***
    i. **Grid refinement and higher-order approximation**
9) ***Accurate KIVA multi-component Spray model***
10) **Eulerian**, with **better/okay *k-ϖ* turbulence modeling**
    i. **Improvement over other 2-equation models**
    ii. **Good Dynamic LES model**
11) ***Conjugate Heat Transfer* is essentially free**
    i. **No assumed heat transfer coefficient**
12) ***hp*-adaptive FEM – exponentially grid convergent**

Error as function(*grid size*)
Traditional KIVA-type method



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

A lot to ask?
How can we get so many numerical win-win-win combinations?
***hp*-Adaptive FEM with local ALE allows this!**

Technical Accomplishments

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-ϖ turbulence modeling***
  - Big improvement over other 2-equation models
  - Conjugate Heat Transfer is essentially free
  - Dynamic LES underdevelopment
- ***Nodal valued Spark Kernel Approximation Model***
- ***Chemistry (KIVA 30+ fuels or ChemKin)***

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

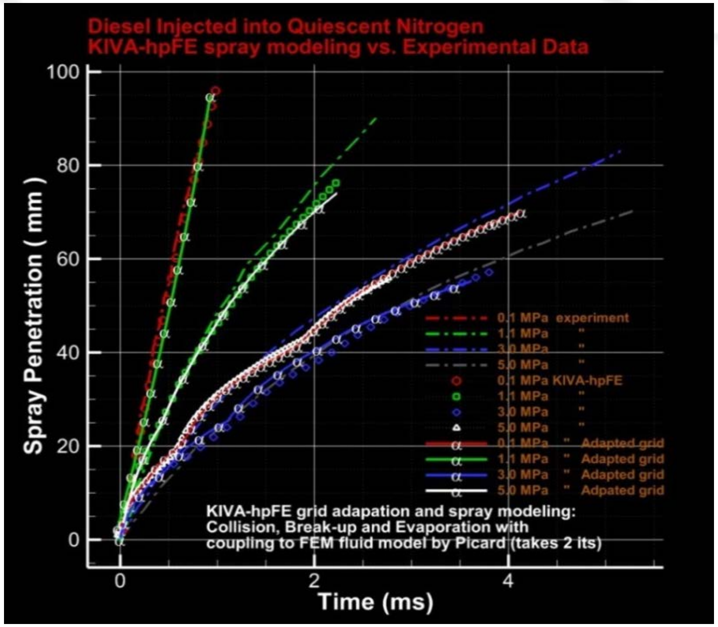
- ***Scotch versus Metis Domain Decomposition – Scotch is preferred***
- ***Efficient MPI with nested OpenMP processing on moderate computer platforms.***
- ***Beam-Warming Method with Parallel Additive Schwartz preconditioning developed for PCG (Joubert & Carey) solver package (integrated).***

KIVA-hpFE spray model

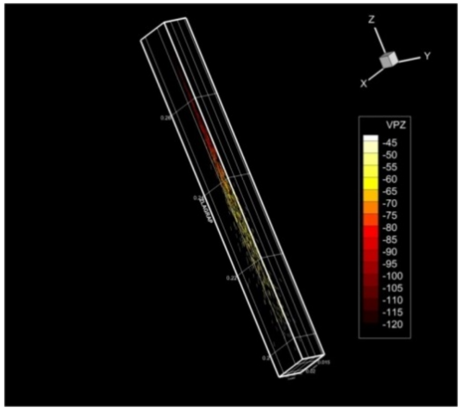
- Mostly the same Los Alamos KIVA Multi-component Spray algorithms by P.J. O'Rourke, Tony Amsden, David J. Torres, John K. Dukowicz
  - Droplet collision, agglomeration & break-up
  - Evaporation employing thermal field in droplets/parcel representation
  - Turbulent diffusion
- **Finite Element Spray** modeling
  - New two-way coupling between fluid and droplets (usually only 2 iterations required)
  - New fast ray-tracing method for associating elements with droplet parcels.
  - Precise measure of fluid and thermal properties at each droplet/parcel location (2nd order or grid scale accuracy) .

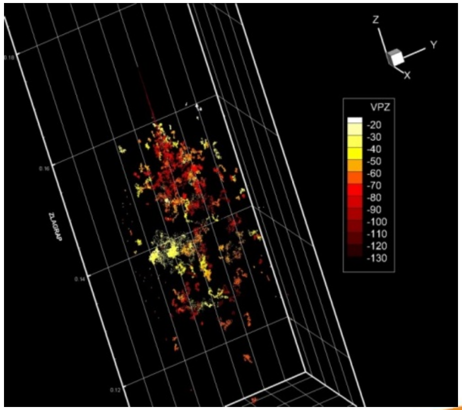
KIVA-hpFE Spray Modeling V&V

- Spatially convergent spray modeling
- KIVA-hpFE
  - hp-adaptive FEM method
  - Turbulent (k-ω) reactive flow
  - Fluid properties & momentum evaluated at each droplet position
- KIVA multicomponent Spray Model



Diesel injected into quiescent Nitrogen
Pressures of 1, 11, 30 and 50 atmos.
Velocity of injected spray
Ranges 85m/s to 115 m/s





Experimental data from **H. Hiroyasu & T. Kadota, "Fuel Droplet Size Distribution in Diesel Combustion Chamber," SAE paper 740715, 1977**

KIVA-hpFE V&V - Subsonic flow regime

NACA 0012 airfoil test

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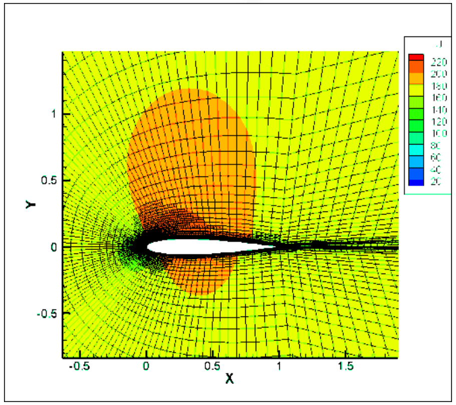
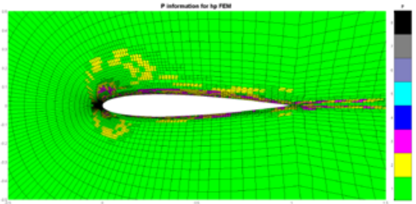
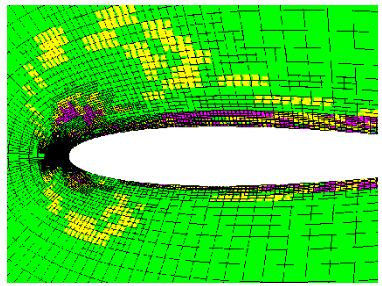
- $M_\infty = 0.502$ $\alpha_\infty = 2.06^0$
- $Re = 2.91 \times 10^6$



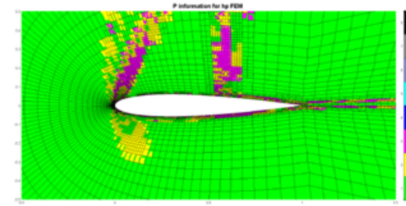
Horizontal Velocity

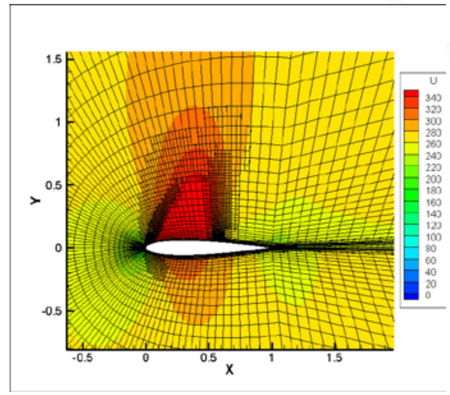




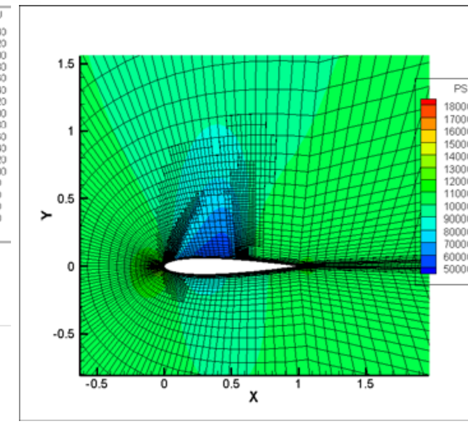
hp-adapted domain

- Mach = 0.75 $\alpha = 2.05^o$
- $Re = 1.0 \times 10^7$

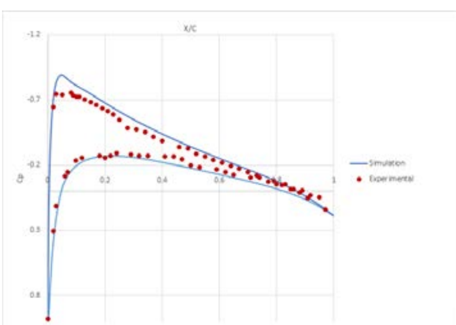




Horizontal Velocity

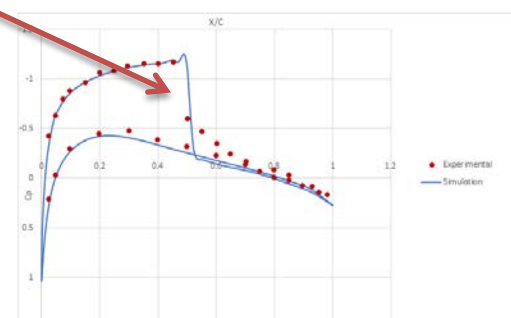


hp-adapted domain



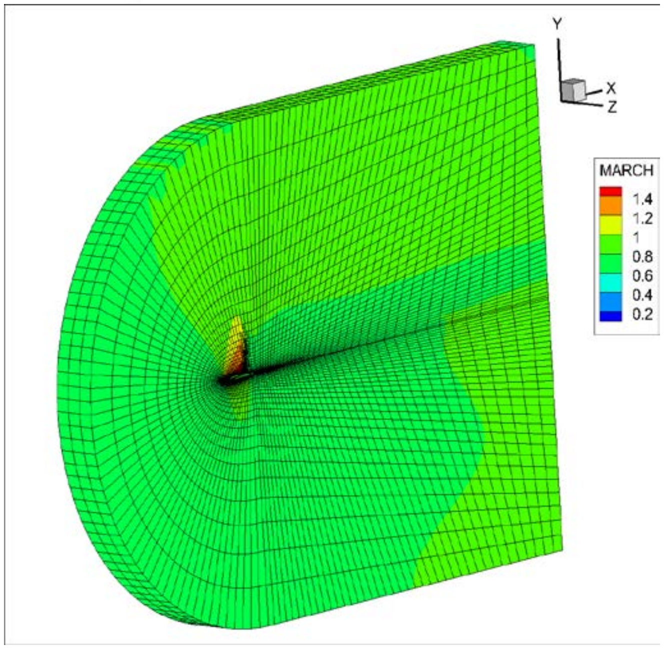
Shock Capture

Coefficient of Pressure
Experimental data
from AGARD

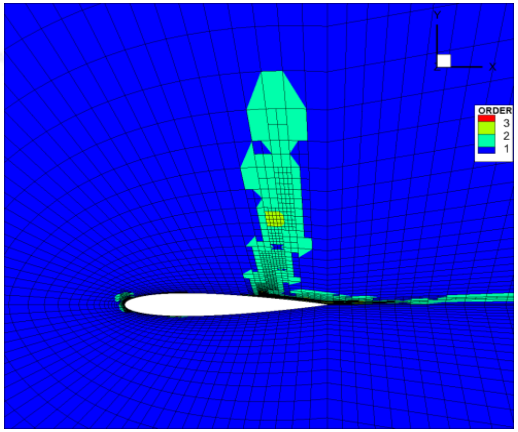


*hp-a*daptive PCS FEM for 3-D NACA Airfoil at Subsonic

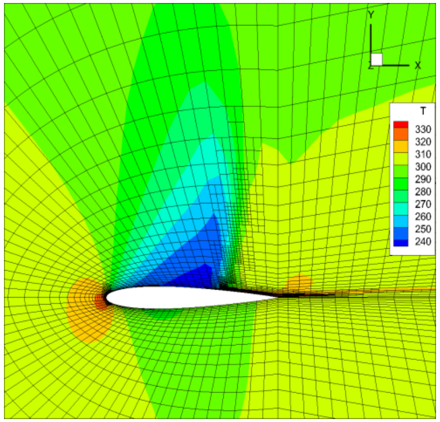
- Mach = 0.8 & attack angle α = 4°
  - Time dependent solution
  - Gambit generated initial grid
  - Agreement with data



Local Mach

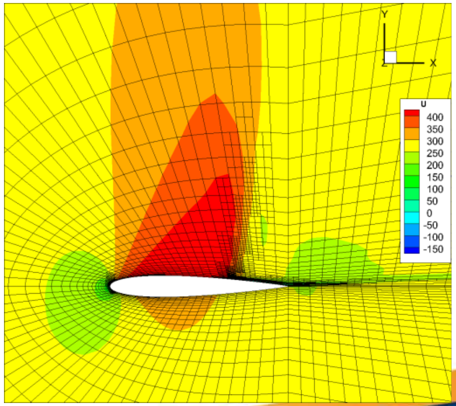


Final mesh *hp*-adaptive
(polynomial order shown in color)



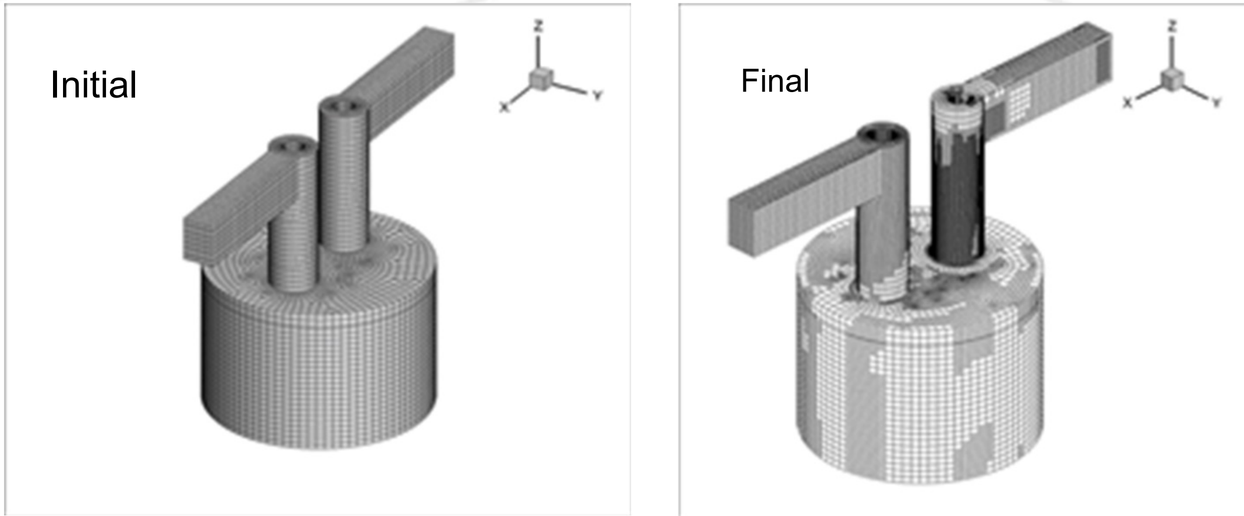
Temperature

Velocity components

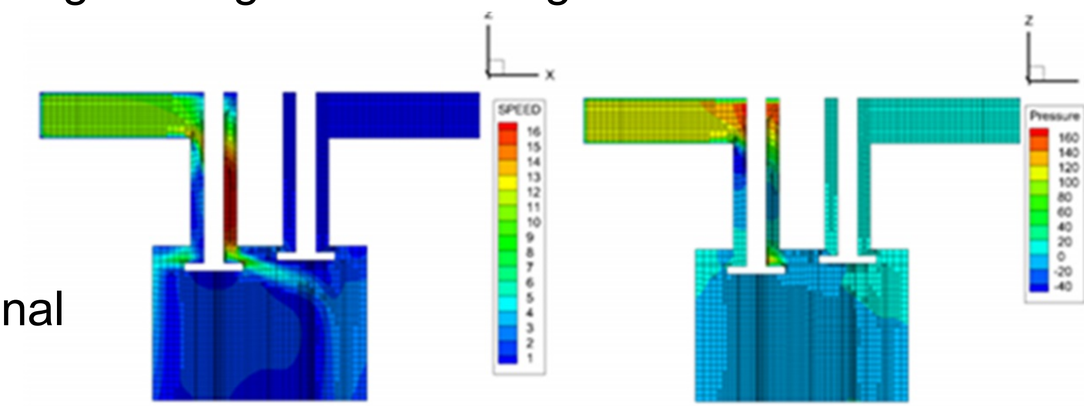


- Also continues to demonstrating Solver Capability
  - Truly curved and complex domains

hp-adaptive PCS FEM on Engine



Initial and final grids at given crank angle



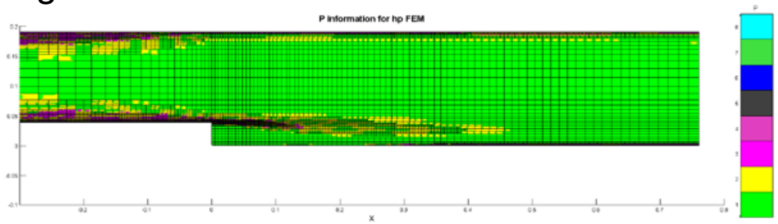
Plane at central meridional
Speed and Pressure

Parallel *hp-a*daptive PCS FEM – MPI & OpenMP

- Mixing OpenMP / MPI version of the code
  - MPI outer level is domain decomposed
  - OpenMP threads on inner level

OpenMP

Backward-facing step simulation with Re=28,000,
15979 elements, 15975 vertex nodes,
60976 high order nodes => 90477 total DOF.



MPI

- Exchange across subdomains with MPI
- Parallel (MPI) PCG Linear equation solver
- Developed and installed
  - in-situ preconditioning methods

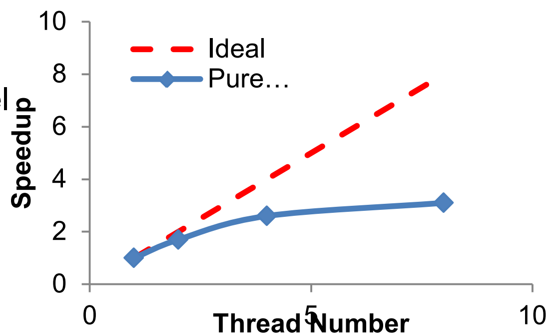
Improved parallel performance over conventional methods

1st step for Parallelizing code: **OpenMP**

OpenMP ~ 2.5x speed-up

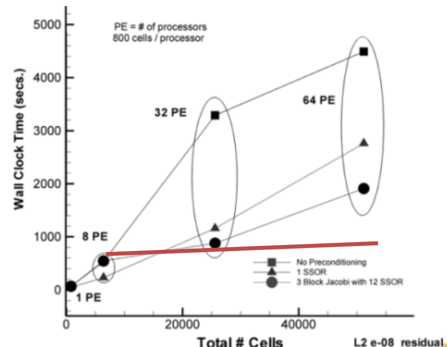
Only a Small Desktop PC for
90477 degrees of freedom

Test run on a Dell PowerEdge R510, 2 Intel Xeon X5672 3.20GHz CPU's



2nd step for Parallelizing code:

- Embed OpenMP (2.5x) in MPI domain decomposition for a 10x speed-up with a 10x increase in resolution for theoretical upper limit speed-up of 100x per cell.



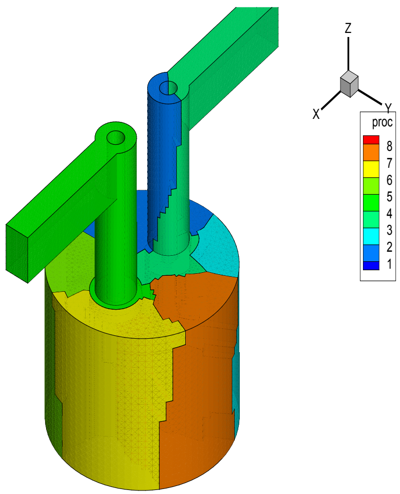
Each traditional MPI parallel scaling (PE=processors) to be reduced by factor of 2.5

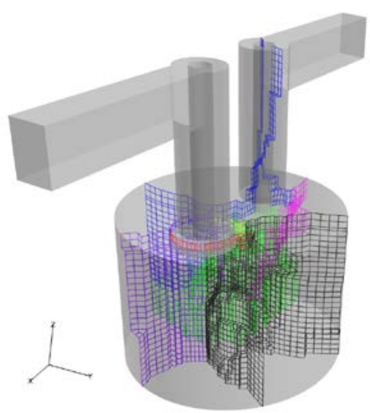
Ideal scaling

Metis vs. Scotch Domain Decomposition of Vertical Valve Engine

Metis

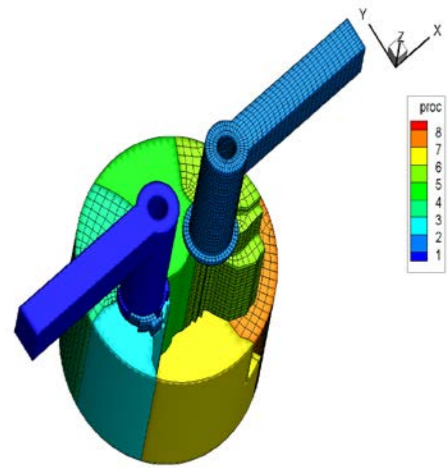
- Metis number of element for the big domain: 45058
    - Max number of cells for the sub-domains = 5801 (2.996% above average 5632.25)

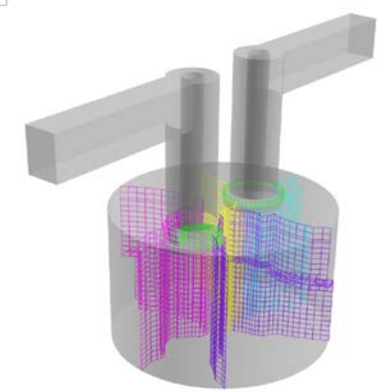




Scotch

- Scotch number of element for the big domain: 45058
    - Max number of cells for the sub-domains = 5688 (0.99% above average 5632.25)

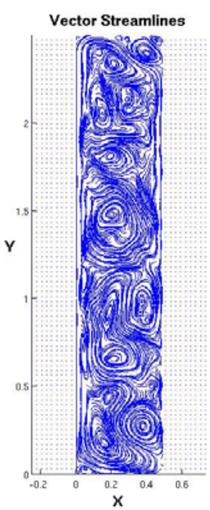


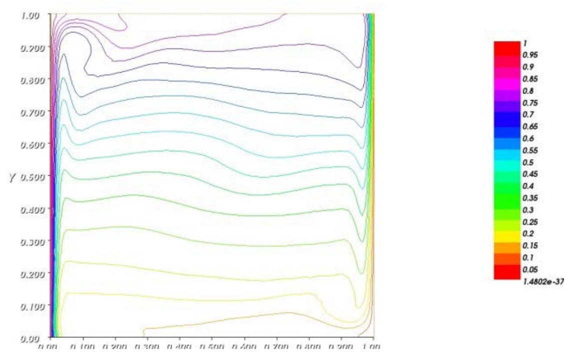


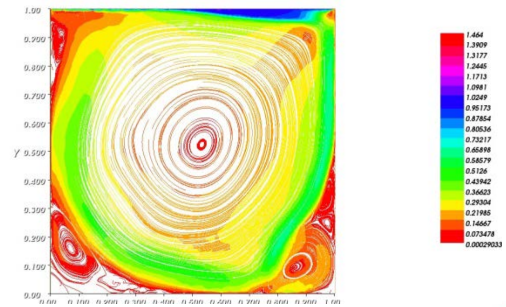
LES - Method Development

- Dynamic method that is:
  - Ideal for wall bounded flows - self-damping at solid walls
  - Dynamic filtering and up-scaling (back-scatter)
  - Spans the laminar and transitional flow to fully turbulent
  - Ideal model for complex flow having multiple flow regimes
  - Ideal model for flow that is continuously developing new regimes

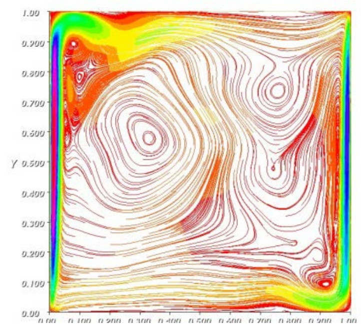
Preliminary Results on various lower Re tests







Spanning Laminar Transition To Turbulent Flow



UNCLASSIFIED

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

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

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

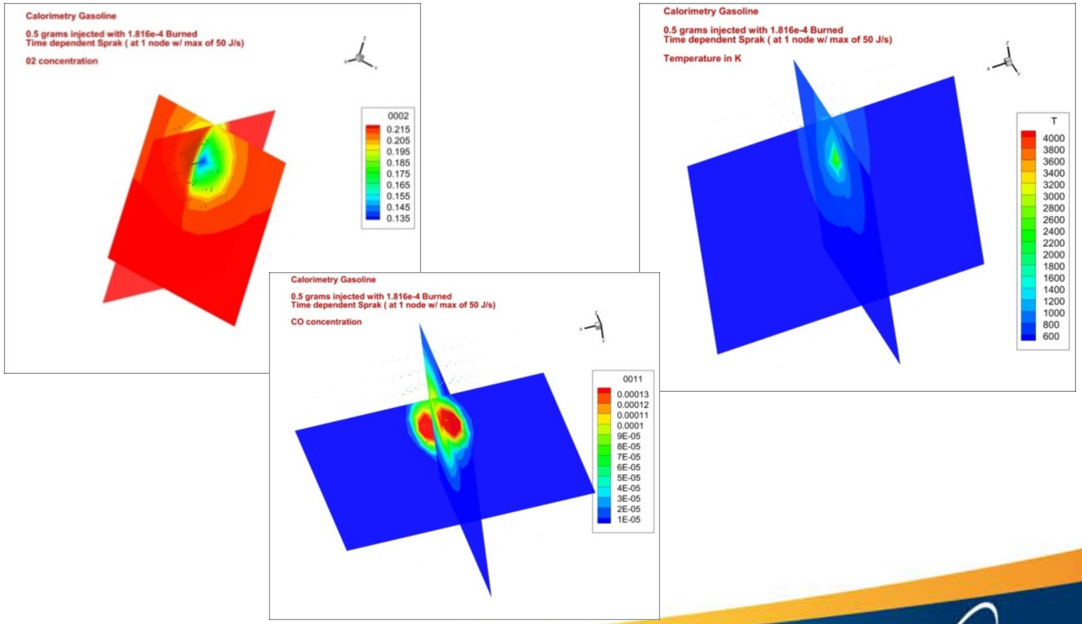
$$\frac{dV_k}{dt} = \frac{\rho_f}{\rho_k} A_k S_{eff} + V_k\left(\frac{1}{T_k}\frac{dT_k}{dt} - \frac{1}{P}\frac{dP}{dt}\right)$$

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

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

Velocity of Flame + Heat diffusion

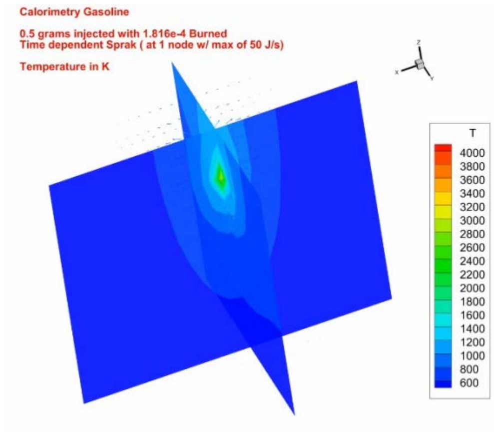
- Calorimetric validation to LHV
  - 0.5 grams Gasoline (KIVA) at 325K injected into Air at 1atm & 296 K
  - Spark at node at max of 50 J/s

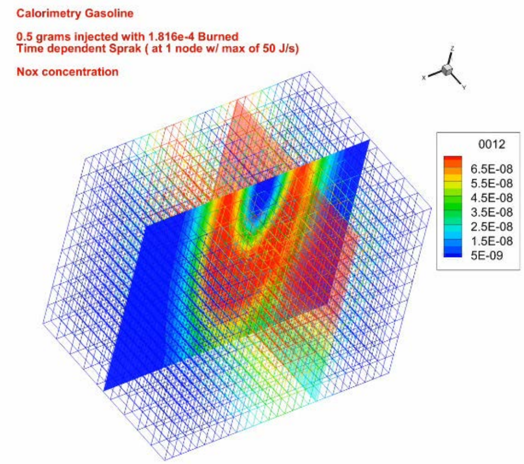


Calorimetric Studies – V&V

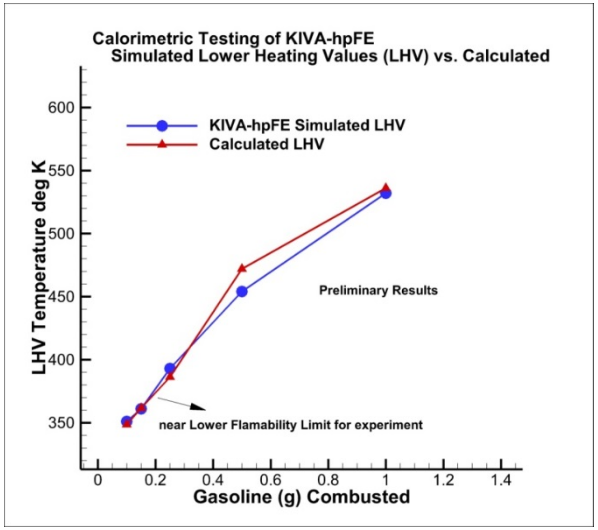
KIVA-hpFE Spray, Chemistry & Spark ignition PCS FEM

- Gasoline (KIVA) at 325K injected into Air at 1 (325K) & 10 atm (525K)
- 0.5 grams injected Time dependent
- Spark Kernel approximation model (node w/ max of 50 J/s)





Steady-State Temperature of Simulation versus Theoretical value

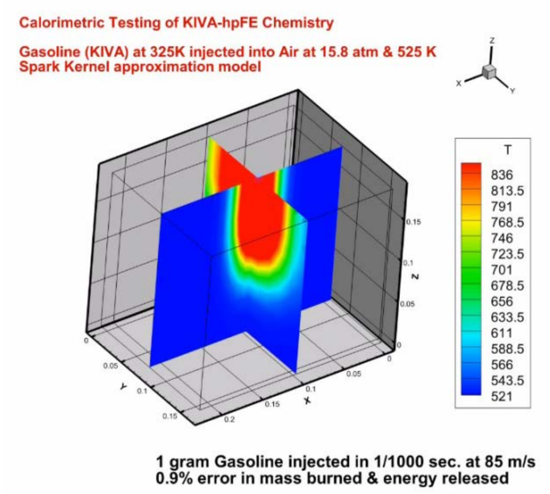


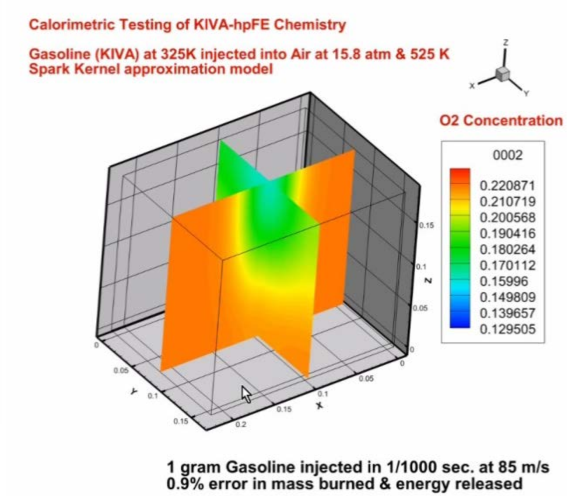
- Calorimetric validation to LHV
  - Spark Ignition of Injected Gasoline

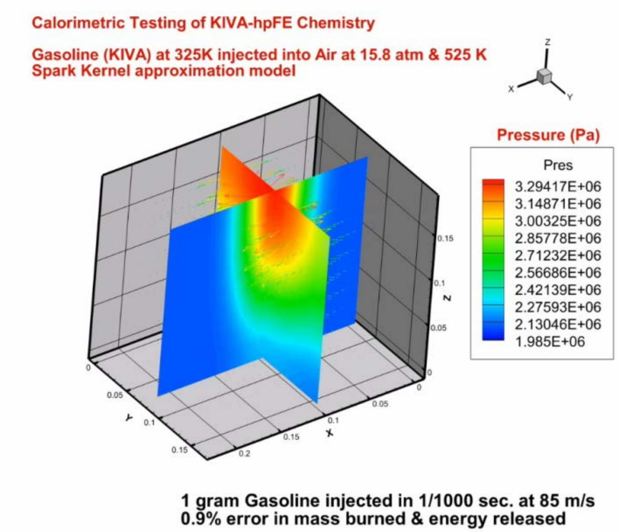
Calorimetric Studies – V&V

KIVA-hpFE Spray, Chemistry & Spark ignition PCS FEM

- Spark/Flame Kernel Approximation Model
  - Gasoline (KIVA) at 325K injected into Air at 15.8 atm & 525 K
  - Spark Kernel approximation model

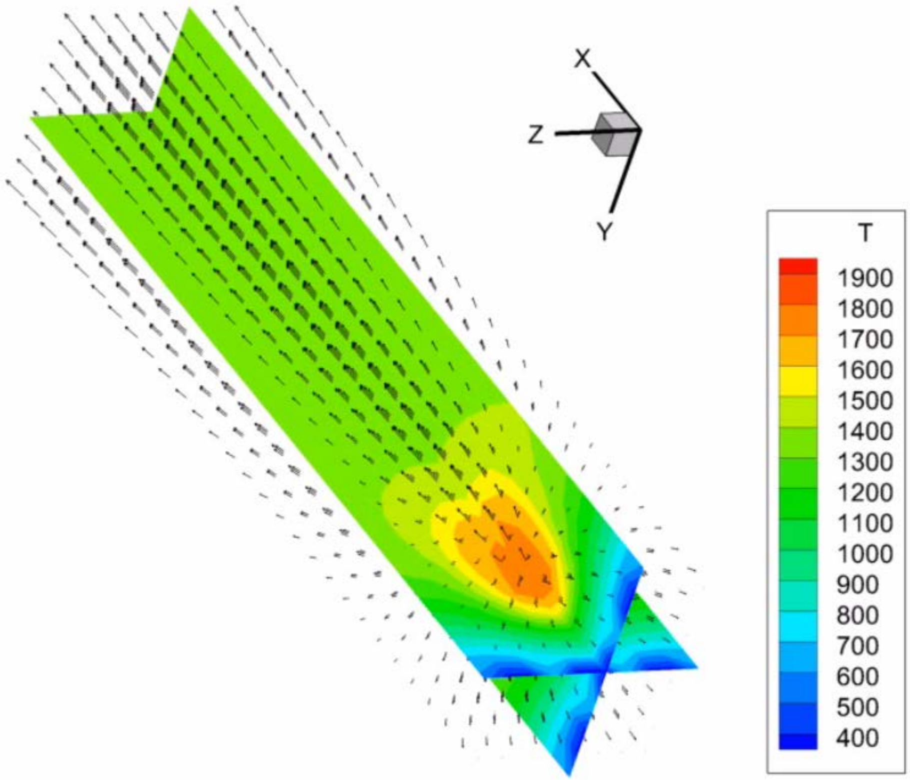






- Calorimetric validation to LHV
  - 1 gram Gasoline injected in 1/1000 sec. at 85 m/s
  - 0.9% error in mass burned & energy released

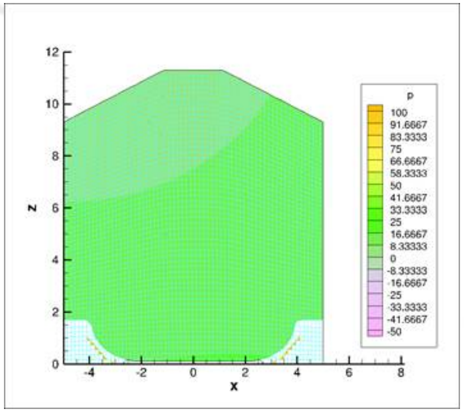
KIVA-hpFE Burner Test



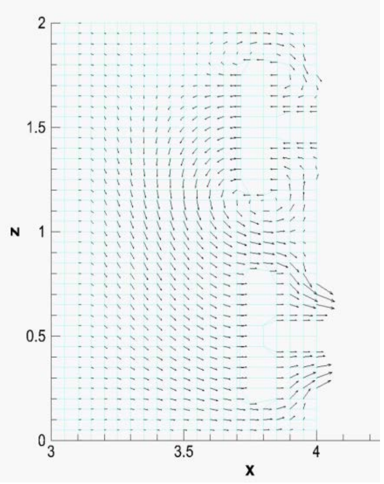
Methane Burner
for Validation comparisons

Local ALE for moving parts on unstructured grids

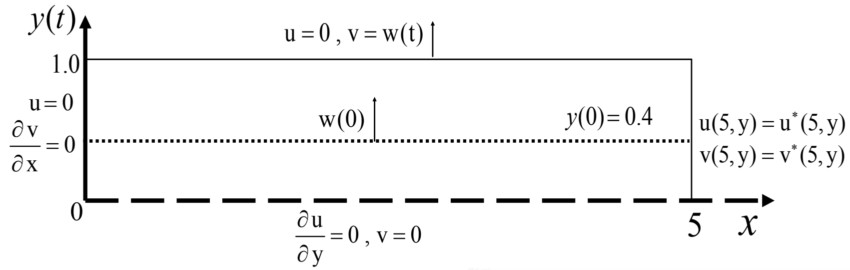
- ***New* local ALE FEM**
  - ***Not often in CFD we even get a win-win situation, here it is a win-win-win!***
- Increase robustness and is 2^{nd} order accurate.
- Simulations with higher resolution.
- Use of overset parts/grids.
- Grid is of body only, fluid only.
- Allows for automatic grid generation by Cubit or ICEM
  - CAD to Engine Grid!

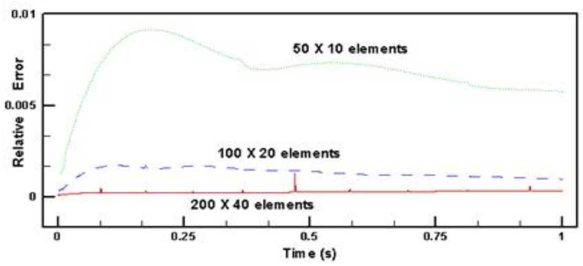


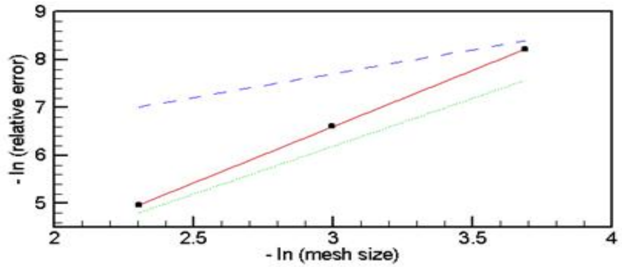
2-D engine type test of ALE



Test Case: Layer of fluid between two plates separating with speed w(t). Height goes from y = 0.4 to 1.0; (u*, v*) is the analytical solution.



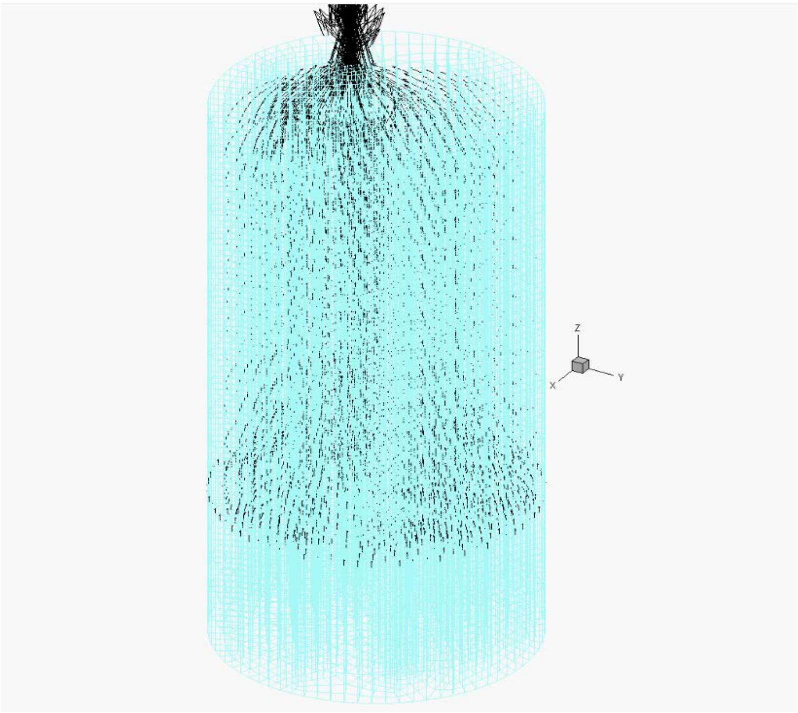


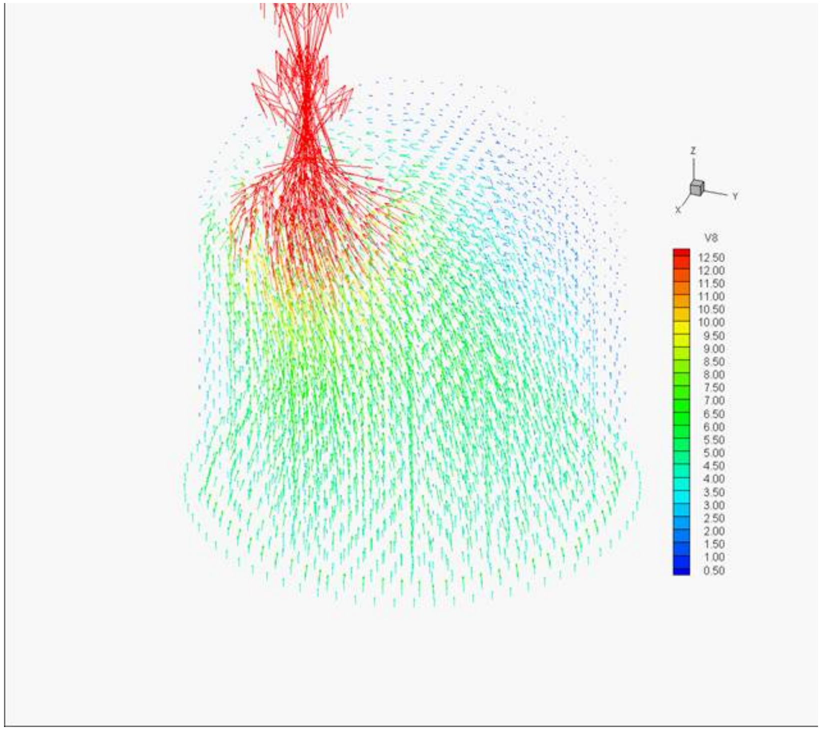


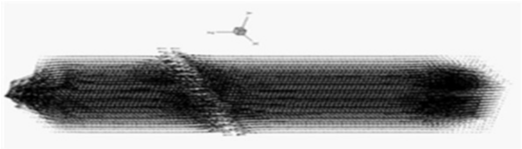
Grid convergence test : Average relative error vs. analytic solution

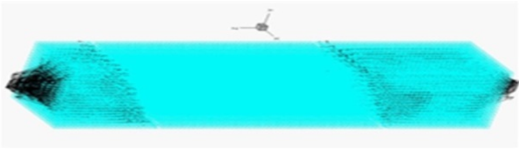
Local 3-D ALE for moving parts on unstructured grids

- Local 3-D local ALE for moving parts on unstructured grids
  - Overlaid actuated parts





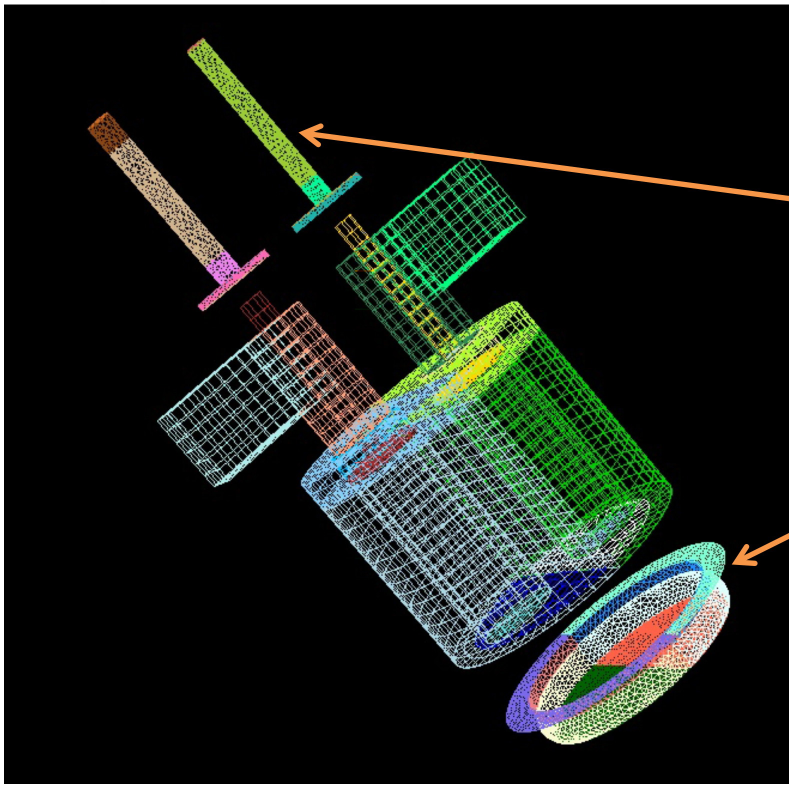




Grid Generation

- 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



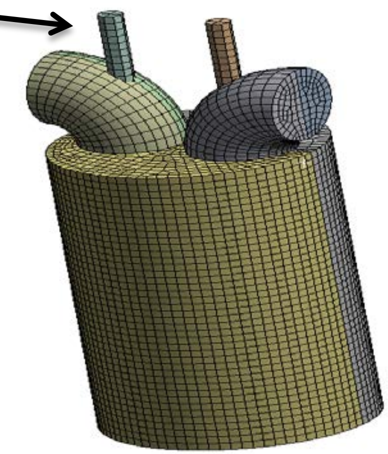
Overlaid valves

Overlaid piston

Cubit Meshing Tool

Test Engine with 3D ALE beginning

ANSYS MeshTool



Program Collaborators

- Purdue, Calumet
  - *hp*-Adaptive FEM with Predictor-Corrector Split (PCS)
  - OpenMP and MPI parallel solution development
  - Turbulence modeling
    - Xiuling Wang and GRA
- University of New Mexico
  - Moving Immersed Body
  - Boundaries Algorithm Development
    - Juan Heinrich, Monayem Mazumder (PostDoc) & Dominic Munoz
- University of Nevada, Las Vegas
  - Dynamic LES
    - Darrell Pepper, JiaJia Waters (PostDoc started April 1), David Fyda (GRA)
- LANL
  - PCS FEM with adaptive methods
  - Parallel Solver MPI development
  - Beam-Warming with PCG package linear algebra solver development
  - Turbulence & spray development, chemistry models and grid incorporation.
    - David Carrington

Challenges and Barriers

- Challenges include:
  - Parallel code development
  - Better turbulence modeling
  - Better spray modeling, primary break-up and interface capture
  - Spark kernel model development
- Barriers include:
  - Proper sub-modeling of the primary break-up and turbulence along with interface tracking system for two-phase flow.

Reviewers' Comments

Reviewers' Comments and *our responses:*

- **A reviewer felt that improved computational modeling is r**equired 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, overall ease of implementation and it currently uses known KIVA code and improved submodels for spray.*
- **A reviewer wanted to see a bomb type problem.**
  - *We have performed calorimetric studies with spray injected fuel with excellent results for heating values of burned fuel.*
- **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 core 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 which are more appropriate for the flow in engines. We are validating the solutions. 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.*
    - *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 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 submodeling of the physics.***
  - *Does SNL's work have robust and accurate moving parts?* **No**, moving parts and combustion (at present) are absent.
  - *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.
- ***Our new code is designed to be easy to use, robust and accurate, without compromising any one critical piece for the another.***

Future or Ongoing effort in FY14 to FY 15 Parallel hp-adaptive PCS FEM with 3d

- V&V of Spray and Combustion Systems (ongoing)
  - Calorimeter type tests for Combustion V&V
  - Approximate Flame Kernel model based on spark current and kernel with heat losses – a simple model from spark plug specifications
  - Flame kernel model for predictive ignition (future)
- Parallel *hp*-adaptive PCS FEM in 3-D (ongoing)
  - OpenMP embedded in MPI Parallel constructions
    - MPI, enhanced by OpenMP
- Local ALE in 3-D (ongoing)
  - V&V and modular installation into KIVA-hpFE all flow speed solver
- LES Turbulence modeling development (ongoing)
  - Dynamic LES, handles transitional flow without law of the wall
- Other turbulence closure (future)
    - Turbulence modeling, Reynolds Stress Modeling –
      - 2^{nd} moment methods
- Spray model development in FEM (future)
  - New algorithms
    - Develop model to predict instabilities and waves in jet near nozzle
    - Volume of Fluid interface tracking (VOF)

Summary

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-ϖ turbulence and great Dynamic LES model***
- Big improvement over other 2-equation models
  - Conjugate Heat Transfer is essentially free
- ***Nodal valued Spark Kernel Model***
- ***Chemistry (KIVA 30+ fuels or ChemKin)***

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

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

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.)

KIVA Program Users

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Many of these engineers and scientist LANL supports with general answer to problems. Those with less familiarity with engines and CFD require more instruction which I provide by correspondences over time as they develop a problem and solution, often those are students at universities. The code requires learning over time by performing problems and analysis.

Also, over **600 free licenses** of executable KIVA-4 code – node limited (45,000) but, fully functional version

Specific Material Properties at Droplet Location

The Finite Element approximation is of the form

$$\hat{\phi}(x_i) = \sum_{i=1}^{n} \phi_i N_i$$

- Term N_i is a polynomial of order *n* (bi-linear for 2nd *O* where n = 8).
- ϕ_i is the trial or determined nodal function value from the solution the governing equations.

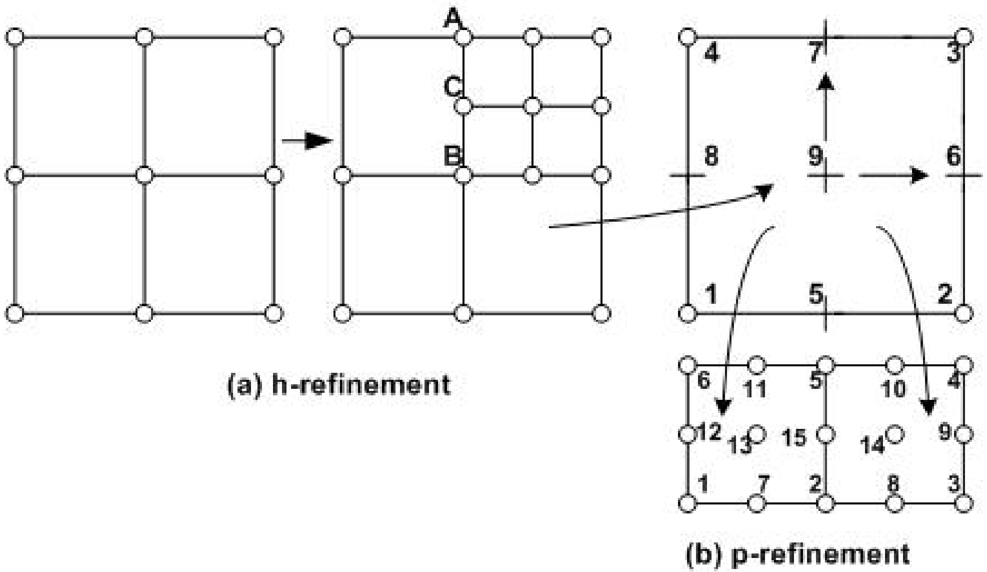
- We seek $\hat{\phi}(x, y, z)$ at some drop location, x, y, z.
- The proper values of N_i make the statement true.
- These global shape functions are evaluated in global coordinates by solving the n x *n* system to determine global interpolation functions yields N_i

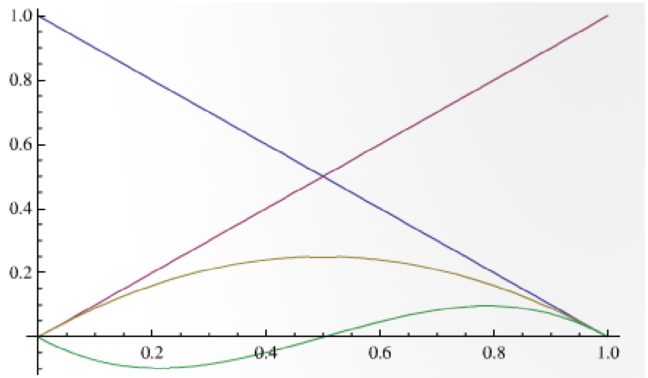
$$\begin{bmatrix} N_1 \\ N_2 \\ N_3 \\ N_4 \\ N_5 \\ N_6 \\ N_7 \\ N_8 \end{bmatrix} = \frac{1}{8} \begin{bmatrix} (1-x)(1-y)(1-z) \\ (1+x)(1-y)(1-z) \\ (1+x)(1+y)(1-z) \\ (1-x)(1+y)(1-z) \\ (1-x)(1-y)(1+z) \\ (1+x)(1-y)(1+z) \\ (1+x)(1+y)(1+z) \\ (1-x)(1+y)(1+z) \end{bmatrix}$$

- **Could transform into natural coordinates**
  - **Would require mapping global to local**

Then simply evaluate properties at the location were the properties are needed: T, *k*,ϖ, c_p, etc…

h and hp Adaptation Methods and shape functions





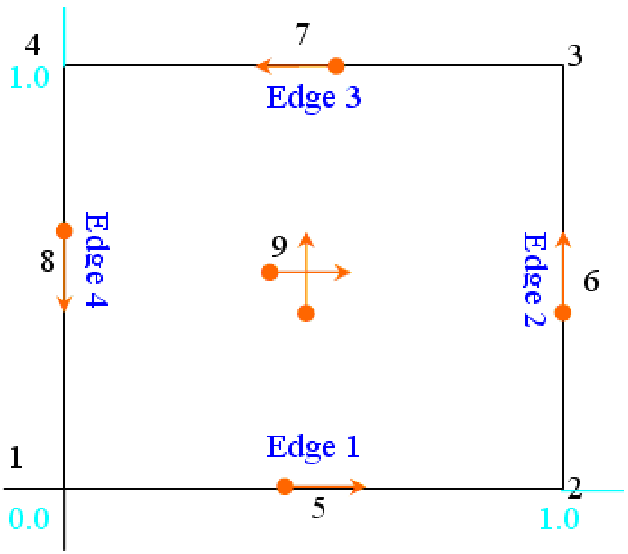
- Using Peano shape functions:

$$P_1 = 1 - \xi \;\; and \;\; P_2 = \xi \qquad \mathrm{P_i} = \mathrm{P_1}(\xi)\mathrm{P_2}(\xi)(2\xi\text{-}1)^{i-3} \;\; \text{for} \;\; \mathrm{i} = 3, \ldots, \mathrm{p}+1$$

- P1 and P2 are vertex shape functions.
- P_i either odd or even bubble functions, i=3,…p+1.
- Tensor product combinations span the space (algebraic products)

Hierarchic shape function

- Enrichment with Peano basis: adding new shape functions to existing.
  - Vertex shape functions and DOF remain same.
  - Add edge and bubble functions via tensor (algebraic) products of P_i



P1 and P2 Vertex shape functions where ξ_i

is vertex point on element side.

$$\begin{cases} \hat\phi_1(\xi_1,\xi_2)=\hat\chi_1(\xi_1)\hat\chi_1(\xi_2)=(1-\xi_1)(1-\xi_2)=P_1(1)P_1(2) \\ \hat\phi_2(\xi_1,\xi_2)=\hat\chi_2(\xi_1)\hat\chi_1(\xi_2)=\xi_1(1-\xi_2)=P_2(1)P_1(2) \\ \hat\phi_3(\xi_1,\xi_2)=\hat\chi_2(\xi_1)\hat\chi_2(\xi_2)=\xi_1\xi_2=P_2(1)P_2(2) \\ \hat\phi_4(\xi_1,\xi_2)=\hat\chi_1(\xi_1)\hat\chi_2(\xi_2)=(1-\xi_1)\xi_2=P_1(1)P_2(2) \end{cases}$$

Mid-edge shape functions P5 to P8:

$$\begin{cases} \hat\phi_{5,j}(\xi_1,\xi_2)=\hat\chi_{2+j}(\xi_1)\hat\chi_1(\xi_2) & j=1,\cdots,p_1-1 \\ \hat\phi_{6,j}(\xi_1,\xi_2)=\hat\chi_2(\xi_1)\hat\chi_{2+j}(\xi_2) & j=1,\cdots,p_2-1 \\ \hat\phi_{7,j}(\xi_1,\xi_2)=\hat\chi_{2+j}(1-\xi_1)\hat\chi_2(\xi_2) & j=1,\cdots,p_3-1 \\ \hat\phi_{8,j}(\xi_1,\xi_2)=\hat\chi_1(\xi_1)\hat\chi_{2+j}(1-\xi_2) & j=1,\cdots,p_4-1 \end{cases}$$

e.g., $\hat\phi_{5,1}(\xi_1,\xi_2)=P_3(\xi_1)P_1(\xi_2)=$
$P_1(\xi_1)P_2(\xi_1)(2\xi_1-1)^0\,P_1(\xi_2)$

Bubble shape functions

(inner area):

$$\hat\phi_{9,i,j}(\xi_1,\xi_2)=\hat\chi_{2+i}(\xi_1)\hat\chi_{2+j}(\xi_2) \quad \begin{cases} i=1,\cdots,p_v-1 \\ j=1,\cdots,p_h-1 \end{cases}$$

Adaptation and Error – the driver for resolution

$$\|e_V\| = \left(\int_\Omega e_V^T e_V \, d\Omega \right)^{1/2}$$ L_2 norm of error measure

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

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

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

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

$$p_{new} = p_{old} \, \xi_i^{1/p}$$ 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!