2012 DOE
Merit Review

2012 KIVA-Development

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Los Alamos National Laboratory
May 15, 2012

Project ID # ACE014

LA-UR-12-20079

Overview

2012 DOE Merit Review

Timeline

- 10/01/09
- 09/01/13
- 60% complete

Budget

- Total project funding to date:
  - 1,780K, 660K in FY 11
  - Contractor (Universities) share 30%
- Funding received in FY12 - 640K

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 engine technology development
  - 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
- Iowa State University - Dr. Song-Charng Kong

FY 09 to FY 13 KIVA-Development

Objectives

- **Robust, Accurate Algorithms in a Modular setting** –
  - Relevance to accurately predicting engine processes to enable better understanding of, flow, thermodynamics, sprays, in easy to use software for moderate computer platforms
    - **More accurate modeling requires new algorithms and their correct implementation.**
      - Developing more robust and accurate algorithms
        - To understand better combustion processes in internal engines
      - Providing a better mainstay tool
        - improving engine efficiencies and
        - 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 under PCCI conditions with strong wall impingement.
        - Providing accurate boundary conditions.
- **Easier and quicker grid generation**
  - **Relevant to minimizing of engine technology development**
    - 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- FY12

06/09 – Started Researching Fractional Step CBS method (switched to Pressure Stabilized PCS with P-G)

09/09 – 2D and 3D P-G Fractional Step (PCS/CBS) Finite Element Algorithm Developed (mathematics, engineering documents and evaluation).

01/10 – *h*-adaptive grid technique/algorithm implement in PCS-FEM method for 2D

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 – Benchmark tests

03/11 – Inserting PCS algorithm/coding **into *hp*-adaptive Framework**.

01/11 – FY11 Engineering documentation and precise algorithm details.

03/11 – *R*unga-Kutta method for 2nd order-in-time

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 – Subsonic and Supersonic Viscous Flow Benchmarks

10/11 – Local ALE for immersed moving parts with overset grid system 2-D

12/11 – Benchmarked Local ALE

12/11 – Parallel Conjugate Heat Transfer in KIVA-4mpi

01/12 – Paper submitted to ICHT and CTS

02/12 – Injection Spray model into the PCS FEM formulation

03/12 – Chemistry model into the PCS FEM formulation

03/12 – Abstract submitted ASME V&V and NHT

02&03/12 – Papers submitted to CTS

Approach

- Approach for Developing Robust and Accurate Numerical Simulation Code:
  - Computational Physics
    - Understanding of the physical processes to be modeled
    - Assumptions inherent in any particular model
      - Ability of the chosen method, the mathematical formulation, and its discretization to model the physical system to within a desired accuracy.
    - The ability of the models to meet and or adjust to users' requirements – modularity, documentation.
    - The ability of the discretization to meet and or adjust to the changing needs of the users.
    - Validation and Verification (V&V) – meeting requirements and data.
    - Effective modeling employs good software engineering practices.

Development Approach and Milestones

- Approach for Robust and Accurate Numerical Simulation:
  - Algorithms and their implementation (discretization) must be of sufficient accuracy and robustness to do be able to perform turbulence and spray modeling in a complex domain.
    - Yes, we need better models for spray and turbulence, on a robust and accurate platform.
  - More accurate modeling requires either 1) altering existing KIVA or 2) new algorithms. We have proceeded on both paths but, with greatest emphasis and promise by using newest algorithms and leveraging recent research.
- Development Process
  - Understanding of the physical processes to be modeled
    - Mathematical representations and evaluation of appropriate models.
    - Guiding engineering documents
      - Assumptions inherent in particular model and methods
      - Ability of hp-adaptive PCS/CBS method, the mathematical formulation, and its discretization to model the physical system to within a desired accuracy.
      - The ability of the models to meet and or adjust to users' requirements – chose
      - The ability of the discretization to meet and or adjust to the changing needs of the users.
      - Effective modeling employs good software engineering practices.
        - Modularity, Documentation, Levelized (under-the-hood)
  - Validation and Verification (V&V) – meeting requirements and data.
    - Verification via known algorithm substitution
    - Validation and development process
      - Benchmark Problems that exercise all code in all flow regimes

FY-12 Technical Accomplishments

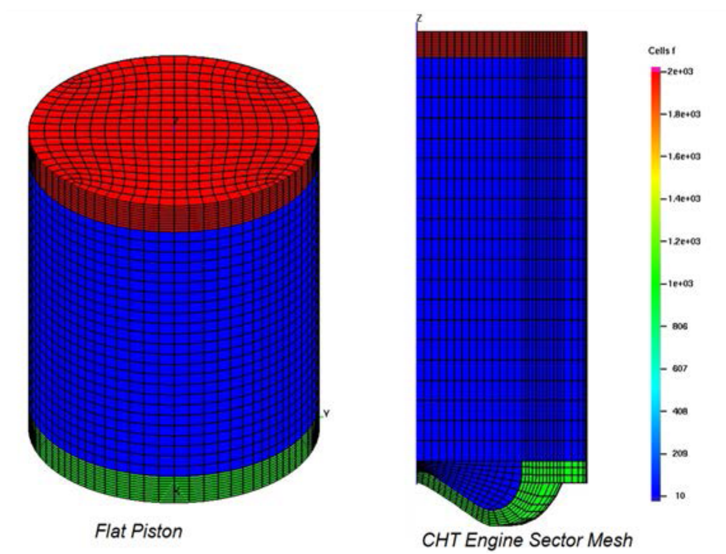
- Developing *hp*-adaptive PCS FEM Discretization for:
  - Accurate and Robust Turbulence Reactive Flow Combustion Modeling
  - 2-D and 3-D PCS *h*-adaptive and *hp*-adpative FEM codes are coded:
    - Modeling –Benefit of Eulerian system with 2nd order-in-time algorithm
    - Performed without large system of linear equations to solve!
    - Petrov-Galerkin Stabilization (P-G) having 3rd order spatial accuracy
    - Essentially no Numerical dispersion – FEM allows for precise measure and removal prior to solution advancement.
    - P-G Stabilization, Pressure Stabilization and can include Runga-Kutta for 2nd order-in-time (FY11)
    - 1 pressure solve per time step : Semi-implicit or an Explicit modality good for multi-core threading.
    - Equal-order isoparametric elements: same basis for pressure and momentum, exactly models curved surfaces.
    - k-ω turbulence model FY-09 & FY-10 (Carrington, et al 2010) *in hp-FEM formulation (FY12)*
    - *k-ε* blended low Reynolds (Wang, Carrington, Pepper 2009) .
    - New wall function system for both 2D and 3D - compressible (variable density in FY11).
    - PCG Solver & in-situ stationary preconditioning (FY 10)
    - Verification complete
      - Via known algorithm substitution and benchmark problems solution
    - *Validation and continued development and error/bug removal via*
      - *Benchmarks Problems*
    - Developed I/O and interfacing similar to KIVA-4 .
- *KIVA Spray model installed* ***with FEM Lagrangian Particle Transport***
- *Cubit grid generation (automatic from scripts) for both KIVA-4 and new KIVA, the hp-adaptive FEM m*ethod
- New accurate & robust local Arbitrary Lagrangian Eulerian (ALE) for moving parts on an Eulerian FEM fluids discretization!
- KIVA-4 Web-based Manual, Wiki KIVA, new KIVA web page, Demonstration code

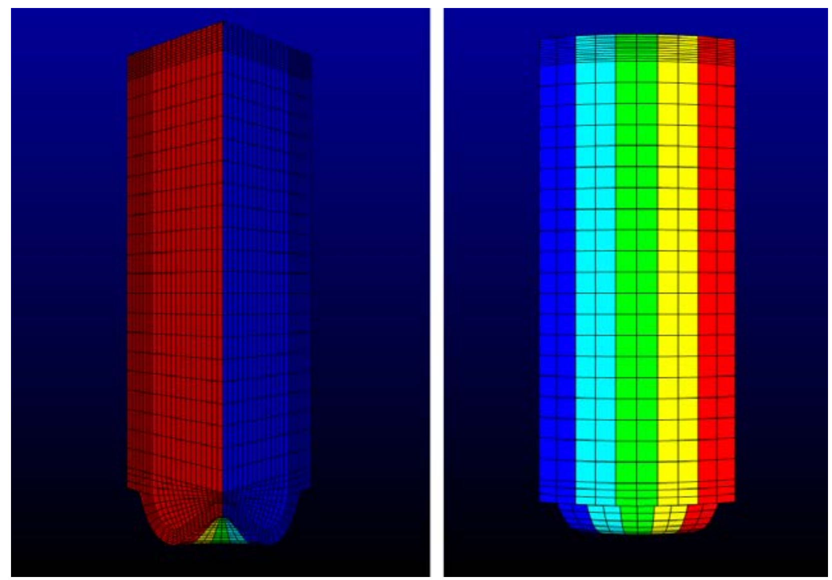
FY-12 Technical Accomplishments

- Conjugate Heat Transfer (CHT) in parallel code KIVA-4mpi
  - Motivation
    - Extend KIVA-4 capability to predict heat conduction in solids.
    - Use KIVA-4 to perform simultaneous simulation of in-cylinder processes and heat conduction in mechanical components.
    - In parallel method for faster turn-around times.
  - Expected outcome
    - Prediction of combustion chamber wall temperature distribution.
    - More accurate prediction of wall film and its effects on combustion and emissions under PCCI conditions with strong wall impingement.
  - Approach
    - Modify KIVA-4 for heat conduction calculation in solid.
    - Extend the computational domain to include both fluid and solid domains.
    - Decompose the domains, both fluid and solid, for parallel processing.
    - Perform integrated thermo-fluids modeling.
    - Energy equation is solved in solids.

Conjugate Heat Transfer (CHT) in parallel with KIVA-4mpi

- Overall combustion and emissions predictions are similar to the baseline case using uniform surface temperatures.
  - In general users are good at specify temperature and making adjustments in the models to produce good results on known systems.
- CHT is able to predict the surface T distribution (thermal loading) in the combustion chamber.
  - More predictive modeling capability.
- The code works for both conventional mesh and CHT mesh

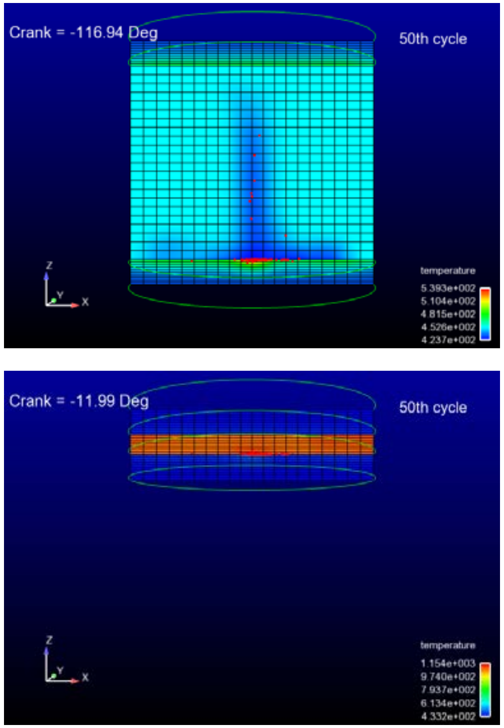




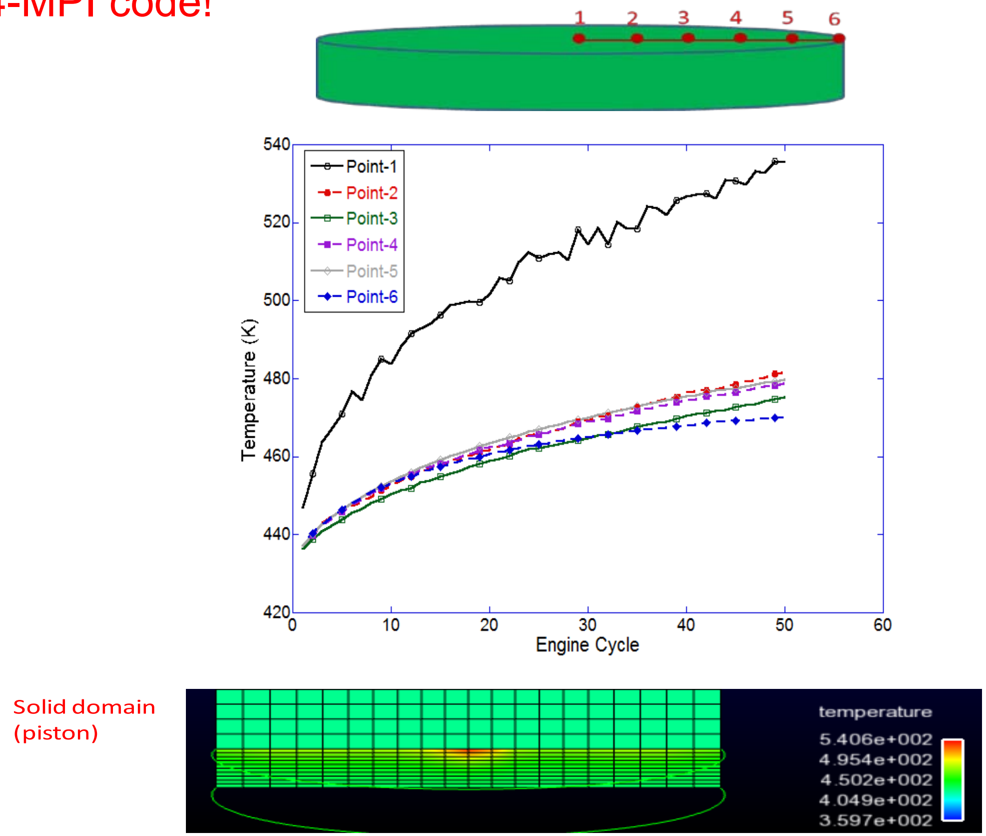
Domain decomposition for five processors for a diesel engine.

Enhancements to KIVA-4 MPI (parallel) for CHT modeling in solids

- Model predicts thermal gradients from heat transfer between in-cylinder gas and solids.
- Highest T occurs where at piston surface where spray combustion takes place most vigorously.
- Model predicts in-cylinder spray combustion and determines Temperature distribution on the solid surface using the improved KIVA-4-MPI code!



Temperature distributions in the gas and solid phases for selected timings at the 50th simulation cycle

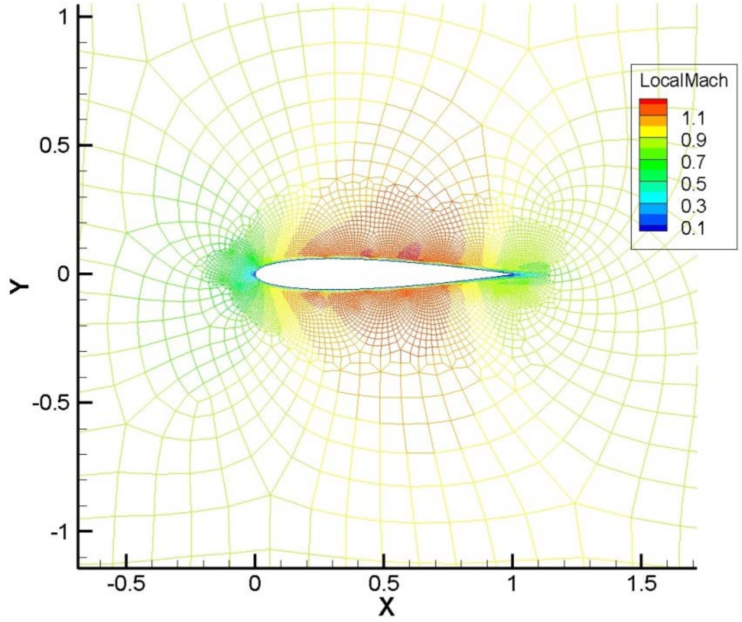


Temperature distributions on the piston surface after 50 simulation cycles

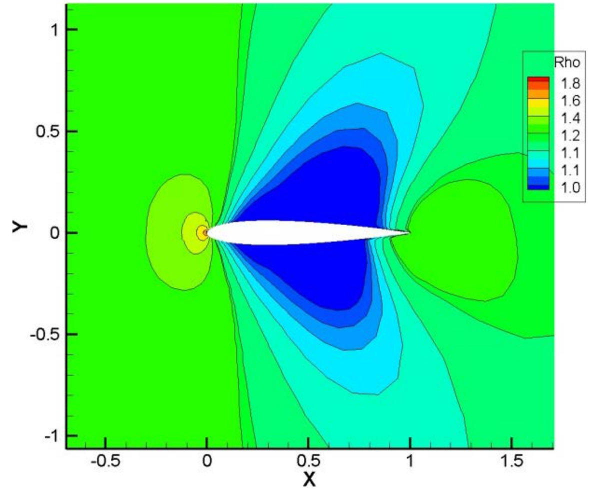
PCS FEM V&V - Subsonic flow regime

NACA 0012 airfoil test

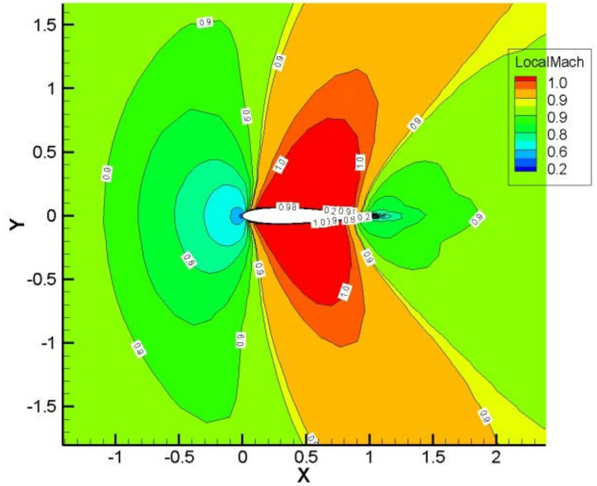
- Mach = 0.85 & α = 0
- Time dependent solution
- P-G stabilization.
- Multi-species testing, 2 species at inlet.
- Adapted grid by Cubit on generation .



~8000 cells and nodes – adapted on boundary



Density



Local Mach Number

Validation of *hp-a*daptive Method for NACA Airfoil at Subsonic

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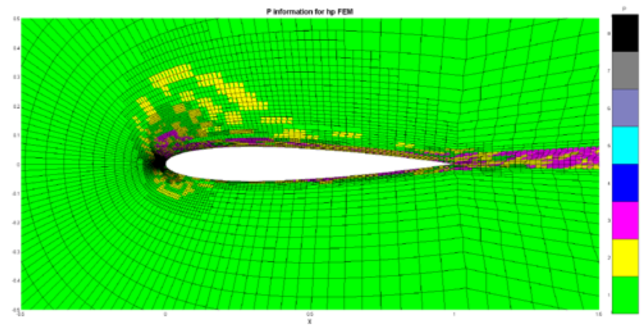
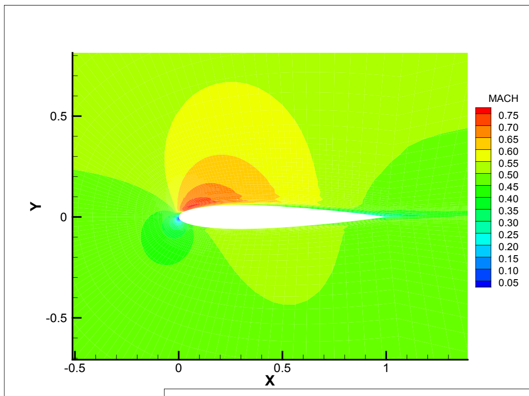
- Mach = 0.5 & attack angle α = 4°
  - Time dependent solution
  - Gambit generated initial grid
  - Agreement with data

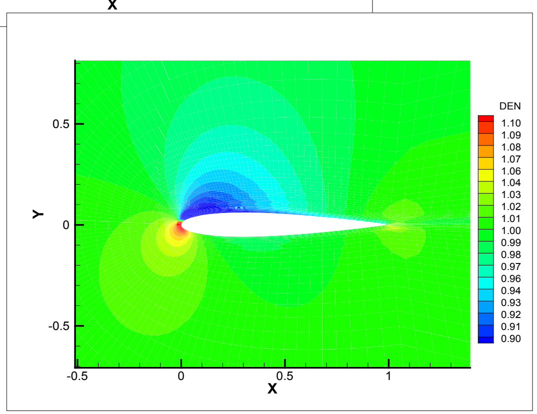


Final mesh *hp*-adaptive
(polynomial order shown in color)

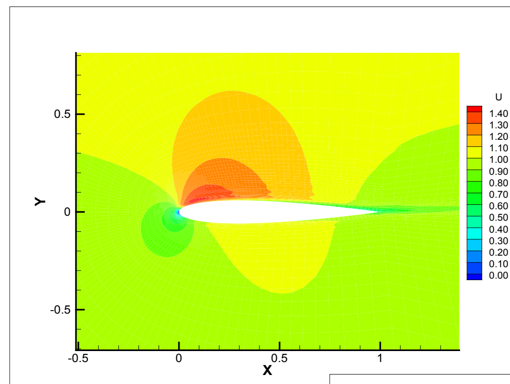
Local Mach

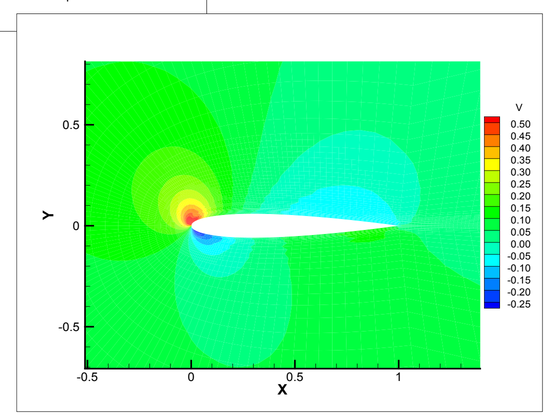


Density



Velocity components



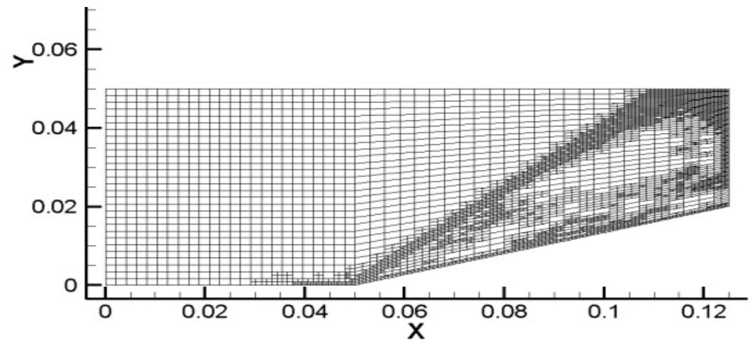


- Also continues to demonstrating Solver Capability
  - Truly curved and complex domains

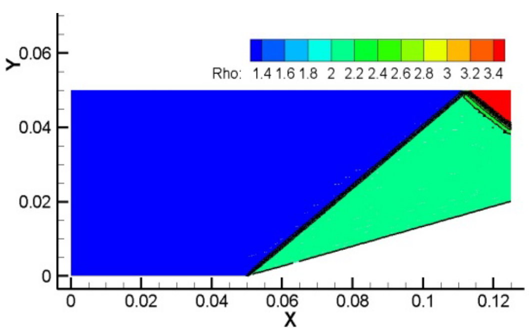
Validation of 2-D *h*-adaptive – PCS FEM

- Invsicid compressible Supersonic flow.
- 15^{o} compression ramp
  - Or moving projectile/scramjet
- Simulation results exactly matches analytic solution

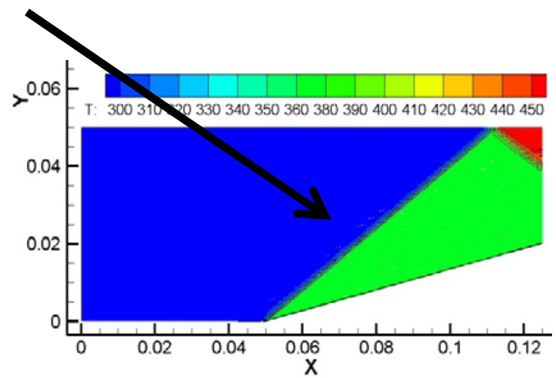
Adapted 20x50 Grid



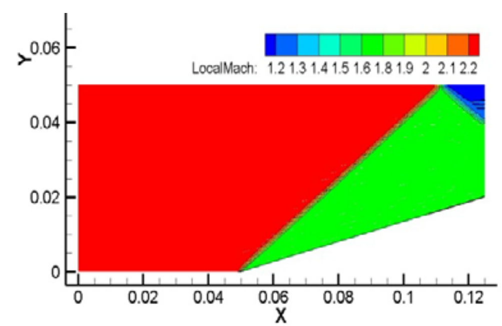
Shock



Density contours



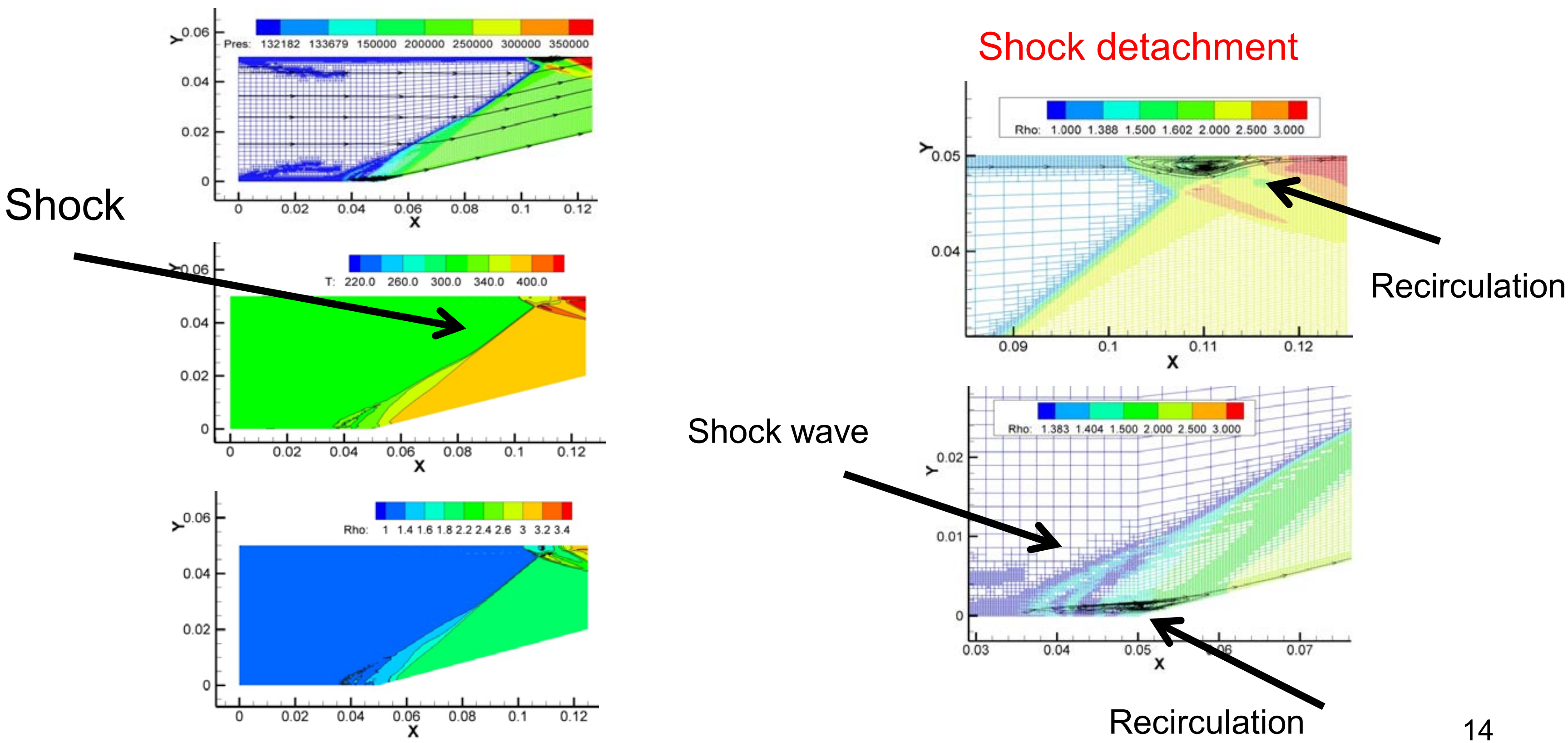
Isotherms



Local Mach contours

V&V - Viscous Flow on 15° Compression Ramp

- 15° compression ramp inlet speed Mach = 2.22
- *h*-adaptive PCS FEM (3 levels tracking the shock front in time.
- Shock angle exactly matches analytic solution
- Boundary layer separation, shock detachment and flow reversal (recirculation) in agreement experiment and other solutions.



Local ALE for immersed moving parts on unstructured grids

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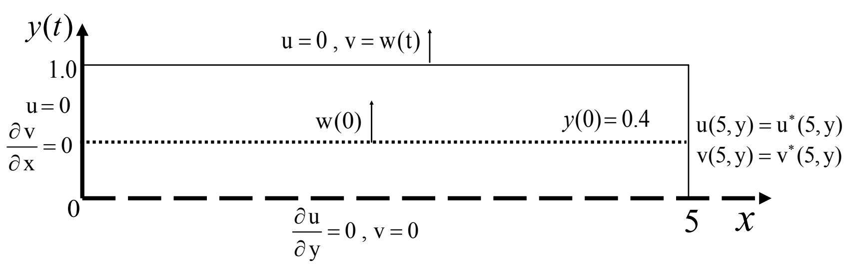
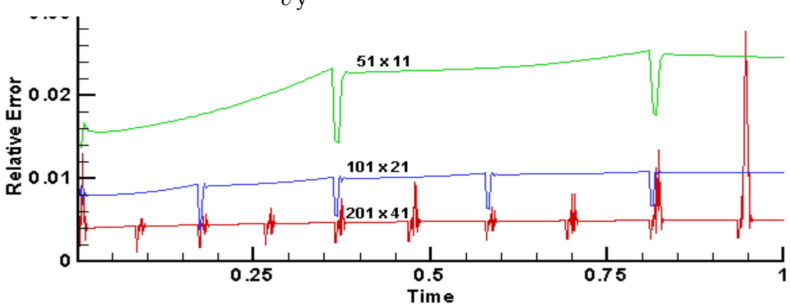
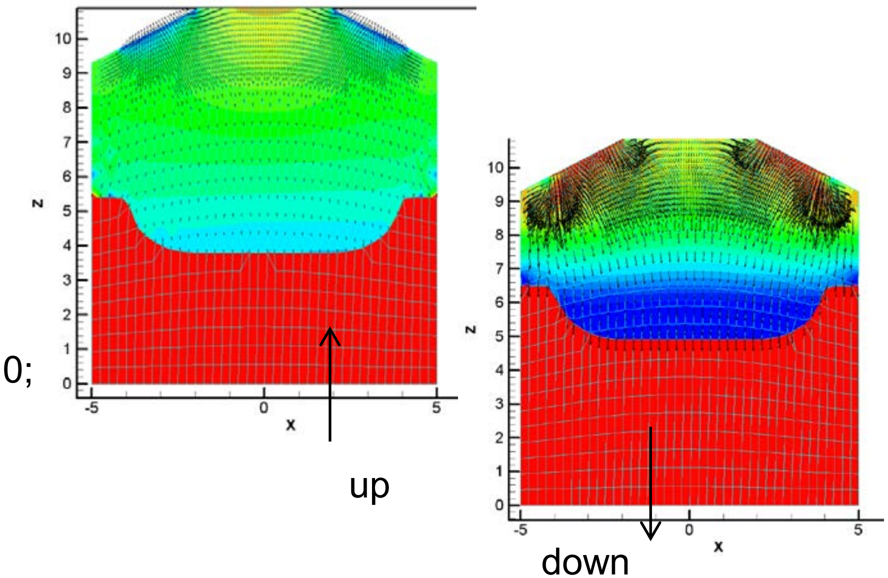
- **New local ALE algorithm**
  - Increase robustness - generic method.
  - Simulations with higher resolution.
  - Use of overset parts/grids.
  - Grid is of body only, fluid only.

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.

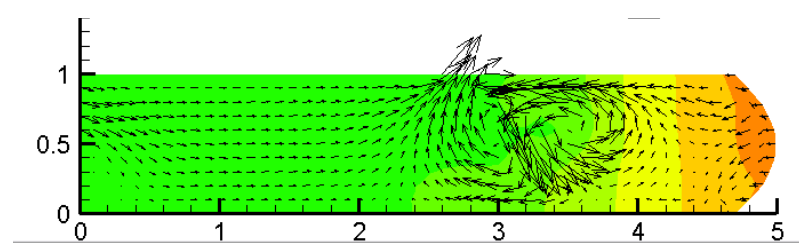




Grid convergence test : Average relative error vs. analytic solution to 2d pump(function of time)



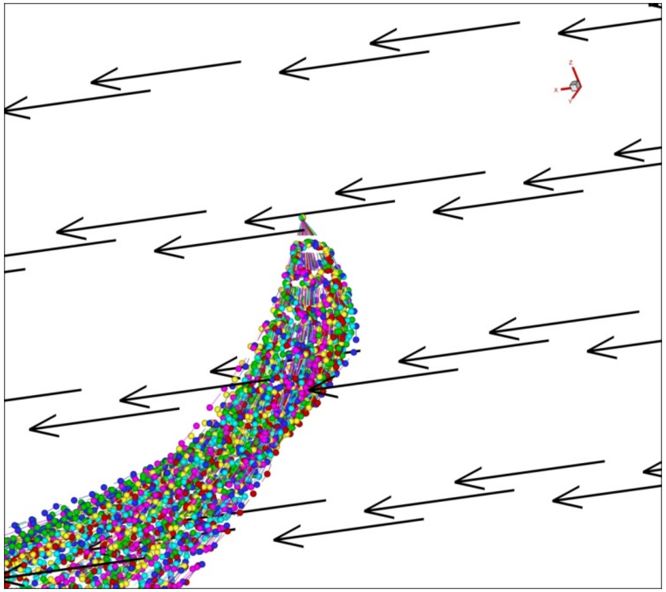
2d engine type test of ALE

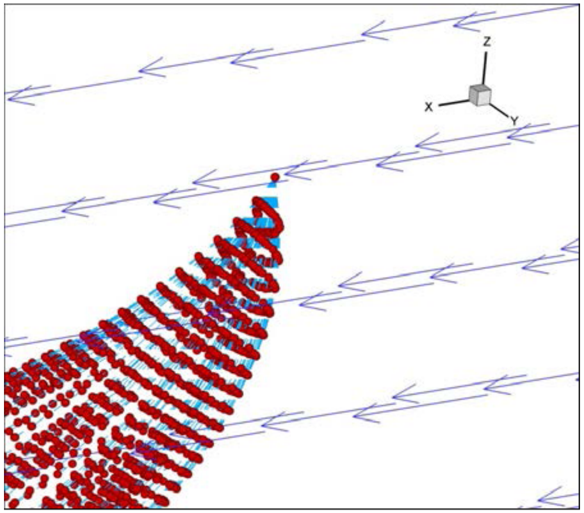


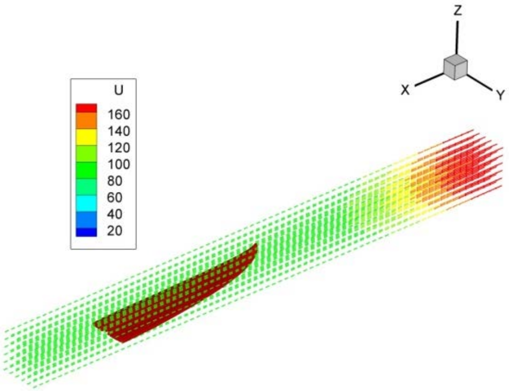
Parabolic Piston
working on incompressible fluid

Injection Spray in FEM (unstructured grids)

- **Improving the current algorithms with FEM**
- **KIVA multi-component spray with:**
  - Increase robustness on FEM
    - Exact location found quickly, robustly.
  - Simulations with higher resolution.
  - Precisely locating particles and associated flow/fluid properties >= 2^{nd} order.
    - 2^{nd} Order Spatial Resolution (minimum)
    - Fluid properties are exactly transferred to the injection spray – grid scale accuracy.



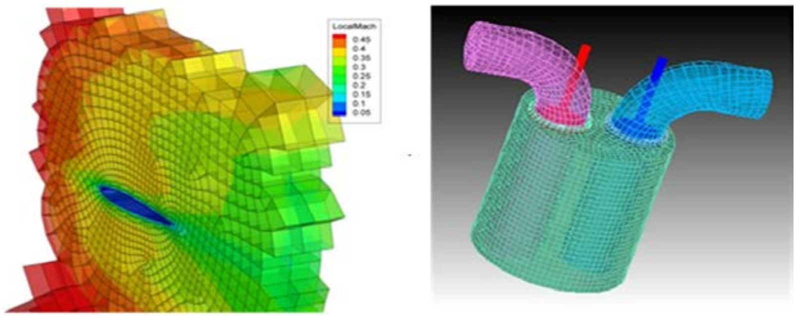




Grid Generation for KIVA-4 and the FEM formulation

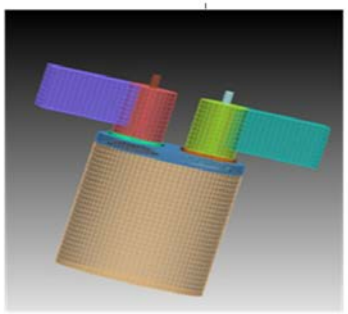
- **Grid generation**
  - **FEM is easy to grid with overset grid &**
    - **And local ALE**
  - **KIVA-4 is problematic but doable once scripts are created and tested**

FEM PCS Grids

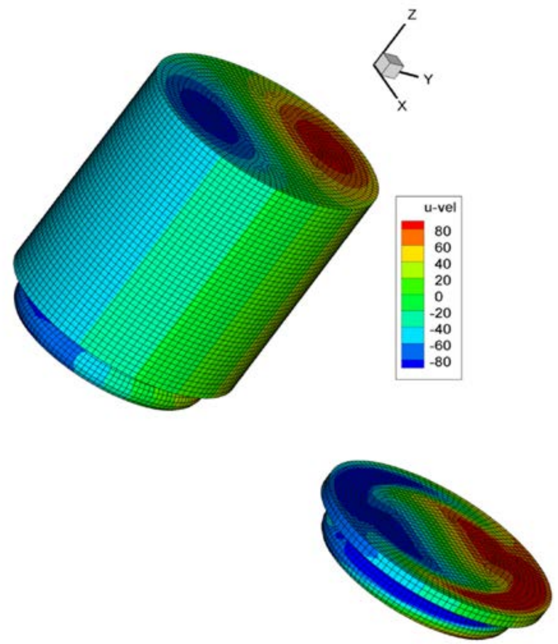


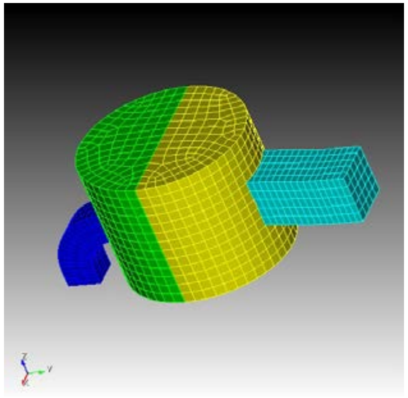
a) 3-D NACA Airfoil b) Engine grid

KIVA-4 Grid



c) Engine grid



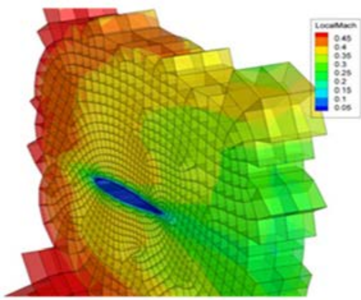


Grid generation using Cubit and only hexahedral cells

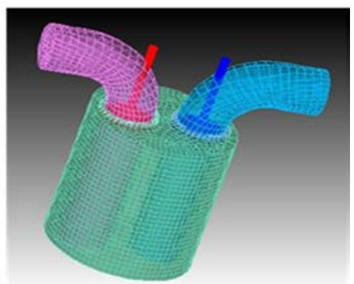
Grid Generation – Cubit and scripting

•Adding more to the program development including:
- In-house Grid Generation capability for both
- KIVA-hpFE and for KIVA-4 using,
  - Cubit for unstructured grids hexahedral engine domains.
- Engine Simulation using Cubit generated grid

FEM PCS Grids

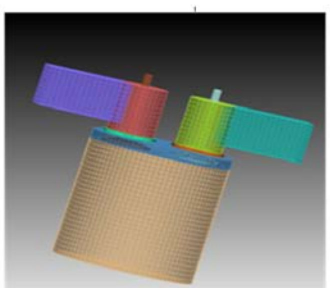


a) 3-D NACA Airfoil



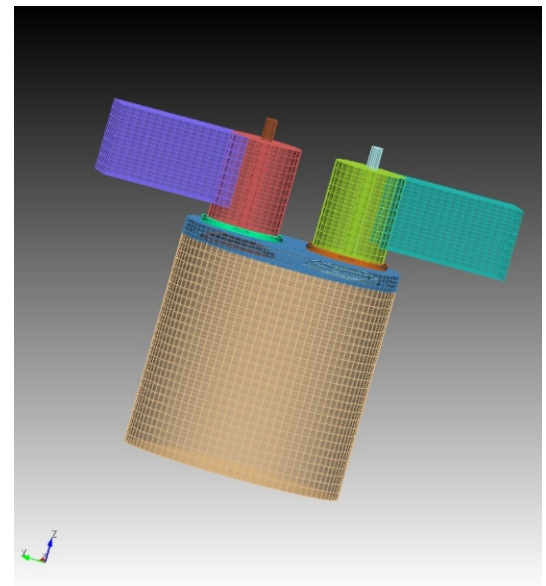
b) Engine grid

KIVA-4 Grid



c) Engine grid

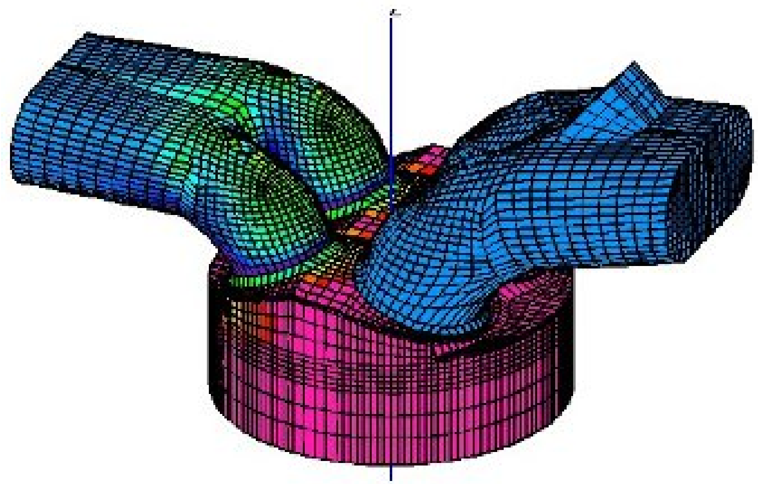
Grids for new
hp-FEM KIVA and KIVA-4



2 valve Engine Simulation using
Cubit generated grid

KIVA-4 Manual and websites

Manual Logo and new KIVA-4 logo (link to manual)



Wiki KIVA website and updated LANL KIVA website:
http://en.wikipedia.org/wiki/KIVA_(software)

http://www.lanl.gov/orgs/t/t3/codes/kiva.shtml

Linkedin KIVA discussion group created.

Demo distribution with automatic download at:
http://www.lanl.gov/orgs/tt/license/software/kiva/index.php

Program Collaborators

- Purdue, Calumet
  - *hp*-Adaptive FEM with Predictor-Corrector Split (PCS)
    - Xiuling Wang (Purdue) and GRA
- University of Nevada, Las Vegas
  - *hp*-Adaptive FEM with PCS split
- University of New Mexico
  - Moving Immersed Body and Boundaries Algorithm Development
    - Juan Heinrich, GRA and Postdoc
- Iowa State University
  - Conjugate Heat Transfer in KIVA-4 and KIVA-4mpi
    - Song-Charng Kong, a GRA and Postdoc (now at Caterpillar).
- LANL – 2 GRA’s in FY 11/12

KIVA Program Users

Licenses issued from LANL since 2010

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Program Users of all KIVA versions

Since Inception of licensing – most from OSTI - ESTSC

AB Volvo Penta Abt. TWT Analytik, Thermo- und Aerodynamik Achates Power LLC Advanced Science & Technology Applications (ASTA) AEA Technology Aerometrics Aerometrics Aerometrics Aeronauticos Universidad Polltecnica de Madrid AFRL/PRRE Air Force Alliance for Sustainable Energy, LLC Alliance for Sustainable Energy, LLC Allied Signal AES Allied-Signal Aerospace Co. Analysis & Design Application Co. Analysis & Design Application Co. Applied Research Associates Applied Thermal Sciences Applied Thermal Sciences Argonne National Laboratory Army Research Laboratory AutoEverSystems Corp. Automated Analysis Corp. Automotive Research Association of India Automotive Research Association of India Automotive Research Association of India AVL - List GmbH AWE AWE AZTI - Tecnalia/Itsas Ikerketa Saila BKM, Inc. 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Virginia Polytechnic Institute & State University Virginia Polytechnic Institute & State University Virginia Tech Von Karman Institute for Fluid Dynamics Warsaw University of Technology Warsaw University of Technology Waseda University Waseda University Waseda University Waseda University Waseda University, Center for Science and Engineering Wayne State University Wayne State University Wayne State University West Virginia University West Virginia University West Virginia University Western Michigan University Westinghouse Electric Corp. Westport Innovations, Inc. Wisconsin Engine Research Consultants Wolfson School of Mechanical and Manufacturing Engineering Woodward Governor Company Woodward Governor Company Yamaguchi University YAMAHA MOTOR CO., LTD. Yonsei University Yoshikawa Lab ZEXEL Corporation Zhejiang University, , Texas Southern , University, **University of Minnesota**

Future or Ongoing effort in FY12 to FY 14 Parallel hp-adaptive PCS FEM with 3d

- PCS-FEM
  - Consolidate research efforts into the main package (All)
  - Test cases: finish tests (LANL & Purdue)
    - Simple unit, various benchmark problems and more complex domains too/
    - Make rigorous comparisons to data and analytics.
      - Publish results in peer reviewed articles (3 papers just recently).
  - Overset Grid method for moving parts. Moving grid – new algorithm development for moving boundaries and immersed bodies. Immersed moving bodies - UNM.
  - Turbulence modeling (LES/RANS) – LANL, Purdue, UNLV.
  - Spray modeling (use of phase space spray model initiation and new algorithms such as Discrete Quadrature Moments Methods), Iowa State, UNLV, and LANL.
  - Parallel constructions – Matrix solver already developed for massively parallel constructions (Purdue and LANL).

Summary

- **Accurate, Robust and well Documented algorithms**
  - Developing and implementing robust and extremely accurate algorithms – Predictor-Corrector *hp-adaptive* FEM.
    - Reducing model's physical and numerical assumptions.
    - Measure of solution error
    - Drives the resolution when and where required.
    - New algorithm requiring less communication
    - no pressure iteration, an option for explicit: newest architectures providing super-linear scaling.
    - Robust and accurate immersed moving parts algorithm (local ALE).
      - 2d completed
      - 3d under development.
  - Conjugate Heat Transfer
    - More accurate prediction in wall film and its effects on combustion and emissions under PCCI conditions with strong wall impingement.
  - Validation in progress for all flow regimes
    - With Multi-Species
    - Beginning spray and chemistry model incorporation.
- **Grid generation**
  - Quickly generate grids from CAD surfaces of complex domains.
    - Cubit Grid interface developed.
    - Cubit supplies rapid generation, from quickly developed scripts.
      - The scripts are the technology now developed which can be easily modified for various engine designs.

Technical Back-Up Slides

(Note: please include this “separator” slide if you are including back-up technical slides (maximum of five). 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.)

Fractional Step or Predictor Corrector Petrov-Galerkin and/or Characteristic Terms

- FEM Discretization for PCS or CBS
  - Velocity predictor

$$\left\{\Delta \mathbf{U}_i^*\right\} = -\Delta t\left[\mathbf{M}_v^{-1}\right]\left[\left[\mathbf{A}_u\right]\left\{\mathbf{U}_i\right\} + \left[\mathbf{K}_{\tau u}\right]\left\{\mathbf{U}_i\right\} - \left\{\mathbf{F}_{v_i}\right\} - \frac{\Delta t}{2}\left(\left[\mathbf{K}_{char}\right]\left\{\mathbf{U}_i\right\} - \left\{\mathbf{F}_{char_i}\right\}\right)\right]^n$$

where $\left\{\Delta U_i^*\right\} = \left\{U_i^*\right\} - \left\{U_i^n\right\}$

  - Velocity corrector (*desire this*)

$$U^{n+1} - U^* = \Delta t \frac{\partial P'}{\partial x_i}$$ and $\left\{U_i^*\right\}$ is an intermediate

  - How do we arrive at a corrector preserving mass/continuity?
    - Continuity

$$\frac{\partial \rho}{\partial t} = -\frac{\partial \rho u_i}{\partial x_i} = -\frac{\partial U_i}{\partial x_i} \qquad \frac{\rho^{n+1} - \rho^n}{\Delta t} = -\frac{\partial U'_i}{\partial x_i}$$

Define $U' = \theta_1 U^{n+1} + \left(1-\theta_1\right)U^n$ with a level of implicitness

Desire $U^{n+1} - U^* = \Delta t \frac{\partial P'}{\partial x_i}$ Let $U'_i = \theta_1\left(-\Delta t \frac{\partial P'}{\partial x_i} + U_i^*\right) + \left(1-\theta_1\right)U_i^n$

Then $$\frac{1}{c^2}\Delta P = \Delta \rho = -\Delta t \frac{\partial U'_i}{\partial x_i} = -\Delta t \frac{\partial}{\partial x_i}\left[\left(\theta_1\left(-\Delta t\right)\frac{\partial P'}{\partial x_i} + \theta_1 U_i^*\right) + \left(1-\theta_1\right)U_i^n\right]$$

Density Solve (Pressure when incompressible flow)

So $$\frac{1}{c^2}\Delta P = \Delta\rho = -\Delta t\frac{\partial U_i^{'}}{\partial x_i} = \left[\left(\Delta t^2\theta_1\frac{\partial^2 P^{'}}{\partial x_i^2} - \Delta t\theta_1\frac{\partial U_i^*}{\partial x_i}\right) - \Delta t\left(1-\theta_1\right)\frac{\partial U_i^n}{\partial x_i}\right]$$

Let $P^{'} = \theta_2 P^{n+1} + (1-\theta_2)P^n$ with some level of implicitness

recall $\Delta U^* = U^* - U^n$

Then $$\frac{1}{c^2}\Delta P = \Delta\rho = -\Delta t\frac{\partial U_i^{'}}{\partial x_i} = \Delta t^2\theta_1\left(\theta_2\frac{\partial^2 P^{n+1}}{\partial x_i^2} + \left(1-\theta_2\right)\frac{\partial^2 P^n}{\partial x_i^2}\right) - \Delta t\left(\theta_1\frac{\partial \Delta U_i^*}{\partial x_i} + \frac{\partial U_i^n}{\partial x_i}\right)$$

and $\Delta P = P^{n+1} - P^n$

Density then $$\Delta\rho - \theta_2\frac{\partial^2\Delta P}{\partial x_i^2} = \frac{1}{c^2}\Delta P - \theta_1\theta_2\frac{\partial^2\Delta P}{\partial x_i^2} = \Delta t^2\theta_1\frac{\partial^2 P^n}{\partial x_i^2} - \Delta t\left(\theta_1\frac{\partial\Delta U_i^*}{\partial x_i} + \frac{\partial U_i^n}{\partial x_i}\right)$$

FEM Matrix form $$\left(\left[\mathbf{M}_p\right] + \Delta t^2 c^2\theta_1\theta_2\mathbf{H}\right)\left\{\Delta\rho_i\right\} = \left(\left[\frac{\mathbf{M}_p}{c^2}\right] + \Delta t^2\theta_1\theta_2\mathbf{H}\right)\left\{\Delta P_i\right\} =$$
$$\Delta t^2\theta_1\mathbf{H}\left\{P_i^n\right\} - \Delta t\left(\theta_1\mathbf{G}\left\{\Delta\mathbf{U}_i^*\right\} + \mathbf{G}\left\{\mathbf{U}_i^n\right\}\right) - \Delta t\left\{\mathbf{F}_{P_i}\right\}$$

Momentum/Velocity Corrector

Now $P^{n+1} = \Delta P + P^n$

recall $P^{'} = \theta_2 P^{n+1} + (1-\theta_2)P^n = \theta_2 \Delta P + P^n$

Then $$\Delta U_i = U^{n+1} - U^n = \Delta U* - \Delta t \frac{\partial P^{'}}{\partial x_i} = \Delta U* - \Delta t \left(\theta_2 \frac{\partial \Delta P}{\partial x_i} + \frac{\partial P^n}{\partial x_i} \right)$$

FEM Matrix form $$\left\{ \Delta \mathbf{U}_i \right\} = \left\{ \Delta \mathbf{U}^* \right\} - \Delta t \left[\mathbf{M}_u^{-1} \right] \left(\theta_2 \left[\mathbf{G} \right] \left\{ \Delta p_i \right\} + \left[\mathbf{G} \right] \left\{ p_i^{\,n} \right\} \right)$$

where $$\left\{ \mathbf{U}_i^{\,n+1} \right\} = \left\{ \Delta \mathbf{U}_i \right\} + \left\{ \mathbf{U}_i^{\,n} \right\}$$

final mass conserving velocity $$u^{n+1} = U^{n+1} / \rho^{n+1}$$

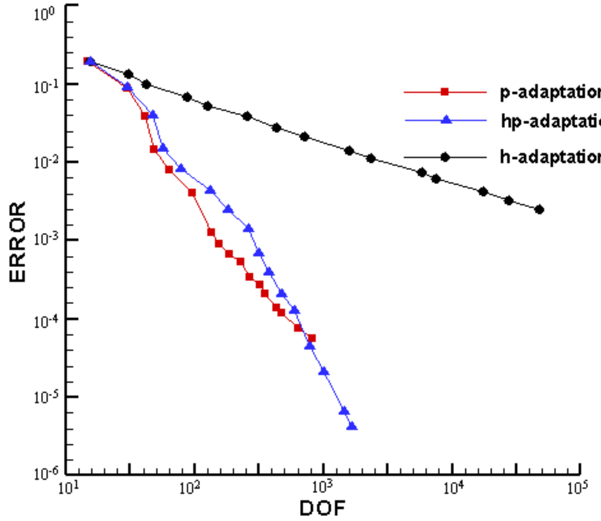
hp-adaptive methods for KIVA a CBS FEM method

- Why *hp*-adaptive grid
  - The use of *h*-adaptation can yield accurate solutions and rapid convergence rates.
    - Important when encountering singularities in the problem geometry.
  - Exponential convergence when higher-order, hp-adaptation
  - Error bounded by the following well known relation

$$\left\| u - u_h \right\|_m \leq c h^{k+1-m} \left\| u \right\|_r$$

'*u*' is assumed smooth in an H^{k+1} Sobolev norm, *m* is norm space, *r*=*k*+1, degree of integrable derivates in *H.*

- Convergence of *hp* about same as *p*. Speed of solution is better for *hp,* since the higher-order polynomials are used judiciously.
  - First perform h, then p for an hp scheme



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

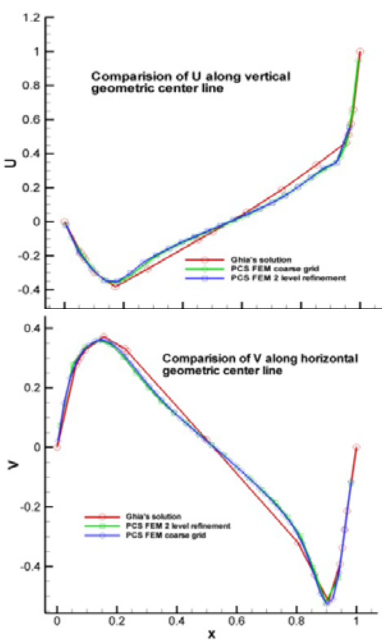
$$p_{new} = p_{old} \, \xi_i^{1/p}$$ Level of polynomial for element

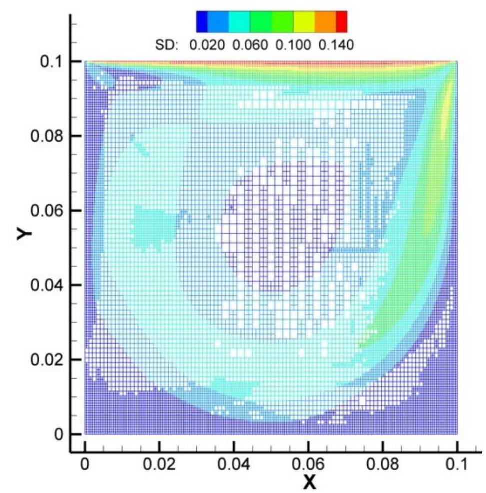
- Error measures:
  - Residual, Stress Error, etc..
- Typical error measures:
  - Zienkiewicz and Zhu Stress
  - Simple Residual
  - Residual measure
    - How far the solution is from true solution.
    - "True" measure in the model being used to form the residual.
    - If model is correct, e.g., Navier-Stokes,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

Validation of 2-D Fractional Step – FEM

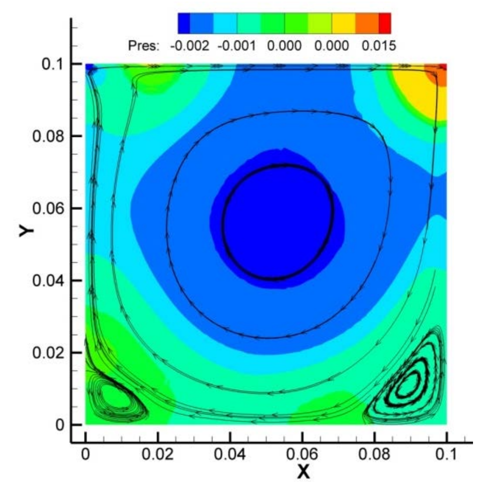
- Driven Cavity Benchmark – Re = 1000
  - **KIVA-4 published solution shows ~45,000 cells** for low Mach equations, an order magnitude larger than PCS or CBS FEM!
    - Adaptation at Pressure singularity in upper corners really helps solution
    - Original Grid 40x50
    - Excellent agreement with benchmark solution of Ghia
      - Ghia's benchmakr data is sparse resulting in poor representation of velocity gradients (curvature)

PCS FEM Comparison to
Ghia's solutions





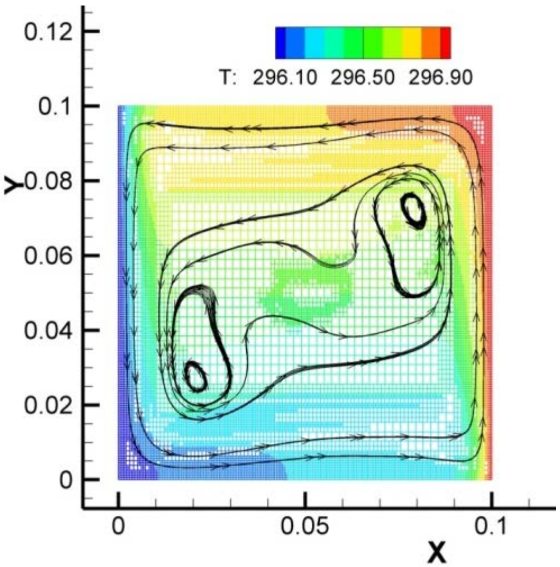
Enriched &
dynamically adapted grid



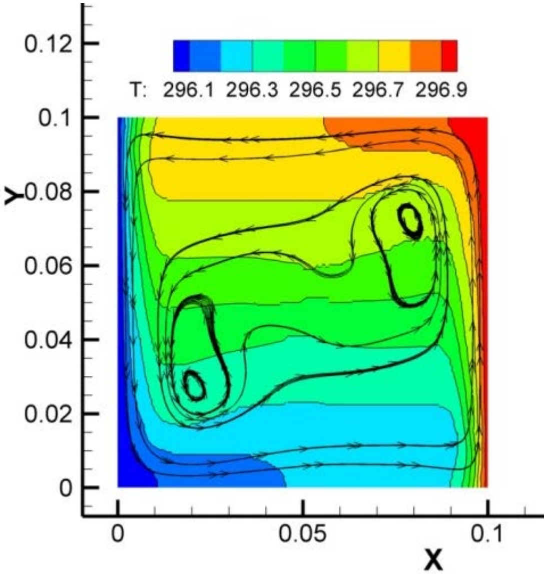
Streamlines & proper
location of recirculation zones

Validation of 2-D Predictor-Corrector PCS – FEM

- Slightly compressible low speed flow.
- Differentially Heated Cavity - Ra = 1.0e06.
- 40x50 Grid original grid density
- The final grid has 21245 nodes & 20037 elements. These nodes are added during automatic refinement as a function of the time dependent solution. The location and amount of refinement various in time.
- Excellent agreement with known benchmark solutions.
- Nusselt number average at hot side is 10.5 in reasonable agreement with other calculations (val Davis)



Adapted grid & streamlines dynamic grid refinement



Isotherms & streamlines