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Title: A Fractional-step h-adaptive Finite Element Method for Turbulent Reactive Flow – Validation for Incompressible Flow Regimes

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# A Fractional-step *h*-adaptive Finite Element Method
# for
# Turbulent Reactive Flow –
# Validation for Incompressible Flow Regimes

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The validation of a new Predictor-Corrector Split (PCS) projection method combining *h*-adaptive mesh refinement in a Finite Element Method (FEM) for combustion modeling is developed in this paper. This PCS system advances the accuracy and range of applicability of the KIVA combustion model and software. In fact, the algorithm combined with current KIVA spray and chemistry models and a moving parts algorithm in development will be the new KIVA generation of software from Los Alamos National Laboratory.

This paper describes the PCS *h*-adaptive FEM model for turbulent reactive flow spanning all velocity regimes and fluids. The method is applicable to Newtonian and non-Newtonian fluids and also for incompressible solids and fluid structure interaction problems. The method produces a minimal amount of computational effort as compared to fully resolved grids at the same accuracy.

The solver with *h*-adaption is validated here for incompressible benchmark problems in the subsonic flow regime as follows: 1) 2-D backward-facing step, 2) 2-D driven cavity, 3) 2-D natural convection in a differentially heat cavity.

The PCS formulation uses a Petrov-Galerkin (P-G) weighting for advection (similar to the Streamline Upwinding Petrov-Galerkin (SUPG)). The method is particularly well suited to changes in implicitness, from nearly implicit to fully explicit. The latter mode easily applied to the newest computers and parallel computing using one or a great many multi-core processors. In fact, the explicit mode is easily parallelized for multi-core processors and has been demonstrated to have super-linear scaling in the CBS stabilization.

The discretization is a conservative system for the compressible and incompressible momentum transport equation along with other transport equations for reactive flow. Error measurement allows the grid to adjust, increasing the spatial accuracy and bringing it under some specified amount. The conservative form also allows for the determination of the exact locations of the shocks. The *h*-adaptive method along with conservative P-G upwinding provides for good shock capturing. We also employ a gradient method shock capturing scheme for the supersonic/transonic flow regimes.

The method described in this paper is generally semi-implicit but, also can be run in explicit mode. In semi-implicit mode, pressure will range from implicit to explicit. The algorithm uses equal-order approximation for the dependent variables similar to much of our research in the field. The solution to the turbulent Navier-Stokes equations is similar to of previous work, using the k-W model. The system solves turbulent Navier-Stokes equations in a multi-component formulation as described by Carrington [1].

[1] Carrington, D.B., (2011) "A Fractional step *hp*-adaptive finite element method for turbulent reactive flow," Los Alamos National Laboratory Report, LA-UR-11-00466.

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# A Fractional-step *h*-adaptive Finite Element Method For Turbulent Reactive Flow – Validation for Incompressible Flow Regimes

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# Approach and Validation for KIVA-hpFE Combustion Code Development

- **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 an engine.
  - More accurate modeling requires either algorithm enhancements or using new algorithms.
    - We have proceeded on both paths –
      - greatest emphasis and promise by using newest algorithms and leveraging recent research and developments.
- **Development Process**
  - Understanding of the physical processes to be modeled
  - Guiding engineering documents
    - Assumptions inherent in a particular model and methods used.
    - Ability of h and 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.
    - 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
- **Validation and Verification** (V&V) – meeting requirements and data.
  - Verification via known algorithm substitution
  - Validation via enough benchmark problems that exercise all code in all flow regimes

# Critical Assumptions and Issues

- **A Fractional-Step Predictor-Correct System (PCS) in FEM algorithm**
  - **PCS *hp*-FEM algorithm removes assumptions and numerical from previous KIVA models. The method incorporates**
    - Variable density boundary layer & 3 zone turbulent wall law.
    - Wall shear stress is solved – not inaccurate power law assumptions.
    - Proper wall conditions for fluid momentum.
    - Ability to measure solution error.
    - Accurate advection, minimized advective dispersion.
    - At a minimum 2$^{nd}$ order-in-space, 3$^{rd}$ order advection
    - At a minimum 2$^{nd}$ order-in-space calculation of spray droplet physics and transport.
      - Ability to precisely bring temp, density, concentration, turbulence viscosity, momentum to each spray droplet quickly
      - Fast and precise location of droplets

# Fractional Step or Predictor Corrector using Petrov-Galerkin stabilization

- **FEM Discretization for PCS**
  - Velocity predictor

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

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

  - Velocity corrector (*desire this*) $U^{n+1} - U^{*} = \Delta t \dfrac{\partial P'}{\partial x_i}$

and $\left\{U_i^{*}\right\}$ is an intermediate

  - How do we arrive at a corrector preserving mass/continuity?
    - Continuity $\dfrac{\partial \rho}{\partial t} = -\dfrac{\partial \rho u_i}{\partial x_i} = -\dfrac{\partial U_i}{\partial x_i}$ $\qquad \dfrac{\rho^{n+1} - \rho^{n}}{\Delta t} = -\dfrac{\partial U'_i}{\partial x_i}$

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

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

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

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

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

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

# Momentum Predictor in Matrix form

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

Advection $$\mathbf{A}_u = \int_\Omega \left\{N_i\right\} u_j \left(\left[\frac{\partial N_k}{\partial x_j}\right]\right)\left\{U_i\right\} d\Omega$$

Stresses $$\mathbf{K}_{\tau u} = -\left(\int_\Omega \left\{N_i\right\}\left[\frac{\partial N_j}{\partial x_i}\right]\left\{\mu_t\right\}\left(\left[\frac{\partial N_j}{\partial x_i}\right] + \frac{1}{3}\left[\frac{\partial N_j}{\partial x_i}\right]\right)\left\{u_j\right\} d\Omega\right)$$

$$+\int_\Omega \left(\left[\mu + \mu_t\right]\left(\left\{\frac{\partial N_i}{\partial x_j}\right\}\left[\frac{\partial N_j}{\partial x_i}\right]\left\{u_i\right\} + \frac{1}{3}\frac{\partial N_j}{\partial x_i}\left\{u_j\right\}\right) - \frac{2}{3}\delta_{ij}\rho k\right) d\Omega$$

Body Force
Spray Force
Boundary stress

$$\mathbf{F}_u = \int_\Omega \left\{N_i\right\}\rho \sum_{k=1}^{NumSpecies}\left[N_j\right]\left\{\Upsilon_k f_k(x_i)\right\} d\Omega + \int_\Omega \left\{N_i\right\}\left[N_j\right]\left\{f_{drop_i}\right\} d\Omega +$$

$$\int_\Gamma \left\{N_i\right\}\left[\mu + \mu_t\right]\mathbf{n}_j \left[\frac{\partial N_j}{\partial x_j}\right]\left\{U_i\right\} d\Gamma$$

Characteristic terms

$$\mathbf{K}_{char} = -\int_\Omega \left[\frac{\partial N_k}{\partial x_l}\right]\left\{u_l\right\}\left(\nabla\left(U_k\left[N_k\right]\right)\right) d\Omega \qquad \mathbf{F}_{char} = \int_\Omega \left[\frac{\partial N_k}{\partial x_l}\right]\left\{u_l\right\}\left\{\rho g_i\right\} d\Omega$$

# Total Energy Matrix Terms

$$\mathbf{A}_e = \int_\Omega \{N_i\} u_j \left( \left[ \frac{\partial N_k}{\partial x_j} \right] \right) \{E_i\}\, d\Omega \qquad \mathbf{C}_p = \int_\Omega \{N_m\}[N_l]\{p_i\} \left[ \frac{\partial N_l}{\partial x_k} \right] \{u_k\}\, d\Omega$$

$$\mathbf{K}_\tau = \int_\Omega \left( \mu \left( \left\{ \frac{\partial N_i}{\partial x_j} \right\} \left[ \frac{\partial N_j}{\partial x_i} \right] - \frac{2}{3}\delta_{ij} \left[ \frac{\partial N_j}{\partial x_i} \right] \right) \{u_i\} - \frac{2}{3}\delta_{ij}\rho k \right) [N_j]\{u_k\}\, d\Omega$$

$$\mathbf{K}_T = \int_\Omega \left\{ \frac{\partial N_i}{\partial x_j} \right\} \left( \kappa + \frac{\mu_\tau}{\mathrm{Pr}_t} \right) \left[ \frac{\partial N_i}{\partial x_j} \right] + \left( \kappa + \frac{\mu_\tau}{\mathrm{Pr}_t} \right) \left\{ \frac{\partial N_i}{\partial x_j} \right\} \left[ \frac{\partial N_i}{\partial x_j} \right] d\Omega$$

$$q_{div} = \int_\Omega \rho \left( \sum_{l=1}^{NumSpecies} H_l D_{l,N} \left\{ \frac{\partial N_i}{\partial x_j} \right\} \left[ \frac{\partial N_i}{\partial x_j} \right] \{\Upsilon_{li}\} \right) d\Omega = \int_\Omega \rho \left( \sum_{l=1}^{NumSpecies} c_{pl} D_{l,N} \left\{ \frac{\partial N_i}{\partial x_j} \right\} \left[ \frac{\partial N_i}{\partial x_j} \right] \{\Upsilon_{li}\} T \right) d\Omega$$

$$\mathbf{Q}_{ss} = -\int_\Omega \{N_i\} \sum_{k=1}^{NumSpecies} \{H_{o,k} w_{k,i}\} d\Omega \qquad \mathbf{Q}_{vs} = \int_\Omega \{N_i\}\{Q_e\}\, d\Omega$$

$$\mathbf{F}_{eb} = \int_\Omega \rho \{N_i\} \left( \sum_{l=1}^{NumSpecies} [N_j]\{U_k\}[N_j]\{\Upsilon_l f_l(x_k)_i\} \right) d\Omega$$

$$\mathbf{F}_{es} = \int_\Gamma \{N_i\} \hat{n} \cdot \left( [N_j]\{q_i\} \right) d\Gamma + \int_\Gamma \{N_i\} \hat{n} \cdot \left( \sum_{k=1}^{NumSpec} \left[ \frac{\partial N_j}{\partial x_i} \right] \{ (D_{kN} \Upsilon_k)_i \} \right) d\Gamma$$

# Species Transport

- Species $\Upsilon_j = {\rho_j}/{\rho}$

$$\rho\frac{\partial \Upsilon_j}{\partial t} = -\rho\frac{\partial}{\partial x_i}\left(\Upsilon_j u_i\right) + \frac{\partial}{\partial x_i}\left[\left(\rho D_{j,N} + \frac{\mu_\tau}{Sc_t}\right)\frac{\partial \Upsilon_j}{\partial x_i}\right] + \Upsilon_j f_j(x_i) + \dot{w}^j_{chem} + \dot{w}^j_{spray}$$

$$\Delta\Upsilon_i^j = -\Delta t\left[\mathbf{M}_\Upsilon^{-1}\right]\left[\left[\mathbf{A}_\Upsilon\right]\left\{\Upsilon_i^j\right\} + \left[\mathbf{K}_\Upsilon\right]\left\{\Upsilon_i^j\right\} + \left\{\mathbf{F}_{\Upsilon s_i^j}\right\} + \left\{\mathbf{Q}_{\mathbf{i}_i}\right\}\right]^n$$

$$\mathbf{A}_\Upsilon = \int_\Omega \{N_i\} u_j \left(\left[\frac{\partial N_k}{\partial x_j}\right]\right)\{\Upsilon_i\}\, d\Omega$$

$$\mathbf{K}_\Upsilon = -\left(\int_\Omega \{N_i\}\left[\frac{\partial N_j}{\partial x_i}\right]\left\{\frac{\mu_t}{Sc_t}\right\}\left[\frac{\partial N_j}{\partial x_i}\right] d\Omega\right) + \int_\Omega \left(\left[D + \frac{\mu_t}{Sc_t}\right]\frac{\partial N_i}{\partial x_j}\frac{\partial N_j}{\partial x_i}\right) d\Omega$$

$$\mathbf{Q}_\Upsilon = \int_\Omega \{N_i\}\left[N_j\right]\left\{\dot{w}^j_{chem}\right\} + \{N_i\}\left[N_j\right]\left\{\dot{w}^j_{spray}\right\} d\Omega$$

$$\mathbf{F}_{\mathbf{i}} = \int_\Omega \{N_i\}\left[N_j\right]\left\{\Upsilon_j f_j(x_i)\right\} d\Omega$$

# 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!

# Incompressible Form - artificial compressibility

- This Pressure Poisson equation can be solved without an artificial compressibility term
  - Severe time step restrictions.
- Using artificial incompressibility for solution of pressure
  - Reduce the time step restrictions

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

- Assume speed of sound is sufficiently low to not need restrictive time step sizes.
- Rewriting for solution of delta pressure

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

An artificial compressibility parameter $\beta$ can be stated:

$$\beta=\max(\varepsilon,vel_{convec},vel_{diff})$$

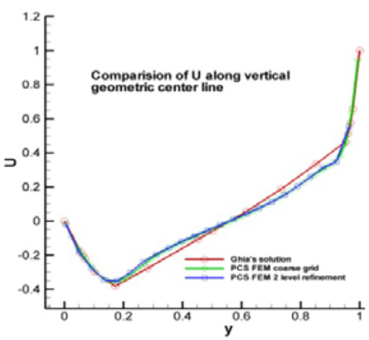
Here $vel_{convec}$ and $vel_{diff}$ are the convection and diffusion velocities, respectively, given as

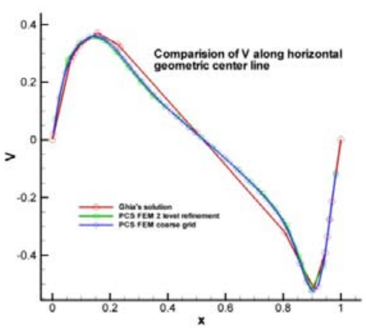
$$vel_{convec}=\|u\|,\ vel_{diff}=\frac{\mu}{\rho h_e}$$

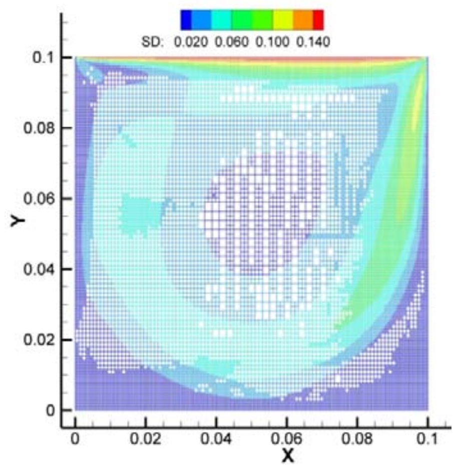
where '$h_e$' is the element size and where ε is a small to ensure $\beta$ is not approaching zero.

# Validation of 2-D Fractional Step – FEM

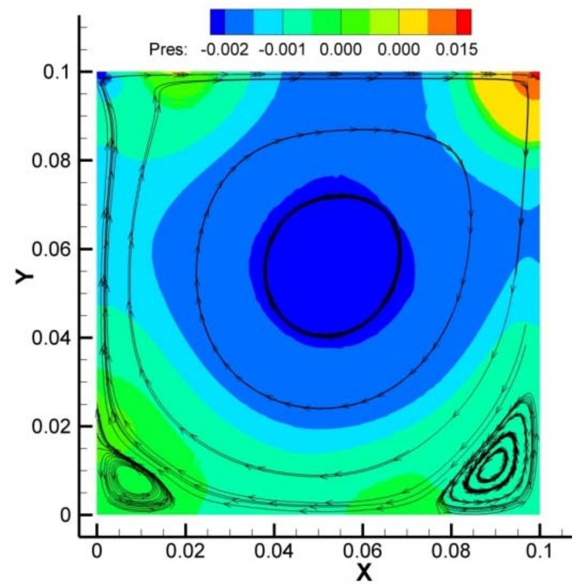
- **Driven Cavity Benchmark – Re = 1000**
  - Adaptation at Pressure singularity in upper corners really helps solution
  - Original Grid 40x50
  - Excellent agreement with benchmark solution of Ghia
    - Ghia's benchmark data is sparse resulting in poor representation of velocity gradients (curvature)
    - Primary circulation corresponds to Ghia's location of <.05313,0.5625>
    - Circulartion bottom left of ~ Ghia's <.00859,0.00781>
    - Circulation bottom right of ~ Ghia's <0.08594,,0.01094>




Enriched & dynamically adapted grid




Streamlines & proper location of recirculation zones

# Validation of Natural Convection in the 2-D Pedictor-Corrector Method

- Slightly compressible low speed flow.
- Differentially Heated Cavity - Ra = 1.0e05.
- 40x50 Grid original grid density
- The final grid has 20014 nodes & 18876 elements. These nodes are added during automatic refinement as a function of the time dependent solution. The location and amount of refinement varies in time.
- Excellent agreement with known benchmark solutions.
- Nusselt number in reasonable agreement with Graham val Davis (*IJNMF*1983):
  - Average on Δx convergence
    - 4.523 to 4.767 on hot wall

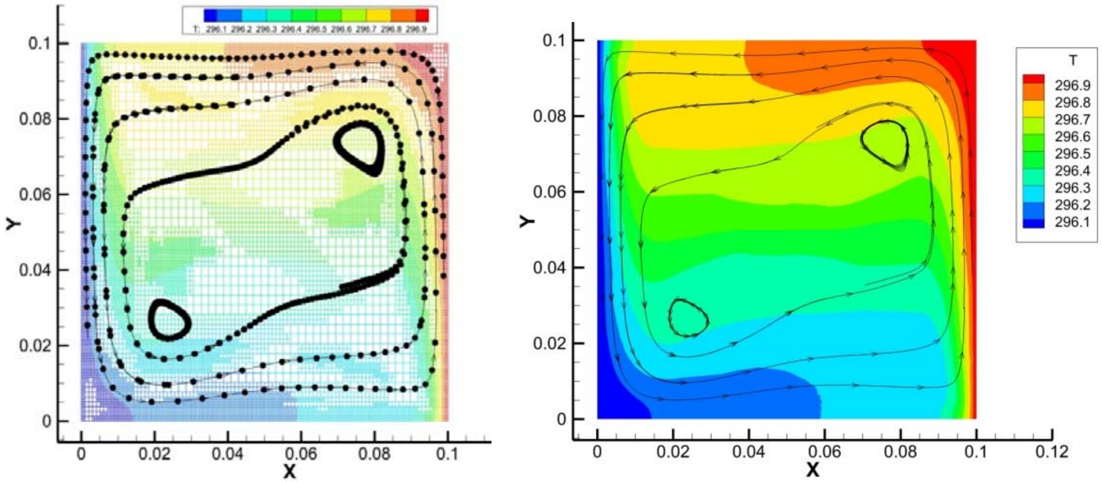
      compares to PCS FEM of

      = 3.4 to 4.1
  - Highest Nusselt
    - 6.538 to 7.905

      compares to FEM of

      6.06 to 8.4 but in the

      proper locations.

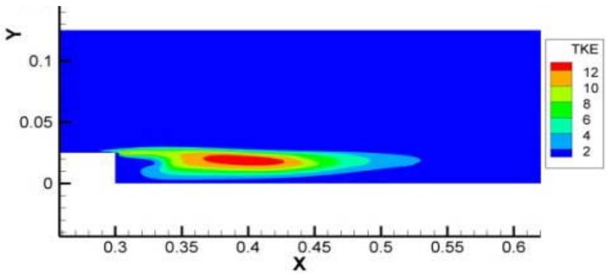



Adapted grid & streamlines dynamic grid refinement

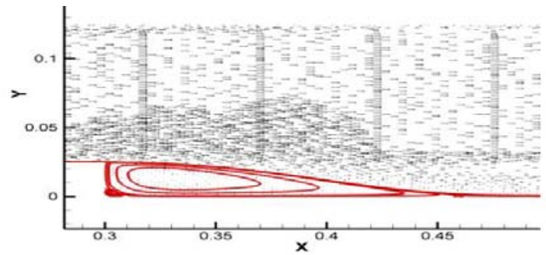
Isotherms & streamlines

# Validation of RANS turbulence model *k-ω* using backward-facing step at Re=28,000

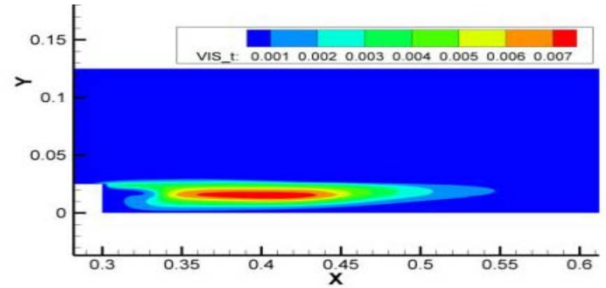
Comparison to Experimental data from Vogel and Eaton (1985)




Turbulent kinetic energy

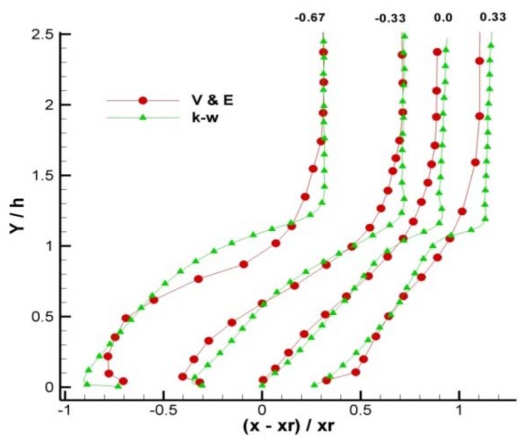



Velocity Vectors and Streamlines, xr = 6.8h



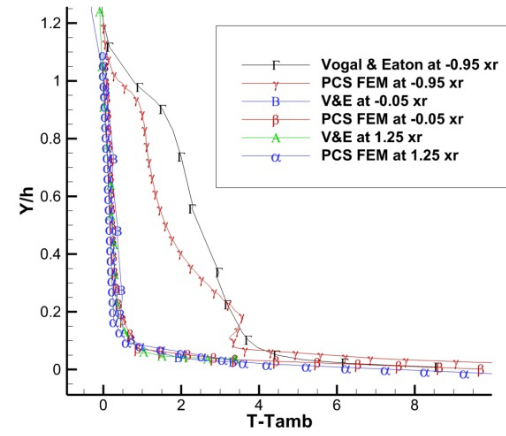

Effective viscosity

xr = recirculation length




U velocity downstream of step vs. experiment at various xr

Also, compares favorably to solution of similar configuration by Ilinca, et al. (1998).




Thermal profile downstream of step vs. experiment at various xr

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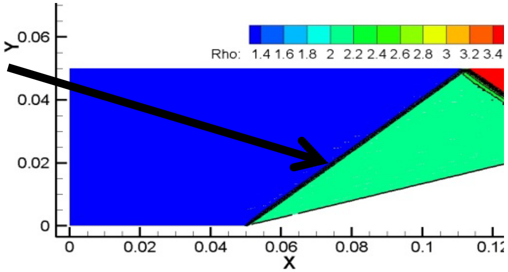
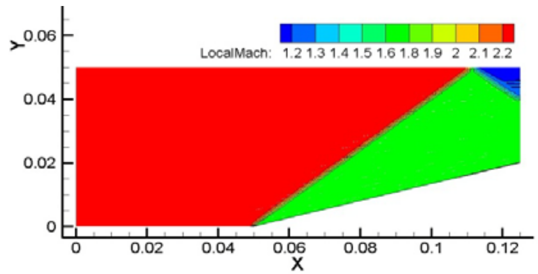
# Ongoing/Future Validation

- Viscous / invisicid compressible supersonic flow.
  - $15^o$ compression ramp

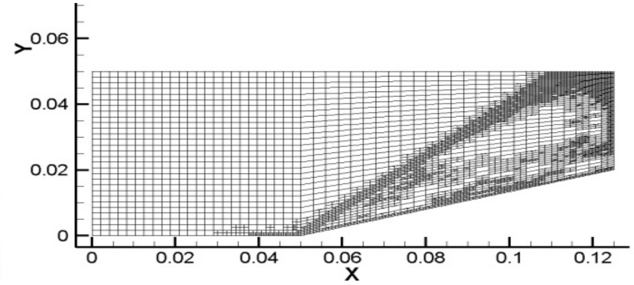
Shock




Density contours

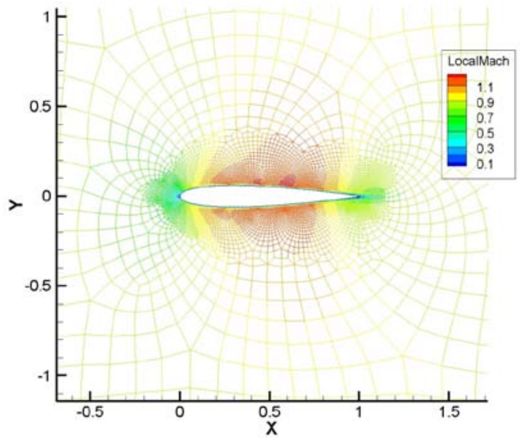


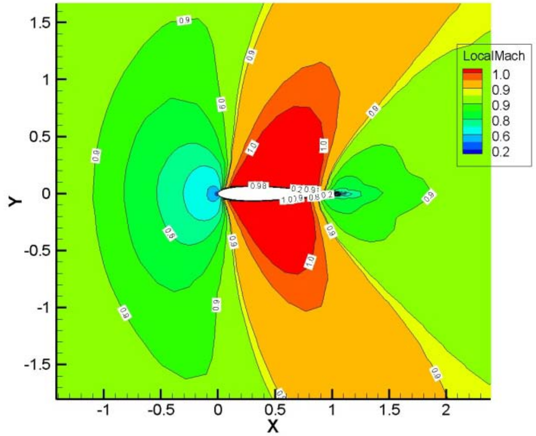

Local Mach contours




Adapted 20x50 Grid

  - NACA 0012 Airfoil for compressible subsonic / transonic flow



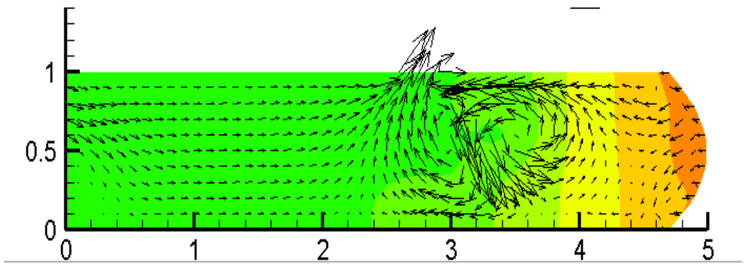




Local Mach Number

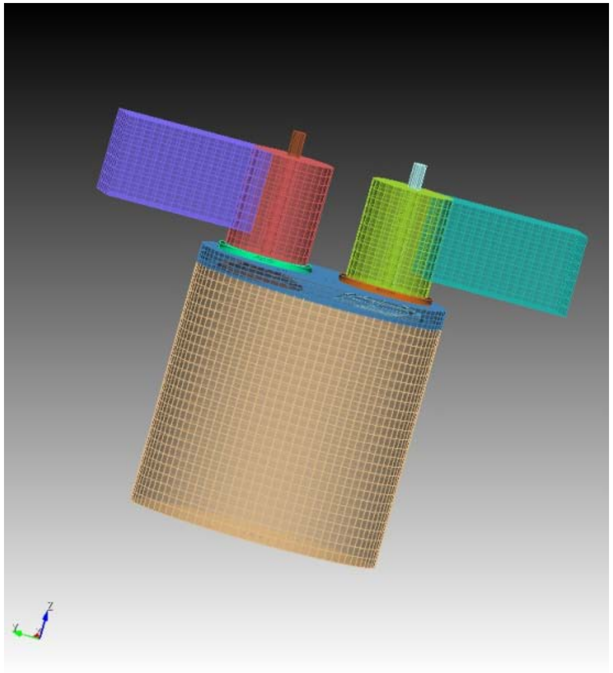
~8000 cells and nodes – adapted on boundary

# Ultimately have Validated Software for engine modeling

The goal for KIVA-hpFE is accurate and robust engine modeling




Parabolic Piston
•An incompressible fluid pump.
•Cubit generated unstructured grid.
**(from Juan Heinrich at UNM)**



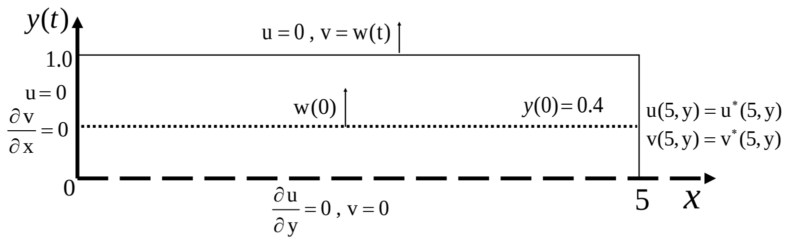
2 valve Engine Simulation using
Cubit generated grid and old ALE algorithms - structured like grid.

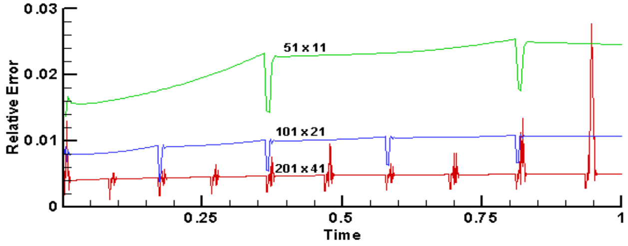
# Ongoing Validation for Local ALE

## -immersed moving parts (piston/valves) on unstructured grids

- **New local ALE algorithm ( from Juan Heinrich at UNM )**
  - 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)

# Program Collaborators

- Purdue, Calumet
  - *hp*-Adaptive FEM with Predictor-Corrector Split (PCS)
    - Xiuling Wang (Purdue) and GRA's
- University of Nevada, Las Vegas
  - FEM and LES with sprays with PCS split
    - Darrell Pepper and looking for a Ph.D. candidate
- University of New Mexico
  - Moving Immersed Body and Boundaries Algorithm Development
    - Juan Heinrich, GRA and looking for a Postdoc
- LANL – 2 GRA's in FY 11/12

# Summary

- **Accurate, Robust and well Documented algorithms**
  - Developing and implementing robust and extremely accurate algorithms
    - Predictor-Corrector *h-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,
      - Option for explicit mode for newest architectures providing super-linear scaling.
  - Validation in progress for all flow regimes
    - Old school comparison to analytic solutions and experiments
    - Various Benchmark problems with known solutions or experimental data.
      - Testing all components in all flow regimes.
      - with Multi-Species transport to test scalar equations and aggregate fluid properties

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- University of New Mexico
- University of Nevada, Las Vegas