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Report

KIVA-Update June 2012

USCAR Working Group Meeting

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T-3 Fluid Dynamics and Solid Mechanics

Abstract

Development of a fractional step, a Predictor-Corrector Split (PCS), or what is often known as a projection method combining *hp*-adaptive system in a Finite Element Method (FEM) for combustion modeling has been achieved. This model will advance the accuracy and range of applicability of the KIVA combustion model and software used typically for internal combustion engine modeling.

This abstract describes a PCS *hp*-adaptive FEM model for turbulent reactive flow spanning all velocity regimes and fluids that is being developed for the new KIVA combustion algorithm, particularly for internal combustion engines. The method and general solver is applicable to Newtonian and non-Newtonian fluids and also for incompressible solids, porous media, solidification modeling, and fluid structure interaction problems. The fuel injection and injector modeling could easily benefit from the capability of solving the fluid structure interaction problem in an injector, helping to understand cycle to cycle variation and cavitation. This is just one example where the new algorithm differs from the old, in addition to handling Conjugate Heat Transfer (CHT), although there a numerous features that makes the new system more robust and accurate. In these ways, the PCS *hp*-adaptive algorithm does not compete with commercial software packages, those often used in conjunction with the currently distributed KIVA codes for engine combustion modeling. In addition, choosing a local ALE method on immersed moving parts represented by overset grid that is 2nd order spatially accurate, allows for easy grid generation from CAD to fluid grid while also provide for robustness in handling any possible moving parts configuration without any code modifications!

The combined methods employed produce a minimal amount of computational effort as compared to fully resolved grids at the same accuracy. We demonstrate the solver on benchmark problems for the all flow regimes as follows: 1) 2-D backward-facing step using h-adaption, 2) 2-D driven cavity, 3) 2-D natural convection in a differentially heat cavity with h-adaptation, 4) NACA 0012 airfoil in 2-D, 4) supersonic flows over compression ramps, 5) 2-D natural convection in a differentially heat cavity with *hp*-adaptation, 6) 3-D natural convection in a differentially heat sphere with *hp*-adaptation.

In addition, we show the new moving parts algorithm for working for a 2-D piston; the immersed moving parts method also for valves and pistons, vanes, etc... The movement is performed using an overset grid method and is 2nd order accurate in space, and never produces a tangle grid, that is, robust system at any resolution and any parts configuration.

We also show CHT for the currently distributed KIVA-4mpi software and some fairly automatic grid generation using Sandia's Cubit unstructured grid generator. A new electronic web-based manual for KIVA-4 has been developed as well.

This abstract is part of a other documents which not only is part of the verification process but an engineering working document, describing the method and how it gets incorporated into the larger combination of spray and chemistry models/modules from (in) KIVA. These document also detail to some extent what has been implemented and what has been verified and validated to date.

The PCS formulation is similar to that described in 2 papers by O.C. Zienkiewicz and R. Codina [1] and O.C. Zienkiewicz et al. [2] where they use a characteristic finite element method (CBS). The difference between systems is use of a Petrov-Galerkin (P-G) method [3] which is similar to the Streamline Upwinding Petrov-Galerkin (SUPG) instead of the CBS scheme. The method is particularly well suited to changes in implicitness, from nearly implicit to fully explicit. The latter mode being well suited for the newest computers and parallel computing using one or a great many multi-core processors (*exascale* computing). 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.

Many examples and description of a P-G method are found in the literature. Some using a characteristic scheme, e.g., Demkowicz and Oden used the characteristic FEM method combined an *h*-adaptive grid method to solve various convection diffusion equations that also employed P-G weighting for stabilization [4]. Using Runga-Kutta (R-K) integration with P-G seems to provide a stable and perhaps more flexible mechanism than just the characteristic formulation for about the same cost. Although without the higher order time integration, found with the CBS or R-K methods, the solver seems to perform well in time for couple solutions (source terms) and since the pressure scheme is stabilized with higher order time terms.

The underlying discretization is a conservative system for the compressible and incompressible momentum transport equation along with other transport equations for reactive flow. This method provides for a measurement of the error in the discretization, and adjusts the spatial accuracy to minimize the error or bring it under some specified amount. The conservative form allows for the determination of the exact locations of the shocks. The *hp*-adaptive method along with conservative P-G upwinding provides for good shock capturing.

The method employs a partially implicit system of equations if desired. The algorithm allows for equal-order approximation similar to much of our research in the field [7][8]. The *hp* scheme generally is constructed as that currently implemented and described by Wang and Pepper [9]. The general FEM method for equal-order projection approximation is detailed in Pepper and Carrington [10], Carrington and Pepper [11], Wang, Carrington and Pepper [12]. The solution to the turbulent Navier-Stokes equations as given by Carrington [13] and Wang, Carrington and Pepper [12], and is somewhat adjusted for the CBS algorithm. The solution to the turbulent Navier-Stokes equations from the original incompressible and compressible codes is somewhat adjusted, but many of the operators we currently employ function in the PCS scheme as outlined by the following. For more detailed turbulence modeling discussion with adaptive FEM and a 2-equation closure please see Carrington, 2007 [13].

A detailed derivation of the underlying numerical method, that is, the FEM discretization and use of the variation residual statements can be found in the references, particularly the following: [2][9][10][11][12][13].

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LA-UR-12-draft

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T-3 Fluid Dynamics and Solid Mechanics

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KIVA-Development: (more) predictive turbulent reactive flow modeling

- **Robust, Accurate Algorithms in a Modular, Modern setting**
  - Robustly & accurately predicting engine processes
    - To enable better understanding of flow, thermodynamics, and sprays.
    - Easy to use reliable software for moderate computer platforms providing reasonalble turn-around.
    - Doesn't compete with commercial software.
  - **More accurate modeling requires new algorithms and their correct implementation.**
    - Developing more robust and accurate algorithms
      - To help in understanding better combustion processes within internal engines
    - Providing a better mainstay tool
      - Better two-equation turbulence models, developing LES
      - Newer and mathematically rigorous algorithms will allow KIVA to meet the future and current needs for combustion modeling and engine design.
      - Developing a fractional step Petrov-Galerkin (P-G) *hp*-adaptive finite element method.
      - Measure of error even without knowing the true solution – **That's Predictability**!
- **Easier and quicker grid generation**
  - **Relevant to minimizing the time it takes for engine technology development**
    - CAD to CFD via Cubit or Gambit Grid Generation Software and FEM using local ALE for parts.
      - Easy CAD to CFD using Cubit or Gambit grid generators
      - *hp*-FEM CFD solver with overset actuated parts and new local ALE in CFD,
        - removes problems with gridding around valves and stems.
        - Grid the fluid domain and simply overlay the parts and still have 2nd order spatial accuracy
      - KIVA-4 engine grid generation (pretty much automatic with *snapper work –round still difficult*).

Developing Robust and Accurate Numerical Simulations:

- 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.

Robust and Accurate Numerical Simulation

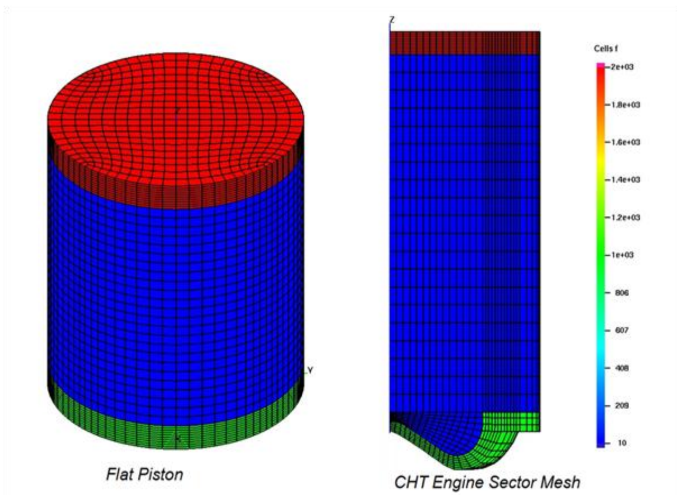
- Sufficiently accurate and robust Algorithms and discretization to allow for good turbulence and spray modeling in a complex domains.
  - Yes, we need better models for spray and turbulence, on a robust and accurate platform.
- More accurate modeling requires either altering existing KIVA or new algorithms.
  - 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 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 (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

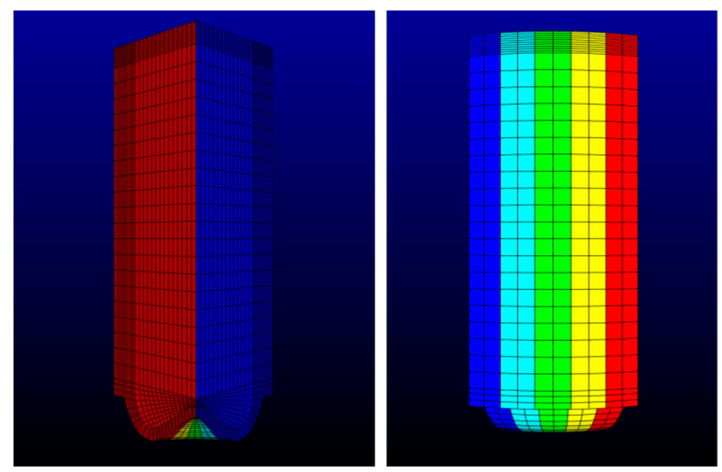
Accomplishments - Accurate and Robust Turbulence Reactive Flow/Combustion

- **Developing *hp*-adaptive PCS FEM Discretization for:**
  - 2-D and 3-D Predictor-Corrector Split (PCS) *h*-adaptive and *hp*-adpative FEM codes are developed:
    - Modeling –Benefit of Eulerian system with 2nd order-in-time algorithm (with Runga-Kutta 2)
    - PCS is performed without large system of linear equations to solve!
    - Petrov-Galerkin Stabilization (P-G) having 3rd order spatial accuracy
    - P-G advection Stabilization & Pressure Stabilized
    - 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 and *k-ε* blended low Reynolds better for wall bounded recirculating flows.
    - Parallel PCG Solver & in-situ stationary preconditioning.
    - *Validation and continued development and error/bug removal via*
      - *Dozens of Benchmarks Problems*
  - *KIVA multi-component Spray model using* ***FEM Lagrangian Particle Transport***
  - *Cubit (automatic from scripts) and Gambit grid generation (automatic) for the PCS FEM m*ethod
  - New local Arbitrary Lagrangian Eulerian (ALE) for moving parts on an Eulerian system
    - Accurate (2nd order in space) ,
    - robust for all designs – no modifications for engine types or parts, ports, vanes, etc…
    - robust for high resolution while maintaining accuracy!
    - Provides for easy automatic grid generation because of the overset grids for parts
- KIVA-4 and KIVA-4mpi
  - KIVA-4 *Web-based* Manual, *Wiki* KIVA, *new KIVA web page*, *Demonstration code*
  - Parallel Conjugate Heat Transfer extended from KIVA-4 to KIVA-4mpi

Conjugate Heat Transfer (CHT) in parallel 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**
  - Decomposed grid made for both solid and fluid parts, collocated nodes and the flux is balance via iteration per time step.

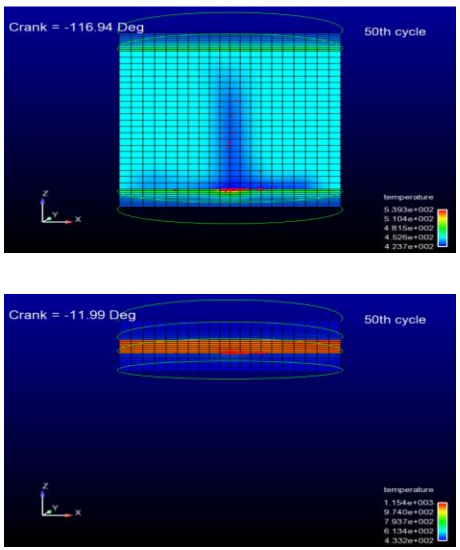




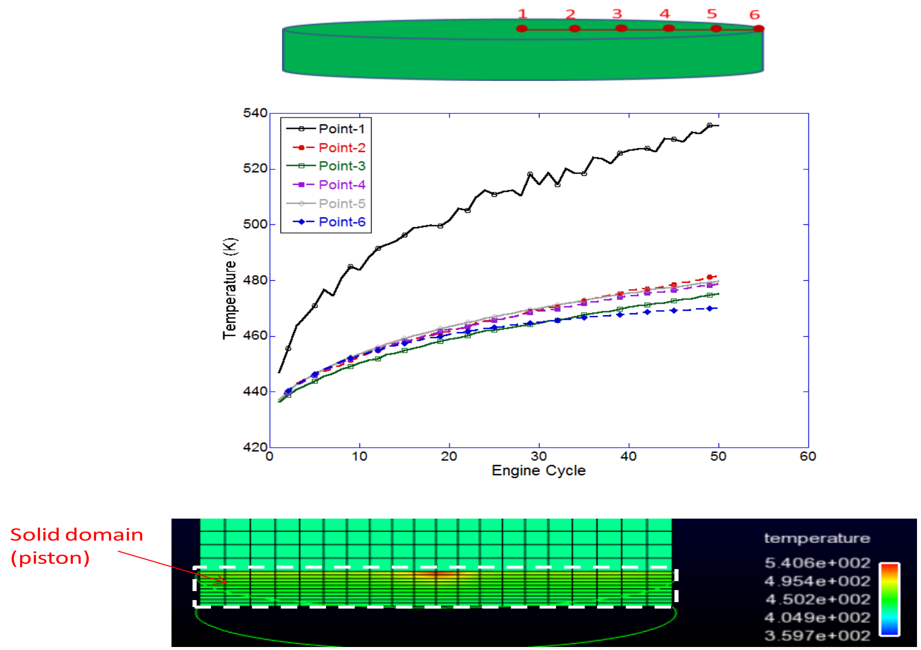
Domain decomposition for five processors for a diesel engine.

Enhancements to KIVA-4 MPI - CHT

- **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

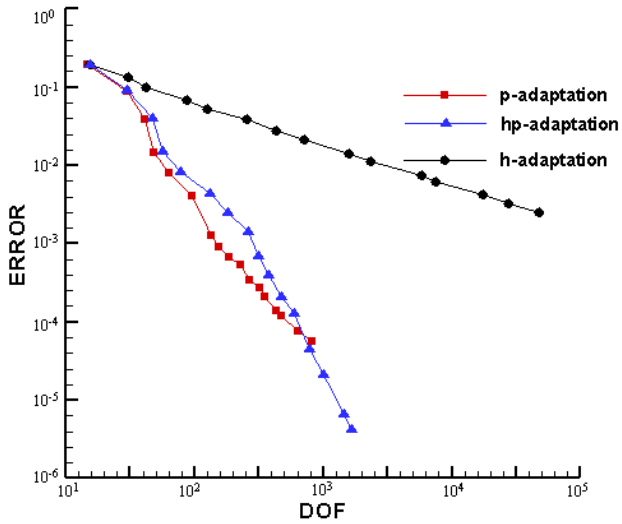
hp-adaptive FEM framework and algorithms

- *hp*-adaptive framework is developed and undergoing changes and PCS method is into the framework.
- Modern coding syntax.
- Under-the-hood system, user and other developers need not deal with the intricacies of the system, upper leveling call structure

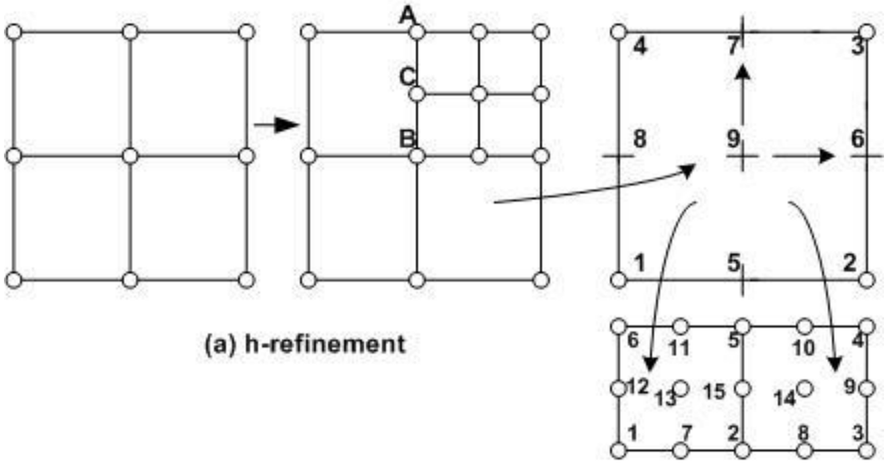
hp-adaptive methods for KIVA a PCS FEM method

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

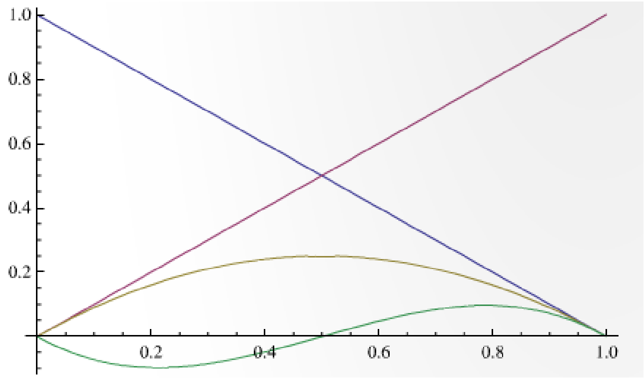


h and hp Adaptation Methods and shape functions



(a) h-refinement

(b) p-refinement



Peano shape functions

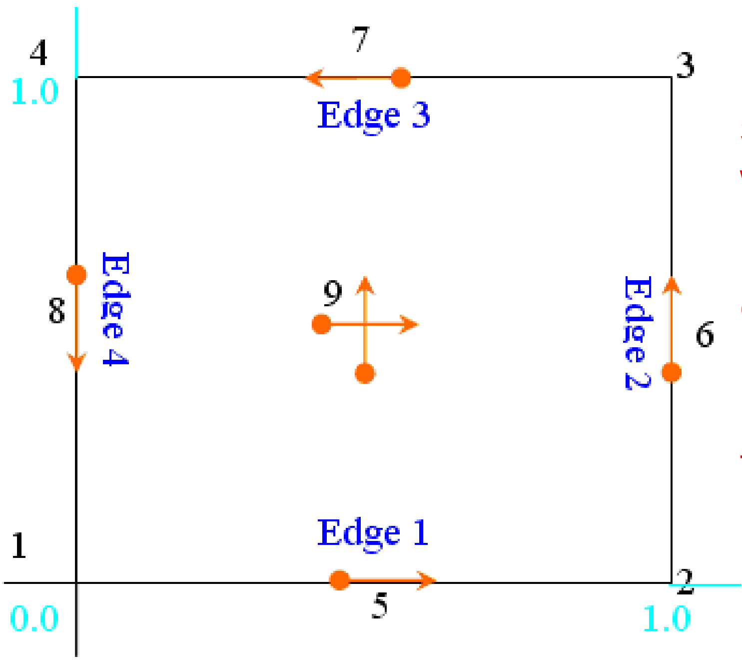
- Using Peano shape functions:

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

- 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

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

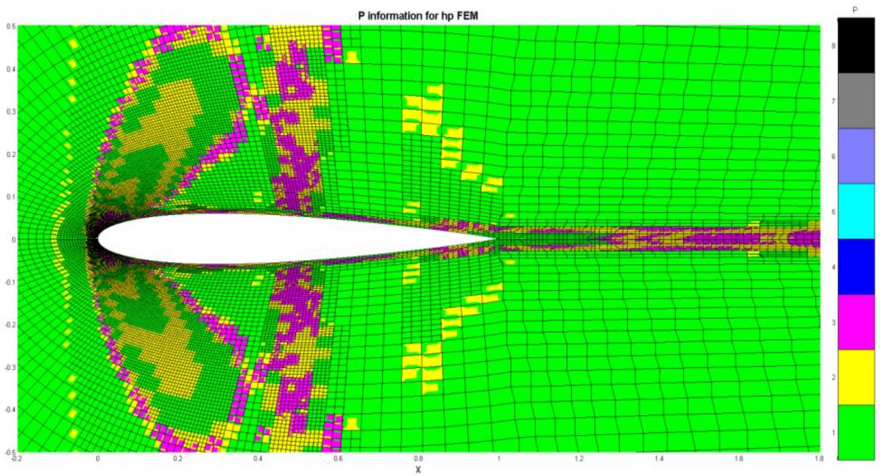
$$\xi_i = \frac{\|e\|_i}{\bar{e}_{avg}}$$ Refinement criteria

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

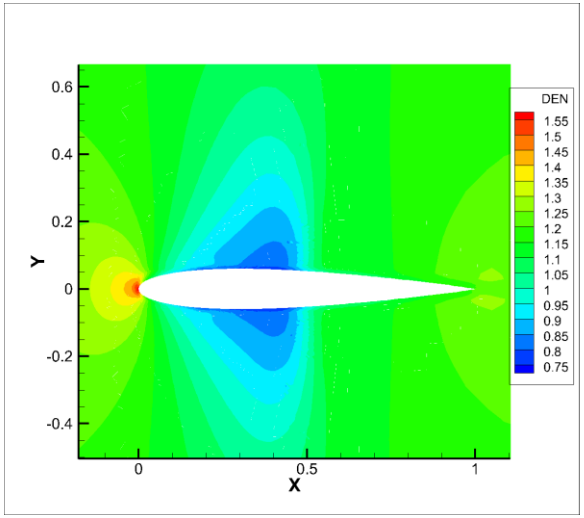
- Error measures:
  - Residual, Stress Error, etc..
- Typical error measures:
  - Zienkiewicz and Zhu Stress
  - Simple Residual
  - Residual measure
    - How far the solution is from true solution.
    - "True" measure in the model being used to form the residual.
    - If model is correct, e.g., Navier-Stokes,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

PCS FEM V&V - Subsonic flow regime

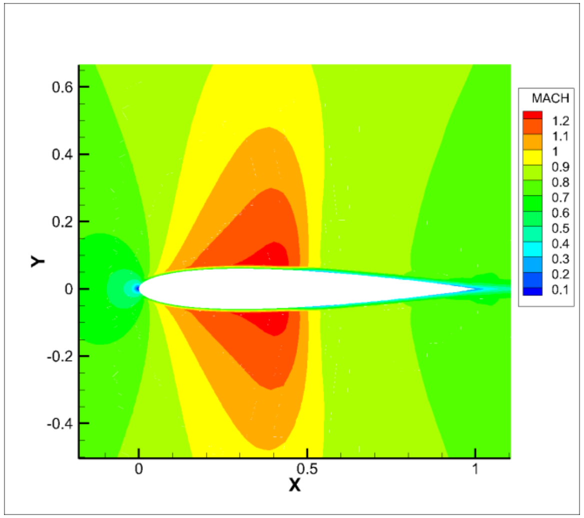
- NACA 0012 airfoil test
  - Mach = 0.8 & α = 0
  - Time dependent solution
  - P-G stabilization.
  - Multi-species testing, 2 species at inlet.



hp-adapted domain



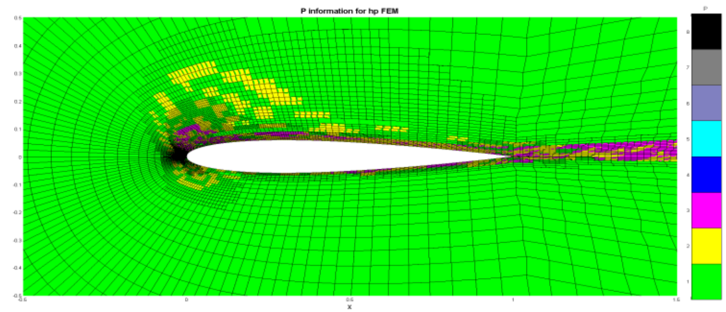
Density



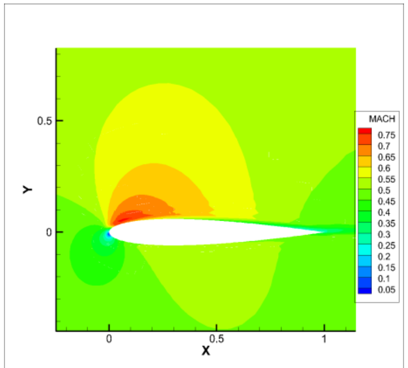
Local Mach Number

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

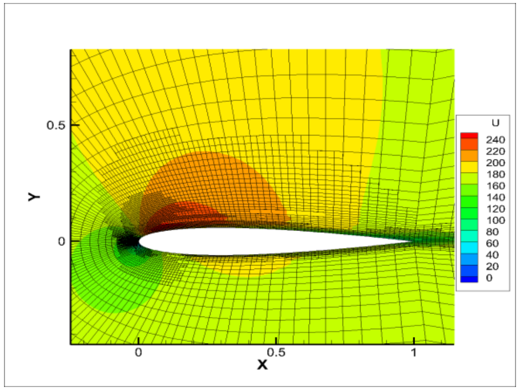
- Mach = 0.5 & attack angle α = 4º
  - Time dependent solution
  - Gambit generated initial grid
  - Agreement with data



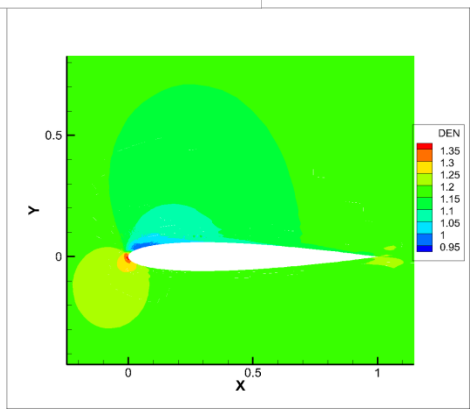
Final mesh *hp*-adaptive
(polynomial order shown in color)



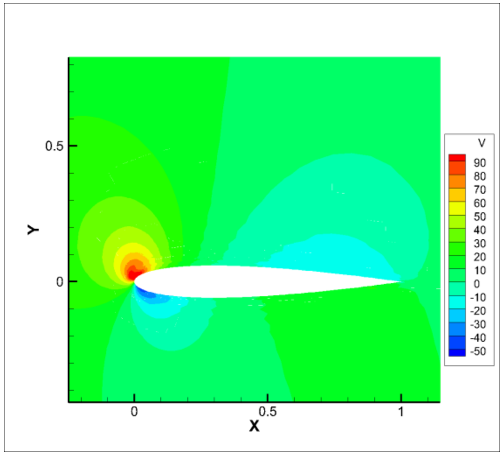
Local Mach



Velocity components



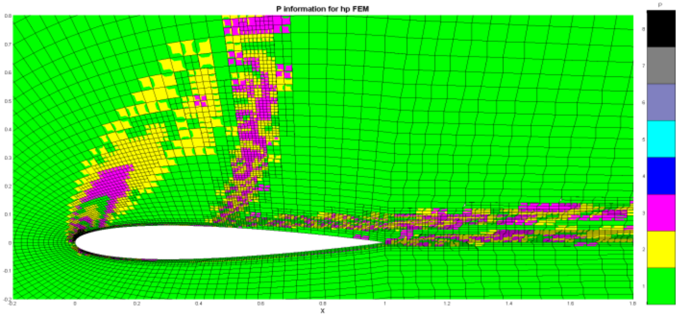
Density



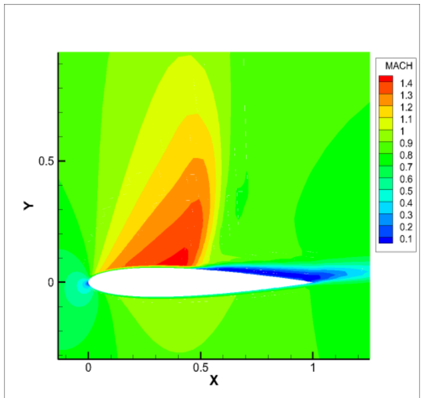
- Demonstrating Solver Capability –
  Truly Curved and complex domains

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

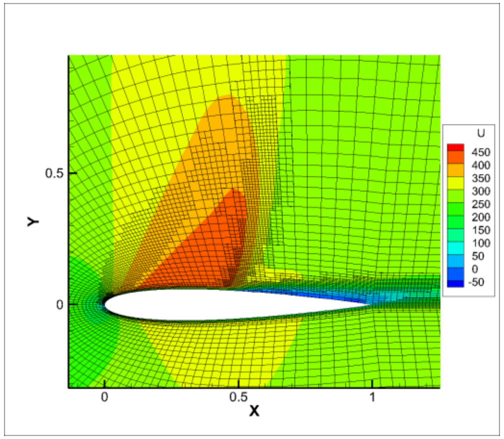
- Mach = 0.8 & attack angle α = 4º
    - Time dependent solution
    - Gambit generated initial grid
    - Agreement with data



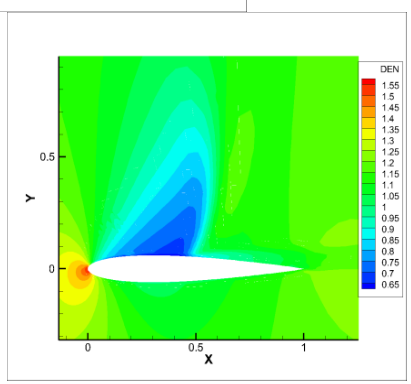
Final mesh *hp*-adaptive
(polynomial order shown in color)



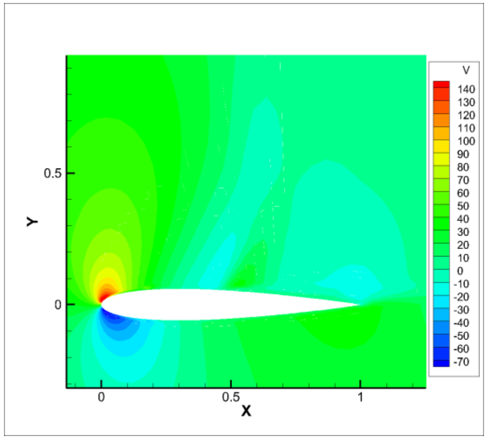
Local Mach



Velocity components



Density

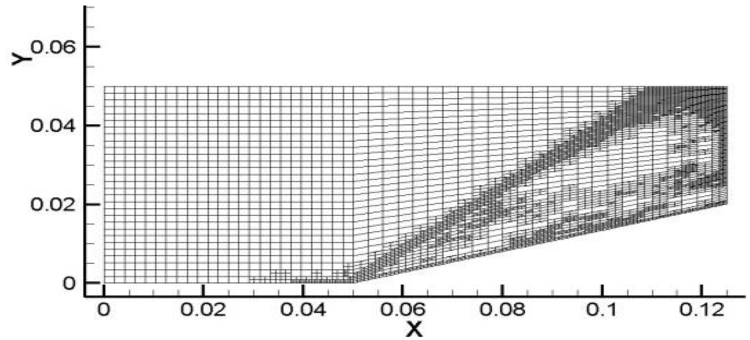


- Also continues to demonstrating Solver Capability
    - Truly curved and complex domains

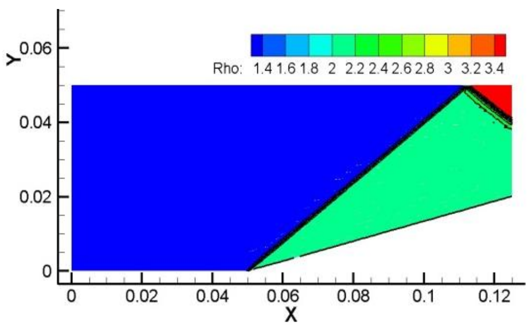
Validation of 2-D *h*-adaptive – PCS FEM

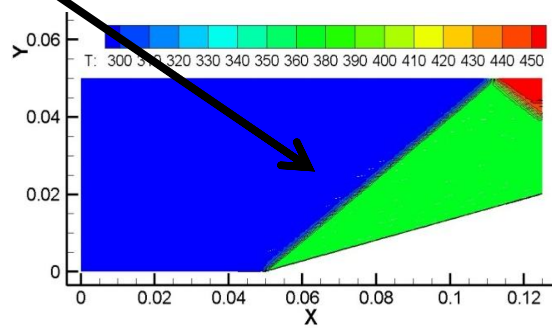
- **Invsicid compressible Supersonic flow.**
- **15º compression ramp**
  - Or moving projectile/scramjet
- **Simulation results exactly matches analytic solution**

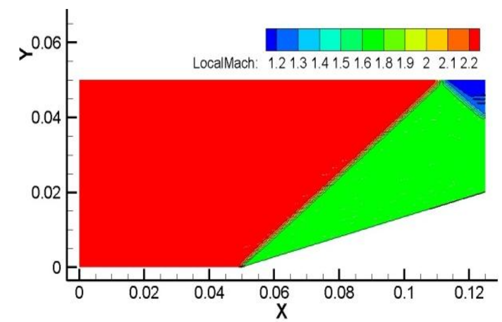
Adapted 20x50 Grid



Shock







Density contours

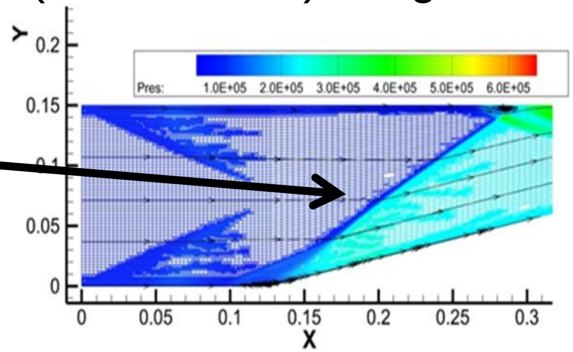
Isotherms

Local Mach contours

V&V - Viscous Flow on 18º Compression Ramp

- 18º compression ramp inlet speed Mach = 2.25
- *h*-adaptive turbulent (*k-ω*) PCS FEM (2 levels tracking the shock front in time).
- Shock angle matches analytic solution
- Boundary layer separation, shock detachment and flow reversal (recirculation) in agreement experiment and other solutions.

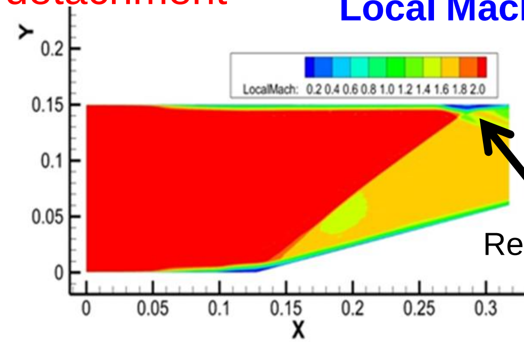
Shock



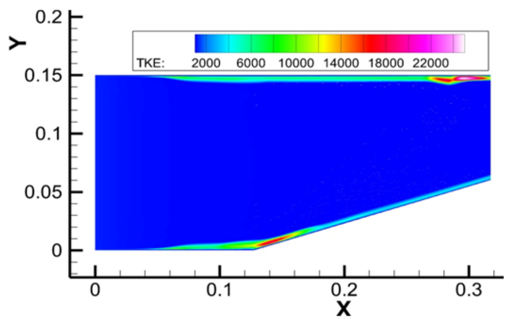
Pressure

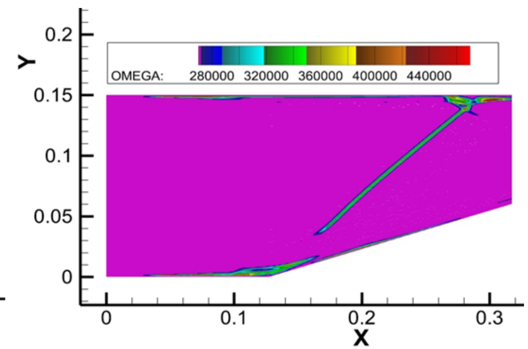
Shock detachment

Local Mach

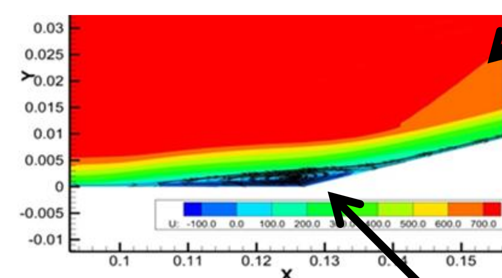


Recirculation





Shock wave



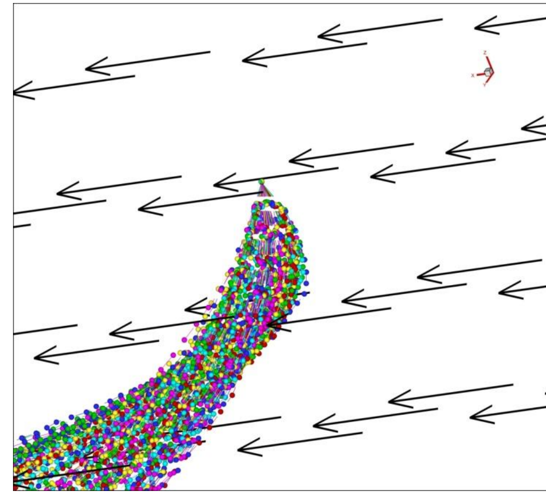
Turbulent Kinetic Energy

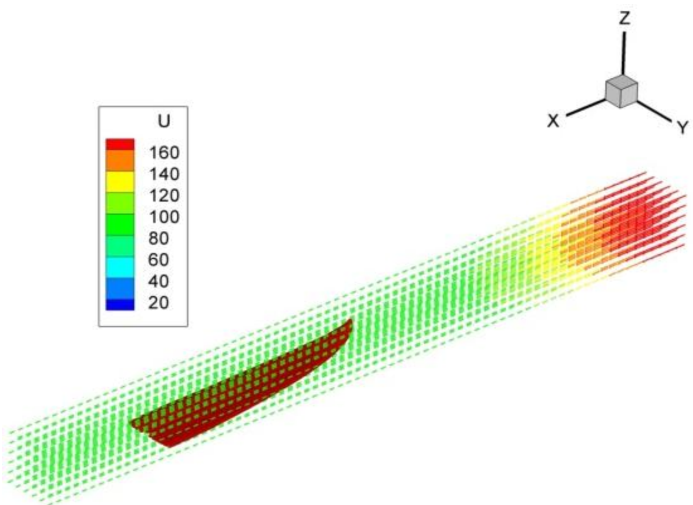
Specific dissipation rate

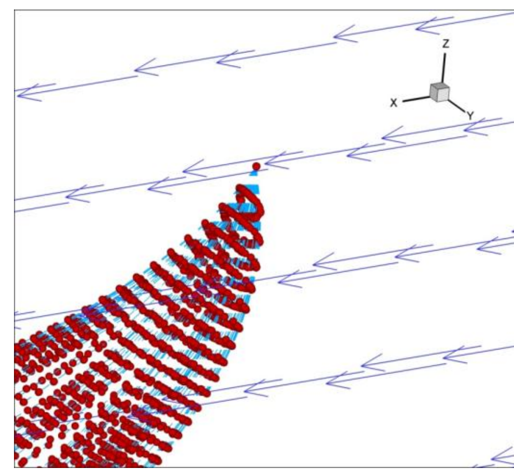
Recirculation

Injection Spray in FEM (unstructured grids)

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



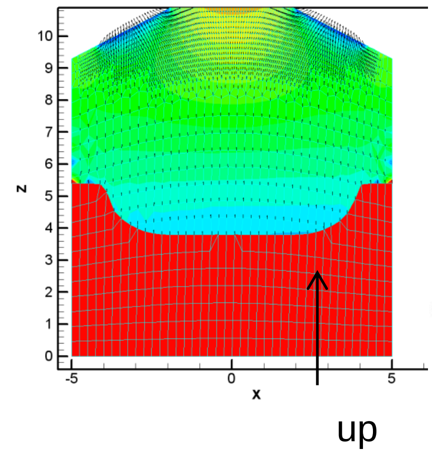


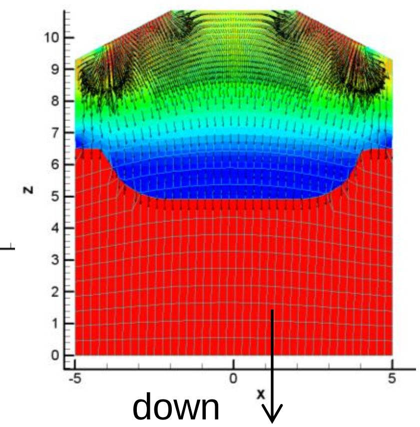


Local ALE for moving parts on unstructured grids

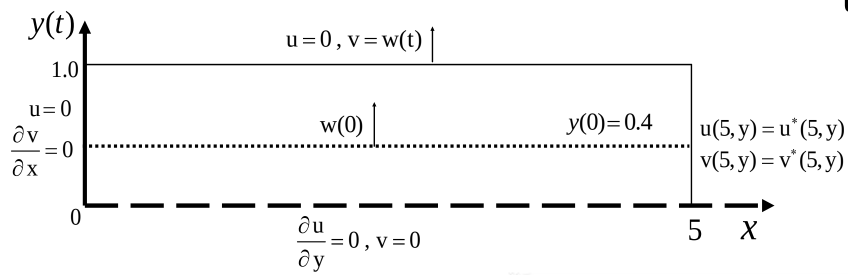
- ***New* local ALE algorithm**
  - Increase robustness - generic method.
  - Simulations with higher resolution.
  - Use of overset parts/grids.
  - Grid is of body only, fluid only.
  - Allows for automatic grid generation by Cubit or ICEM –
    - CAD to Engine Grid!

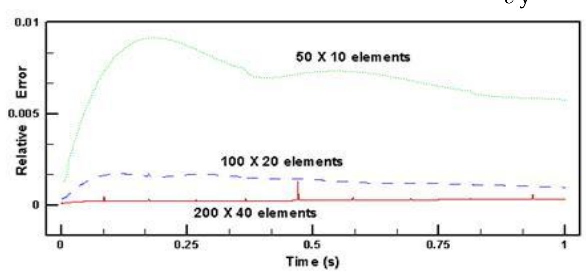
2-D engine type test of ALE

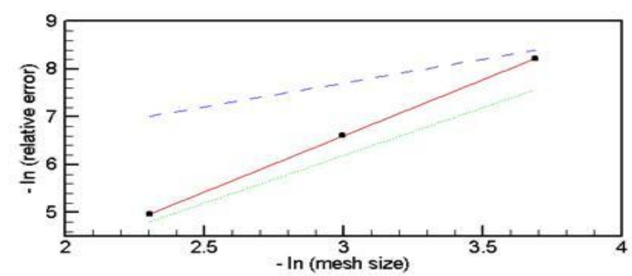




Test Case: Layer of fluid between two plates separating with speed w(t). Height goes from y = 0.4 to 1.0; (u*, v*) is the analytical solution.





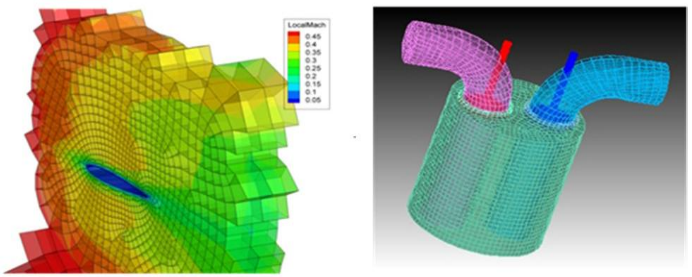


Grid convergence test : Average relative error vs. analytic solution to 2d pump(function of time) and having of 2^{nd} order spatial accuracy.

Grid Generation for KIVA-4 vs. the local ALE FEM

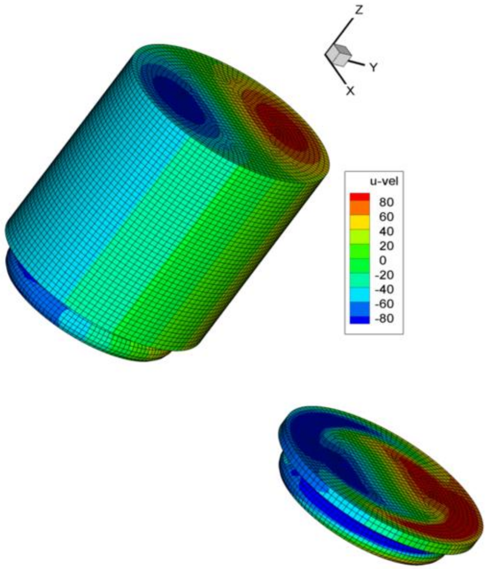
- **Grid generation**
  - ***hp*-adaptive FEM is EASY to grid with overset grid & and use of local ALE**
    - **Robust and 2nd order spatial accuracy.**
  - **KIVA-4 is very problematic but doable once scripts are created and tested.**

FEM PCS Grids

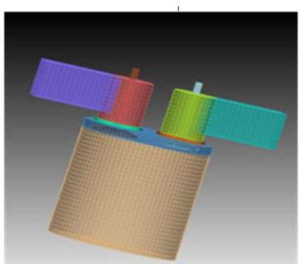


a) 3-D NACA Airfoil b) Engine grid

Overlaying parts for easy/automatic grid generation.

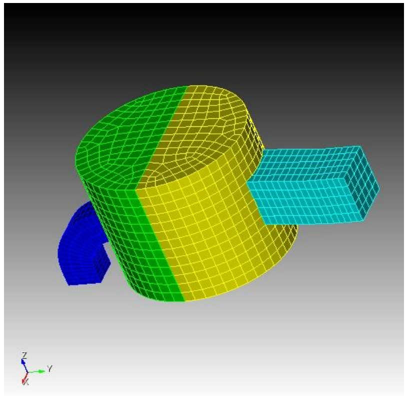


KIVA-4 Grid



c) Engine grid

Parts have to be incorporated into fluid domain - problematic.

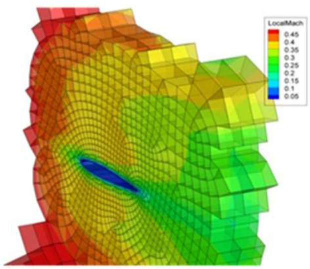


Grid generation using Cubit and only hexahedral cells

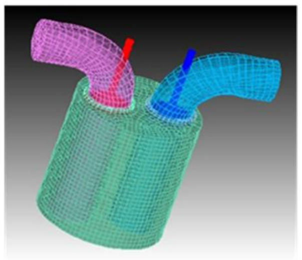
Grid Generation – Cubit and scripting

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

FEM PCS Grids



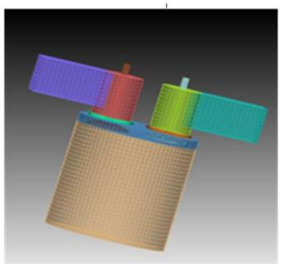
a) 3-D NACA Airfoil



b) Engine grid

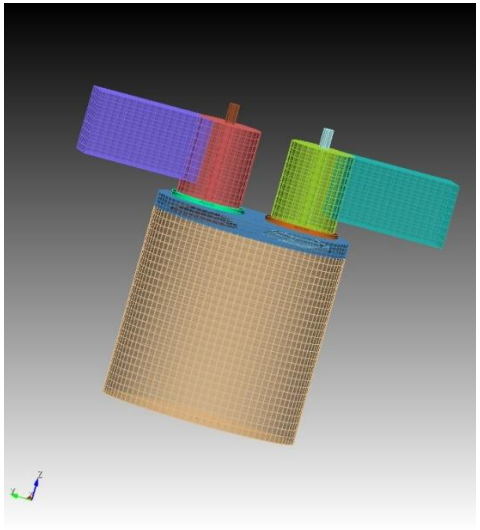
Overlaying parts for easy/automatic grid generation.

KIVA-4 Grid



c) Engine grid

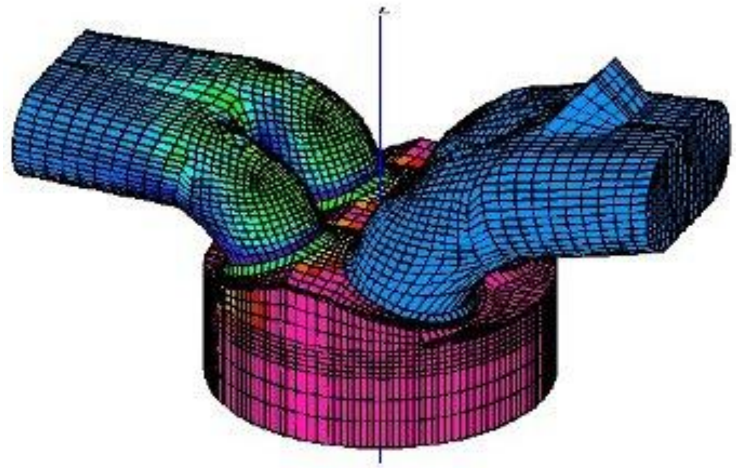
Grids for new
hp-FEM KIVA and KIVA-4



2 valve KIVA-4 Engine Simulation
Using Cubit generated grid

KIVA-4 Manual and websites

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



KIVA-4

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

Current Program Contributors & Collaborators

- University of New Mexico
  - *ALE* for Moving Immersed Bodies & Boundaries Algorithm Development
  - Juan Heinrich, GRA & Post Doctorial Staff
- Purdue, Calumet
  - *hp*-adaptive FEM with Predictor-Corrector Split (PCS) & *parallel*
  - Xiuling Wang & GRAs
- University of Nevada, Las Vegas
  - *LES* and spray interaction
  - Darrell Pepper & Ph.D. GRA
- **T-3** at LANL
  - Spray, Chemistry, PCS algorithm development, *hp*-adaptive & parallel
  - Dave Carrington & 2 GRA's in part of FY 11/12 and Ph.D. GRA summer FY12

Ongoing and Future effort

- **Parallel *hp*-adaptive PCS FEM in 3-D**
  - Parallel constructions
    - matrix solver already developed for massively parallel constructions.
- **Local ALE in 3-D and parallel solution**
- **LES development (as a template for others at least)**
- **Other turbulence closure**
  - Turbulence modeling (Higher moment methods)
- **Spray model development in FEM**
  - Use phase space information from fine grain solutions of injector.
  - New algorithms such as Eulerian frame Discrete Quadrature Moments Methods
- **Test cases: finish tests**
    - Make rigorous comparisons to data and analytics.
      - Publish results in peer reviewed articles (3 papers just recently).

Acknowledgements

- Funding provided by the DOE EERE office of Vehicle Technologies Program -- Advanced Combustion Engines – Gurpreet Singh.
- University of Purdue, Calumet
- University of New Mexico
- University of Iowa, Ames
- University of Nevada, Las Vegas
-

Summary – A paradigm shift

- **Accurate, Robust and well Documented algorithms**
  - Developing 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.
  - 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 and Gambit supply rapid generation, from quickly developed scripts and GUI tools.
    - Overlay moving parts on unstructured grid,
      - no need to grid around immersed moving parts because of *new* local ALE method.
      - easy and quick grid generation for unstructured grids and still have 2nd order or better accuracy throughout the domain.

- **Back up slides for additional information follow this spacer**

Fractional Step or Predictor Corrector

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

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

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

  - Velocity corrector (*desire this*)

$$U^{n+1} - U^{*} = \Delta t \frac{\partial P'}{\partial x_i}$$ and U_i^{*} 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 $U' = \theta_1 U^{n+1} + (1-\theta_1) U^{n}$ with a level of implicitness

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

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

Density Solve (Pressure when incompressible flow)

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

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

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

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

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

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

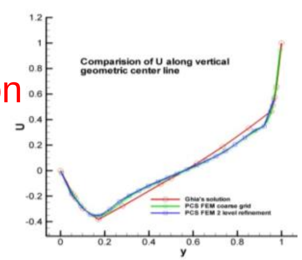
where $$\mathbf{U}_i^{n+1} = \Delta \mathbf{U}_i + \mathbf{U}_i^{n}$$

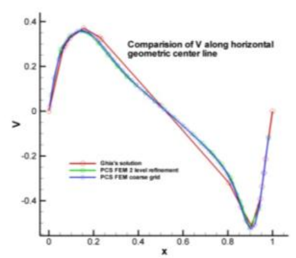
final mass conserving velocity $$u^{n+1} = U^{n+1} / \rho^{n+1}$$

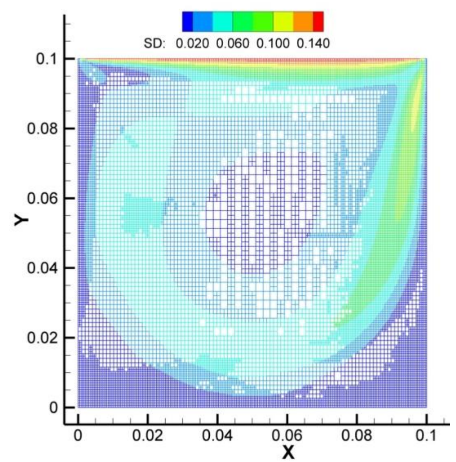
Validation of 2-D Fractional Step – FEM

- **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 benchmark data is sparse resulting in poor representation of velocity gradients (curvature)

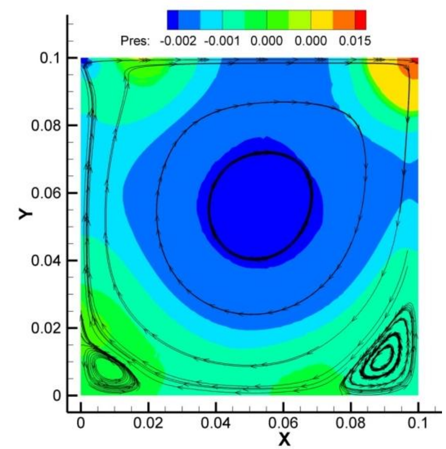
PCS FEM Comparison to Ghia's solutions







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 = 1.0e05.**
- **40x50 Grid original grid density**
- **The final grid has 20,014 nodes & 18,876 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.**

- Average Nusselt # on Δx convergence
  - 4.523 to 4.767 on hot wall

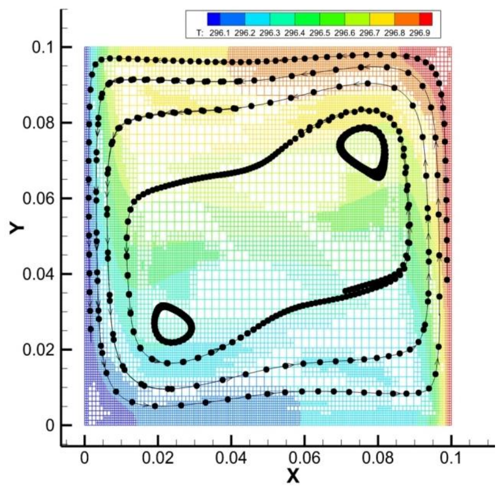
    compares to PCS FEM of

    = 3.4 to 4.1
- Highest Nusselt #
  - 6.538 to 7.905 on hot wall

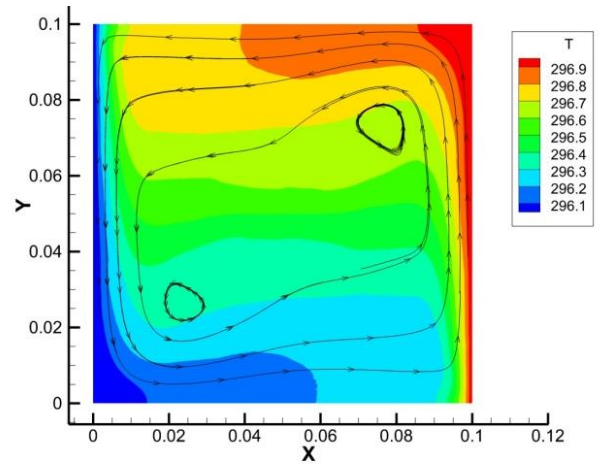
    compares to FEM of

    6.06 to 8.4 & in the

    proper locations.



Adapted grid & streamlines dynamic grid refinement



Isotherms & streamlines

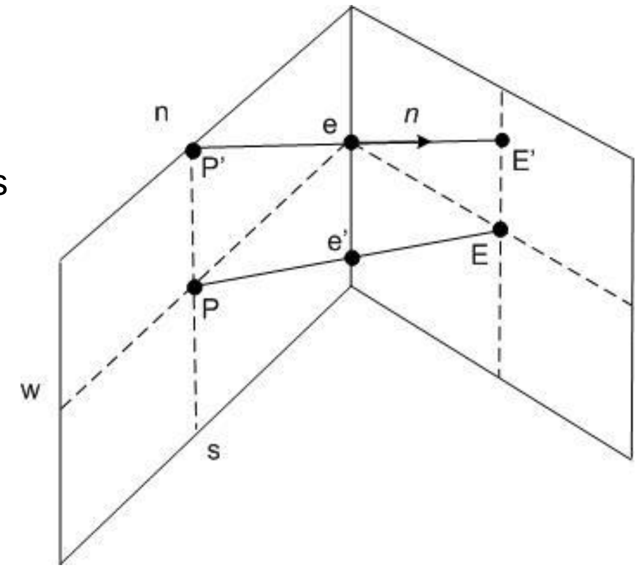
FEM Fractional Step for Turbulent Reactive Flow

- **Finite Element Method (FEM) formulation for discretization –**
  - Predictor-Corrector Split (PCS)
  - Petrov-Galerkin (P-G) stabilization
- **The *hp*-adaptive FEM:**
  - **LBB compliant *with Equal-Order*** approximating polynomials.
  - **Spatially accurate to any degree**. Higher-order – 3rd or higher
  - **2nd order accuracy in time as needed**.
  - **Conservative both *locally* and globally**.
  - Pressure is C_o continuous - not piecewise constant as with current KIVA.
  - 1 pressure solve per time step – Poisson equation in semi-implicit mode.
  - **No pressure Poisson matrix solve in explicit mode – good for new computer architectures**.
  - Resolution when and where required via hp-adaptive method!
  - **Hooks** to models **nearly the same**
    - We supply models which can be changed or enhanced to help further development.
  - FEM provides **a integration over each element without concern for neighboring** information - except at boundary**, a very good feature**!
  - FEM easily provides accuracy of gradients on adapted grids.

Current KIVA vs. New FEM formulation

- **In *hp*-FEM there is**
  - No Virtual volume creation for each node into surrounding cells.
  - No Flux calculations & normal vectors within the domain unless desired.
  - No Need for 6 neighboring cell data.
  - No Cumbersome stencils, associated combining use of h-adaptation.

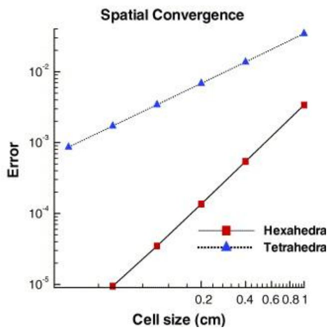
- **KIVA discretization not necessarily 2nd order accurate in space**
  - At the point *e'* yes, but not at mid-point *e* .
  - No adjustment to produce 2nd order at point *e*
    - A Simpson's like integration although
      - Flux not found at edge/vertex - across face
        - average of nodal values of adjacent cells
      - Uses value at point P, E, without adjustments
      - Edge values my degenerate from 2nd *O* also
    - Could use
      - Shape functions to interpolate to P, E
      - Or $\phi_{P'} = \phi_P + \nabla\phi_P \bullet (r_{P'} - r_P)$
      - where location of P' $r_{P'} = r_e - \left[(r_e - r_p) \bullet n \right] n$



KIVA-4 Spatial Convergence vs. FEM on Regular Grids

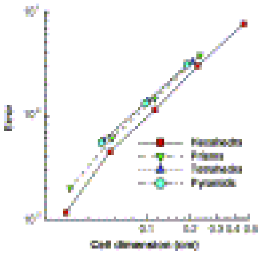
KIVA-4*

1-D diffusion

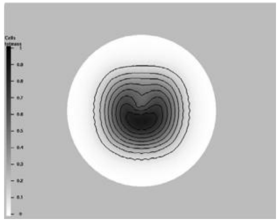


Slope tets ~ 1

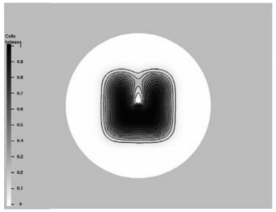
Rotating notch



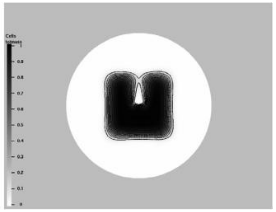
Slope ~ 1



1,456 prisms

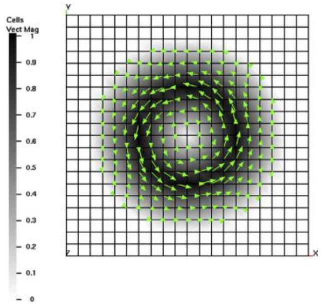


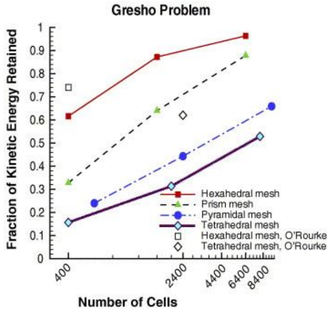
6,000 prisms



88,000 prisms

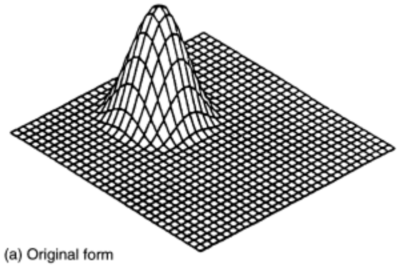
Gresho momentum flux



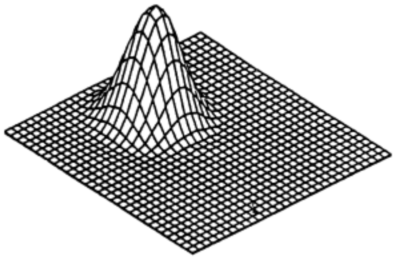


FEM- CBS**

Rotating Cosine hill similar to rotating notch



(a) Original form



(b) Form after one revolution using consistent M matrix

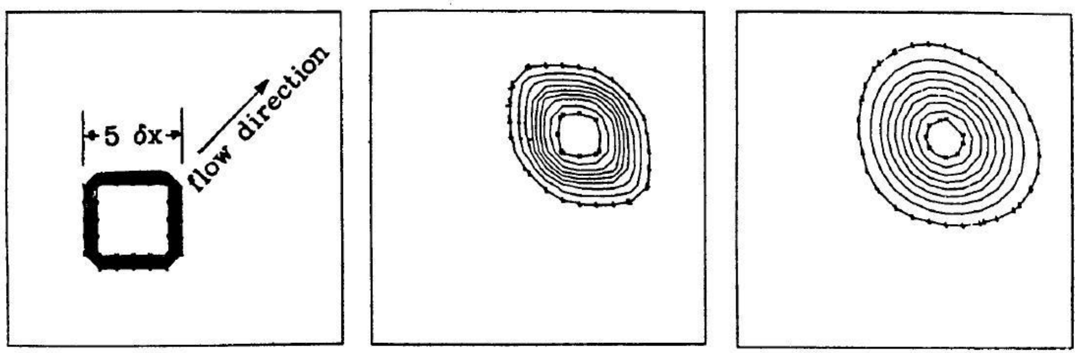
~225 cells

*from - Torres & Trujillo, KIVA-4: An unstructured ALE code for compressible gas flow with sprays, JCP, 219, 2006, pp. 943-975.

**from - Finite Element Method for Fluid Dynamics (6th Edition) , Zienkiewicz, O.C.; Taylor, R.L.; Nithiarasu, P. © 2005 Elsevier

Eulerian advection: Current KIVA vs. FEM on Regular Grids

Current KIVA advective Flux*



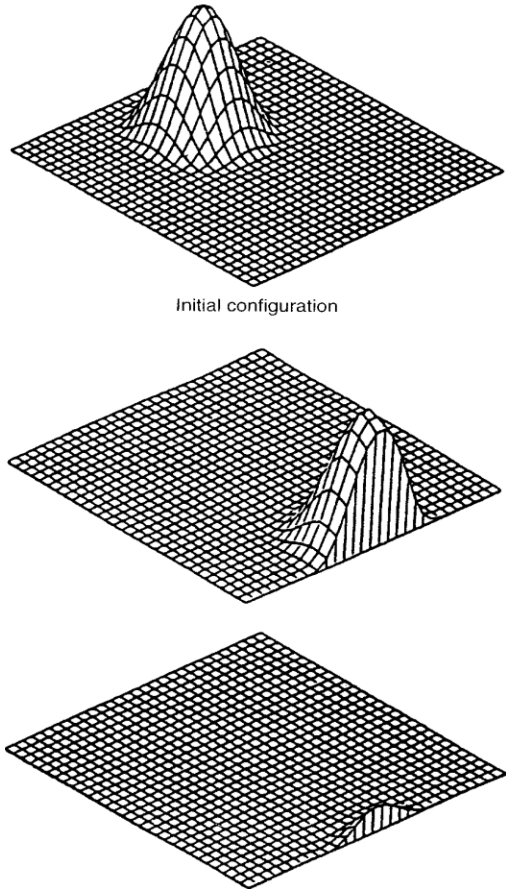
Initial Condition
Max = 1.0
Min = 0.0

QSOU
$u\Delta t_c/\Delta x = 0.2$
Max = 0.87 Min = 0.0
Error = 0.36

Donor Cell
$u\Delta t_c/\Delta x = 0.2$
Max = 0.63 Min = 0.0
Error = 0.53

Phase C advective flux is very diffusive

CBS-FEM Advection**



Advection is nearly exact

*from – Amsden, et al., KIVA-II: A Computer Program for Chemically Reacting Flows with Sprays, LA-11560-MS, Los Alamos Scientific Report, 1989.

**from - Finite Element Method for Fluid Dynamics (6th Edition) , Zienkiewicz, O.C.; Taylor, R.L.; Nithiarasu, P. © 2005 Elsevier

Fractional Step or Predictor Corrector

- **FEM Discretization for PCS or Characteristic Split (CBS)**
  - Velocity predictor

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

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

  - Velocity corrector (*desire this*)

$$U^{n+1} - U^{*} = \Delta t \frac{\partial P'}{\partial x_i}$$ and U_i^{*} 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 $U' = \theta_1 U^{n+1} + 1 - \theta_1 \quad U^n$ with a level of implicitness

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

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

Pressure Solve

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

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

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

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

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

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

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

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

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

Momentum Predictor in Matrix form

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

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

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

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

Body Force
Spray Force
Boundary stress

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

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

Characteristic terms

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

Total Energy Transport (compressible flow)

Total energy is mass and specific total energy
(includes kinetic and internal energy)

$$E = \rho\, e_{Total}$$

In conservative form total energy is

$$\frac{\partial E}{\partial t} = -\frac{\partial}{\partial x_i} \; Eu_i + pu_i \; + \frac{\partial}{\partial x_i}\left(\kappa + \frac{\mu_\tau}{\mathrm{Pr}_t}\right)\frac{\partial T}{\partial x_i} + \frac{\partial}{\partial x_i} \; t_{ij} + \tau_{ij} \; u_j$$
$$+ \frac{\partial}{\partial x_i}\left[\rho \sum_{k=1}^{NumSpecies} \bar{H}_k \left(D_k + \frac{\mu_\tau}{Sc_t}\right)\frac{\partial \Upsilon_k}{\partial x_i}\right] + \rho \sum_{j=1}^{NumSpecies} \Upsilon_j f_j(x_i) \bullet U_i - \sum_{k=1}^{NumSpecies} H_{o,k} w_k$$

Weak form matrix equation

$$\Delta E_{\mathbf{i}} = -\Delta t \left[\mathbf{M}_e^{\,\mathbf{-1}}\right] \begin{bmatrix} \mathbf{A}_e \;\; \mathbf{E}_{\mathbf{i}} + \mathbf{C}_P \;\; p_{\mathbf{i}} + \mathbf{K}_{\mathbf{T}} \;\; \mathbf{T}_{\mathbf{i}} + \mathbf{K}_\tau \;\; u_{\mathbf{i}} + \mathbf{F}_{eb} + \mathbf{Q}_{ss} + \mathbf{Q}_{vs} - \\ \Delta t \;\; \mathbf{K}_{uE} \;\; \mathbf{E}_{\mathbf{i}} + \left[\mathbf{K}_{up}\right] p_{\mathbf{i}} + \mathbf{F}_{es} + \mathbf{Q}_{ss} + \mathbf{Q}_{vs} \end{bmatrix}^n$$

Total Energy Matrix Terms

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

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

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

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

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

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

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

Species Transport

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

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

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

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

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

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

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

Turbulence Closure

- Turbulence Closure – *k-ω (not showing characteristic terms)*

$$\Delta k_{\mathbf{i}} = +\Delta \mathbf{t}\left[\mathbf{M}^{-1}\right]\begin{bmatrix} \mathbf{F}_k + \mathbf{P}_k + \beta^* \mathbf{k}\,\mathbf{w} - \\ \mathbf{K}_k \quad k - \mathbf{A}_v \quad k \end{bmatrix}^n$$

$$\Delta \boldsymbol{\omega}_{\mathbf{i}} = -\Delta \mathbf{t}\left[\mathbf{M}^{-1}\right]\begin{bmatrix} \mathbf{F}_{\varpi} + \alpha \, \mathbf{k}/\boldsymbol{\omega} \quad \mathbf{P}_k + \beta \mathbf{w}^2 - \\ \mathbf{K}_{\varpi} \quad \omega - \mathbf{A}_v \quad \varpi \end{bmatrix}^n$$

$$\mathbf{K}_k = -\left(\int_{\Omega} N_i \left[\frac{\partial N_j}{\partial x_i}\right] \sigma^* \mu_t \left[\frac{\partial N_j}{\partial x_i}\right] d\Omega\right) + \int_{\Omega}\left(\left[\mu + \sigma^* \mu_t\right]\frac{\partial N_i}{\partial x_j}\frac{\partial N_i}{\partial x_j}\right) d\Omega$$

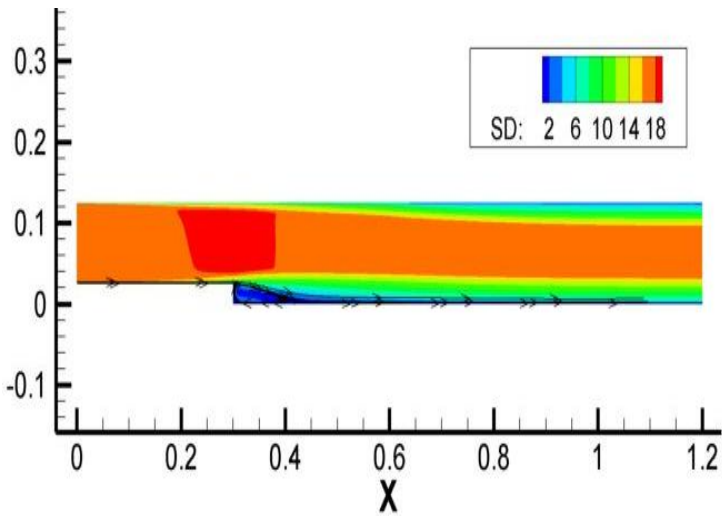
$$\mathbf{K}_{\varpi} = -\left(\int_{\Omega} N_i \left[\frac{\partial N_j}{\partial x_i}\right] \sigma \, \mu_t \left[\frac{\partial N_j}{\partial x_i}\right] d\Omega\right) + \int_{\Omega}\left(\mu + \sigma \, \mu_t \frac{\partial N_i}{\partial x_j}\frac{\partial N_i}{\partial x_j}\right) d\Omega$$

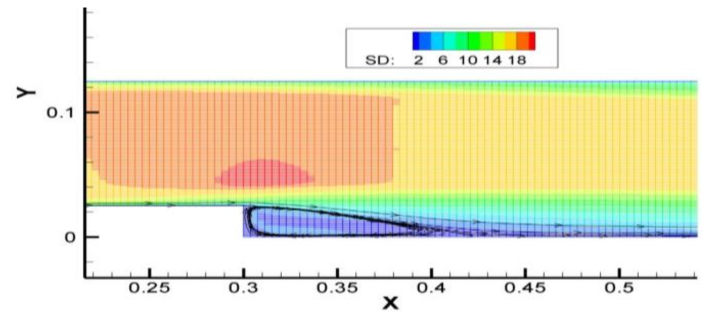
$$\mathbf{P}_k = \int_{\Omega}\left[N_j \quad \mu_{t_i} \left(\left[\frac{\partial N_j}{\partial x_i}\right] u_i + \left[\frac{\partial N_i}{\partial x_j}\right] u_i - \frac{2}{3}\frac{\partial N_k}{\partial x_k} u_k \quad \delta_{ij}\right) - \delta_{ij}\frac{2}{3}\rho\left[N_j\right] k_i \right] d\Omega$$

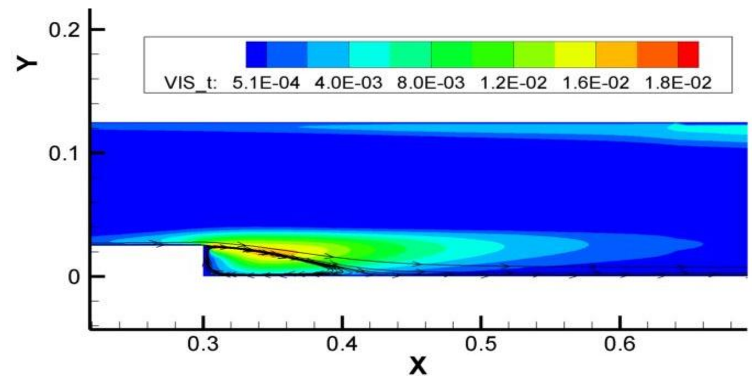
$$\mathbf{F}_T = \left(\int_{\Gamma} N_i \left[N_j\right] q_i \quad d\Gamma\right)$$

PCS *h*-adaptive Validation
Unsteady Turbulence Modeling with *h*-adaptive Grid

- Turbulent convective flow over a backward-facing step (current KIVA can't do well!).
- Re=28,000, inflow is 17m/s (Mach number ~0.05) matches data. This is around the lower velocity in a typical internal combustion engine.
- 2 species at inlet with different mass fractions, both are air.
- 1 specie at t=0.
  - k-ω closure model
  - currently recirculation ~6.0h

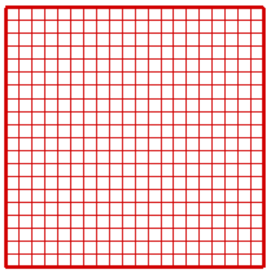




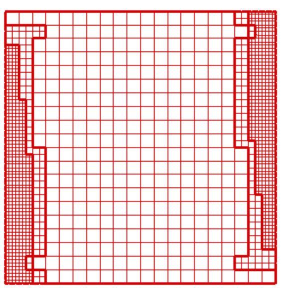


2-D Natural convection within square enclosure*

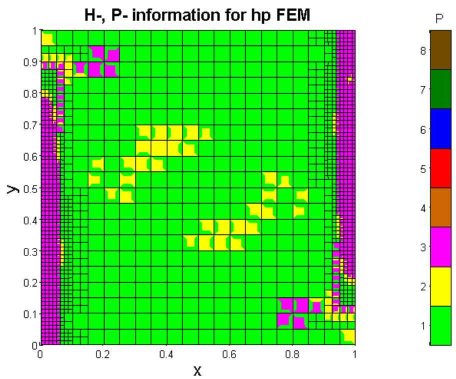
hp-adaptive mesh for Ra=10^6



(a) Initial mesh 400 elements and 441 DOFs

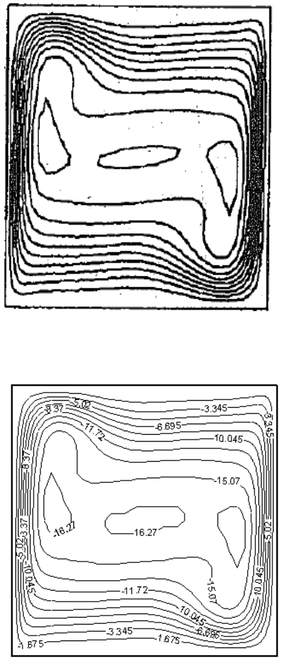


(b) Intermediate mesh 1372 elements and 1541 DOFs

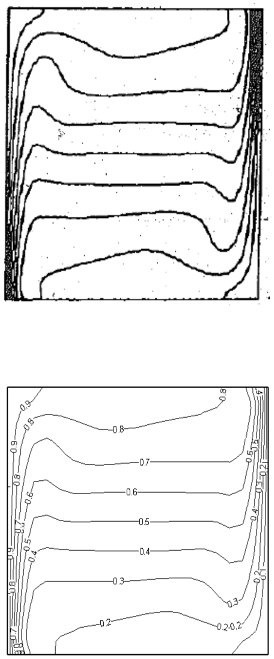


(c) Final mesh (1372 elements and 6529 DOFs)

Comparison with benchmark



(a) Streamlines at -16.27 and -15.07 to 0 in 1.675 intervals

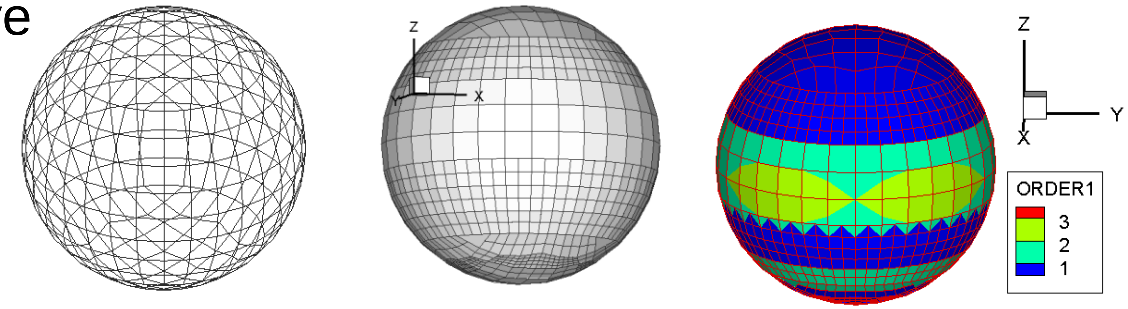


(b) Isotherms ranges from 0 to 1 in 0.1 intervals

*from - Wang, X. and Pepper, D. W. (2007), "Application of an *hp*-adaptive FEM for Solving Thermal Flow Problems," *AIAA Journal of Thermophysics and Heat Transfer*, Vol.21, No.1, pp. 190 – 198.

Natural Convection in a Differentially Heated Sphere

hp-adaptive FEM*



Ra=10^4

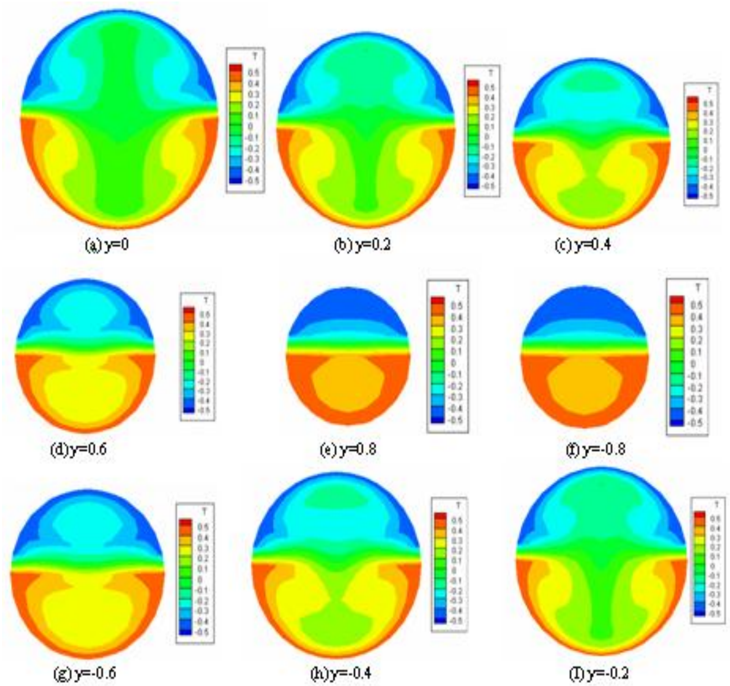
(a) initial mesh on truly curve surface

(b) intermediate *h*-adaptive mesh

(c) final *hp*-adaptive mesh

$$-1 \leq R \leq 1$$

2-D planar isotherms at
-0.8, -0.6, -0.4, -0.2, 0.0, 0.2, 0.4, 0.6, 0.8
along major axis in x-z planes



*from - WANG, X. AND PEPPER, D. W. (2007), "APPLICATION OF AN *HP*-ADAPTIVE FEM FOR SOLVING THERMAL FLOW PROBLEMS," *AIAA JOURNAL OF THERMOPHYSICS AND HEAT TRANSFER*, VOL.21, NO.1, PP. 190 – 198.