2011 DOE Merit Review

2011 DOE Vehicle Technologies KIVA-Development

David Carrington Los Alamos National Laboratory May 10, 2011

LA-UR-11-10120

Project ID # ACE014

This presentation does not contain any proprietary, confidential, or otherwise restricted information

Overview

Timeline

- 10/01/09
- 09/01/13
- 40% complete

Budget

- Total project funding to date:
 - 1,140K
 - Contractor share 30%
- Funding received in FY10
 - 580K
 - Funding for FY11 660K
 - Received only 1/3
 - Continuing Resolution restricting ability to meet milestones and progress

Barriers

- Improve understanding of the fundamentals of fuel injection, fuel-air mixing, thermodynamic combustion losses, and incylinder 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

Partners

- Iowa State University Dr. Song-Charng Kong (under funded)
- University of Nevada, Las Vegas Dr. Darrell
 W. Pepper (not yet contracted FY 11)
- University of Purdue, Calumet Dr. Xiuling Wang (under funded)
- University of New Mexico- Dr. Juan Heinrich (FY 11 - not yet contracted)

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, etc....
 - Developing more robust and accurate algorithms for helping to understand better combustion processes in internal engines
 - Providing a better mainstay tool for improving engine efficiencies and help in reducing undesirable combustion products.
 - Newer and mathematically rigorous algorithms will allow KIVA to meet the needs of future and current combustion modelers and designers.
 - Developing Fractional Step (PCS) Petrov-Galerkin (P-G) and Characteristic-Based Split (CBS) *hp*-adaptive finite element method
 - Conjugate Heat Transfer for 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
 - Cut-Cell grid implementation: CAD to CFD
 - Cut-cell output to KIVA-4 via Cubit and Cubit to KIVA converter.

Milestones for FY 10- FY11

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- **06/09- Started Researching** Fractional Step CBS method developed some research coding and altering/combining with existing Projection code and *h*-adaptive algorithms.
- **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/CBS-FEM method for 2D
- 02/10 *h*-adaptive grid technique/algorithm implement in PCS/CBS-FEM method for 3D
- 02/10 *hp*-adaptive FEM Algorithm & Framework: continued development and changes.

02/10 thru 09/10 –

Successful at meeting standard benchmark problems in the incompressible regime using CBS Fractional Step (PCS) and P-G stabilization without CBS stabilization.

- **04/10 New algorithm** for **Cut-Cell** grid generation started more robust algorithm.
- 05/10 Multi-Species Transport testing in PCS/CBS-FEM algorithm.
- **09/10 2D and 3D Characteristic-based Split** (CBS) stabilization extended to turbulence closure routines. Continue debugging CBS and combination of CBS and PG capabilities.
- 10/10 P-G found to be more flexible than CBS stabilization via benchmark comparisons.
- 12/10 Start looking into Runga-Kutta method for 2nd order-in-time in P-G only Fractional Step.
- 12/10 Benchmark tests of PCS and CBS and begin comparing results.
 Find CBS a bit less flexible the P-G but, does provide good solution, and can be used with P-G.
- 12/10 Inserting PCS/CBS algorithm/coding into hp-adaptive Framework.
- 01/11 FY11 Engineering documentation and precise algorithm details.
- 02/11 Continue working the PCS/CBS method in the compressible flow regimes.
- 02/11 Discussions with Sandia on Cut-cell (our algorithm) & incorporation into Cubit software.

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:
- Development Process
 - Understanding of the physical processes to be modeled
 - Mathematical representations and evaluation of appropriate methods and 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

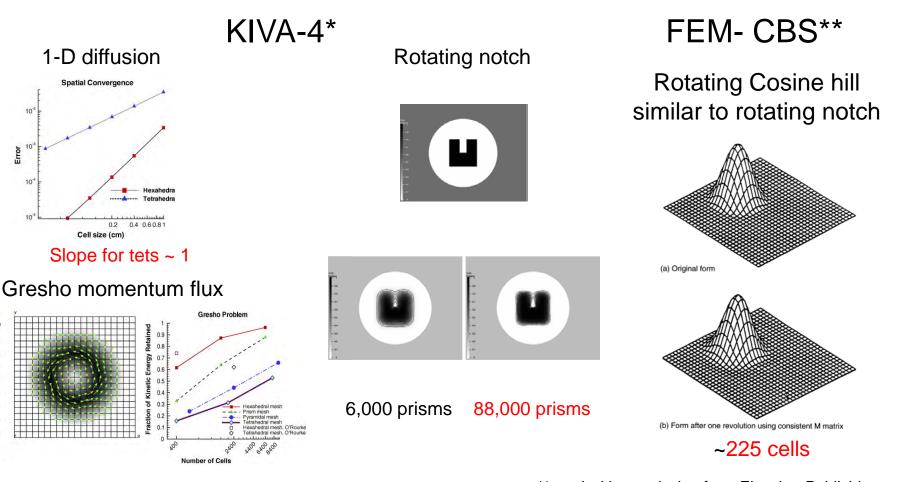
FY-11 Technical Accomplishments

- Developing *hp*-adaptive PCS/CBS FEM Discretization for: Accurate and Robust Turbulence Reactive Flow Modeling – Combustion Modeling
- 2-D and 3-D PCS/CBS *h*-adaptive FEM codes are coded:
 - Benefit of Eulerian system with 2nd order-in-time algorithm
 - Performed without large system of linear equations to solve!
 - CBS or Petrov-Galerkin Stabilization (P-G) having 3rd order spatial accuracy
 - Numerical dispersion precisely measured and removed prior to solution advancement.
 - Various choices of Stabilizing Modes:
 - P-G with CBS for 2nd order-in-time or use CBS alone for 2nd order-in-time
 - 1 pressure solve per time step : Semi-implicit or an Explicit modality.
 - Equal-order: same basis for pressure and momentum (if desired).
 - *h*-adaptive with Residual error & Gradient control (incorporated FY 09).
 - *k-ω* turbulence model FY-09 & FY-10
 - *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)
 - New MAKE system (FY10).
 - Stochastic particle model now porting KIVA-4 model to FEM method FY11/12.
 - Verification complete
 - Via known algorithm substitution and benchmark problems solution
 - · Validation and continued development and error/bug removal via
 - Benchmarks Problems

FY-11 Technical Accomplishments

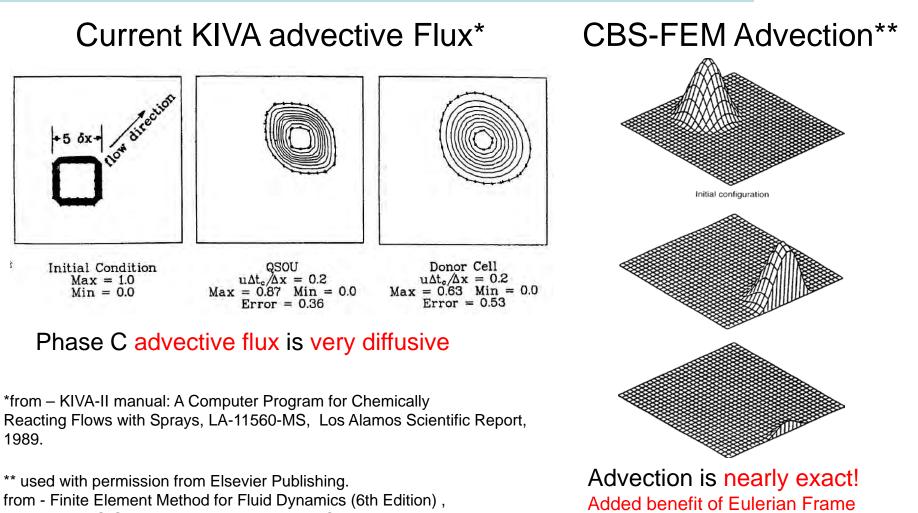
- Conjugate Heat Transfer (CHT)
 - Motivation
 - Extend KIVA-4 capability to predict heat conduction in solids.
 - Use KIVA-4 to perform simultaneous simulation of in-cylinder processes and heat conduction in mechanical components.
 - Expected outcome
 - Prediction of combustion chamber wall temperature 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.
 - Perform integrated thermo-fluids modeling in one simulation using the same code.
 - Applicable energy equation is solved for temperature distribution in solids

Why Do We Need New Method? Accuracy & Robustness KIVA-4 Spatial Convergence vs. FEM on Regular Grids 2011 DOE Merit Review



*used with permission from Dave Torres.

**used with permission from Elsevier Publishing-Finite Element Method for Fluid Dynamics (6th Edition), Zienkiewicz, O.C.; Taylor, R.L.; Nithiarasu, P. © 2005 Elsevier Why Do We Need New Method? Accuracy & Robustness Eulerian advection: Current KIVA vs. FEM on Regular Grids 2011 DOE Merit Review



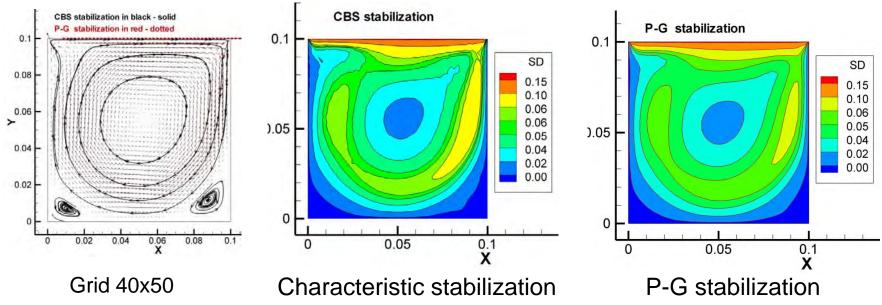
Zienkiewicz, O.C.; Taylor, R.L.; Nithiarasu, P. © 2005 Elsevier

large linear equations to solve.

along with 2nd order-in-time without

Validation of 2-D Fractional Step – FEM

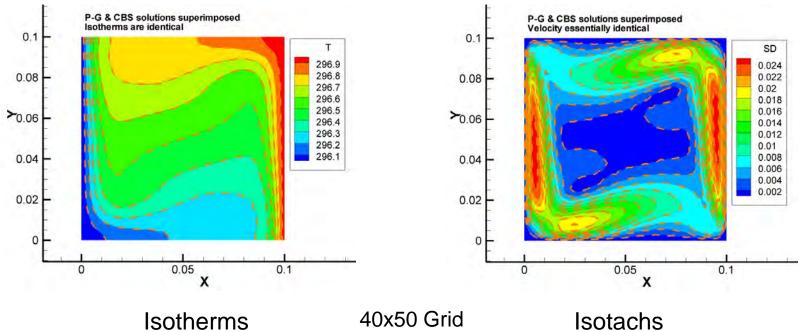
- Driven Cavity Benchmark Re = 1000
 - Semi-implicit solve pressure Poisson equation
 - KIVA-4 published solution shows ~45,000 cells for low Mach equations, an order magnitude larger than PCS or CBS FEM!
 - Characteristic vs. P-G :
 - P-G is more flexible, has good adjustment of element size h_e
 - Characteristic has 2nd O in time inherent in scheme
 - Adaptation at Pressure singularity in upper corners really helps solution



Validation of 2-D Characteristic-Based Split – FEM

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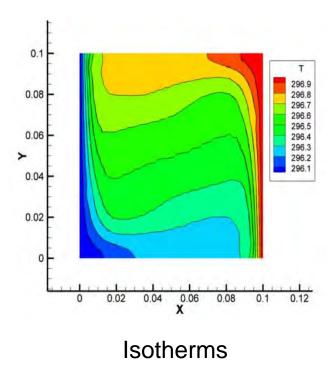
- Slightly compressible low speed flow.
- Differentially Heated Cavity Ra = 1.0e06.
- Pressure Poisson matrix solved.
- Identical results between CBS and P-G stabilization
 - Source Term (Boussinesq approximation) helps 1st order –in-time scheme be as accurate as 2nd order CBS method.

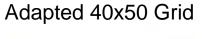


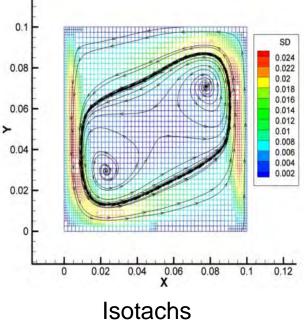
2 solutions: P-G and CBS stabilization

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

- Slightly compressible low speed flow.
- Differentially Heated Cavity Ra = 1.0e06.
- Pressure explicit mode.
- P-G stabilization

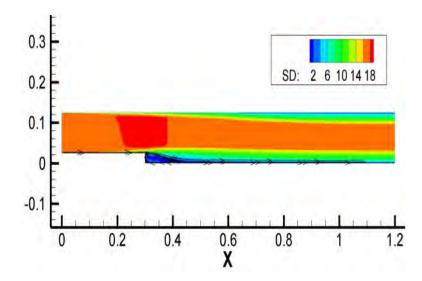


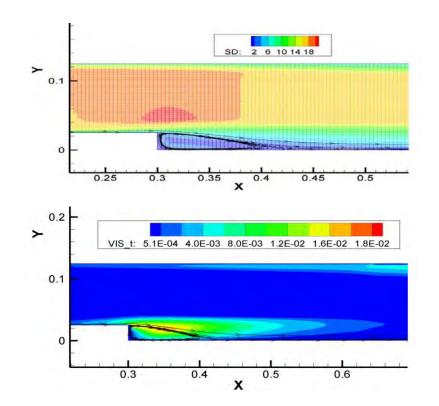




CBS/PG h-adaptive Validation

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





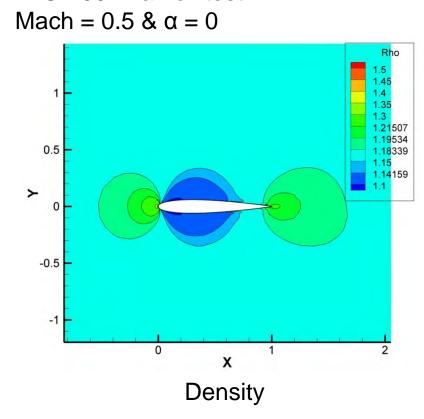
Subsonic flow regime

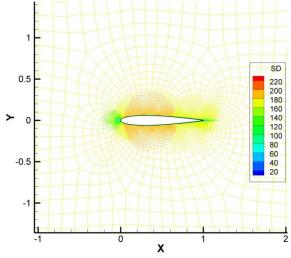
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Time dependent solution

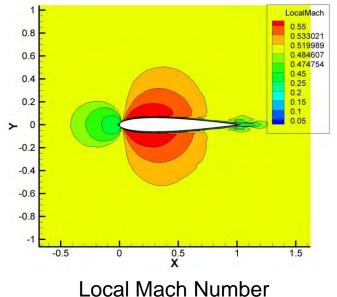
NACA 0012 airfoil test

- CBS and P-G combined system.
- Multi-species testing, 2 species at inlet.





~8000 cells and nodes - adapted on boundary



Density Contour on a Planar 15° Ramp at M=2.28

outflow a lax = t

- 15° compression ramp
- *h*-adaptive P-G FEM
 - Explicit scheme with Runga-Kutta 2
- Time dependent solution
 - Our research code identical to CBS system in explicit mode.

aV/an = 0

aV/an = 0

15*

Mach = 2.28 at inlet

inflow

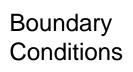
1.0

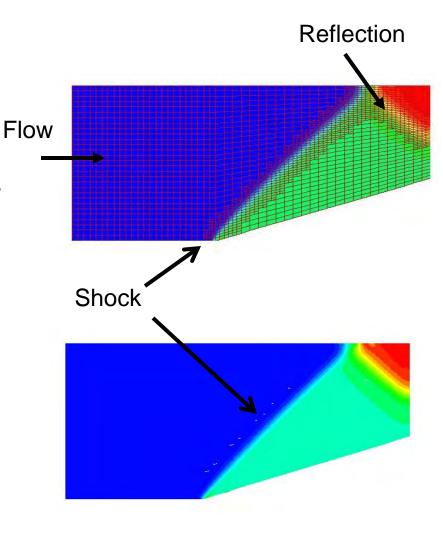
o=1

v=0

T=1 M=2.28

1.0



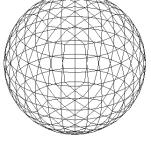


Natural Convection in a Differentially Heated Sphere

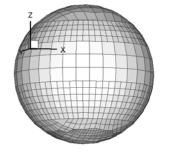
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Ra=10⁴

hp-adaptive FEM*



(a) initial mesh



(b) intermediate *h*-adaptive mesh

ORDER1

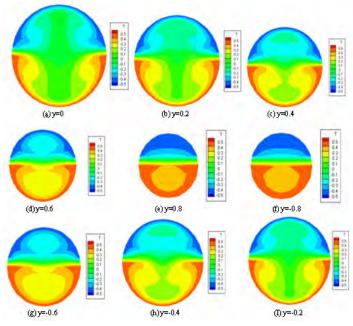
(c) final hp-adaptive mesh

7

•Demonstrating Solver Capability •Truly curved and complex domains

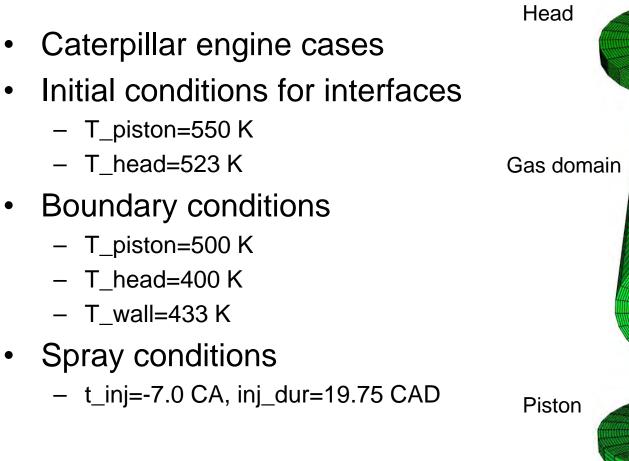
2-D planar isotherms at $-1 \le R \le 1$ -0.8, -0.6, -0.4, -0.2, 0.0, 0.2, 0.4, 0.6, 0.8 along major axis in x-z planes

*used with permission from Wang, X. and Pepper, D. W.



CHT Modeling – Current Progress

•



CHT - Cat Engine Test Results

- 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.

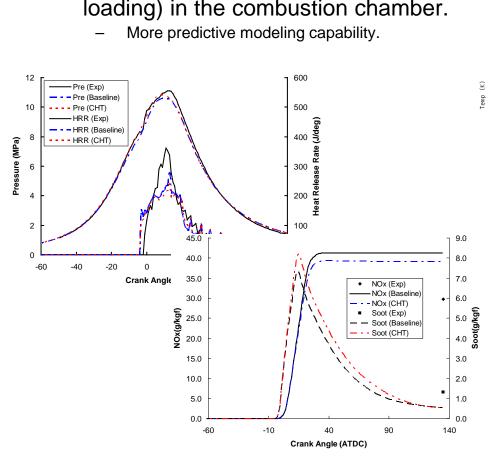
600

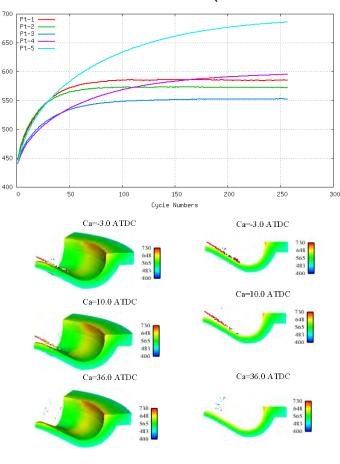
550

500

450

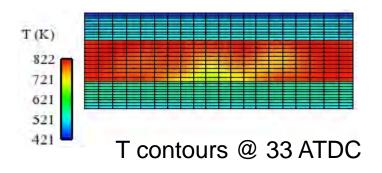
Nonetheless, CHT is able to predict the surface T distribution (thermal ٠ loading) in the combustion chamber. 700 Pt-1

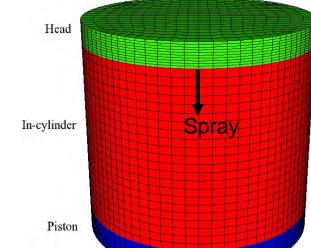


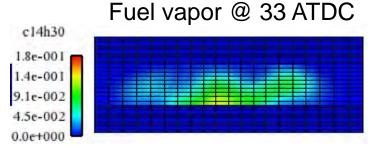


Enhancements to KIVA-4 MPI for CHT modeling in solids

- •The code can run for both conventional mesh and CHT mesh
- •CHT model validated via known analytic solution
 - Flat piston and cylinder head
 - Initial conditions for interfaces
 - T_piston=550 K; T_head=523 K
 - Boundary conditions
 - T_piston=500 K; T_head=400 K
 - Spray conditions
 - t_inj=-9.0 CA, inj_dur=19.75 CAD
 - m_f=28 mg







Program Collaborators

- LLNL collaborating
 - providing great feedback and reporting on KIVA-4mpi
- Iowa State University
 - Conjugate Heat Transfer in KIVA-4 and KIVA-4mpi
 - Song-Charng Kong & GRA and Postdoc.
- Purdue, Calumet
 - hp-Adaptive FEM with Characteristic-Based Split (CBS)
 - Xiuling Wang (Purdue) and GRA
- University of Nevada, Las Vegas
 - *hp*-Adaptive FEM with Characteristic-Based Split (CBS)
 - Darrell Pepper (UNLV) and GRA.
- University of New Mexico
 - Moving Immersed Body and Boundaries Algorithm Development
 - Juan Heinrich and Graduate Student

Future or Ongoing effort in FY11 to FY 13

- PCS/CBS-FEM
 - 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.
 - Develop KIVA type I/O and interfacing.
 - Incorporate the injection/spray model and reactive chemistry coding.
 - Overset Grid method for moving parts. Moving grid new algorithm development for moving boundaries and immersed bodies. Immersed moving bodies - UNM.
 - Mixed element types UNLV.
 - Turbulence modeling LANL, Purdue, UNLV.
 - Parallel constructions Matrix solver already developed for massively parallel constructions (All).
- Conjugate Heat Transfer (CHT) modeling
 - Develop partitioning algorithms for solid domain for parallel computing
 - Perform simulation using multiple processors
 - Conduct combustion modeling
 - Test the code in practical bowl-in-piston geometry challenges in partitioning complex geometry of the solid domain

Future – New Immersed and Moving Boundary Algorithm

Improving the current algorithms

Increase robustness - generic method.

•Simulations with higher resolution.

·Use of overset parts/grids.

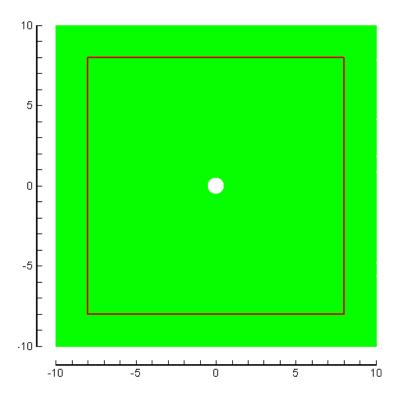
•Good candidate:Unstructured grid, precisely locate body.

•2nd Order in space.

Grid is of body only, fluid only.Boundary condition update

Movie of ball/fluid interaction*

•Juan Heinrich (University of New Mexico).



*Used with permission from Juan Heinrich

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Summary

• Accurate, Robust and well Documented algorithms

- Developing and implementing robust and extremely accurate algorithms in KIVA-4 architecture – PCS/CBS *hp-adaptive* FEM.
- Reducing model's physical and numerical assumptions.
- Measure of solution error: resolution when and where required.
- New algorithm requiring less communication, no pressure iteration, an option for explicit: newest architectures providing super-linear scaling.
- More robust and accurate moving parts algorithms in development.
 - Lagrangian Frame for grid movement.
- 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
 - Starting spray and chemistry model incorporation.

Cut-Cell grid Generation and Implementation

- Quickly generate grids from CAD surfaces of complex domains. New algorithm has been developed, more generic
- Cubit Grid interface being developed for boundary conditions implementation.
- Discussions with Sandia about incorporating LANL cut-cell ideas into Cubit

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

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

Then
$$\frac{1}{c^2}\Delta P = \Delta \rho = -\Delta t \frac{\partial U_i}{\partial x_i} = -\Delta t \frac{\partial}{\partial x_i} \left[\left(\theta_1 \left(-\Delta t \right) \frac{\partial P}{\partial x_i} + \theta_1 U_i^* \right) + \left(1 - \theta_1 \right) U_i^n \right]$$
26

Density Solve (Pressure when incompressible flow)

So
$$\frac{1}{c^{2}}\Delta P = \Delta \rho = -\Delta t \frac{\partial U_{i}^{'}}{\partial x_{i}} = \left[\left(\Delta t^{2} \theta_{1} \frac{\partial^{2} P_{i}^{'}}{\partial x_{i}^{2}} - \Delta t \theta_{1} \frac{\partial U_{i}^{*}}{\partial x_{i}} \right) - \Delta t (1 - \theta_{1}) \frac{\partial U_{i}^{n}}{\partial x_{i}} \right]$$
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 $\left(\left[\mathbf{M}_{p} \right] + \Delta t^{2} c^{2} \theta_{1} \theta_{2} \mathbf{H} \right) \left\{ \Delta \rho_{i} \right\} = \left(\left[\frac{\mathbf{M}_{p}}{c^{2}} \right] + \Delta t^{2} \theta_{1} \theta_{2} \mathbf{H} \right) \left\{ \Delta P_{i} \right\} = \Delta t^{2} \theta_{1} \theta_{1} \mathbf{G} \left\{ \Delta \mathbf{U}_{i}^{*} \right\} + \mathbf{G} \left\{ \mathbf{U}_{i}^{n} \right\} - \Delta t \left\{ \mathbf{F}_{p} \right\}$

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

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

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

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

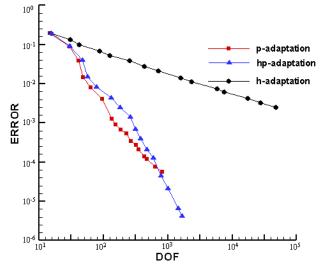
Error bounded by the following well known relation

$$\left\|u-u_{h}\right\|_{m}\leq ch^{k+1-m}\left\|u\right\|_{r}$$

'*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

 $||e_v|| = \left(\int_{\Omega} e_v^T e_v d\Omega\right)^{1/2}$ L₂ norm of error measure Error measures: $\|e_V\|^2 = \sum_{v=1}^m \|e_V\|^2$ Element error Residual, Stress Error, etc.. Typical error measures: $\eta_{V} = \left(\frac{\|e_{V}\|^{2}}{\|V^{*}\|^{2} + \|e_{V}\|^{2}}\right)^{1/2} \times 100\% \quad \text{Error distribution}$ Zienkiewicz and Zhu Stress Simple Residual Residual measure How far the solution is from $\overline{e}_{avg} = \overline{\eta}_{max} \left| \frac{\left(\left\| V^* \right\|^2 + \left\| e_V \right\|^2 \right)}{m} \right|^{\frac{1}{2}} \quad \text{Error average}$ true solution. •"True" measure in the model being used to form the residual. $\xi_i = \frac{\|e\|_i}{\overline{e}}$ Refinement criteria •If model is correct, e.g., Navier-Stokes, then this is a measure how far solution is $p_{new} = p_{old} \xi_i^{1/p}$ Level of polynomial for element from the actual physics!

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