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A Reflection of Recent ASC Milestones in Support of the Abnormal/Thermal Environment

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Exceptional service in the national interest

Sandia National Laboratories

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Outline

Advanced Simulation and Computing (ASC) Project's Driving Principle

Abnormal/Thermal Environment

FY12 and FY13 Milestone Efforts

Conclusions

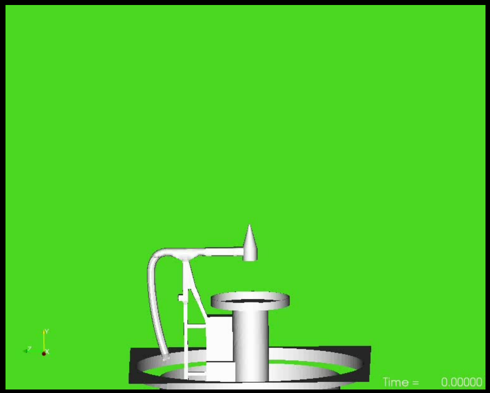
ASC Enables Science-based Stockpile Stewardship

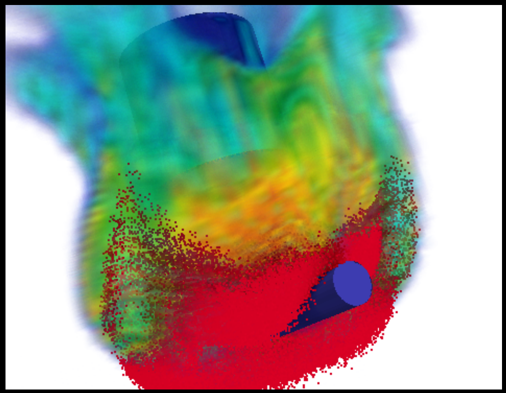
…Production ready

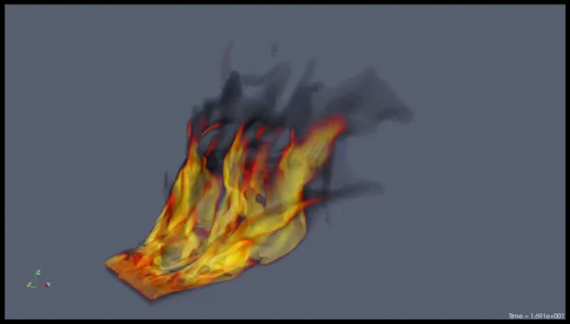
…Verification and Validation (V&V) pedigree established

Abnormal/Thermal Environment Complexity: Turbulent Reacting Flow with PMR

10 meter outdoor JP-8



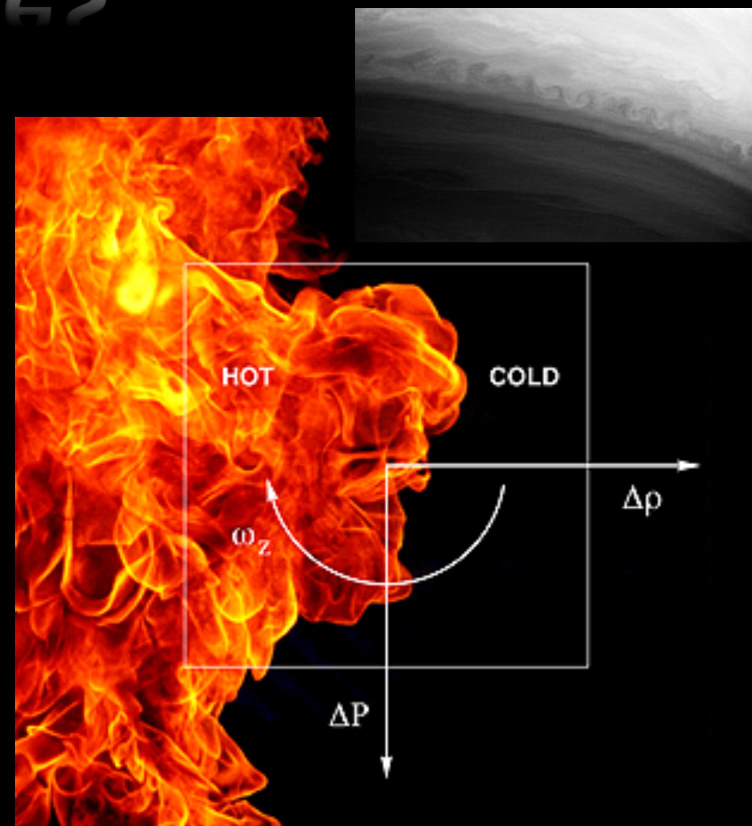




Unique multi-physics coupling

Abnormal/Thermal Environment Challenge: Capture Transient Small Scale Instabilities

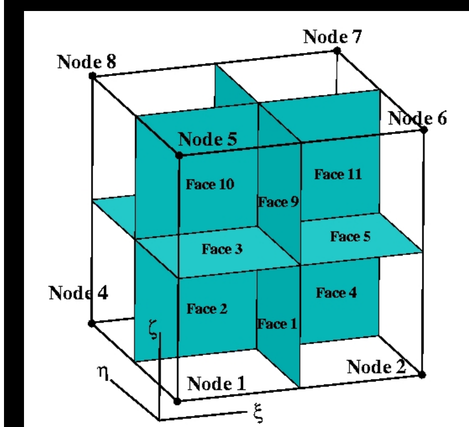
Time-averaged (inset transient)

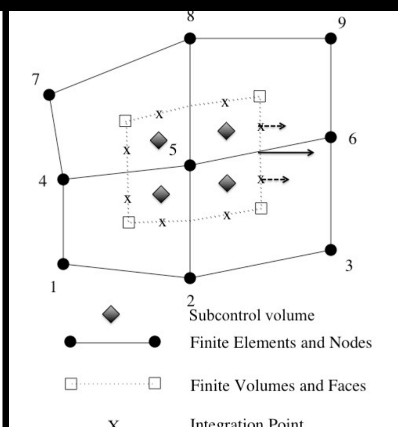


Vorticity generation

Low Mach Equation Set with PMR: ~60-130 Degree-of-Freedom (dof) System

- Variable density, unity Lewis#, *incompressible* equation set (pressure–projection)





Discretization

Control Volume Finite Element (CVFEM);L

Edge-based Vertex Centered (EBVC);R

$$\frac{\partial\bar{\rho}}{\partial t}+\frac{\partial\bar{\rho}\tilde{u}_j}{\partial x_j}=0$$

$$s_j^k\frac{\partial\overline{I^k}}{\partial x_j}+\overline{\mu_a}\,\overline{I^k}=\frac{\overline{\mu_a\sigma T^4}}{\pi}$$

$$\frac{\partial\bar{\rho}Y_k}{\partial t}+\frac{\partial\bar{\rho}\tilde{u}_j\tilde{Y}_k}{\partial x_j}=\frac{\partial}{\partial x_j}\left(\frac{\mu}{\mathrm{Pr}}\frac{\partial\tilde{Y}_k}{\partial x_j}-\tau_{Y_k u_j}\right)-\overline{\rho\varpi_k}$$

$$\frac{\partial\bar{\rho}\tilde{h}}{\partial t}+\frac{\partial\bar{\rho}\tilde{u}_j\tilde{h}}{\partial x_j}=\frac{\partial}{\partial x_j}\left(\frac{\mu}{\mathrm{Pr}}\frac{\partial\tilde{h}}{\partial x_j}-\tau_{hu_j}\right)-\frac{\partial q_j}{\partial x_j}$$

$$\frac{\partial\bar{\rho}\tilde{u}_i}{\partial t}+\frac{\partial\bar{\rho}\tilde{u}_j\tilde{u}_i}{\partial x_j}=-\frac{\partial}{\partial x_i}p+\frac{\partial}{\partial x_j}\left(\overline{\tau_{ij}}-\tau_{u_iu_j}\right)+(\bar{\rho}-\rho^r)g_i$$

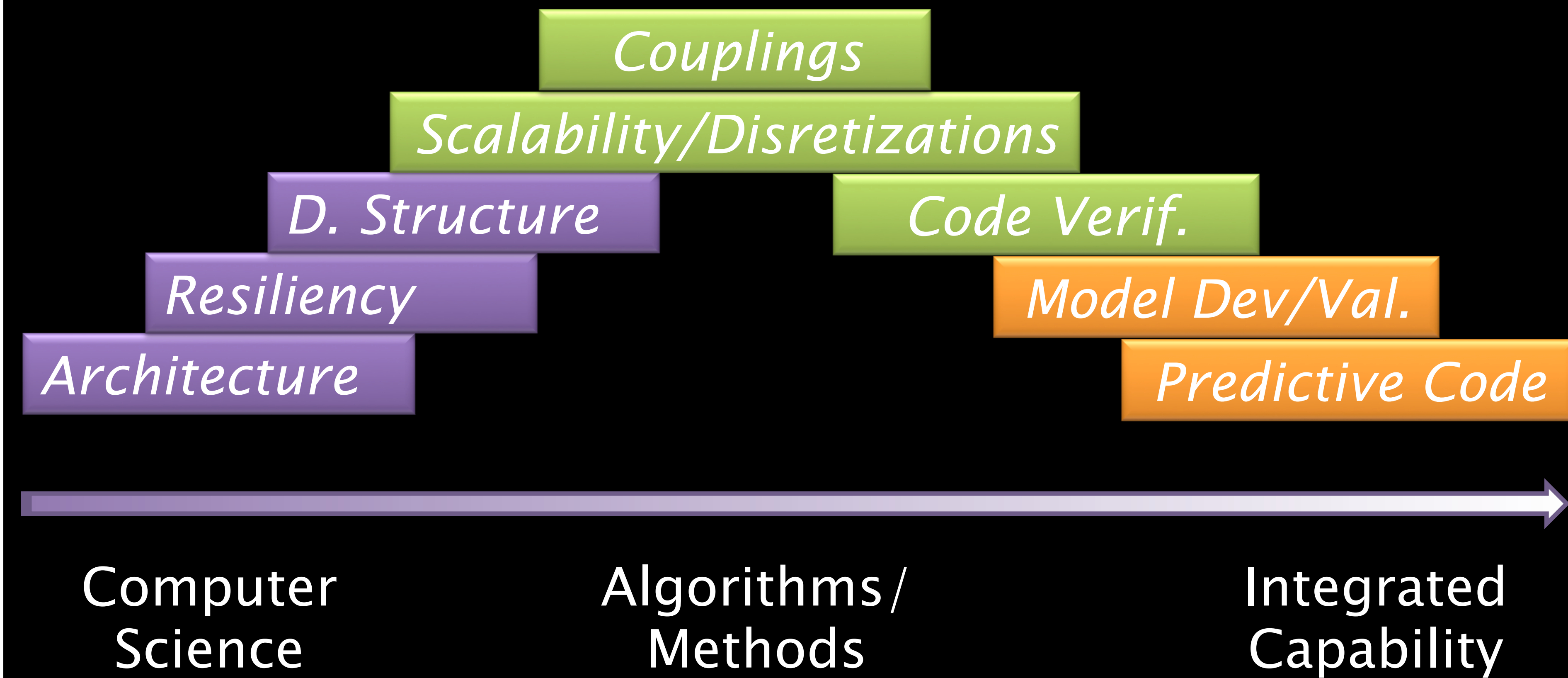
Subgrid closure models

ASC Mechanism to Drive Capability Development and Deployment: Milestones

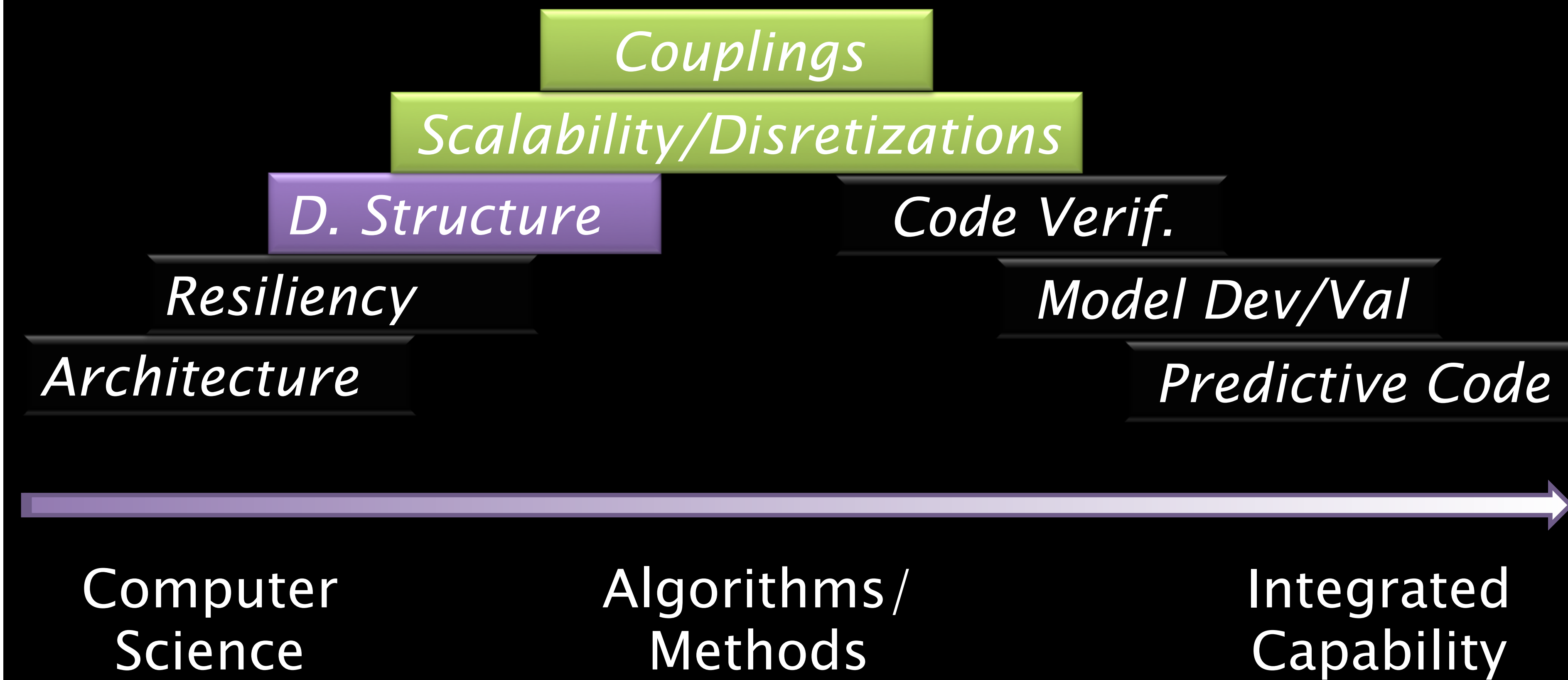
Provides concentrated alignment to NW mission space

Focus on the positive *and* the negative

Milestone Spectrum: CS-based->Capability-based



FY12 and FY13 Milestone: Tend Towards the "Middle-Left"

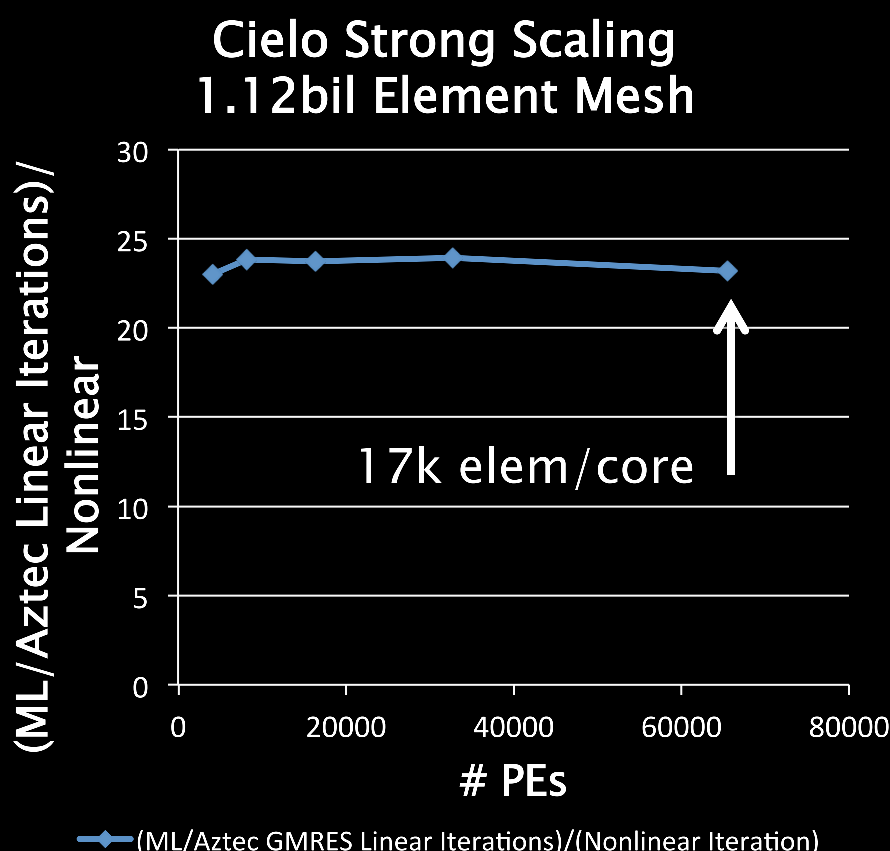


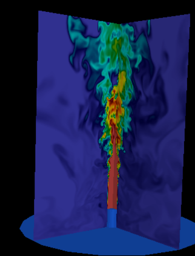
ASC FY12 L2: Performance-based Code Assessment for low Mach Large Eddy Simulation (LES)

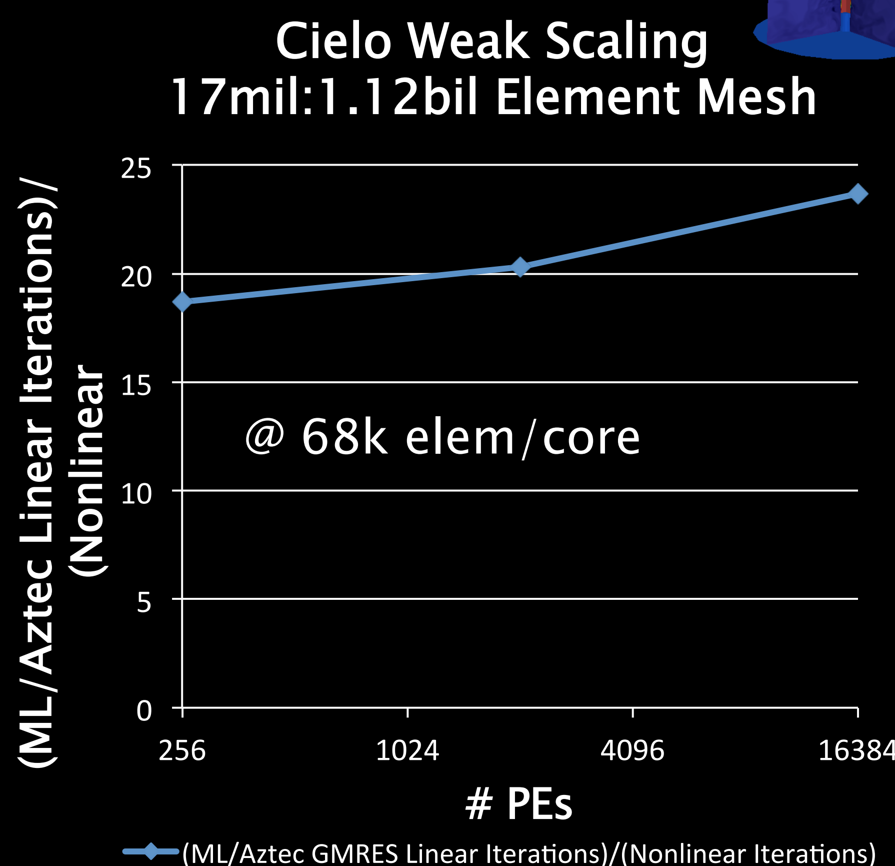
Goal: Drive code performance and scalability for next generation Abnormal/ Thermal LES support

Success Metric: Demonstrated weak and strong scaling studies on tens of thousands of cores; push towards upper 32-bit limit

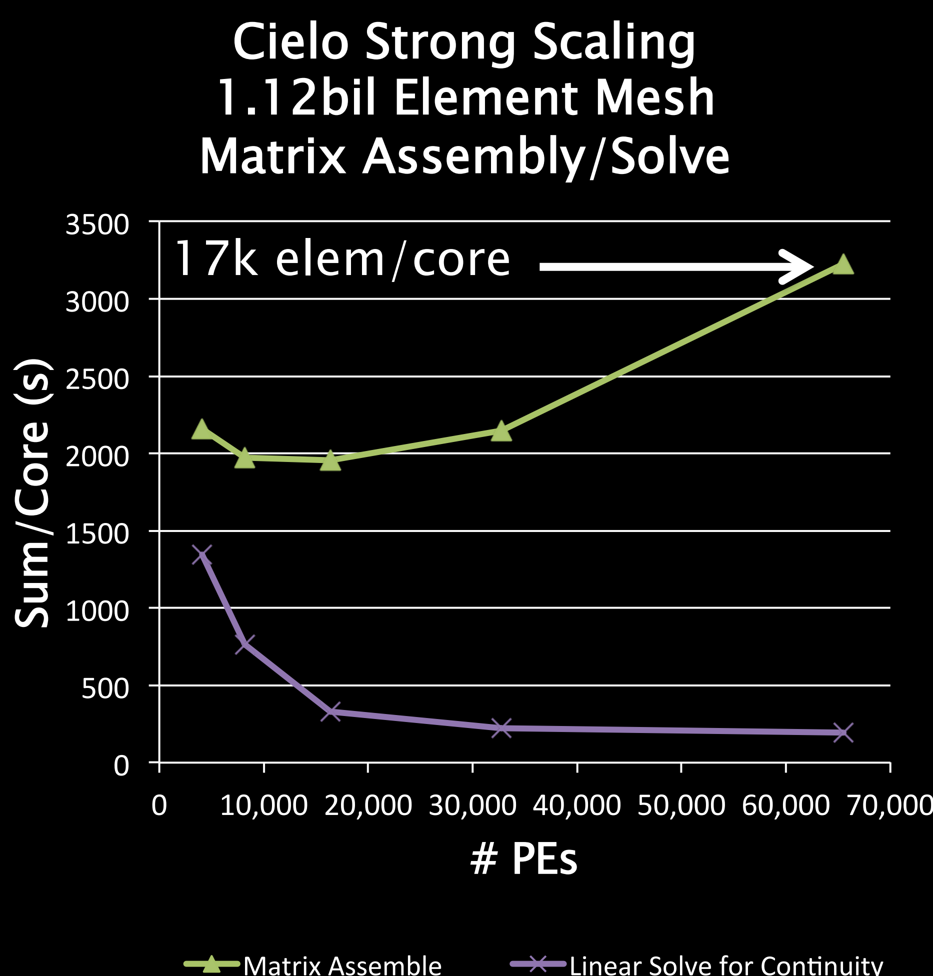
FY12 Overview: Ideal Algorithmic Solver Scalability

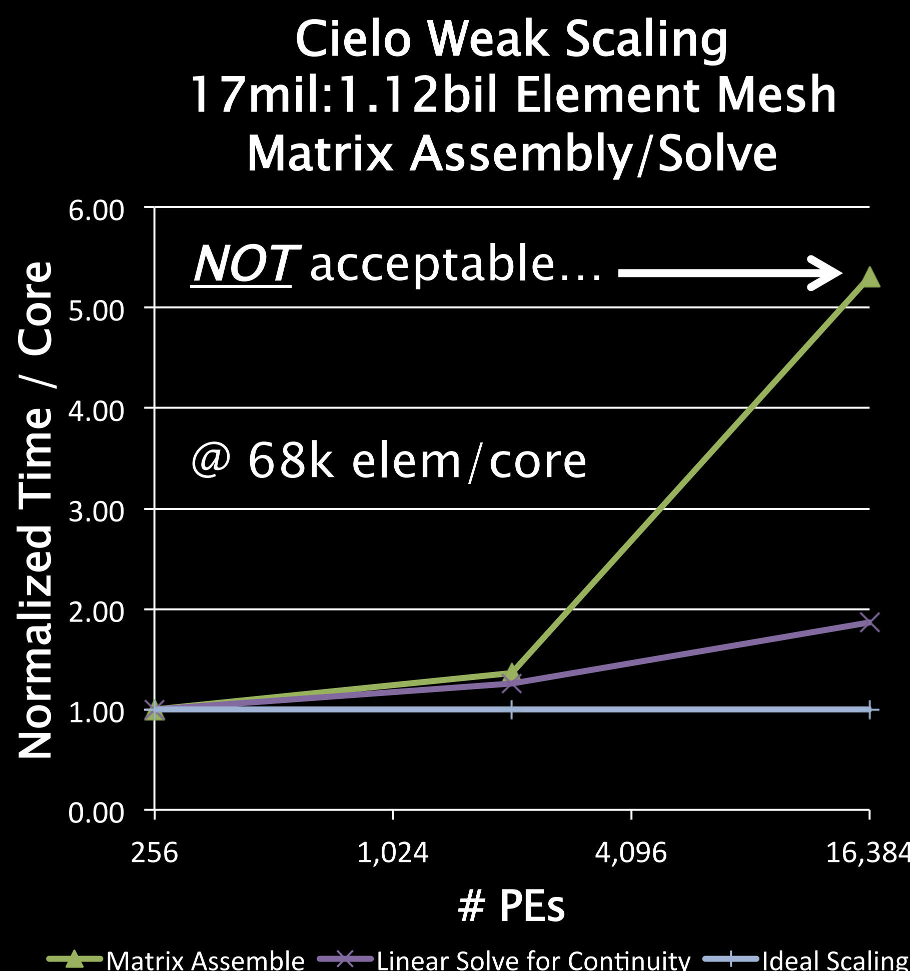




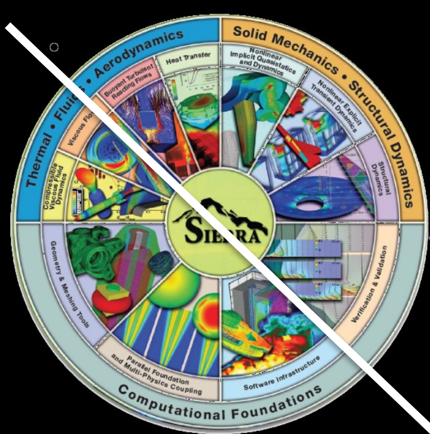


FY12 Challenges: Non-optimal Matrix Assemble Scaling



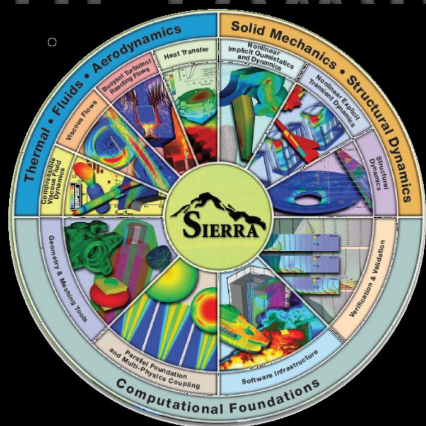


FY12 Challenges: 64-Bit Call Stack Compliance



FEI

FY13 Effort:
Beyond 32-bit
Path Towards New Architectures



+ ASC IC
Investments

()

Sierra Toolkit/Trilinos TPetra
MPI+X parallelism
Arbitrary data types
Support for new architectures

ASC FY13 L2: New Trilinos Scalable Solver Stack Deployed to Low Mach Thermal/Fluids Application

Goal: Drive code performance and scalability for next generation Trilinos/Tpetra solver stack, which includes design principles that support advanced architectures, in support of the Abnormal/Thermal LES application space

Success Metric: Integration of Trilinos/Tpetra into Sierra low Mach fluids code base, demonstrated code performance improvements and systems solved of size > 2.2 billion dof

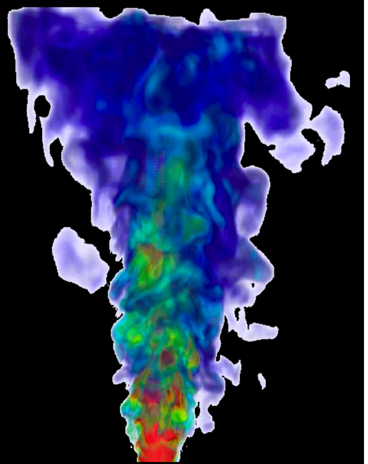
Demonstrated Unstructured Extreme-Scale CFD: Successful 9 Billion Element Mesh Simulations

Unstructured hexahedral mesh (Abdel et al) turbulent open jet

Panel: Please note literature review in the supplemental slides section

Demonstrated simulation on >65k core

Equation System	Size	DOF	Solver / Toolkit Stack
Momentum	3x3	27 billion	Trilinos Tpetra / STK
Pressure	1x1	9 billion	Trilinos Tpetra / STK
Ksgs	1x1	9 billion	Trilinos Tpetra / STK
Z	1x1	9 billion	Trilinos Tpetra / STK



VR Z-field

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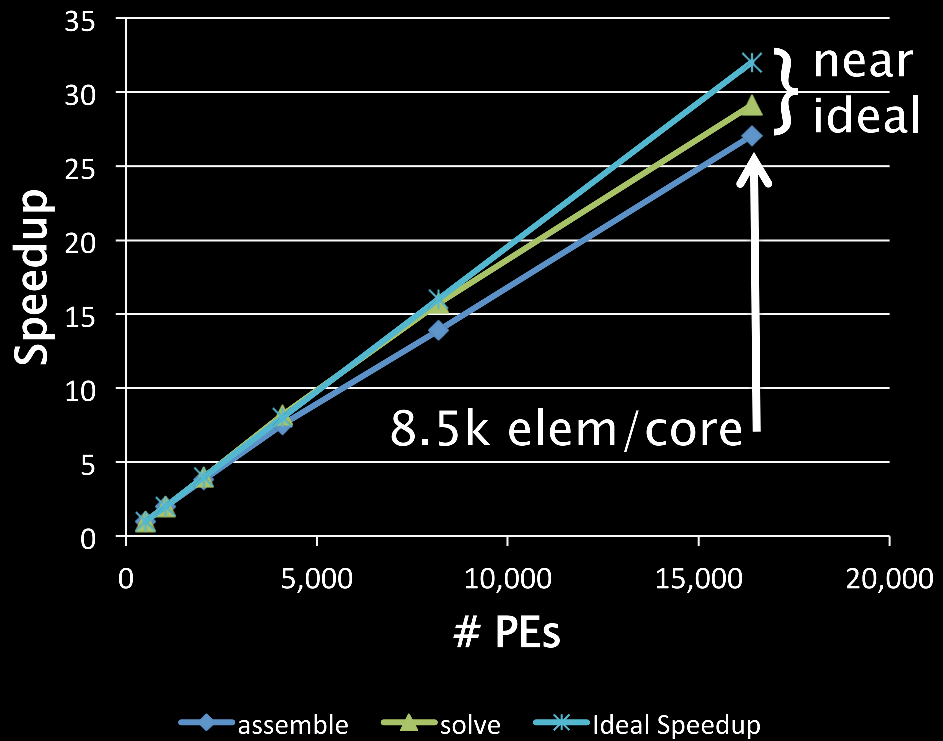
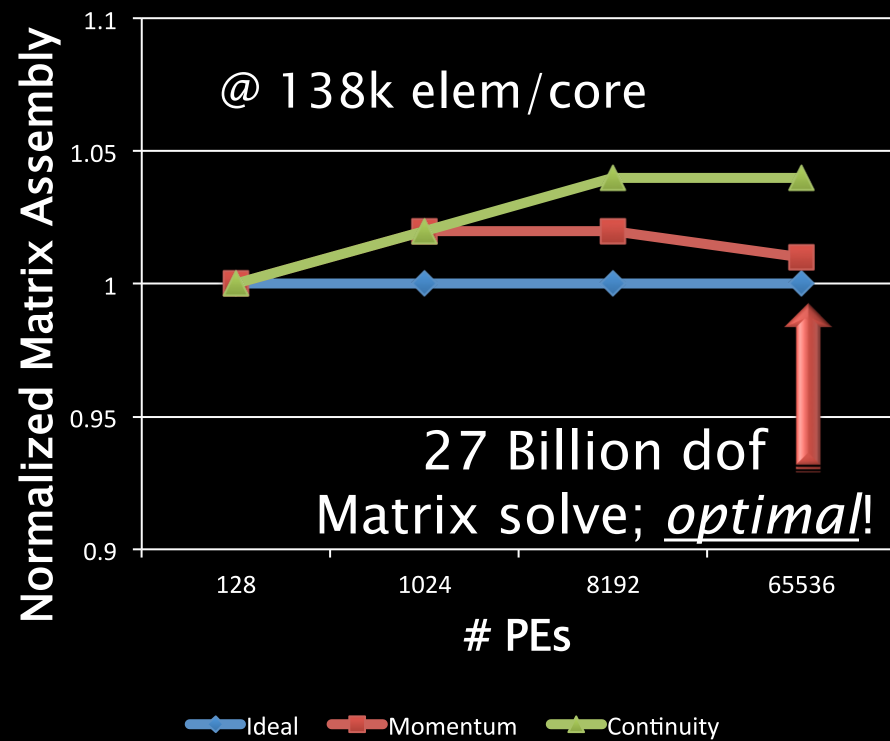
FY13 Accomplishments: Near Optimal Scaling Demonstrated

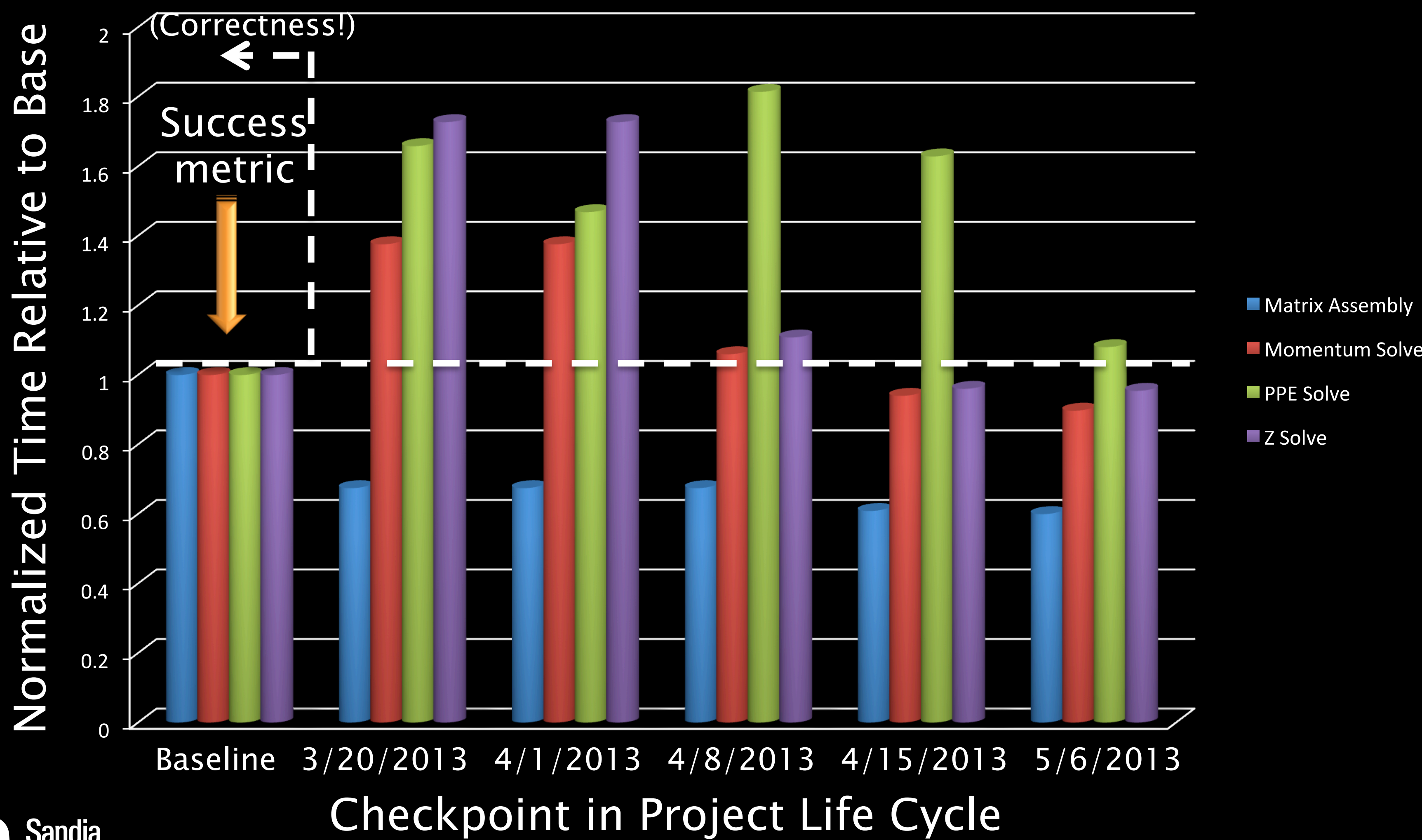
Cielo Strong Scaling
140mil Element Mesh
Coupled Momentum Solve



Cielo Weak Scaling
17mil:9bil Element Mesh
Matrix assembly



Evolution of Code Performance: Faster & Enables Path to Exascale



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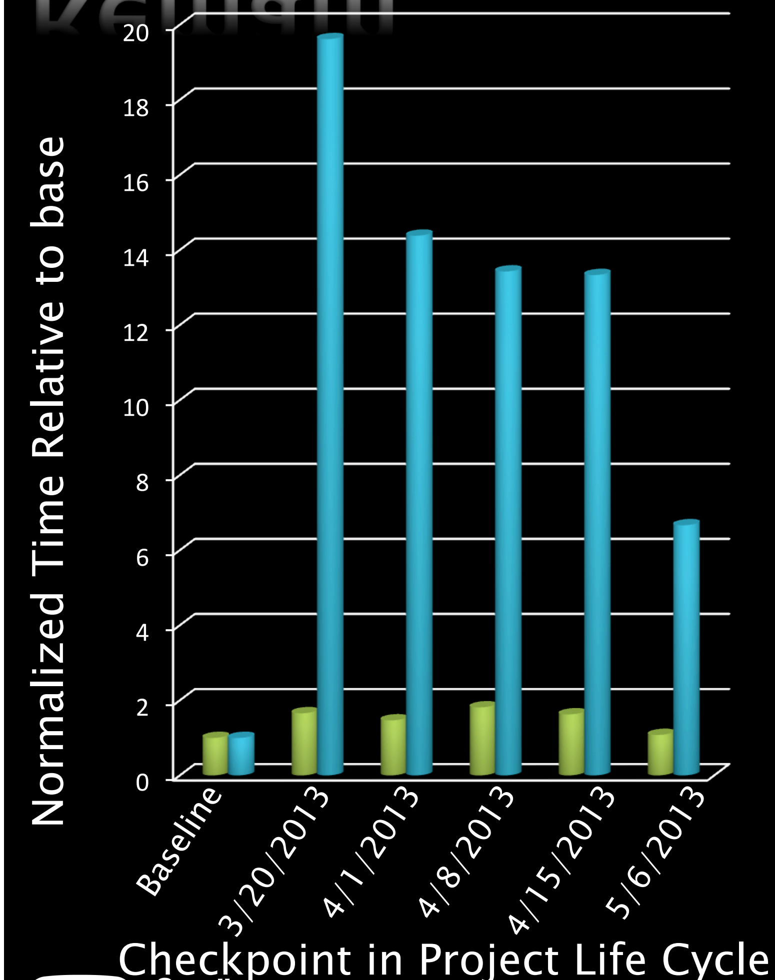
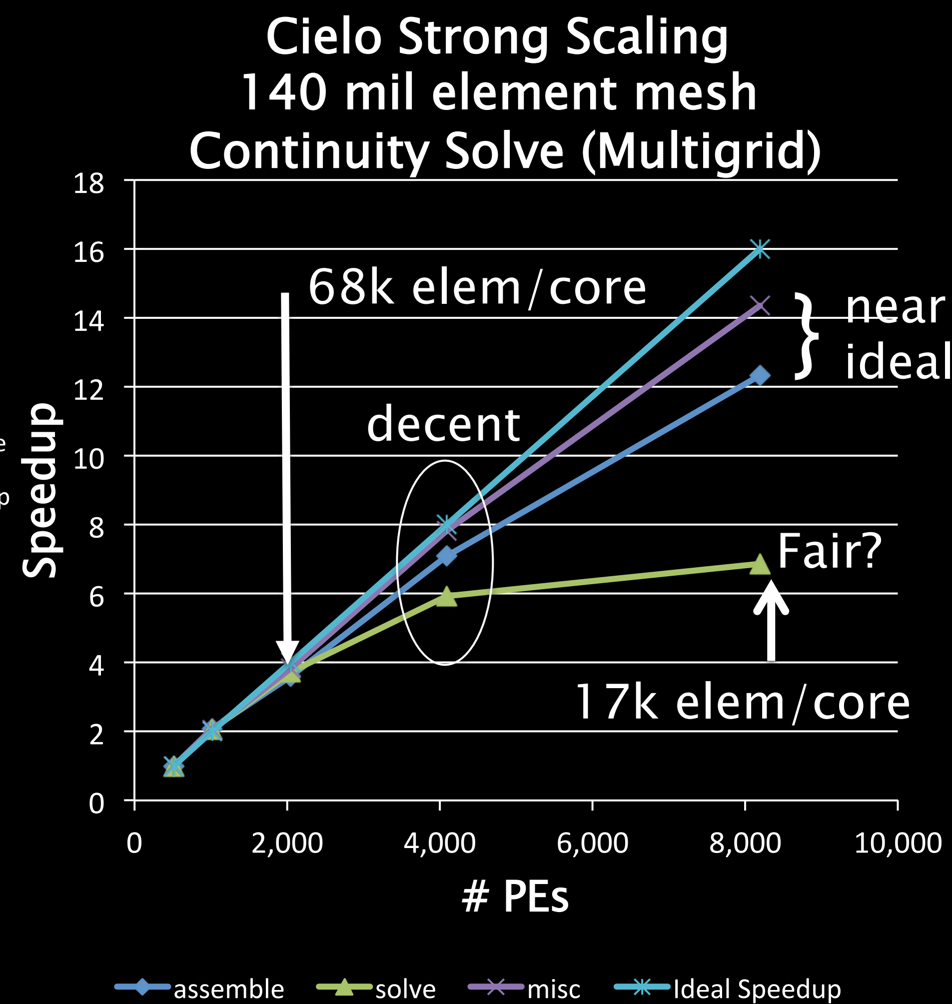
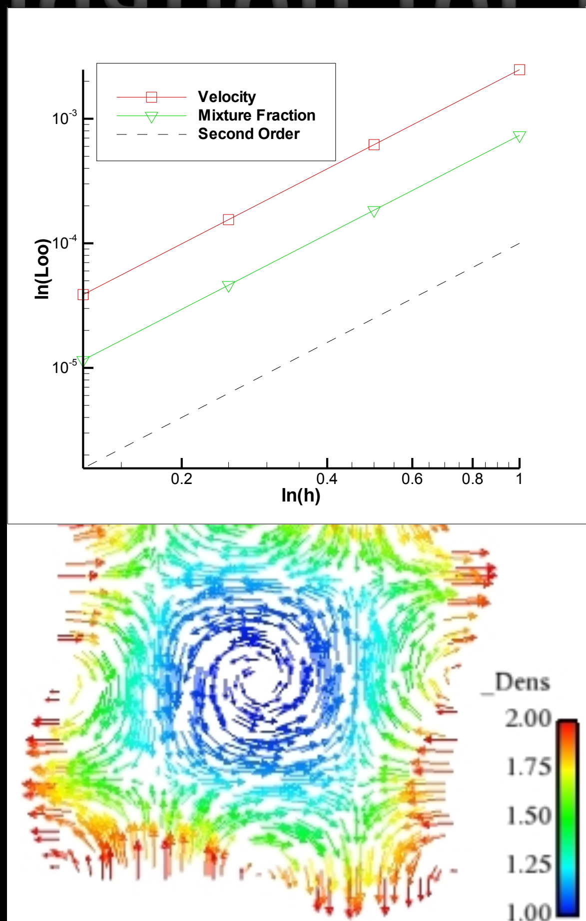
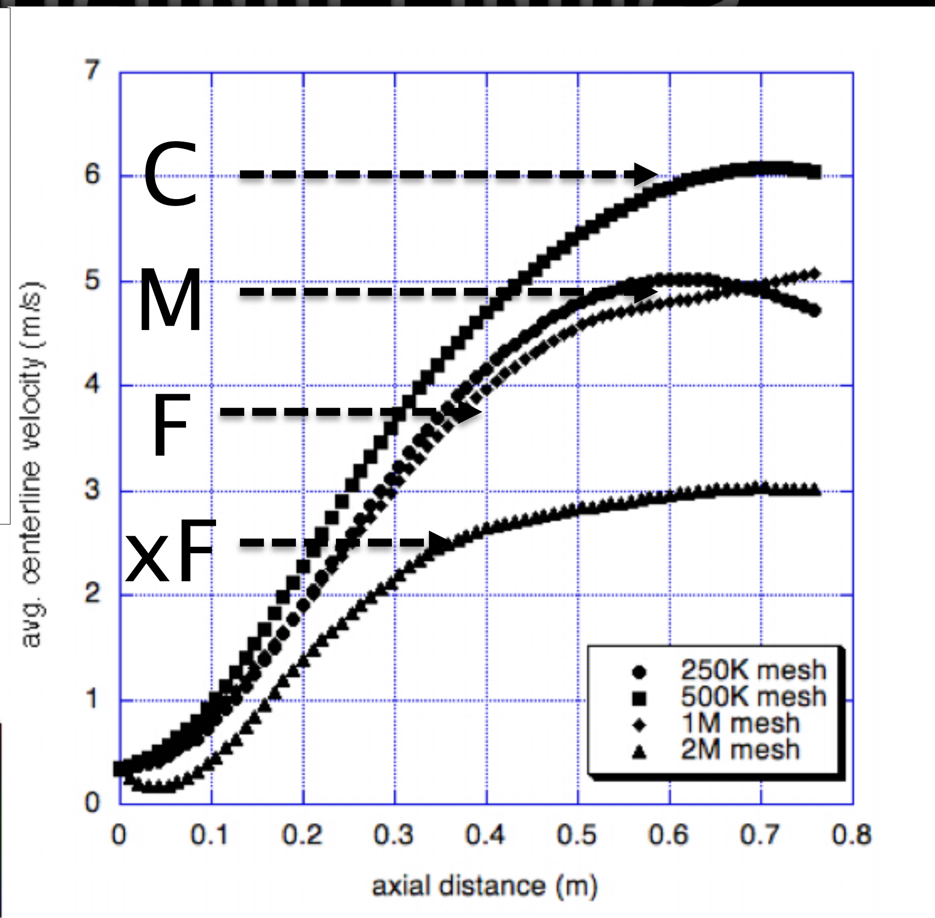
Multi-level Pre-conditioner: Performance Improvements Remain





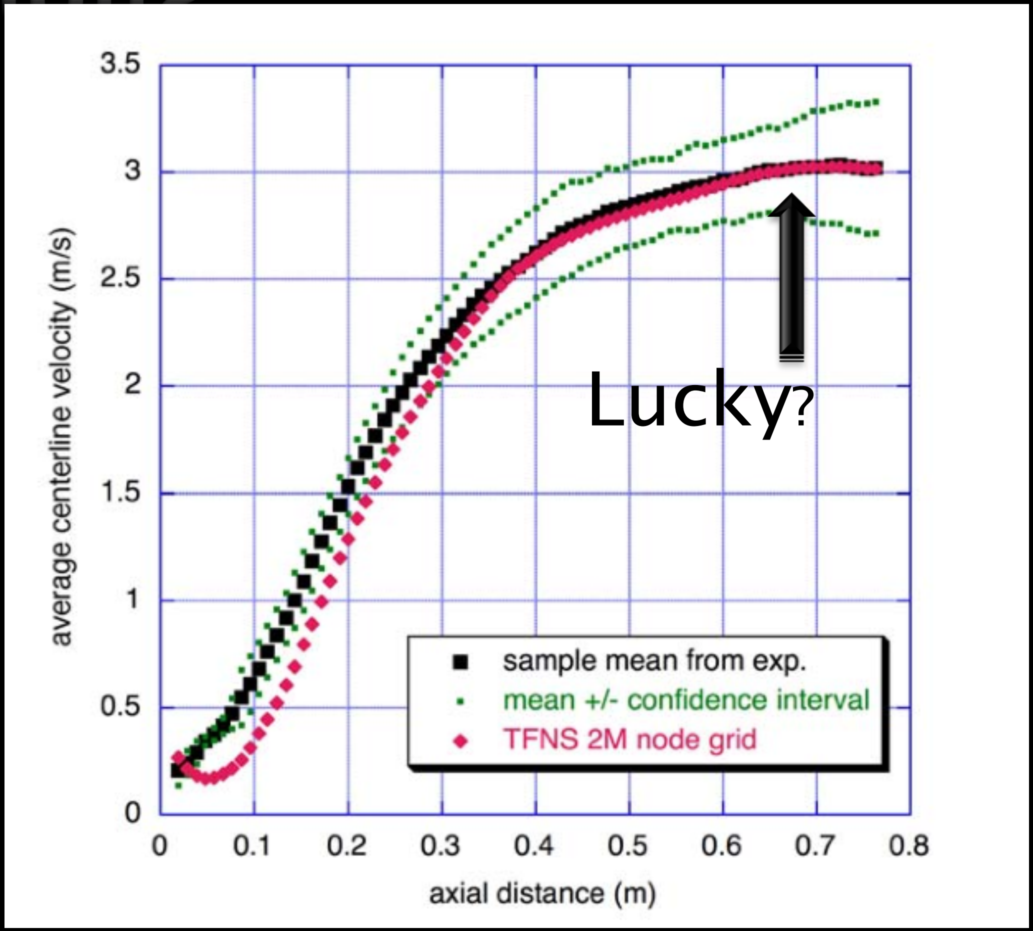
Enabling the NW Mission Space: Extend Verification and & Validation for Helium Plumes



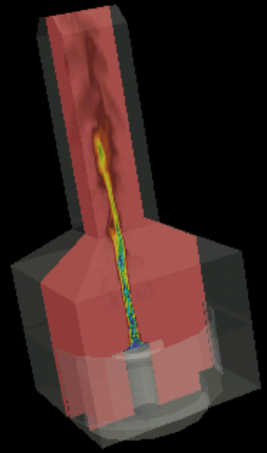


Previous V&V Results, Verification (L)/Validation (R)

Enabling the NW Mission Space: Resolve Solution Verification Questions



Previous V&V Results (comparison to data)



FLAME Facility Simulation

Unprecedented Validation Effort For low Mach Buoyant Plumes in FLAME Planned…

Enabling the NW Mission Space: New STK/Tpetra-Based Code is 2-4x Faster…

Helium Plume FLAME Facility Production Runs

Code	2 million	18 million
Fuego; elem (Aztec/ML with reinit.)	1 (3550s)	1 (12100s)
stk_nalu; elem (Tpetra/Epetra ML with out reinit.)	0.62 (2196s)	0.50 (6092)
stk_nalu; elem (Tpetra/Epetra ML with reinit.)	0.68 (2430s)	0.59 (7173s)
stk_nalu; elem (Tpetra/Tpetra Muelu no-reinit.)	0.61 (2188s)	0.51 (6211s)
stk_nalu; edge (Tpetra/Tpetra Muelu no-reinit.)	0.31 (1101s)	0.23 (2782s)

< 1 is *FASTER*

Conclusions

A new scale of scientific computing for unstructured implicit low Mach simulations has been demonstrated; 60 *billion* dof physics set with excellent scalability

Current effort provides foundation for production code deployment on advanced architectures

Amazing accomplishments to enable the NW mission space can be realized when ASC Milestones are strategic and aligned

The success of these milestones reflect the creation of high performing teams from a set of highly diverse personnel

Cross Cutting FY13 L2 Team:
Engineering Sciences/Computing Research/ Information Solutions & Services

Matt Bettencourt (1426)
Ryan Bond (1541)
Eric Cyr (1426)
Stefan Domino (1541)
Travis Fisher (1541)
Jeremie Gaidamour (1426)
Mike Glass (1545)
Mike Heroux (1426)
Rob Hoekstra (1426)
Mark Hoemmen (1426)
Jonathan Hu (1426)
Paul Lin (1426)
Kyran Mish (1542)
Pat Notz (1541)
Brent Perschbacher (9515)
Eric Phipps (1441)
Andrey Prokopenko (1426)
Siva Rajamanickam (1445)
Chris Siefert (1443)
Jim Willenbring (1426)
Alan Williams (1543)

A very talented team with a wide range of expertise

Backup Slides

Acronym/Abbreviations Used

Cielo Details

Code Names

Discretizations

Literature Survey

Acronym/Abbreviation Definitions

ASC: Advanced Simulation and Computing
Bil: Billion, 1e9
CVFEM: Control Volume Finite Element
CS: Computer Science
D: Data structure
Dev: Development
DNS: Direct Numerical Simulation
DOF: Degree-of-freedom
EBVC: Edge-based Vertex Centered
Elem: Element
FEI: Finite Element Interface
FLAME: Fire Lab for Accreditation of Modeling by Experiment
IC: Integrated Codes
K: Turbulent kinetic energy
NS: Navier Stokes
LES: Large Eddy Simulation
Mil: Million, 1e6
PPE: Pressure Projection Equation
PMR: Participating Media Radiation
Reinit: Re-initialization
SGS: Subgrid-scale
STK: Sierra Toolkit
TFNS: Temporally filtered NS
UQ: Uncertainty and Quantification
Verif: Verification
V&V: Verification and Validation
Val: Validation
VR: Volume-rendered
Z: Mixture fraction

Cielo Details

Cielo; a NNSA DOE resource ~1.37 petaflop Cray-based machine (XE6) built in Spring of 2010

- 2 GB per core
- Cray Gemini high-speed interconnect

PGI, Cray, Intel and GNU compiler suites

Design, procurement and deployment were accomplished by the NNSA's New Mexico Alliance for Computing at Extreme Scale (ACES)

- Joint partnership between Los Alamos National Laboratory and Sandia National Laboratories

Code Names/Brief Descriptions

Epetra: Fundamental construction routines and services to support massively parallel Linear Algebra libraries within Trilinos

Fuego: The Sierra-Framework low Mach fluids model internal code name. Uses a CVFEM pressure projection scheme that supports the Nuclear Weapons mission space for the Abnormal/Thermal environment

ML/Muelu: Multi-level preconditioner built on Epetra/Tpetra, respectively

Nalu: The Sierra Toolkit low Mach fluids internal code name. Supports both CVFEM and EBVC discretizations

Tpetra: Fundamental construction routines and [templated] services to support massively parallel Linear Algebra libraries within Trilinos on advanced platforms on > 2.14 billion dof systems

Trilinos: The Sandia solver library

CVFEM Discretization

The core discretization used in the low Mach code base has been the Control Volume Finite Element Method, CVFEM

An elemental basis is defined from which interpolation and gradients within the element are determined

The test function is defined to be piece-wise constant

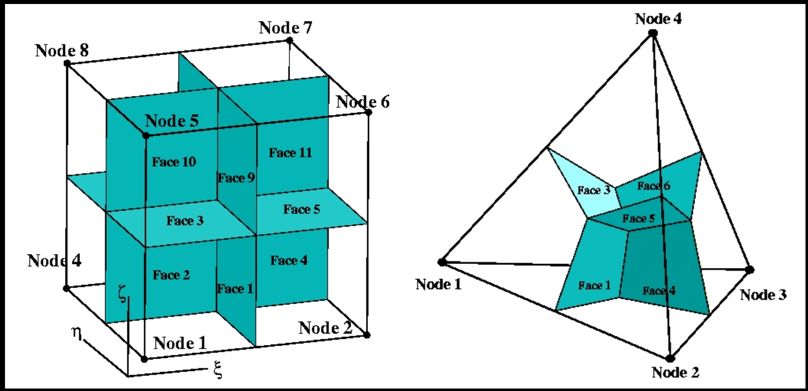
This method can best be described as a Petrov-Galerkin method

The canonical 27-point stencil is recovered

$$\int w \frac{\partial \bar{\rho}\tilde{u}_j\tilde{\phi}}{\partial x_j} d\Omega = -\int \bar{\rho}\tilde{u}_j\tilde{\phi}\frac{\partial w}{\partial x_j} d\Omega + \int w\bar{\rho}\tilde{u}_j\phi n_j \, d\Gamma$$

$$w = w_I ; \frac{\partial w_I}{\partial x_j} = -\delta(x - x_{scs})$$

$$\int w \frac{\partial \bar{\rho}\tilde{u}_j\tilde{\phi}}{\partial x_j} d\Omega = \sum_{ip} \left(\bar{\rho}\tilde{u}_j\right)_{ip} \tilde{\phi}_{ip} n_j dS = \sum_{ip} \dot{m}_{ip}\tilde{\phi}_{ip}$$



Hexahedral Dual Mesh (L)
Tetrahedral Dual Mesh (R)

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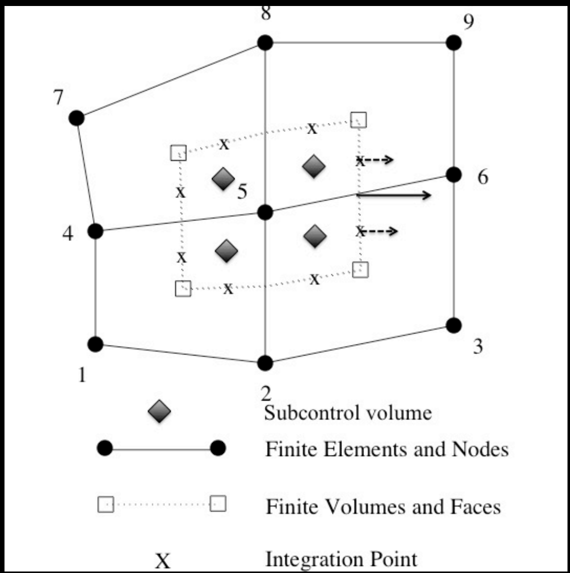
Edge-based Vertex Centered Discretization

In this method, the dual mesh is defined to establish geometric values at the edge midpoint (area vector) and node (volume)



Quadrature points for edge-based scheme

- Ramifications for the edge-based finite volume (EBFV)structure are as follows:
  - Reduced stencil (27-point to 7-point for structured hex)
  - Simple L/R data structure allows for simple interpolation and orthogonal gradient contributions
  - Lack of elemental basis requires a diffusion operator in terms of orthogonal to the edge and non-orthogonal correction that requires projected nodal gradients
  - Better accuracy on orthogonal mesh; worse on unstructured
  - 2-4x faster than CVFEM/FEM

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Finite Element Discretization

ASC

- Classic Equal Order Interpolation with explicit pressure stabilization
- Monolithic or approximate pressure projection couplings exist
- Pressure stabilization can be similar to segregated approach (2nd or 4th order) or PSPG
- Advection stabilization obtained via SUPG

$$\tilde{w} = w + \tau u_j \frac{\partial}{\partial x_j} w$$

- Ramifications for the FEM method:
  - Canonical 27-point stencil for structured hex
  - Full elemental diffusion operator (issues with diffusion operator monotonicity exists for aspect ratios greater than sqrt(2))
  - Galerkin method not regularly used due to the need for residual-based stabilization thus making most implementations a Petrov-Galerkin method
  - VMS foundation replaces classic SUPG and PSPG approach

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Literature Survey (Brief)

Simulation problem scale of interest depends on modeling technique, i.e., Direct Numerical Simulation (DNS) or Large Eddy Simulation (LES), the choice of structured vs. unstructured and, finally, implicit or explicit coupling strategies. The following contains a brief summary of the leaders in the field based on the extreme algorithm scales of interest

Explicit DNS of reacting flow on structured meshes are led by Jackie Chen of Sandia National Laboratories within the Combustion Research Center. Here, DNS simulations of reacting jet in cross flows, e.g., Kolla et al, Comb. & Flame, 159(8), (2012), and LES simulations of flame wrinkling, e.g., Hawkes et al, Comb. & Flame, 159(8), (2012) have been demonstrated on structured meshes of up to seven billion elements on 120k core.

Implicit LES of reacting flow on un-structured meshes are led by CORIA-CNRS (University of Rouen and the Institute of Applied Sciences) where both DNS and LES reacting flow simulations of swirl burners, Moureau et al, Comb. & Flame, 158(7), (2011), have been performed on up to 2.6 billion unstructured tet meshes. Simulations at the 20 billion tet meshes have been performed (personal communication with V. Moureau during the 2012 CTR Summer Program)