SAND2007-1842C

ADVANCED SIMULATION & COMPUTING™

Code and Solution Verification in a Parallel Finite Element Code

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14th International Conference on Finite Elements in Flow Problems
March 28, 2007

Sandia National Laboratories

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

NNSA
National Nuclear Security Administration

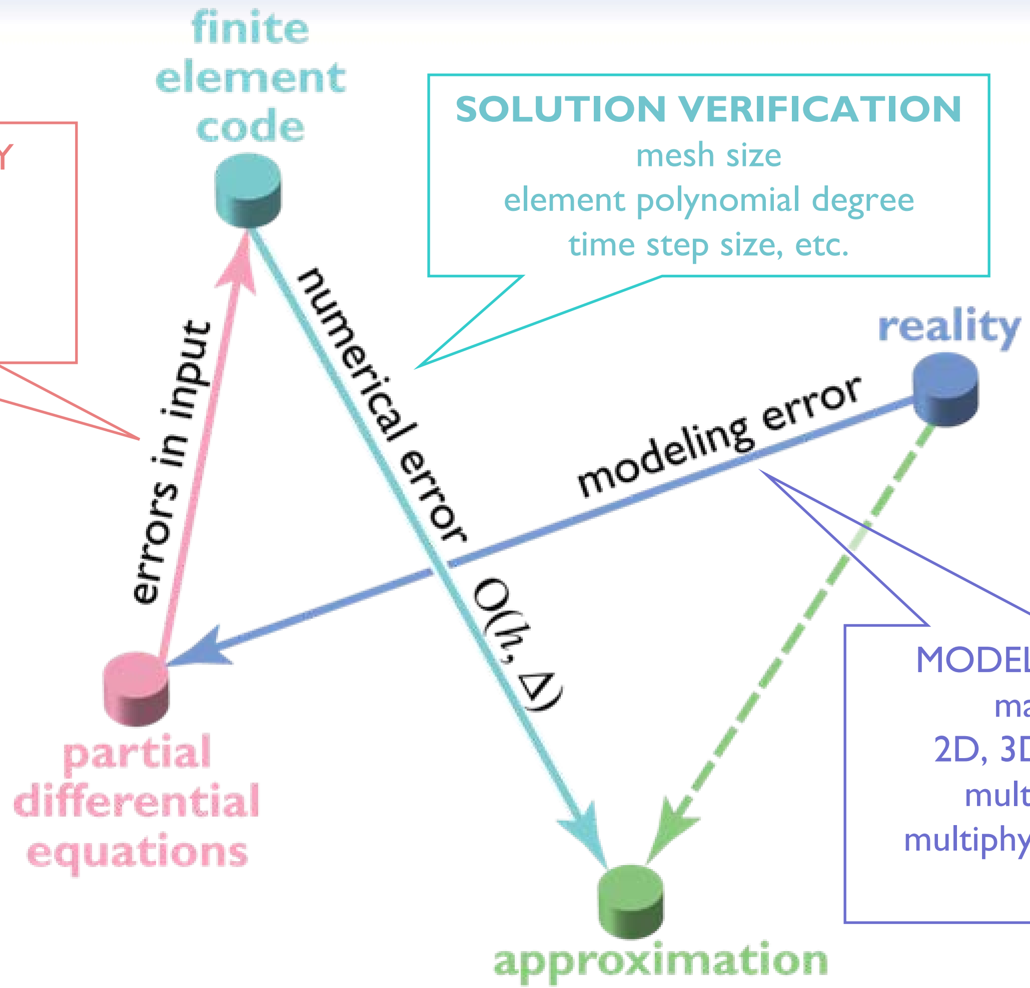
Code Verification

Is your code free of defects?

Are the algorithms implemented correctly?

- Order of Accuracy Tests
  - Comparison with analytic solutions on mesh sequences
  - H^1, L^2, L^∞ Norms most sensitive to defects in code/platform
  - Developer must be aware of regularity assumptions
  - Portable, parallel, and automatic–installed with executable
- Code Coverage Metrics
  - Smaller tests for function coverage and line coverage not enough: "system" tests or "integration" tests
  - If boundary condition A and B work alone, it does not imply that they work together
  - Link requirements to test cases, and add requirements coverage as a code quality metric.
  - A metric that expresses coverage in terms of the functionality required for a particular problem space: Phenomena Identification and Ranking Table (PIRT)

Solution Verification



INPUT UNCERTAINTY
errors in geometry
material properties
boundary conditions
etc.

SOLUTION VERIFICATION
mesh size
element polynomial degree
time step size, etc.

MODEL VALIDATION
material laws
2D, 3D, beams/shells
multiscale effects
multiphysics assumptions
etc.

A schematic of the sum effect of all errors/uncertainties in an FE approximation. The errors may cancel, or have synergistic effects.

part I

Coda

A Verification Toolkit

Coda – verification toolkit

Product of ASC Algorithms: **Error Estimation and Adaptivity**

Goals:

- Tools for enabling predictive simulation
- Help manage the tradeoff of resources vs. accuracy

Tools:

- Functions and Continuous Differencing
- Norms
- Refinement Markers
- Curved Geometry Representation
- Error Indicators (Flux jump, ZZ-like)
- Adaptive Mesh Refinement
- A posteriori Error Estimators

Coda – verification toolkit

Meets the need for offline code and solution verification

- Enables manufactured solutions
- Enables convergence studies in global norms, other functionals
- Inputs can be Exodus II files, which are not specific to SIERRA codes

Abstracts Concept of Functions:

- Simulation fields
- String definitions in input file: u = “x + z”
- User subroutines

Enables Post-processing at Continuous Level

- Differencing of solutions on sequences of meshes
- Norms, L2, L-inf, H1
- Functionals of solution: pressure on boundary, etc.
- Richardson Extrapolation

part 2

Thermal Contact

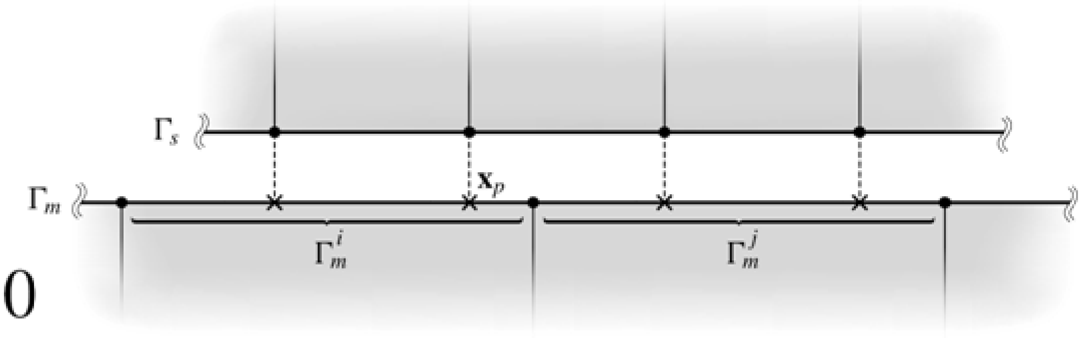
Unaligned Meshes and Gap Resistances

Thermal Contact in *Calore*

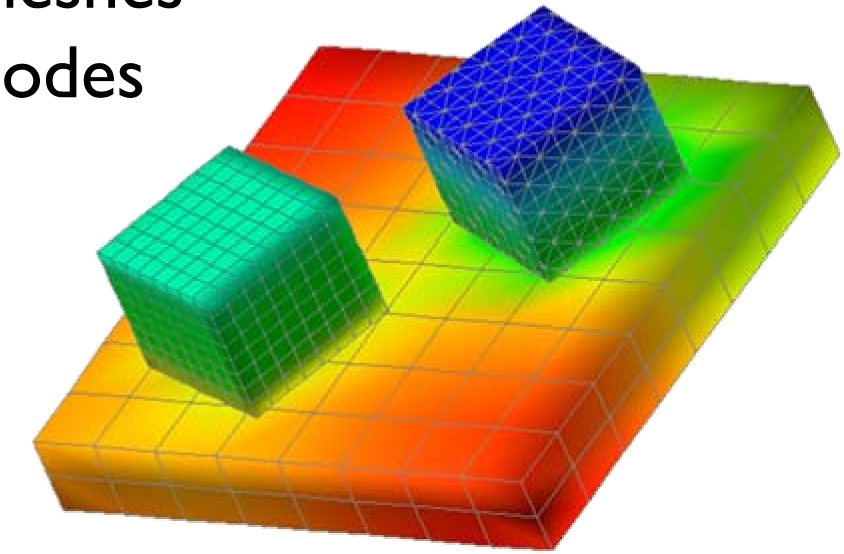
Tied contact:

- Enforced with Lagrange multipliers

$$u\Big|_{\partial\Omega_i} - u\Big|_{\partial\Omega_j} = 0$$



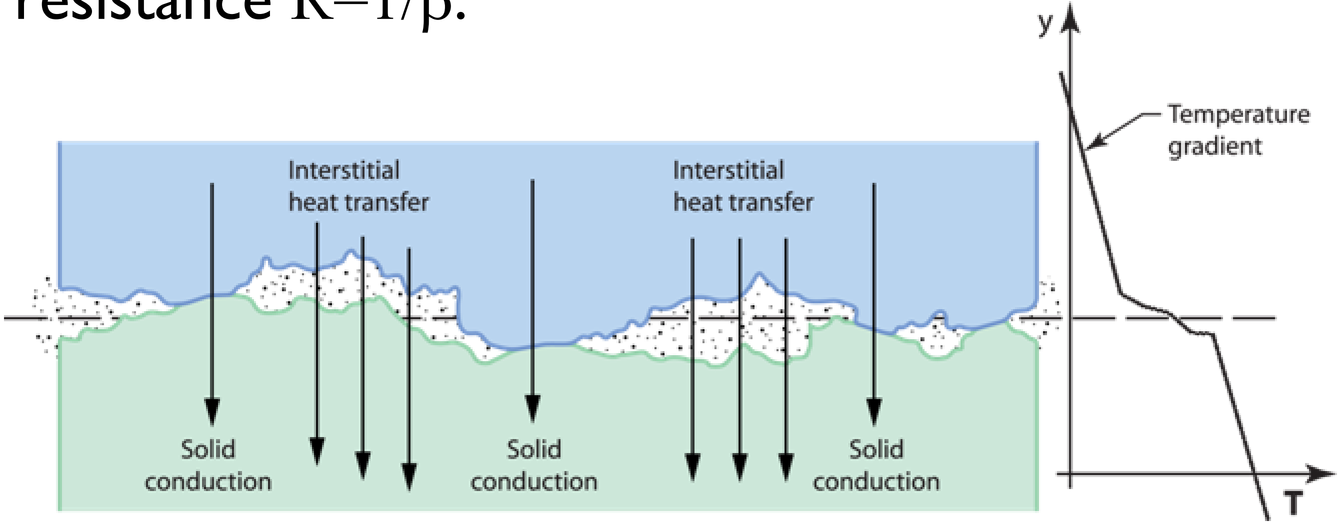
- Non-matching meshes with unaligned nodes



Thermal Contact in *Calore*

Imperfect Contact

- A finite contact resistance between two conducting media resulting from imperfect contact.
  - Surface roughness
  - Poor conduction in gas filled interstices
  - Inefficient radiation across gaps
- The key parameter is the thermal conductance β or resistance $R=1/\beta$.



Generalized Contact Model

- Our numerical model for contact handles both zero and finite contact resistance.
- When $[u] = 0$, the exact solution satisfies

$$(a\,\nabla u, \nabla v)_\Omega \quad - \langle \{\nabla u\} \cdot n, [v] \rangle_\Gamma \\ + \underbrace{\langle \beta_h\,[u], [v] \rangle_\Gamma}_{=0, \quad \forall \beta_h} = (f, v)_\Omega, \qquad \forall v$$

- The FE model is a (Discontinuous Galerkin) DG model

$$(a\,\nabla u_h, \nabla v_h)_\Omega \quad - \langle \alpha_h\,\{\nabla u_h\} \cdot n, [v_h] \rangle_\Gamma \\ + \langle \beta_h\,[u_h], [v_h] \rangle_\Gamma = (f, v_h)_\Omega$$

Parameters for the Contact Model

- Parameters for zero resistance

$$\alpha_h \equiv 1 \qquad \beta_h \equiv C\{a\}/h$$

(DG + penalty)

- Parameters for finite resistance

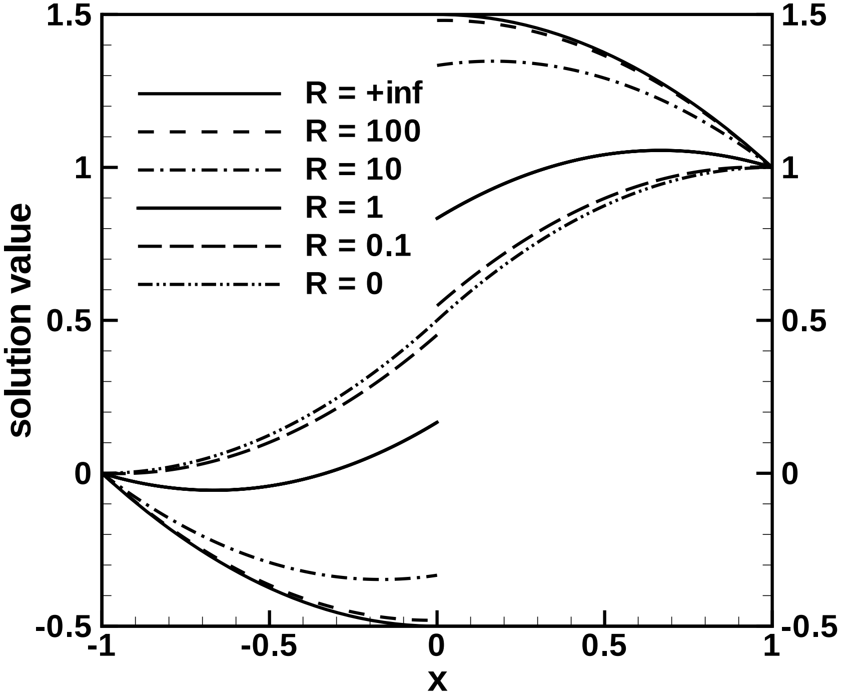
$$H \equiv \beta/(C\,\{a\}/h) = \frac{\beta\, h}{C\,\{a\}} = O(h)$$

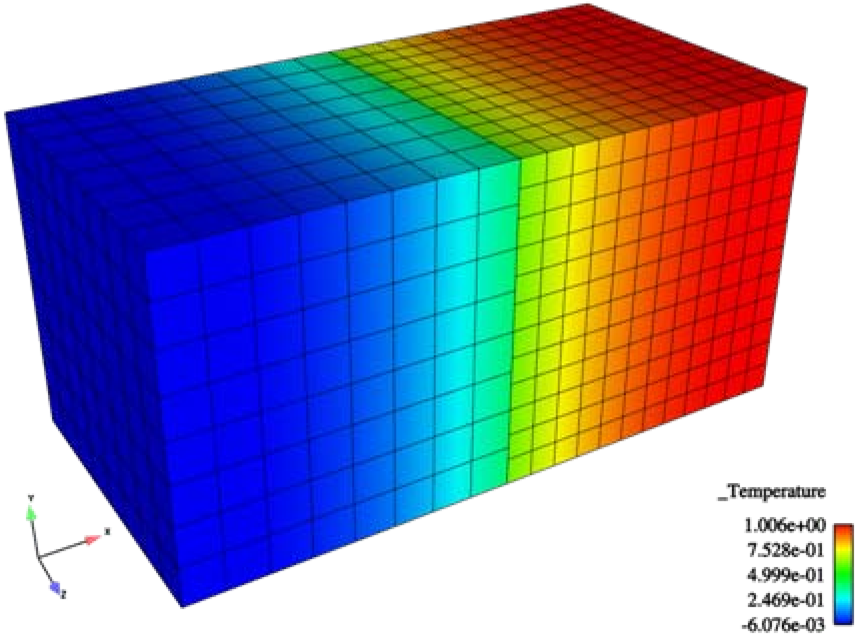
$$\alpha_h \equiv \begin{cases} 1 - 1/H, & H \geq 1 \\ 0, & H \leq 1 \end{cases}$$

$$\beta_h \equiv \begin{cases} C\{a\}/h, & H \geq 1 \\ \beta, & H \leq 1 \end{cases}$$

Example 1: 1D Solution Verification

- Analytical 1D solution with resistance:





R = 0.25

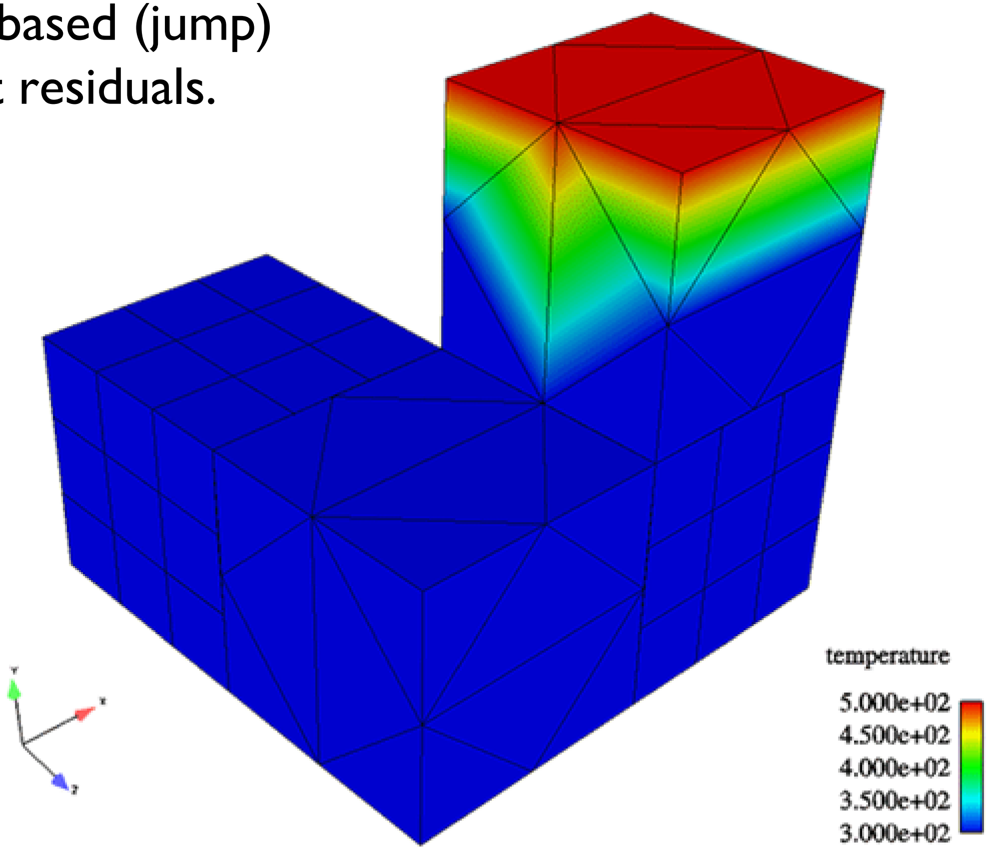
Example 1: 1D Solution Verification

- We compared the generalized contact algorithm with another algorithm that is based on nodal constraints (tied contact).
- The generalized contact had optimal convergence rates for linear and quadratic elements, for aligned and unaligned meshes, and for both hex and tet elements.
- The tied contact had suboptimal convergence rates when the meshes were not perfectly aligned.
- The rates for tied contact degenerated to zero as the mesh scales of the two surfaces in contact became more disparate.
- Finally, tied contact appeared to be unsuitable for adaptivity, since new nodes appearing on the master side were not properly constrained as hanging nodes.

Example 2: 3D Adaptive Transient

- Generalized contact with $R = 0$ and unaligned linear hex/tet meshes.
- Adaptivity based on a residual-based (jump) estimator that includes contact residuals.

- Contact search $O(N \log N)$ is recomputed after each mesh refinement.
- Generalized contact appears to be well suited for adaptive mesh refinement, because of the symmetric nature of the contact interactions.



part 3

Transient Heat Transfer

Convergence in Time and Space

Transient Heat Transfer

- Parabolic PDE

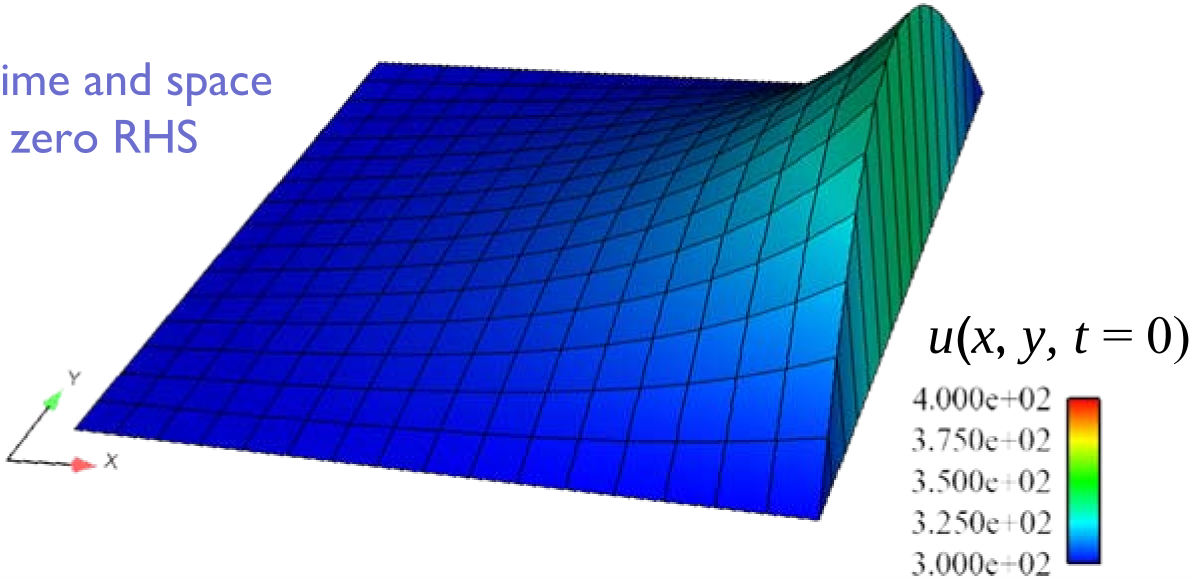
Find temperature $u = u(\mathbf{x}, t)$ such that

$$\rho c \frac{\partial u}{\partial t} - \nabla \cdot (\mathbf{K} \nabla u) = \dot{q} \qquad \forall\, \mathbf{x} \in \{\Omega_i \,|\, \Omega_i \in \mathscr{S}\};\, t > t_0,$$

- Analytic exact solution

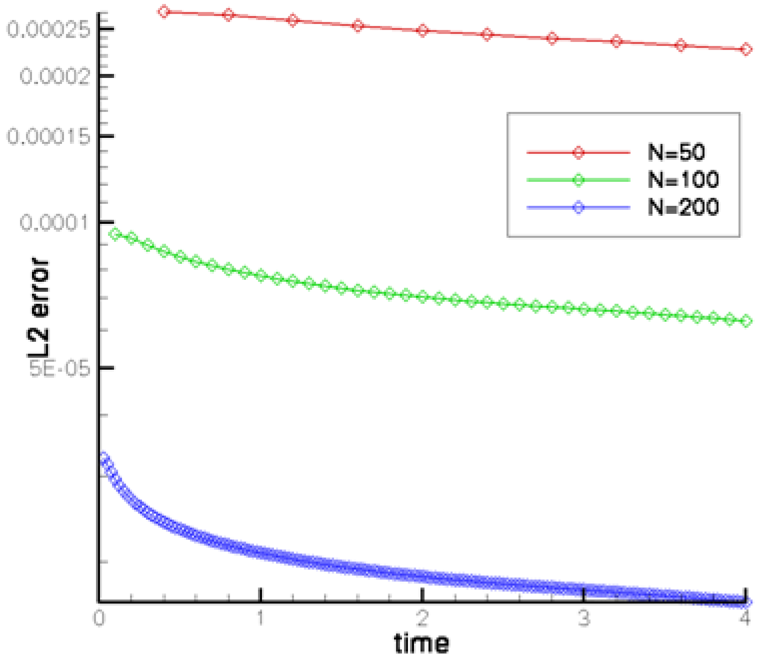
$$u(x, y, t) = 300 + 100\ \mathrm{e}^{-t}\ \operatorname{csch}\left(\sqrt{\pi^2 - 1}\right) \sin(\pi y) \sinh\left(x\sqrt{\pi^2 - 1}\right)$$

Smooth in time and space
Exhibits zero RHS

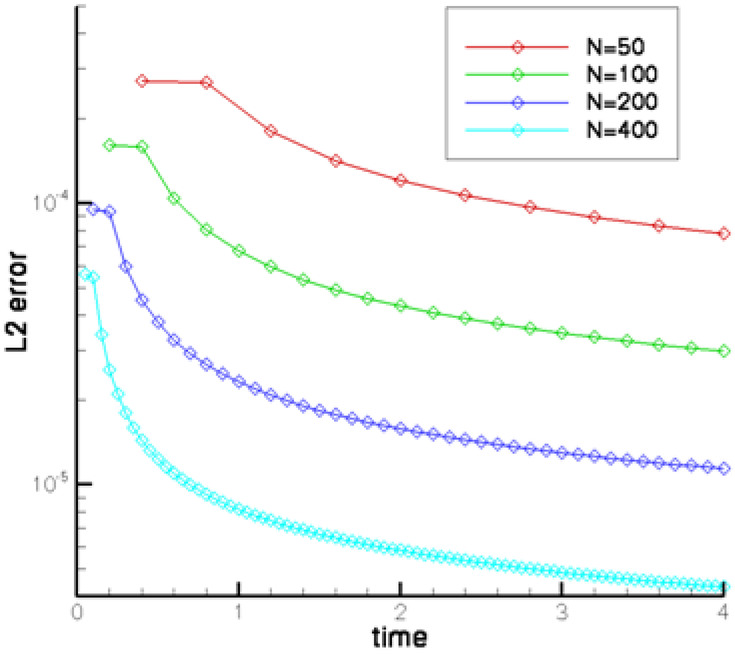


Order Verification for Transient Solution

- Convergence of space time mesh sequences: $\{\Delta t, h\}$



Implicit rule: constant $\Delta t / h^2$



Trapezoid rule: constant $\Delta t / h$

part 4

Enclosure Radiation

Loose Coupling with Conduction

Radiation

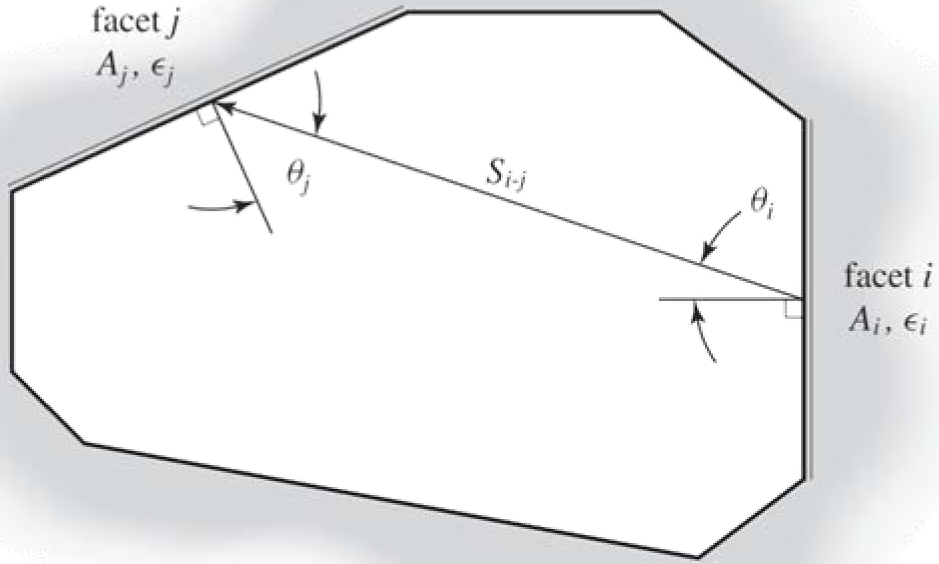
Radiative flux on facet *i*

$$q_n = \underbrace{\sigma \epsilon u^4}_{\text{emitted}} - \underbrace{\epsilon G_i}_{\text{absorbed}}$$

where

$$G_i = \sum_{j=1}^{E} \overset{\text{geometric viewfactor}}{F_{ij}} \underset{\text{radiosity of surface } j}{J_j}$$

F_{ij} = fraction of energy
that leaves facet *i*
and arrives at facet *j*



Coupled Conduction and Radiation

- Thermal radiation within an enclosure is significant in many problems at Sandia.
- Given emitted thermal radiation E, the radiation equations determine the emitted radiation, or radiosity J, and the incident radiation G:

$$J - \rho \mathcal{F} J = E, \qquad G \equiv \mathcal{F} J$$

reflectivity

surface integral operator on the enclosure

- These equations couple to the conduction on the enclosure surface:

$$-(k\,\nabla u)\cdot n = \epsilon\,\sigma u^4 - \alpha\, G, \qquad E \equiv \epsilon\,\sigma u^4$$

conductivity

emissivity

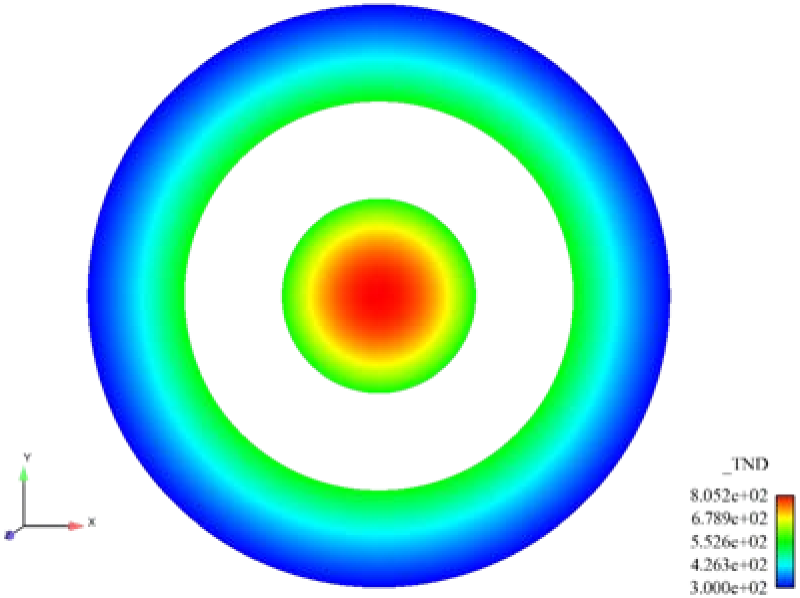
Stefan-Boltzmann constant

absorptivity

incident radiation

Analytic Solution for Verification

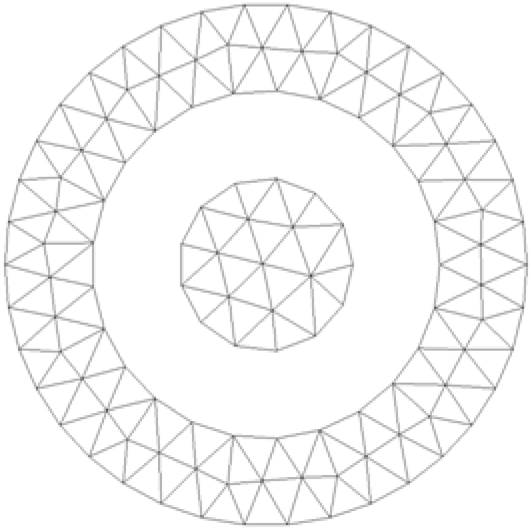
- Analytic solution in a 2D radially symmetric geometry.
- Heat source in cylinder
- Enclosure radiation between cylinder and annulus
- Prescribed temperature exterior boundary
- The temperatures at the interfaces are calculated using the radiation equations and the energy balance



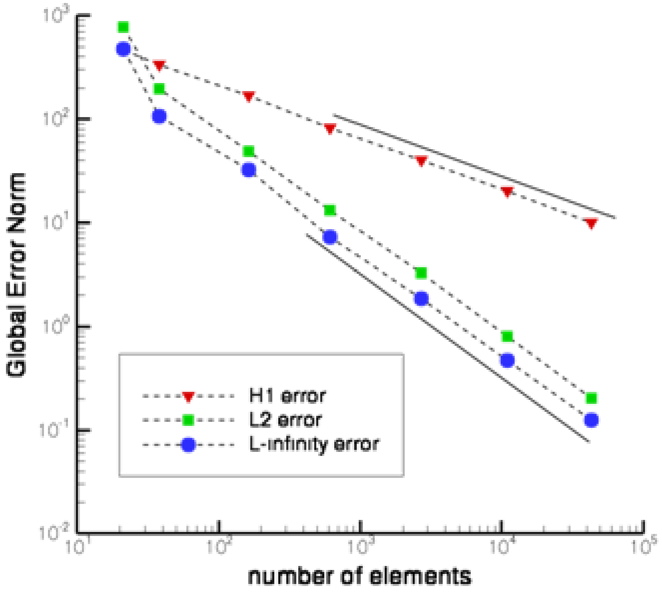
$$u(r) = \begin{cases} u_0 - \frac{r^2}{4\,k_1} Q, & 0 \le r \le r_1, \\ u_3 + \ln(r/r_3)\,\frac{(u_2 - u_3)}{\ln r_2/r_3}, & r_2 \le r \le r_3. \end{cases}$$

Verification for Tri3 Elements

- For 2D problems, Calore uses linear (tri3/quad4) or quadratic (tri6/quad9) elements; Chaparral (enclosure radiation solver) always uses piecewise constant elements.
- This results in an O(*h*) error in the radiative flux in Calore.



coarse Tri3 mesh

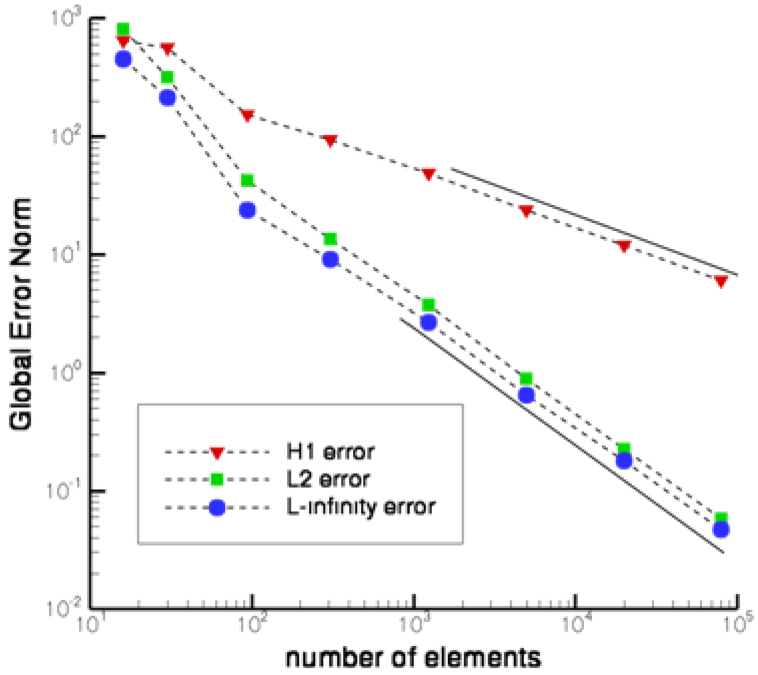


error rates for Tri3 meshes

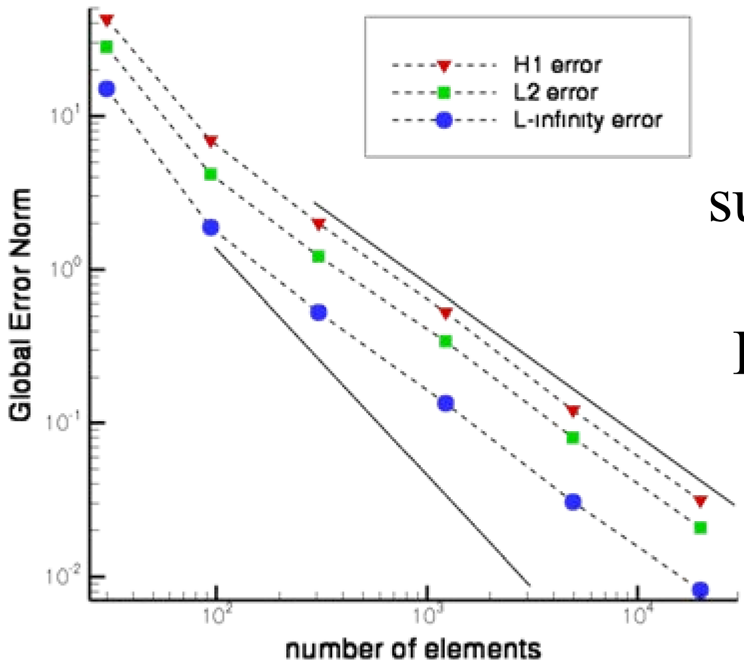
Optimal rates for all norms

Verification for Quad4/Quad9 Elements

- For the linear Quad4 element, all rates are optimal.
- For the quadratic Quad9 element, the H^1 error is optimal $O(h^2)$, but the L^2 and L^∞ rates are limited to $O(h^2)$.



error rates for Quad4 meshes



error rates for Quad9 meshes

suboptimal
rates for
L2, L-inf

Conclusions

- Coda, a shared code-base for
  - Mesh refinement parallel verification toolkit
- Code Verification
  - Compare with simple analytical solutions (no infinite series!)
  - Automat your order verification test suite
  - Report a test metric that targets specific problem domains
  - Standard global norms with sufficient quadrature
- Solution Verification
  - Compute on sequences of meshes
  - Comparison with overkill solutions, or imposed manufactured solution on same domain
  - Know when regularity assumptions apply for your PDE