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Verification of the *Calore* Thermal Analysis Code

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

Calore Thermal Analysis Code

- *Calore* is general purpose transient 3-D finite element code that models
  - Anisotropic heat conduction
  - Capacitance or energy storage
  - Energy source (may be driven by chemical kinetics)
  - Enclosure radiation with non participating medium

Verification Before Validation

- Code Verification-process of insuring that the implemented model equations are solved correctly
  - Assure expected convergence rates ("Bug" check)
  - Study/quantify discretization errors relevant for the code users
- Verification will primarily rely on analytical solutions (both classical and manufactured)
- Both local and global error norms will be considered

Code Verification Coverage Test Suite

- All paths through code must be tested; this requires consultation with code authors
- It is not necessary to test all combinations of all options; this would be an insurmountable task
  - This assumes that element level conduction routines can be tested with or without capacitance
- Focus will be on testing various terms in PDE
  - Conduction, Capacitance and Source
- Boundary condition types
  - Specified temperature, specified flux, convection, far field radiation, and enclosure radiation
- Properly chosen verification problems can also be used as code confirmation problems

Analytical Solution Techniques

- **Classical methods (Separation of Variables, Green's functions, …)**
  - **Funded work at MSU on development of software to evaluate Green's function solution in parallelepiped**
  - **Boundary conditions must be uniform on six faces but can have any combination of specified flux, specified temperature, and convection (initial version with non-uniform/time dependence complete)**
  - **Software potentially contains thousands of independent analytical solutions**
  - **Solution for both Temperature and Heat Flux**
  - **Accuracy demonstrated to be (at least) 8 significant figures**
  - **Internal verification of analytical solution**
  - **Combined with a transformation to address nonlinear problems**

Analytical Solution Techniques (con't)

- **Manufactured solutions**
  - **Substitute analytical solution into energy equation with source term**
  - **Solve for source term consistent with analytical solution and boundary/initial conditions**
  - **Source term may be complex analytical function**
  - **Determine boundary/initial conditions directly from proposed analytical solution**
  - **Implement *calore* user defined source subroutine**
  - **Usually requires user defined subroutines for BC's/IC's**

Global Error Norms

- *Calore* uses Linear Galerkin FEM
- Theoretical error (linear elements)

$$\|e\|_s \equiv \left\|T - T^{Num}\right\|_s \leq Ch^{\mu} \|T\|_r \qquad 0 \leq s \leq m$$

  - μ = min(2-s,r-s)
  - s – highest derivative in the norm
  - m=1 – C^0 elements
- Assuming integrable 2nd derivative for the analytical solution $(r \geq 2)$

$$\|e\|_0 \leq Ch^2 \|T\|_2 = C'h^2 \qquad \|e\|_\infty \leq Ch^2 |\log h| \|T\|_{k+1,\infty}$$

$$\|e\|_1 \leq Ch^1 \|T\|_2 = C'h^1$$

Calore has the capability to calculate all three norms given a user provided analytical solution

Engineering Error Norms

- **Engineering analysts prefer maximum error (at a given location)**
- **Theory not as well developed but useful computational results are being produced**

$$e = \left| T(\mathbf{x}_e, t) - T^{Num}(\mathbf{x}_e, t) \right|$$

$$\mathbf{x}_e - \text{location of interest}$$

- **All verification problems presented will have engineering error norm results; some also have global error norm results**

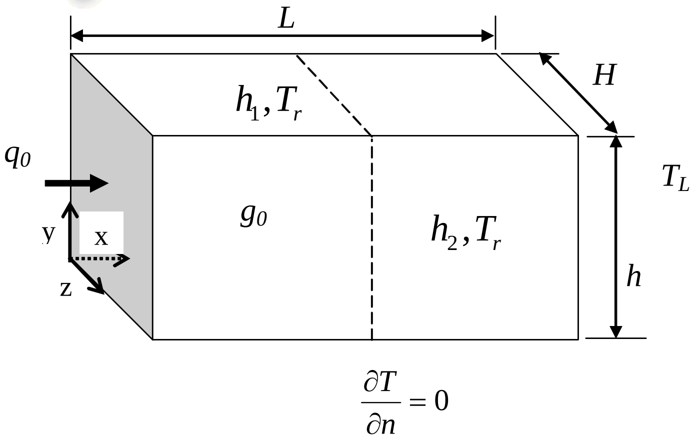
General Description of Verification Problems

- A recurring theme at Sandia is "weapon in a fire"
- Temperature range for these problems is about 300-1300K
- Verification problem temperature range generally consistent with "weapon in a fire"
- Error norm results could be made dimensionless
- Instead, problems were left dimensional so that results will be useful for both code developers and thermal analysts

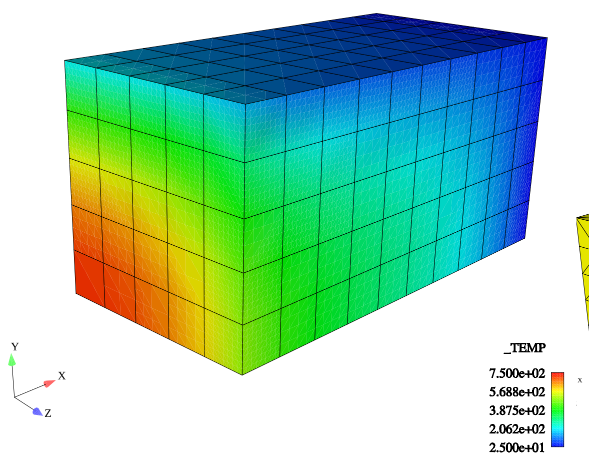
Calore Verification Suite

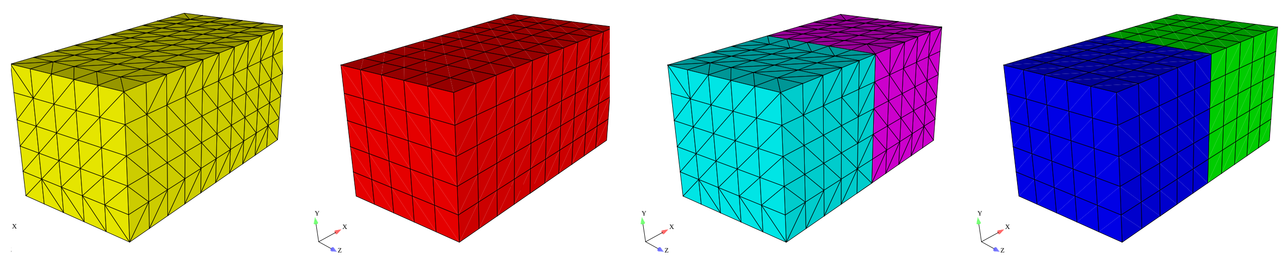
Model Eqn	Comments
Geometric	Volume errors in Cyl/Sph region
Conduction	SS Linear, 1D Cyl/Sph, T-BCs SS Linear, 1D Cyl, Vol Src, T-BCs SS Linear, 2D Rect, Vol Src, (T, q, h) BCs SS Linear, 3D Rect, Vol Src, (T, q, h) BCs, Contact, Adaptivity SS Linear, 2D Rect, Anisotropic, user Vol Src., T-BCs Trans Linear, 1D Rect, q-BCs Trans Nonlinear, 1D Rect, *k(T),* user q-BCs Trans Nonlinear, 1D Rect, *Cp(T),* user q-BCs Trans Nonlinear, 1D Rect, k(T), *Cp(T),* q-BCs
Chemical Kinetics (interfaced with Conduction)	2-reactions, isothermal
Conduction/ Contact Resistance	SS Linear, 1D
Conduction/ Enclosure Radiation	SS Conduction, 1D Concen. Sph Shell, T-BCs

Suite of Verification Cases

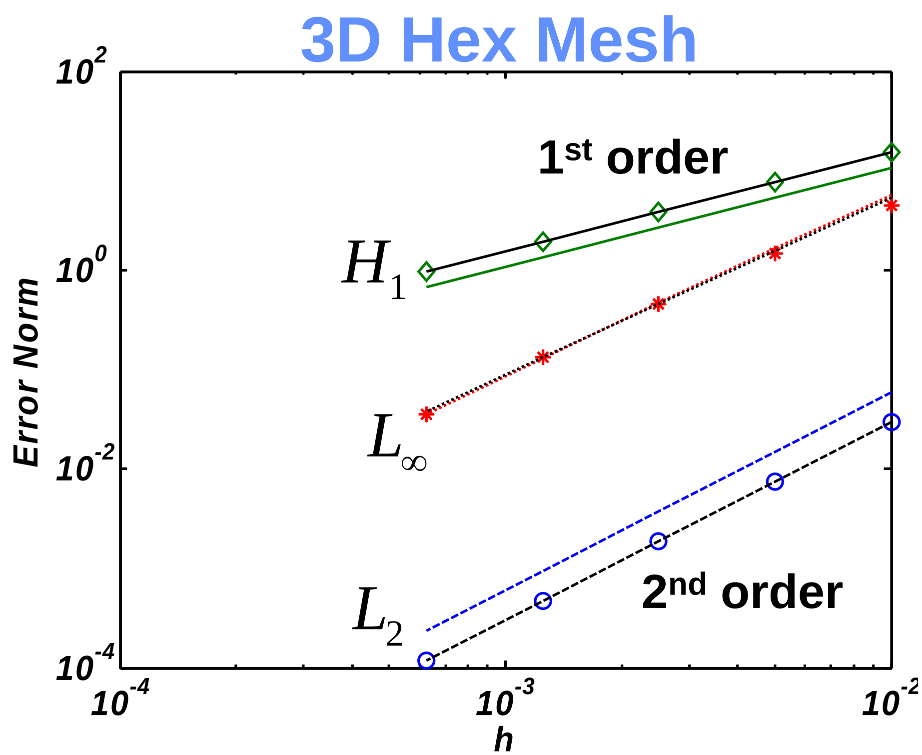


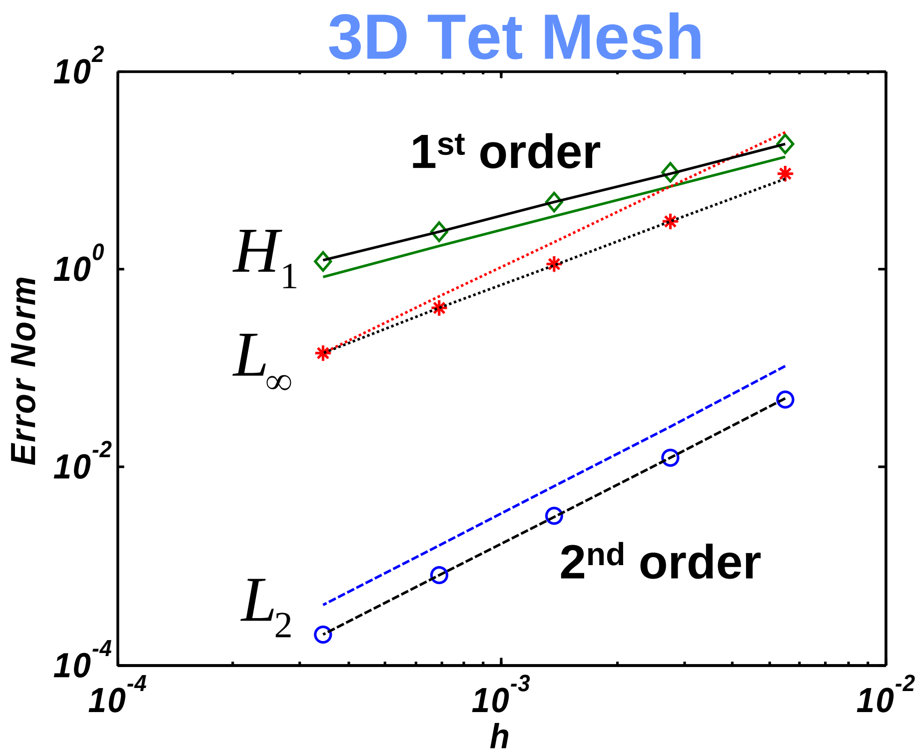
Case	PDE		Mesh		Contact		Refine	
	Steady	Trans	Hex	Tet	None	Tied	Uniform	Adp
1	x		x		x		x	
2	x			x	x		x	
3		x(2nd)	x		x		x	
4		x(2nd)		x	x		x	
5		x(1st)		x	x		x	
6	x		x			x	x	
7	x			x		x	x	
8	x		x			x	x	
9		x(2nd)		x		x	x	
10	x		x		x			x
11	x			x	x			x
12		x(2nd)	x		x			x
13		x(2nd)		x	x			x
14	x		x			x		x





All cases with Tet elements had less than 2nd order convergence for L_∞ Norm





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Convergence rate obtained for L_∞ Norm with Tet elements was less than 2nd order

- Expected convergence (for linear elements)

$$L_\infty \leq h^2 \left|\log(h)\right|$$

- Other norms (L_2 and H_1) exhibit expected convergence for Tet elements
- L_∞ exhibits expected convergence for Hex elements
- Various possible explanations for non optimal convergence with Tet elements have been examined
  - Analytical solution has been checked
  - Calculation of the norm has been independently verified
  - 2D case exhibits same outcome
    - » Tris give less than optimal, Quad give optimal convergence
  - Mesh quality has been investigated (2D case)

Why would the L_∞ Norm not follow expected convergence for Tet mesh while other norms do??

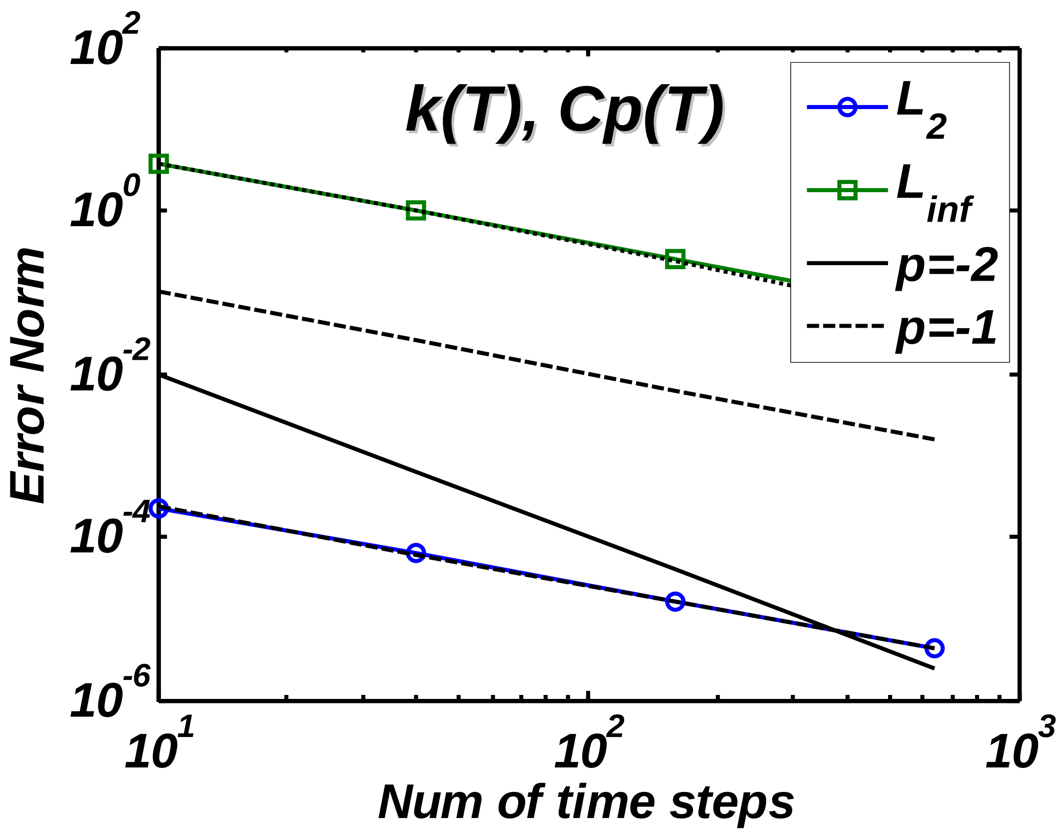
Verification of Nonlinear Transient Heat Conduction

- **Nonlinearity due to temperature dependence of the thermal properties (thermal conductivity, *k*, and specific heat, C_p)**

$$\frac{\partial}{\partial x}\left(k\,\frac{\partial T}{\partial x}\right) = \rho C_p\,\frac{\partial T}{\partial t}$$

- **Suite of Verification problems conducted**
  - *k*-constant, C_p-constant
  - *k(T)*, C_p-constant
  - *k*-constant, $C_p(T)$
  - *k(T)*, $C_p(T)$
- **Temp Depend of properties was linear (range selected to give significant property variation for T variation)**
- **Space and time discretization refined simultaneously**
  - 2nd order time integrator ($\Delta t/h$ =*constant*)
  - 1st order time integrator ($\Delta t/h^2$=*constant*)

Implicit (1^{st} order) time integrator shows expected convergence rates for all problems



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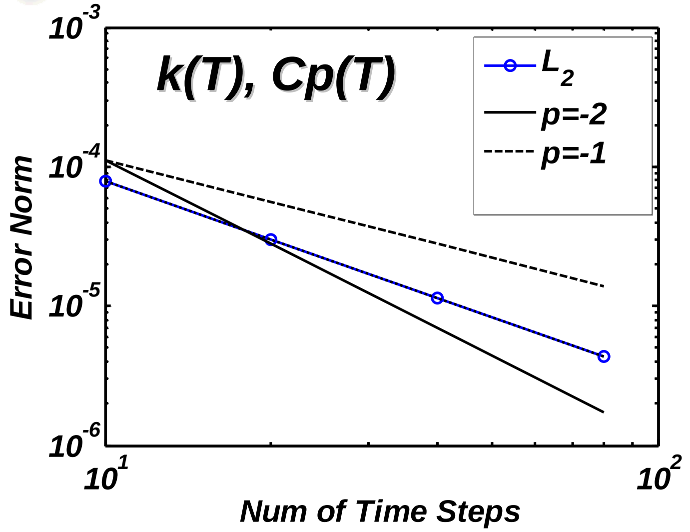
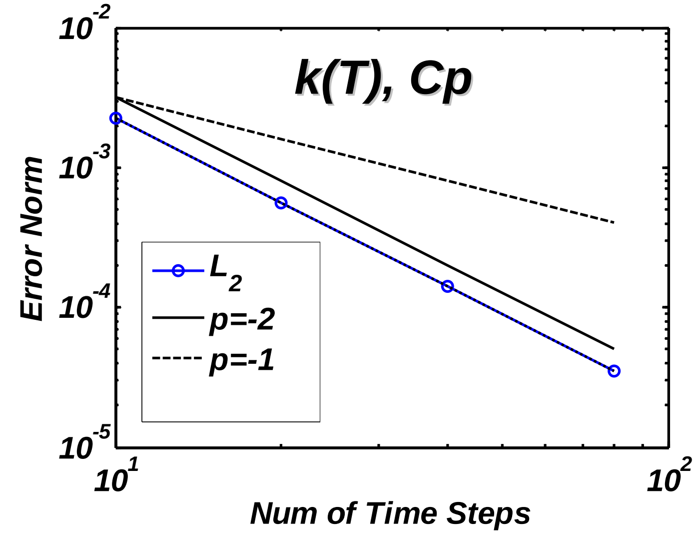
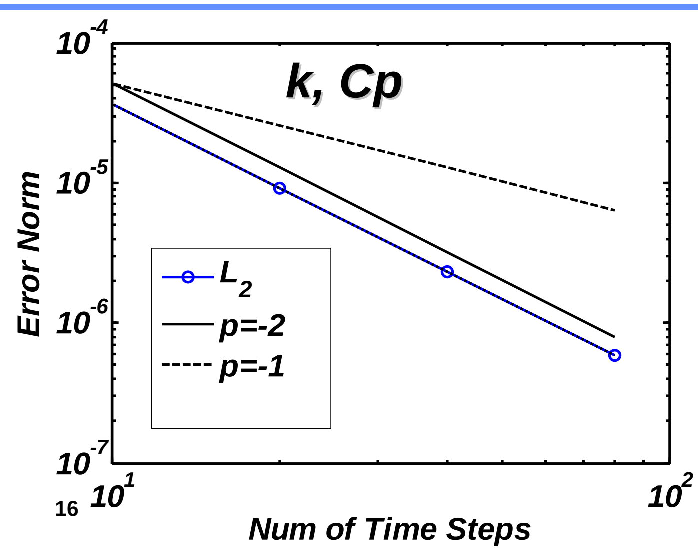
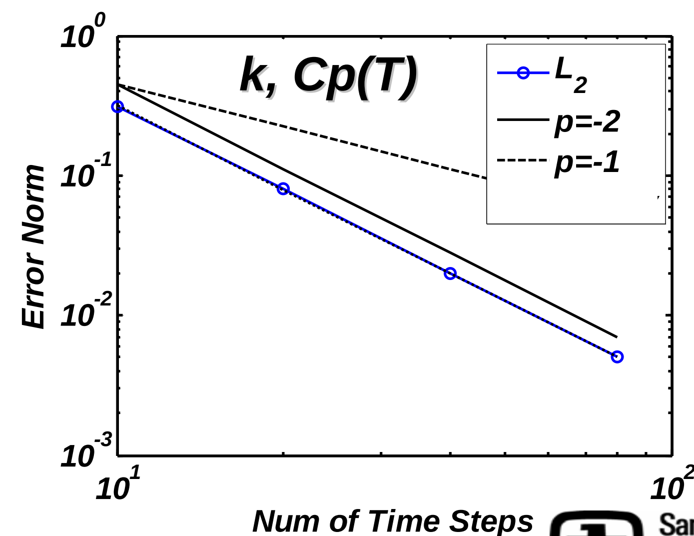
Trapezoid (2nd order) time integrator shows unexpected convergence rates when both properties temp depend









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Summary of Verification for Nonlinear Heat Conduction

- **Implicit time integrator is 1st order for all problems studied**
- **Fully nonlinear problem (both *k(T),Cp(T)*) has less than 2nd order convergence (p=1.4)**
- **Linear and partially nonlinear problems (*k(T) or Cp(T)*) demonstrate 2nd order convergence**
- **Process has been checked to insure accuracy of analytical solution and norm calculation**
- **Fully nonlinear problem has been run in two other codes – one gives 2nd order, one doesn't**
- **Additional problem has shown 2nd order convergence for the Trapezoid integrator**

Should we expect 2nd order convergence for the Trapezoid time integrator for the Fully nonlinear problems???

Summary of Calore Verification

- Order of convergence is a sensitive metric for code verification
  - L_∞ has shown to be the most sensitive
- When expected convergence rates are not obtained all parts of the process must be checked
  - Analytical solution
  - Norm calculation
  - Basis for the expected convergence (theory)

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