SANDIA REPORT

SAND2019-12297

Printed October 9, 2019

Sandia National Laboratories

Sierra/Aria 4.54 Verification Manual

Brian R. Carnes

Prepared by
Sandia National Laboratories
Albuquerque, New Mexico 87185
Livermore, California 94550

Issued by Sandia National Laboratories, operated for the United States Department of Energy by National Technology & Engineering Solutions of Sandia, LLC.

ABSTRACT

Presented in this document is a portion of the tests that exist in the Sierra Thermal/Fluids verification test suite. Each of these tests is run nightly with the Sierra/TF code suite and the results of the test checked under mesh refinement against the correct analytic result. For each of the tests presented in this document the test setup, derivation of the analytic solution, and comparison of the code results to the analytic solution is provided. This document can be used to confirm that a given code capability is verified or referenced as a compilation of example problems.

ACKNOWLEDGMENTS

This document's authors acknowledge the help of the Sierra/TF team in creating and maintaining these verification tests.

CONTENTS

LIST OF FIGURES

LIST OF TABLES

1. INTRODUCTION

The Sierra/TF Verification Manual is divided into chapters based on related capabilities. Each section of a chapter represents a distinct verification test. Some problems that are not yet fully documented are listed at the end of each chapter.

All of these verification tests are run nightly by the development team to continually verify code accuracy under mesh refinement. The graphics and charts in this document are automatically generated by the nightly test runs.

The test files for these problems may be found in the Sierra regression test repository. Most are in the sub-directory called "verification."

```
aria_rtest/verification
```

All tests are assigned the keyword "verification". Those that appear in this document also have the keyword "self-documenting".

For each test, the approximate finite element solution T_h is compared to the exact solution T using several global norms, and in some cases using response quantities of interest. This is repeated over a series of uniformly refined meshes (not necessarily nested) with mesh sizes $\{h_i\}$, giving a sequence of errors $\{E_i\}$. For each pair of meshes, a convergence rate is estimated using the formula

$$r_i \equiv \log(E_i/E_{i-1})/\log(h_i/h_{i-1}). \tag{1.1}$$

The convergence of r_i to the expected rate is monitored as the mesh is refined. A test passes if all of the estimated convergence rates on the finest pair of meshes are within a given tolerance of the expected rates.

2. BASIC THERMAL TESTS

2.1. STEADY HEAT CONDUCTION: HEX8 MESHES

This problem tests basic steady state heat conduction in a 3D domain. The geometry consists of a unit cube. A variety of different source terms and boundary conditions are simultaneously applied. The exact solution is a manufactured solution.

2.1.1. Features Tested

Basic heat conduction on Hex8 meshes; dirichlet, heat flux, and convective flux boundary conditions; constant source terms; heat flux and source term from Encore user subroutines.

2.1.2. Boundary Conditions

At surfaces 4 and 6, the temperature is prescribed as a constant value. On surfaces 3 and 5, a heat flux condition is prescribed using a sum of a constant heat flux and a heat flux from an Encore function (user subroutine). On surfaces 1 and 2, heat flux condition is prescribed using a sum of a convective flux boundary condition (with constant flux and convective coefficient) and a heat flux from an Encore function (user subroutine). Within the domain a source term is prescribed using a sum of a constant source and an Encore function (user subroutine).

2.1.3. Material Parameters

The values of density, thermal conductivity, and specific heat are all constant, equal to one in both blocks.

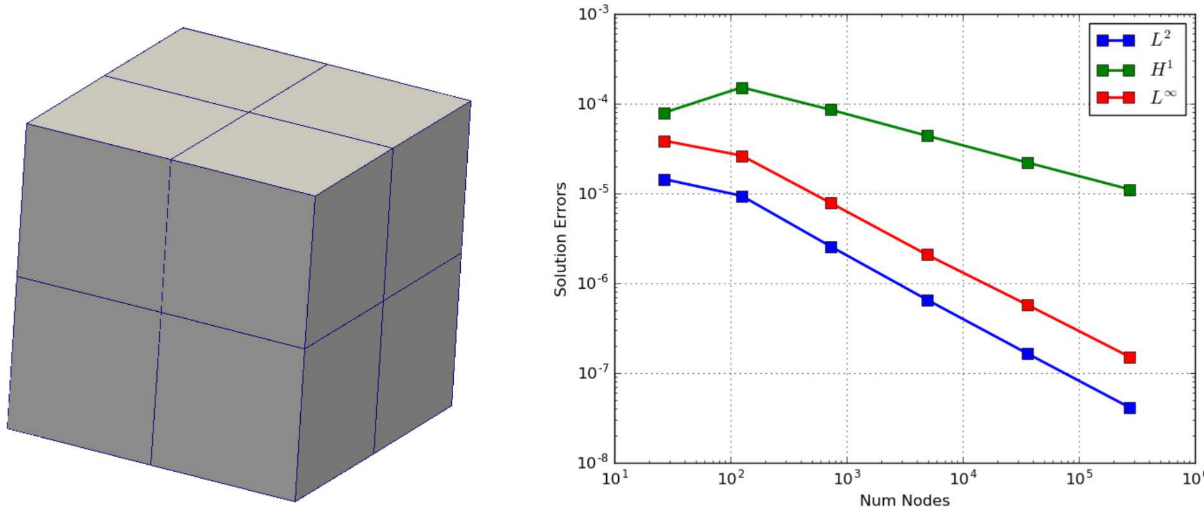
2.1.4. Verification of Solution

A manufactured solution is chosen as

$$T(x, y, z) = 1 + (x - x^2)^2(y - y^2)^2(z - z^2)^2.$$

The source and heat flux user subroutines are chosen so that the solution satisfies the heat equation with the correct boundary conditions.

For each mesh, the errors in the temperature solution are computed in the L^2, L^∞ and H^1 norms. The test passes, only if the observed rates of convergence in these norms are 2, 2, and 1, respectively (within a tolerance).



Coarse Mesh Error Norms

Figure 2.1-1.. Steady Heat Conduction: Hex8 Meshes

Table 2.1-1.. Steady Heat Conduction: Convergence Rates for Hex8 Meshes

Num Dofs	L^2	H^1	L^∞
125	0.83	-1.27	0.74
729	2.20	0.98	2.07
4913	2.15	1.05	2.08
35940	2.08	1.03	1.94
274600	2.05	1.02	1.97

For input decks see Appendix 12.1.1.

2.2. STEADY HEAT CONDUCTION: HEX20 MESHES

This problem tests basic steady state heat conduction in a 3D domain. The geometry consists of a unit cube. A variety of different source terms and boundary conditions are simultaneously applied. The exact solution is a manufactured solution.

2.2.1. Features Tested

Basic heat conduction on Hex20 meshes; dirichlet, heat flux, and convective flux boundary conditions; constant source terms; heat flux and source term from Encore user subroutines.

2.2.2. Boundary Conditions

At surfaces 4 and 6, the temperature is prescribed as a constant value. On surfaces 3 and 5, a heat flux condition is prescribed using a sum of a constant heat flux and a heat flux from an Encore function (user subroutine). On surfaces 1 and 2, heat flux condition is prescribed using a sum of a convective flux boundary condition (with constant flux and convective coefficient) and a heat flux from an Encore function (user subroutine). Within the domain a source term is prescribed using a sum of a constant source and an Encore function (user subroutine).

2.2.3. Material Parameters

The values of density, thermal conductivity, and specific heat are all constant, equal to one in both blocks.

2.2.4. Verification of Solution

A manufactured solution is chosen as

$$T(x, y, z) = 1 + (x - x^2)^2(y - y^2)^2(z - z^2)^2.$$

The source and heat flux user subroutines are chosen so that the solution satisfies the heat equation with the correct boundary conditions.

For each mesh, the errors in the temperature solution are computed in the L^2, L^∞ and H^1 norms. The test passes, only if the observed rates of convergence in these norms are 2, 2, and 1, respectively (within a tolerance).

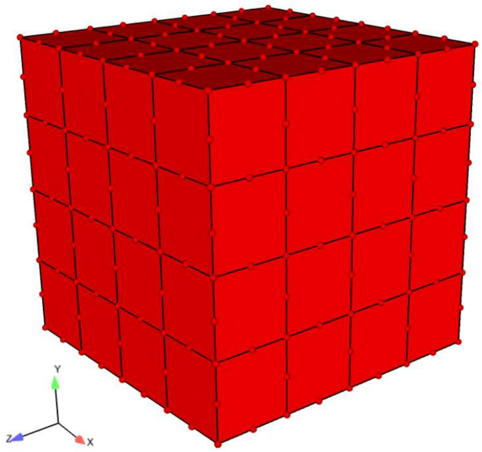
Table 2.2-1.. Steady Heat Conduction: Convergence Rates for Hex20 Meshes

Num Dofs	L^2	H^1	L^∞
2673	3.39	2.32	3.52
18780	3.19	2.15	3.13
60620	3.11	2.08	3.04
140500	3.08	2.06	3.01

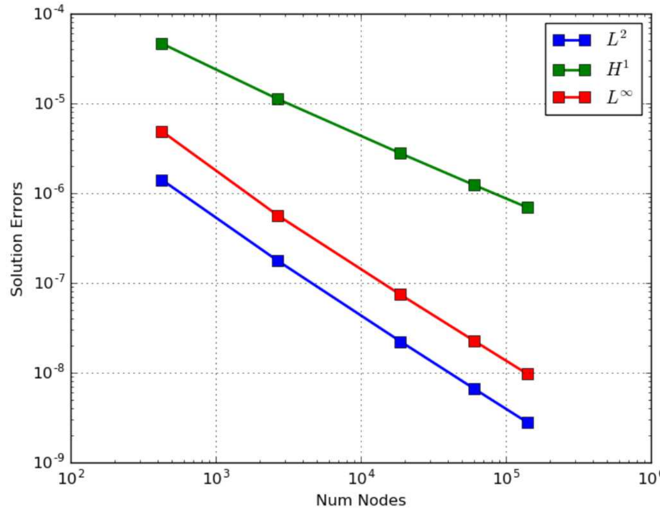
For input decks see Appendix 12.1.2.

2.3. STEADY HEAT CONDUCTION: HEX27 MESHES

This problem tests basic steady state heat conduction in a 3D domain. The geometry consists of a unit cube. A variety of different source terms and boundary conditions are simultaneously applied. The exact solution is a manufactured solution.



Coarse Mesh



Error Norms

Figure 2.2-1.. Steady Heat Conduction: Hex20 Meshes

2.3.1. Features Tested

Basic heat conduction on Hex27 meshes; dirichlet, heat flux, and convective flux boundary conditions; constant source terms; heat flux and source term from Encore user subroutines.

2.3.2. Boundary Conditions

At surfaces 4 and 6, the temperature is prescribed as a constant value. On surfaces 3 and 5, a heat flux condition is prescribed using a sum of a constant heat flux and a heat flux from an Encore function (user subroutine). On surfaces 1 and 2, heat flux condition is prescribed using a sum of a convective flux boundary condition (with constant flux and convective coefficient) and a heat flux from an Encore function (user subroutine). Within the domain a source term is prescribed using a sum of a constant source and an Encore function (user subroutine).

2.3.3. Material Parameters

The values of density, thermal conductivity, and specific heat are all constant, equal to one in both blocks.

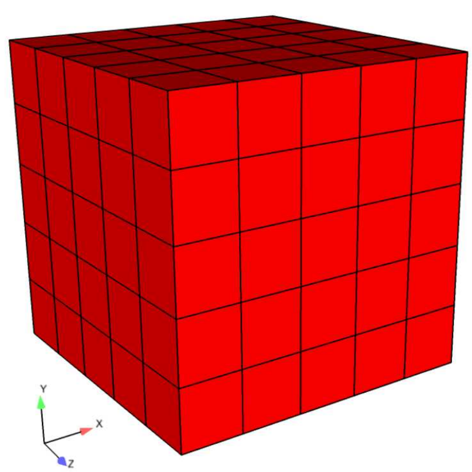
2.3.4. Verification of Solution

A manufactured solution is chosen as

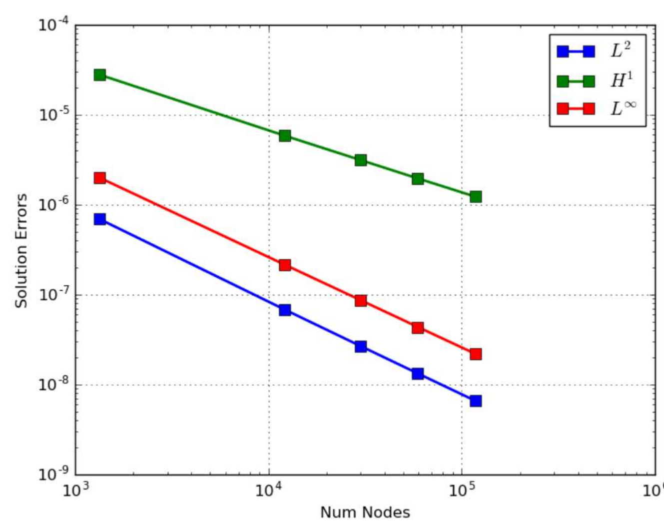
$$T(x, y, z) = 1 + (x - x^2)^2(y - y^2)^2(z - z^2)^2.$$

The source and heat flux user subroutines are chosen so that the solution satisfies the heat equation with the correct boundary conditions.

For each mesh, the errors in the temperature solution are computed in the L^2, L^∞ and H^1 norms. The test passes, only if the observed rates of convergence in these norms are 2, 2, and 1, respectively (within a tolerance).



Coarse Mesh



Error Norms

Figure 2.3-1.. Steady Heat Conduction: Hex27 Meshes

Table 2.3-1.. Steady Heat Conduction: Convergence Rates for Hex27 Meshes

Num Dofs	L^2	H^1	L^∞
12170	3.15	2.12	3.03
29790	3.10	2.07	3.01
59320	3.08	2.06	3.02
117600	3.07	2.05	3.01

For input decks see Appendix 12.1.3.

2.4. STEADY HEAT CONDUCTION: TET4 MESHES

This problem is identical to the one in Section 2.1 except that unstructured Tet4 meshes are used instead. The meshes are obtained from Cubit.

2.4.1. Features Tested

Basic heat conduction on Tet4 meshes; dirichlet, heat flux, and convective flux boundary conditions; constant source terms; heat flux and source term from Encore user subroutines.

2.4.2. Boundary Conditions

Same as in Section 2.1.

2.4.3. Material Parameters

The values of density, thermal conductivity, and specific heat are all constant, equal to one in both blocks.

2.4.4. Verification of Solution

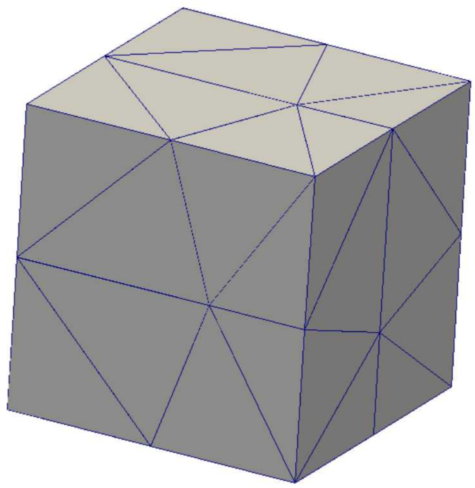
Same as in Section 2.1.

Unlike the Hex8 case, we have observed in many cases, and in this test, that the convergence rate for the temperature in the L^∞ norm is somewhat less than 2, in this case about 1.9. The exact reason for this behavior is unclear.

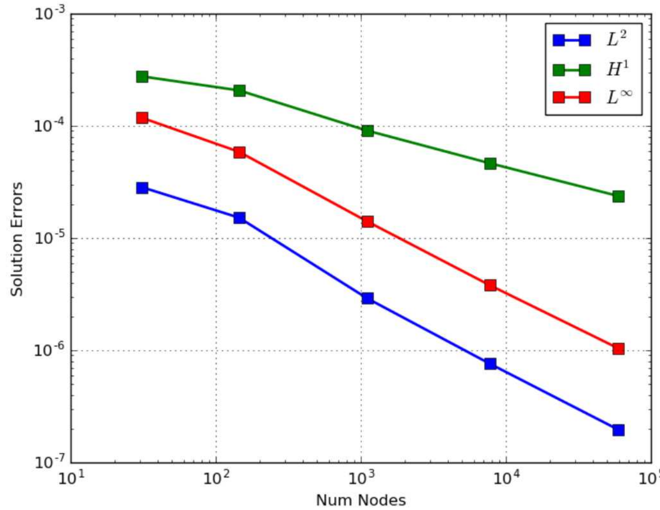
Table 2.4-1.. Steady Heat Conduction: Convergence Rates for Tet4 Meshes

Num Dofs	L^2	H^1	L^∞
145	1.21	0.56	1.36
1104	2.45	1.22	2.10
7725	2.07	1.03	2.02
59640	1.99	0.99	1.91

For input decks see Appendix 12.1.4.



Coarse Mesh



Error Norms

Figure 2.4-1.. Steady Heat Conduction: Tet4 Meshes

2.5. STEADY HEAT CONDUCTION: TET4TET10 MESHES

This problem is identical to the one in Section 2.1 with the exception of constant thermal conductivity and use of unstructured Tet10 meshes. The meshes are obtained from Cubit.

2.5.1. Features Tested

Basic heat conduction with Tet4 solution on Tet10 meshes; dirichlet, heat flux, and convective flux boundary conditions; constant source terms; heat flux and source term from Encore user subroutines.

2.5.2. Boundary Conditions

Same as in Section 2.1.

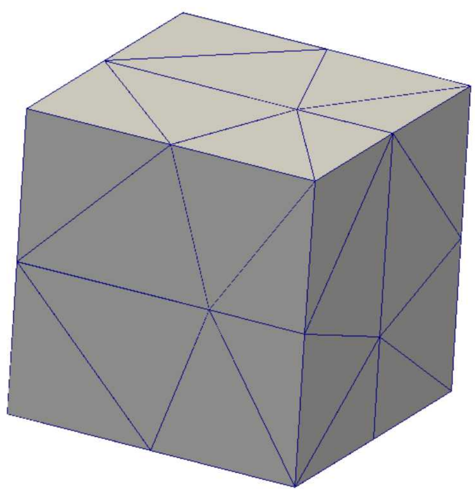
2.5.3. Material Parameters

The values of density, thermal conductivity, and specific heat are all constant, equal to one in both blocks.

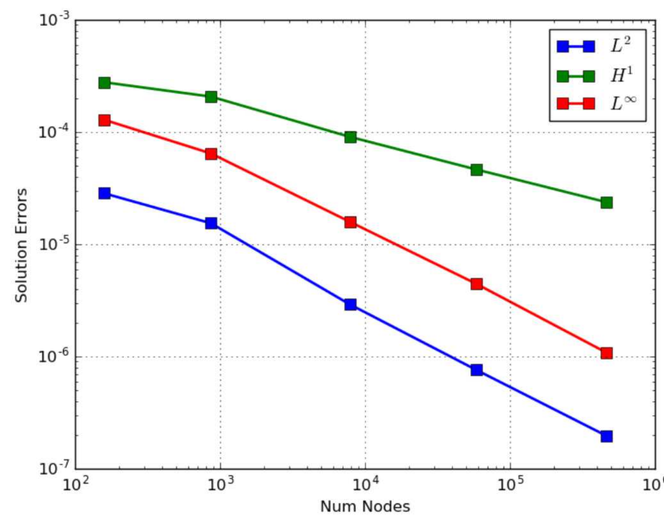
2.5.4. Verification of Solution

Same as in Section 2.1.

Unlike the Hex8 case, we have observed in many cases, and in this test, that the convergence rate for the temperature in the L^∞ norm is somewhat less than 2, in this case about 1.9. The exact reason for this behavior is unclear.



Coarse Mesh



Error Norms

Figure 2.5-1.. Steady Heat Conduction: Tet4 Solutions on Tet10 Meshes

Table 2.5-1.. Steady Heat Conduction: Convergence Rates for Tet4Tet10 Meshes

Num Dofs	L^2	H^1	L^∞
865	1.09	0.52	1.22
7831	2.26	1.12	1.90
58210	2.01	1.00	1.90
464400	1.96	0.98	2.05

For input decks see Appendix 12.1.5.

2.6. STEADY HEAT CONDUCTION: TET10 MESHES

This problem is identical to the one in Section 2.1 except that unstructured Tet10 meshes are used instead. The meshes are obtained from Cubit.

2.6.1. Features Tested

Basic heat conduction on Tet10 meshes; dirichlet, heat flux, and convective flux boundary conditions; constant source terms; heat flux and source term from Encore user subroutines.

2.6.2. Boundary Conditions

Same as in Section 2.1.

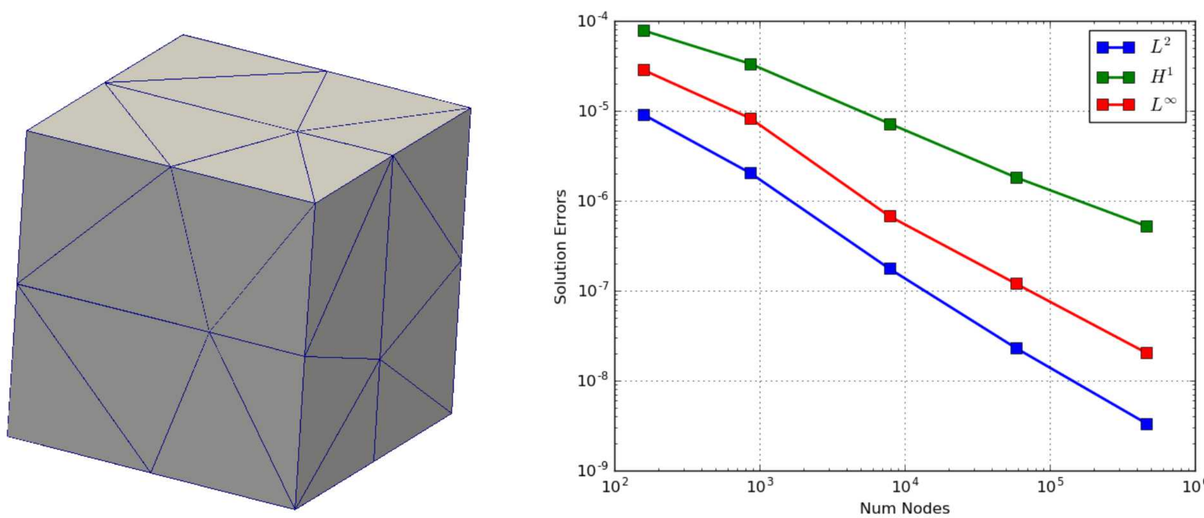
2.6.3. Material Parameters

The values of density, thermal conductivity, and specific heat are all constant, equal to one in both blocks.

2.6.4. Verification of Solution

Same as in Section 2.1.

Unlike the Hex8 case, we have observed in many cases, and in this test, that the convergence rate for the temperature in the L^∞ norm is somewhat less than 3, in this case about 2.7. The exact reason for this behavior is unclear.



Coarse Mesh | Error Norms

Figure 2.6-1.. Steady Heat Conduction: Tet10 Meshes

For input decks see Appendix 12.1.6.

Table 2.6-1.. Steady Heat Conduction: Convergence Rates for Tet10 Meshes

Num Dofs	L^2	H^1	L^∞
865	2.65	1.51	2.19
7831	3.32	2.08	3.41
58210	3.04	2.07	2.58
464400	2.80	1.80	2.57

2.7. TRANSIENT HEAT CONDUCTION: HEX8 MESHES

This problem tests basic transient heat conduction in a 3D domain. The geometry consists of a unit cube.

2.7.1. Features Tested

Basic transient heat conduction on Hex8 meshes; dirichlet, heat flux, and convective flux boundary conditions; constant source terms; heat flux and source term from Encore user subroutines.

2.7.2. Boundary Conditions

At surfaces 4 and 6, the temperature is prescribed as a constant value. On surfaces 3 and 5, a heat flux condition is prescribed using a sum of a constant heat flux and a heat flux from an Encore function (user subroutine). On surfaces 1 and 2, heat flux condition is prescribed using a sum of a convective flux boundary condition (with constant flux and convective coefficient) and a heat flux from an Encore function (user subroutine). Within the domain a source term is prescribed using a sum of a constant source and an Encore function (user subroutine).

2.7.3. Material Parameters

The values of density, thermal conductivity, and specific heat are all constant, equal to one in both blocks.

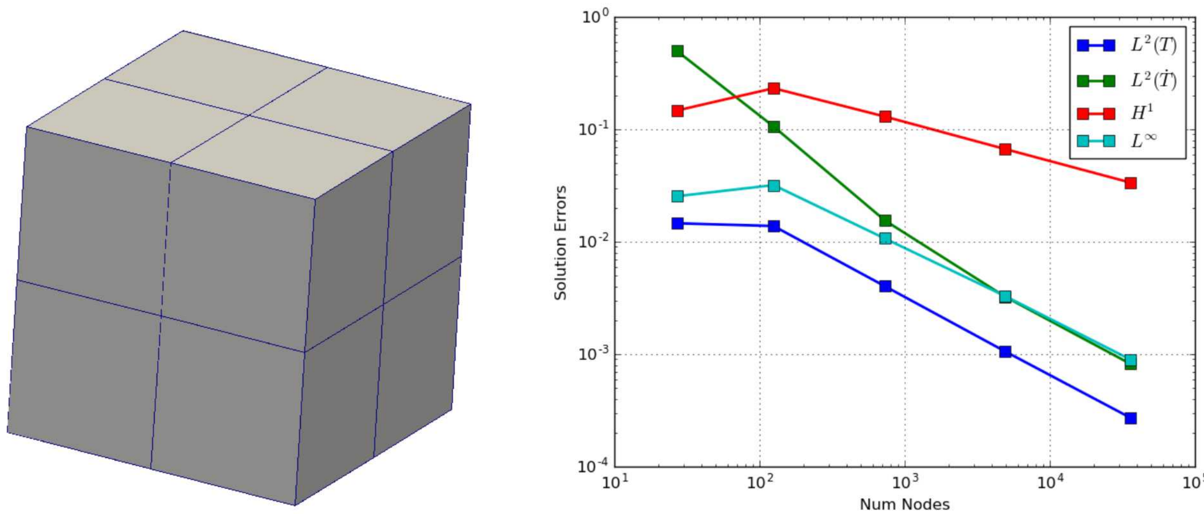
2.7.4. Verification of Solution

A manufactured solution is chosen as

$$T(x, y, z, t) = (x - x^2)^2\,(y - y^2)^2\,(z - z^2)^2 m(t) + 1,$$
$$m(t) = 10^4\,(1 - \exp(-t) + t\,\exp(-(t-1)^2))$$

The source and heat flux user subroutines are chosen so that the solution satisfies the heat equation with the correct boundary conditions.

For each mesh, the errors in the temperature solution at final time are computed in the L^2 norm of T and $\dot{T}$, L^∞ and H^1 norms. The test passes, only if the observed rates of convergence in these norms are 2, 2, 2 and 1, respectively (within a tolerance).



Coarse Mesh Error Norms

Figure 2.7-1.. Transient Heat Conduction: Hex8 Meshes

Table 2.7-1.. Transient Heat Conduction: Convergence Rates for Hex8 Meshes

Num Dofs	$L^2(T)$	$L^2(\dot{T})$	H^1	L^∞
125	0.12	3.02	-0.89	-0.45
729	2.09	3.28	0.98	1.85
4913	2.09	2.46	1.05	1.86
35940	2.06	2.07	1.04	1.96

For input decks see Appendix 12.1.7.

2.8. TRANSIENT HEAT CONDUCTION: TET4 MESHES

This problem tests basic transient heat conduction in a 3D domain as in Section 2.7. The geometry consists of a unit cube and a single bulk fluid element.

2.8.1. Features Tested

Basic transient heat conduction on Tet4 meshes; dirichlet, heat flux, and convective flux boundary conditions; constant source terms; bulk fluid element; heat flux and source term from Encore user subroutines.

2.8.2. Boundary Conditions

Identical to Section 2.7 except one convective flux boundary condition is now connected to a bulk fluid element.

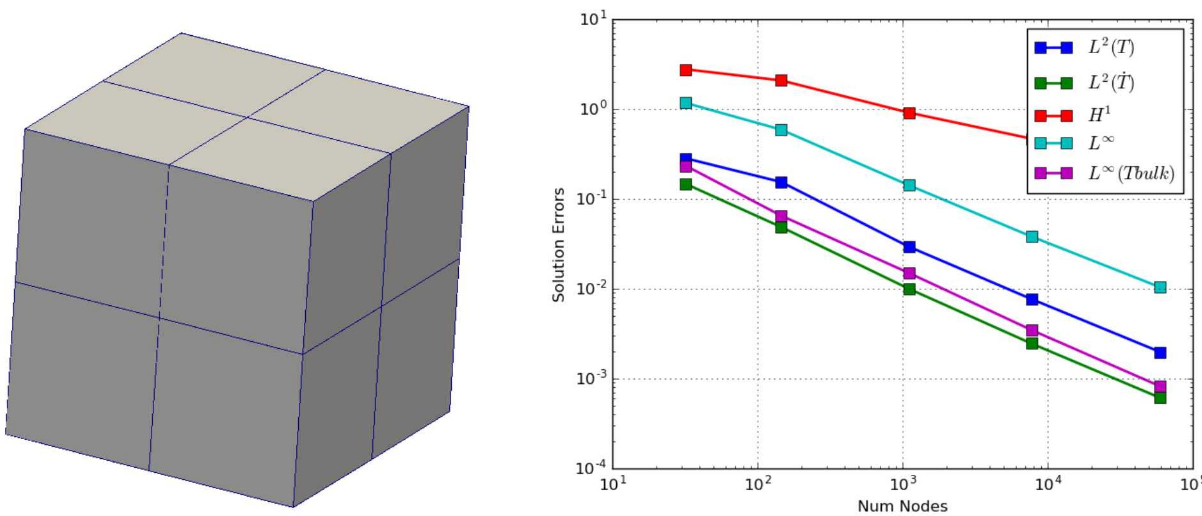
2.8.3. Material Parameters

The values of density, thermal conductivity, and specific heat are all constant, equal to one in both blocks.

2.8.4. Verification of Solution

A manufactured solution is chosen as in Section 2.7.

For each mesh, the errors in the temperature solution at final time are computed in the L^2 norm of T and $\dot{T}$, L^∞ and H^1 norms. As in Section 2.4, we see convergence rates for L^∞ that are slightly less than 2.



Coarse Mesh Error Norms

Figure 2.8-1.. Transient Heat Conduction: Tet4 Meshes

Table 2.8-1.. Transient Heat Conduction: Convergence Rates for Tet4 Meshes

Num Dofs	$L^2(T)$	$L^2(\dot{T})$	H^1	L^∞	$L^\infty(Tbulk)$
146	1.20	2.19	0.57	1.36	2.53
1105	2.45	2.34	1.22	2.11	2.17
7726	2.07	2.16	1.03	2.02	2.26
59640	1.99	2.04	0.99	1.91	2.12

For input decks see Appendix 12.1.8.

2.9. TRANSIENT HEAT CONDUCTION: TET4TET10 MESHES

This problem tests basic transient heat conduction in a 3D domain as in Section 2.8. The geometry consists of a unit cube.

2.9.1. Features Tested

Basic transient heat conduction Tet4 analysis on Tet10 meshes; dirichlet, heat flux, and convective flux boundary conditions; constant source terms; heat flux and source term from Encore user subroutines.

2.9.2. Boundary Conditions

Identical to Section 2.8

2.9.3. Material Parameters

The values of density, thermal conductivity, and specific heat are all constant, equal to one in both blocks.

2.9.4. Verification of Solution

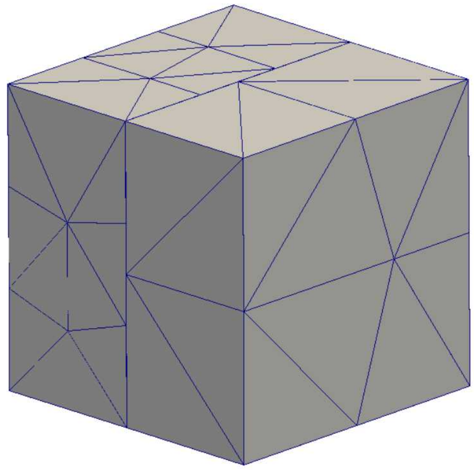
A manufactured solution is chosen as in Section 2.8.

For each mesh, the errors in the temperature solution at final time are computed in the L^2 norm of T and $\dot{T}$, L^∞ and H^1 norms. As in Section 2.8, we see convergence rates for L^∞ that are slightly less than 2.

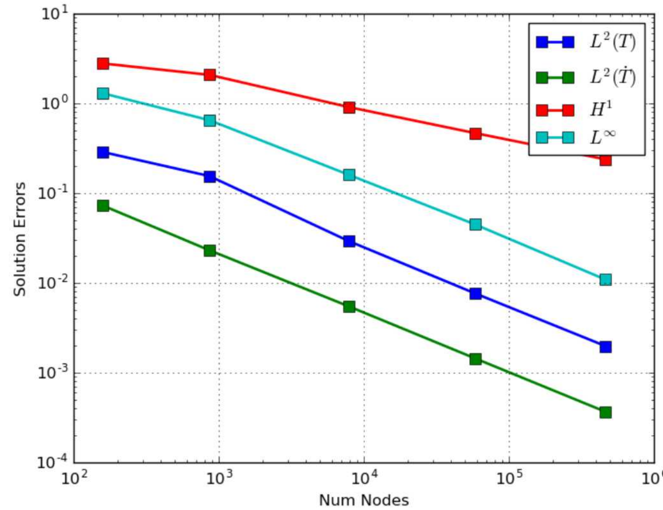
Table 2.9-1.. Transient Heat Conduction: Convergence Rates for Tet4 Solution on Tet10 Meshes

Num Dofs	$L^2(T)$	$L^2(\dot{T})$	H^1	L^∞
865	1.09	2.03	0.52	1.22
7831	2.26	1.95	1.12	1.90
58210	2.01	2.00	1.00	1.90
464400	1.96	1.98	0.98	2.05

For input decks see Appendix 12.1.9.



Coarse Mesh



Error Norms

Figure 2.9-1.. Transient Heat Conduction: Tet4 Solution on Tet10 Meshes

2.10. TRANSIENT HEAT CONDUCTION: TET10 MESHES

This problem tests basic transient heat conduction in a 3D domain as in Section 2.7. The geometry consists of a unit cube.

2.10.1. Features Tested

Basic transient heat conduction on Tet10 meshes; dirichlet, heat flux, and convective flux boundary conditions; constant source terms; heat flux and source term from Encore user subroutines.

2.10.2. Boundary Conditions

Identical to Section 2.7

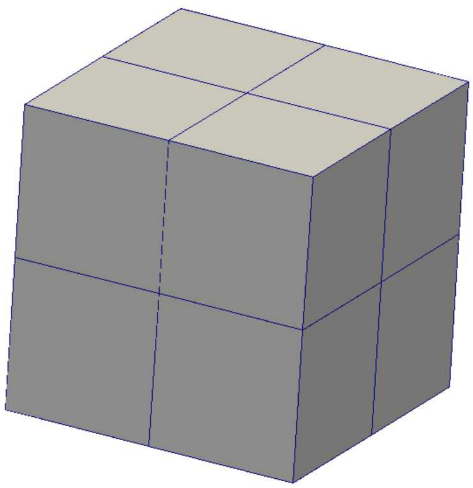
2.10.3. Material Parameters

The values of density, thermal conductivity, and specific heat are all constant, equal to one in both blocks.

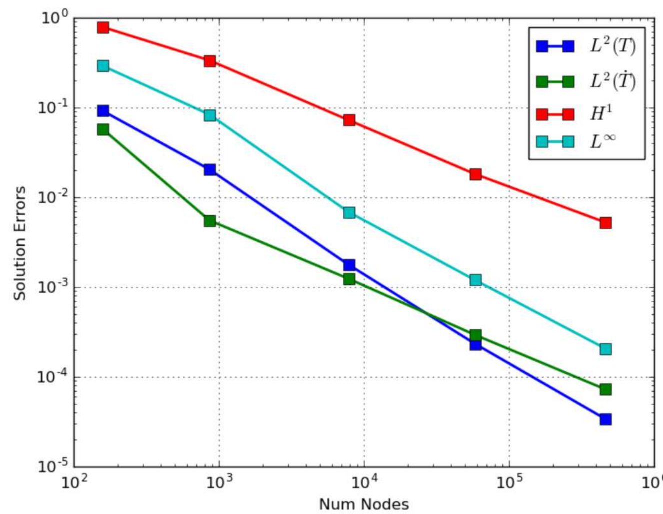
2.10.4. Verification of Solution

A manufactured solution is chosen as in Section 2.7.

For each mesh, the errors in the temperature solution at final time are computed in the L^2 norm of T and $\dot{T}$, L^∞ and H^1 norms. As in Section 2.6, we see convergence rates for L^∞ that are slightly less than 2.



Coarse Mesh



Error Norms

Figure 2.10-1.. Transient Heat Conduction: Tet10 Meshes

Table 2.10-1.. Transient Heat Conduction: Convergence Rates for Tet10 Meshes

Num Dofs	$L^2(T)$	$L^2(\dot{T})$	H^1	L^∞
865	2.66	4.15	1.51	2.21
7831	3.32	2.04	2.08	3.40
58210	3.03	2.15	2.07	2.61
464400	2.79	2.02	1.80	2.55

For input decks see Appendix 12.1.10.

2.11. POSTPROCESS MIN/MAX

2.11.1. Problem Description

This problem tests the min/max postprocessors in Aria.

2.11.2. Features Tested

min max postprocessors

2.11.3. Boundary Conditions

Dirichlet BCs are specified using the exact solution on surfaces 1-4.

A source term is applied within all blocks based on substituting the exact solution into the heat conduction operator.

2.11.4. Material Parameters

The values of density, thermal conductivity, and specific heat are all constant.

2.11.5. Verification of Solution

The manufactured solution is

$$\sin(7x)\sin(8y).$$

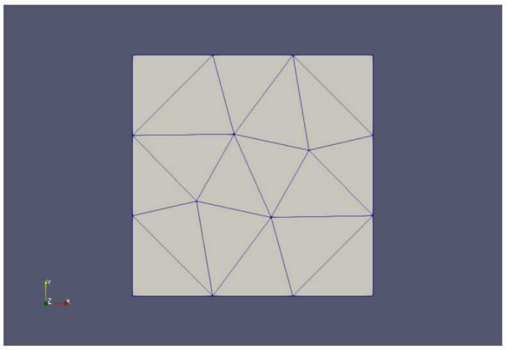
For each uniformly refined mesh, the errors in the temperature solution are computed in the L^2, H^1, and L^∞ norms and for various postprocessors. Additionally, the nodal maximum and minimum values on both block 1 and surface 2 are computed using Encore postprocessors and the convergence of these values is compared as well. Since the maximum and minimums are nodal, the location of the nodes will reflect the max/min values produced for a given mesh. Provided that the mesh is uniformly refined (without smoothing that may shift the nodal locations), every mesh refinement will produce a better result, dependent on how much closer to the maximum/minimum true solution the new nodes are.

Table 2.11-1.. Min Max Postprocess: Convergence Rates

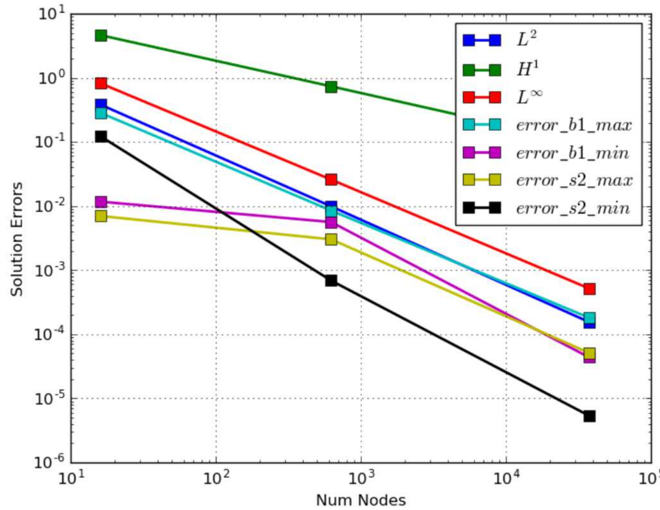
Num Dofs	L^2	H^1	L^∞	$error\_b1\_max$	$error\_b1\_min$	$error\_s2\_max$	$error\_s2\_min$
625	2.00	1.00	1.89	1.92	0.40	0.46	2.83
37249	2.03	1.02	1.91	1.88	2.37	1.99	2.37

2.12. ADAPTIVITY

This problem is identical to the one in Section 2.4 except that we use adaptive mesh refinement to refine from a coarse base mesh obtained from Cubit.



Coarse Mesh



Error Norms

Figure 2.11-1.. Min Max Postprocess

2.12.1. Features Tested

Basic heat conduction on Tet4 meshes; dirichlet, heat flux, and convective flux boundary conditions; constant source terms; heat flux and source term from Encore user subroutines; adaptive mesh refinement; local error indicators based on jump in heat flux.

2.12.2. Boundary Conditions

Same as in Section 2.1.

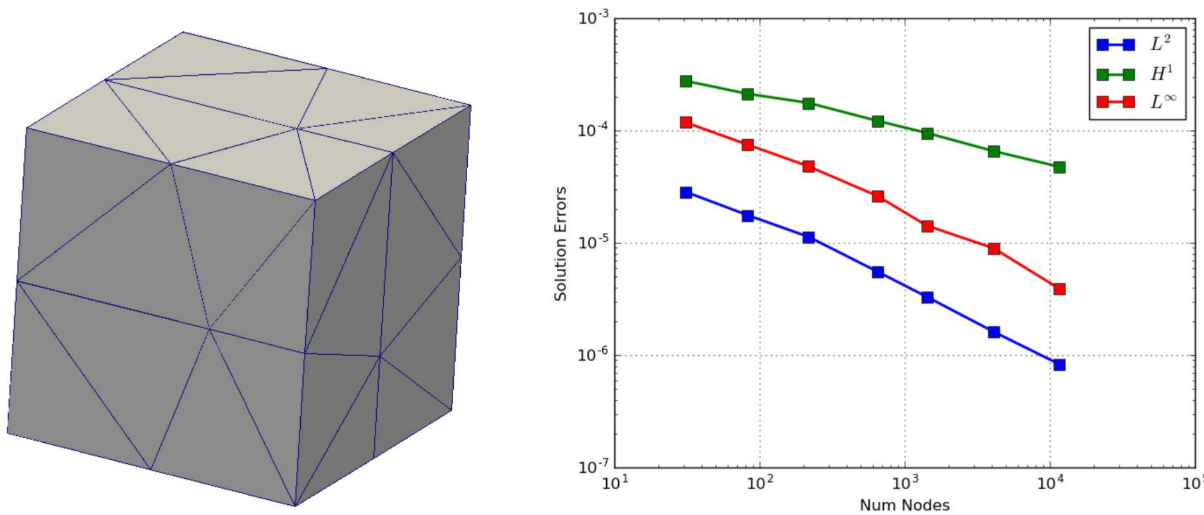
2.12.3. Material Parameters

The values of density, thermal conductivity, and specific heat are all constant, equal to one in both blocks.

2.12.4. Verification of Solution

The mesh is adapted using code from Sierra/Percept that refines tetrahedral meshes without any hanging nodes (conformal meshes only). The element error indicator is computed using a residual-based error indicator in Encore, that computes the integrated jump in the normal heat flux across inter-element faces. The input file is configured to refine elements so that the sum of the error in the refined elements is approximately 75% of the total error in all elements.

Because of variability in the meshes, we expect the error reduction to be noisy. In this case, we use linear least squares to estimate the slope of the error on a log-log plot against mesh size. Since the solution is smooth we also expect the meshes to eventually refine everywhere. We estimate convergence in the usual error norms and observe rates close to the theoretical ones (second order convergence for the L^2 and L^∞ norms and first order convergence for the H^1 norm). Mesh size is estimated using the formula $h \approx N^{-1/3}$, where N is the number of nodes in the mesh.



Coarse Mesh | Error Norms

Figure 2.12-1.. Steady Heat Conduction: Tet4 Meshes (Adaptive Mesh Refinement)

Documentation for the following tests is in progress:

```
nlin_verify1/1dnonlin_verify1.test|np8
o_2d/aniso_2d.test|np8
o_3d/aniso_3d.test|np8
shell_2d/cyl_shell_2d.test|np8
shell_3d/cyl_shell_3d.test|np8
in_C_fi/nonlin_C_fi.test|np1
in_C_trap/nonlin_C_trap.test|np1
ce_parab/source_parab.test|np1
ce_parab_2d/source_parab_2d.test|np1
shell_axi/sph_shell_axi.test|np1
rical_shell/spherical_shell.test|np4
11_nonlin/x11b11_nonlin.test|np1
```

3. THERMAL BOUNDARY CONDITIONS

3.1. RADIATIVE HEAT FLUX

This problem tests the radiative flux boundary condition under steady state heat conduction in a 2D domain. The geometry consists of a unit square.

3.1.1. Features Tested

Basic heat conduction on Quad4 meshes; radiative flux boundary conditions with constant emissivity and reference temperature; radiation form factor from C-style user subroutine; temperature boundary conditions from C-style user subroutine and constant values.

3.1.2. Boundary Conditions

At surface 3, the temperature is prescribed from a C-style user subroutine. On surfaces 2 and 4, a constant temperatre boundary condition is used. On surface 1, a radiative heat flux condition is prescribed. No source term is needed.

3.1.3. Material Parameters

The values of density, thermal conductivity, and specific heat are all constant.

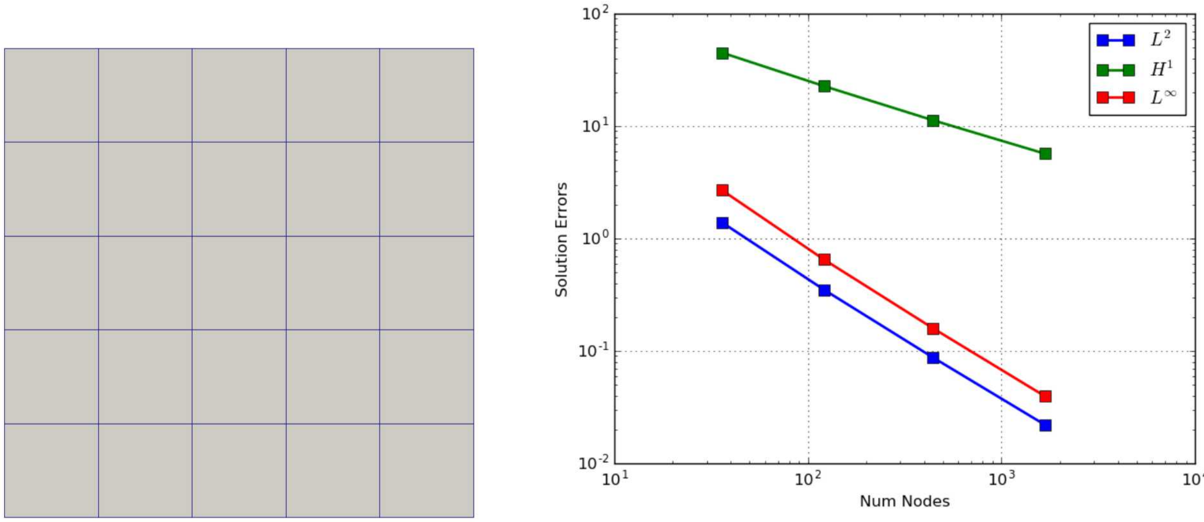
3.1.4. Verification of Solution

A manufactured solution is chosen as

$$T(x, y) = 200\ \exp(-\pi y)\ \sin(\pi x) + 600$$

For each mesh, the errors in the temperature solution are computed in the L^2, H^1 and L^∞ norms. The test passes, only if the observed rates of convergence in these norms are 2, 1, and 2, respectively (within a tolerance).

For input decks see Appendix 12.2.1.



Coarse Mesh Error Norms

Figure 3.1-1.. Radiative Heat Flux

Table 3.1-1.. Radiative Heat Flux: Convergence Rates for Hex8 Meshes

Num Dofs	L^2	H^1	L^∞
121	2.27	1.13	2.34
441	2.14	1.07	2.17
1681	2.07	1.04	2.09

3.2. RADIATIVE HEAT FLUX FROM FORTRAN USER SUBROUTINE

This test verifies that a user-supplied subroutine for convective coefficient and reference temperature (restricted to a surface patch) produces the same results as the equivalent input syntax with constant values. The user subroutine is applied to the entire exterior surface, while the case using constant values must be applied only to specific sidesets that span a portion of the exterior surface.

3.2.1. Features Tested

Basic heat conduction on a Hex8 mesh; convective and radiative flux BCs, Fortran user subroutines.

3.2.2. Boundary Conditions

Convective and radiative flux BCs are applied to the exterior boundary.

3.2.3. Material Parameters

The values of density, thermal conductivity, emissivity and specific heat are all constant.

3.2.4. Verification of Solution

The test compares Exodus output between two input files. The first does not use any user subroutines and instead relies on sidesets to apply the correct convective and radiative boundary conditions with constant coefficients. The second uses a single convective boundary condition with user subroutines for both the convective coefficient and reference temperature. The two input files produce results that agree to the default tolerances in the exodiff script.

For input decks see Appendix 12.2.2.

3.3. CONVECTIVE HEAT FLUX

This problem tests the convective flux boundary condition under transient heat conduction in a 2D domain. The geometry consists of a unit square.

3.3.1. Features Tested

Transient heat conduction on Quad4 meshes; convective flux boundary conditions with user subroutines for convective coefficient and reference temperature; temperature boundary conditions from C-style user subroutine and constant values.

3.3.2. Boundary Conditions

At surface 3, the temperature is prescribed from a C-style user subroutine. On surfaces 2 and 4, a constant temperature boundary condition is used. On surface 1, a convective heat flux condition is prescribed. No source term is needed. The initial condition is provided by a C-style user subroutine

3.3.3. Material Parameters

The values of density, thermal conductivity, and specific heat are all constant.

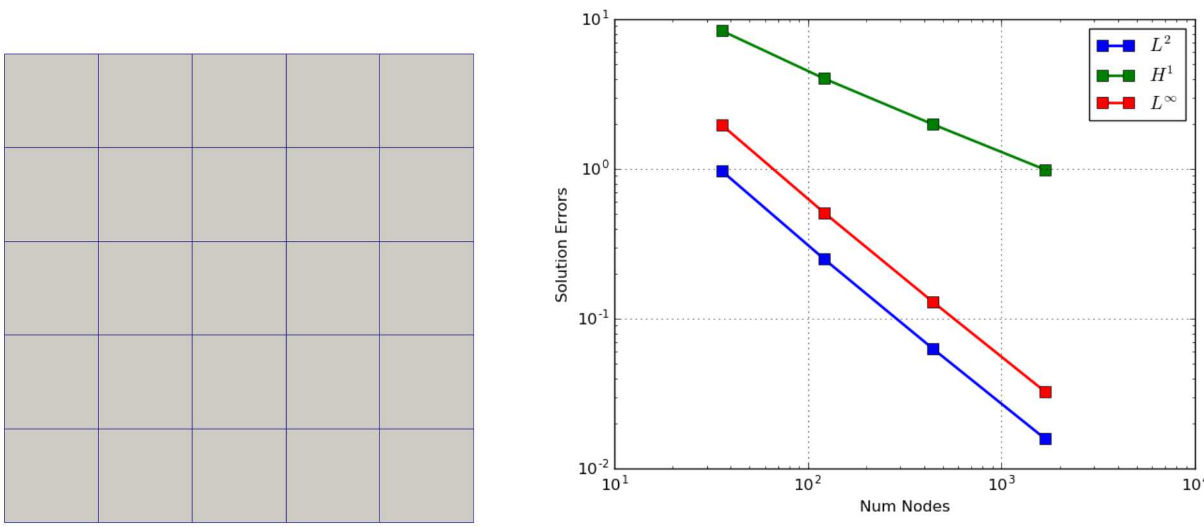
3.3.4. Verification of Solution

A manufactured solution is chosen as

$$T(x,y,t) = 100\ \exp(-2\pi^2 t)\ \sin(\pi x)\,(\cos(\pi y) + \sin(\pi y))$$

Because the solution is based on eigenfunctions, it satisfies the heat equation with no source term.

For each mesh, the errors in the temperature solution are computed in the L^2, L^∞ and H^1 norms. The test passes, only if the observed rates of convergence in these norms are 2, 2, and 1, respectively (within a tolerance).



Coarse Mesh Error Norms

Figure 3.3-1.. Convective Heat Flux

Table 3.3-1.. Convective Heat Flux: Convergence Rates for Hex8 Meshes

Num Dofs	L^2	H^1	L^∞
121	2.22	1.21	2.22
441	2.13	1.09	2.12
1681	2.07	1.04	2.07

For input decks see Appendix 12.2.3.

3.4. THERMAL CONVECTIVE FLUX (FORTRAN SUB-ROUTINE)

3.4.1. Problem Description

This problem tests the convective flux boundary condition with a convective coefficient Fortran subroutine for a steady thermal problem in a 3D domain whose geometry consists of a unit-sized cube.

3.4.2. Features Tested

Convective Flux BC, Convective Coefficient Fortran Subroutine, user subroutine, integrated flux, integrated power

3.4.3. Boundary Conditions

Convective flux boundary conditions are imposed on surfaces 1 and 2. Dirichlet BCs are specified using the exact solution on surfaces 3-6. A source term is applied within all blocks based on substituting the exact solution into the heat conduction operator.

3.4.4. Material Parameters

The values of density, thermal conductivity, and specific heat are all constant.

3.4.5. Verification of Solution

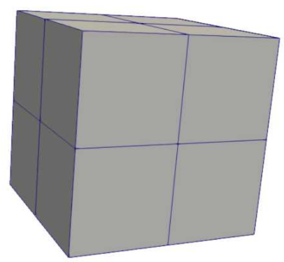
The manufactured solution is

$$T(x, y, z) = (x - x^2)^2(y - y^2)^2(z - z^2)^2 + (z + z^2).$$

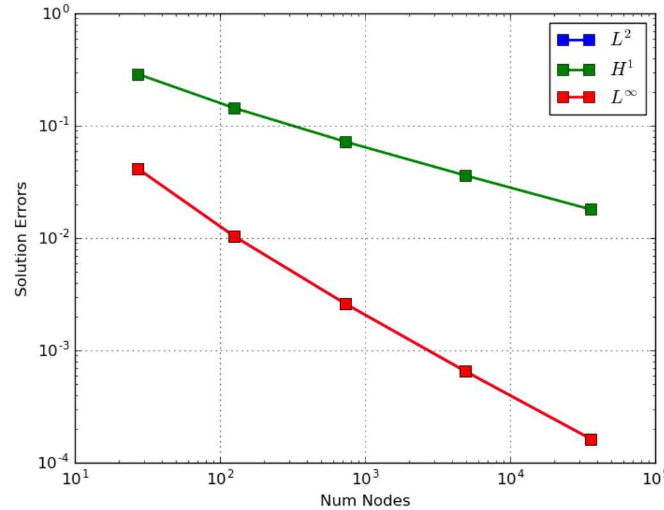
For each mesh, the errors in the temperature solution are computed in the L^2, H^1, and L^∞ norms.

Table 3.4-1.. Thermal Convective BC: Convergence Rates

Num Dofs	L^2	H^1	L^∞
125	2.71	1.36	2.71
729	2.36	1.18	2.36
4913	2.18	1.09	2.18
35940	2.09	1.04	2.09



Coarse Mesh



Error Norms

Figure 3.4-1.. Convergence for 3D thermal steady convective flux BCs.

3.5. THERMAL CONVECTIVE FLUX (USER FIELD FROM EXODUS READ-IN)

3.5.1. Problem Description

This problem evalutates a convective flux boundary condition with a convective coefficient and a reference temperature from an exodus file for a steady thermal problem in a 3D domain whose geometry consists of a unit-sized cube.

3.5.2. Features Tested

Convective Flux BC, Convective Coefficient, transfers, user subroutine, integrated flux, integrated power

3.5.3. Boundary Conditions

Convective flux boundary conditions are imposed on surfaces 1 and 2. Dirichlet BCs are specified using the exact solution on surfaces 3-6. A source term is applied within all blocks based on substituting the exact solution into the heat conduction operator.

3.5.4. Material Parameters

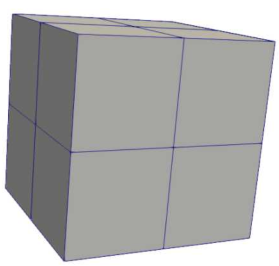
The values of density, thermal conductivity, and specific heat are all constant.

3.5.5. Verification of Solution

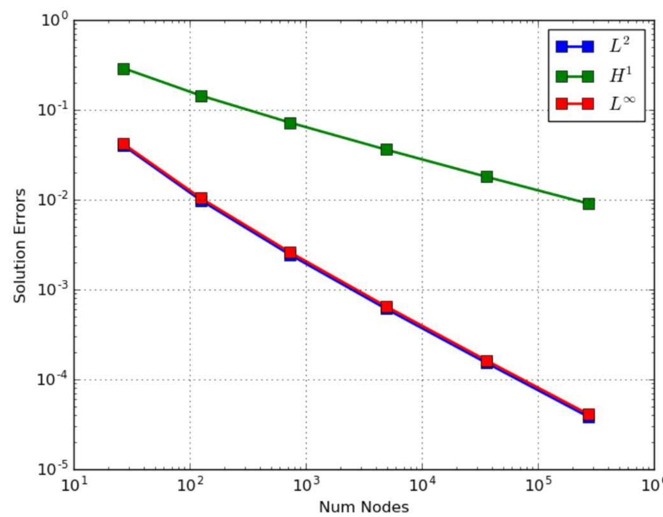
The manufactured solution is

$$T(x,y,z) = (x - x^2)^2(y - y^2)^2(z - z^2)^2 + (z^2 + z).$$

For each mesh, the errors in the temperature solution are computed in the L^2, H^1, and L^∞ norms.



Coarse Mesh



Error Norms

Figure 3.5-1.. Convergence for 3D thermal steady convective flux BCs.

Table 3.5-1.. Thermal Convective BC: Convergence Rates

Num Dofs	L^2	H^1	L^∞
125	2.74	1.36	2.71
729	2.36	1.18	2.36
4913	2.18	1.09	2.18
35940	2.09	1.05	2.09
274600	2.05	1.02	2.05

3.6. THERMAL HEAT FLUX

3.6.1. Thermal Heat Flux (Basic)

3.6.1.1. Problem Description

This problem tests a steady thermal solution on a unit cube with heat flux boundary conditions imposed on one of the six surfaces. The mesh uses Hex8 elements.

3.6.1.2. Features Tested

Basic heat conduction, Calore style heat flux BCs, Integrated Flux Output, Integrated Power Output, Hex8 meshes, user functions.

3.6.1.3. Boundary Conditions

Dirichlet BCs are specified using the exact solution on surfaces 2-6. On surface 1, a heat flux BC is specified, using a heat flux of $2 - \exp(1)$. A source term is applied within all blocks based on substituting the exact solution into the heat conduction operator. The integrated flux and power are calculated and output as global variables, which should both be equal for a surface with area of 1 and equal to $2 - \exp(1)$ for all meshes considered.

3.6.1.4. Material Parameters

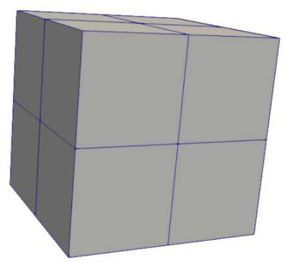
The values of density, thermal conductivity, and specific heat are all constant with the same value for both blocks.

3.6.1.5. Verification of Solution

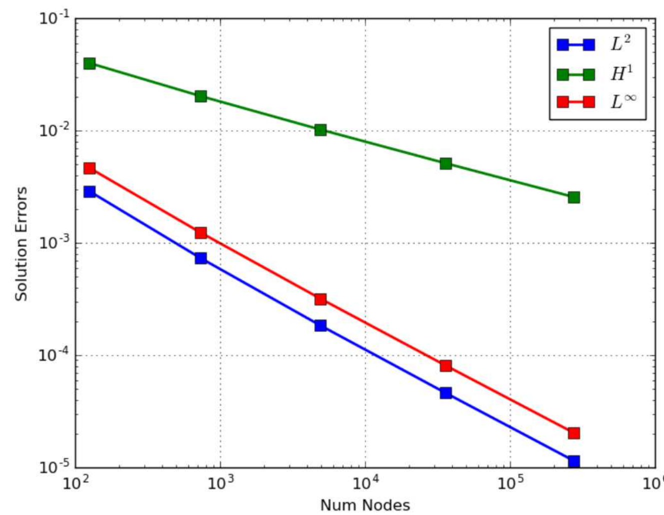
The manufactured solution is

$$T(x, y, x) = (x - x^2)^2(y - y^2)^2(z - z^2)^2 + z^2 \exp(z).$$

For each mesh, the errors in the temperature solution are computed in the L^2, H^1, and L^∞ norms. The test passes, only if the observed rates of convergence are 2 (except for the L^∞ norm, with convergence order 1).



Coarse Mesh



Error Norms

Figure 3.6-1.. Thermal Heat Flux BC

Table 3.6-1.. Thermal Heat Flux BC: Convergence Rates

Num Dofs	L^2	L^∞	H^1
729	2.33	1.15	2.25
4913	2.17	1.08	2.13
35940	2.09	1.04	2.07
274600	2.04	1.02	2.04

3.6.2. Thermal Heat Flux (Flux node variable user field)

3.6.2.1. Problem Description

This problem tests a steady thermal solution on a unit cube with heat flux boundary conditions imposed on one of the six surfaces. The mesh uses Hex8 elements.

3.6.2.2. Features Tested

Basic heat conduction, Calore style heat flux BCs, Flux Node Variable, User field, Field Scaling, Hex8 meshes, user functions, transfer.

3.6.2.3. Boundary Conditions

Dirichlet BCs are specified using the exact solution on surfaces 1 and 3-6. On surface 2, a heat flux BC is specified, using a flux node variable user field. A source term is applied within all blocks based on substituting the exact solution into the heat conduction operator. Transfers are specified at the surface.

3.6.2.4. Material Parameters

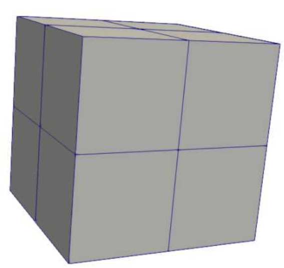
The values of density, thermal conductivity, and specific heat are all constant with the same value for both blocks.

3.6.2.5. Verification of Solution

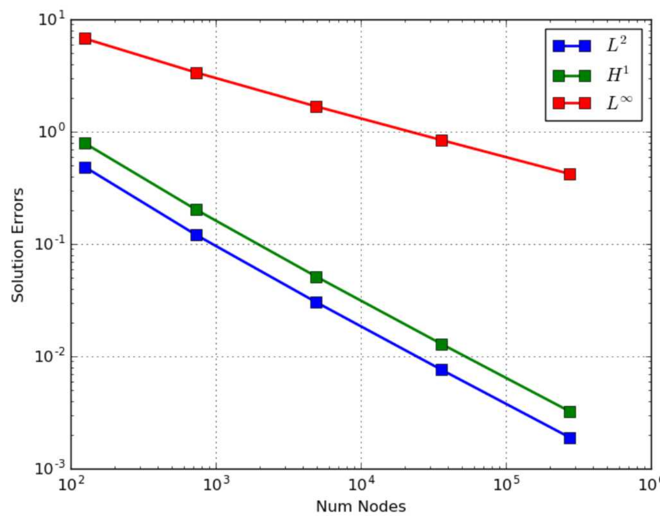
The manufactured solution is

$$T(x, y, x) = (x - x^2)^2(y - y^2)^2(z - z^2)^2 + 20 * (z^2 - z) * (1 + x + y + xy).$$

For each mesh, the errors in the temperature solution are computed in the L^2, H^1, and L^∞ norms. The test passes, only if the observed rates of convergence are 2 (except for the L^∞ norm, with convergence order 1).



Coarse Mesh



Error Norms

Figure 3.6-2.. Thermal Heat Flux BC

3.6.3. Thermal Heat Flux (Flux node variable user field)

3.6.3.1. Problem Description

This problem tests a steady thermal solution on a unit cube with heat flux boundary conditions imposed on one of the six surfaces. The mesh uses Hex8 elements.

Table 3.6-2.. Thermal Heat Flux BC: Convergence Rates

Num Dofs	L^2	L^∞	H^1
729	2.36	2.31	1.18
4913	2.18	2.16	1.09
35940	2.09	2.08	1.04
274600	2.05	2.04	1.02

3.6.3.2. *Features Tested*

Basic heat conduction, Calore style heat flux BCs, User field real nodal vector, Hex8 meshes, user functions, transfers.

3.6.3.3. *Boundary Conditions*

Dirichlet BCs are specified using the exact solution on surfaces 1 and 3-6. On surface 2, a heat flux BC is specified, using a flux vector node variable defined as a user field. A source term is applied within all blocks based on substituting the exact solution into the heat conduction operator.

3.6.3.4. *Material Parameters*

The values of density, thermal conductivity, and specific heat are all constant with the same value for both blocks.

3.6.3.5. *Verification of Solution*

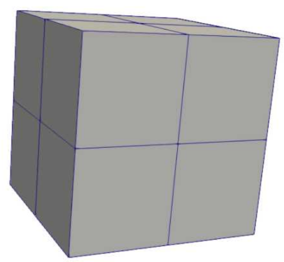
The manufactured solution is

$$T(x, y, x) = (x - x^2)^2(y - y^2)^2(z - z^2)^2 + 20 * (z^2 - z) * (1 + x + y + xy).$$

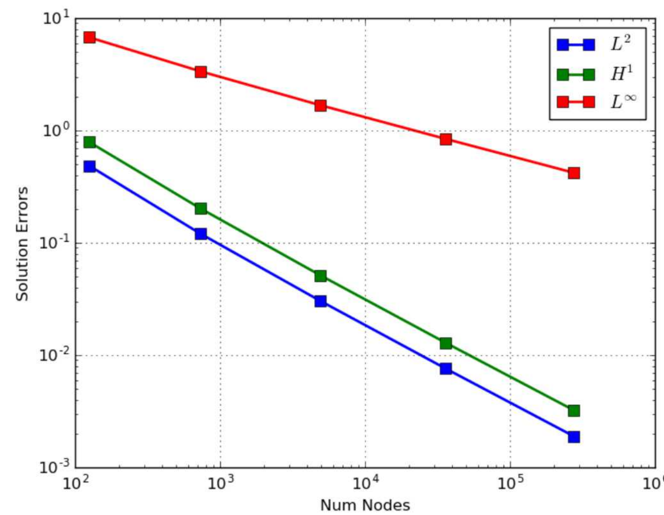
For each mesh, the errors in the temperature solution are computed in the L^2, H^1, and L^∞ norms. The test passes, only if the observed rates of convergence are 2 (except for the L^∞ norm, with convergence order 1).

Table 3.6-3.. Thermal Heat Flux BC: Convergence Rates

Num Dofs	L^2	L^∞	H^1
729	2.36	2.31	1.18
4913	2.18	2.16	1.09
35940	2.09	2.08	1.04
274600	2.05	2.04	1.02



Coarse Mesh



Error Norms

Figure 3.6-3.. Thermal Heat Flux BC

3.6.4. Thermal Heat Flux (Fortran Subroutine)

3.6.4.1. Problem Description

This problem tests a steady thermal solution on a unit cube with heat flux boundary conditions imposed on one of the six surfaces. The mesh uses Hex8 elements.

3.6.4.2. Features Tested

Basic heat conduction, Calore style heat flux BCs, Integrated Flux Output, Integrated Power Output, Fortran subroutine, Hex8 meshes, user plugin.

3.6.4.3. Boundary Conditions

Dirichlet BCs are specified using the exact solution on surfaces 3-6. On surfaces 1 and 2, heat flux BCs are specified, using Fortran subroutines. A source term is applied within all blocks based on substituting the exact solution into the heat conduction operator.

3.6.4.4. Material Parameters

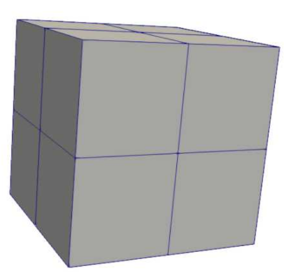
The values of density, thermal conductivity, and specific heat are all constant with the same value for both blocks.

3.6.4.5. *Verification of Solution*

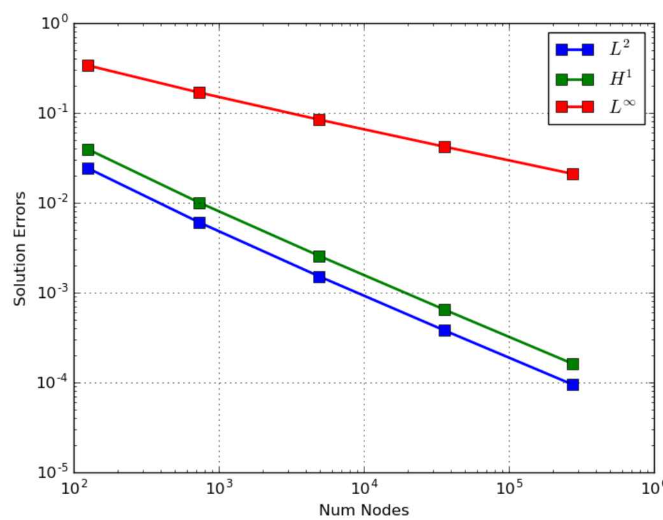
The manufactured solution is

$$T(x,y,x) = (x - x^2)^2(y - y^2)^2(z - z^2)^2 + (z^2 + z) * (1 + x + y + xy).$$

For each mesh, the errors in the temperature solution are computed in the L^2, H^1, and L^∞ norms. The test passes, only if the observed rates of convergence are 2 (except for the L^∞ norm, with convergence order 1).



Coarse Mesh



Error Norms

Figure 3.6-4.. Thermal Heat Flux BC

Table 3.6-4.. Thermal Heat Flux BC: Convergence Rates

Num Dofs	L^2	L^∞	H^1
729	2.36	2.31	1.18
4913	2.18	2.16	1.09
35940	2.09	2.08	1.05
274600	2.05	2.04	1.02

3.7. THERMAL RADIATIVE HEAT FLUX

3.7.1. Basic Calore-Style BC

3.7.1.1. *Problem Description*

This problem evaluates a steady thermal solution with radiative heat flux boundary conditions on a 3D unit cube domain.

3.7.1.2. *Features Tested*

Basic heat conduction, Calore style radiative heat flux BCs, Integrated Flux Output, Integrated Power Output, Hex8 meshes.

3.7.1.3. *Boundary Conditions*

Dirichlet BCs are specified using the exact solution on surfaces 2-6. On surface 1, a radiative heat flux BC is specified with constant emissivity and a radiation form factor of 0.2. A source term is applied within all blocks based on substituting the exact solution into the heat conduction operator.

3.7.1.4. *Material Parameters*

The values of density, thermal conductivity, specific heat, and emissivity are all constant values.

3.7.1.5. *Verification of Solution*

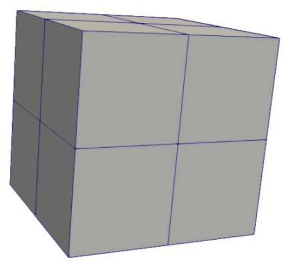
The manufactured solution is

$$T(x,y,x) = (x-x^2)^2(y-y^2)^2(z-z^2)^2 + T - \frac{\partial T}{\partial n}(z^2-z).$$

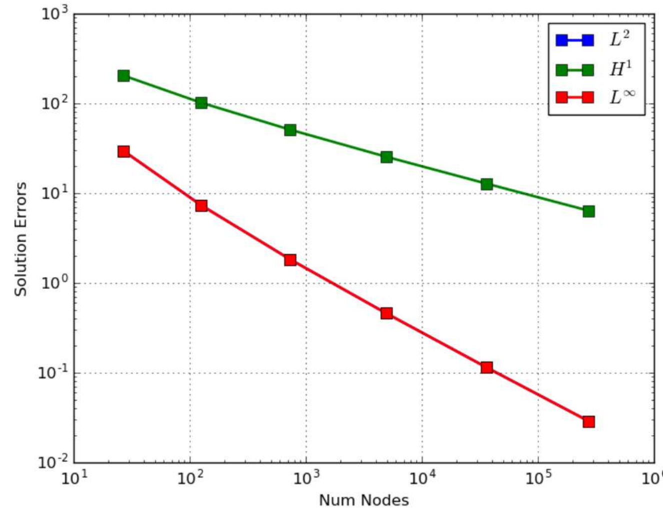
For each discretization, the errors in the temperature solution are computed in the L^2, H^1, and L^∞ norms. The observed rates of convergence are 2 (except for the L^∞ norm, with convergence order 1).

Table 3.7-1.. Thermal Radiative Flux BC: Convergence Rates

Num Dofs	L^2	L^∞	H^1
125	2.71	1.36	2.71
729	2.36	1.18	2.36
4913	2.18	1.09	2.18
35940	2.09	1.04	2.09
274600	2.05	1.02	2.05



Coarse Mesh



Error Norms

Figure 3.7-1.. Thermal Radiative Flux

3.7.2. With Fortran Subroutines

3.7.2.1. Problem Description

This problem evaluates a steady thermal solution with radiative heat flux boundary conditions using Fortran subroutines on a 3D unit cube domain.

3.7.2.2. Features Tested

Basic heat conduction, Calore style radiative heat flux BCs, Integrated Flux Output, Integrated Power Output, Hex8 meshes, Fortran subroutines.

3.7.2.3. Boundary Conditions

Dirichlet BCs are specified using the exact solution on surfaces 2-6. On surface 1, a radiative heat flux BC is specified with emissivity, reference temperature, and radiation form factor of provided by Fortran subroutines. A source term is applied within all blocks based on substituting the exact solution into the heat conduction operator.

3.7.2.4. Material Parameters

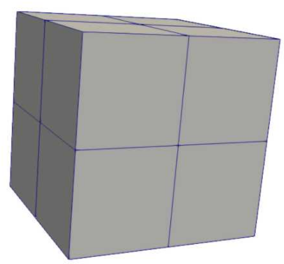
The values of density, thermal conductivity, specific heat, and emissivity are all constant values.

3.7.2.5. Verification of Solution

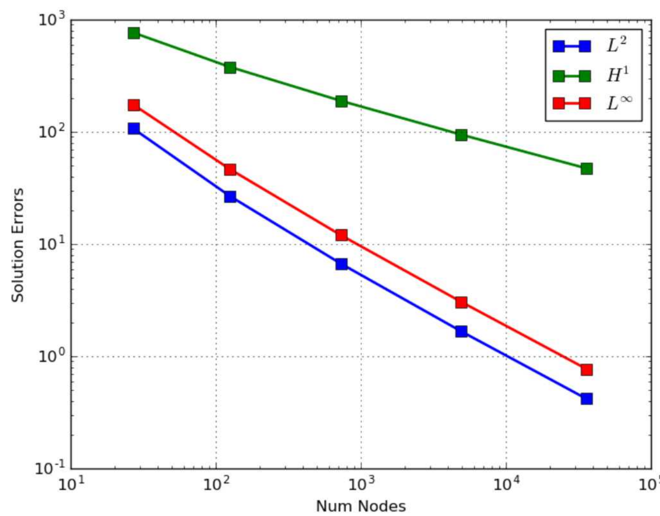
The manufactured solution is

$$T(x,y,x) = (x-x^2)^2(y-y^2)^2(z-z^2)^2 + T - \frac{\partial T}{\partial n}(z^2-z).$$

For each discretization, the errors in the temperature solution are computed in the L^2, H^1, and L^∞ norms. The observed rates of convergence are 2 (except for the L^∞ norm, with convergence order 1).



Coarse Mesh



Error Norms

Figure 3.7-2.. Thermal Radiative Flux

Table 3.7-2.. Thermal Radiative Flux BC: Convergence Rates

Num Dofs	L^2	L^∞	H^1
125	2.72	1.38	2.59
729	2.36	1.18	2.30
4913	2.18	1.09	2.15
35940	2.09	1.05	2.08

3.7.3. With User Subroutines

3.7.3.1. Problem Description

This problem evaluates a steady thermal solution with radiative heat flux boundary conditions with user subroutines on a 3D unit cube domain.

3.7.3.2. Features Tested

Basic heat conduction, Calore style radiative heat flux BCs, Integrated Flux Output, Integrated Power Output, Hex8 meshes, user subroutines.

3.7.3.3. Boundary Conditions

Dirichlet BCs are specified using the exact solution on surfaces 2-6. On surface 1, a radiative heat flux BC is specified with emissivity, reference termperature and radiation form factor provided by user subroutines. A source term is applied within all blocks based on substituting the exact solution into the heat conduction operator.

3.7.3.4. Material Parameters

The values of density, thermal conductivity, specific heat, and emissivity are all constant values.

3.7.3.5. Verification of Solution

The manufactured solution is

$$T(x, y, x) = (x - x^2)^2(y - y^2)^2(z - z^2)^2 + T - \frac{\partial T}{\partial n}(z^2 - z).$$

For each discretization, the errors in the temperature solution are computed in the L^2, H^1, and L^∞ norms. The observed rates of convergence are 2 (except for the L^∞ norm, with convergence order 1).

Table 3.7-3.. Thermal Radiative Flux BC: Convergence Rates

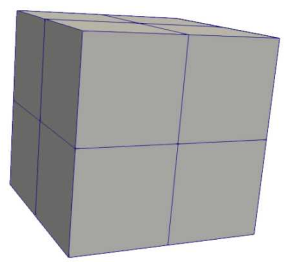
Num Dofs	L^2	L^∞	H^1
125	2.72	1.38	2.59
729	2.36	1.18	2.30
4913	2.18	1.09	2.15
35940	2.09	1.05	2.08

3.8. ADVECTIVE BAR

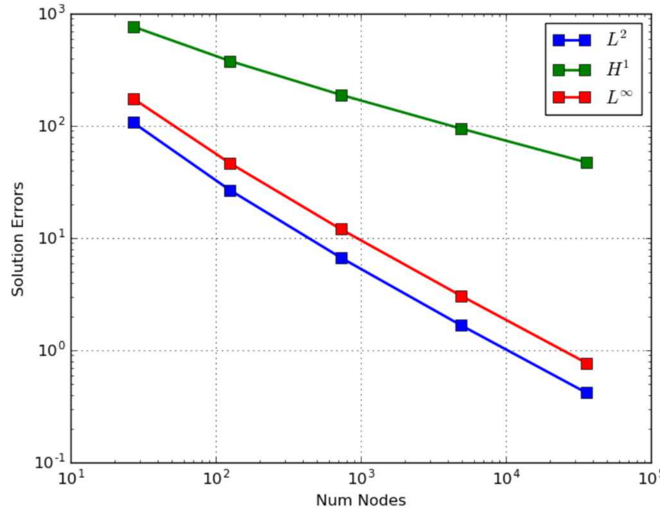
Advective bar model verification tests.

3.8.1. Steady Advection-Diffusion

The three dimensional Bar2 meshes of one element block are generated in Cubit.



Coarse Mesh



Error Norms

Figure 3.7-3.. Thermal Radiative Flux

3.8.2. Features Tested

Steady heat conduction on 3D Bar2 meshes, Dirichlet boundary conditions, constant source term, advection and SUPG stabilization.

3.8.3. Boundary Conditions

$$T(0) = T(1) = 0$$

3.8.4. Material Parameters

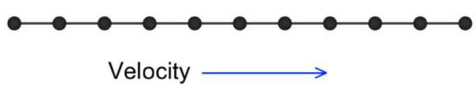
The values of density, thermal conductivity, and specific heat are all constant, equal to one in the block.

3.8.5. Verification of Solution

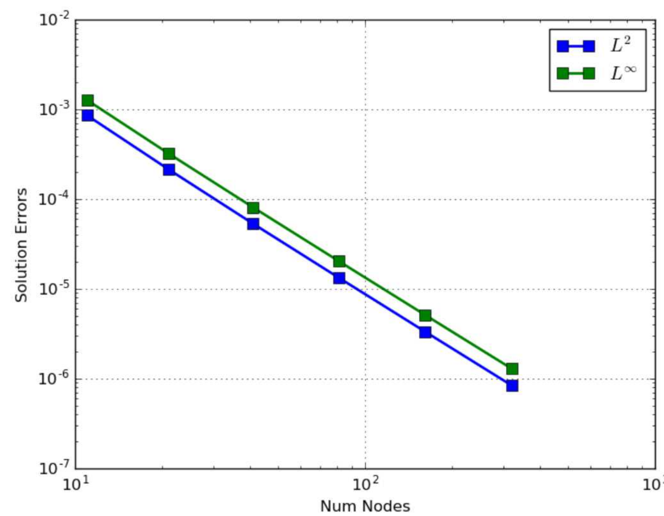
Solution verification is carried out by computing the error in the numerical solution based upon comparison with the analytic solution.

$$T(x) = \frac{1}{\rho C V}\left[x - \frac{1-\exp(x\gamma)}{1-\exp(\gamma)}\right]$$

where $\gamma = \rho CV/k$ where ρ is the density, C is specific heat, k is the thermal conductivity and V is the advection velocity. In this test, we find that the convergence rate for the temperature in the L^∞ and L^2 norms are 2.



Coarse Mesh



Error Norms

Figure 3.8-1.. Steady Advective Conduction: 3D Bar2 Meshes

Table 3.8-1.. Steady Advective Conduction: Convergence Rates for 3D Bar2 Meshes

Num Dofs	L^2	L^∞
21	2.14	2.11
41	2.07	2.06
81	2.04	2.03
161	2.02	2.01
321	2.01	2.01

3.8.6. Transient Advection-Diffusion

The three dimensional Bar2 meshes of one element block are generated in Cubit.

3.8.7. Features Tested

Transient heat conduction on 3D Bar2 meshes, Dirichlet boundary conditions and Encore function source term.

3.8.8. Boundary Conditions

Dirichlet boundary conditions on the bar ends based upon the manufactured solution $T(x)$

$$T(0) = T(1) = T_i$$

3.8.9. Material Parameters

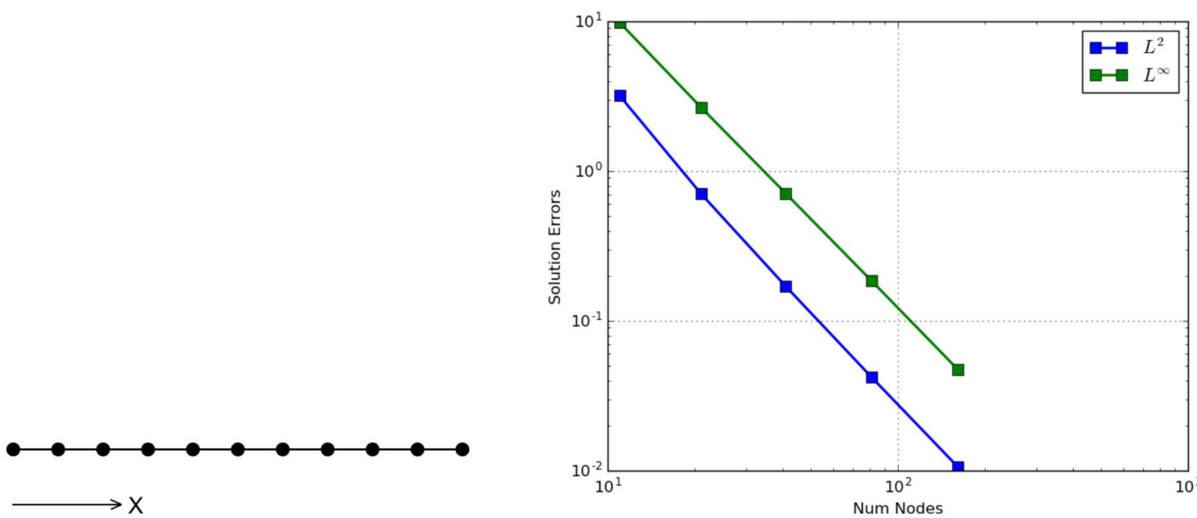
The values of density, thermal conductivity, and specific heat are all constant, equal to one in the bar block.

3.8.10. Verification of Solution

Solution verification is carried out by computing the error in the numerical solution based upon comparison with the analytic solution.

$$T(x) = T_i + Atx(x-1)\exp(-Bt)\exp(-Bx)$$

In this test, we find that the convergence rate for the temperature in the L^∞ and L^2 norms are 2.



Coarse Mesh Error Norms

Figure 3.8-2.. Transient Heat Conduction: 3D Bar2 Meshes

3.8.11. Transient Advection-Diffusion in 2D

The two dimensional Bar2 meshes of one elment block are generated in Cubit.

Table 3.8-2.. Transient Heat Conduction: Convergence Rates for 3D Bar2 Meshes

Num Dofs	L^2	L^∞
21	2.33	2.02
41	2.12	1.97
81	2.05	1.98
161	2.02	1.99

3.8.12. Features Tested

Transient heat conduction on 2D Bar2 meshes, Dirichlet boundary conditions and Encore function source term.

3.8.13. Boundary Conditions

Dirichlet boundary conditions on the bar ends

$$T(0) = T(1) = T_i$$

3.8.14. Material Parameters

The values of density, thermal conductivity, and specific heat are all constant, equal to one in the bar block.

3.8.15. Verification of Solution

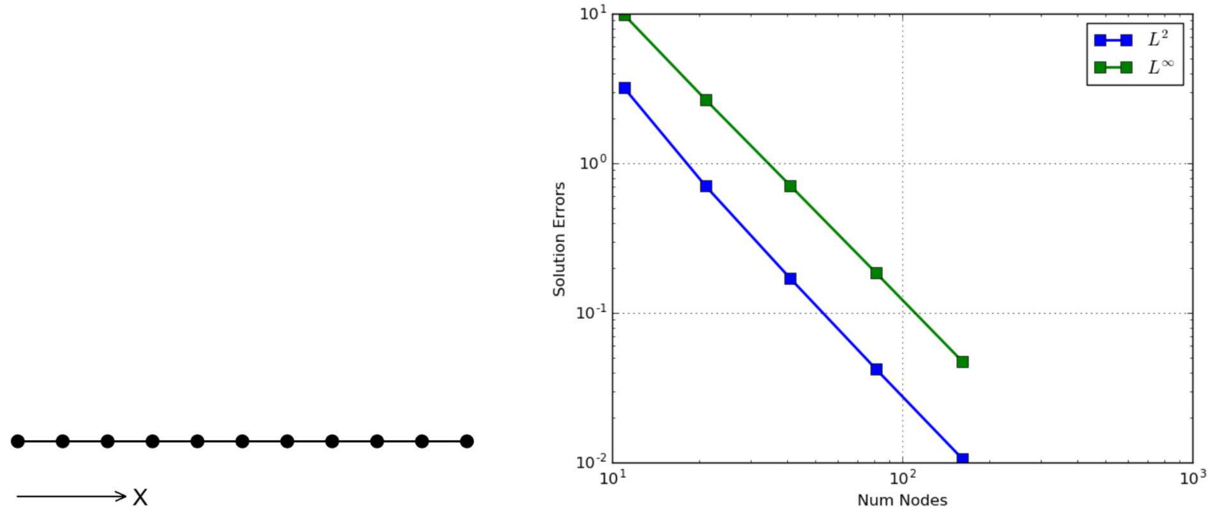
Solution verification is carried out by computing the error in the numerical solution based upon comparison with the analytic solution.

$$T(x) = T_i + Atx(x-1)\exp(-Bt)\exp(-Bx)$$

In this test, we find that the convergence rate for the temperature in the L^∞ and L^2 norms are 2.

Table 3.8-3.. Transient Heat Conduction: Convergence Rates for 2D Bar2 Meshes

Num Dofs	L^2	L^∞
21	2.33	2.02
41	2.12	1.97
81	2.05	1.98
161	2.02	1.99



Coarse Mesh | Error Norms

Figure 3.8-3.. Transient Heat Conduction: Bar2 Meshes

3.9. SOLUTION VERIFICATION

This test is for a Mock AFF (including a metal case, foam, mock components, and temperature-dependent properties) that uses extrapolation to determine an approximation to the exact solution as a function of the results from three levels of meshes.

3.9.1. Features Tested

Extrapolation, Radiative flux boundary condition

3.9.2. Material Parameters

Constant density, emissivity. Temperature dependent user functions for specific hear and thermal conductivity.

3.9.3. Verification of Solution

Quantities of interest are the maximum, minimum, and average temperatures on both blocks and points. There is no manufactured solution in this case, instead an extrapolated solution is calculated and used to measure convergence and approximate the absolute error for a given mesh resolution.

Documentation for the following tests is in progress:

```
nic_material_decomposition/organic_material_decomposition.test|np4
```

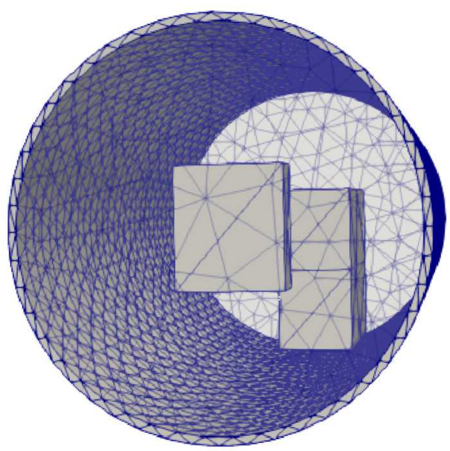


Figure 3.9-1.. Mock AFF Solution Verification

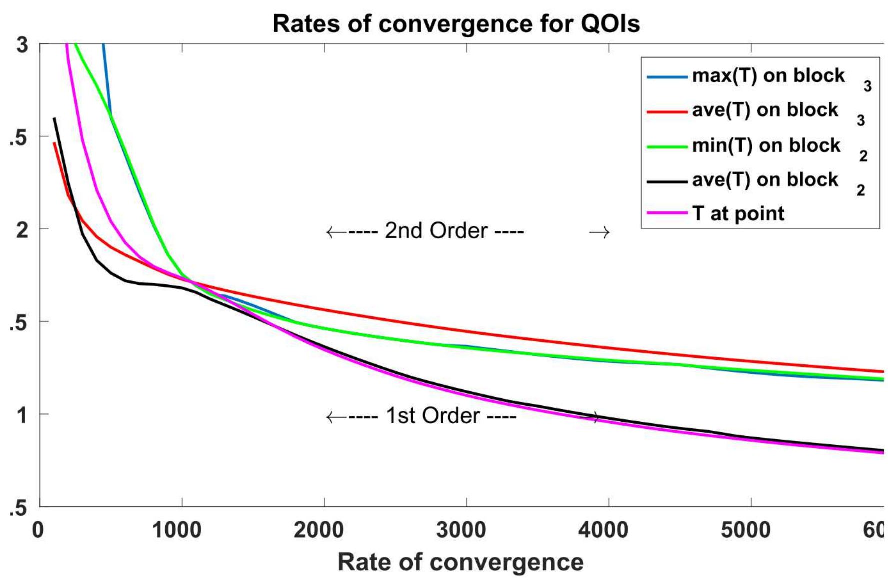


Figure 3.9-2.. The convergence rates can vary over time and between QOIs

4. THERMAL CONTACT

4.1. 1D FLAT CONTACT

This problem tests thermal contact along a flat surface using 3D domains. The geometry consists of two thick blocks, which are in contact along a common flat surface. The mesh nodes on either side of the contact surface are not aligned in general.

In this problem we observe sub-optimal convergence rates in the L^∞ norm when using Tet elements. This is a known issue with unknown cause.

The contact search tolerances are fixed for all meshes, with a zero tangential and normal tolerances.

4.1.1. Features Tested

Basic heat conduction, tied and resistance thermal contact between non-matching meshes (Hex-Hex, Tet-Tet, Hex-Tet).

4.1.2. Boundary Conditions

The interface between the two blocks is a thermal contact boundary condition. Both tied contact and resistance contact (with finite contact resistance) are tested. The left and right boundary conditions are prescribed using constant values. The remaining boundary conditions are adiabatic. A constant source term is applied in each block (with different signs).

4.1.3. Material Parameters

The values of density, thermal conductivity, and specific heat are all constant, equal to one in both blocks.

4.1.4. Verification of Solution

A manufactured solution is chosen based on the contact interface at $x = 0$:

$$T(x,y,z) = \begin{cases} \frac{1}{2}(1+x)(\gamma+x), & x<0, \\ 1+\frac{1}{2}(1-x)(-\gamma+x), & x>0 \end{cases}$$

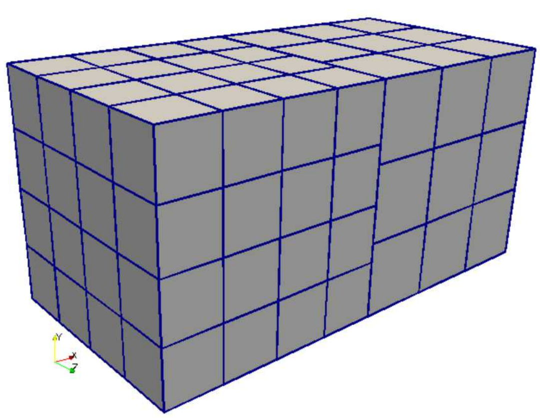
where $\gamma = (2-R)/(2+R)$ is a constant depending on the thermal contact resistance R. Here R is the inverse of the contact conductance that is provided as a code input. In the case of tied contact, $R = 0$ and therefore $\gamma = 1$. We note that when $R > 0$, this exact solution exhibits a jump in temperature across the contact interface.

For each mesh, the errors in the temperature solution are computed in the L^2, L^∞ and H^1 norms. The test passes, only if the observed rates of convergence in these norms are 2, 2, and 1, respectively (within a tolerance).

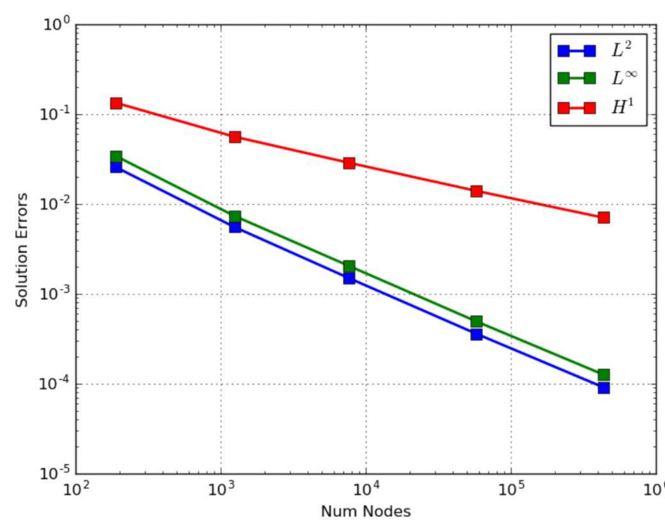
These rates are observed for the Hex-Hex case; however, both of the cases involving Tet meshes exhibit a reduced order of convergence in the L^∞ norms (convergence rate about 1.7).

For input decks see Appendix 12.3.1.

4.1.5. Results: Hex8 Tied



Coarse Mesh



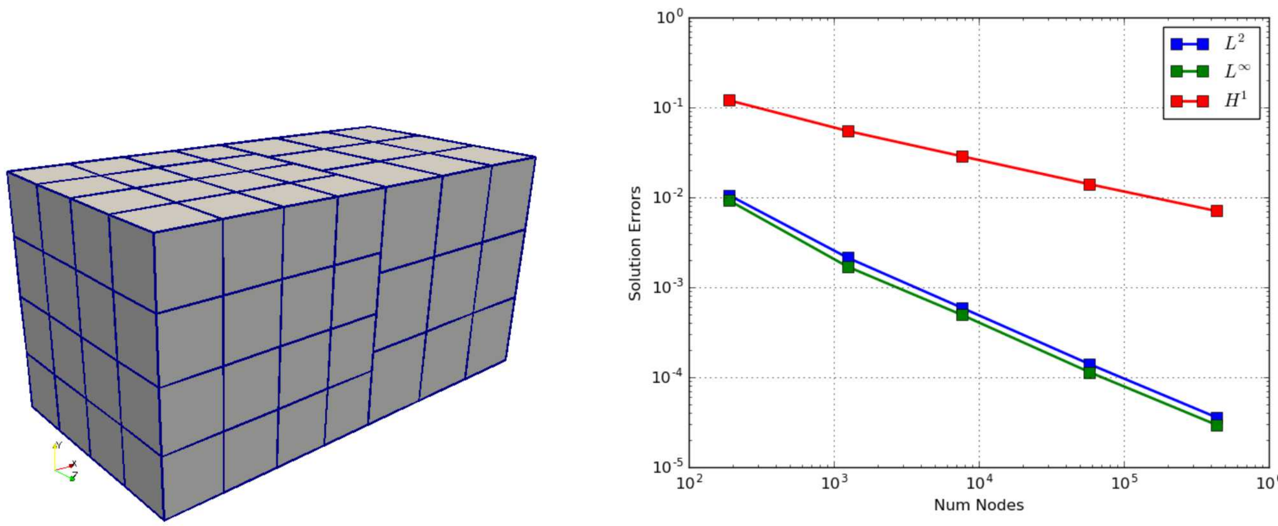
Error Norms

Figure 4.1-1.. 1D Flat Contact: Hex8 Tied

4.1.6. Results: Hex8 Resistance

Table 4.1-1.. 1D Flat Contact: Convergence Rates for Hex8 Tied

Num Dofs	L^2	L^∞	H^1
1241	2.45	2.44	1.38
7657	2.17	2.12	1.10
57890	2.11	2.11	1.07
432100	2.04	2.03	1.02



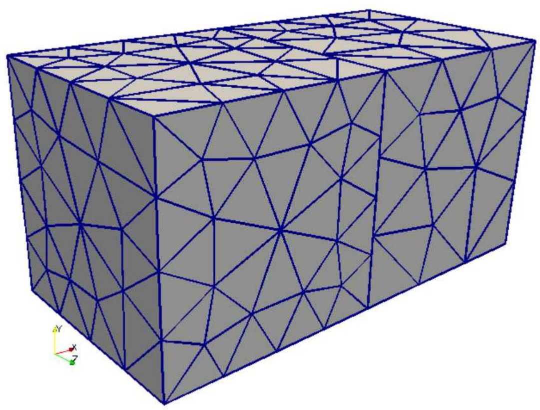
Coarse Mesh Error Norms

Figure 4.1-2.. 1D Flat Contact: Hex8 Resistance

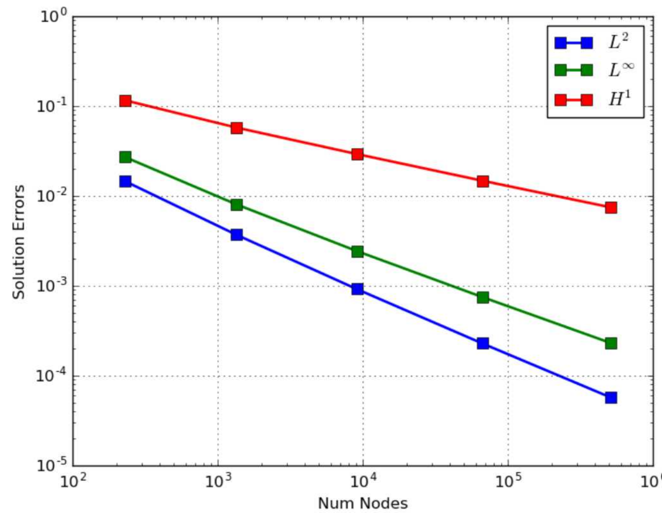
Table 4.1-2.. 1D Flat Contact: Convergence Rates for Hex8 Resistance

Num Dofs	L^2	L^∞	H^1
1241	2.55	2.70	1.25
7657	2.12	2.04	1.07
57890	2.13	2.17	1.06
432100	2.03	2.01	1.02

4.1.7. Results: Tet4 Tied



Coarse Mesh



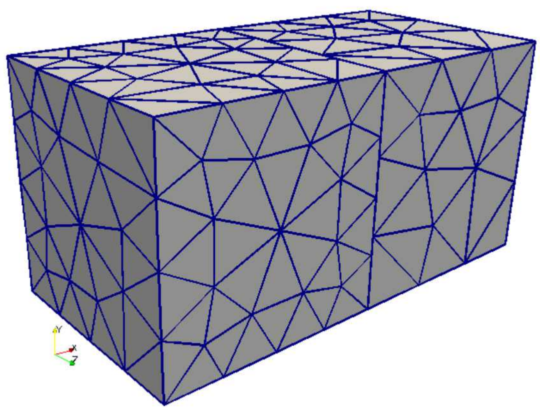
Error Norms

Figure 4.1-3.. 1D Flat Contact: Tet4 Tied

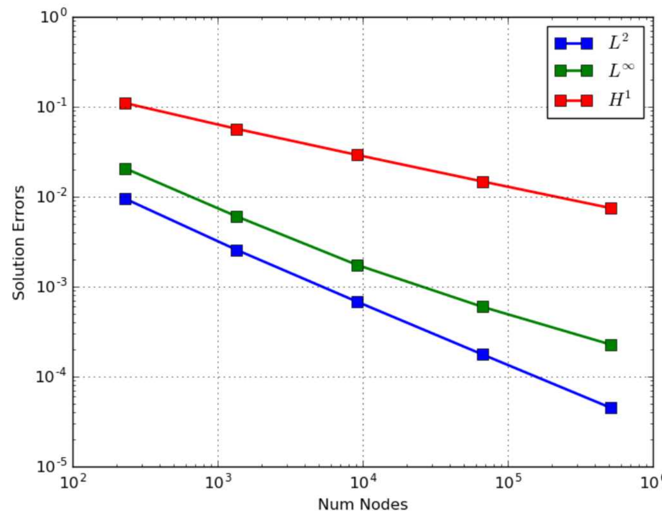
Table 4.1-3.. 1D Flat Contact: Convergence Rates for Tet4 Tied

Num Dofs	L^2	L^∞	H^1
1348	2.33	2.06	1.18
9102	2.19	1.88	1.06
66620	2.09	1.78	1.03
509200	2.04	1.73	1.01

4.1.8. Results: Tet4 Resistance



Coarse Mesh



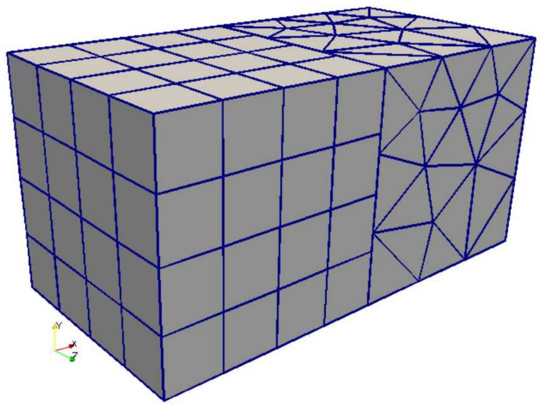
Error Norms

Figure 4.1-4.. 1D Flat Contact: Tet4 Resistance

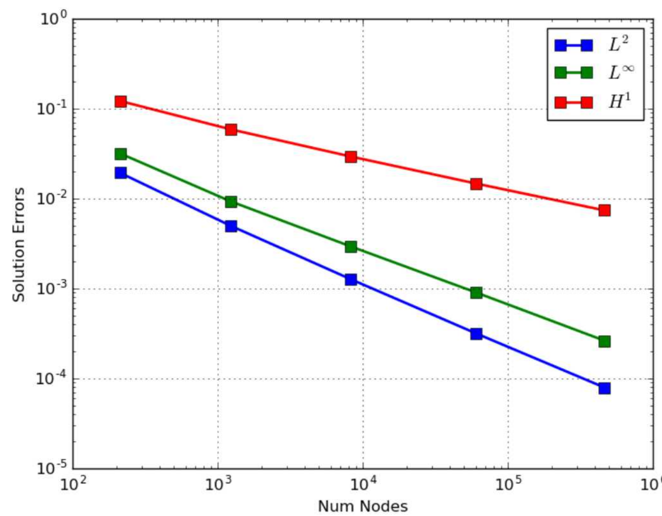
Table 4.1-4.. 1D Flat Contact: Convergence Rates for Tet4 Resistance

Num Dofs	L^2	L^∞	H^1
1348	2.22	2.09	1.12
9102	2.08	1.95	1.05
66620	2.04	1.62	1.02
509200	2.01	1.42	1.01

4.1.9. Results: Hex8-Tet4 Tied



Coarse Mesh



Error Norms

Figure 4.1-5.. 1D Flat Contact: Hex8-Tet4 Tied

Table 4.1-5.. 1D Flat Contact: Convergence Rates for Hex8-Tet4 Tied

Num Dofs	L^2	L^∞	H^1
1231	2.32	2.10	1.24
8284	2.16	1.82	1.09
60570	2.09	1.78	1.04
462800	2.04	1.82	1.02

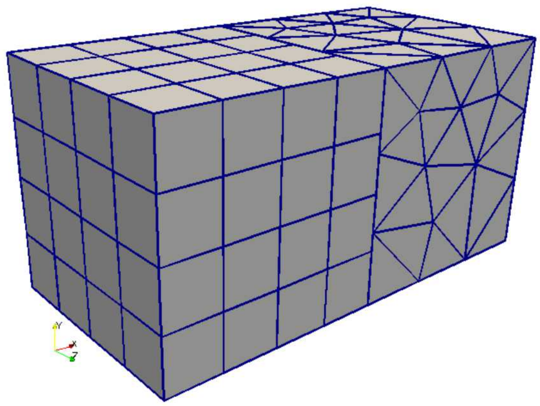
4.1.10. Results: Hex8-Tet4 Resistance

4.2. 3D CURVED CONTACT

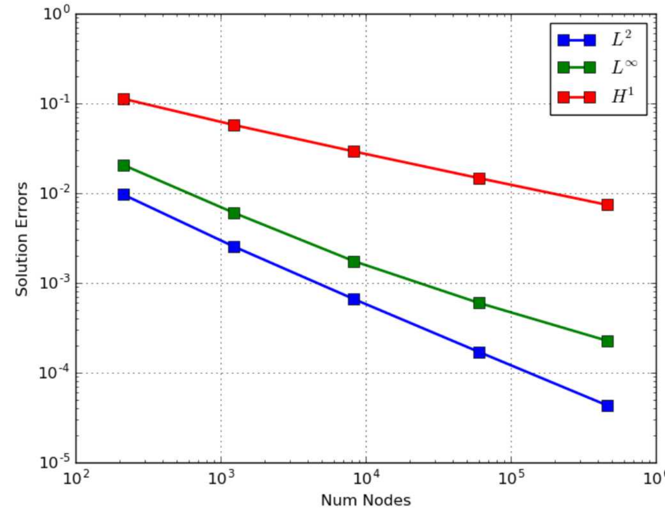
This problem tests thermal contact along a curved surface in 3D. The geometry consists of two thick spherical shells, which are in contact along a shared surface. The mesh nodes on either side of the contact surface are not aligned in general.

In this problem we observe sub-optimal convergence rates in the L^∞ norm when using tet elements. This is a known issue with unknown cause.

The contact search tolerances are fixed for all meshes, with a zero tangential tolerance and a normal tolerance large enough to insure a proper contact search on the coarsest mesh.



Coarse Mesh



Error Norms

Figure 4.1-6.. 1D Flat Contact: Hex8-Tet4 Resistance

Table 4.1-6.. 1D Flat Contact: Convergence Rates for Hex8-Tet4 Resistance

Num Dofs	L^2	L^∞	H^1
1231	2.28	2.10	1.15
8284	2.12	1.95	1.07
60570	2.05	1.62	1.03
462800	2.02	1.43	1.01

4.2.1. Features Tested

Basic heat conduction, tied thermal contact between non-matching meshes (hex-hex, tet-tet, hex-tet).

4.2.2. Boundary Conditions

The interface between the two blocks is a tied thermal contact boundary condition. The outer and inner boundary conditions are prescribed at the nodes using the analytic solution.

4.2.3. Material Parameters

The values of density, thermal conductivity, and specific heat are all constant, equal to one in both blocks.

4.2.4. Verification of Solution

A manufactured solution is chosen as

$$T(x, y, z) = -3x^2 z - 3y^2 z + 2z^3$$

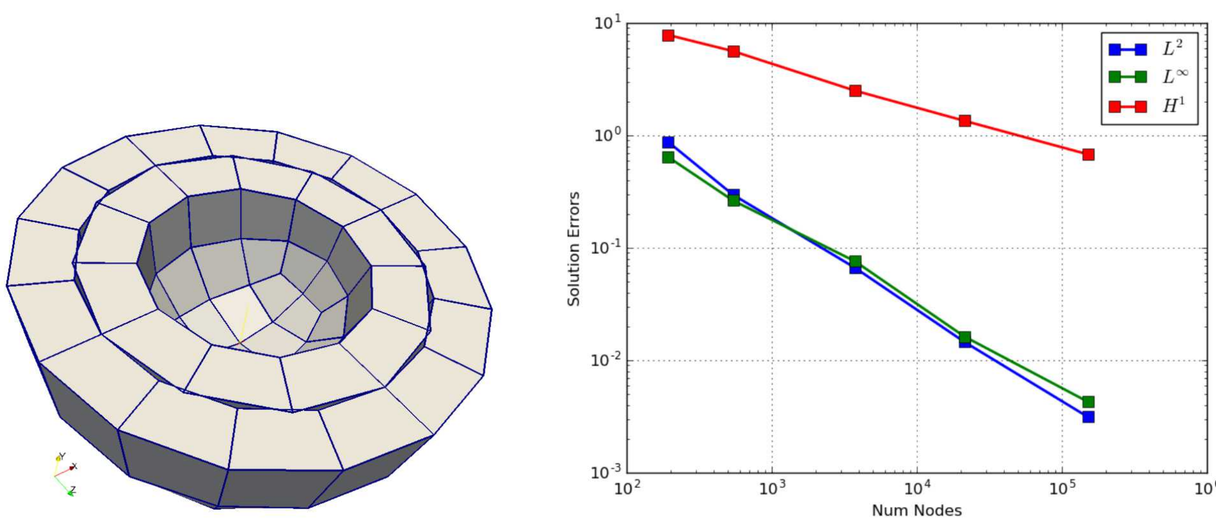
This solution is harmonic, implying that no source term is needed for the steady state heat equation with constant conductivity.

For each mesh, the errors in the temperature solution are computed in the L^2, L^∞ and H^1 norms. The test passes, only if the observed rates of convergence in these norms are 2, 2, and 1, respectively (within a tolerance).

These rates are observed for the hex-hex case; however, both of the cases involving tet meshes exhibit a reduced order of convergence in the L^∞ norms (convergence rate about 1.7).

For input decks see Appendix 12.3.2.

4.2.5. Results: Hex8-Hex8 Contact



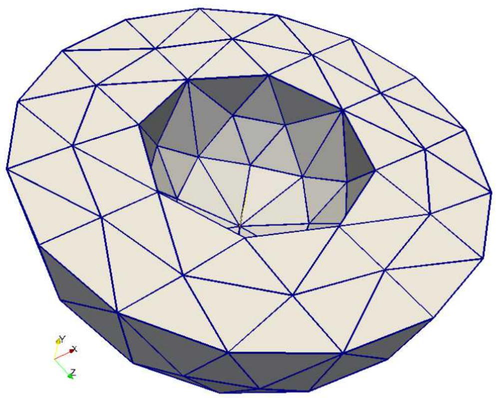
Coarse Mesh Error Norms

Figure 4.2-1.. 3D Curved Contact: Hex8-Hex8 Case

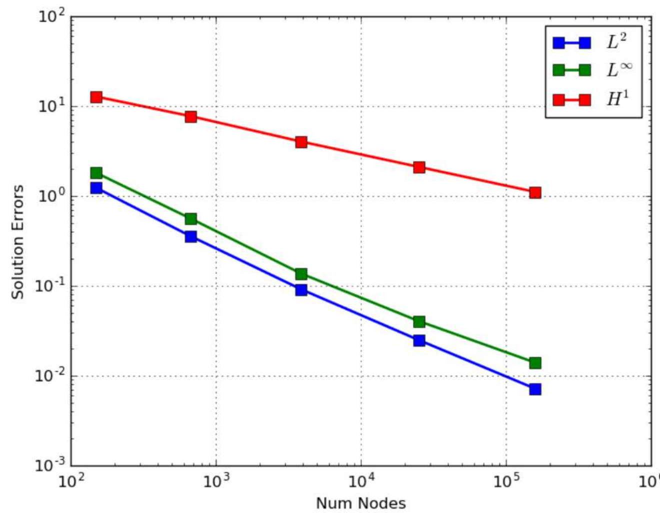
Table 4.2-1.. 3D Curved Contact: Convergence Rates for Hex8-Hex8

Num Dofs	L^2	L^∞	H^1
540	3.16	2.60	0.96
3752	2.32	1.93	1.25
21220	2.62	2.66	1.07
150700	2.35	2.05	1.06

4.2.6. Results: Tet4-Tet4 Contact



Coarse Mesh



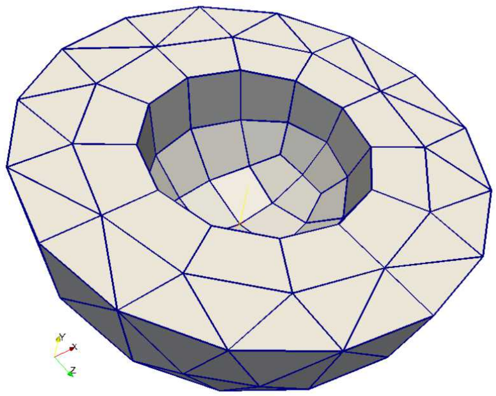
Error Norms

Figure 4.2-2.. 3D Curved Contact: Tet4-Tet4 Case

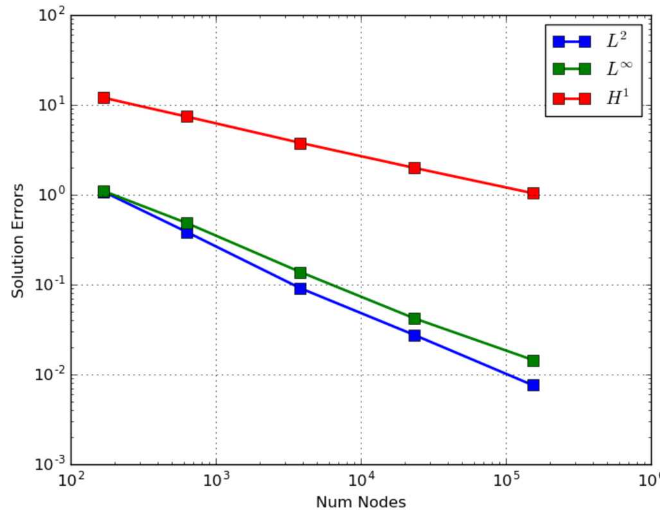
Table 4.2-2.. 3D Curved Contact: Convergence Rates for Tet4-Tet4

Num Dofs	L^2	L^∞	H^1
674	2.47	2.34	1.00
3881	2.33	2.41	1.11
25010	2.09	1.96	1.04
159100	2.02	1.73	1.04

4.2.7. Results: Hex8-Tet4 Contact



Coarse Mesh



Error Norms

Figure 4.2-3.. 3D Curved Contact: Hex8-Tet4 Case

Table 4.2-3.. 3D Curved Contact: Convergence Rates for Hex8-Tet4

Num Dofs	L^2	L^∞	H^1
630	2.34	1.87	1.11
3830	2.40	2.09	1.12
23420	1.98	1.97	1.06
153700	2.06	1.70	1.04

4.3. STEADY HEX8 CONTACT

This problem tests basic steady state heat conduction in a 3D domain. The geometry consists of a unit cube.

4.3.1. Features Tested

Basic heat conduction on Hex8 meshes; dirichlet, heat flux, and convective flux boundary conditions; constant source terms; heat flux and source term from Encore user subroutines.

4.3.2. Boundary Conditions

At surfaces 4 and 6, the temperature is prescribed as a constant value. On surfaces 3 and 5, a heat flux condition is prescribed using a sum of a constant heat flux and a heat flux from an Encore function (user subroutine). On surfaces 1 and 2, heat flux condition is prescribed using a sum of a convective flux boundary condition (with constant flux and convective coefficient) and a heat flux from an Encore function (user subroutine). Within the domain a source term is prescribed using a sum of a constant source and an Encore function (user subroutine).

4.3.3. Material Parameters

The values of density, thermal conductivity, and specific heat are all constant, equal to one in both blocks.

4.3.4. Verification of Solution

A manufactured solution is chosen as

$$T(x, y, z) = 1 + (x - x^2)^2(y - y^2)^2(z - z^2)^2.$$

The source and heat flux user subroutines are chosen so that the solution satisfies the heat equation with the correct boundary conditions.

For each mesh, the errors in the temperature solution are computed in the L^2, L^∞ and H^1 norms. The test passes, only if the observed rates of convergence in these norms are 2, 2, and 1, respectively (within a tolerance).

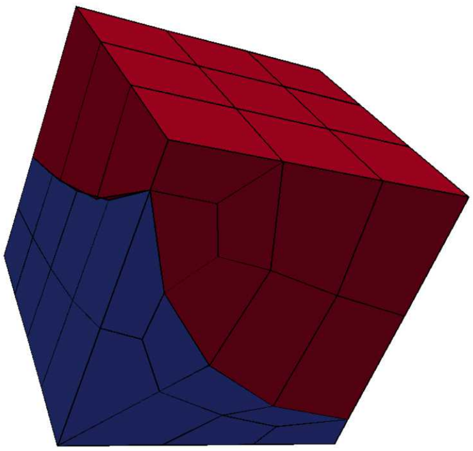
Table 4.3-1.. Steady Tied Contact: Convergence Rates for Hex8 Meshes

Num Dofs	L^2	H^1	L^∞
192	0.86	-0.44	0.60
982	2.22	0.97	2.39
6419	2.31	1.07	2.28
46280	2.06	1.04	1.71
350600	1.95	1.02	2.08

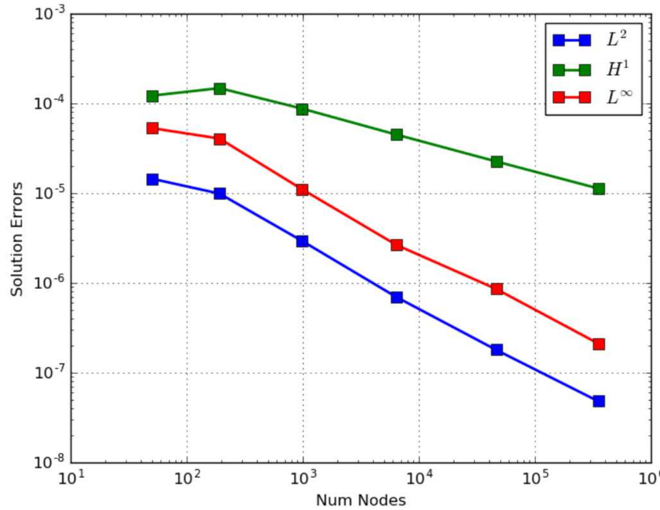
For input decks see Appendix 12.3.3.

4.4. STEADY HEX20 CONTACT

This problem tests basic steady state heat conduction in a 3D domain. The geometry consists of a unit cube. A variety of different source terms and boundary conditions are simultaneously applied. The exact solution is a manufactured solution.



Coarse Mesh



Error Norms

Figure 4.3-1.. Steady Tied Contact: Hex8 Meshes

4.4.1. Features Tested

Basic heat conduction on Hex20 meshes; dirichlet, heat flux, and convective flux boundary conditions; constant source terms; heat flux and source term from Encore user subroutines.

4.4.2. Boundary Conditions

At surfaces 4 and 6, the temperature is prescribed as a constant value. On surfaces 3 and 5, a heat flux condition is prescribed using a sum of a constant heat flux and a heat flux from an Encore function (user subroutine). On surfaces 1 and 2, heat flux condition is prescribed using a sum of a convective flux boundary condition (with constant flux and convective coefficient) and a heat flux from an Encore function (user subroutine). Within the domain a source term is prescribed using a sum of a constant source and an Encore function (user subroutine).

4.4.3. Material Parameters

The values of density, thermal conductivity, and specific heat are all constant, equal to one in both blocks.

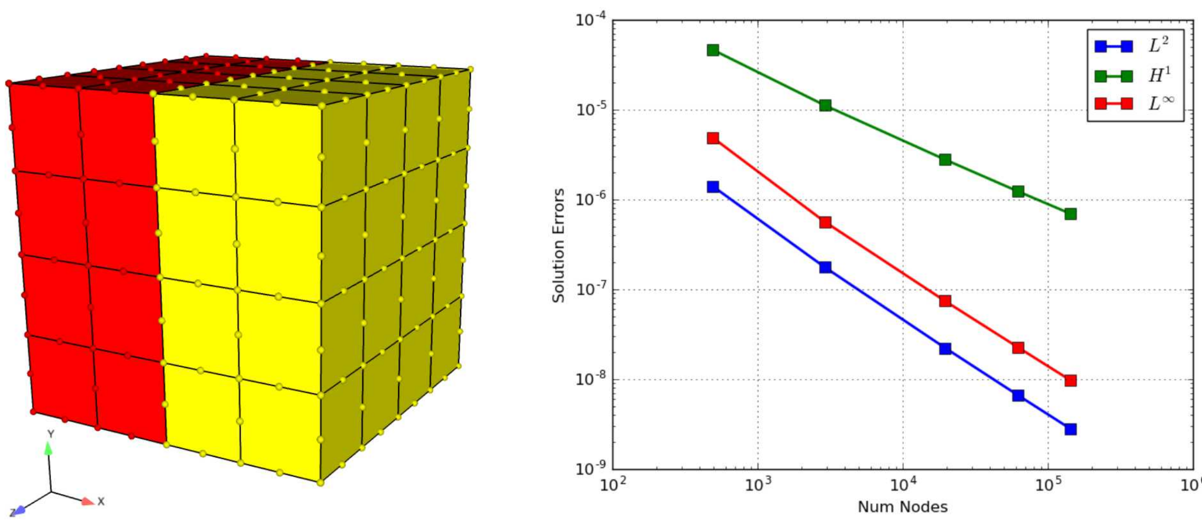
4.4.4. Verification of Solution

A manufactured solution is chosen as

$$T(x, y, z) = 1 + (x - x^2)^2(y - y^2)^2(z - z^2)^2.$$

The source and heat flux user subroutines are chosen so that the solution satisfies the heat equation with the correct boundary conditions.

For each mesh, the errors in the temperature solution are computed in the L^2, L^∞ and H^1 norms. The test passes, only if the observed rates of convergence in these norms are 2, 2, and 1, respectively (within a tolerance).



Coarse Mesh   Error Norms

Figure 4.4-1.. Steady Heat Conduction: Hex20 Meshes

Table 4.4-1.. Steady Heat Conduction: Convergence Rates for Hex20 Meshes

Num Dofs	L^2	H^1	L^∞
2898	3.50	2.40	3.64
19620	3.25	2.19	3.19
62450	3.15	2.10	3.08
143700	3.10	2.07	3.04

For input decks see Appendix 12.3.4.

4.5. STEADY HEX27 CONTACT

This problem tests basic steady state heat conduction in a 3D domain. The geometry consists of a unit cube. A variety of different source terms and boundary conditions are simultaneously applied. The exact solution is a manufactured solution.

4.5.1. Features Tested

Basic heat conduction on Hex27 meshes; dirichlet, heat flux, and convective flux boundary conditions; constant source terms; heat flux and source term from Encore user subroutines.

4.5.2. Boundary Conditions

At surfaces 4 and 6, the temperature is prescribed as a constant value. On surfaces 3 and 5, a heat flux condition is prescribed using a sum of a constant heat flux and a heat flux from an Encore function (user subroutine). On surfaces 1 and 2, heat flux condition is prescribed using a sum of a convective flux boundary condition (with constant flux and convective coefficient) and a heat flux from an Encore function (user subroutine). Within the domain a source term is prescribed using a sum of a constant source and an Encore function (user subroutine).

4.5.3. Material Parameters

The values of density, thermal conductivity, and specific heat are all constant, equal to one in both blocks.

4.5.4. Verification of Solution

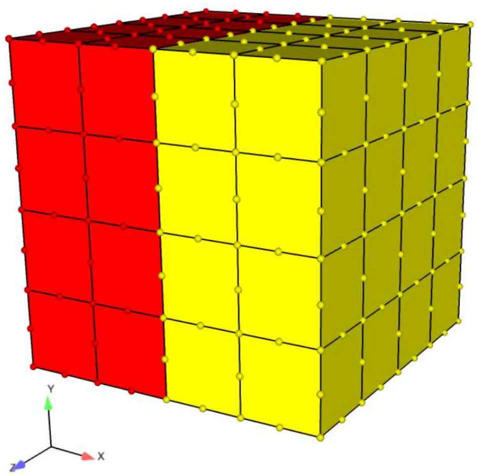
A manufactured solution is chosen as

$$T(x, y, z) = 1 + (x - x^2)^2(y - y^2)^2(z - z^2)^2.$$

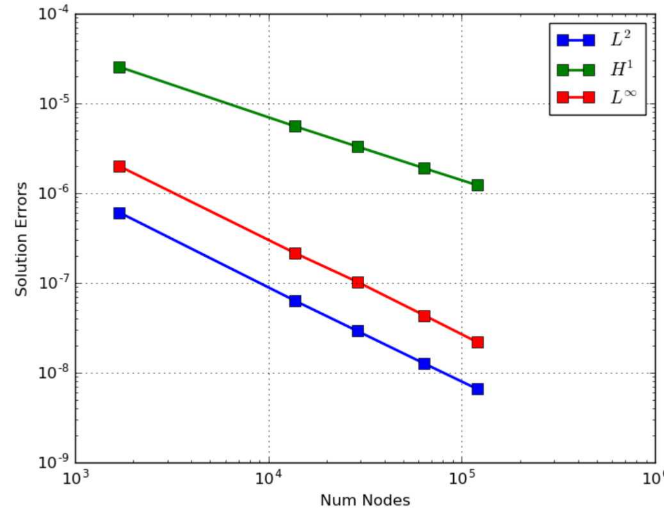
The source and heat flux user subroutines are chosen so that the solution satisfies the heat equation with the correct boundary conditions.

For each mesh, the errors in the temperature solution are computed in the L^2, L^∞ and H^1 norms. The test passes, only if the observed rates of convergence in these norms are 2, 2, and 1, respectively (within a tolerance).

For input decks see Appendix 12.3.5.



Coarse Mesh



Error Norms

Figure 4.5-1.. Steady Heat Conduction: Hex27 Meshes

Table 4.5-1.. Steady Heat Conduction: Convergence Rates for Hex27 Meshes

Num Dofs	L^2	H^1	L^∞
13750	3.25	2.18	3.19
28830	3.13	2.10	2.97
63880	3.14	2.09	3.25
120000	3.11	2.07	3.26

4.6. STEADY TET4 CONTACT

This problem is identical to the one in Section 2.1 except that unstructured Tet4 meshes are used instead.

4.6.1. Features Tested

Basic heat conduction on Tet4 meshes; dirichlet, heat flux, and convective flux boundary conditions; constant source terms; heat flux and source term from Encore user subroutines.

4.6.2. Boundary Conditions

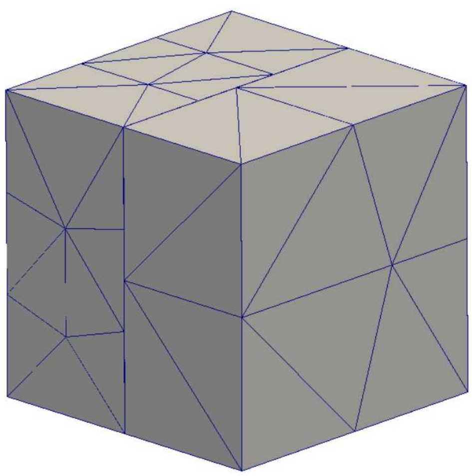
Same as in Section 2.1.

4.6.3. Material Parameters

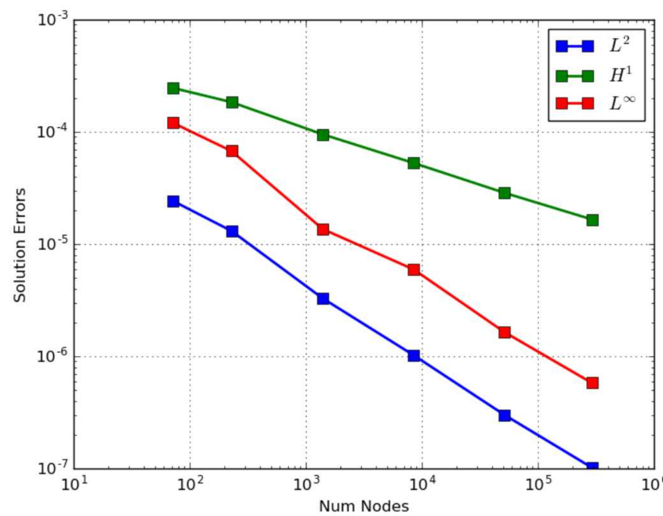
The values of density, thermal conductivity, and specific heat are all constant, equal to one in both blocks.

4.6.4. Verification of Solution

Same as in Section 2.1.



Coarse Mesh



Error Norms

Figure 4.6-1.. Steady Tied Contact: Tet4 Meshes

Table 4.6-1.. Steady Tied Contact: Convergence Rates for Tet4 Meshes

Num Dofs	L^2	H^1	L^∞
229	1.60	0.76	1.48
1402	2.29	1.09	2.65
8535	1.93	0.98	1.38
51620	2.05	1.02	2.14
291200	1.88	0.94	1.81

For input decks see Appendix 12.3.6.

4.7. STEADY TET4TET10 CONTACT

This problem is identical to the one in Section 2.1 except that unstructured Tet4 meshes are used instead.

4.7.1. Features Tested

Basic heat conduction on Tet4 meshes; dirichlet, heat flux, and convective flux boundary conditions; constant source terms; heat flux and source term from Encore user subroutines.

4.7.2. Boundary Conditions

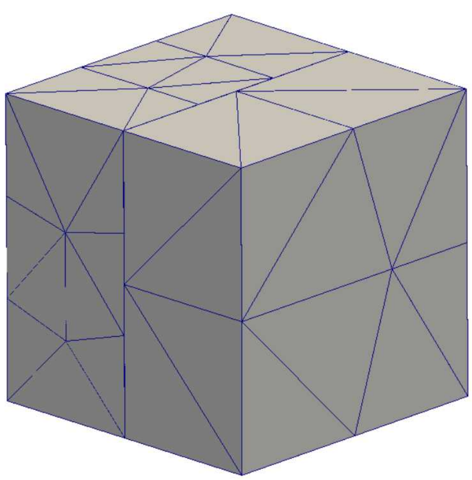
Same as in Section 2.1.

4.7.3. Material Parameters

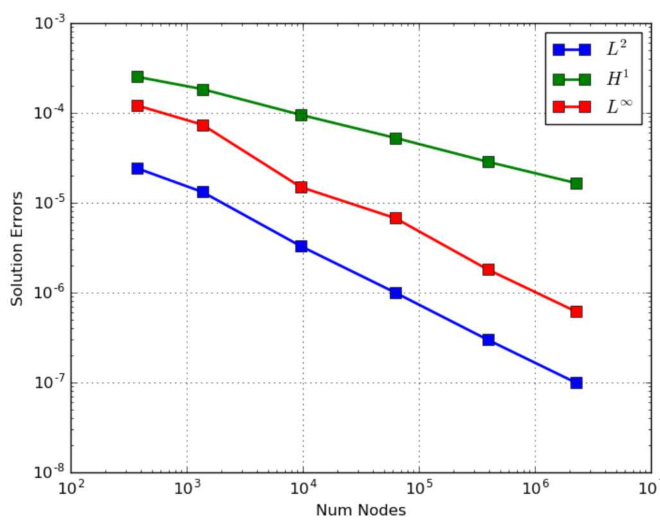
The values of density, thermal conductivity, and specific heat are all constant, equal to one in both blocks.

4.7.4. Verification of Solution

Same as in Section 2.1.



Coarse Mesh



Error Norms

Figure 4.7-1.. Steady Tied Contact: Tet4 Meshes

For input decks see Appendix 12.3.7.

Table 4.7-1.. Steady Tied Contact: Convergence Rates for Tet4 Meshes

Num Dofs	L^2	H^1	L^∞
1364	1.40	0.72	1.13
9663	2.14	1.02	2.46
62720	1.90	0.94	1.27
392000	1.98	1.00	2.16
2250000	1.89	0.93	1.84

4.8. STEADY TET10 CONTACT

This problem is identical to the one in Section 2.1 except that unstructured Tet10 meshes are used instead.

4.8.1. Features Tested

Basic heat conduction on Tet10 meshes; dirichlet, heat flux, and convective flux boundary conditions; constant source terms; heat flux and source term from Encore user subroutines.

4.8.2. Boundary Conditions

Same as in Section 2.1.

4.8.3. Material Parameters

The values of density, thermal conductivity, and specific heat are all constant, equal to one in both blocks.

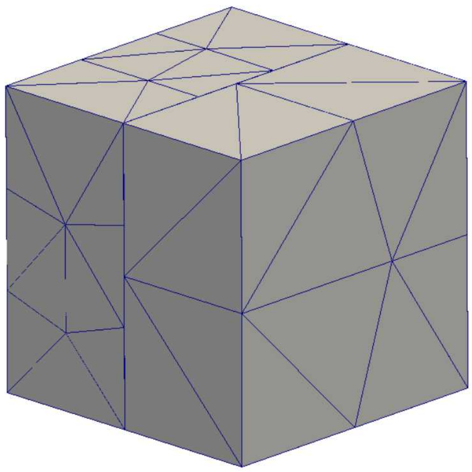
4.8.4. Verification of Solution

Same as in Section 2.1.

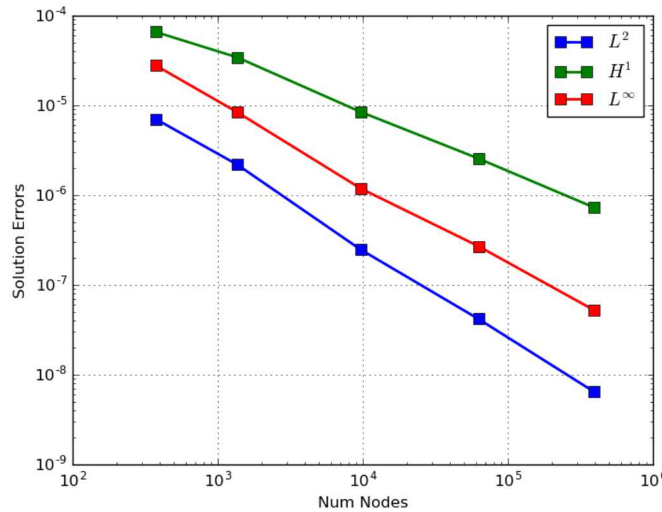
Table 4.8-1.. Steady Tied Contact: Convergence Rates for Tet10 Meshes

Num Dofs	L^2	H^1	L^∞
1364	2.71	1.51	2.78
9663	3.34	2.14	2.99
62720	2.86	1.92	2.39
392000	3.06	2.05	2.68

For input decks see Appendix 12.3.8.



Coarse Mesh



Error Norms

Figure 4.8-1.. Steady Tied Contact: Tet10 Meshes

4.9. STEADY TET10 DASH CONTACT

This problem is identical to the one in Section 2.1 except that unstructured Tet10 meshes are used instead.

4.9.1. Features Tested

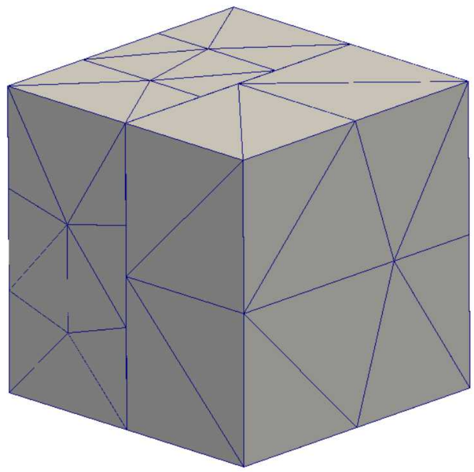
Basic heat conduction on Tet10 meshes; dirichlet, heat flux, and convective flux boundary conditions; constant source terms; heat flux and source term from Encore user subroutines.

4.9.2. Boundary Conditions

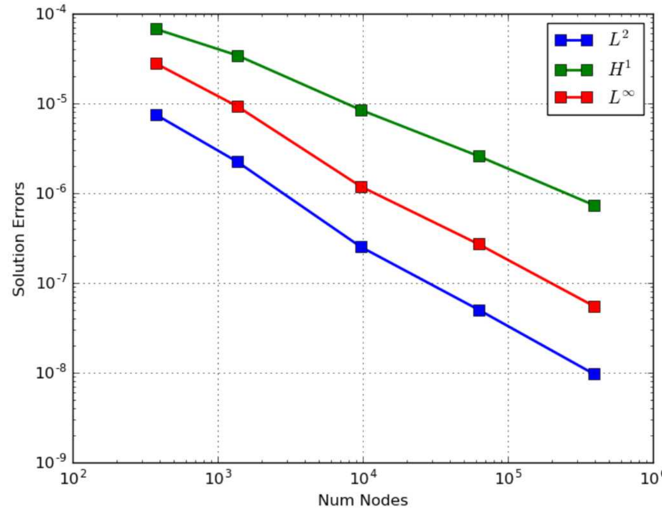
Same as in Section 2.1.

4.9.3. Material Parameters

The values of density, thermal conductivity, and specific heat are all constant, equal to one in both blocks.



Coarse Mesh



Error Norms

Figure 4.9-1.. Steady Tied Dash Contact: Tet10 Meshes

Table 4.9-1.. Steady Tied DASH Contact: Convergence Rates for Tet10 Meshes

Num Dofs	L^2	H^1	L^∞
1364	2.80	1.57	2.55
9663	3.34	2.14	3.14
62720	2.59	1.91	2.38
392000	2.70	2.06	2.61

4.9.4. Verification of Solution

Same as in Section 2.1.

For input decks see Appendix 12.3.9.

4.10. TRANSIENT TET4TET10 CONTACT

This problem tests basic transient heat conduction with contact in a 3D domain. The geometry consists of two halves of a unit cube meshed with Tet10 elements. The problem is solved using Tet4 interpolation and applying thermal contact at the common interface between the two domains.

4.10.1. Features Tested

Basic heat conduction on Tet10 meshes; dirichlet, heat flux, and convective flux boundary conditions; constant source terms; heat flux and source term from Encore user subroutines.

4.10.2. Boundary Conditions

Using a manufactured solution, Dirichlet boundary conditions are applied on all the non-contact exposed faces.

4.10.3. Material Parameters

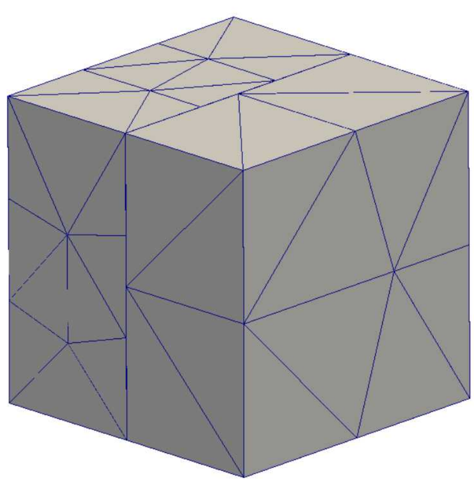
The values of density, thermal conductivity, and specific heat are all constant, equal to one in both blocks.

4.10.4. Verification of Solution

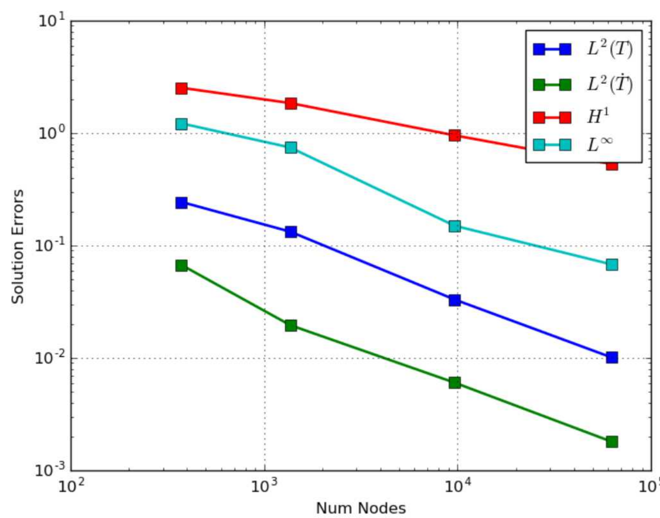
A manufactured solution is chosen as

$$
\begin{aligned}
T(x,y,z,t) &= (x-x^2)^2\,(y-y^2)^2\,(z-z^2)^2 m(t) + 1, \\
m(t) &= 10^4\,\left[1. - \exp(-t) + t * \exp(-(t-1.0)*(t-1.0))\right];
\end{aligned}
$$

The source and heat flux user subroutines are chosen so that the solution satisfies the heat equation with the correct boundary conditions.



Coarse Mesh



Error Norms

Figure 4.10-1.. Transient Tied Contact: Tet10 Meshes

For input decks see Appendix 12.3.10.

Table 4.10-1.. Transient Tied Contact: Convergence Rates for Tet10 Meshes

Num Dofs	$L^2(T)$	$L^2(\dot{T})$	H^1	L^∞
1364	1.41	2.85	0.72	1.14
9663	2.13	1.81	1.02	2.46
62720	1.90	1.94	0.94	1.27

4.11. TRANSIENT TET10 CONTACT

This problem tests basic transient heat conduction with contact in a 3D domain. The geometry consists of two halves of a unit cube meshed with Tet10 elements. The problem is solved by applying thermal contact at the common interface between the two domains.

4.11.1. Features Tested

Basic heat conduction on Tet10 meshes; dirichlet, heat flux, and convective flux boundary conditions; constant source terms; heat flux and source term from Encore user subroutines.

4.11.2. Boundary Conditions

Using a manufactured solution, Dirichlet boundary conditions are applied on all the non-contact exposed faces.

4.11.3. Material Parameters

The values of density, thermal conductivity, and specific heat are all constant, equal to one in both blocks.

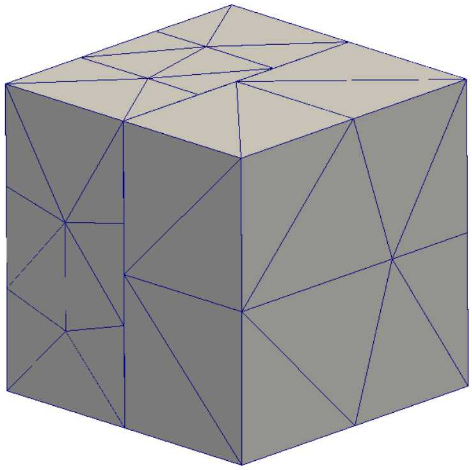
4.11.4. Verification of Solution

A manufactured solution is chosen as

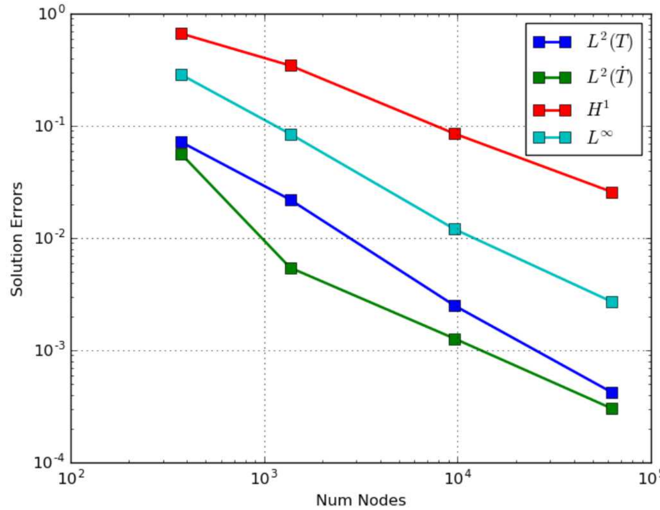
$$\begin{aligned} T(x,y,z,t) &= (x-x^2)^2\,(y-y^2)^2\,(z-z^2)^2 m(t) + 1, \\ m(t) &= 10^4\,\left[1. - \exp(-t) + t * \exp(-(t-1.0)*(t-1.0))\right]; \end{aligned}$$

The source and heat flux user subroutines are chosen so that the solution satisfies the heat equation with the correct boundary conditions.

For input decks see Appendix 12.3.11.



Coarse Mesh



Error Norms

Figure 4.11-1.. Transient Tied Contact: Tet10 Meshes

Table 4.11-1.. Transient Tied Contact: Convergence Rates for Tet10 Meshes

Num Dofs	$L^2(T)$	$L^2(\dot{T})$	H^1	L^∞
1364	2.73	5.40	1.51	2.81
9663	3.33	2.23	2.14	3.00
62720	2.85	2.30	1.92	2.39

4.12. TRANSIENT HEX8 TIED CONTACT

This problem tests transient heat conduction on a 3D domains with a nonconformal mesh between two blocks. Tied temperature (generalized contact) is used for matching the energy equation between nonconformal blocks. The geometry consists of a unit cube.

4.12.1. Features Tested

Transient heat conduction on Hex8 meshes; dirichlet, heat flux, and convective flux boundary conditions, Tied Contact, Nonconformal; constant source terms; heat flux and source term from Encore user subroutines.

4.12.2. Boundary Conditions

At surfaces 4 and 6, the temperature is prescribed as a constant value. On surfaces 3 and 5, a heat flux condition is prescribed using a sum of a constant heat flux and a heat flux from an Encore function (user subroutine). On surfaces 1 and 2, heat flux condition is prescribed using a sum of a convective flux boundary condition (with constant flux and convective coefficient) and a heat flux from an Encore function (user subroutine). Within the domain a source term is prescribed using a sum of a constant source and an Encore function (user subroutine). On the two interior surfaces connecting the nonconformal blocks (surfaces 7 and 8), a contact definition is defined as tied temperature.

4.12.3. Material Parameters

The values of density, thermal conductivity, and specific heat are all constant, equal to one in both blocks.

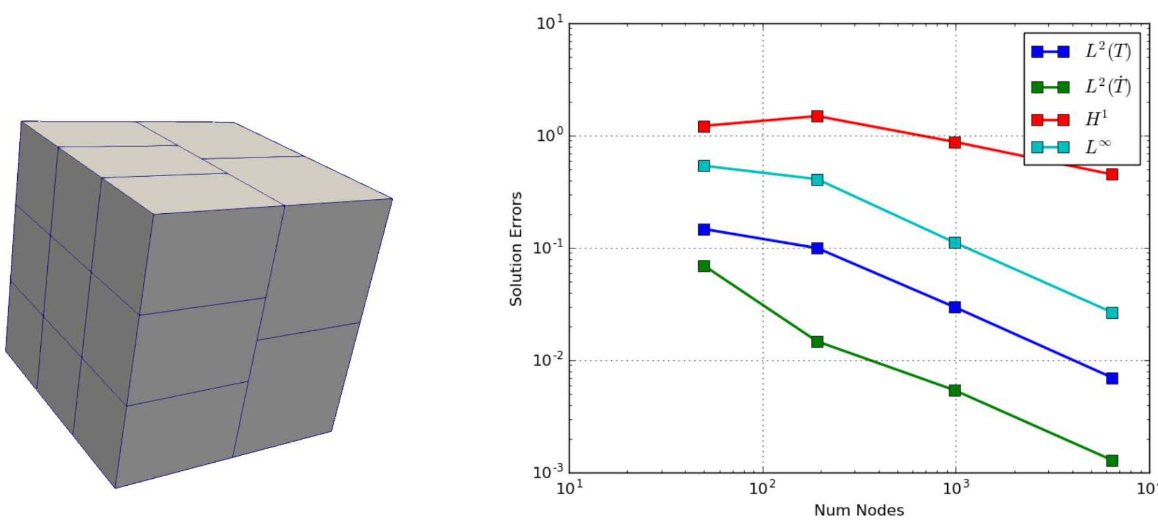
4.12.4. Verification of Solution

A manufactured solution is chosen as

$$
\begin{aligned}
T(x,y,z,t) &= (x-x^2)^2\,(y-y^2)^2\,(z-z^2)^2 m(t) + 1,\\
m(t) &= 10^4\,(1-\exp(-t) + t\,\exp(-(t-1)^2))
\end{aligned}
$$

The source and heat flux user subroutines are chosen so that the solution satisfies the heat equation with the correct boundary conditions.

For each mesh, the errors in the temperature solution at final time are computed in the L^2 norm of T and $\dot{T}$, L^∞ and H^1 norms. The test passes, only if the observed rates of convergence in these norms are 2, 2, 2 and 1, respectively (within a tolerance).



Coarse Mesh Error Norms

Figure 4.12-1.. Tied Contact Transient Heat Conduction: Hex8 Meshes

Table 4.12-1.. Tied Contact Transient Heat Conduction: Convergence Rates for Hex8 Meshes

Num Dofs	$L^2(T)$	$L^2(\dot{T})$	H^1	L^∞
192	0.88	3.46	-0.44	0.61
982	2.22	1.84	0.97	2.39
6419	2.31	2.30	1.07	2.29

4.13. TRANSIENT TET4 TIED CONTACT

This problem tests transient heat conduction and tied thermal contact in a 3D domain as in Section 2.7. The geometry consists of a unit cube that is split along the plane at $x = 0.5$.

4.13.1. Features Tested

Basic transient heat conduction on Tet4 meshes; non-conformal tied thermal contact; dirichlet, heat flux, and convective flux boundary conditions; constant source terms; heat flux and source term from Encore user subroutines.

4.13.2. Boundary Conditions

Identical to Section 2.7.

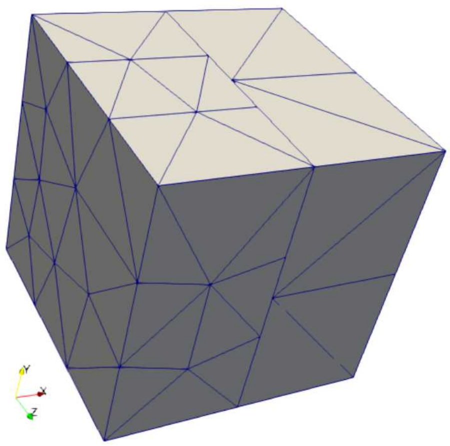
4.13.3. Material Parameters

The values of density, thermal conductivity, and specific heat are all constant, equal to one in both blocks.

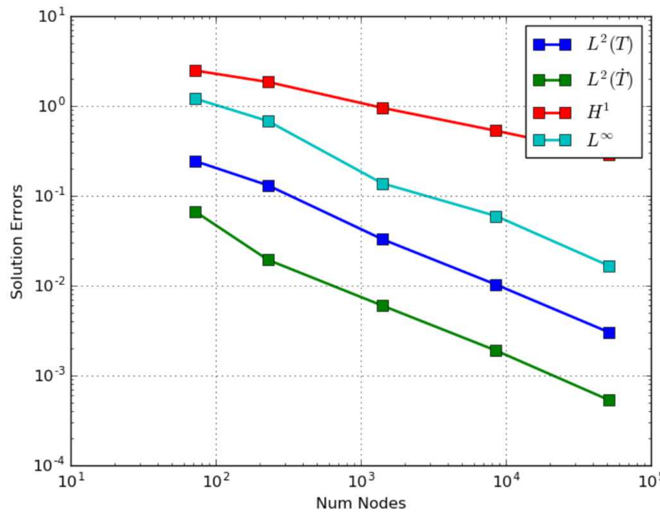
4.13.4. Verification of Solution

A manufactured solution is chosen as in Section 2.7.

For each mesh, the errors in the temperature solution at final time are computed in the L^2 norm of T and $\dot{T}$, L^∞ and H^1 norms. We see convergence rates for $\dot{T}$ that are slightly greater than two.



Coarse Mesh



Error Norms

Figure 4.13-1.. Transient Heat Conduction with Tied Contact: Tet4 Meshes

Table 4.13-1.. Transient Heat Conduction with Tied Contact: Convergence Rates for Tet4 Meshes

Num Dofs	$L^2(T)$	$L^2(\dot{T})$	H^1	L^∞
229	1.61	3.22	0.76	1.49
1402	2.29	1.94	1.10	2.64
8535	1.93	1.91	0.98	1.39
51620	2.05	2.12	1.02	2.14

5. ELEMENT DEATH

5.1. CDFEM ELEMENT DEATH (HEAT FLUX)

This problem tests transient conduction and CDFEM element death using 2D and 3D domains. The geometry consists of a thick 1/4 cylindrical or 1/8 spherical shell.

5.1.1. Features Tested

Transient heat conduction, adaptive second order time integration (BDF2), CDFEM element death, temperature and heat flux boundary conditions, Tri3 and Tet4 meshes.

5.1.2. Boundary Conditions

On one surface, the exact solution is used to specify a time-varying temperature. At the other surface, an analytic heat flux is applied using the exact solution. The erosion of the volume from CDFEM element death causes the surface with the heat flux BC to gradually recede as the material is removed.

5.1.3. Material Parameters

The values of density, thermal conductivity, and specific heat are all constant, equal to one in both blocks.

5.1.4. Verification of Solution

A manufactured solution T and exact source term S are chosen in 2D to be:

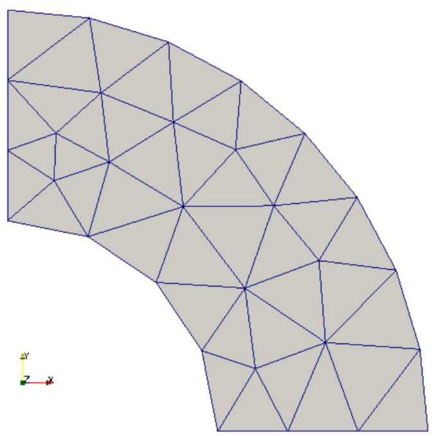
$$T(r,t) = \frac{\ln(r)}{\ln(2-t)}, \quad S(r,t) = \frac{\ln(r)}{(\ln(2-t))^2(2-t)}$$

and in 3D to be:

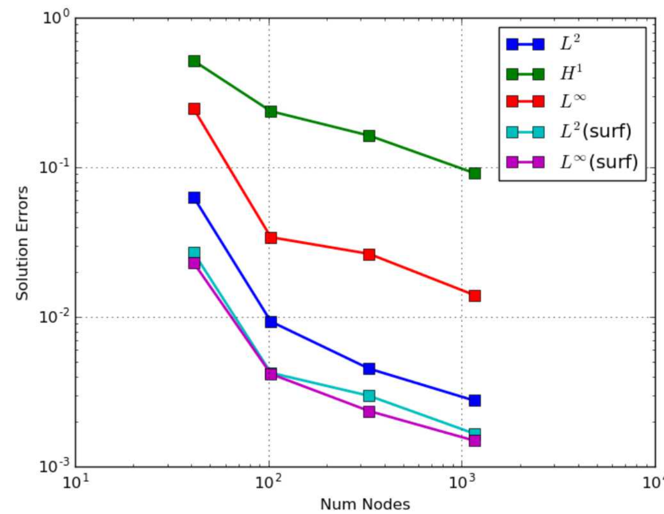
$$T(r,t) = (1+t)/r, \quad S(r,t) = 1/r.$$

For each mesh, the errors in the temperature solution are computed in the L^2, L^∞ and H^1 norms over the volume, and in the L^2 and L^∞ norms over the outer surface. The test passes, only if the observed rates of convergence in these norms are one (within a tolerance). First order convergence is expected in this case, due to the nature of the coupling of the CDFEM mesh decomposition and the heat conduction solve.

5.1.5. Results: Tri3



Coarse Mesh



Error Norms

Figure 5.1-1.. CDFEM Element Death (Heat Flux): Tri3

Table 5.1-1.. CDFEM Element Death (Heat Flux): Convergence Rates for Tri3

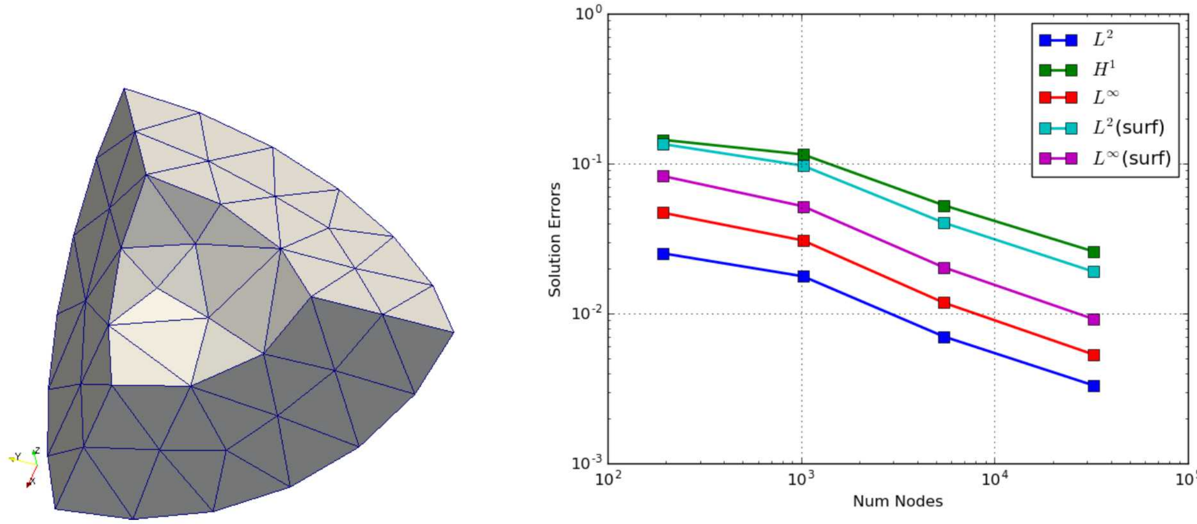
Num Dofs	L^2	H^1	L^∞	L^2(surf)	L^∞(surf)
103	4.16	1.69	4.30	4.03	3.73
332	1.24	0.64	0.44	0.60	0.98
1163	0.78	0.93	1.01	0.93	0.73

5.1.6. Results: Tet4

Table 5.1-2.. CDFEM Element Death (Heat Flux): Convergence Rates for Tet4

Num Dofs	L^2	H^1	L^∞	L^2(surf)	L^∞(surf)
1024	0.63	0.39	0.76	0.60	0.83
5470	1.66	1.40	1.71	1.57	1.68
32588	1.27	1.19	1.34	1.27	1.34

For input decks see Appendix 12.4.1.



Coarse Mesh Error Norms

Figure 5.1-2.. CDFEM Element Death (Heat Flux): Tet4

5.2. 3D SPHERICAL SHELL ENCLOSURE

5.2.1. Problem Description

This problem tests transient conduction, enclosure radiation, and CDFEM element death. The initial geometry of this problem is a hollow sphere (block 2) inside and in contact with a second hollow sphere (block 1). The geometry is such that the solution maintains radial symmetry. The inner sphere decomposes at a specific failure temperature, resulting in a changing enclosure geometry.

5.2.2. Features Tested

Transient heat conduction, enclosure radiation, CDFEM element death, Tet4 meshes.

5.2.3. Boundary and Initial Conditions

The initial condition is a piecewise steady state temperature distribution defined below in (5.1). The boundary conditions specify the temperature T_4 at the outer surface (4) of the outer sphere and T_1 at the inner surface (1) of the inner sphere. The inner temperature T_1 will be gradually increased, while T_4 remains constant in time.

An enclosure is defined initially using the outer surface of the inner volume (surface 2 of block 2) and the inner surface of the outer volume (surface 3 of block 1). The erosion of the inner volume (block 2) from CDFEM element death causes surface 2 to gradually recede as the material within block 2 is removed.

Dimensions are defined in Table 5.2-1.

Table 5.2-1.. Dimensions of problem

radius of surface_1	r_1	0.01
radius of surface_2	r_2	0.02
radius of surface_3	r_3	0.03
radius of surface_4	r_4	0.04

5.2.4. Material Parameters

Material properties are shown in Table 5.2-2.

Table 5.2-2.. Material properties

Thermal conductivity	κ	1.0
Density	ρ	7682.0
Specific heat	C_p	10.0
emissivity (inner)	ϵ_2	0.6
emissivity (outer)	ϵ_3	0.7
Stefan-Boltzmann constant	σ	5.6704e-8
failure temperature (block 2)	T_c	867.011674920813

5.2.5. Verification of Solution

The solution after failure occurs is specified using inner and outer temperature solutions of the form:

$$T_i(r) \equiv T_1 + (T_c - T_1)\frac{1/r - 1/r_1}{1/r_2 - 1/r_1}, \quad r_1 \le r \le r_2, \tag{5.1}$$

$$T_o(r) \equiv C_o + (T_4 - C_o)\frac{1/r - 1/r_3}{1/r_4 - 1/r_3}, \quad r_3 \le r \le r_4 \tag{5.2}$$

Here all parameters are known except r_2 and C_o, which will vary with time. The initial value of r_2 is given in Table 5.2-1; the initial value of C_o is chosen to satisfy the enclosure radiation equilibrium equations below.

To complete the solution, we now derive a system of two nonlinear equations to solve for r_2 and C_o. These are the energy balances on the outer and inner enclosure surfaces, given by

$$R_2 \equiv q_2 - \sigma\epsilon_2 T_2^4 + \epsilon_2(F_{22}J_2 + F_{23}J_3) \tag{5.3}$$

$$R_3 \equiv -q_3 - \sigma\epsilon_3 T_3^4 + \epsilon_3(F_{32}J_2 + F_{33}J_3) \tag{5.4}$$

where the three terms in each equation represent fluxes from conduction, radiative emission, and radiative reflection. The conductive fluxes are defined by Fourier's law as

$$
\begin{aligned}
q_2 &= -\kappa_2 \frac{\partial T_i}{\partial r}|_{r=r_2} = \kappa_2 \frac{T_c - T_1}{r_1^2(1/r_2 - 1/r_1)} &(5.5)\\
q_3 &= -\kappa_3 \frac{\partial T_o}{\partial r}|_{r=r_3} = \kappa_3 \frac{T_4 - C_o}{r_3^2(1/r_4 - 1/r_3)} &(5.6)
\end{aligned}
$$

The surface temperatures are

$$T_2 \equiv T_i|_{r=r_2} = T_c, \quad T_3 \equiv T_o|_{r=r_3} = C_o$$

The radiosities are obtained by solving the linear system for enclosure radiation

$$\begin{bmatrix} 1-(1-\epsilon_2)F_{22} & -(1-\epsilon_2)F_{23} \\ -(1-\epsilon_3)F_{32} & 1-(1-\epsilon_3)F_{33} \end{bmatrix} \begin{bmatrix} J_2 \\ J_3 \end{bmatrix} = \begin{bmatrix} \sigma\epsilon_2 T_2^4 \\ \sigma\epsilon_3 T_3^4 \end{bmatrix}$$

to obtain

$$\begin{bmatrix} J_2 \\ J_3 \end{bmatrix} = \frac{1}{\mathrm{a}} \begin{bmatrix} 1-(1-\epsilon_3)F_{33} & (1-\epsilon_2)F_{23} \\ (1-\epsilon_3)F_{32} & 1-(1-\epsilon_2)F_{22} \end{bmatrix} \begin{bmatrix} \sigma\epsilon_2 T_2^4 \\ \sigma\epsilon_3 T_3^4 \end{bmatrix}$$

where a is the determinant

$$a = (1-(1-\epsilon_2)F_{22})(1-(1-\epsilon_3)F_{33}) - (1-\epsilon_2)F_{23}(1-\epsilon_3)F_{32}$$

The viewfactor coefficients F_{ij} are given by

$$F_{22} = 0, \quad F_{23} = 1, \quad F_{32} = (r_2/r_3)^2, \quad F_{33} = 1 - F_{32}$$

The specific function we choose for $T_1(t)$ is

$$T_1(t) \equiv T_1 + 400(1 - \cos(\pi t))/2$$

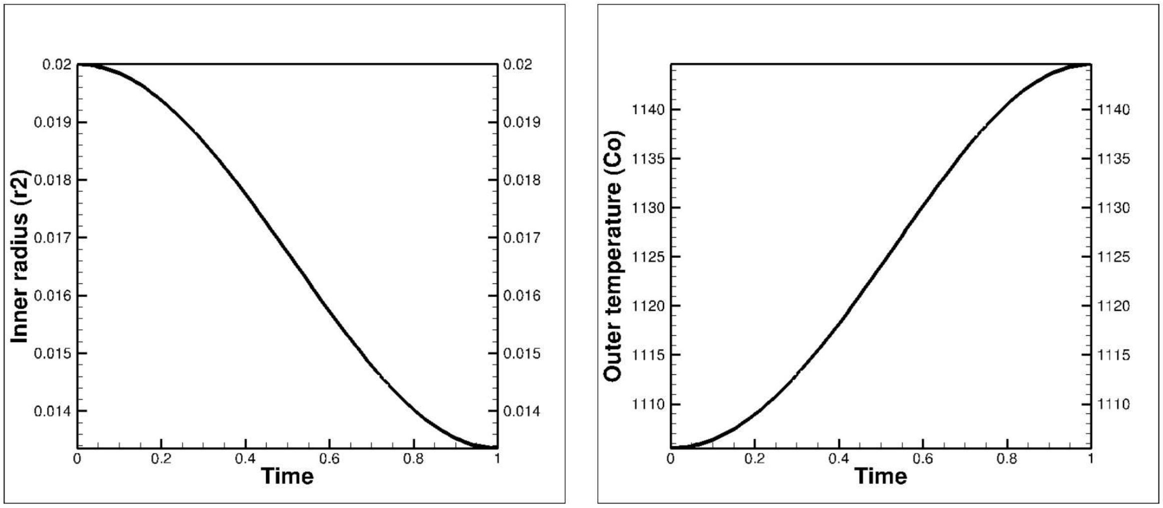
The time histories of r_2 and C_o are shown in Figure 5.2-1.

In order to derive the source term, the time derivatives of r_2 and C_o are computed once the pair of nonlinear equations is solved using Newton's method. Since the spatial part of the piecewise solution is harmonic, the source terms become just $\rho c_p \partial_t T$, where

$$
\begin{aligned}
\partial_t T_i &\equiv \dot{T}_1 + (T_c - \dot{T}_1)\frac{1/r - 1/r_1}{1/r_2 - 1/r_1} + (T_c - T_1)\frac{\dot{r}_2(1/r - 1/r_1)}{r_2^2(1/r_2 - 1/r_1)^2}, \quad r_1 \le r \le r_2, &(5.7)\\
\partial_t T_o &\equiv \dot{C}_o(1 - \frac{1/r - 1/r_3}{1/r_4 - 1/r_3}), \quad r_3 \le r \le r_4 &(5.8)
\end{aligned}
$$

5.2.6. Results

Results are presented running the problem on three meshes up to time $t = 0.9$.



$r_2(t)$ $C_o(t)$

Figure 5.2-1.. Evolution of parameters r_2 and C_o.

Table 5.2-3.. Convergence Rates at $t = 0.9$

Num Dofs	$L^2(T)$	$L^2(\dot{T})$	L^∞	H^1
4307	2.11	2.09	0.83	1.03
25590	2.25	1.52	2.15	1.05
178700	2.03	1.49	1.87	0.99

For input decks see Appendix 12.4.2.

5.3. STANDARD ELEMENT DEATH (HEAT FLUX)

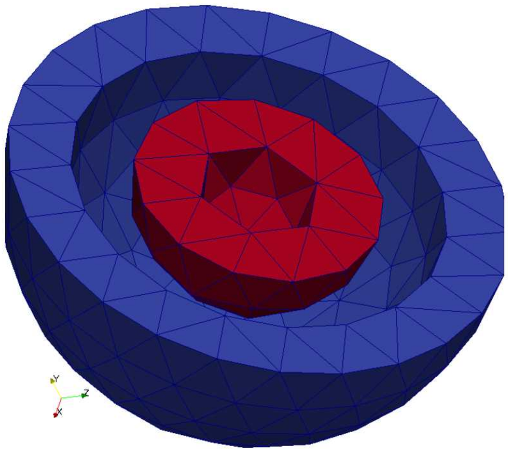
This problem tests transient conduction with standard element death on a 2D square domain than is essentially a 1D problem.

5.3.1. Features Tested

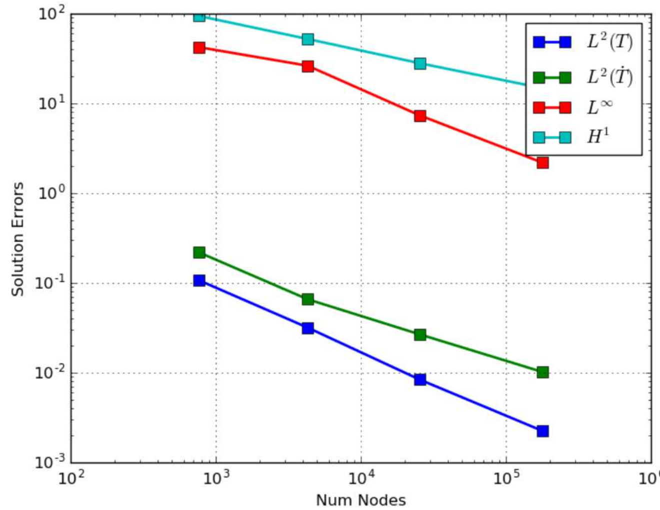
Transient heat conduction, adaptive second order time integration (BDF2), standard element death, temperature and heat flux boundary conditions, Tri3, Hex8 and Quad4 meshes.

5.3.2. Boundary Conditions

On one surface, the exact solution is used to specify a time-varying temperature. At the other surface, an analytic heat flux is applied using the exact solution. The erosion of the volume from element death causes the surface with the heat flux BC to recede element by element as the material is removed.



Coarse Mesh



Error Norms ($t = 0.9$)

5.3.3. Material Parameters

The values of density, thermal conductivity, and specific heat are all constant, equal to one in both blocks.

5.3.4. Verification of Solution

A manufactured solution T and exact source term S are chosen to be:

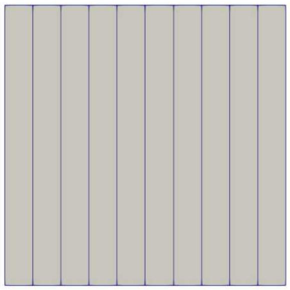
$$T(r, t) = \exp(t - x).$$

For each mesh, the errors in the temperature solution are computed in the L^2, L^∞ and H^1 norms over the area. The test passes, only if the observed rates of convergence in these norms are one (within a tolerance). First order convergence is expected in this case.

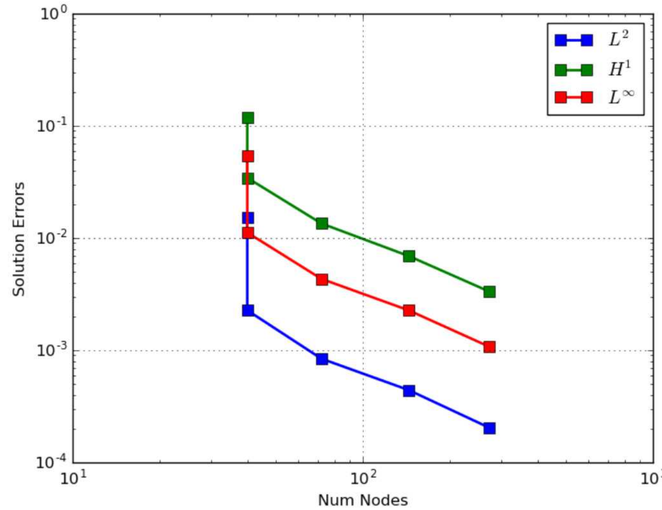
5.3.5. Results: 1D Hex8

Table 5.3-1.. Element Death (Heat Flux): Convergence Rates for Hex8

Num Dofs	Var1	Var2	Var3
40	nan	nan	nan
72	1.69	1.59	1.62
144	0.93	0.96	0.93
272	1.21	1.14	1.17



Coarse Mesh



Error Norms

Figure 5.3-1.. Element Death (Heat Flux): Hex8

5.3.6. Results: 1D Quad4

Table 5.3-2.. Element Death (Heat Flux): Convergence Rates for Quad4

Num Dofs	Var1	Var2	Var3
22	1.38	1.38	1.34
36	1.85	1.52	1.66
68	1.16	1.12	1.13
134	1.09	1.09	1.09

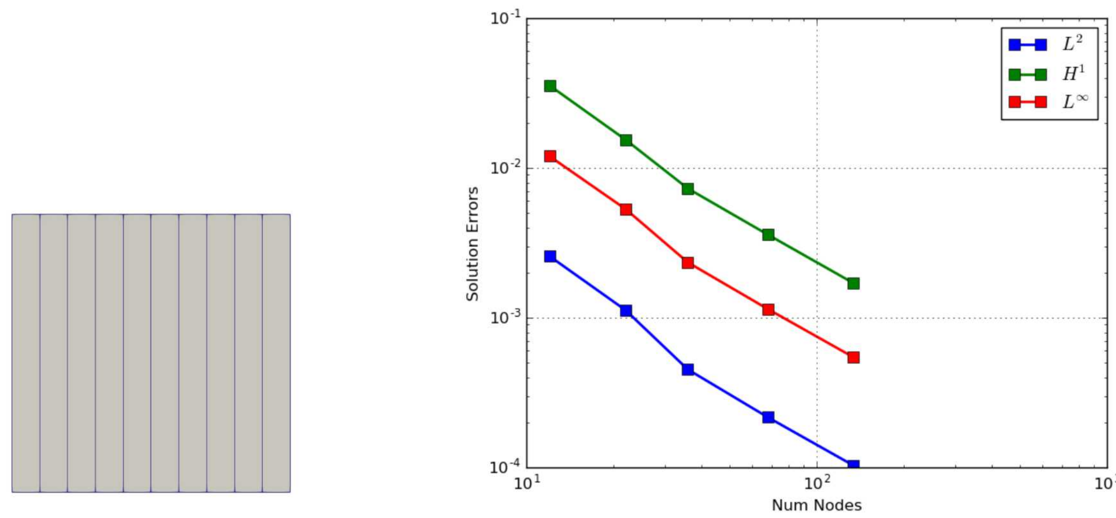
5.3.7. Results: 1D Tri3

Table 5.3-3.. Element Death (Heat Flux): Convergence Rates for Tri3

Num Dofs	Var1	Var2	Var3
20	nan	nan	nan
38	1.43	1.44	1.40
73	1.09	1.04	1.04
138	1.19	1.12	1.17

5.3.8. Results: 2D Quad4

This problem tests transient conduction with standard element death on a 2D quarter slice of an annulus.



Coarse Mesh Error Norms

Figure 5.3-2.. Element Death (Heat Flux): Quad4

5.3.9. Features Tested

Transient heat conduction, fixed first order time integration, standard element death, Quad4 mesh.

5.3.10. Boundary Conditions

On one surface, the exact solution is used to specify a time-varying temperature. On the other surfaces, the exact source solution is provided as the flux boundary condition. The erosion of the volume from element death is caused by having a minimum nodal value of temperature less than 1.

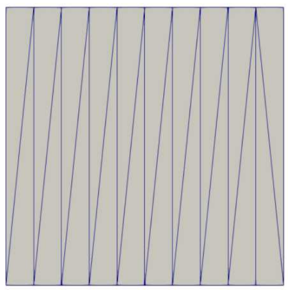
5.3.11. Material Parameters

The values of density, thermal conductivity, and specific heat are all constant, equal to one in both blocks.

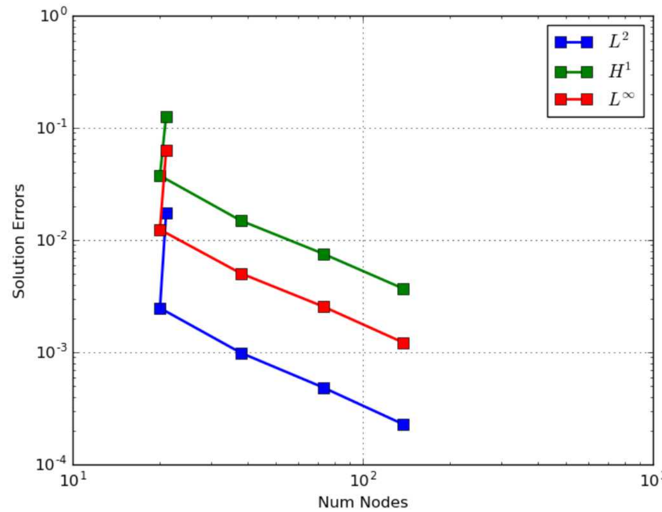
5.3.12. Verification of Solution

A manufactured solution T and exact source term S are chosen to be:

$$T(r,t) = \ln(\sqrt{x^2+y^2})(1/\ln(2-t)).$$



Coarse Mesh



Error Norms

Figure 5.3-3.. Element Death (Heat Flux): Tri3

For each mesh, the errors in the temperature solution are computed in the L^2, L^∞ and H^1 norms over the area. The test passes, only if the observed rates of convergence in these norms are one (within a tolerance). First order convergence is expected in this case.

Table 5.3-4.. 2D Element Death (Heat Flux): Convergence Rates for Quad4

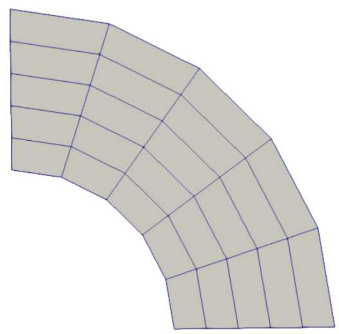
Num Dofs	Var1	Var2	Var3	Var4	Var5
63	4.53	2.35	3.28	16.25	nan
246	0.79	1.10	0.91	-5.66	nan
810	1.45	1.25	1.32	1.16	1.16
2898	1.12	1.02	1.04	1.10	1.08

5.3.13. Results: 3D Hex8

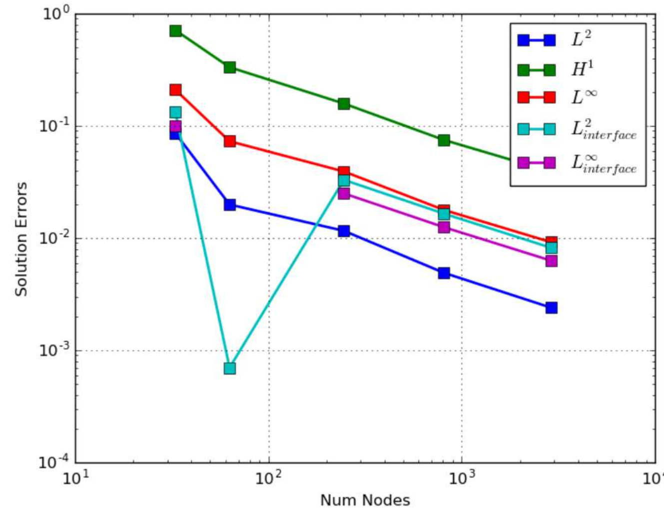
This problem evaluates transient conduction with standard element death on a 3D quarter of a hollow sphere geometry.

5.3.14. Features Tested

Transient heat conduction, fixed first order time integration, standard element death, Hex8 mesh.



Coarse Mesh



Error Norms

Figure 5.3-4.. Element Death (Heat Flux): Quad4

5.3.15. Boundary Conditions

On surface 2, the exact solution is used to specify a time-varying temperature. On all remaining surfaces, a heat flux boundary condition is imposed with a flux time function specified. The erosion of the volume from element death is caused by having a maximum nodal value of temperature greater than 1.

5.3.16. Material Parameters

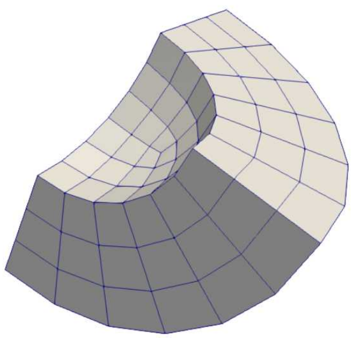
The values of density, thermal conductivity, and specific heat are all constant, equal to one in both blocks.

5.3.17. Verification of Solution

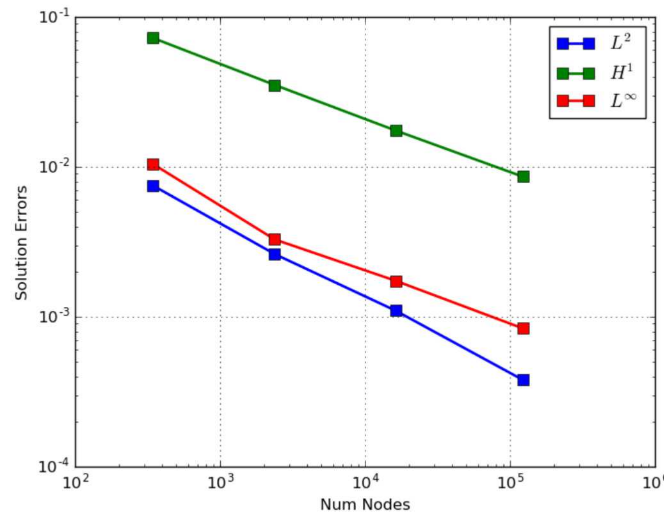
A manufactured solution T and exact source term S are chosen to be:

$$T(r,t) = \frac{1+t}{\sqrt{x^2+y^2+z^2}}.$$

For each mesh, the errors in the temperature solution are computed in the L^2, L^∞ and H^1 norms over the area. The observed rates of convergence in these norms are one (within a tolerance). First order convergence is expected in this case.



Coarse Mesh



Error Norms

Figure 5.3-5.. Element Death (Heat Flux): Hex8

Table 5.3-5.. Element Death (Heat Flux): Convergence Rates for Hex8

Num Dofs	L^2	H^1	L^∞
2382	1.64	1.12	1.80
16214	1.36	1.10	1.00
122892	1.57	1.05	1.08

6. TIME INTEGRATION

6.1. ADAPTIVE TIME INTEGRATION

This problem tests the various implicit time integrators using both fixed and adaptive time stepping. The integrators are first order (Backward Euler), second order (Crank-Nicolson) and BDF2. The geometry is a 2D square.

6.1.1. Features Tested

Transient heat conduction, time integrators, adaptive time stepping, polynomial temperature dependence of density and thermal conductivity.

6.1.2. Boundary Conditions

The boundary conditions are prescribed at the nodes using the analytic solution. The initial condition is specified using an Encore function evaluated at the nodes.

6.1.3. Material Parameters

The specific heat is constant. The density and thermal conductivity are linear polynomials in the temperature.

6.1.4. Verification of Solution

A manufactured solution is chosen as

$$T(x, y, t) = \sin(C_1 t) + 2x\cos(C_2 t) + 3y\sin(C_3 t) + 4xy\cos(C_4 t) + 5x^2\sin(C_5 t) + 6y^2\cos(C_6 t)$$

which requires a source term. This solution is designed to have a non-trivial time-dependence using constants:

$$C_1 = \pi, \quad C_2 = 2\pi, \quad C_3 = 3\pi, \quad C_4 = \pi, \quad C_5 = 2.5\pi, \quad C_6 = 0.5\pi$$

For each mesh, the errors in the temperature solution are computed in the L^2, L^∞ and H^1 norms. The L^2 error in the temperature time derivative is also computed. The test passes, only if the observed rates of convergence in these norms are 1 for H^1 and 2 for all other norms (within a tolerance).

Because the adaptive meshes use less time steps, we use time step size instead of mesh size for estimation of the convergence rates. We also include the L^2 error in the time derivative of the temperature.

For input decks see Appendix 12.5.1.

6.1.5. Results: First Order Fixed

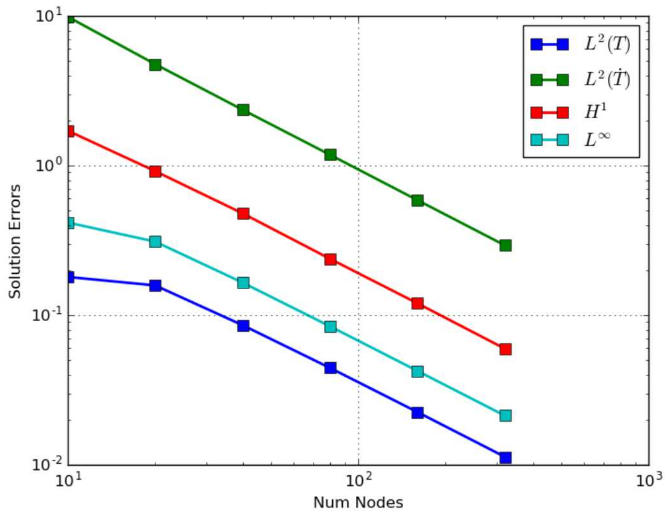


Figure 6.1-1.. Adaptive Time Integration: Errors for First Order Fixed

Table 6.1-1.. Adaptive Time Integration: Convergence Rates for First Order Fixed

Num Dofs	$L^2(T)$	$L^2(\dot{T})$	H^1	L^∞
20	0.18	1.05	0.89	0.43
40	0.89	1.01	0.94	0.91
80	0.95	1.01	1.01	0.97
160	0.98	1.00	0.99	0.99
320	0.99	1.00	1.00	0.99

6.1.6. Results: First Order Adaptive

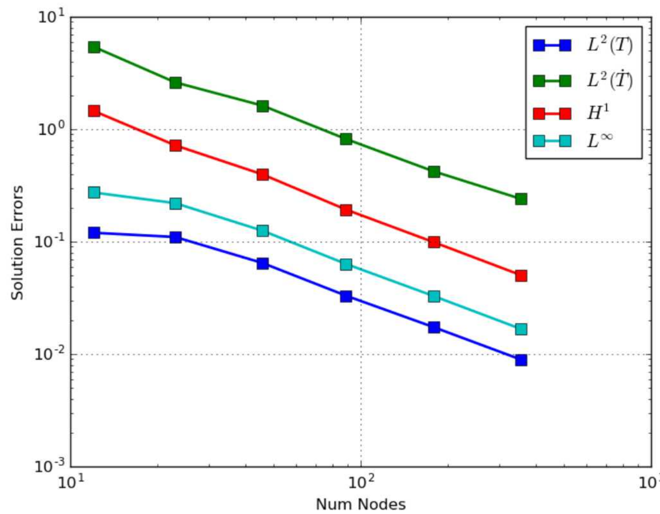


Figure 6.1-2.. Adaptive Time Integration: Errors for First Order Adaptive

Table 6.1-2.. Adaptive Time Integration: Convergence Rates for First Order Adaptive

Num Dofs	$L^2(T)$	$L^2(\dot{T})$	H^1	L^∞
23	0.13	1.13	1.09	0.34
46	0.77	0.68	0.86	0.81
89	1.01	1.04	1.09	1.03
178	0.93	0.95	0.96	0.95
355	0.96	0.81	0.98	0.97

6.1.7. Results: Second Order Fixed

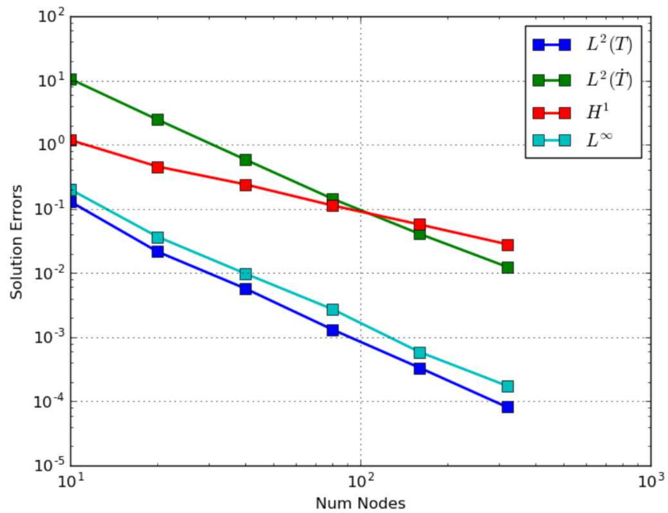


Figure 6.1-3.. Adaptive Time Integration: Errors for Second Order Fixed

Table 6.1-3.. Adaptive Time Integration: Convergence Rates for Second Order Fixed

Num Dofs	$L^2(T)$	$L^2(\dot{T})$	H^1	L^∞
20	2.59	2.11	1.37	2.46
40	1.90	2.06	0.92	1.90
80	2.13	2.03	1.10	1.85
160	1.98	1.82	0.99	2.22
320	2.03	1.71	1.02	1.75

6.1.8. Results: Second Order Adaptive

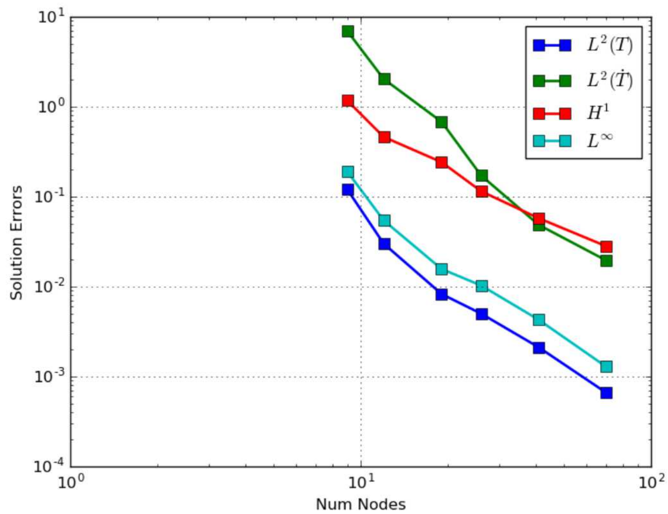


Figure 6.1-4.. Adaptive Time Integration: Errors for Second Order Adaptive

Table 6.1-4.. Adaptive Time Integration: Convergence Rates for Second Order Adaptive

Num Dofs	$L^2(T)$	$L^2(\dot{T})$	H^1	L^∞
12	4.81	4.26	3.24	4.34
19	2.81	2.39	1.41	2.71
26	1.61	4.38	2.38	1.35
41	1.88	2.77	1.51	1.92
70	2.17	1.70	1.34	2.24

6.1.9. Results: BDF2 Fixed

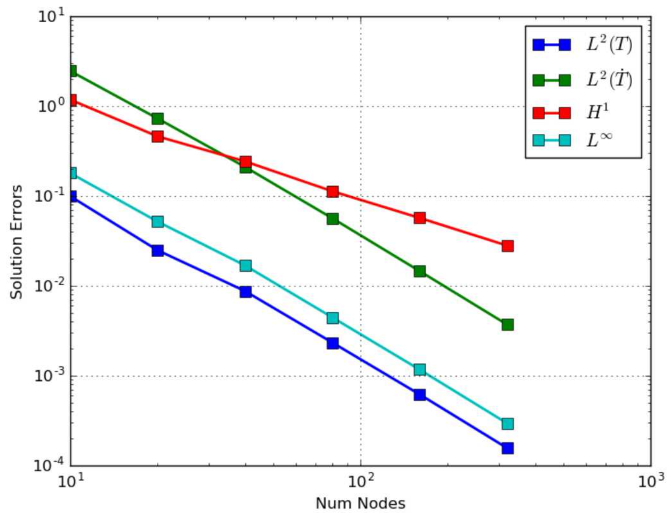


Figure 6.1-5.. Adaptive Time Integration: Errors for BDF2 Fixed

Table 6.1-5.. Adaptive Time Integration: Convergence Rates for BDF2 Fixed

Num Dofs	$L^2(T)$	$L^2(\dot{T})$	H^1	L^∞
20	2.00	1.75	1.36	1.80
40	1.51	1.79	0.92	1.61
80	1.90	1.90	1.10	1.93
160	1.92	1.95	0.99	1.93
320	1.98	1.98	1.02	1.98

6.1.10. Results: BDF2 Adaptive

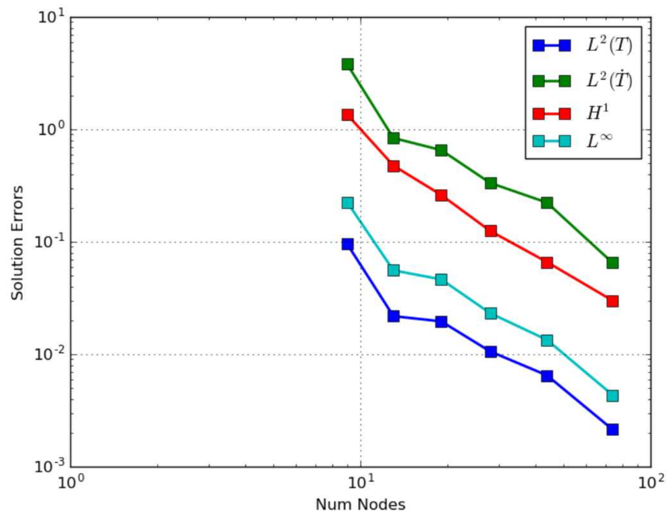


Figure 6.1-6.. Adaptive Time Integration: Errors for BDF2 Adaptive

Table 6.1-6.. Adaptive Time Integration: Convergence Rates for BDF2 Adaptive

Num Dofs	$L^2(T)$	$L^2(\dot{T})$	H^1	L^∞
13	4.03	4.12	2.86	3.80
19	0.27	0.65	1.58	0.49
28	1.59	1.73	1.89	1.78
44	1.09	0.90	1.42	1.22
74	2.13	2.37	1.51	2.17

7. ENCLOSURE RADIATION

7.1. 2D CYLINDRICAL SHELL ENCLOSURE

7.1.1. Problem Description

This problem tests steady state coupled conduction and enclosure radiation. The geometry of this problem is a hollow cylinder (block 2) inside a second hollow cylinder (block 1), which is a radially symmetric problem.

7.1.2. Features Tested

Basic heat conduction, enclosure radiation, Quad4/Tri3 meshes.

7.1.3. Boundary Conditions

The boundary conditions specify the temperature of the outer surface of the outer sphere ($T(r_4) = T_4$) and the inner surface of the inner sphere ($T(r_1) = T_1$).

The problem is steady state but is initialized with a constant temperature of 300 in both blocks. The inner surface temperature T_1 is set to 300. The outer surface temperature T_4 is set to 1300.

Dimensions are defined in Table 7.1-1.

Table 7.1-1.. Dimensions of problem

radius of surface_1	r_1	0.01
radius of surface_2	r_2	0.02
radius of surface_3	r_3	0.03
radius of surface_4	r_4	0.04

7.1.4. Material Parameters

Material properties are shown in Table 7.1-2.

Table 7.1-2.. Material properties

Thermal conductivity (block_1)	κ_1	2.0
Thermal conductivity (block_2)	κ_2	0.35
Density	ρ	1.0
Specific heat	C_p	1.0
emissivity (surface_2)	ϵ_2	0.50
emissivity (surface_3)	ϵ_3	0.55
Stefan-Boltzmann constant	σ	5.6704e-8

7.1.5. Verification of Solution

In cylindrical coordinates, the temperature is independent of θ and z. Integrating this equation twice with respect to the radius r, we obtain the general solution in either hollow cylinder to be

$$T(r) = C_1 \log(r) + C_2,$$

for arbitrary constants C_1 and C_2. We will use $r_i, i = 1, \ldots, 4$ to denote the location of the four surfaces of constant r, numbered from inside to outside. Unless specified otherwise, we will use these subscripts for other quantities which are evaluated at one of the four surfaces.

Including the boundary conditions into the solution allows us to eliminate two constants and gives

$$T_{inner}(r) = T_1 + c_I \log(r/r_1) \text{ for } r_1 < r < r_2 \tag{7.1}$$

$$T_{outer}(r) = T_4 + c_O \log(r/r_4) \text{ for } r_3 < r < r_4 \tag{7.2}$$

To solve for c_I and c_O we compute the temperatures at the enclosure surfaces r_2 and r_3, defined as $T_2 = T_{inner}(r_2)$ and $T_3 = T_{outer}(r_3)$:

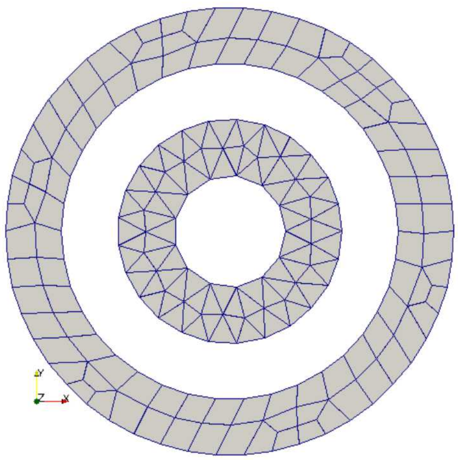
7.1.6. Results

The exact temperatures at the enclosure surfaces (to six digits precision) are $T_2 = 444.7977$ and $T_3 = 956.5915$. From these values we can compute the values of c_O and c_I and thus the exact solution.

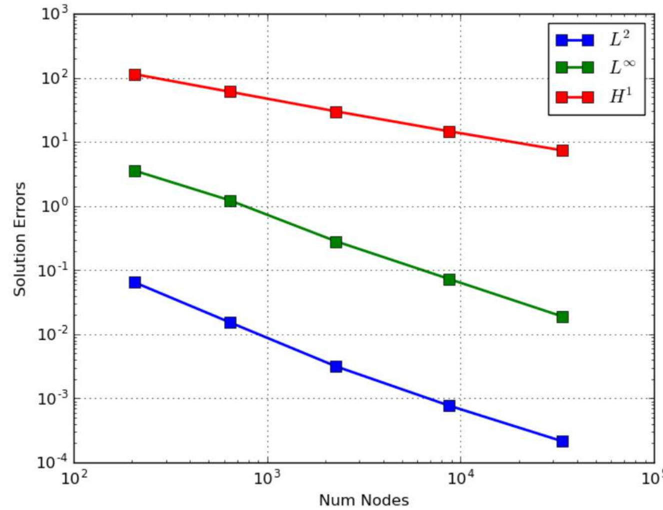
For each mesh, the errors in the temperature solution are computed in the L^2, L^∞ and H^1 norms. The test passes, only if the observed rates of convergence in these norms are 2, 2, and 1, respectively (within a tolerance).

These optimal rates are observed in this test.

For input decks see Appendix 12.6.1.



Coarse Mesh



Error Norms

Figure 7.1-1.. Enclosure Radiation 2D

Table 7.1-3.. Enclosure Radiation 2D: Convergence Rates

Num Dofs	L^2	L^∞	H^1
640	2.54	1.88	1.11
2276	2.50	2.33	1.11
8673	2.10	2.01	1.07
33500	1.90	2.00	1.02

7.2. 2D ANNULAR ENCLOSURE

7.2.1. Problem Description

This problem tests steady state coupled conduction and enclosure radiation. The geometry is an annulus with a crack.

7.2.2. Features Tested

Basic heat conduction, enclosure radiation, Tri3 mesh.

7.2.3. Boundary Conditions

The outer and crack boundary conditions are prescribed at the nodes using the analytic solution. The inner boundary uses an enclosure boundary condition.

7.2.4. Material Parameters

The values of density, thermal conductivity, and specific heat are all constant.

7.2.5. Verification of Solution

The manufactured solution is

$$
\begin{aligned}
J(\theta) &= k_1 + k_2\sqrt{\varepsilon}\cos\left(\frac{\sqrt{\varepsilon}\theta}{2}\right) / \sin\left(\sqrt{\frac{\varepsilon}{\pi}2}\right), \\
H(\theta) &= k_1 + k_2(\frac{\sqrt{\varepsilon}}{1-\varepsilon})\left(\cos\left(\frac{\sqrt{\varepsilon}\theta}{2}\right) / \sin\left(\frac{\sqrt{\varepsilon}\pi}{2}\right) - \sqrt{\varepsilon}\cos\left(\frac{\theta}{2}\right)\right), \\
q(\theta) &= J(\theta) - H(\theta), \\
\beta(\theta) &= \left(\frac{k_1 + k_2\cos\left(\frac{\theta}{2}\right)}{\sigma}\right)^{1/4}, \\
T(r,\theta) &= r\beta(\theta) + (r - r_{\text{cyl}})\left(\frac{q(\theta)}{\kappa} - \beta(\theta)\right),
\end{aligned}
$$

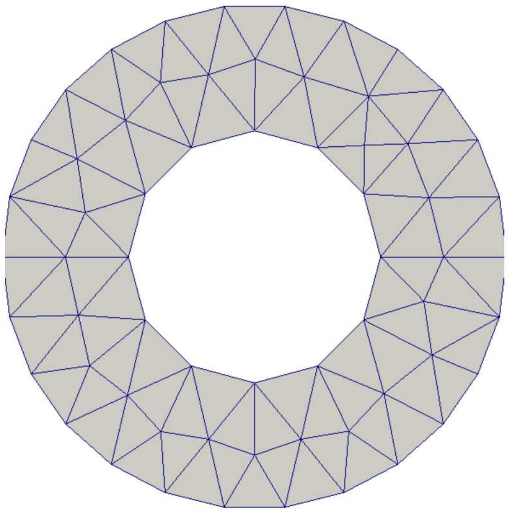
where J is the radiosity, H is the irradiance, q is the flux, and

$$
\begin{aligned}
\sigma &= 5.6704 \times 10^{-8}, \\
\kappa &= 1, \\
r_{\text{cyl}} &= 1, \\
\varepsilon &= 0.9, \\
k_1 &= 8000, \\
k_2 &= 400.
\end{aligned}
$$

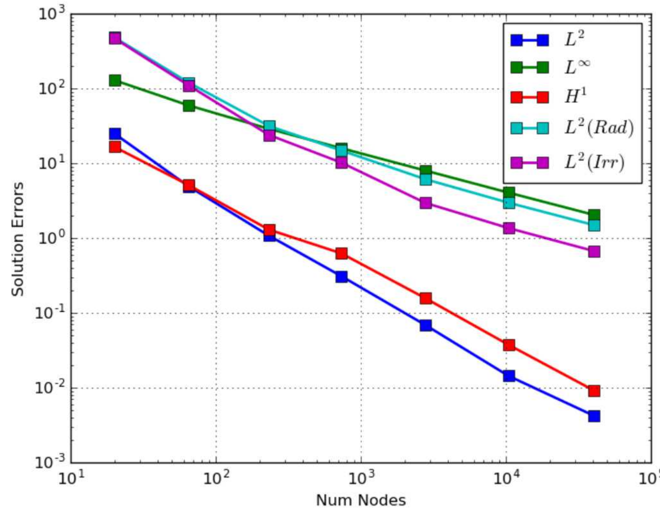
For each mesh, the errors in the temperature solution are computed in the L^2, L^∞ and H^1 norms. The test passes, only if the observed rates of convergence in these norms are 2, 2, and 1, respectively (within a tolerance). Additionally, the errors in the radiosity and irradiance are computed in the L^2 norms and be 1 (within a tolerance).

These optimal rates are observed in this test.

For input decks see Appendix 12.6.2.



Coarse Mesh



Error Norms

Figure 7.2-1.. 2D Full Enclosure Radiation

Table 7.2-1.. 2D Full Enclosure Radiation: Convergence Rates

Num Dofs	L^2	L^∞	H^1	$L^2(Rad)$	$L^2(Irr)$
65	2.76	1.31	2.00	2.36	2.46
232	2.38	1.13	2.15	2.10	2.40
734	2.18	1.04	1.27	1.32	1.49
2788	2.26	1.03	2.07	1.32	1.85
10420	2.37	1.03	2.17	1.09	1.18
40530	1.81	1.01	2.08	1.01	1.04

7.3. 3D SPHERICAL SHELL ENCLOSURE

7.3.1. Problem Description

This problem tests steady state coupled conduction and enclosure radiation. The geometry of this problem is a hollow sphere (block 2) inside a second hollow sphere (block 1), which is a radially symmetric problem.

7.3.2. Features Tested

Basic heat conduction, enclosure radiation, Hex8 meshes.

7.3.3. Boundary Conditions

The boundary conditions specify the temperature of the outer surface of the outer sphere ($T(r_4) = T_4$) and the inner surface of the inner sphere ($T(r_1) = T_1$).

The problem is steady state but is initialized with a constant temperature of 300 in both blocks. The inner surface temperature T_1 is set to 300. The outer surface temperature T_4 is set to 1300.

Dimensions are defined in Table 7.3-1.

Table 7.3-1.. Dimensions of problem

radius of surface_1	r_1	0.01
radius of surface_2	r_2	0.02
radius of surface_3	r_3	0.03
radius of surface_4	r_4	0.04

7.3.4. Material Parameters

Material properties are shown in Table 7.3-2.

Table 7.3-2.. Material properties

Thermal conductivity (block_1)	κ_1	2.0
Thermal conductivity (block_2)	κ_2	0.35
Density	ρ	1.0
Specific heat	C_p	1.0
emissivity (surface_2)	ϵ_2	0.50
emissivity (surface_3)	ϵ_3	0.55
Stefan-Boltzmann constant	σ	5.6704e-8

7.3.5. Verification of Solution

In spherical coordinates, the temperature is independent of θ and ϕ. Integrating this equation twice with respect to the radius r, we obtain the general solution in either hollow sphere to be

$$T(r) = C_1 r^{-1} + C_2,$$

for arbitrary constants C_1 and C_2. We will use $r_i, i = 1, \ldots, 4$ to denote the location of the four surfaces of constant r, numbered from inside to outside. Unless specified otherwise, we will use these subscripts for other quantities which are evaluated at one of the four surfaces.

Including the boundary conditions into the solution allows us to eliminate two constants and gives

$$T_{inner}(r) = T_1 + c_I\left(\frac{1}{r} - \frac{1}{r_4}\right) \text{ for } r_1 < r < r_2 \tag{7.3}$$

$$T_{outer}(r) = T_4 + c_O\left(\frac{1}{r} - \frac{1}{r_1}\right) \text{ for } r_3 < r < r_4 \tag{7.4}$$

To solve for c_I and c_O we compute the temperatures at the enclosure surfaces r_2 and r_3, defined as $T_2 = T_{inner}(r_2)$ and $T_3 = T_{outer}(r_3)$:

$$T_2 = T_1 + c_I\left(\frac{1}{r_2} - \frac{1}{r_4}\right) \tag{7.5}$$

$$T_3 = T_4 + c_O\left(\frac{1}{r_3} - \frac{1}{r_1}\right) \tag{7.6}$$

The fluxes at the surfaces between the two hollow spheres are

$$q_2 = \left(-\kappa \left.\frac{\partial T}{\partial r}\right|_{r=r_3}\right) \cdot \mathbf{n} = \frac{\kappa_1 c_I}{r_2^2}$$

$$q_3 = \left(-\kappa \left.\frac{\partial T}{\partial r}\right|_{r=r_2}\right) \cdot \mathbf{n} = \frac{\kappa_2 c_O}{r_3^2}$$

Here we have used κ_1 and κ_2 to denote the thermal conductivity of the inner and outer blocks, respectively.

These normal conductive fluxes are included in the total energy balance at the enclosure surfaces using the radiative transport equations (for grey diffuse surfaces):

$$q_2 = \sigma\epsilon_2 T_2^4 - \epsilon_2 \sum_j F_{2j} J_j$$

$$q_3 = \sigma\epsilon_3 T_3^4 - \epsilon_3 \sum_j F_{3j} J_j$$

where σ is the Stefan Boltzmann constant, ϵ is the emissivity, F_{ij} is the geometric viewfactor of surface i with respect to surface j and J_j is the radiosity for surface j.

The viewfactor coefficient F_{ij} is the fraction of energy that leaves surface i and arrives at surface j. For this geometric setup, no point on the inner surface at r_2 can “see” itself (no straight line can be drawn from a point on its surface onto itself) and so $F_{22} = 0$. By viewfactor reciprocity

$$\sum_j F_{ij} = 1$$

we must have $F_{23} = 1$. The outer-to-inner view factor F_{32} can be computed analytically to be

$$F_{32} = \frac{r_2^2}{r_3^2}$$

and again by viewfactor reciprocity

$$F_{33} = 1 - F_{32} = 1 - \frac{r_2^2}{r_3^2}$$

The system of equations that must be solved for the radiosities at the inner and outer surfaces is given by

$$\begin{aligned} J_2 &= \epsilon_2 \sigma T_2^4 + (1 - \epsilon_2)[F_{22} J_2 + F_{23} J_3] \\ J_3 &= \epsilon_3 \sigma T_3^4 + (1 - \epsilon_3)[F_{32} J_2 + F_{33} J_3] \end{aligned}$$

Solving this system of equations, we can write J_2 and J_3 in terms of temperature, and plug this back into the equation for the surface flux. We then get a system of two nonlinear equations to solve for T_2 and T_3, the temperatures of the adjacent surfaces without Dirichlet boundary conditions. For our given set of parameters, these equations are solved iteratively in Matlab using the fsolve function.

7.3.6. Results

The exact temperatures at the enclosure surfaces (to six digits precision) are $T_2 = 564.783$ and $T_3 = 1047.825$. From these values we can compute the values of c_O and c_I and thus the exact solution.

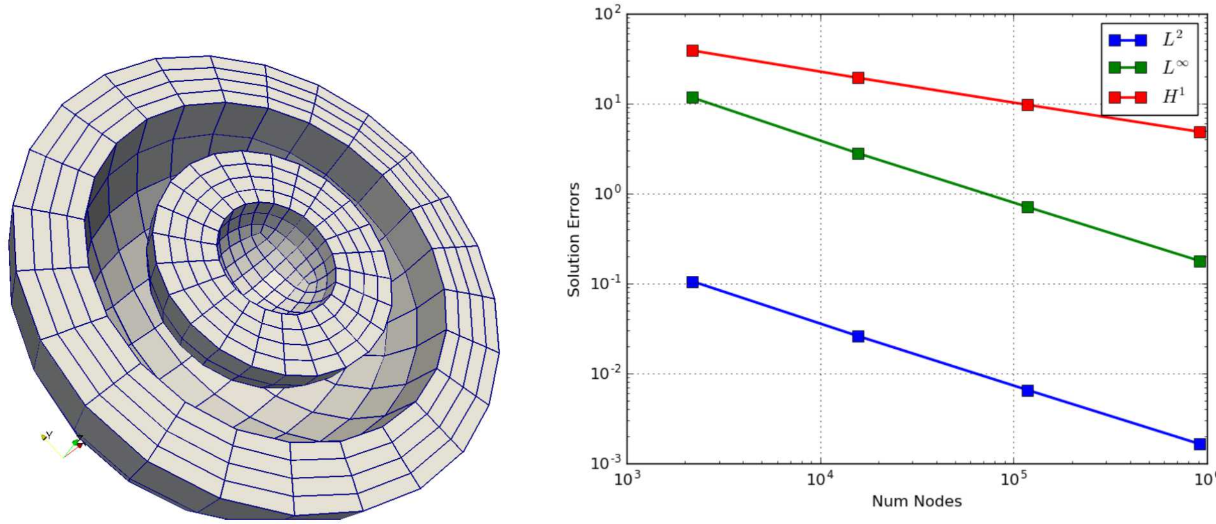
For each mesh, the errors in the temperature solution are computed in the L^2, L^∞ and H^1 norms. The test passes, only if the observed rates of convergence in these norms are 2, 2, and 1, respectively (within a tolerance).

These optimal rates are observed in this test.

Table 7.3-3.. Enclosure Radiation: Convergence Rates

Num Dofs	L^2	L^∞	H^1
15590	2.14	2.17	1.06
117600	2.05	2.05	1.03
912500	2.02	2.02	1.01

For input decks see Appendix 12.6.3.



Coarse Mesh | Error Norms

Figure 7.3-1.. Enclosure Radiation

7.4. 3D SPHERICAL SHELL PARTIAL ENCLOSURE

7.4.1. Problem Description

This problem tests coupled conduction and enclosure radiation with a partial enclosure. The geometry consists of two thick spherical shells separated by a gap. The outer shell has a section removed so that the enclosure is only partial.

7.4.2. Features Tested

Basic heat conduction, enclosure radiation with partial enclosure, Hex8 meshes.

7.4.3. Boundary Conditions

The outer and inner boundary conditions are prescribed at the nodes using the analytic solution. The analytic solution is used to set the boundary conditions on the cutaway face near the opening in the outer shell.

7.4.4. Material Parameters

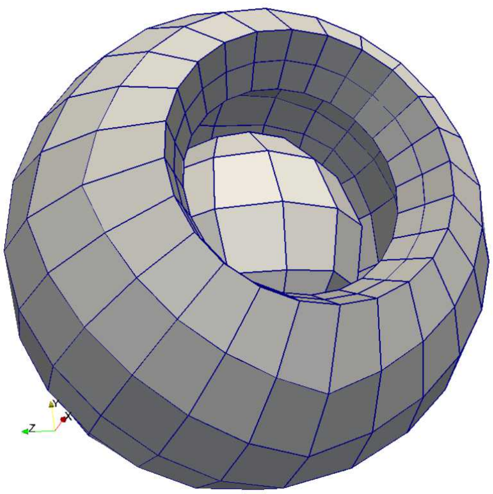
The values of density, thermal conductivity, and specific heat are all constant within each element block; however, the values differ between blocks.

7.4.5. Verification of Solution

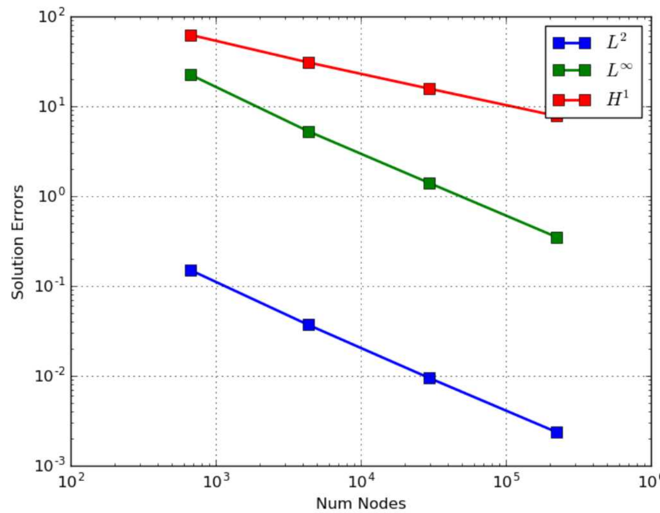
The analytic solution is identical to Section 7.3. The area for the partial enclosure is computed analytically.

For each mesh, the errors in the temperature solution are computed in the L^2, L^∞ and H^1 norms. The test passes, only if the observed rates of convergence in these norms are 2, 2, and 1, respectively (within a tolerance).

These optimal rates are observed in this test.



Coarse Mesh



Error Norms

Figure 7.4-1.. Partial Enclosure Radiation

Table 7.4-1.. Partial Enclosure Radiation: Convergence Rates

Num Dofs	L^2	L^∞	H^1
4338	2.26	2.32	1.13
29690	2.13	2.07	1.06
223200	2.06	2.06	1.03

For input decks see Appendix 12.6.4.

8. CHEMISTRY

8.1. FIRST ORDER REACTION (SPATIALLY VARYING TEMPERATURE)

This problem tests the interface to the CHEMEQ solver under the assumption that the temperature remains is variable in space but remains constant in time. The geometry consists of a unit cube meshed with Hex8 elements refined only in one direction (x).

8.1.1. Features Tested

CHEMEQ solver; source term from chemistry; nonlinear solver; second order time integrator with fixed time steps; constant initial temperature; constant temperature boundary condition.

8.1.2. Boundary Conditions

A constant temperature is applied on surface 1. The initial temperature is provided by an Encore user subroutine and the initial species values are $A = 1$ and $B = 0$.

8.1.3. Material Parameters

The values of density, thermal conductivity, and specific heat are all constant, equal to one in both blocks. The CHEMEQ parameters are chosen to model a single first order reaction $A \rightarrow B$ with constant values of pre-exponential factor and activation energy.

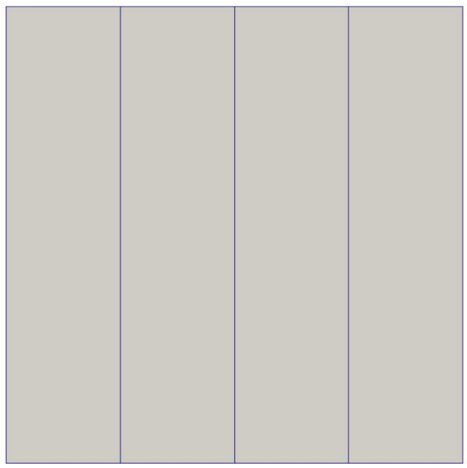
8.1.4. Verification of Solution

A manufactured solution is chosen as

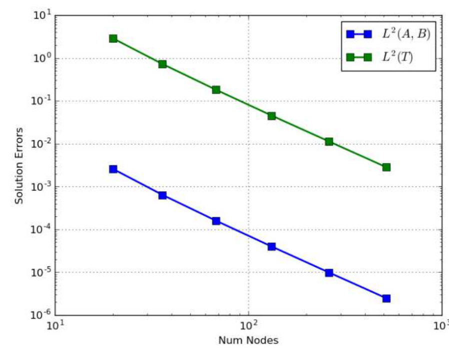
$$\begin{aligned} T(x) &= 400\,(1 + 0.2\cos(\pi\,x)), \\ A(x,t) &= \exp\left\{ -\exp(5)\ \exp(-\frac{1000}{R\,T(x)})\,t \right\}, \\ B(x,t) &= 1 - A(x,t) \end{aligned}$$

where $R = 1.9872$ is the ideal gas constant. A source term is used to insure that the temperature does not vary in time.

For each mesh, the errors in the temperature and species A and B are computed in the L^2 norm. The test passes, only if the observed rates of convergence in these norms are 2 (within a tolerance).



Coarse Mesh



Error Norms

Figure 8.1-1.. First Order Reaction (Spatially Varying Temperature)

Table 8.1-1.. First Order Reaction (Spatially Varying Temperature): Convergence Rates for Hex8 Meshes

Num Dofs	$L^2(A, B)$	$L^2(T)$
36	2.37	2.34
68	2.18	2.18
132	2.09	2.09
260	2.04	2.04
516	2.02	2.02

For input decks see Appendix 12.7.2.

8.2. FIRST ORDER REACTION

This problem tests the interface to the CHEMEQ solver under a temperature field that is variable in space and time. The geometry consists of a unit cube meshed with Hex8 elements refined only in one direction.

8.2.1. Features Tested

CHEMEQ solver; source term from chemistry; nonlinear solver; second order time integrator with fixed time steps; initial temperature from user sub; constant temperature boundary condition.

8.2.2. Boundary Conditions

The initial temperature and the temperature boundary condition on surface 1 are provided by an Encore user subroutine and the initial species values are $A = 1$ and $B = 0$.

8.2.3. Material Parameters

The values of density, thermal conductivity, and specific heat are all constant, equal to one in both blocks. The CHEMEQ parameters are chosen to model a single first order reaction $A \rightarrow B$ with constant values of pre-exponential factor and activation energy.

8.2.4. Verification of Solution

A manufactured solution is chosen as

$$\begin{aligned}
\phi(x,t) &= \exp(a - E/(RT_0))(1 + 0.1\sin(x))\exp(t), \\
\Phi(x,t) &= \exp(a - E/(RT_0))(1 + 0.1\sin(x))(\exp(t) - 1), \\
T(x,t) &= (E/R)/(a - \ln(\phi(x,t))), \\
A(x,t) &= \exp(-\Phi(x,t)), \\
B(x,t) &= 1 - A(x,t)
\end{aligned}$$

where a is the log pre-exponential factor, R is the ideal gas constant, E is the activation energy, and T_0 is a reference temperature value. The form of the solution is contrived so that

$$\begin{aligned}
\partial_t A(x,t) = -\partial_t B(x,t) &= -\phi(x,t)\, A(x,t) \\
\phi(x,t) &= \exp(a)\exp(-\frac{E}{RT(x,t)})
\end{aligned}$$

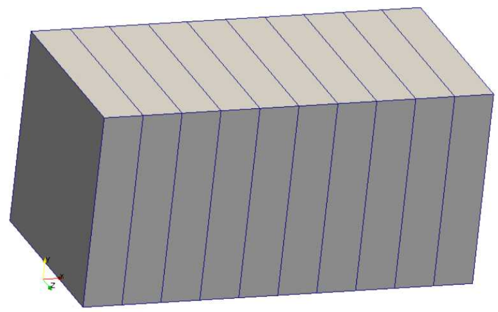
This allows the chemistry ODEs to be satisfied exactly, but a source term is needed in the energy equation.

For each mesh, the errors in the temperature and species A and B are computed in the L^2 norm. The test passes, only if the observed rates of convergence in these norms are 1 (within a tolerance). Currently it is not clear why the convergence rates are only first order.

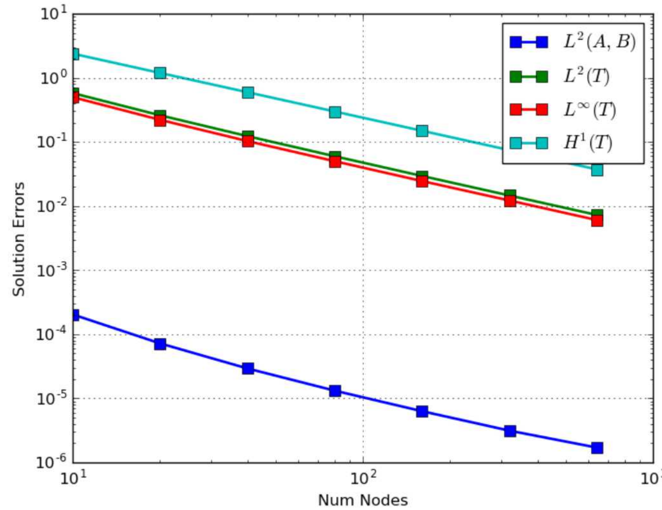
For input decks see Appendix 12.7.3.

8.3. DAE AND PRESSURE TEST

This test runs CHEMEQ with a kinetics model that includes both pressure dependence and distributed activation energy for a single element mesh with uniform temperature and pressure.



Coarse Mesh



Error Norms

Figure 8.2-1.. First Order Reaction

Table 8.2-1.. First Order Reaction: Convergence Rates for Hex8 Meshes

Num Dofs	$L^2(A,B)$	$L^2(T)$	$L^\infty(T)$	$H^1(T)$
20	1.50	1.15	1.17	1.00
40	1.30	1.08	1.10	1.00
80	1.15	1.04	1.05	1.00
160	1.07	1.02	1.03	1.00
320	1.00	1.01	1.01	1.00
640	0.88	1.01	1.01	1.00

8.3.1. Features Tested

Basic heat conduction on a Hex8 mesh; CHEMEQ solver with pressure dependence and distributed activation energy.

8.3.2. Boundary Conditions

No boundary conditions are prescribed, resulting in an adiabatic flux BC.

8.3.3. Material Parameters

The values of density, thermal conductivity, and specific heat are all constant.

8.3.4. Verification of Solution

The analytic solution for the concentration of species A as a function of time for the constant values used in this test case is

$$A(t) = \frac{1}{2}\mathrm{erfc}(\frac{1}{6}(\sqrt{(}2) - 6\mathrm{erf}^{-1}(1 - 45t/(2\exp(\frac{61}{18})))))$$

The test compares the temperature errors against a gold file of the error at each time step. The exact solution for the concentration of A is also output to the exodus file and a comparison plotting that and the solved for concentration as a function of time has them lying on top of one another.

For input decks see Appendix 12.7.4.

8.4. PMDI PLUGIN TEST

This test verifies that the PMDI plugin calculates the correct pressure and effective conductivity based on the auxiliary variable values.

8.4.1. Features Tested

Basic heat conduction on a Hex8 mesh; CHEMEQ solver with pressure dependence and a user plugin to model a seven-species PDMI foam decomposition reaction.

8.4.2. Boundary Conditions

No boundary conditions are prescribed, resulting in an adiabatic flux BC.

8.4.3. Material Parameters

The values of density, emissivity and specific heat are all constant. The thermal conductivity is computed using a C-style user subroutine contained within the foam model.

8.4.4. Verification of Solution

The initial conditions are specified as follows: The test includes a Mathematica notebook file (ExpectedSolution.nb) for calculation of expected pressure which is 1.15125e7 Pa or 1669.75 psi.

For input decks see Appendix 12.7.5.

Table 8.4-1.. PMDI Plugin Test: Initial Conditions

Variable	Value	Units
Bulk Density	321.4432249	kg/m^3
Initial condensed density	1500	
Initial porosity	0.786301	
Mass fraction of all ChemEQ species	1/7	
Temperature	599.8	
Initial gas pressure (N2)	101325	
Initial gas temperature	299.9	

9. MISCELLANEOUS

9.1. THERMAL POSTPROCESSING

9.1.1. Problem Description

This problem tests basic thermal postprocessors in Aria.

9.1.2. Features Tested

Basic heat conduction, thermal postprocessors, Hex8 meshes.

9.1.3. Boundary Conditions

Dirichlet BCs are specified using the exact solution on surface 1. On surface 2, a natural convection BC is specified, using the exact solution as the reference temperature and a constant heat transfer coefficient. Similarly, a radiative flux BC is applied on surface 3, with constant values of emissivity and radiation form factor. A source term is applied within all blocks based on substituting the exact solution into the heat conduction operator.

9.1.4. Material Parameters

The values of density, thermal conductivity, and specific heat are all constant with the same value for both blocks.

9.1.5. Verification of Solution

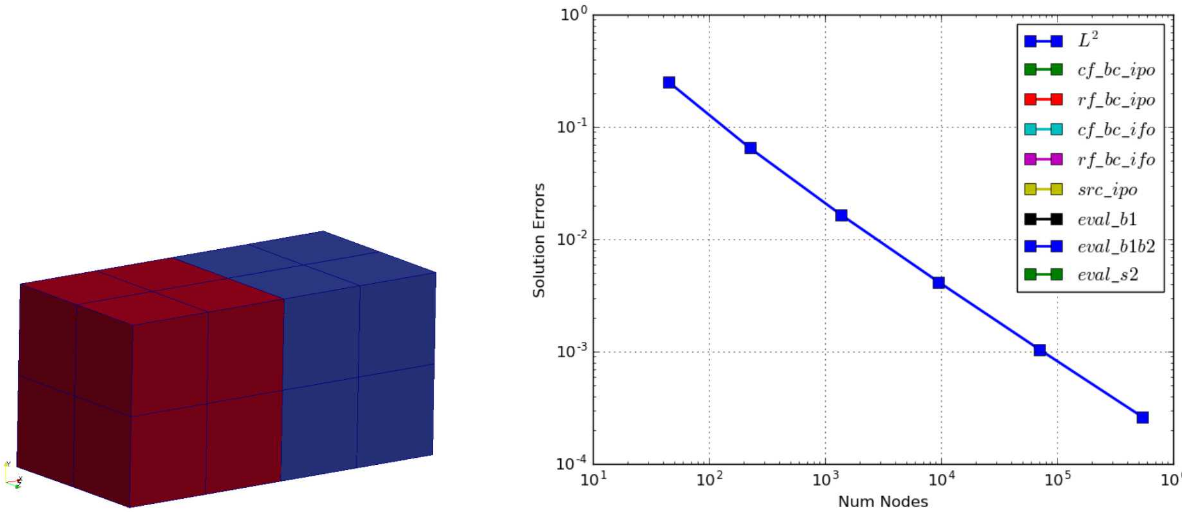
The manufactured solution is

$$T_0 + \exp(C_0(x^2 - 1) + C_1(y^2 - 0.25) + C_2(z^2 - 0.25) + C_3 t).$$

Postprocessors are computed for the integrated power output for convective and radiative BCs (cf_bc_ipo, rf_bc_ipo), the integrated flux output for convective and radiative BCs (cf_bc_ifo, rf_bc_ifo), the integrated power output for volume source terms (src_ipo), and several point evaluations (eval_b1, eval_b1b2, eval_s2).

For each mesh, the errors in the temperature solution are computed in the L^2 norm and for various postprocessors. The test passes, only if the observed rates of convergence are 2 (except for the integrated power output for source terms, which convergences with order 4).

These optimal rates are observed in this test clearly in most cases. However, for the point evaluation cases, a large amount of variability exists in the convergence rates.



Coarse Mesh | Error Norms

Figure 9.1-1.. Thermal Postprocess

Table 9.1-1.. Thermal Postprocess: Convergence Rates

Num Dofs	L^2	cf_bc_ipo	rf_bc_ipo	cf_bc_ifo	rf_bc_ifo	src_ipo	$eval\_b1$	$eval\_b1b2$	$eval\_s2$
225	2.52	2.88	2.83	2.88	2.83	4.62	2.21	1.94	2.56
1377	2.27	2.52	2.48	2.52	2.48	4.44	2.83	3.47	5.75
9537	2.14	2.27	2.25	2.27	2.25	4.26	1.71	1.98	-0.16
70785	2.07	2.13	2.12	2.13	2.12	4.14	2.15	2.05	2.37
545025	2.04	2.06	2.05	2.06	2.05	4.07	2.20	1.57	2.44

For input decks see Appendix 12.8.1.

9.2. LOCAL COORDINATES: CARTESIAN

This problem tests the use of a local Cartesian coordinate system in a material model. The geometry is a 3D cube that has been rotated.

9.2.1. Features Tested

Steady heat conduction, time integrators, tensor thermal conductivity, local Cartesian coordinates in a material model.

9.2.2. Boundary Conditions

The boundary conditions are prescribed at the nodes using the analytic solution. The initial condition is specified using an Encore function evaluated at the nodes.

9.2.3. Material Parameters

The specific heat is constant. The density and thermal conductivity are constant, with a diagonal (tensor) thermal conductivity in the local coordinate space of the material.

9.2.4. Verification of Solution

A manufactured solution is chosen as

$$T(X, Y, Z) = T_0 + T_1 \cos(x_k X) \cos(y_k Y) \cos(z_k Z)$$

where (X, Y, Z) are the local material coordinates, which are related to the Cartesian coordinates (x, y, z) by a rotation matrix consisting of a product of rotations (22.5 deg around the z-axis and 45 deg around the x-axis).

For each mesh, the errors in the temperature solution are computed in the L^2, L^∞ and H^1 norms. The test passes, only if the observed rates of convergence in these norms are 1 for H^1 and 2 for all other norms (within a tolerance).

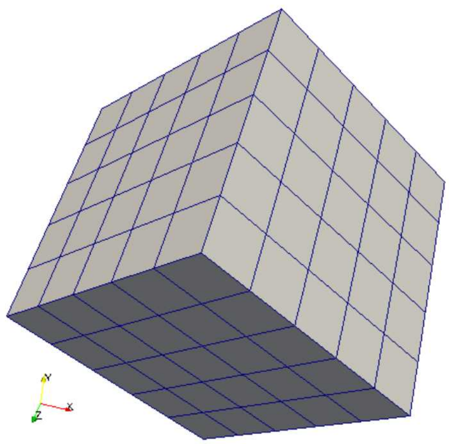
Table 9.2-1.. Local Cartesian Coordinate System: Convergence Rates

Num Dofs	L^2	L^∞
1331	2.29	2.27
9261	2.15	2.14

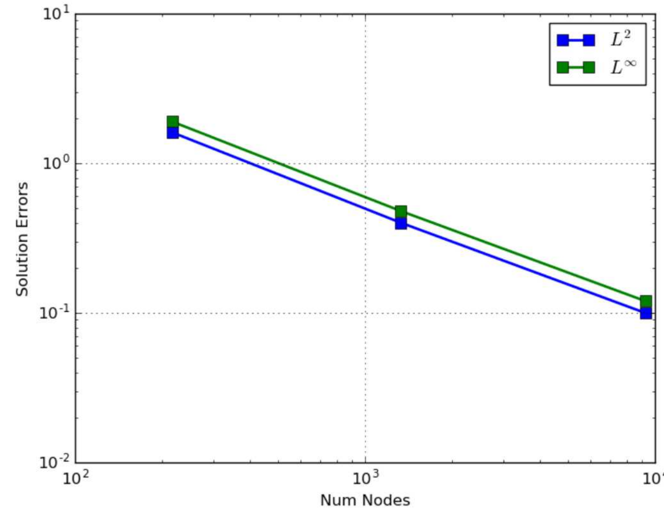
For input decks see Appendix 12.8.3.

9.3. LOCAL COORDINATES: CYLINDRICAL

This problem tests the use of a local cylindrical coordinate system in a material model. The geometry is a 3D cube that has been rotated.



Coarse Mesh



Error Norms

Figure 9.2-1.. Local Cartesian Coordinate System

9.3.1. Features Tested

Steady heat conduction, time integrators, tensor thermal conductivity, local coordinates in a material model.

9.3.2. Boundary Conditions

The boundary conditions are prescribed at the nodes using the analytic solution. The initial condition is specified using an Encore function evaluated at the nodes.

9.3.3. Material Parameters

The specific heat and density are constant. The diagonal (tensor) components of the thermal conductivity are specified using constant values in the local coordinate space of the material.

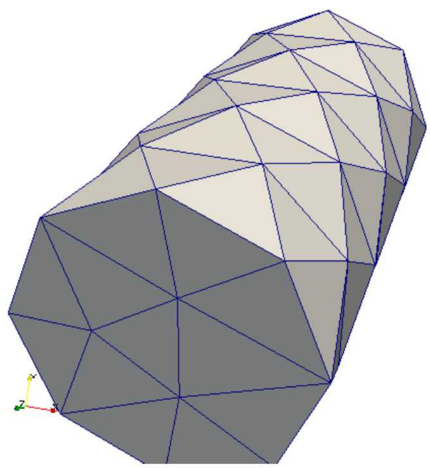
9.3.4. Verification of Solution

A manufactured solution is chosen as

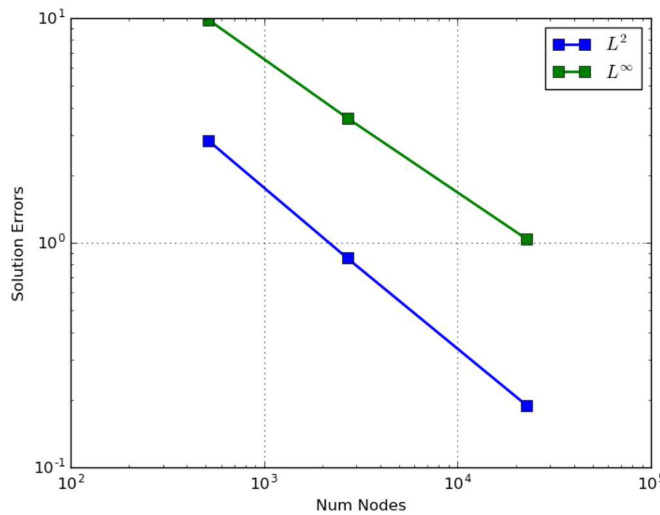
$$T(X, Y, Z) = T_0 + T_1(2R)^3 \cos(\theta) \cos(z_k Z)$$

where (R, Θ, Z) are the local cylindrical material coordinates, which are related to the standard cylindrical coordinates (x, y, z) by a rotation matrix consisting of a product of rotations (22.5 deg around the z-axis and 45 deg around the x-axis).

For each mesh, the errors in the temperature solution are computed in the L^2, L^∞ and H^1 norms. The test passes, only if the observed rates of convergence in these norms are 1 for H^1 and 2 for all other norms (within a tolerance).



Coarse Mesh



Error Norms

Figure 9.3-1.. Local Cylindrical Coordinate System

Table 9.3-1.. Local Cylindrical Coordinate System: Convergence Rates

Num Dofs	L^2	L^∞
2692	2.19	1.83
22723	2.12	1.74

For input decks see Appendix 12.8.4.

10. LOW-MACH FLUID FLOW

Documentation for the following tests is in progress:

```
_rtest/aria/cvfemConvTaylorVortex/cvfemConvTaylorVortex.test|np4
_rtest/aria/gfemConvTaylorVortex/gfemConvTaylorVortex.test|np4
_rtest/aria/hfemConvTaylorVortex/hfemConvTaylorVortex.test|np4
mConvTaylorVortex/cvfemConvTaylorVortex.test|np8
mSteadyTaylorVortex/cvfemSteadyTaylorVortex.test|np8
mSteadyTaylorVortexKeps/cvfemSteadyTaylorVortexKeps.test|np8
m_couette_flow/cdfem_couette_flow.test|cdfem_couette_flow_tri3
m_couette_flow/cdfem_couette_flow.test|cdfem_couette_flow_tri6
ConvTaylorVortex/gfemConvTaylorVortex.test|np8
SteadyTaylorVortex/gfemSteadyTaylorVortex.test|np8
```

11. HOW TO BUILD THIS DOCUMENT

You need to have Sierra developer access (through WebCars). Then you should clone the Sierra Git repository containing the tests to a location with adequate memory (currently more than 80GB), using a command like this:

```
git clone sierra-git:/git/tests
```

Then you need to assign the verification tests, running the following command from your local tests repository:

```
assign --path aria_rtest/verification
```

This will produce a text file called assigned.tests containing the list of all tests to run. You should edit the second line of this file to indicate the remote location (accessible from the HPC machine where you will run the tests). For example, I might have something like this:

```
# Created by assign at Fri Sep 19 09:52:09 2014
#@ /gscratch1/bcarnes/TESTS
aria_rtest/verification/1dnonlin_verify1/1dnonlin_verify1.test|np8
aria_rtest/verification/cyl_shell_2d/cyl_shell_2d.test|np8
aria_rtest/verification/cyl_shell_3d/cyl_shell_3d.test|np8
...
```

Next you need to copy the test files and the assigned.test file to the remote location (here it is "/gscratch1/bcarnes/TESTS/"):

```
rsync -azv aria_rtest/verification redsky:/gscratch1/bcarnes/TESTS/aria_rtest
scp assigned.tests redsky:/gscratch1/bcarnes/TESTS/
```

Here I am only copying the verification test sub-directory, since I do not want to run any other tests.

On the HPC machine, you will need to load a pre-built version of the code such as the nightly master build:

```
module load sierra/master
```

To see where the executables are located, you can run something like:

```
[bcarnes@redsky-login9 ~]$ which aria
/projects/sierra/redsky/install/master/bin/aria
```

Finally, to run the tests, you use the testrun script, with a few additional arguments. The first locates the source code needed to compile the various user subroutines (which we just found from running "which aria"), the second enables tests to run as long as needed, the third uses the queue, and the fourth saves the results so you can use them in the manual.

```
testrun --user sourcedir=/projects/sierra/tlcc2/install/master/ \
        --allow-multipliers=time \
        --queued \
        --save-all-results
```

It may take 1-2 hours to run all the tests. Note that if the tests start to fail with an error associated with the ACCOUNT not being set, you may need to set it using your WCID:

```
export ACCOUNT=fyXXXXX
```

To view your available WCIDs, run the following command:

```
mywcid
```

To build this manual, you should clone the Sierra Git repository containing the documentation files using a command like this:

```
git clone sierra-git:/git/docs
```

Then go to the directory within your local repository containing the Aria Verification Manual files:

```
cd aria/doc/verification_manual
```

Once the tests have all ran successfully, you should sync the results from the remote location back to this directory:

```
rsync -azv redsky:/gscratch1/bcarnes/TESTS/results .
```

Then run the a script to execute any local postprocessing needed to create the plots for the tests:

```
python ariaPostprocess.py
```

Finally you can create the manual using pdflatex:

```
pdflatex Aria_Verification_Manual.tex
```

which should create a new PDF output file.

12. INPUT DECKS FOR VERIFICATION PROBLEMS

12.1. BASIC THERMAL TESTS

12.1.1. Steady Heat Conduction: Hex8 Meshes

```
BEGIN SIERRA myJob

  begin definition for function kxx
    type = piecewise linear
    begin values
       0.0 0.5
       1.0 2.0
       2.0 8.0
      end values
   end

  begin definition for function kyy
    type = piecewise linear
    begin values
       0.0 0.2
       1.0 1.2
       2.0 2.1
       20.0 20.2
      end values
   end

  begin definition for function kzz
    type = piecewise linear
    begin values
       0.0 1.0
       1.0 2.0
       2.0 3.0
       20.0 21.0
     end values
     scale by 2.0
   end

   BEGIN ARIA MATERIAL Kryptonite
     Density              = Constant rho=1
     tensor thermal conductivity = user_function X = temperature name_xx = kxx name_yy = kyy name_zz = kzz
     Specific Heat        = Constant cp=1
     heat conduction      = Generalized
   END ARIA MATERIAL Kryptonite

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  DIRECT_SOLVER
      BEGIN SUPERLU SOLVER
      END
    END TPETRA EQUATION SOLVER
{else}
```

```
    Begin Trilinos Equation Solver Direct_Solver
      Solution Method = amesos-superlu
    End
{endif}

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  ITERATIVE_SOLVER
      BEGIN CG SOLVER
        BEGIN JACOBI PRECONDITIONER
        END
        MAXIMUM ITERATIONS = 1000
        RESIDUAL SCALING = NONE
        CONVERGENCE TOLERANCE = 1.000000e-14
      END
    END TPETRA EQUATION SOLVER
{else}
    Begin Trilinos Equation Solver Iterative_Solver
      Solution Method = CG
      Preconditioning Method = Jacobi
      Maximum Iterations = 1000
      Residual Norm Scaling = None
      Residual Norm Tolerance = 1.0e-14
    End
{endif}

   BEGIN FINITE ELEMENT MODEL cube
      database name = cube_h{N}_hex8.e
      coordinate system is cartesian
      decomposition method = rcb

      BEGIN PARAMETERS FOR BLOCK block_1
 material Kryptonite
      END PARAMETERS FOR BLOCK block_1

   END FINITE ELEMENT MODEL cube

   Begin User Function exact_soln
     Load From File ./exact.so Using Function registerExactSoln
   End

   Begin User Function exact_src
     Load From File ./exact.so Using Function registerExactSrc
   End

   Begin User Function flux_surface_3
     Load From File ./exact.so Using Function registerFlux_Surface_3
   End

   Begin User Function flux_surface_5
     Load From File ./exact.so Using Function registerFlux_Surface_5
   End

   Begin User Function flux_surface_1
     Load From File ./exact.so Using Function registerFlux_Surface_1
   End

   Begin User Function flux_surface_2
     Load From File ./exact.so Using Function registerFlux_Surface_2
   End

   Begin Norm Postprocessor l2
     Use Function exact_soln
     Subtract Function nonlinear_solution->TEMPERATURE
     Compute Norms L2
   End

   Begin Norm Postprocessor h1
     Use Function exact_soln
```

```
    Subtract Function nonlinear_solution->TEMPERATURE
    Compute Norms H1
  End

  Begin Norm Postprocessor linf
    Use Function exact_soln
    Subtract Function nonlinear_solution->TEMPERATURE
    Compute Norms LInfinity
  End

  Begin Postprocessor Output Control pp_out
    Comment Character Is %
     Write To File errors_thermal_steady_hex8_h{N}.dat
    Floating Point Precision Is 3
    Floating Point Format Is Scientific
  End

  BEGIN PROCEDURE myAriaProcedure

     Begin Solution Control Description
Use System Main
Begin System Main
   Begin Sequential The_Time_Block
      Advance myRegion
   End
      Simulation Start Time = 0
   Simulation Termination Time = 1
End
     End

     BEGIN ARIA REGION myRegion

Nonlinear Solution Strategy = Newton
        Maximum Nonlinear Iterations = 10
        Nonlinear Residual Tolerance = 1.0e-12
        Nonlinear Correction Tolerance = 1.0e-12
        Nonlinear Relaxation Factor  = 1.0
        use dof averaged nonlinear residual

use finite element model cube
        Use Linear Solver Iterative_Solver #Direct_Solver

EQ ENERGY for TEMPERATURE on block_1 using Q1 with DIFF SRC

# surface_4: x=0
# surface_6: x=1

# surface_3: y=0
# surface_5: y=1

# surface_1: z=1
# surface_2: z=0

# const Temp BC (x)
        BC const dirichlet at surface_4 Temperature = 1.0
        BC const dirichlet at surface_6 Temperature = 1.0

# const flux BC (y)
BC FLUX for Energy on surface_3  = constant flux = 3
BC FLUX for Energy on surface_5  = constant flux = 5

BC FLUX for Energy on surface_3  = Encore_Function Name=flux_surface_3
BC FLUX for Energy on surface_5  = Encore_Function Name=flux_surface_5

# convective flux BC with const Temp and H (z)
        BC Flux for Energy on surface_1 = Nat_Conv T_Ref=1 H=1
        BC Flux for Energy on surface_2 = Nat_Conv T_Ref=2 H=2
```

```
 BC FLUX for Energy on surface_1  = Encore_Function Name=flux_surface_1
 BC FLUX for Energy on surface_2  = Encore_Function Name=flux_surface_2

 #  const source term
 Source For ENERGY on block_1 = Constant value=1

 Source For ENERGY on block_1 = Encore_Function Name=exact_src

    Output Number of Nodes

 Evaluate Postprocessor l2
 Evaluate Postprocessor h1
 Evaluate Postprocessor linf

 BEGIN RESULTS OUTPUT LABEL diffusion output
           database Name = thermal_steady_hex8_h{N}.e
    at step 1, increment = 1
    # time interval is 1.0
    title Aria cube test
    nodal variables = nonlinear_solution->TEMPERATURE as T
 END RESULTS OUTPUT LABEL diffusion output

      END ARIA REGION myRegion

   END PROCEDURE myAriaProcedure

END SIERRA myJob
```

12.1.2. Steady Heat Conduction: Hex20 Meshes

```
BEGIN SIERRA myJob

   load user plugin file ./exact.so

  begin definition for function kxx
    type = piecewise linear
    begin values
       0.0 0.5
       1.0 2.0
       2.0 8.0
      end values
   end

  begin definition for function kyy
    type = piecewise linear
    begin values
       0.0 0.2
       1.0 1.2
       2.0 2.1
       20.0 20.2
      end values
   end

  begin definition for function kzz
    type = piecewise linear
    begin values
       0.0 1.0
       1.0 2.0
       2.0 3.0
       20.0 21.0
     end values
     scale by 2.0
   end

   BEGIN ARIA MATERIAL Kryptonite
     Density              = Constant rho=1
```

```
      tensor thermal conductivity = user_function X = temperature name_xx = kxx name_yy = kyy name_zz = kzz
      Specific Heat        = Constant cp=1
      heat conduction      = Generalized
    END ARIA MATERIAL Kryptonite

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  DIRECT_SOLVER
      BEGIN SUPERLU SOLVER
      END
    END TPETRA EQUATION SOLVER
{else}
    Begin Trilinos Equation Solver Direct_Solver
      Solution Method = amesos-superlu
    End
{endif}

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  ITERATIVE_SOLVER
      BEGIN CG SOLVER
        BEGIN JACOBI PRECONDITIONER
        END
        MAXIMUM ITERATIONS = 1000
        RESIDUAL SCALING = NONE
        CONVERGENCE TOLERANCE = 1.000000e-14
      END
    END TPETRA EQUATION SOLVER
{else}
    Begin Trilinos Equation Solver Iterative_Solver
      Solution Method = CG
      Preconditioning Method = Jacobi
      Maximum Iterations = 1000
      Residual Norm Scaling = None
      Residual Norm Tolerance = 1.0e-14
    End
{endif}

   BEGIN FINITE ELEMENT MODEL cube
      database name = cube_h{N}_hex20.g
      coordinate system is cartesian
      decomposition method = rcb

      BEGIN PARAMETERS FOR BLOCK block_1
         material Kryptonite
      END PARAMETERS FOR BLOCK block_1

   END FINITE ELEMENT MODEL cube

   Begin User Function exact_soln
     Load From File ./exact.so Using Function registerExactSoln
   End

   Begin User Function exact_src
     Load From File ./exact.so Using Function registerExactSrc
   End

   Begin User Function flux_surface_3
     Load From File ./exact.so Using Function registerFlux_Surface_3
   End

   Begin User Function flux_surface_5
     Load From File ./exact.so Using Function registerFlux_Surface_5
   End

   Begin User Function flux_surface_1
     Load From File ./exact.so Using Function registerFlux_Surface_1
   End

   Begin User Function flux_surface_2
```

```
  Load From File ./exact.so Using Function registerFlux_Surface_2
 End

 Begin Norm Postprocessor l2
   Use Function exact_soln
   Subtract Function nonlinear_solution->TEMPERATURE
   Compute Norms L2
 End

 Begin Norm Postprocessor h1
   Use Function exact_soln
   Subtract Function nonlinear_solution->TEMPERATURE
   Compute Norms H1
 End

 Begin Norm Postprocessor linf
   Use Function exact_soln
   Subtract Function nonlinear_solution->TEMPERATURE
   Compute Norms LInfinity
 End

 Begin Postprocessor Output Control pp_out
   Comment Character Is %
Write To File errors_thermal_steady_hex20_h{N}.dat
   Floating Point Precision Is 3
   Floating Point Format Is Scientific
 End

 BEGIN PROCEDURE myAriaProcedure

    Begin Solution Control Description
       Use System Main
       Begin System Main
          Begin Sequential The_Time_Block
             Advance myRegion
          End
            Simulation Start Time = 0
          Simulation Termination Time = 1
       End
    End

    BEGIN ARIA REGION myRegion

       Nonlinear Solution Strategy = Newton
       Maximum Nonlinear Iterations = 10
       Nonlinear Residual Tolerance = 1.0e-12
       Nonlinear Correction Tolerance = 1.0e-12
       Nonlinear Relaxation Factor  = 1.0
       use dof averaged nonlinear residual

       use finite element model cube
       Use Linear Solver Iterative_Solver #Direct_Solver

       EQ ENERGY for TEMPERATURE on block_1 using Q2S with DIFF SRC

       # surface_4: x=0
       # surface_6: x=1

       # surface_3: y=0
       # surface_5: y=1

       # surface_1: z=1
       # surface_2: z=0

       # const Temp BC (x)
       BC const dirichlet at surface_4 Temperature = 1.0
       BC const dirichlet at surface_6 Temperature = 1.0
```

```
        # const flux BC (y)
        BC FLUX for Energy on surface_3  = constant flux = 3
        BC FLUX for Energy on surface_5  = constant flux = 5

        BC FLUX for Energy on surface_3  = Encore_Function Name=flux_surface_3
        BC FLUX for Energy on surface_5  = Encore_Function Name=flux_surface_5

        # convective flux BC with const Temp and H (z)
        BC Flux for Energy on surface_1 = Nat_Conv T_Ref=1 H=1
        BC Flux for Energy on surface_2 = Nat_Conv T_Ref=2 H=2

        BC FLUX for Energy on surface_1  = Encore_Function Name=flux_surface_1
        BC FLUX for Energy on surface_2  = Encore_Function Name=flux_surface_2

        #  const source term
        Source For ENERGY on block_1 = Constant value=1

        Source For ENERGY on block_1 = Encore_Function Name=exact_src

          Output Number of Nodes

        Evaluate Postprocessor l2
        Evaluate Postprocessor h1
        Evaluate Postprocessor linf

        BEGIN RESULTS OUTPUT LABEL diffusion output
           database Name = thermal_steady_hex20_h{N}.e
           at step 1, increment = 1
           # time interval is 1.0
           title Aria cube test
           nodal variables = nonlinear_solution->TEMPERATURE as T
        END RESULTS OUTPUT LABEL diffusion output

     END ARIA REGION myRegion

   END PROCEDURE myAriaProcedure

END SIERRA myJob
```

12.1.3. Steady Heat Conduction: Hex27 Meshes

```
BEGIN SIERRA myJob

   load user plugin file ./exact.so

  begin definition for function kxx
    type = piecewise linear
    begin values
       0.0 0.5
       1.0 2.0
       2.0 8.0
     end values
   end

  begin definition for function kyy
    type = piecewise linear
    begin values
       0.0 0.2
       1.0 1.2
       2.0 2.1
       20.0 20.2
     end values
   end

  begin definition for function kzz
    type = piecewise linear
```

```
    begin values
       0.0 1.0
       1.0 2.0
       2.0 3.0
       20.0 21.0
     end values
     scale by 2.0
   end

   BEGIN ARIA MATERIAL Kryptonite
     Density              = Constant rho=1
     tensor thermal conductivity = user_function X = temperature name_xx = kxx name_yy = kyy name_zz = kzz
     Specific Heat        = Constant cp=1
     heat conduction      = Generalized
   END ARIA MATERIAL Kryptonite

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  DIRECT_SOLVER
      BEGIN SUPERLU SOLVER
      END
    END TPETRA EQUATION SOLVER
{else}
    Begin Trilinos Equation Solver Direct_Solver
      Solution Method = amesos-superlu
    End
{endif}

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  ITERATIVE_SOLVER
      BEGIN CG SOLVER
        BEGIN JACOBI PRECONDITIONER
        END
        MAXIMUM ITERATIONS = 1000
        RESIDUAL SCALING = NONE
        CONVERGENCE TOLERANCE = 1.000000e-14
      END
    END TPETRA EQUATION SOLVER
{else}
    Begin Trilinos Equation Solver Iterative_Solver
      Solution Method = CG
      Preconditioning Method = Jacobi
      Maximum Iterations = 1000
      Residual Norm Scaling = None
      Residual Norm Tolerance = 1.0e-14
    End
{endif}

   BEGIN FINITE ELEMENT MODEL cube
      database name = cube_h{N}_hex27.g
      coordinate system is cartesian
      decomposition method = rcb

      BEGIN PARAMETERS FOR BLOCK block_1
         material Kryptonite
      END PARAMETERS FOR BLOCK block_1

   END FINITE ELEMENT MODEL cube

   Begin User Function exact_soln
     Load From File ./exact.so Using Function registerExactSoln
   End

   Begin User Function exact_src
     Load From File ./exact.so Using Function registerExactSrc
   End

   Begin User Function flux_surface_3
     Load From File ./exact.so Using Function registerFlux_Surface_3
```

```
 End

 Begin User Function flux_surface_5
   Load From File ./exact.so Using Function registerFlux_Surface_5
 End

 Begin User Function flux_surface_1
   Load From File ./exact.so Using Function registerFlux_Surface_1
 End

 Begin User Function flux_surface_2
   Load From File ./exact.so Using Function registerFlux_Surface_2
 End

 Begin Norm Postprocessor l2
   Use Function exact_soln
   Subtract Function nonlinear_solution->TEMPERATURE
   Compute Norms L2
 End

 Begin Norm Postprocessor h1
   Use Function exact_soln
   Subtract Function nonlinear_solution->TEMPERATURE
   Compute Norms H1
 End

 Begin Norm Postprocessor linf
   Use Function exact_soln
   Subtract Function nonlinear_solution->TEMPERATURE
   Compute Norms LInfinity
 End

 Begin Postprocessor Output Control pp_out
   Comment Character Is %
Write To File errors_thermal_steady_hex27_h{N}.dat
   Floating Point Precision Is 3
   Floating Point Format Is Scientific
 End

 BEGIN PROCEDURE myAriaProcedure

    Begin Solution Control Description
       Use System Main
       Begin System Main
          Begin Sequential The_Time_Block
             Advance myRegion
          End
            Simulation Start Time = 0
          Simulation Termination Time = 1
       End
    End

    BEGIN ARIA REGION myRegion

       Nonlinear Solution Strategy = Newton
       Maximum Nonlinear Iterations = 10
       Nonlinear Residual Tolerance = 1.0e-12
       Nonlinear Correction Tolerance = 1.0e-12
       Nonlinear Relaxation Factor  = 1.0
       use dof averaged nonlinear residual

       use finite element model cube
       Use Linear Solver Iterative_Solver #Direct_Solver

       EQ ENERGY for TEMPERATURE on block_1 using Q2 with DIFF SRC

       # surface_4: x=0
       # surface_6: x=1
```

```
        # surface_3: y=0
        # surface_5: y=1

        # surface_1: z=1
        # surface_2: z=0

        # const Temp BC (x)
        BC const dirichlet at surface_4 Temperature = 1.0
        BC const dirichlet at surface_6 Temperature = 1.0

        # const flux BC (y)
        BC FLUX for Energy on surface_3  = constant flux = 3
        BC FLUX for Energy on surface_5  = constant flux = 5

        BC FLUX for Energy on surface_3  = Encore_Function Name=flux_surface_3
        BC FLUX for Energy on surface_5  = Encore_Function Name=flux_surface_5

        # convective flux BC with const Temp and H (z)
        BC Flux for Energy on surface_1 = Nat_Conv T_Ref=1 H=1
        BC Flux for Energy on surface_2 = Nat_Conv T_Ref=2 H=2

        BC FLUX for Energy on surface_1  = Encore_Function Name=flux_surface_1
        BC FLUX for Energy on surface_2  = Encore_Function Name=flux_surface_2

        #  const source term
        Source For ENERGY on block_1 = Constant value=1

        Source For ENERGY on block_1 = Encore_Function Name=exact_src

          Output Number of Nodes

        Evaluate Postprocessor l2
        Evaluate Postprocessor h1
        Evaluate Postprocessor linf

        BEGIN RESULTS OUTPUT LABEL diffusion output
           database Name = thermal_steady_hex27_h{N}.e
           at step 1, increment = 1
           # time interval is 1.0
           title Aria cube test
           nodal variables = nonlinear_solution->TEMPERATURE as T
        END RESULTS OUTPUT LABEL diffusion output

      END ARIA REGION myRegion

   END PROCEDURE myAriaProcedure

END SIERRA myJob
```

12.1.4. Steady Heat Conduction: Tet4 Meshes

```
BEGIN SIERRA myJob

   load user plugin file ./exact.so

   BEGIN ARIA MATERIAL Kryptonite
     Density              = Constant rho=1
     Thermal Conductivity = constant k=1
     Specific Heat        = Constant cp=1
     heat conduction      = basic
   END ARIA MATERIAL Kryptonite

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  DIRECT_SOLVER
      BEGIN SUPERLU SOLVER
```

```
      END
    END TPETRA EQUATION SOLVER
{else}
    Begin Trilinos Equation Solver Direct_Solver
      Solution Method = amesos-superlu
    End
{endif}

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  ITERATIVE_SOLVER
      BEGIN CG SOLVER
        BEGIN JACOBI PRECONDITIONER
        END
        MAXIMUM ITERATIONS = 1000
        RESIDUAL SCALING = NONE
        CONVERGENCE TOLERANCE = 1.000000e-14
      END
    END TPETRA EQUATION SOLVER
{else}
    Begin Trilinos Equation Solver Iterative_Solver
      Solution Method = CG
      Preconditioning Method = Jacobi
      Maximum Iterations = 1000
      Residual Norm Scaling = None
      Residual Norm Tolerance = 1.0e-14
    End
{endif}

   BEGIN FINITE ELEMENT MODEL cube
      database name = cube_h{N}_tet4.e
      coordinate system is cartesian
      decomposition method = rcb

      BEGIN PARAMETERS FOR BLOCK block_1
 material Kryptonite
      END PARAMETERS FOR BLOCK block_1

   END FINITE ELEMENT MODEL cube

   Begin User Function exact_soln
     Load From File ./exact.so Using Function registerExactSoln
   End

   Begin User Function exact_soln_dot
     Load From File ./exact.so Using Function registerExactSolnDot
   End

   Begin User Function exact_src
     Load From File ./exact.so Using Function registerExactSrc
   End

   Begin User Function flux_surface_3
     Load From File ./exact.so Using Function registerFlux_Surface_3
   End

   Begin User Function flux_surface_5
     Load From File ./exact.so Using Function registerFlux_Surface_5
   End

   Begin User Function flux_surface_1
     Load From File ./exact.so Using Function registerFlux_Surface_1
   End

   Begin User Function flux_surface_2
     Load From File ./exact.so Using Function registerFlux_Surface_2
   End

   Begin Norm Postprocessor l2
```

```
    Use Function exact_soln
    Subtract Function nonlinear_solution->TEMPERATURE
    Compute Norms L2
  End

  Begin Norm Postprocessor h1
    Use Function exact_soln
    Subtract Function nonlinear_solution->TEMPERATURE
    Compute Norms H1
  End

  Begin Norm Postprocessor linf
    Use Function exact_soln
    Subtract Function nonlinear_solution->TEMPERATURE
    Compute Norms LInfinity
  End

  Begin Postprocessor Output Control pp_out
    Comment Character Is %
 Write To File errors_h{N}.dat
    Floating Point Precision Is 3
    Floating Point Format Is Scientific
  End

  BEGIN PROCEDURE myAriaProcedure

     Begin Solution Control Description
Use System Main
Begin System Main
   Begin Sequential The_Time_Block
      Advance myRegion
   End
      Simulation Start Time = 0
   Simulation Termination Time = 1
End
     End

     BEGIN ARIA REGION myRegion

Nonlinear Solution Strategy = Newton
        Maximum Nonlinear Iterations = 10
        Nonlinear Residual Tolerance = 1.0e-12
        Nonlinear Correction Tolerance = 1.0e-12
        Nonlinear Relaxation Factor  = 1.0
        use dof averaged nonlinear residual

use finite element model cube
        Use Linear Solver Iterative_Solver #Direct_Solver

EQ ENERGY for TEMPERATURE on block_1 using Q1 with DIFF SRC

# surface_4: x=0
# surface_6: x=1

# surface_3: y=0
# surface_5: y=1

# surface_1: z=1
# surface_2: z=0

# const Temp BC (x)
        BC const dirichlet at surface_4 Temperature = 1.0
        BC const dirichlet at surface_6 Temperature = 1.0

# const flux BC (y)
BC FLUX for Energy on surface_3  = constant flux = 3
BC FLUX for Energy on surface_5  = constant flux = 5
```

```
 BC FLUX for Energy on surface_3  = Encore_Function Name=flux_surface_3
 BC FLUX for Energy on surface_5  = Encore_Function Name=flux_surface_5

 # convective flux BC with const Temp and H (z)
         BC Flux for Energy on surface_1 = Nat_Conv T_Ref=1 H=1
         BC Flux for Energy on surface_2 = Nat_Conv T_Ref=2 H=2

 BC FLUX for Energy on surface_1  = Encore_Function Name=flux_surface_1
 BC FLUX for Energy on surface_2  = Encore_Function Name=flux_surface_2

 #  const source term
 Source For ENERGY on block_1 = Constant value=1

 Source For ENERGY on block_1 = Encore_Function Name=exact_src

    Output Number of Nodes

 Evaluate Postprocessor l2
 Evaluate Postprocessor h1
 Evaluate Postprocessor linf

 BEGIN RESULTS OUTPUT LABEL diffusion output
    database Name = thermal_steady_tet4_h{N}.e
    at step 1, increment = 1
    # time interval is 1.0
    title Aria cube test
    nodal variables = nonlinear_solution->TEMPERATURE as T
 END RESULTS OUTPUT LABEL diffusion output

      END ARIA REGION myRegion

   END PROCEDURE myAriaProcedure

END SIERRA myJob
```

12.1.5. Steady Heat Conduction: Tet4Tet10 Meshes

```
BEGIN SIERRA myJob

   load user plugin file ./exact.so

   BEGIN ARIA MATERIAL Kryptonite
     Density              = Constant rho=1
     Thermal Conductivity = constant k=1
     Specific Heat        = Constant cp=1
     heat conduction      = basic
   END ARIA MATERIAL Kryptonite

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  DIRECT_SOLVER
      BEGIN SUPERLU SOLVER
      END
    END TPETRA EQUATION SOLVER
{else}
    Begin Trilinos Equation Solver Direct_Solver
      Solution Method = amesos-superlu
    End
{endif}

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  ITERATIVE_SOLVER
      BEGIN CG SOLVER
        BEGIN JACOBI PRECONDITIONER
        END
        MAXIMUM ITERATIONS = 1000
        RESIDUAL SCALING = NONE
```

```
        CONVERGENCE TOLERANCE = 1.000000e-14
      END
    END TPETRA EQUATION SOLVER
{else}
    Begin Trilinos Equation Solver Iterative_Solver
      Solution Method = CG
      Preconditioning Method = Jacobi
      Maximum Iterations = 1000
      Residual Norm Scaling = None
      Residual Norm Tolerance = 1.0e-14
    End
{endif}

   BEGIN FINITE ELEMENT MODEL cube
      database name = cube_h{N}_tet10.e
      coordinate system is cartesian
      decomposition method = rcb

      BEGIN PARAMETERS FOR BLOCK block_1
 material Kryptonite
      END PARAMETERS FOR BLOCK block_1

   END FINITE ELEMENT MODEL cube

   Begin User Function exact_soln
     Load From File ./exact.so Using Function registerExactSoln
   End

   Begin User Function exact_soln_dot
     Load From File ./exact.so Using Function registerExactSolnDot
   End

   Begin User Function exact_src
     Load From File ./exact.so Using Function registerExactSrc
   End

   Begin User Function flux_surface_3
     Load From File ./exact.so Using Function registerFlux_Surface_3
   End

   Begin User Function flux_surface_5
     Load From File ./exact.so Using Function registerFlux_Surface_5
   End

   Begin User Function flux_surface_1
     Load From File ./exact.so Using Function registerFlux_Surface_1
   End

   Begin User Function flux_surface_2
     Load From File ./exact.so Using Function registerFlux_Surface_2
   End

   Begin Norm Postprocessor l2
     Use Function exact_soln
     Subtract Function nonlinear_solution->TEMPERATURE
     Compute Norms L2
   End

   Begin Norm Postprocessor h1
     Use Function exact_soln
     Subtract Function nonlinear_solution->TEMPERATURE
     Compute Norms H1
   End

   Begin Norm Postprocessor linf
     Use Function exact_soln
     Subtract Function nonlinear_solution->TEMPERATURE
     Compute Norms LInfinity
```

```
  End

  Begin Postprocessor Output Control pp_out
    Comment Character Is %
 Write To File errors_thermal_steady_tet4_h{N}.dat
    Floating Point Precision Is 3
    Floating Point Format Is Scientific
  End

  BEGIN PROCEDURE myAriaProcedure

     Begin Solution Control Description
Use System Main
Begin System Main
   Begin Sequential The_Time_Block
      Advance myRegion
   End
      Simulation Start Time = 0
   Simulation Termination Time = 1
End
     End

     BEGIN ARIA REGION myRegion

Nonlinear Solution Strategy = Newton
        Maximum Nonlinear Iterations = 10
        Nonlinear Residual Tolerance = 1.0e-12
        Nonlinear Correction Tolerance = 1.0e-12
        Nonlinear Relaxation Factor  = 1.0
        use dof averaged nonlinear residual

use finite element model cube
        Use Linear Solver Iterative_Solver #Direct_Solver

EQ ENERGY for TEMPERATURE on block_1 using Q1 with DIFF SRC

# surface_4: x=0
# surface_6: x=1

# surface_3: y=0
# surface_5: y=1

# surface_1: z=1
# surface_2: z=0

# const Temp BC (x)
        BC const dirichlet at surface_4 Temperature = 1.0
        BC const dirichlet at surface_6 Temperature = 1.0

# const flux BC (y)
BC FLUX for Energy on surface_3  = constant flux = 3
BC FLUX for Energy on surface_5  = constant flux = 5

BC FLUX for Energy on surface_3  = Encore_Function Name=flux_surface_3
BC FLUX for Energy on surface_5  = Encore_Function Name=flux_surface_5

# convective flux BC with const Temp and H (z)
        BC Flux for Energy on surface_1 = Nat_Conv T_Ref=1 H=1
        BC Flux for Energy on surface_2 = Nat_Conv T_Ref=2 H=2

BC FLUX for Energy on surface_1  = Encore_Function Name=flux_surface_1
BC FLUX for Energy on surface_2  = Encore_Function Name=flux_surface_2

#  const source term
Source For ENERGY on block_1 = Constant value=1

Source For ENERGY on block_1 = Encore_Function Name=exact_src
```

```
    Output Number of Nodes

 Evaluate Postprocessor l2
 Evaluate Postprocessor h1
 Evaluate Postprocessor linf

 BEGIN RESULTS OUTPUT LABEL diffusion output
    database Name = thermal_steady_tet4_h{N}.e
    at step 1, increment = 1
    # time interval is 1.0
    title Aria cube test
    nodal variables = nonlinear_solution->TEMPERATURE as T
 END RESULTS OUTPUT LABEL diffusion output

      END ARIA REGION myRegion

   END PROCEDURE myAriaProcedure

END SIERRA myJob
```

12.1.6. Steady Heat Conduction: Tet10 Meshes

```
BEGIN SIERRA myJob

   load user plugin file ./exact.so

   BEGIN ARIA MATERIAL Kryptonite
     Density              = Constant rho=1
     Thermal Conductivity = constant k=1
     Specific Heat        = Constant cp=1
     heat conduction      = basic
   END ARIA MATERIAL Kryptonite

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  DIRECT_SOLVER
      BEGIN SUPERLU SOLVER
      END
    END TPETRA EQUATION SOLVER
{else}
    Begin Trilinos Equation Solver Direct_Solver
      Solution Method = amesos-superlu
    End
{endif}

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  ITERATIVE_SOLVER
      BEGIN CG SOLVER
        BEGIN JACOBI PRECONDITIONER
        END
        MAXIMUM ITERATIONS = 1000
        RESIDUAL SCALING = NONE
        CONVERGENCE TOLERANCE = 1.000000e-14
      END
    END TPETRA EQUATION SOLVER
{else}
    Begin Trilinos Equation Solver Iterative_Solver
      Solution Method = CG
      Preconditioning Method = Jacobi
      Maximum Iterations = 1000
      Residual Norm Scaling = None
      Residual Norm Tolerance = 1.0e-14
    End
{endif}

   BEGIN FINITE ELEMENT MODEL cube
      database name = cube_h{N}_tet10.e
```

```
     coordinate system is cartesian
     decomposition method = rcb

     BEGIN PARAMETERS FOR BLOCK block_1
material Kryptonite
     END PARAMETERS FOR BLOCK block_1

  END FINITE ELEMENT MODEL cube

  Begin User Function exact_soln
    Load From File ./exact.so Using Function registerExactSoln
  End

  Begin User Function exact_soln_dot
    Load From File ./exact.so Using Function registerExactSolnDot
  End

  Begin User Function exact_src
    Load From File ./exact.so Using Function registerExactSrc
  End

  Begin User Function flux_surface_3
    Load From File ./exact.so Using Function registerFlux_Surface_3
  End

  Begin User Function flux_surface_5
    Load From File ./exact.so Using Function registerFlux_Surface_5
  End

  Begin User Function flux_surface_1
    Load From File ./exact.so Using Function registerFlux_Surface_1
  End

  Begin User Function flux_surface_2
    Load From File ./exact.so Using Function registerFlux_Surface_2
  End

  Begin Norm Postprocessor l2
    Use Function exact_soln
    Subtract Function nonlinear_solution->TEMPERATURE
    Compute Norms L2
  End

  Begin Norm Postprocessor h1
    Use Function exact_soln
    Subtract Function nonlinear_solution->TEMPERATURE
    Compute Norms H1
  End

  Begin Norm Postprocessor linf
    Use Function exact_soln
    Subtract Function nonlinear_solution->TEMPERATURE
    Compute Norms LInfinity
  End

  Begin Postprocessor Output Control pp_out
    Comment Character Is %
 Write To File errors_thermal_steady_tet10_h{N}.dat
    Floating Point Precision Is 3
    Floating Point Format Is Scientific
  End

  BEGIN PROCEDURE myAriaProcedure

     Begin Solution Control Description
Use System Main
Begin System Main
   Begin Sequential The_Time_Block
```

```
      Advance myRegion
   End
      Simulation Start Time = 0
   Simulation Termination Time = 1
End
     End

     BEGIN ARIA REGION myRegion

Nonlinear Solution Strategy = Newton
        Maximum Nonlinear Iterations = 10
        Nonlinear Residual Tolerance = 1.0e-12
        Nonlinear Correction Tolerance = 1.0e-12
        Nonlinear Relaxation Factor  = 1.0
        use dof averaged nonlinear residual

use finite element model cube
        Use Linear Solver Iterative_Solver #Direct_Solver

EQ ENERGY for TEMPERATURE on block_1 using Q2 with DIFF SRC

# surface_4: x=0
# surface_6: x=1

# surface_3: y=0
# surface_5: y=1

# surface_1: z=1
# surface_2: z=0

# const Temp BC (x)
        BC const dirichlet at surface_4 Temperature = 1.0
        BC const dirichlet at surface_6 Temperature = 1.0

# const flux BC (y)
BC FLUX for Energy on surface_3  = constant flux = 3
BC FLUX for Energy on surface_5  = constant flux = 5

BC FLUX for Energy on surface_3  = Encore_Function Name=flux_surface_3
BC FLUX for Energy on surface_5  = Encore_Function Name=flux_surface_5

# convective flux BC with const Temp and H (z)
        BC Flux for Energy on surface_1 = Nat_Conv T_Ref=1 H=1
        BC Flux for Energy on surface_2 = Nat_Conv T_Ref=2 H=2

BC FLUX for Energy on surface_1  = Encore_Function Name=flux_surface_1
BC FLUX for Energy on surface_2  = Encore_Function Name=flux_surface_2

#  const source term
Source For ENERGY on block_1 = Constant value=1

Source For ENERGY on block_1 = Encore_Function Name=exact_src

   Output Number of Nodes

Evaluate Postprocessor l2
Evaluate Postprocessor h1
Evaluate Postprocessor linf

BEGIN RESULTS OUTPUT LABEL diffusion output
   database Name = thermal_steady_tet10_h{N}.e
   at step 1, increment = 1
   # time interval is 1.0
   title Aria cube test
   nodal variables = nonlinear_solution->TEMPERATURE as T
END RESULTS OUTPUT LABEL diffusion output

     END ARIA REGION myRegion
```

```
   END PROCEDURE myAriaProcedure

END SIERRA myJob
```

12.1.7. Transient Heat Conduction: Hex8 Meshes

```
BEGIN SIERRA myJob

   load user plugin file ./exact_transient.so

# L = { L = 10 }
# rho = { rho = 1 }
# Cp = { Cp = 1 }
   BEGIN ARIA MATERIAL Kryptonite
     Density              = Constant rho={rho}
     Thermal Conductivity = constant k=1
     Specific Heat        = Constant cp={Cp}
     heat conduction      = basic
     latent heat = constant value={L}
   END ARIA MATERIAL Kryptonite

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  DIRECT_SOLVER
      BEGIN SUPERLU SOLVER
      END
    END TPETRA EQUATION SOLVER
{else}
    Begin Trilinos Equation Solver Direct_Solver
      Solution Method = amesos-superlu
    End
{endif}

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  ITERATIVE_SOLVER
      BEGIN CG SOLVER
        BEGIN JACOBI PRECONDITIONER
        END
        MAXIMUM ITERATIONS = 1000
        RESIDUAL SCALING = NONE
        CONVERGENCE TOLERANCE = 1.000000e-12
      END
    END TPETRA EQUATION SOLVER
{else}
    Begin Trilinos Equation Solver Iterative_Solver
      Solution Method = CG
      Preconditioning Method = Jacobi
      Maximum Iterations = 1000
      Residual Norm Scaling = None
      Residual Norm Tolerance = 1.0e-12
    End
{endif}

   BEGIN FINITE ELEMENT MODEL cube
      database name = cube_h{N}_hex8.e
      coordinate system is cartesian
      decomposition method = rcb

      BEGIN PARAMETERS FOR BLOCK block_1
 material Kryptonite
      END PARAMETERS FOR BLOCK block_1

   END FINITE ELEMENT MODEL cube

   Begin User Function exact_soln
     Load From File ./exact_transient.so Using Function registerExactSoln
```

```
    End

    Begin User Function exact_soln_dot
      Load From File ./exact_transient.so Using Function registerExactSolnDot
    End

    Begin User Function exact_src
      Load From File ./exact_transient.so Using Function registerExactSrc
    End

    Begin User Function flux_surface_3
      Load From File ./exact_transient.so Using Function registerFlux_Surface_3
    End

    Begin User Function flux_surface_5
      Load From File ./exact_transient.so Using Function registerFlux_Surface_5
    End

    Begin User Function flux_surface_1
      Load From File ./exact_transient.so Using Function registerFlux_Surface_1
    End

    Begin User Function flux_surface_2
      Load From File ./exact_transient.so Using Function registerFlux_Surface_2
    End

# Ts = { Ts = 0.5 }
# Tl = { Tl = 1.5 }
# Tm = { Tm = 0.5 * (Ts + Tl) }
# sigma = { sigma =  0.429858 * (Tm - Ts) }

    Begin Norm Postprocessor l2
      Use Function exact_soln
      Subtract Function nonlinear_solution->TEMPERATURE
      Compute Norms L2
    End

    Begin Norm Postprocessor l2_dot
      Use Function exact_soln_dot
      Subtract Function time_derivative_at_time->TEMPERATURE
      Compute Norms L2
    End

    Begin Norm Postprocessor h1
      Use Function exact_soln
      Subtract Function nonlinear_solution->TEMPERATURE
      Compute Norms H1
    End

    Begin Norm Postprocessor linf
      Use Function exact_soln
      Subtract Function nonlinear_solution->TEMPERATURE
      Compute Norms LInfinity
    End

    Begin Postprocessor Output Control pp_out
      Comment Character Is %
      Write To File errors{N}.dat
      Floating Point Precision Is 3
      Floating Point Format Is Scientific
    End

    BEGIN PROCEDURE myAriaProcedure

       Begin Solution Control Description
 Use System Main
 Begin System Main
    Begin Transient The_Time_Block
```

```
      Advance myRegion
   End
      Simulation Start Time = 0
   Simulation Termination Time = 3
End
Begin Parameters For Transient The_Time_Block
   Begin Parameters For Aria Region myRegion
     Initial Time Step Size = {0.5/2**N}
     Time Integration Method = Second_Order
     Time Step Variation = fixed
  End
End
     End

     BEGIN ARIA REGION myRegion

Nonlinear Solution Strategy = Newton
        Maximum Nonlinear Iterations = 10
        Nonlinear Residual Tolerance = 1.0e-12
        Nonlinear Correction Tolerance = 1.0e-12
        Nonlinear Relaxation Factor  = 1.0
        use dof averaged nonlinear residual

use finite element model cube
        Use Linear Solver Iterative_Solver #Direct_Solver

EQ ENERGY for TEMPERATURE on block_1 using Q1 with MASS DIFF SRC

        IC for temperature on block_1 = encore_function name=exact_soln

# surface_4: x=0
# surface_6: x=1

# surface_3: y=0
# surface_5: y=1

# surface_1: z=1
# surface_2: z=0

# const Temp BC (x)
        BC const dirichlet at surface_4 Temperature = 1.0
        BC const dirichlet at surface_6 Temperature = 1.0

# const flux BC (y)
BC FLUX for Energy on surface_3  = constant flux = 3

        Begin Heat Flux Boundary Condition hfbc2
  Add Surface surface_5
          Flux = -5
        End

BC FLUX for Energy on surface_3  = Encore_Function Name=flux_surface_3
BC FLUX for Energy on surface_5  = Encore_Function Name=flux_surface_5

# convective flux BC with const Temp and H (z)
        BC Flux for Energy on surface_1 = Nat_Conv T_Ref=1 H=1

        Begin Convective Flux Boundary Condition cfbc2
  Add Surface surface_2
          Convective Coefficient = 2
          Reference Temperature = 2
        End

BC FLUX for Energy on surface_1  = Encore_Function Name=flux_surface_1
BC FLUX for Energy on surface_2  = Encore_Function Name=flux_surface_2

#  const source term
        Begin Volume Heating vh1
```

```
          Add Volume block_1
          Value = 1
        End

        Source for Energy on block_1 = melting Ts={Ts} Tl={Tl}

 Source For ENERGY on block_1 = Encore_Function Name=exact_src

    Output Number of Nodes

 Evaluate Postprocessor l2
 Evaluate Postprocessor l2_dot
 Evaluate Postprocessor h1
 Evaluate Postprocessor linf

 BEGIN RESULTS OUTPUT LABEL diffusion output
    database Name = output{N}.e
    at step 0, increment = {2**N}
    #at step 0, increment = 1
    title Aria cube test
    nodal variables = solution->TEMPERATURE as T
    nodal variables = time_derivative_at_time->TEMPERATURE as TDOT
 END RESULTS OUTPUT LABEL diffusion output

      END ARIA REGION myRegion

   END PROCEDURE myAriaProcedure

END SIERRA myJob
```

12.1.8. Transient Heat Conduction: Tet4 Meshes

```
BEGIN SIERRA myJob

   load user plugin file ./exact_transient.so

   BEGIN ARIA MATERIAL Kryptonite
     Density              = Constant rho=1
     Thermal Conductivity = constant k=1
     Specific Heat        = Constant cp=1
     heat conduction      = basic
   END ARIA MATERIAL Kryptonite

   BEGIN ARIA MATERIAL Air
     Density              = Constant rho=1
     Thermal Conductivity = constant k=1
     Specific Heat        = Constant cp=1
     heat conduction      = basic
   END ARIA MATERIAL

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  DIRECT_SOLVER
      BEGIN SUPERLU SOLVER
      END
    END TPETRA EQUATION SOLVER
{else}
    Begin Trilinos Equation Solver Direct_Solver
      Solution Method = amesos-superlu
    End
{endif}

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  ITERATIVE_SOLVER
      BEGIN CG SOLVER
        BEGIN JACOBI PRECONDITIONER
        END
```

```
        MAXIMUM ITERATIONS = 1000
        RESIDUAL SCALING = NONE
        CONVERGENCE TOLERANCE = 1.000000e-12
      END
    END TPETRA EQUATION SOLVER
{else}
    Begin Trilinos Equation Solver Iterative_Solver
      Solution Method = CG
      Preconditioning Method = Jacobi
      Maximum Iterations = 1000
      Residual Norm Scaling = None
      Residual Norm Tolerance = 1.0e-12
    End
{endif}

   BEGIN FINITE ELEMENT MODEL cube
      database name = cube_h{N}_tet4.e
      coordinate system is cartesian
      decomposition method = rcb

      BEGIN PARAMETERS FOR BLOCK block_1
 material Kryptonite
      END PARAMETERS FOR BLOCK block_1

   END FINITE ELEMENT MODEL cube

   Begin User Function exact_soln
     Load From File ./exact_transient.so Using Function registerExactSoln
   End

   Begin User Function exact_soln_dot
     Load From File ./exact_transient.so Using Function registerExactSolnDot
   End

   Begin User Function exact_src
     Load From File ./exact_transient.so Using Function registerExactSrc
   End

   Begin User Function flux_surface_3
     Load From File ./exact_transient.so Using Function registerFlux_Surface_3
   End

   Begin User Function flux_surface_5
     Load From File ./exact_transient.so Using Function registerFlux_Surface_5
   End

   Begin User Function flux_surface_1
     Load From File ./exact_transient.so Using Function registerFlux_Surface_1
   End

   Begin User Function flux_surface_2
     Load From File ./exact_transient.so Using Function registerFlux_Surface_2
   End

   # T0 = { T0 = 2 }
   # h = { h = 2 }
   # rho = { rho = 1 }
   # cp = { cp = 1 }
   # omega = { omega = PI }
   # bn_vol = { bn_vol = 0.5 }
   Begin String Function bulk_node_exact_solution
      Value is "{T0} * (sin({omega} * t) + 1)"
   End
   Begin String Function bulk_node_source
      use function bulk_node_exact_solution as Tb
      Value is "{rho * cp * omega * T0} * cos({omega} * t) - ({h} * (1 - Tb))/{bn_vol}"
   End
   Begin String Function bulk_node_flux_bc_corr
```

```
      use function bulk_node_exact_solution as Tb
      Value is "({h} * (Tb - 2))"
   End

   Begin Norm Postprocessor l2
     Use Function exact_soln
     Subtract Function nonlinear_solution->TEMPERATURE
     Compute Norms L2
     volumes block_1
   End

   Begin Norm Postprocessor l2_dot
     Use Function exact_soln_dot
     Subtract Function time_derivative_at_time->TEMPERATURE
     Compute Norms L2
     volumes block_1
   End

   Begin Norm Postprocessor h1
     Use Function exact_soln
     Subtract Function nonlinear_solution->TEMPERATURE
     Compute Norms H1
     volumes block_1
   End

   Begin Norm Postprocessor linf
     Use Function exact_soln
     Subtract Function nonlinear_solution->TEMPERATURE
     Compute Norms LInfinity
     volumes block_1
   End

   Begin Norm Postprocessor linf_bulk_node
     Use Function bulk_node_exact_solution
     Subtract Function nonlinear_solution->TEMPERATURE
     Compute Norms Nodal LInfinity
     volumes block_for_abulknode
   End

   Begin Postprocessor Output Control pp_out
     Comment Character Is %
     Write To File errors{N}.dat
     Floating Point Precision Is 3
     Floating Point Format Is Scientific
   End

   BEGIN PROCEDURE myAriaProcedure

      Begin Solution Control Description
 Use System Main
 Begin System Main
    Begin Transient The_Time_Block
       Advance myRegion
    End
       Simulation Start Time = 0
    Simulation Termination Time = 3
 End
 Begin Parameters For Transient The_Time_Block
    Begin Parameters For Aria Region myRegion
             Initial Time Step Size = {0.5/2**N}
      Time Integration Method = Second_Order
      Time Step Variation = fixed
   End
 End
      End

      BEGIN ARIA REGION myRegion
```

```
Nonlinear Solution Strategy = Newton
        Minimum Nonlinear Solves = 1
        Maximum Nonlinear Iterations = 10
        Nonlinear Residual Tolerance = 1.0e-12
        nonlinear residual minimum convergence rate = 0.999 number of steps = 3
        Nonlinear Correction Tolerance = 1.0e-12
        Nonlinear Relaxation Factor  = 1.0
        use dof averaged nonlinear residual

use finite element model cube
        Use Linear Solver Iterative_Solver #Direct_Solver

EQ ENERGY for TEMPERATURE on block_1 using Q1 with MASS DIFF SRC

        IC const on block_1 temperature = 1.0

# surface_4: x=0
# surface_6: x=1

# surface_3: y=0
# surface_5: y=1

# surface_1: z=1
# surface_2: z=0

# const Temp BC (x)
        BC const dirichlet at surface_4 Temperature = 1.0
        BC const dirichlet at surface_6 Temperature = 1.0

# const flux BC (y)
BC FLUX for Energy on surface_3  = constant flux = 3
BC FLUX for Energy on surface_5  = constant flux = 5

BC FLUX for Energy on surface_3  = Encore_Function Name=flux_surface_3
BC FLUX for Energy on surface_5  = Encore_Function Name=flux_surface_5

# convective flux BC with const Temp and H (z)
        BC Flux for Energy on surface_1 = Nat_Conv T_Ref=1 H=1

        Begin Bulk Fluid Element aBulkNode
          material = Air
          bulk element volume = constant v = {bn_vol}
          initial temperature = {T0}
          bulk eq energy for temperature using p0 with mass src
          bulk source for energy = encore_function name=bulk_node_source
        End
        Begin Convective Flux Boundary Condition bulk_flux
          add surface surface_2
          use bulk element aBulkNode
          convective coefficient = {h}
        End
        BC Flux for Energy on surface_2 = encore_function name=bulk_node_flux_bc_corr

BC FLUX for Energy on surface_1  = Encore_Function Name=flux_surface_1
BC FLUX for Energy on surface_2  = Encore_Function Name=flux_surface_2

#  const source term
Source For ENERGY on block_1 = Constant value=1

Source For ENERGY on block_1 = Encore_Function Name=exact_src

   Output Number of Nodes

Evaluate Postprocessor l2
Evaluate Postprocessor l2_dot
Evaluate Postprocessor h1
Evaluate Postprocessor linf
Evaluate Postprocessor linf_bulk_node
```

```
 BEGIN RESULTS OUTPUT LABEL diffusion output
           database Name = output{N}.e
    at step 0, increment = {2**N}
    title Aria cube test
    nodal variables = solution->TEMPERATURE as T
    nodal variables = time_derivative_at_time->TEMPERATURE as TDOT
      global variables = abulknode_T
 END RESULTS OUTPUT LABEL diffusion output

      END ARIA REGION myRegion

   END PROCEDURE myAriaProcedure

END SIERRA myJob
```

12.1.9. Transient Heat Conduction: Tet4Tet10 Meshes

```
BEGIN SIERRA myJob

   load user plugin file ./exact_transient.so

   BEGIN ARIA MATERIAL Kryptonite
     Density              = Constant rho=1
     Thermal Conductivity = constant k=1
     Specific Heat        = Constant cp=1
     heat conduction      = basic
   END ARIA MATERIAL Kryptonite

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  DIRECT_SOLVER
      BEGIN SUPERLU SOLVER
      END
    END TPETRA EQUATION SOLVER
{else}
    Begin Trilinos Equation Solver Direct_Solver
      Solution Method = amesos-superlu
    End
{endif}

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  ITERATIVE_SOLVER
      BEGIN CG SOLVER
        BEGIN JACOBI PRECONDITIONER
        END
        MAXIMUM ITERATIONS = 1000
        RESIDUAL SCALING = NONE
        CONVERGENCE TOLERANCE = 1.000000e-12
      END
    END TPETRA EQUATION SOLVER
{else}
    Begin Trilinos Equation Solver Iterative_Solver
      Solution Method = CG
      Preconditioning Method = Jacobi
      Maximum Iterations = 1000
      Residual Norm Scaling = None
      Residual Norm Tolerance = 1.0e-12
    End
{endif}

   BEGIN FINITE ELEMENT MODEL cube
      database name = cube_h{N}_tet10.e
      coordinate system is cartesian
      decomposition method = rcb

      BEGIN PARAMETERS FOR BLOCK block_1
```

```
material Kryptonite
     END PARAMETERS FOR BLOCK block_1

  END FINITE ELEMENT MODEL cube

  Begin User Function exact_soln
    Load From File ./exact_transient.so Using Function registerExactSoln
  End

  Begin User Function exact_soln_dot
    Load From File ./exact_transient.so Using Function registerExactSolnDot
  End

  Begin User Function exact_src
    Load From File ./exact_transient.so Using Function registerExactSrc
  End

  Begin User Function flux_surface_3
    Load From File ./exact_transient.so Using Function registerFlux_Surface_3
  End

  Begin User Function flux_surface_5
    Load From File ./exact_transient.so Using Function registerFlux_Surface_5
  End

  Begin User Function flux_surface_1
    Load From File ./exact_transient.so Using Function registerFlux_Surface_1
  End

  Begin User Function flux_surface_2
    Load From File ./exact_transient.so Using Function registerFlux_Surface_2
  End

  Begin Norm Postprocessor l2
    Use Function exact_soln
    Subtract Function nonlinear_solution->TEMPERATURE
    Compute Norms L2
  End

  Begin Norm Postprocessor l2_dot
    Use Function exact_soln_dot
    Subtract Function time_derivative_at_time->TEMPERATURE
    Compute Norms L2
  End

  Begin Norm Postprocessor h1
    Use Function exact_soln
    Subtract Function nonlinear_solution->TEMPERATURE
    Compute Norms H1
  End

  Begin Norm Postprocessor linf
    Use Function exact_soln
    Subtract Function nonlinear_solution->TEMPERATURE
    Compute Norms LInfinity
  End

  Begin Postprocessor Output Control pp_out
    Comment Character Is %
    Write To File errors{N}.dat
    Floating Point Precision Is 3
    Floating Point Format Is Scientific
  End

  BEGIN PROCEDURE myAriaProcedure

     Begin Solution Control Description
Use System Main
```

```
Begin System Main
   Begin Transient The_Time_Block
      Advance myRegion
   End
      Simulation Start Time = 0
   Simulation Termination Time = 3
End
Begin Parameters For Transient The_Time_Block
   Begin Parameters For Aria Region myRegion
             Initial Time Step Size = {0.5/2**N}
     Time Integration Method = Second_Order
     Time Step Variation = fixed
  End
End
     End

     BEGIN ARIA REGION myRegion

Nonlinear Solution Strategy = Newton
        Maximum Nonlinear Iterations = 10
        Nonlinear Residual Tolerance = 1.0e-12
        Nonlinear Correction Tolerance = 1.0e-12
        Nonlinear Relaxation Factor  = 1.0
        use dof averaged nonlinear residual

use finite element model cube
        Use Linear Solver Iterative_Solver #Direct_Solver

EQ ENERGY for TEMPERATURE on block_1 using Q1 with MASS DIFF SRC

        IC const on block_1 temperature = 1.0

# surface_4: x=0
# surface_6: x=1

# surface_3: y=0
# surface_5: y=1

# surface_1: z=1
# surface_2: z=0

# const Temp BC (x)
        BC const dirichlet at surface_4 Temperature = 1.0
        BC const dirichlet at surface_6 Temperature = 1.0

# const flux BC (y)
BC FLUX for Energy on surface_3  = constant flux = 3
BC FLUX for Energy on surface_5  = constant flux = 5

BC FLUX for Energy on surface_3  = Encore_Function Name=flux_surface_3
BC FLUX for Energy on surface_5  = Encore_Function Name=flux_surface_5

# convective flux BC with const Temp and H (z)
        BC Flux for Energy on surface_1 = Nat_Conv T_Ref=1 H=1
        BC Flux for Energy on surface_2 = Nat_Conv T_Ref=2 H=2

BC FLUX for Energy on surface_1  = Encore_Function Name=flux_surface_1
BC FLUX for Energy on surface_2  = Encore_Function Name=flux_surface_2

#  const source term
Source For ENERGY on block_1 = Constant value=1

Source For ENERGY on block_1 = Encore_Function Name=exact_src

   Output Number of Nodes

Evaluate Postprocessor l2
Evaluate Postprocessor l2_dot
```

```
 Evaluate Postprocessor h1
 Evaluate Postprocessor linf

 BEGIN RESULTS OUTPUT LABEL diffusion output
           database Name = output{N}.e
    at step 0, increment = {2**N}
    title Aria cube test
    nodal variables = solution->TEMPERATURE as T
    nodal variables = time_derivative_at_time->TEMPERATURE as TDOT
 END RESULTS OUTPUT LABEL diffusion output

      END ARIA REGION myRegion

   END PROCEDURE myAriaProcedure

END SIERRA myJob
```

12.1.10. Transient Heat Conduction: Tet10 Meshes

```
BEGIN SIERRA myJob

   load user plugin file ./exact_transient.so

   BEGIN ARIA MATERIAL Kryptonite
     Density              = Constant rho=1
     Thermal Conductivity = constant k=1
     Specific Heat        = Constant cp=1
     heat conduction      = basic
   END ARIA MATERIAL Kryptonite

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  DIRECT_SOLVER
      BEGIN SUPERLU SOLVER
      END
    END TPETRA EQUATION SOLVER
{else}
    Begin Trilinos Equation Solver Direct_Solver
      Solution Method = amesos-superlu
    End
{endif}

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  ITERATIVE_SOLVER
      BEGIN CG SOLVER
        BEGIN JACOBI PRECONDITIONER
        END
        MAXIMUM ITERATIONS = 1000
        RESIDUAL SCALING = NONE
        CONVERGENCE TOLERANCE = 1.000000e-12
      END
    END TPETRA EQUATION SOLVER
{else}
    Begin Trilinos Equation Solver Iterative_Solver
      Solution Method = CG
      Preconditioning Method = Jacobi
      Maximum Iterations = 1000
      Residual Norm Scaling = None
      Residual Norm Tolerance = 1.0e-12
    End
{endif}

   BEGIN FINITE ELEMENT MODEL cube
      database name = cube_h{N}_tet10.e
      coordinate system is cartesian
      decomposition method = rcb
```

```
      BEGIN PARAMETERS FOR BLOCK block_1
material Kryptonite
      END PARAMETERS FOR BLOCK block_1

   END FINITE ELEMENT MODEL cube

   Begin User Function exact_soln
     Load From File ./exact_transient.so Using Function registerExactSoln
   End

   Begin User Function exact_soln_dot
     Load From File ./exact_transient.so Using Function registerExactSolnDot
   End

   Begin User Function exact_src
     Load From File ./exact_transient.so Using Function registerExactSrc
   End

   Begin User Function flux_surface_3
     Load From File ./exact_transient.so Using Function registerFlux_Surface_3
   End

   Begin User Function flux_surface_5
     Load From File ./exact_transient.so Using Function registerFlux_Surface_5
   End

   Begin User Function flux_surface_1
     Load From File ./exact_transient.so Using Function registerFlux_Surface_1
   End

   Begin User Function flux_surface_2
     Load From File ./exact_transient.so Using Function registerFlux_Surface_2
   End

   Begin Norm Postprocessor l2
     Use Function exact_soln
     Subtract Function nonlinear_solution->TEMPERATURE
     Compute Norms L2
   End

   Begin Norm Postprocessor l2_dot
     Use Function exact_soln_dot
     Subtract Function time_derivative_at_time->TEMPERATURE
     Compute Norms L2
   End

   Begin Norm Postprocessor h1
     Use Function exact_soln
     Subtract Function nonlinear_solution->TEMPERATURE
     Compute Norms H1
   End

   Begin Norm Postprocessor linf
     Use Function exact_soln
     Subtract Function nonlinear_solution->TEMPERATURE
     Compute Norms LInfinity
   End

   Begin Postprocessor Output Control pp_out
     Comment Character Is %
     Write To File errors{N}.dat
     Floating Point Precision Is 3
     Floating Point Format Is Scientific
   End

   BEGIN PROCEDURE myAriaProcedure

      Begin Solution Control Description
```

```
Use System Main
Begin System Main
   Begin Transient The_Time_Block
      Advance myRegion
   End
      Simulation Start Time = 0
   Simulation Termination Time = 3
End
Begin Parameters For Transient The_Time_Block
   Begin Parameters For Aria Region myRegion
             Initial Time Step Size = {0.5/2**N}
     Time Integration Method = Second_Order
     Time Step Variation = fixed
  End
End
     End

     BEGIN ARIA REGION myRegion

Nonlinear Solution Strategy = Newton
        Maximum Nonlinear Iterations = 10
        Nonlinear Residual Tolerance = 1.0e-12
        Nonlinear Correction Tolerance = 1.0e-12
        Nonlinear Relaxation Factor  = 1.0
        use dof averaged nonlinear residual

use finite element model cube
        Use Linear Solver Iterative_Solver #Direct_Solver

EQ ENERGY for TEMPERATURE on block_1 using Q2 with MASS DIFF SRC

        IC const on block_1 temperature = 1.0

# surface_4: x=0
# surface_6: x=1

# surface_3: y=0
# surface_5: y=1

# surface_1: z=1
# surface_2: z=0

# const Temp BC (x)
        BC const dirichlet at surface_4 Temperature = 1.0
        BC const dirichlet at surface_6 Temperature = 1.0

# const flux BC (y)
BC FLUX for Energy on surface_3  = constant flux = 3
BC FLUX for Energy on surface_5  = constant flux = 5

BC FLUX for Energy on surface_3  = Encore_Function Name=flux_surface_3
BC FLUX for Energy on surface_5  = Encore_Function Name=flux_surface_5

# convective flux BC with const Temp and H (z)
        BC Flux for Energy on surface_1 = Nat_Conv T_Ref=1 H=1
        BC Flux for Energy on surface_2 = Nat_Conv T_Ref=2 H=2

BC FLUX for Energy on surface_1  = Encore_Function Name=flux_surface_1
BC FLUX for Energy on surface_2  = Encore_Function Name=flux_surface_2

#  const source term
Source For ENERGY on block_1 = Constant value=1

Source For ENERGY on block_1 = Encore_Function Name=exact_src

   Output Number of Nodes

Evaluate Postprocessor l2
```

```
 Evaluate Postprocessor l2_dot
 Evaluate Postprocessor h1
 Evaluate Postprocessor linf

 BEGIN RESULTS OUTPUT LABEL diffusion output
            database Name = output{N}.e
    at step 0, increment = {2**N}
    title Aria cube test
    nodal variables = solution->TEMPERATURE as T
    nodal variables = time_derivative_at_time->TEMPERATURE as TDOT
 END RESULTS OUTPUT LABEL diffusion output

      END ARIA REGION myRegion

    END PROCEDURE myAriaProcedure

END SIERRA myJob
```

12.2. THERMAL BOUNDARY CONDITIONS

12.2.1. Radiative Heat Flux 3.1

```
BEGIN SIERRA Aria

  Title Radiation Form Factor Flux User_Sub

  Begin Global Constants
    Stefan Boltzmann constant = 5.6704E-8
  End Global Constants

  load user plugin file ./FormFactor.so
  load user plugin file ./DirichletBC.so

   Begin User Function exact_soln
     Load From File ./Exact_Solution.so Using Function registerExactSoln
   End

   Begin Norm Postprocessor l2
     Use Function exact_soln
     Subtract Function nonlinear_solution->TEMPERATURE
     Compute Norms L2
   End

   Begin Norm Postprocessor h1
     Use Function exact_soln
     Subtract Function nonlinear_solution->TEMPERATURE
     Compute Norms H1
   End

   Begin Norm Postprocessor linf
     Use Function exact_soln
     Subtract Function nonlinear_solution->TEMPERATURE
     Compute Norms LInfinity
   End

   Begin Postprocessor Output Control pp_out
     Comment Character Is %
     Write To File errors{N}.dat
     Floating Point Precision Is 3
     Floating Point Format Is Scientific
   End

  Begin Aria Material mat1
    density = constant rho = 0.1
    thermal conductivity = constant k = 1.0
    specific heat = constant cp = 1.0
    heat conduction = basic
  End Aria Material mat1

  Begin Aria Material mat_s1
    emissivity = constant e = 0.8
    bc rad reference temperature = constant t_ref = 500
    radiation form factor = calore_user_sub name = form_factor type = element
  End

  Begin Finite Element Model myModel
    Database Name = mesh{N}.g
    Coordinate System = Cartesian
    decomposition method = rcb
    Database Type = EXODUSII
    Use Material mat1 for block_1
    Use Material mat_s1 for surface_1
  End Finite Element Model myModel
```

```
{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  SOLVE_TEMPERATURE
      BEGIN CG SOLVER
        BEGIN JACOBI PRECONDITIONER
        END
        MAXIMUM ITERATIONS = 1000
        RESIDUAL SCALING = R0
        CONVERGENCE TOLERANCE = 1.000000e-12
      END
    END TPETRA EQUATION SOLVER
{else}
    begin aztec equation solver solve_temperature
      solution method = cg
      preconditioning method = jacobi
      maximum iterations = 1000
      residual norm tolerance = 1.0e-12
      residual norm scaling = r0
    end aztec equation solver solve_temperature
{endif}

  begin procedure myProcedure

     Begin Solution Control Description
        Use System Main
        Begin System Main
           Begin Sequential MySolveBlock
              Advance myRegion
           End
        End
     End

    begin Aria region myRegion

     Use Finite Element Model myModel
     Use Linear Solver solve_temperature

     Nonlinear Solution Strategy = Newton

     Maximum nonlinear iterations = 10
     Nonlinear residual tolerance = 1.0e-10
     Nonlinear correction tolerance = 1.0e-10
     Nonlinear relaxation factor  = 1.0

     EQ ENERGY for TEMPERATURE on block_1 using Q1 with DIFF

     BC dirichlet for temperature on surface_3 = calore_user_sub name = localCoord_bc type=node

#     Begin Radiative Flux Boundary Condition fraction
#       Add surface surface_1
#       Emissivity = 0.8
#       Reference Temperature = 500.0
#       Radiation Form Factor Subroutine = form_factor
#     End

     BC Flux for Energy at surface_1 = generalized_rad

     BC const DIRICHLET at surface_2 temperature = 600.0
     BC const DIRICHLET at surface_4 temperature = 600.0

     Output Number of Nodes
     Evaluate Postprocessor l2
     Evaluate Postprocessor h1
     Evaluate Postprocessor linf

     Begin Results Output Label diffusion output
       database Name = output{N}.e
       At Step 1, Increment = 1
       Timestep Adjustment Interval = 1
```

```
      Title Radiative Flux BC User Sub Test
      Nodal Variables = solution->temperature as T
    End Results Output Label diffusion output

   end Aria region myRegion

 end procedure myProcedure

end sierra Aria
```

12.2.2. Radiative Heat Flux From Fortran User Subroutine

```
begin sierra FandI_VnVtest

   title Verification of Fire and Ice BC subroutine, AKA Directed Heating User Sub \$
   Simplified model with sidesets to check that BCs are applied to faces specified \$

Load User Plugin File ./FireAndIceBC.so USING function conv_subs_register

###################################################
######## Material property definitions ############
###################################################

  begin aria material VnVmat
    heat conduction = basic
    density = constant rho = 8000.0 # Approximate value for VnV study
    emissivity = constant e = 0.30 # Approximate value for VnV study
    specific heat = constant cp = 550 # Approximate value for VnV study
    thermal conductivity = constant k = 20 # Approximate value for VnV study
  end aria material VnVmat

#####################################################################
############ UPDATE THE FINITE ELEMENT MODEL #######################
#####################################################################

   begin finite element model fem
      database name = VnVmesh2.g
      database type = exodusII
      use material VnVmat for block_1

      # - Block id 10 had name 10
      use material VnVmat for block_10

      # - Block id 11 had name 11
      use material VnVmat for block_11

      # - Block id 12 had name 12
      use material VnVmat for block_12

      # - Block id 13 had name 13
      use material VnVmat for block_13

      # - Block id 2 had name 2
      use material VnVmat for block_2

      # - Block id 3 had name 3
      use material VnVmat for block_3

      # - Block id 4 had name 4
      use material VnVmat for block_4

      # - Block id 5 had name 5
      use material VnVmat for block_5

      # - Block id 6 had name 6
      use material VnVmat for block_6
```

```
      # - Block id 7 had name 7
      use material VnVmat for block_7

      # - Block id 8 had name 8
      use material VnVmat for block_8

      # - Block id 9 had name 9
      use material VnVmat for block_9
   end finite element model fem

###################################################

  begin global constants
    stefan boltzmann constant = 5.67e-8
  end global constants

################################################

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  TRILINOS_SOLVE
      BEGIN GMRES SOLVER
        BEGIN DD-ILUT PRECONDITIONER
          DROP TOLERANCE = 0
          FILL FRACTION = 5.000000e+00
        END
        MAXIMUM ITERATIONS = 1000
        RESTART ITERATIONS = 100
        RESIDUAL SCALING = R0
        CONVERGENCE TOLERANCE = 1.000000e-12
      END
      MATRIX SCALING = ONE_NORM
    END TPETRA EQUATION SOLVER
{else}
    Begin TRILINOS Equation Solver trilinos_solve
      Solution Method = GMRES
      Preconditioning Method = DD-ILUT
      Maximum Iterations = 1000
      Matrix Scaling = row-sum
      Residual Norm Tolerance = 1.0e-12
      Residual Norm Scaling = R0
      Restart Iterations is 100
      preconditioning steps is 1
      Param-Real AZ_ilut_fill value 5.0
      polynomial order = 300
      ilu threshold = 1.0e-6
    End TRILINOS Equation Solver trilinos_solve
{endif}

  begin procedure aria_procedure

    begin solution control description

      Use System Main

      Begin System Main
        Simulation Max Global Iterations = 10000
        Simulation Start Time           = 0.0
        #Simulation Termination Time      = 3600.0

        Begin Transient Main
          Advance myRegion
        End

      End

      Begin Parameters For Transient Main
        Start Time = 0.0
```

```
        Termination Time = 0.1

        Begin Parameters for Aria Region myRegion
#         --------------------------------------#
          Time Integration Method = Second_Order  #Second_Order
#         --------------------------------------#
          Time Step Variation     = Adaptive
          Initial Time Step Size  = 0.01
          Minimum Time Step Size  = 0.01
          Maximum Time Step Size  = 0.01
          #Minimum Resolved Time Step Size = 0.001
          Predictor-Corrector Tolerance = 1.0e-08
        End
      End

    End  #solution control

#######################################################

    begin aria region myRegion
       # solve energy equation for temperature at the nodes (1st order) with diffusion
       EQ ENERGY for TEMPERATURE on all_blocks using Q1 with lumped_mass Diff

      use finite element model fem

      nonlinear solution strategy = newton
      use dof averaged nonlinear residual
      accept solution after maximum nonlinear iterations = true
      use linear solver trilinos_solve
      nonlinear relaxation factor = 1.0

      nonlinear residual tolerance = 1.0e-10  # for transient
      maximum nonlinear iterations = 10  # for transient
      #nonlinear residual tolerance = 1.0e-15 # for steady state
      #maximum nonlinear iterations = 150 # for steady state

#########################################################
############## Initial Conditions ######################
#########################################################

      IC Const on all_blocks temperature = 300.0

#########################################################
########### Convective Boundary Conditions ##############
#########################################################
#
        begin convective flux boundary condition FireAndIceBC

          add surface surface_1   surface_2   surface_3   surface_4
          add surface surface_5   surface_6   surface_7   surface_8
          add surface surface_9   surface_10  surface_11  surface_12
          add surface surface_13  surface_14  surface_15  surface_16
          add surface surface_17  surface_18  surface_19  surface_20
          add surface surface_21  surface_22  surface_23  surface_24
          add surface surface_25 # All external surfaces

# User Sub Integer Input Constants:
#   cosdistA=idat(1), for x < xA
#   cosdistAB=idat(2), for xA <= x <= xB
#   cosdistB=idat(3), for x > xB

# User Sub Real Input Constants:
#   xoffset=rdat(1), such that abs(xnosetip-xoffset)=0
#   xA=rdat(2), distance from nosetip to position A (xA>0)
#   xB=rdat(3), distance from nosetip to position B (xB>0)
#   hA1=rdat(4), convective htc for x < xA for azimuthal section 1
#   hAB1=rdat(5), convective htc for xA <= x <= xB for section 1
#   hB1=rdat(6), convective htc for x > xB for azimuthal section 1
```

```
#   TrefA1=rdat(7), Tref for x < xA for azimuthal section 1
#   TrefAB1=rdat(8), Tref for xA <= x <= xB for azimuthal section 1
#   TrefB1=rdat(9), Tref for x > xB for azimuthal section 1
#   emisA1=rdat(10), emis for x < xA for azimuthal section 1
#   emisAB1=rdat(11), emis for xA <= x <= xB for azimuthal section 1
#   emisB1=rdat(12), emis for x > xB for azimuthal section 1
#   hA2=rdat(13), convective htc for x < xA for azimuthal section 2
#   hAB2=rdat(14), convective htc for xA <= x <= xB for azimuthal section 2
#   hB2=rdat(15), convective htc for x > xB for azimuthal section 2
#   TrefA2=rdat(16), Tref for x < xA for azimuthal section 2
#   TrefAB2=rdat(17), Tref for xA <= x <= xB for azimuthal section 2
#   TrefB2=rdat(18), Tref for x > xB for azimuthal section 2
#   emisA2=rdat(19), emis for x < xA for azimuthal section 2
#   emisAB2=rdat(20), emis for xA <= x <= xB for azimuthal section 2
#   emisB2=rdat(21), emis for x > xB for azimuthal section 2
#   thetaA=rdat(22),  azimuthal reference angle (degrees) for section 1 of region A
#   thetaAB=rdat(23), azimuthal reference angle (degrees) for section 1 of region AB
#   thetaB=rdat(24), azimuthal reference angle (degrees) for section 1 of region B
#   dphiA=rdat(25), subtended angle (degrees) for section 1 of region A
#   dphiAB=rdat(26), subtended angle (degrees) for section 1 of region AB
#   dphiB=rdat(27), subtended angle (degrees) for section 1 of region B
# notes:
#   if cosdistA (or AB,or B) set to 1 then impose cosine distribution on radiative htc
#    otherwise, distribution is uniform (convective distribution is always uniform)
#   x coordinate assumed to lie on centerline of bomb
#   htc_total = convective htc + effective radiative htc
#   effective radiative htc = sigma*emis*(Twall+Tref)*(Twall^2+Tref^2)
#   emissivities should be the same as associated material emissivities, but
#    can be set to zero to eliminate radiative heat transfer from a region
#   set convective htc to zero to eliminate convective heat tranfer from a region
#   set both convective htc and emis to zero for an adiabatic (insulated) surface
#   a zero-degree angle corresponds to the y axis
#   angle is positive in clockwise direction when looking in the positive x axis direction
#   theta is the angle for the center of the azimuthal section and dphi is the delta angle
#    with section 1 extending from theta-dphi/2 to theta+dphi/2, centered on theta
#   section 2 is opposite section 1 and can be empty if dphi = 360 degrees.

            convective coefficient fortran subroutine is coef_directed_angle
            reference temperature fortran subroutine is tref_directed_angle
            integer data 0 0 0
              #       xoffset  xA   xB
              #   hA1     hAB1     hB1
              #   TrefA1  TrefAB1  TrefB1
              #   emisA1  emisAB1  emisB1
              #   hA2     hAB2     hB2
              #   TrefA2  TrefAB2  TrefB2
              #   emisA2  emisAB2  emisB2
              #       thetaA  thetaAB  thetaB
              #       dphiA   dphiAB   dphiB
            real data -1.5 0.5 1.0  \$
                  0.0 50.0    0  \$
                  300.0  1000.0  300.0  \$
                  0.0    0.8    0.0  \$
                  0.0 0.0    100.0  \$
                  300.0  300.0  900.0  \$
                  0.0    0.0    0.0  \$
                      0.0   300.0   240.  \$
                      0.0 120.0 240.0
#                                                                                     +theta
#          xA     xB   azimuthal section 1                -dphi/2        ^           ^   |
#      A    |  AB  |     B   axial (x axis) regions        |             y|          y|   V
#   ==============================  surfaces              0-theta        |_ _ > x    |_ _ >z
#           |      |                                       |
#          xA     xB   azimuthal section 2                 dphi/2     z out of page  x into page
#
            integrated power output qFireIce
            integrated flux output fluxFireIce
```

```
        end convective flux boundary condition FireAndIceBC


#######################################################
############# Results ################################
#######################################################
#######################################################

      Begin user variable HTC
        type is face real length = 1
        initial value = 0.0
        add part surface_1   surface_2   surface_3   surface_4
        add part surface_5   surface_6   surface_7   surface_8
        add part surface_9   surface_10  surface_11  surface_12
        add part surface_13  surface_14  surface_15  surface_16
        add part surface_17  surface_18  surface_19  surface_20
        add part surface_21  surface_22  surface_23  surface_24
        add part surface_25
      End

      Begin user variable SurfFlux
        type is face real length = 1
        initial value = 0.0
         add part surface_1   surface_2   surface_3   surface_4
         add part surface_5   surface_6   surface_7   surface_8
         add part surface_9   surface_10  surface_11  surface_12
         add part surface_13  surface_14  surface_15  surface_16
         add part surface_17  surface_18  surface_19  surface_20
         add part surface_21  surface_22  surface_23  surface_24
         add part surface_25
      End

      Begin user variable Tref  #for checking only
        type is face real length = 1
        initial value = 0.0
         add part surface_1   surface_2   surface_3   surface_4
         add part surface_5   surface_6   surface_7   surface_8
         add part surface_9   surface_10  surface_11  surface_12
         add part surface_13  surface_14  surface_15  surface_16
         add part surface_17  surface_18  surface_19  surface_20
         add part surface_21  surface_22  surface_23  surface_24
         add part surface_25
     End


      Begin Results Output NodalTdata
        Title VnVtest Nodal Temperature Data
        database name = VnVinputTest.e
        Nodal Variables = solution->temperature as T
        #nodal variables = temperaturedot as Tdot
        #Face Variables = HTC SurfFlux Tref #costheta
        Global Variables = time_step as timestep

#         Global Variables = PEinterior_T as PEinterior_T

        Timestep Adjustment Interval is 1
        At Time 0.0, Increment = 0.01  #

      End

#######################################################

      end aria region myRegion

  end procedure aria_procedure

end sierra FandI_VnVtest
```

12.2.3. Convective Heat Flux 3.3

```
Begin SIERRA Aria

  load user plugin file ./Exact_Solution.so

  Begin User Function exact_soln
    Load From File ./Exact_Solution.so Using Function registerExactSoln
  End

   Begin Norm Postprocessor l2_norm
     Use Function exact_soln
     Subtract Function nonlinear_solution->temperature
     Compute Norms L2
   End

   Begin Norm Postprocessor h1_norm
     Use Function exact_soln
     Subtract Function nonlinear_solution->temperature
     Compute Norms H1
   End

   Begin Norm Postprocessor linf_norm
     Use Function exact_soln
     Subtract Function nonlinear_solution->temperature
     Compute Norms LInfinity
   End

  Begin Postprocessor Output Control pp_out
     Comment Character Is %
     Write To File errors{N}.dat
     Floating Point Precision Is 3
     Floating Point Format Is Scientific
  End

  load user plugin file ./FluxBC.so
  load user plugin file ./DirichletBC.so
  load user plugin file ./Init.so

  Begin Aria Material M_Block
    density              = constant rho = 1.
    specific heat        = constant cp = 1.
    heat conduction      = basic
    Thermal conductivity = constant k = 1.
  End

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  SOLVE_TEMPERATURE
      BEGIN GMRES SOLVER
        BEGIN DD-ILU PRECONDITIONER
        END
        MAXIMUM ITERATIONS = 1000
        RESIDUAL SCALING = NONE
        CONVERGENCE TOLERANCE = 1.000000e-12
      END
    END TPETRA EQUATION SOLVER
{else}
    Begin AZTEC Equation Solver solve_temperature
      Solution Method = gmres
      Preconditioning Method = dd-ilu
      Maximum Iterations = 1000
      Residual Norm Tolerance = 1e-12
      Residual Norm Scaling = NONE
    End
{endif}

  Begin Finite Element Model myModel
```

```
  Database Name = mesh{N}.g
  Coordinate System = cartesian
  decomposition method = rcb
  Use Material M_Block for block_1
End

Begin procedure myProcedure

  Begin solution control description
    Use System Main
    Begin System Main
      Simulation Start Time            = 0.0
      Simulation Termination Time      = 0.1
      Simulation Max Global Iterations = 100
      Begin Transient Time_Block
advance myRegion
      End
    End System Main

    Begin parameters for transient Time_Block
      Start Time = 0.0
      Begin parameters for aria Region myRegion
        time step variation = fixed # adaptive
        initial time step size = {0.008*0.5**(N)}
        time integration method = second_order
        predictor-corrector tolerance = 1.0E-5
      End
    End
  End Solution Control Description

  begin aria region myRegion

    Use Finite Element Model myModel
    Use Linear Solver solve_temperature

    nonlinear solution strategy = newton
    nonlinear residual tolerance = 1.0e-10
    maximum nonlinear iterations = 10
    Nonlinear Relaxation Factor = 1.0

    EQ energy for temperature on block_1 using Q1 with diff mass

    BC const dirichlet on surface_2 Temperature = 0.0

    Begin Temperature Boundary Condition s4
      Add Surface surface_4
      Temperature = 0.0
    End

    BC dirichlet for temperature on surface_3 = calore_user_sub name = localCoord_bc type=node
    IC for temperature on block_1 = calore_user_sub name = localCoord_ic type=node

    Output Number of Nodes
    Evaluate Postprocessor l2_norm
    Evaluate Postprocessor h1_norm
    Evaluate Postprocessor linf_norm

    Begin Convective Flux Boundary Condition internal
      Add Surface surface_1  #y=1, 0<x<1, normal=(0,1)
      Reference Temperature Subroutine = tref_coeff
      Convective Coefficient Subroutine = convec_coeff
    End

    Begin Results Output output
      Database Name = output{N}.e
      AT STEP 0, INCREMENT = {2**(N)}
      TITLE Aria Heat Convective Flux BC Condition
      Nodal Variables = nonlinear_solution->temperature as T
```

```
      End

    end aria region myRegion

  End procedure myProcedure

End sierra Aria
```

12.3. THERMAL CONTACT

12.3.1. 1D Flat Contact 4.1

12.3.1.1. Hex8 Tied

```
#{R=0.0}
begin sierra Aria

    title Adaptive Square

    load user plugin file ./Exact_solution.so

    BEGIN ARIA MATERIAL M1
        Density              = Constant rho=1
        Thermal Conductivity = constant k=1
        Specific Heat        = Constant cp=1
        heat conduction      = basic
    END

    BEGIN ARIA MATERIAL M2
        Density              = Constant rho=1
        Thermal Conductivity = constant k=1
        Specific Heat        = Constant cp=1
        heat conduction      = basic
    END

    Begin Finite Element Model bar
        Database Name = 2blocks_contact_unaligned_hex8_h{N}.g
        Begin parameters for block block_1
            material M1
        End
        Begin parameters for block block_2
            material M2
        End
    End Finite Element Model bar

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  DIRECT_SOLVER
      BEGIN UMFPACK SOLVER
      END
    END TPETRA EQUATION SOLVER
{else}
    begin trilinos equation solver direct_solver
      solution method = amesos-umfpack
    end trilinos equation solver direct_solver
{endif}

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  ITERATIVE_SOLVER
      BEGIN GMRES SOLVER
        BEGIN JACOBI PRECONDITIONER
        END
        MAXIMUM ITERATIONS = 20000
        RESIDUAL SCALING = R0
        CONVERGENCE TOLERANCE = 1.000000e-12
      END
    END TPETRA EQUATION SOLVER
{else}
    Begin Trilinos Equation Solver Iterative_Solver
      Solution Method = GMRES
      Preconditioning Method = Jacobi
      Maximum Iterations = 20000
      Residual Norm Scaling = R0
      Residual Norm Tolerance = 1.0e-12
    End
```

```
{endif}

    Begin Field Function ffunc
        Use Nodal Field solution->temperature As Value
    End

    Begin User Function exact_soln
        Load From File ./Exact_solution.so Using Function registerExactSolution
        Parameter R = {R}
    End

    Begin Norm Postprocessor l2
        Use Function exact_soln
        Subtract Function ffunc
        Compute Norms L2
        Store in l2_err
    End

    Begin Norm Postprocessor linf
        Use Function exact_soln
        Subtract Function ffunc
        Compute Norms LInfinity
        Store in linf_err
    End

    Begin Norm Postprocessor h1
        Use Function exact_soln
        Subtract Function ffunc
        Compute Norms H1
        Store in h1_err
    End

    Begin Postprocessor Output Control pp_out
        Comment Character Is %
        Write To File errors_tied_h{N}.dat
        Floating Point Precision Is 3
        Floating Point Format Is Scientific
    End

    begin procedure myProcedure

        Begin Solution Control Description
            Use System Main
            Begin System Main
                Begin Sequential The_Time_Block
                    Advance myRegion
                End
                Simulation Start Time = 0
                Simulation Termination Time = 1
            End
        End

        begin Aria region myRegion

            Nonlinear Solution Strategy = Newton
            Maximum Nonlinear Iterations = 10
            Nonlinear Residual Tolerance = 1.0e-12
            Nonlinear Correction Tolerance = 1.0e-12
            Nonlinear Relaxation Factor  = 1.0
            use dof averaged nonlinear residual

            use finite element model bar
            use linear solver Iterative_Solver #Direct_Solver #

            EQ ENERGY for TEMPERATURE on all_blocks using Q1 with DIFF SRC

            Begin  TEMPERATURE BOUNDARY CONDITION xm1
                add surface surface_1
```

```
                TEMPERATURE = 0.
            End

            Begin  TEMPERATURE BOUNDARY CONDITION xp1
                add surface surface_2
                TEMPERATURE = 1.
            End

            Begin VOLUME HEATING sm
                add volume block_1
                VALUE = -1.
            End

            Begin VOLUME HEATING sp
                add volume block_2
                VALUE = 1.
            End

            begin contact definition res1
                contact surface surf_1 contains surface_3
                contact surface surf_2 contains surface_4

                begin interaction inter_1
                    surfaces = surf_1 surf_2
                end interaction inter_1

                begin enforcement enf_1
                    Enforcement for Energy = Tied_Temperature
                end enforcement

            end contact definition res1

            Output Number of Nodes
            Evaluate Postprocessor l2
            Evaluate Postprocessor linf
            Evaluate Postprocessor h1

            Begin Results Output Label diffusion output
                database Name = 2blocks_tied_h{N}.e
                At Step 1, Increment = 1
                Title Calore Two Blocks
                Nodal Variables = solution->temperature as T
                Element Variables = l2_err linf_err h1_err
            End

        end

    end

end
```

12.3.1.2. Hex8 Resistance

```
#{R=4.0}
begin sierra Aria

    title Adaptive Square

    BEGIN ARIA MATERIAL M1
        Density              = Constant rho=1
        Thermal Conductivity = constant k=1
        Specific Heat        = Constant cp=1
        heat conduction      = basic
    END

    BEGIN ARIA MATERIAL M2
```

```
        Density              = Constant rho=1
        Thermal Conductivity = constant k=1
        Specific Heat        = Constant cp=1
        heat conduction      = basic
    END

    Begin Finite Element Model bar
        Database Name = 2blocks_contact_unaligned_hex8_h{N}.g
        Begin parameters for block block_1
            material M1
        End
        Begin parameters for block block_2
            material M2
        End
    End Finite Element Model bar

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  DIRECT_SOLVER
      BEGIN UMFPACK SOLVER
      END
    END TPETRA EQUATION SOLVER
{else}
    begin trilinos equation solver direct_solver
      solution method = amesos-umfpack
    end trilinos equation solver direct_solver
{endif}

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  ITERATIVE_SOLVER
      BEGIN GMRES SOLVER
        BEGIN JACOBI PRECONDITIONER
        END
        MAXIMUM ITERATIONS = 20000
        RESIDUAL SCALING = R0
        CONVERGENCE TOLERANCE = 1.000000e-12
      END
    END TPETRA EQUATION SOLVER
{else}
    Begin Trilinos Equation Solver Iterative_Solver
      Solution Method = GMRES
      Preconditioning Method = Jacobi
      Maximum Iterations = 20000
      Residual Norm Scaling = R0
      Residual Norm Tolerance = 1.0e-12
    End
{endif}

    Begin Field Function ffunc
        Use Nodal Field solution->temperature As Value
    End

    Begin User Function exact_soln
        Load From File ./Exact_solution.so Using Function registerExactSolution
        Parameter R = {R}
    End

    Begin Norm Postprocessor l2
        Use Function exact_soln
        Subtract Function ffunc
        Compute Norms L2
        Store in l2_err
    End

    Begin Norm Postprocessor linf
        Use Function exact_soln
        Subtract Function ffunc
        Compute Norms LInfinity
        Store in linf_err
```

```
End

Begin Norm Postprocessor h1
    Use Function exact_soln
    Subtract Function ffunc
    Compute Norms H1
    Store in h1_err
End

Begin Postprocessor Output Control pp_out
    Comment Character Is %
    Write To File errors_res_h{N}.dat
    Floating Point Precision Is 3
    Floating Point Format Is Scientific
End

begin procedure myProcedure

    Begin Solution Control Description
        Use System Main
        Begin System Main
            Begin Sequential The_Time_Block
                Advance myRegion
            End
            Simulation Start Time = 0
            Simulation Termination Time = 1
        End
    End

    begin Aria region myRegion

        Nonlinear Solution Strategy = Newton
        Maximum Nonlinear Iterations = 10
        Nonlinear Residual Tolerance = 1.0e-12
        Nonlinear Correction Tolerance = 1.0e-12
        Nonlinear Relaxation Factor  = 1.0
        use dof averaged nonlinear residual

        use finite element model bar
        use linear solver Iterative_Solver #Direct_Solver #

        EQ ENERGY for TEMPERATURE on all_blocks using Q1 with DIFF SRC

        Begin  TEMPERATURE BOUNDARY CONDITION xm1
            add surface surface_1
            TEMPERATURE = 0.
        End

        Begin  TEMPERATURE BOUNDARY CONDITION xp1
            add surface surface_2
            TEMPERATURE = 1.
        End

        Begin VOLUME HEATING sm
            add volume block_1
            VALUE = -1.
        End

        Begin VOLUME HEATING sp
            add volume block_2
            VALUE = 1.
        End

        begin contact definition res1
            contact surface surf_1 contains surface_3
            contact surface surf_2 contains surface_4

            begin interaction inter_1
```

```
                surfaces = surf_1 surf_2
            end interaction inter_1

            begin enforcement enf_1
                conductance coefficient= {1.0/R}
                Enforcement for Energy = gap_conductance
            end enforcement

        end contact definition res1

        Output Number of Nodes

        Evaluate Postprocessor l2
        Evaluate Postprocessor linf
        Evaluate Postprocessor h1

        Begin Results Output Label diffusion output
            database Name = 2blocks_res_h{N}.e
            At Step 1, Increment = 1
            Title Calore Two Blocks
            Nodal Variables = solution->temperature as T
            Element Variables = l2_err linf_err h1_err
        End

    end

  end

end
```

12.3.1.3. Tet4 Tied

```
#{R=0.0}
begin sierra Aria

  title Adaptive Square

  load user plugin file ./Exact_solution.so

  BEGIN ARIA MATERIAL M1
    Density              = Constant rho=1
    Thermal Conductivity = constant k=1
    Specific Heat        = Constant cp=1
    heat conduction      = basic
  END

  BEGIN ARIA MATERIAL M2
    Density              = Constant rho=1
    Thermal Conductivity = constant k=1
    Specific Heat        = Constant cp=1
    heat conduction      = basic
  END

  Begin Finite Element Model bar
    Database Name = 2blocks_contact_unaligned_tet4_h{N}.g
    Begin parameters for block block_1
      material M1
    End
    Begin parameters for block block_2
      material M2
    End
  End Finite Element Model bar

{if(useTpetra)}
  BEGIN TPETRA EQUATION SOLVER  DIRECT_SOLVER
   BEGIN UMFPACK SOLVER
```

```
      END
    END TPETRA EQUATION SOLVER
{else}
    begin trilinos equation solver direct_solver
      solution method = amesos-umfpack
    end trilinos equation solver direct_solver
{endif}

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  ITERATIVE_SOLVER
      BEGIN GMRES SOLVER
        BEGIN DD-ILU PRECONDITIONER
        END
        MAXIMUM ITERATIONS = 200
        RESIDUAL SCALING = R0
        CONVERGENCE TOLERANCE = 1.000000e-12
      END
    END TPETRA EQUATION SOLVER
{else}
    Begin Trilinos Equation Solver Iterative_Solver
      Solution Method = GMRES
      Preconditioning Method = dd-ilu
      Maximum Iterations = 200
      Residual Norm Scaling = R0
      Residual Norm Tolerance = 1.0e-12
    End
{endif}

    Begin Field Function ffunc
        Use Nodal Field solution->temperature As Value
    End

    Begin User Function exact_soln
        Load From File ./Exact_solution.so Using Function registerExactSolution
        Parameter R = {R}
    End

    Begin Norm Postprocessor l2
        Use Function exact_soln
        Subtract Function ffunc
        Compute Norms L2
        Store in l2_err
    End

    Begin Norm Postprocessor linf
        Use Function exact_soln
        Subtract Function ffunc
        Compute Norms LInfinity
        Store in linf_err
    End

    Begin Norm Postprocessor h1
        Use Function exact_soln
        Subtract Function ffunc
        Compute Norms H1
        Store in h1_err
    End

    Begin Postprocessor Output Control pp_out
        Comment Character Is %
        Write To File errors_tied_h{N}.dat
        Floating Point Precision Is 3
        Floating Point Format Is Scientific
    End

    begin procedure myProcedure

        Begin Solution Control Description
```

```
    Use System Main
    Begin System Main
        Begin Sequential The_Time_Block
            Advance myRegion
        End
        Simulation Start Time = 0
        Simulation Termination Time = 1
    End
End

begin Aria region myRegion

    Nonlinear Solution Strategy = Newton
    Maximum Nonlinear Iterations = 10
    Nonlinear Residual Tolerance = 1.0e-12
    Nonlinear Correction Tolerance = 1.0e-12
    Nonlinear Relaxation Factor  = 1.0
    use dof averaged nonlinear residual

    use finite element model bar
    use linear solver Iterative_Solver #Direct_Solver #

    EQ ENERGY for TEMPERATURE on all_blocks using Q1 with DIFF SRC

    Begin  TEMPERATURE BOUNDARY CONDITION xm1
        add surface surface_1
        TEMPERATURE = 0.
    End

    Begin  TEMPERATURE BOUNDARY CONDITION xp1
        add surface surface_2
        TEMPERATURE = 1.
    End

    Begin VOLUME HEATING sm
        add volume block_1
        VALUE = -1.
    End

    Begin VOLUME HEATING sp
        add volume block_2
        VALUE = 1.
    End

    begin contact definition res1
        contact surface surf_1 contains surface_3
        contact surface surf_2 contains surface_4

        begin interaction inter_1
            surfaces = surf_1 surf_2
        end interaction inter_1

        begin enforcement enf_1
            Enforcement for Energy = Tied_Temperature
        end enforcement

    end contact definition res1

    Output Number of Nodes

    Evaluate Postprocessor l2
    Evaluate Postprocessor linf
    Evaluate Postprocessor h1

    Begin Results Output Label diffusion output
        database Name = 2blocks_tied_h{N}.e
        At Step 1, Increment = 1
        Title Calore Two Blocks
```

```
                Nodal Variables = solution->temperature as T
                Element Variables = l2_err linf_err h1_err
            End

        end

    end

end
```

12.3.1.4. Tet4 Resistance

```
#{R=4.0}
begin sierra Aria

    title Adaptive Square

    BEGIN ARIA MATERIAL M1
        Density              = Constant rho=1
        Thermal Conductivity = constant k=1
        Specific Heat        = Constant cp=1
        heat conduction      = basic
    END

    BEGIN ARIA MATERIAL M2
        Density              = Constant rho=1
        Thermal Conductivity = constant k=1
        Specific Heat        = Constant cp=1
        heat conduction      = basic
    END

    Begin Finite Element Model bar
        Database Name = 2blocks_contact_unaligned_tet4_h{N}.g
        Begin parameters for block block_1
            material M1
        End
        Begin parameters for block block_2
            material M2
        End
    End Finite Element Model bar

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  DIRECT_SOLVER
      BEGIN UMFPACK SOLVER
      END
    END TPETRA EQUATION SOLVER
{else}
    begin trilinos equation solver direct_solver
      solution method = amesos-umfpack
    end trilinos equation solver direct_solver
{endif}

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  ITERATIVE_SOLVER
      BEGIN GMRES SOLVER
        BEGIN DD-ILU PRECONDITIONER
        END
        MAXIMUM ITERATIONS = 200
        RESIDUAL SCALING = R0
        CONVERGENCE TOLERANCE = 1.000000e-12
      END
    END TPETRA EQUATION SOLVER
{else}
    Begin Trilinos Equation Solver Iterative_Solver
      Solution Method = GMRES
      Preconditioning Method = dd-ilu
```

```
      Maximum Iterations = 200
      Residual Norm Scaling = R0
      Residual Norm Tolerance = 1.0e-12
    End
{endif}

    Begin Field Function ffunc
        Use Nodal Field solution->temperature As Value
    End

    Begin User Function exact_soln
        Load From File ./Exact_solution.so Using Function registerExactSolution
        Parameter R = {R}
    End

    Begin Norm Postprocessor l2
        Use Function exact_soln
        Subtract Function ffunc
        Compute Norms L2
        Store in l2_err
    End

    Begin Norm Postprocessor linf
        Use Function exact_soln
        Subtract Function ffunc
        Compute Norms LInfinity
        Store in linf_err
    End

    Begin Norm Postprocessor h1
        Use Function exact_soln
        Subtract Function ffunc
        Compute Norms H1
        Store in h1_err
    End

    Begin Postprocessor Output Control pp_out
        Comment Character Is %
        Write To File errors_res_h{N}.dat
        Floating Point Precision Is 3
        Floating Point Format Is Scientific
    End

    begin procedure myProcedure

        Begin Solution Control Description
            Use System Main
            Begin System Main
                Begin Sequential The_Time_Block
                    Advance myRegion
                End
                Simulation Start Time = 0
                Simulation Termination Time = 1
            End
        End

        begin Aria region myRegion

            Nonlinear Solution Strategy = Newton
            Maximum Nonlinear Iterations = 10
            Nonlinear Residual Tolerance = 1.0e-12
            Nonlinear Correction Tolerance = 1.0e-12
            Nonlinear Relaxation Factor  = 1.0
            use dof averaged nonlinear residual

            use finite element model bar
            use linear solver Iterative_Solver #Direct_Solver #
```

```
            EQ ENERGY for TEMPERATURE on all_blocks using Q1 with DIFF SRC

            Begin  TEMPERATURE BOUNDARY CONDITION xm1
                add surface surface_1
                TEMPERATURE = 0.
            End

            Begin  TEMPERATURE BOUNDARY CONDITION xp1
                add surface surface_2
                TEMPERATURE = 1.
            End

            Begin VOLUME HEATING sm
                add volume block_1
                VALUE = -1.
            End

            Begin VOLUME HEATING sp
                add volume block_2
                VALUE = 1.
            End

            begin contact definition res1
                contact surface surf_1 contains surface_3
                contact surface surf_2 contains surface_4

                begin interaction inter_1
                    surfaces = surf_1 surf_2
                end interaction inter_1

                begin enforcement enf_1
                    conductance coefficient= {1.0/R}
                    Enforcement for Energy = gap_conductance
                end enforcement

            end contact definition res1

            Output Number of Nodes

            Evaluate Postprocessor l2
            Evaluate Postprocessor linf
            Evaluate Postprocessor h1

            Begin Results Output Label diffusion output
                database Name = 2blocks_res_h{N}.e
                At Step 1, Increment = 1
                Title Calore Two Blocks
                Nodal Variables = solution->temperature as T
                Element Variables = l2_err linf_err h1_err
            End

        end

    end

end
```

12.3.1.5. *Hex8-Tet4 Tied*

```
#{R=0.0}
begin sierra Aria

    title Adaptive Square

    load user plugin file ./Exact_solution.so
```

```
    BEGIN ARIA MATERIAL M1
        Density              = Constant rho=1
        Thermal Conductivity = constant k=1
        Specific Heat        = Constant cp=1
        heat conduction      = basic
    END

    BEGIN ARIA MATERIAL M2
        Density              = Constant rho=1
        Thermal Conductivity = constant k=1
        Specific Heat        = Constant cp=1
        heat conduction      = basic
    END

    Begin Finite Element Model bar
        Database Name = 2blocks_contact_unaligned_hex8_tet4_h{N}.g
        Begin parameters for block block_1
            material M1
        End
        Begin parameters for block block_2
            material M2
        End
    End Finite Element Model bar

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  DIRECT_SOLVER
      BEGIN UMFPACK SOLVER
      END
    END TPETRA EQUATION SOLVER
{else}
    begin trilinos equation solver direct_solver
      solution method = amesos-umfpack
    end trilinos equation solver direct_solver
{endif}

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  ITERATIVE_SOLVER
      BEGIN GMRES SOLVER
        BEGIN DD-ILU PRECONDITIONER
        END
        MAXIMUM ITERATIONS = 200
        RESIDUAL SCALING = R0
        CONVERGENCE TOLERANCE = 1.000000e-12
      END
    END TPETRA EQUATION SOLVER
{else}
    Begin Trilinos Equation Solver Iterative_Solver
      Solution Method = GMRES
      Preconditioning Method = dd-ilu
      Maximum Iterations = 200
      Residual Norm Scaling = R0
      Residual Norm Tolerance = 1.0e-12
    End
{endif}

    Begin Field Function ffunc
        Use Nodal Field solution->temperature As Value
    End

    Begin User Function exact_soln
        Load From File ./Exact_solution.so Using Function registerExactSolution
        Parameter R = {R}
    End

    Begin Norm Postprocessor l2
        Use Function exact_soln
        Subtract Function ffunc
        Compute Norms L2
```

```
    Store in l2_err
End

Begin Norm Postprocessor linf
    Use Function exact_soln
    Subtract Function ffunc
    Compute Norms LInfinity
    Store in linf_err
End

Begin Norm Postprocessor h1
    Use Function exact_soln
    Subtract Function ffunc
    Compute Norms H1
    Store in h1_err
End

Begin Postprocessor Output Control pp_out
    Comment Character Is %
    Write To File errors_tied_h{N}.dat
    Floating Point Precision Is 3
    Floating Point Format Is Scientific
End

begin procedure myProcedure

    Begin Solution Control Description
        Use System Main
        Begin System Main
            Begin Sequential The_Time_Block
                Advance myRegion
            End
            Simulation Start Time = 0
            Simulation Termination Time = 1
        End
    End

    begin Aria region myRegion

        Nonlinear Solution Strategy = Newton
        Maximum Nonlinear Iterations = 10
        Nonlinear Residual Tolerance = 1.0e-12
        Nonlinear Correction Tolerance = 1.0e-12
        Nonlinear Relaxation Factor  = 1.0
        use dof averaged nonlinear residual

        use finite element model bar
        use linear solver Iterative_Solver #Direct_Solver #

        EQ ENERGY for TEMPERATURE on all_blocks using Q1 with DIFF SRC

        Begin  TEMPERATURE BOUNDARY CONDITION xm1
            add surface surface_1
            TEMPERATURE = 0.
        End

        Begin  TEMPERATURE BOUNDARY CONDITION xp1
            add surface surface_2
            TEMPERATURE = 1.
        End

        Begin VOLUME HEATING sm
            add volume block_1
            VALUE = -1.
        End

        Begin VOLUME HEATING sp
            add volume block_2
```

```
            VALUE = 1.
        End

        begin contact definition res1
            contact surface surf_1 contains surface_3
            contact surface surf_2 contains surface_4

            begin interaction inter_1
                surfaces = surf_1 surf_2
            end interaction inter_1

            begin enforcement enf_1
                Enforcement for Energy = Tied_Temperature
            end enforcement

        end contact definition res1

        Output Number of Nodes

        Evaluate Postprocessor l2
        Evaluate Postprocessor linf
        Evaluate Postprocessor h1

        Begin Results Output Label diffusion output
            database Name = 2blocks_tied_h{N}.e
            At Step 1, Increment = 1
            Title Calore Two Blocks
            Nodal Variables = solution->temperature as T
            Element Variables = l2_err linf_err h1_err
        End

    end

  end

end
```

12.3.1.6. Hex8-Tet4 Resistance

```
#{R=4.0}
begin sierra Aria

  title Adaptive Square

  BEGIN ARIA MATERIAL M1
    Density              = Constant rho=1
    Thermal Conductivity = constant k=1
    Specific Heat        = Constant cp=1
    heat conduction      = basic
  END

  BEGIN ARIA MATERIAL M2
    Density              = Constant rho=1
    Thermal Conductivity = constant k=1
    Specific Heat        = Constant cp=1
    heat conduction      = basic
  END

  Begin Finite Element Model bar
    Database Name = 2blocks_contact_unaligned_hex8_tet4_h{N}.g
    Begin parameters for block block_1
        material M1
    End
    Begin parameters for block block_2
        material M2
    End
```

```
    End Finite Element Model bar

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  DIRECT_SOLVER
      BEGIN UMFPACK SOLVER
      END
    END TPETRA EQUATION SOLVER
{else}
    begin trilinos equation solver direct_solver
      solution method = amesos-umfpack
    end trilinos equation solver direct_solver
{endif}

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  ITERATIVE_SOLVER
      BEGIN GMRES SOLVER
        BEGIN DD-ILU PRECONDITIONER
        END
        MAXIMUM ITERATIONS = 200
        RESIDUAL SCALING = R0
        CONVERGENCE TOLERANCE = 1.000000e-12
      END
    END TPETRA EQUATION SOLVER
{else}
    Begin Trilinos Equation Solver Iterative_Solver
      Solution Method = GMRES
      Preconditioning Method = dd-ilu
      Maximum Iterations = 200
      Residual Norm Scaling = R0
      Residual Norm Tolerance = 1.0e-12
    End
{endif}

    Begin Field Function ffunc
        Use Nodal Field solution->temperature As Value
    End

    Begin User Function exact_soln
        Load From File ./Exact_solution.so Using Function registerExactSolution
        Parameter R = {R}
    End

    Begin Norm Postprocessor l2
        Use Function exact_soln
        Subtract Function ffunc
        Compute Norms L2
        Store in l2_err
    End

    Begin Norm Postprocessor linf
        Use Function exact_soln
        Subtract Function ffunc
        Compute Norms LInfinity
        Store in linf_err
    End

    Begin Norm Postprocessor h1
        Use Function exact_soln
        Subtract Function ffunc
        Compute Norms H1
        Store in h1_err
    End

    Begin Postprocessor Output Control pp_out
        Comment Character Is %
        Write To File errors_res_h{N}.dat
        Floating Point Precision Is 3
        Floating Point Format Is Scientific
```

```
End

begin procedure myProcedure

    Begin Solution Control Description
        Use System Main
        Begin System Main
            Begin Sequential The_Time_Block
                Advance myRegion
            End
            Simulation Start Time = 0
            Simulation Termination Time = 1
        End
    End

    begin Aria region myRegion

        Nonlinear Solution Strategy = Newton
        Maximum Nonlinear Iterations = 10
        Nonlinear Residual Tolerance = 1.0e-12
        Nonlinear Correction Tolerance = 1.0e-12
        Nonlinear Relaxation Factor  = 1.0
        use dof averaged nonlinear residual

        use finite element model bar
        use linear solver Iterative_Solver #Direct_Solver #

        EQ ENERGY for TEMPERATURE on all_blocks using Q1 with DIFF SRC

        Begin  TEMPERATURE BOUNDARY CONDITION xm1
            add surface surface_1
            TEMPERATURE = 0.
        End

        Begin  TEMPERATURE BOUNDARY CONDITION xp1
            add surface surface_2
            TEMPERATURE = 1.
        End

        Begin VOLUME HEATING sm
            add volume block_1
            VALUE = -1.
        End

        Begin VOLUME HEATING sp
            add volume block_2
            VALUE = 1.
        End

        begin contact definition res1
            contact surface surf_1 contains surface_3
            contact surface surf_2 contains surface_4

            begin interaction inter_1
                surfaces = surf_1 surf_2
            end interaction inter_1

            begin enforcement enf_1
                conductance coefficient= {1.0/R}
                Enforcement for Energy = gap_conductance
            end enforcement

        end contact definition res1

        Output Number of Nodes

        Evaluate Postprocessor l2
        Evaluate Postprocessor linf
```

```
            Evaluate Postprocessor h1

            Begin Results Output Label diffusion output
                database Name = 2blocks_res_h{N}.e
                At Step 1, Increment = 1
                Title Calore Two Blocks
                Nodal Variables = solution->temperature as T
                Element Variables = l2_err linf_err h1_err
            End

        end

    end

end
```

12.3.2. 3D Curved Contact 4.2

12.3.2.1. Hex8-Hex8 Case

12.3.2.2. Tet4-Tet4 Case

12.3.2.3. Hex8-Tet4 Case

12.3.3. Steady Hex8 Contact

```
#N={N=5}
BEGIN SIERRA myJob

   BEGIN ARIA MATERIAL Kryptonite
     Density              = Constant rho=1
     Thermal Conductivity = constant k=1
     Specific Heat        = Constant cp=1
     heat conduction      = basic
   END ARIA MATERIAL Kryptonite

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  DIRECT_SOLVER
      BEGIN SUPERLU SOLVER
      END
    END TPETRA EQUATION SOLVER
{else}
    Begin Trilinos Equation Solver Direct_Solver
      Solution Method = amesos-superlu
    End
{endif}

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  ITERATIVE_SOLVER
      BEGIN GMRES SOLVER
        BEGIN JACOBI PRECONDITIONER
        END
        MAXIMUM ITERATIONS = 1000
        RESIDUAL SCALING = NONE
        CONVERGENCE TOLERANCE = 1.000000e-15
      END
    END TPETRA EQUATION SOLVER
{else}
    Begin Trilinos Equation Solver Iterative_Solver
      Solution Method = GMRES
      Preconditioning Method = Jacobi
      Maximum Iterations = 1000
      Residual Norm Scaling = None
```

```
      Residual Norm Tolerance = 1.0e-15
    End
{endif}

   BEGIN FINITE ELEMENT MODEL cube
      database name = cube_contact_h{N}_hex8.e
      coordinate system is cartesian
      decomposition method = rcb

      BEGIN PARAMETERS FOR BLOCK block_1
 material Kryptonite
      END PARAMETERS FOR BLOCK block_1

      BEGIN PARAMETERS FOR BLOCK block_2
 material Kryptonite
      END PARAMETERS FOR BLOCK block_2

   END FINITE ELEMENT MODEL cube

   Begin User Function exact_soln
     Load From File ./exact.so Using Function registerExactSoln
   End

   Begin User Function exact_soln_dot
     Load From File ./exact.so Using Function registerExactSolnDot
   End

   Begin User Function exact_src
     Load From File ./exact.so Using Function registerExactSrc
   End

   Begin User Function flux_surface_3
     Load From File ./exact.so Using Function registerFlux_Surface_3
   End

   Begin User Function flux_surface_5
     Load From File ./exact.so Using Function registerFlux_Surface_5
   End

   Begin User Function flux_surface_1
     Load From File ./exact.so Using Function registerFlux_Surface_1
   End

   Begin User Function flux_surface_2
     Load From File ./exact.so Using Function registerFlux_Surface_2
   End

   Begin Norm Postprocessor l2
     Use Function exact_soln
     Subtract Function nonlinear_solution->TEMPERATURE
     Compute Norms L2
     store in l2_error
   End

   Begin Norm Postprocessor h1
     Use Function exact_soln
     Subtract Function nonlinear_solution->TEMPERATURE
     Compute Norms H1
     store in h1_error
   End

   Begin Norm Postprocessor linf
     Use Function exact_soln
     Subtract Function nonlinear_solution->TEMPERATURE
     Compute Norms LInfinity
     store in linf_error
   End
```

```
  Begin Postprocessor Output Control pp_out
    Comment Character Is %
    Write To File errors_h{N}.dat
    Floating Point Precision Is 3
    Floating Point Format Is Scientific
  End

  BEGIN PROCEDURE myAriaProcedure

     Begin Solution Control Description
Use System Main
Begin System Main
   Begin Sequential The_Time_Block
      Advance myRegion
   End
      Simulation Start Time = 0
   Simulation Termination Time = 1
End
     End

     BEGIN ARIA REGION myRegion

Nonlinear Solution Strategy = Newton
        Maximum Nonlinear Iterations = 10
        Nonlinear Residual Tolerance = 1.0e-12
        Nonlinear Correction Tolerance = 1.0e-12
        Nonlinear Relaxation Factor  = 1.0
        use dof averaged nonlinear residual

use finite element model cube
        Use Linear Solver Iterative_Solver #Direct_Solver

EQ ENERGY for TEMPERATURE on block_1 using Q1 with DIFF SRC
EQ ENERGY for TEMPERATURE on block_2 using Q1 with DIFF SRC

# surface_4: x=0
# surface_6: x=1

# surface_3: y=0
# surface_5: y=1

# surface_1: z=1
# surface_2: z=0

# const Temp BC (x)
        BC const dirichlet at surface_4 Temperature = 1.0
        BC const dirichlet at surface_6 Temperature = 1.0

# const flux BC (y)
BC FLUX for Energy on surface_3  = constant flux = 3
BC FLUX for Energy on surface_5  = constant flux = 5

BC FLUX for Energy on surface_3  = Encore_Function Name=flux_surface_3
BC FLUX for Energy on surface_5  = Encore_Function Name=flux_surface_5

# convective flux BC with const Temp and H (z)
        BC Flux for Energy on surface_1 = Nat_Conv T_Ref=1 H=1
        BC Flux for Energy on surface_2 = Nat_Conv T_Ref=2 H=2

BC FLUX for Energy on surface_1  = Encore_Function Name=flux_surface_1
BC FLUX for Energy on surface_2  = Encore_Function Name=flux_surface_2

#  const source term
Source For ENERGY on block_1 = Constant value=1
Source For ENERGY on block_2 = Constant value=1

Source For ENERGY on block_1 = Encore_Function Name=exact_src
Source For ENERGY on block_2 = Encore_Function Name=exact_src
```

```
        begin contact definition mpc1
          contact surface surf_1 contains surface_7
          contact surface surf_2 contains surface_8

          output rule = summary

          begin interaction inter_1
            surfaces = surf_1 surf_2
            normal tolerance = 0.01
          end
          begin enforcement enf_1
            Enforcement for Energy = Tied_Temperature
          end
        end

   Output Number of Nodes

 Evaluate Postprocessor l2
 Evaluate Postprocessor h1
 Evaluate Postprocessor linf

 BEGIN RESULTS OUTPUT LABEL diffusion output
    database Name = thermal_steady_hex8_tied_contact_h{N}.e
    at step 1, increment = 1
    # time interval is 1.0
    title Aria cube test
    nodal variables = nonlinear_solution->TEMPERATURE as T
            element variables = l2_error h2_error linf_error
 END RESULTS OUTPUT LABEL diffusion output

      END ARIA REGION myRegion

   END PROCEDURE myAriaProcedure

END SIERRA myJob
```

12.3.4. Steady Hex20 Contact

```
BEGIN SIERRA myJob

   load user plugin file ./exact.so

  begin definition for function kxx
    type = piecewise linear
    begin values
       0.0 0.5
       1.0 2.0
       2.0 8.0
      end values
   end

  begin definition for function kyy
    type = piecewise linear
    begin values
       0.0 0.2
       1.0 1.2
       2.0 2.1
       20.0 20.2
      end values
   end

  begin definition for function kzz
    type = piecewise linear
    begin values
       0.0 1.0
```

```
      1.0 2.0
      2.0 3.0
      20.0 21.0
    end values
    scale by 2.0
  end

  BEGIN ARIA MATERIAL Kryptonite
    Density              = Constant rho=1
    tensor thermal conductivity = user_function X = temperature name_xx = kxx name_yy = kyy name_zz = kzz
    Specific Heat        = Constant cp=1
    heat conduction      = Generalized
  END ARIA MATERIAL Kryptonite

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  DIRECT_SOLVER
      BEGIN SUPERLU SOLVER
      END
    END TPETRA EQUATION SOLVER
{else}
    Begin Trilinos Equation Solver Direct_Solver
      Solution Method = amesos-superlu
    End
{endif}

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  ITERATIVE_SOLVER
      BEGIN GMRES SOLVER
        BEGIN JACOBI PRECONDITIONER
        END
        MAXIMUM ITERATIONS = 1000
        RESIDUAL SCALING = NONE
        CONVERGENCE TOLERANCE = 1.000000e-14
      END
    END TPETRA EQUATION SOLVER
{else}
    Begin Trilinos Equation Solver Iterative_Solver
      Solution Method = GMRES
      Preconditioning Method = Jacobi
      Maximum Iterations = 1000
      Residual Norm Scaling = None
      Residual Norm Tolerance = 1.0e-14
    End
{endif}

  BEGIN FINITE ELEMENT MODEL cube
     database name = cube_contact_h{N}_hex20.g
     coordinate system is cartesian
     decomposition method = rcb

     BEGIN PARAMETERS FOR BLOCK block_1
        material Kryptonite
     END PARAMETERS FOR BLOCK block_1

     BEGIN PARAMETERS FOR BLOCK block_2
        material Kryptonite
     END PARAMETERS FOR BLOCK block_2

  END FINITE ELEMENT MODEL cube

  Begin User Function exact_soln
    Load From File ./exact.so Using Function registerExactSoln
  End

  Begin User Function exact_src
    Load From File ./exact.so Using Function registerExactSrc
  End
```

```
 Begin User Function flux_surface_3
   Load From File ./exact.so Using Function registerFlux_Surface_3
 End

 Begin User Function flux_surface_5
   Load From File ./exact.so Using Function registerFlux_Surface_5
 End

 Begin User Function flux_surface_1
   Load From File ./exact.so Using Function registerFlux_Surface_1
 End

 Begin User Function flux_surface_2
   Load From File ./exact.so Using Function registerFlux_Surface_2
 End

 Begin Norm Postprocessor l2
   Use Function exact_soln
   Subtract Function nonlinear_solution->TEMPERATURE
   Compute Norms L2
 End

 Begin Norm Postprocessor h1
   Use Function exact_soln
   Subtract Function nonlinear_solution->TEMPERATURE
   Compute Norms H1
 End

 Begin Norm Postprocessor linf
   Use Function exact_soln
   Subtract Function nonlinear_solution->TEMPERATURE
   Compute Norms LInfinity
 End

 Begin Postprocessor Output Control pp_out
   Comment Character Is %
Write To File errors_thermal_steady_hex20_h{N}.dat
   Floating Point Precision Is 3
   Floating Point Format Is Scientific
 End

 BEGIN PROCEDURE myAriaProcedure

    Begin Solution Control Description
       Use System Main
       Begin System Main
          Begin Sequential The_Time_Block
             Advance myRegion
          End
            Simulation Start Time = 0
          Simulation Termination Time = 1
       End
    End

    BEGIN ARIA REGION myRegion

       Nonlinear Solution Strategy = Newton
       Maximum Nonlinear Iterations = 10
       Nonlinear Residual Tolerance = 1.0e-12
       Nonlinear Correction Tolerance = 1.0e-12
       Nonlinear Relaxation Factor  = 1.0
       use dof averaged nonlinear residual

       use finite element model cube
       Use Linear Solver Iterative_Solver #Direct_Solver

       EQ ENERGY for TEMPERATURE on block_1 using Q2S with DIFF SRC
       EQ ENERGY for TEMPERATURE on block_2 using Q2S with DIFF SRC
```

```
    # surface_4: x=0
    # surface_6: x=1

    # surface_3: y=0
    # surface_5: y=1

    # surface_1: z=1
    # surface_2: z=0

    # const Temp BC (x)
    BC const dirichlet at surface_4 Temperature = 1.0
    BC const dirichlet at surface_6 Temperature = 1.0

    # const flux BC (y)
    BC FLUX for Energy on surface_3  = constant flux = 3
    BC FLUX for Energy on surface_5  = constant flux = 5

    BC FLUX for Energy on surface_3  = Encore_Function Name=flux_surface_3
    BC FLUX for Energy on surface_5  = Encore_Function Name=flux_surface_5

    # convective flux BC with const Temp and H (z)
    BC Flux for Energy on surface_1 = Nat_Conv T_Ref=1 H=1
    BC Flux for Energy on surface_2 = Nat_Conv T_Ref=2 H=2

    BC FLUX for Energy on surface_1  = Encore_Function Name=flux_surface_1
    BC FLUX for Energy on surface_2  = Encore_Function Name=flux_surface_2

    #  const source term
    Source For ENERGY on block_1 = Constant value=1

    Source For ENERGY on block_1 = Encore_Function Name=exact_src

    Source For ENERGY on block_2 = Constant value=1

    Source For ENERGY on block_2 = Encore_Function Name=exact_src

    begin contact definition mpc1
      contact surface surf_1 contains surface_7
      contact surface surf_2 contains surface_8

      begin interaction inter_1
        surfaces = surf_1 surf_2
      end
      begin enforcement enf_1
        Enforcement for Energy = Tied_Temperature
      end
    end


    Output Number of Nodes

    Evaluate Postprocessor l2
    Evaluate Postprocessor h1
    Evaluate Postprocessor linf

    BEGIN RESULTS OUTPUT LABEL diffusion output
       database Name = thermal_steady_hex20_tied_contact_h{N}.e
       at step 1, increment = 1
       # time interval is 1.0
       title Aria cube test
       nodal variables = nonlinear_solution->TEMPERATURE as T
    END RESULTS OUTPUT LABEL diffusion output

  END ARIA REGION myRegion

END PROCEDURE myAriaProcedure
```

```
END SIERRA myJob
```

12.3.5. Steady Hex27 Contact

```
BEGIN SIERRA myJob

   load user plugin file ./exact.so

  begin definition for function kxx
    type = piecewise linear
    begin values
       0.0 0.5
       1.0 2.0
       2.0 8.0
      end values
   end

  begin definition for function kyy
    type = piecewise linear
    begin values
       0.0 0.2
       1.0 1.2
       2.0 2.1
       20.0 20.2
      end values
   end

  begin definition for function kzz
    type = piecewise linear
    begin values
       0.0 1.0
       1.0 2.0
       2.0 3.0
       20.0 21.0
     end values
     scale by 2.0
   end

   BEGIN ARIA MATERIAL Kryptonite
     Density              = Constant rho=1
     tensor thermal conductivity = user_function X = temperature name_xx = kxx name_yy = kyy name_zz = kzz
     Specific Heat        = Constant cp=1
     heat conduction      = Generalized
   END ARIA MATERIAL Kryptonite

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  DIRECT_SOLVER
      BEGIN SUPERLU SOLVER
      END
    END TPETRA EQUATION SOLVER
{else}
    Begin Trilinos Equation Solver Direct_Solver
      Solution Method = amesos-superlu
    End
{endif}

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  ITERATIVE_SOLVER
      BEGIN GMRES SOLVER
        BEGIN JACOBI PRECONDITIONER
        END
        MAXIMUM ITERATIONS = 1000
        RESIDUAL SCALING = NONE
        CONVERGENCE TOLERANCE = 1.000000e-14
      END
    END TPETRA EQUATION SOLVER
```

```
{else}
    Begin Trilinos Equation Solver Iterative_Solver
      Solution Method = GMRES
      Preconditioning Method = Jacobi
      Maximum Iterations = 1000
      Residual Norm Scaling = None
      Residual Norm Tolerance = 1.0e-14
    End
{endif}

   BEGIN FINITE ELEMENT MODEL cube
      database name = cube_contact_h{N}_hex27.g
      coordinate system is cartesian
      decomposition method = rcb

      BEGIN PARAMETERS FOR BLOCK block_1
         material Kryptonite
      END PARAMETERS FOR BLOCK block_1

      BEGIN PARAMETERS FOR BLOCK block_2
         material Kryptonite
      END PARAMETERS FOR BLOCK block_2

   END FINITE ELEMENT MODEL cube

   Begin User Function exact_soln
     Load From File ./exact.so Using Function registerExactSoln
   End

   Begin User Function exact_src
     Load From File ./exact.so Using Function registerExactSrc
   End

   Begin User Function flux_surface_3
     Load From File ./exact.so Using Function registerFlux_Surface_3
   End

   Begin User Function flux_surface_5
     Load From File ./exact.so Using Function registerFlux_Surface_5
   End

   Begin User Function flux_surface_1
     Load From File ./exact.so Using Function registerFlux_Surface_1
   End

   Begin User Function flux_surface_2
     Load From File ./exact.so Using Function registerFlux_Surface_2
   End

   Begin Norm Postprocessor l2
     Use Function exact_soln
     Subtract Function nonlinear_solution->TEMPERATURE
     Compute Norms L2
   End

   Begin Norm Postprocessor h1
     Use Function exact_soln
     Subtract Function nonlinear_solution->TEMPERATURE
     Compute Norms H1
   End

   Begin Norm Postprocessor linf
     Use Function exact_soln
     Subtract Function nonlinear_solution->TEMPERATURE
     Compute Norms LInfinity
   End

   Begin Postprocessor Output Control pp_out
```

```
   Comment Character Is %
Write To File errors_thermal_steady_hex27_h{N}.dat
   Floating Point Precision Is 3
   Floating Point Format Is Scientific
 End

 BEGIN PROCEDURE myAriaProcedure

    Begin Solution Control Description
       Use System Main
       Begin System Main
          Begin Sequential The_Time_Block
             Advance myRegion
          End
            Simulation Start Time = 0
          Simulation Termination Time = 1
       End
    End

    BEGIN ARIA REGION myRegion

       Nonlinear Solution Strategy = Newton
       Maximum Nonlinear Iterations = 10
       Nonlinear Residual Tolerance = 1.0e-12
       Nonlinear Correction Tolerance = 1.0e-12
       Nonlinear Relaxation Factor  = 1.0
       use dof averaged nonlinear residual

       use finite element model cube
       Use Linear Solver Iterative_Solver #Direct_Solver

       EQ ENERGY for TEMPERATURE on block_1 using Q2 with DIFF SRC
       EQ ENERGY for TEMPERATURE on block_2 using Q2 with DIFF SRC

       # surface_4: x=0
       # surface_6: x=1

       # surface_3: y=0
       # surface_5: y=1

       # surface_1: z=1
       # surface_2: z=0

       # const Temp BC (x)
       BC const dirichlet at surface_4 Temperature = 1.0
       BC const dirichlet at surface_6 Temperature = 1.0

       # const flux BC (y)
       BC FLUX for Energy on surface_3  = constant flux = 3
       BC FLUX for Energy on surface_5  = constant flux = 5

       BC FLUX for Energy on surface_3  = Encore_Function Name=flux_surface_3
       BC FLUX for Energy on surface_5  = Encore_Function Name=flux_surface_5

       # convective flux BC with const Temp and H (z)
       BC Flux for Energy on surface_1 = Nat_Conv T_Ref=1 H=1
       BC Flux for Energy on surface_2 = Nat_Conv T_Ref=2 H=2

       BC FLUX for Energy on surface_1  = Encore_Function Name=flux_surface_1
       BC FLUX for Energy on surface_2  = Encore_Function Name=flux_surface_2

       #  const source term
       Source For ENERGY on block_1 = Constant value=1

       Source For ENERGY on block_1 = Encore_Function Name=exact_src

       Source For ENERGY on block_2 = Constant value=1
```

```
         Source For ENERGY on block_2 = Encore_Function Name=exact_src

         begin contact definition mpc1
           contact surface surf_1 contains surface_7
           contact surface surf_2 contains surface_8

           begin interaction inter_1
             surfaces = surf_1 surf_2
           end
           begin enforcement enf_1
             Enforcement for Energy = Tied_Temperature
           end
         end


         Output Number of Nodes

         Evaluate Postprocessor l2
         Evaluate Postprocessor h1
         Evaluate Postprocessor linf

         BEGIN RESULTS OUTPUT LABEL diffusion output
            database Name = thermal_steady_hex27_tied_contact_h{N}.e
            at step 1, increment = 1
            # time interval is 1.0
            title Aria cube test
            nodal variables = nonlinear_solution->TEMPERATURE as T
         END RESULTS OUTPUT LABEL diffusion output

      END ARIA REGION myRegion

   END PROCEDURE myAriaProcedure

END SIERRA myJob
```

12.3.6. Steady Tet4 Contact

```
#N={N=5}
BEGIN SIERRA myJob

   BEGIN ARIA MATERIAL Kryptonite
     Density              = Constant rho=1
     Thermal Conductivity = constant k=1
     Specific Heat        = Constant cp=1
     heat conduction      = basic
   END ARIA MATERIAL Kryptonite

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  DIRECT_SOLVER
      BEGIN SUPERLU SOLVER
      END
    END TPETRA EQUATION SOLVER
{else}
    Begin Trilinos Equation Solver Direct_Solver
      Solution Method = amesos-superlu
    End
{endif}

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  ITERATIVE_SOLVER
      BEGIN GMRES SOLVER
        BEGIN JACOBI PRECONDITIONER
        END
        MAXIMUM ITERATIONS = 1000
        RESIDUAL SCALING = NONE
        CONVERGENCE TOLERANCE = 1.000000e-15
```

```
      END
    END TPETRA EQUATION SOLVER
{else}
    Begin Trilinos Equation Solver Iterative_Solver
      Solution Method = GMRES
      Preconditioning Method = Jacobi
      Maximum Iterations = 1000
      Residual Norm Scaling = None
      Residual Norm Tolerance = 1.0e-15
    End
{endif}

   BEGIN FINITE ELEMENT MODEL cube
      database name = cube_contact_h{N}_tet4.e
      coordinate system is cartesian
      decomposition method = rcb

      BEGIN PARAMETERS FOR BLOCK block_1
 material Kryptonite
      END PARAMETERS FOR BLOCK block_1

      BEGIN PARAMETERS FOR BLOCK block_2
 material Kryptonite
      END PARAMETERS FOR BLOCK block_2

   END FINITE ELEMENT MODEL cube

   Begin User Function exact_soln
     Load From File ./exact.so Using Function registerExactSoln
   End

   Begin User Function exact_soln_dot
     Load From File ./exact.so Using Function registerExactSolnDot
   End

   Begin User Function exact_src
     Load From File ./exact.so Using Function registerExactSrc
   End

   Begin User Function flux_surface_3
     Load From File ./exact.so Using Function registerFlux_Surface_3
   End

   Begin User Function flux_surface_5
     Load From File ./exact.so Using Function registerFlux_Surface_5
   End

   Begin User Function flux_surface_1
     Load From File ./exact.so Using Function registerFlux_Surface_1
   End

   Begin User Function flux_surface_2
     Load From File ./exact.so Using Function registerFlux_Surface_2
   End

   Begin Norm Postprocessor l2
     Use Function exact_soln
     Subtract Function nonlinear_solution->TEMPERATURE
     Compute Norms L2
     Store In l2_error
   End

   Begin Norm Postprocessor h1
     Use Function exact_soln
     Subtract Function nonlinear_solution->TEMPERATURE
     Compute Norms H1
     Store In h1_error
   End
```

```
  Begin Norm Postprocessor linf
    Use Function exact_soln
    Subtract Function nonlinear_solution->TEMPERATURE
    Compute Norms LInfinity
    Store In linf_error
  End

  Begin Postprocessor Output Control pp_out
    Comment Character Is %
    Write To File errors_h{N}.dat
    Floating Point Precision Is 3
    Floating Point Format Is Scientific
  End

  BEGIN PROCEDURE myAriaProcedure

     Begin Solution Control Description
Use System Main
Begin System Main
   Begin Sequential The_Time_Block
      Advance myRegion
   End
      Simulation Start Time = 0
   Simulation Termination Time = 1
End
     End

     BEGIN ARIA REGION myRegion

Nonlinear Solution Strategy = Newton
        Maximum Nonlinear Iterations = 10
        Nonlinear Residual Tolerance = 1.0e-12
        Nonlinear Correction Tolerance = 1.0e-12
        Nonlinear Relaxation Factor  = 1.0
        use dof averaged nonlinear residual

use finite element model cube
        Use Linear Solver Iterative_Solver #Direct_Solver

EQ ENERGY for TEMPERATURE on block_1 using Q1 with DIFF SRC
EQ ENERGY for TEMPERATURE on block_2 using Q1 with DIFF SRC

# surface_4: x=0
# surface_6: x=1

# surface_3: y=0
# surface_5: y=1

# surface_1: z=1
# surface_2: z=0

# const Temp BC (x)
        BC const dirichlet at surface_4 Temperature = 1.0
        BC const dirichlet at surface_6 Temperature = 1.0

# const flux BC (y)
BC FLUX for Energy on surface_3  = constant flux = 3
BC FLUX for Energy on surface_5  = constant flux = 5

BC FLUX for Energy on surface_3  = Encore_Function Name=flux_surface_3
BC FLUX for Energy on surface_5  = Encore_Function Name=flux_surface_5

# convective flux BC with const Temp and H (z)
        BC Flux for Energy on surface_1 = Nat_Conv T_Ref=1 H=1
        BC Flux for Energy on surface_2 = Nat_Conv T_Ref=2 H=2

BC FLUX for Energy on surface_1  = Encore_Function Name=flux_surface_1
```

```
 BC FLUX for Energy on surface_2  = Encore_Function Name=flux_surface_2

 #  const source term
 Source For ENERGY on block_1 = Constant value=1
 Source For ENERGY on block_2 = Constant value=1

 Source For ENERGY on block_1 = Encore_Function Name=exact_src
 Source For ENERGY on block_2 = Encore_Function Name=exact_src

         begin contact definition mpc1
           contact surface surf_1 contains surface_7
           contact surface surf_2 contains surface_8

           begin interaction inter_1
             surfaces = surf_1 surf_2
           end
           begin enforcement enf_1
             Enforcement for Energy = Tied_Temperature
           end
         end

    Output Number of Nodes

 Evaluate Postprocessor l2
 Evaluate Postprocessor h1
 Evaluate Postprocessor linf

 BEGIN RESULTS OUTPUT LABEL diffusion output
    database Name = thermal_steady_tet4_tied_contact_h{N}.e
    at step 1, increment = 1
    # time interval is 1.0
    title Aria cube test
    nodal variables = nonlinear_solution->TEMPERATURE as T
            element variables = l2_error h1_error linf_error
 END RESULTS OUTPUT LABEL diffusion output

      END ARIA REGION myRegion

   END PROCEDURE myAriaProcedure

END SIERRA myJob
```

12.3.7. Steady Tet4Tet10 Contact

```
#N={N=5}
BEGIN SIERRA myJob

   BEGIN ARIA MATERIAL Kryptonite
     Density              = Constant rho=1
     Thermal Conductivity = constant k=1
     Specific Heat        = Constant cp=1
     heat conduction      = basic
   END ARIA MATERIAL Kryptonite

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  DIRECT_SOLVER
      BEGIN SUPERLU SOLVER
      END
    END TPETRA EQUATION SOLVER
{else}
    Begin Trilinos Equation Solver Direct_Solver
      Solution Method = amesos-superlu
    End
{endif}

{if(useTpetra)}
```

```
    BEGIN TPETRA EQUATION SOLVER  ITERATIVE_SOLVER
      BEGIN GMRES SOLVER
        BEGIN JACOBI PRECONDITIONER
        END
        MAXIMUM ITERATIONS = 1000
        RESIDUAL SCALING = NONE
        CONVERGENCE TOLERANCE = 1.000000e-15
      END
    END TPETRA EQUATION SOLVER
{else}
    Begin Trilinos Equation Solver Iterative_Solver
      Solution Method = GMRES
      Preconditioning Method = Jacobi
      Maximum Iterations = 1000
      Residual Norm Scaling = None
      Residual Norm Tolerance = 1.0e-15
    End
{endif}

   BEGIN FINITE ELEMENT MODEL cube
      database name = cube_contact_h{N}_tet10.e
      coordinate system is cartesian
      decomposition method = rcb

      BEGIN PARAMETERS FOR BLOCK block_1
 material Kryptonite
      END PARAMETERS FOR BLOCK block_1

      BEGIN PARAMETERS FOR BLOCK block_2
 material Kryptonite
      END PARAMETERS FOR BLOCK block_2

   END FINITE ELEMENT MODEL cube

   Begin User Function exact_soln
     Load From File ./exact.so Using Function registerExactSoln
   End

   Begin User Function exact_soln_dot
     Load From File ./exact.so Using Function registerExactSolnDot
   End

   Begin User Function exact_src
     Load From File ./exact.so Using Function registerExactSrc
   End

   Begin User Function flux_surface_3
     Load From File ./exact.so Using Function registerFlux_Surface_3
   End

   Begin User Function flux_surface_5
     Load From File ./exact.so Using Function registerFlux_Surface_5
   End

   Begin User Function flux_surface_1
     Load From File ./exact.so Using Function registerFlux_Surface_1
   End

   Begin User Function flux_surface_2
     Load From File ./exact.so Using Function registerFlux_Surface_2
   End

   Begin Norm Postprocessor l2
     Use Function exact_soln
     Subtract Function nonlinear_solution->TEMPERATURE
     Compute Norms L2
     Store In l2_error
   End
```

```
  Begin Norm Postprocessor h1
    Use Function exact_soln
    Subtract Function nonlinear_solution->TEMPERATURE
    Compute Norms H1
    Store In h1_error
  End

  Begin Norm Postprocessor linf
    Use Function exact_soln
    Subtract Function nonlinear_solution->TEMPERATURE
    Compute Norms LInfinity
    Store In linf_error
  End

  Begin Postprocessor Output Control pp_out
    Comment Character Is %
    Write To File errors_h{N}.dat
    Floating Point Precision Is 3
    Floating Point Format Is Scientific
  End

  BEGIN PROCEDURE myAriaProcedure

     Begin Solution Control Description
Use System Main
Begin System Main
   Begin Sequential The_Time_Block
      Advance myRegion
   End
      Simulation Start Time = 0
   Simulation Termination Time = 1
End
     End

     BEGIN ARIA REGION myRegion

Nonlinear Solution Strategy = Newton
        Maximum Nonlinear Iterations = 10
        Nonlinear Residual Tolerance = 1.0e-12
        Nonlinear Correction Tolerance = 1.0e-12
        Nonlinear Relaxation Factor  = 1.0
        use dof averaged nonlinear residual

use finite element model cube
        Use Linear Solver Iterative_Solver #Direct_Solver

EQ ENERGY for TEMPERATURE on block_1 using Q1 with DIFF SRC
EQ ENERGY for TEMPERATURE on block_2 using Q1 with DIFF SRC

# surface_4: x=0
# surface_6: x=1

# surface_3: y=0
# surface_5: y=1

# surface_1: z=1
# surface_2: z=0

# const Temp BC (x)
        BC const dirichlet at surface_4 Temperature = 1.0
        BC const dirichlet at surface_6 Temperature = 1.0

# const flux BC (y)
BC FLUX for Energy on surface_3  = constant flux = 3
BC FLUX for Energy on surface_5  = constant flux = 5

BC FLUX for Energy on surface_3  = Encore_Function Name=flux_surface_3
```

```
 BC FLUX for Energy on surface_5  = Encore_Function Name=flux_surface_5

 # convective flux BC with const Temp and H (z)
         BC Flux for Energy on surface_1 = Nat_Conv T_Ref=1 H=1
         BC Flux for Energy on surface_2 = Nat_Conv T_Ref=2 H=2

 BC FLUX for Energy on surface_1  = Encore_Function Name=flux_surface_1
 BC FLUX for Energy on surface_2  = Encore_Function Name=flux_surface_2

 #  const source term
 Source For ENERGY on block_1 = Constant value=1
 Source For ENERGY on block_2 = Constant value=1

 Source For ENERGY on block_1 = Encore_Function Name=exact_src
 Source For ENERGY on block_2 = Encore_Function Name=exact_src

         begin contact definition mpc1
           contact surface surf_1 contains surface_7
           contact surface surf_2 contains surface_8

           begin interaction inter_1
             surfaces = surf_1 surf_2
           end
           begin enforcement enf_1
             Enforcement for Energy = Tied_Temperature
           end
         end

    Output Number of Nodes

 Evaluate Postprocessor l2
 Evaluate Postprocessor h1
 Evaluate Postprocessor linf

 BEGIN RESULTS OUTPUT LABEL diffusion output
    database Name = thermal_steady_tet4_tied_contact_h{N}.e
    at step 1, increment = 1
    # time interval is 1.0
    title Aria cube test
    nodal variables = nonlinear_solution->TEMPERATURE as T
            element variables = l2_error h1_error linf_error
 END RESULTS OUTPUT LABEL diffusion output

      END ARIA REGION myRegion

   END PROCEDURE myAriaProcedure

END SIERRA myJob
```

12.3.8. Steady Tet10 Contact

```
#N={N=5}
BEGIN SIERRA myJob

   BEGIN ARIA MATERIAL Kryptonite
     Density              = Constant rho=1
     Thermal Conductivity = constant k=1
     Specific Heat        = Constant cp=1
     heat conduction      = basic
   END ARIA MATERIAL Kryptonite

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  DIRECT_SOLVER
      BEGIN SUPERLU SOLVER
      END
    END TPETRA EQUATION SOLVER
```

```
{else}
    Begin Trilinos Equation Solver Direct_Solver
      Solution Method = amesos-superlu
    End
{endif}

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  ITERATIVE_SOLVER
      BEGIN GMRES SOLVER
        BEGIN JACOBI PRECONDITIONER
        END
        MAXIMUM ITERATIONS = 1000
        RESIDUAL SCALING = NONE
        CONVERGENCE TOLERANCE = 1.000000e-15
      END
    END TPETRA EQUATION SOLVER
{else}
    Begin Trilinos Equation Solver Iterative_Solver
      Solution Method = GMRES
      Preconditioning Method = Jacobi
      Maximum Iterations = 1000
      Residual Norm Scaling = None
      Residual Norm Tolerance = 1.0e-15
    End
{endif}

   BEGIN FINITE ELEMENT MODEL cube
      database name = cube_contact_h{N}_tet10.e
      coordinate system is cartesian
      decomposition method = rcb

      BEGIN PARAMETERS FOR BLOCK block_1
 material Kryptonite
      END PARAMETERS FOR BLOCK block_1

      BEGIN PARAMETERS FOR BLOCK block_2
 material Kryptonite
      END PARAMETERS FOR BLOCK block_2

   END FINITE ELEMENT MODEL cube

   Begin User Function exact_soln
     Load From File ./exact.so Using Function registerExactSoln
   End

   Begin User Function exact_soln_dot
     Load From File ./exact.so Using Function registerExactSolnDot
   End

   Begin User Function exact_src
     Load From File ./exact.so Using Function registerExactSrc
   End

   Begin User Function flux_surface_3
     Load From File ./exact.so Using Function registerFlux_Surface_3
   End

   Begin User Function flux_surface_5
     Load From File ./exact.so Using Function registerFlux_Surface_5
   End

   Begin User Function flux_surface_1
     Load From File ./exact.so Using Function registerFlux_Surface_1
   End

   Begin User Function flux_surface_2
     Load From File ./exact.so Using Function registerFlux_Surface_2
   End
```

```
  Begin Norm Postprocessor l2
    Use Function exact_soln
    Subtract Function nonlinear_solution->TEMPERATURE
    Compute Norms L2
    Store In l2_error
  End

  Begin Norm Postprocessor h1
    Use Function exact_soln
    Subtract Function nonlinear_solution->TEMPERATURE
    Compute Norms H1
    Store In h1_error
  End

  Begin Norm Postprocessor linf
    Use Function exact_soln
    Subtract Function nonlinear_solution->TEMPERATURE
    Compute Norms LInfinity
    Store In linf_error
  End

  Begin Postprocessor Output Control pp_out
    Comment Character Is %
    Write To File errors_h{N}.dat
    Floating Point Precision Is 3
    Floating Point Format Is Scientific
  End

  BEGIN PROCEDURE myAriaProcedure

     Begin Solution Control Description
Use System Main
Begin System Main
   Begin Sequential The_Time_Block
      Advance myRegion
   End
      Simulation Start Time = 0
   Simulation Termination Time = 1
End
     End

     BEGIN ARIA REGION myRegion

Nonlinear Solution Strategy = Newton
        Maximum Nonlinear Iterations = 10
        Nonlinear Residual Tolerance = 1.0e-12
        Nonlinear Correction Tolerance = 1.0e-12
        Nonlinear Relaxation Factor  = 1.0
        use dof averaged nonlinear residual

use finite element model cube
        Use Linear Solver Iterative_Solver #Direct_Solver

EQ ENERGY for TEMPERATURE on block_1 using Q2 with DIFF SRC
EQ ENERGY for TEMPERATURE on block_2 using Q2 with DIFF SRC

# surface_4: x=0
# surface_6: x=1

# surface_3: y=0
# surface_5: y=1

# surface_1: z=1
# surface_2: z=0

# const Temp BC (x)
        BC const dirichlet at surface_4 Temperature = 1.0
```

```
        BC const dirichlet at surface_6 Temperature = 1.0

 # const flux BC (y)
 BC FLUX for Energy on surface_3  = constant flux = 3
 BC FLUX for Energy on surface_5  = constant flux = 5

 BC FLUX for Energy on surface_3  = Encore_Function Name=flux_surface_3
 BC FLUX for Energy on surface_5  = Encore_Function Name=flux_surface_5

 # convective flux BC with const Temp and H (z)
        BC Flux for Energy on surface_1 = Nat_Conv T_Ref=1 H=1
        BC Flux for Energy on surface_2 = Nat_Conv T_Ref=2 H=2

 BC FLUX for Energy on surface_1  = Encore_Function Name=flux_surface_1
 BC FLUX for Energy on surface_2  = Encore_Function Name=flux_surface_2

 #  const source term
 Source For ENERGY on block_1 = Constant value=1
 Source For ENERGY on block_2 = Constant value=1

 Source For ENERGY on block_1 = Encore_Function Name=exact_src
 Source For ENERGY on block_2 = Encore_Function Name=exact_src

        begin contact definition mpc1
          contact surface surf_1 contains surface_7
          contact surface surf_2 contains surface_8

          begin interaction inter_1
            surfaces = surf_1 surf_2
          end
          begin enforcement enf_1
            Enforcement for Energy = Tied_Temperature
          end
        end

   Output Number of Nodes

 Evaluate Postprocessor l2
 Evaluate Postprocessor h1
 Evaluate Postprocessor linf

 BEGIN RESULTS OUTPUT LABEL diffusion output
   database Name = thermal_steady_tet10_tied_contact_h{N}.e
   at step 1, increment = 1
   # time interval is 1.0
   title Aria cube test
   nodal variables = nonlinear_solution->TEMPERATURE as T
           element variables = l2_error h1_error linf_error
 END RESULTS OUTPUT LABEL diffusion output

     END ARIA REGION myRegion

  END PROCEDURE myAriaProcedure

END SIERRA myJob
```

12.3.9. Steady Tet10 Dash Contact

```
#N={N=4}
BEGIN SIERRA myJob

  BEGIN ARIA MATERIAL Kryptonite
    Density               = Constant rho=1
    Thermal Conductivity = constant k=1
    Specific Heat         = Constant cp=1
    heat conduction       = basic
```

```
   END ARIA MATERIAL Kryptonite

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  DIRECT_SOLVER
      BEGIN SUPERLU SOLVER
      END
    END TPETRA EQUATION SOLVER
{else}
    Begin Trilinos Equation Solver Direct_Solver
      Solution Method = amesos-superlu
    End
{endif}

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  ITERATIVE_SOLVER
      BEGIN GMRES SOLVER
        BEGIN JACOBI PRECONDITIONER
        END
        MAXIMUM ITERATIONS = 1000
        RESIDUAL SCALING = NONE
        CONVERGENCE TOLERANCE = 1.000000e-15
      END
    END TPETRA EQUATION SOLVER
{else}
    Begin Trilinos Equation Solver Iterative_Solver
      Solution Method = GMRES
      Preconditioning Method = Jacobi
      Maximum Iterations = 1000
      Residual Norm Scaling = None
      Residual Norm Tolerance = 1.0e-15
    End
{endif}

   BEGIN FINITE ELEMENT MODEL cube
      database name = cube_contact_h{N}_tet10.e
      coordinate system is cartesian
      decomposition method = rcb

      BEGIN PARAMETERS FOR BLOCK block_1
 material Kryptonite
      END PARAMETERS FOR BLOCK block_1

      BEGIN PARAMETERS FOR BLOCK block_2
 material Kryptonite
      END PARAMETERS FOR BLOCK block_2

   END FINITE ELEMENT MODEL cube

   Begin User Function exact_soln
     Load From File ./exact.so Using Function registerExactSoln
   End

   Begin User Function exact_soln_dot
     Load From File ./exact.so Using Function registerExactSolnDot
   End

   Begin User Function exact_src
     Load From File ./exact.so Using Function registerExactSrc
   End

   Begin User Function flux_surface_3
     Load From File ./exact.so Using Function registerFlux_Surface_3
   End

   Begin User Function flux_surface_5
     Load From File ./exact.so Using Function registerFlux_Surface_5
   End
```

```
  Begin User Function flux_surface_1
    Load From File ./exact.so Using Function registerFlux_Surface_1
  End

  Begin User Function flux_surface_2
    Load From File ./exact.so Using Function registerFlux_Surface_2
  End

  Begin Norm Postprocessor l2
    Use Function exact_soln
    Subtract Function nonlinear_solution->TEMPERATURE
    Compute Norms L2
    Store In l2_error
  End

  Begin Norm Postprocessor h1
    Use Function exact_soln
    Subtract Function nonlinear_solution->TEMPERATURE
    Compute Norms H1
    Store In h1_error
  End

  Begin Norm Postprocessor linf
    Use Function exact_soln
    Subtract Function nonlinear_solution->TEMPERATURE
    Compute Norms LInfinity
    Store In linf_error
  End

  Begin Postprocessor Output Control pp_out
    Comment Character Is %
    Write To File errors_h{N}.dat
    Floating Point Precision Is 3
    Floating Point Format Is Scientific
  End

  BEGIN PROCEDURE myAriaProcedure

     Begin Solution Control Description
Use System Main
Begin System Main
   Begin Sequential The_Time_Block
      Advance myRegion
   End
      Simulation Start Time = 0
   Simulation Termination Time = 1
End
     End

     BEGIN ARIA REGION myRegion

Nonlinear Solution Strategy = Newton
        Maximum Nonlinear Iterations = 10
        Nonlinear Residual Tolerance = 1.0e-12
        Nonlinear Correction Tolerance = 1.0e-12
        Nonlinear Relaxation Factor  = 1.0
        use dof averaged nonlinear residual

use finite element model cube
        Use Linear Solver Iterative_Solver #Direct_Solver

EQ ENERGY for TEMPERATURE on block_1 using Q2 with DIFF SRC
EQ ENERGY for TEMPERATURE on block_2 using Q2 with DIFF SRC

# surface_4: x=0
# surface_6: x=1

# surface_3: y=0
```

```
# surface_5: y=1

# surface_1: z=1
# surface_2: z=0

# const Temp BC (x)
        BC const dirichlet at surface_4 Temperature = 1.0
        BC const dirichlet at surface_6 Temperature = 1.0

# const flux BC (y)
BC FLUX for Energy on surface_3  = constant flux = 3
BC FLUX for Energy on surface_5  = constant flux = 5

BC FLUX for Energy on surface_3  = Encore_Function Name=flux_surface_3
BC FLUX for Energy on surface_5  = Encore_Function Name=flux_surface_5

# convective flux BC with const Temp and H (z)
        BC Flux for Energy on surface_1 = Nat_Conv T_Ref=1 H=1
        BC Flux for Energy on surface_2 = Nat_Conv T_Ref=2 H=2

BC FLUX for Energy on surface_1  = Encore_Function Name=flux_surface_1
BC FLUX for Energy on surface_2  = Encore_Function Name=flux_surface_2

#  const source term
Source For ENERGY on block_1 = Constant value=1
Source For ENERGY on block_2 = Constant value=1

Source For ENERGY on block_1 = Encore_Function Name=exact_src
Source For ENERGY on block_2 = Encore_Function Name=exact_src

        begin contact definition mpc1

         skin all blocks = on

         search = dash

         begin interaction defaults
           general contact = on
         end interaction defaults

         begin dash options
           interaction definition scheme = explicit
           search length scaling = 0.75
         end dash options

          begin enforcement enf_1
            Enforcement for Energy = Dash_Tied
          end
        end

   Output Number of Nodes

Evaluate Postprocessor l2
Evaluate Postprocessor h1
Evaluate Postprocessor linf

BEGIN RESULTS OUTPUT LABEL diffusion output
   database Name = thermal_steady_tet10_tied_dash_contact_h{N}.e
   at step 1, increment = 1
   # time interval is 1.0
   title Aria cube test
   nodal variables = nonlinear_solution->TEMPERATURE as T
           element variables = l2_error h1_error linf_error
END RESULTS OUTPUT LABEL diffusion output

     END ARIA REGION myRegion

  END PROCEDURE myAriaProcedure
```

```
END SIERRA myJob
```

12.3.10. Transient Tet4Tet10 Contact

```
#N={N=5}
BEGIN SIERRA myJob

   BEGIN ARIA MATERIAL Kryptonite
     Density              = Constant rho=1
     Thermal Conductivity = constant k=1
     Specific Heat        = Constant cp=1
     heat conduction      = basic
   END ARIA MATERIAL Kryptonite

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  DIRECT_SOLVER
      BEGIN SUPERLU SOLVER
      END
    END TPETRA EQUATION SOLVER
{else}
    Begin Trilinos Equation Solver Direct_Solver
      Solution Method = amesos-superlu
    End
{endif}

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  ITERATIVE_SOLVER
      BEGIN GMRES SOLVER
        BEGIN JACOBI PRECONDITIONER
        END
        MAXIMUM ITERATIONS = 1000
        RESIDUAL SCALING = NONE
        CONVERGENCE TOLERANCE = 1.000000e-15
      END
    END TPETRA EQUATION SOLVER
{else}
    Begin Trilinos Equation Solver Iterative_Solver
      Solution Method = GMRES
      Preconditioning Method = Jacobi
      Maximum Iterations = 1000
      Residual Norm Scaling = None
      Residual Norm Tolerance = 1.0e-15
    End
{endif}

   BEGIN FINITE ELEMENT MODEL cube
      database name = cube_contact_h{N}_tet10.e
      coordinate system is cartesian
      decomposition method = rcb

      BEGIN PARAMETERS FOR BLOCK block_1
 material Kryptonite
      END PARAMETERS FOR BLOCK block_1

      BEGIN PARAMETERS FOR BLOCK block_2
 material Kryptonite
      END PARAMETERS FOR BLOCK block_2

   END FINITE ELEMENT MODEL cube

   Begin User Function exact_soln
     Load From File ./exact_transient.so Using Function registerExactSoln
   End

   Begin User Function exact_soln_dot
```

```
    Load From File ./exact_transient.so Using Function registerExactSolnDot
  End

  Begin User Function exact_src
    Load From File ./exact_transient.so Using Function registerExactSrc
  End

  Begin User Function flux_surface_3
    Load From File ./exact_transient.so Using Function registerFlux_Surface_3
  End

  Begin User Function flux_surface_5
    Load From File ./exact_transient.so Using Function registerFlux_Surface_5
  End

  Begin User Function flux_surface_1
    Load From File ./exact_transient.so Using Function registerFlux_Surface_1
  End

  Begin User Function flux_surface_2
    Load From File ./exact_transient.so Using Function registerFlux_Surface_2
  End

  Begin Norm Postprocessor l2
    Use Function exact_soln
    Subtract Function nonlinear_solution->TEMPERATURE
    Compute Norms L2
  End

  Begin Norm Postprocessor l2_dot
    Use Function exact_soln_dot
    Subtract Function time_derivative_at_time->TEMPERATURE
    Compute Norms L2
  End

  Begin Norm Postprocessor h1
    Use Function exact_soln
    Subtract Function nonlinear_solution->TEMPERATURE
    Compute Norms H1
  End

  Begin Norm Postprocessor linf
    Use Function exact_soln
    Subtract Function nonlinear_solution->TEMPERATURE
    Compute Norms LInfinity
  End

  Begin Postprocessor Output Control pp_out
    Comment Character Is %
    Write To File errors_h{N}.dat
    Floating Point Precision Is 3
    Floating Point Format Is Scientific
  End

  BEGIN PROCEDURE myAriaProcedure

     Begin Solution Control Description
Use System Main
Begin System Main
   Begin Transient The_Time_Block
      Advance myRegion
   End
      Simulation Start Time = 0
   Simulation Termination Time = 3
End
Begin Parameters For Transient The_Time_Block
   Begin Parameters For Aria Region myRegion
     Initial Time Step Size = {0.5/2**N}
```

```
     Time Integration Method = Second_Order
     Time Step Variation = fixed
  End
End
     End

     BEGIN ARIA REGION myRegion

Nonlinear Solution Strategy = Newton
        Maximum Nonlinear Iterations = 10
        Nonlinear Residual Tolerance = 1.0e-12
        Nonlinear Correction Tolerance = 1.0e-12
        Nonlinear Relaxation Factor  = 1.0
        use dof averaged nonlinear residual

use finite element model cube
        Use Linear Solver Iterative_Solver #Direct_Solver

EQ ENERGY for TEMPERATURE on block_1 using Q1 with MASS DIFF SRC
EQ ENERGY for TEMPERATURE on block_2 using Q1 with MASS DIFF SRC

        IC const on block_1 temperature = 1.0
        IC const on block_2 temperature = 1.0

# surface_4: x=0
# surface_6: x=1

# surface_3: y=0
# surface_5: y=1

# surface_1: z=1
# surface_2: z=0

# const Temp BC (x)
        BC const dirichlet at surface_4 Temperature = 1.0
        BC const dirichlet at surface_6 Temperature = 1.0

# const flux BC (y)
BC FLUX for Energy on surface_3  = constant flux = 3
BC FLUX for Energy on surface_5  = constant flux = 5

BC FLUX for Energy on surface_3  = Encore_Function Name=flux_surface_3
BC FLUX for Energy on surface_5  = Encore_Function Name=flux_surface_5

# convective flux BC with const Temp and H (z)
        BC Flux for Energy on surface_1 = Nat_Conv T_Ref=1 H=1
        BC Flux for Energy on surface_2 = Nat_Conv T_Ref=2 H=2

BC FLUX for Energy on surface_1  = Encore_Function Name=flux_surface_1
BC FLUX for Energy on surface_2  = Encore_Function Name=flux_surface_2

#  const source term
Source For ENERGY on block_1 = Constant value=1
Source For ENERGY on block_2 = Constant value=1

Source For ENERGY on block_1 = Encore_Function Name=exact_src
Source For ENERGY on block_2 = Encore_Function Name=exact_src

        begin contact definition mpc1
          contact surface surf_1 contains surface_7
          contact surface surf_2 contains surface_8

          begin interaction inter_1
            surfaces = surf_1 surf_2
          end
          begin enforcement enf_1
            Enforcement for Energy = Tied_Temperature
          end
```

```
         end

      Output Number of Nodes

   Evaluate Postprocessor l2
   Evaluate Postprocessor l2_dot
   Evaluate Postprocessor h1
   Evaluate Postprocessor linf

   BEGIN RESULTS OUTPUT LABEL diffusion output
      database Name = thermal_transient_tet10_tied_contact_h{N}.e
      at step 0, increment = {2**N}
      title Aria cube test
      nodal variables = solution->TEMPERATURE as T
      nodal variables = time_derivative_at_time->TEMPERATURE as TDOT
   END RESULTS OUTPUT LABEL diffusion output

        END ARIA REGION myRegion

     END PROCEDURE myAriaProcedure

END SIERRA myJob
```

12.3.11. Transient Tet10 Contact

```
#N={N=5}
BEGIN SIERRA myJob

   BEGIN ARIA MATERIAL Kryptonite
     Density              = Constant rho=1
     Thermal Conductivity = constant k=1
     Specific Heat        = Constant cp=1
     heat conduction      = basic
   END ARIA MATERIAL Kryptonite

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  DIRECT_SOLVER
      BEGIN SUPERLU SOLVER
      END
    END TPETRA EQUATION SOLVER
{else}
    Begin Trilinos Equation Solver Direct_Solver
      Solution Method = amesos-superlu
    End
{endif}

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  ITERATIVE_SOLVER
      BEGIN GMRES SOLVER
        BEGIN JACOBI PRECONDITIONER
        END
        MAXIMUM ITERATIONS = 1000
        RESIDUAL SCALING = NONE
        CONVERGENCE TOLERANCE = 1.000000e-15
      END
    END TPETRA EQUATION SOLVER
{else}
    Begin Trilinos Equation Solver Iterative_Solver
      Solution Method = GMRES
      Preconditioning Method = Jacobi
      Maximum Iterations = 1000
      Residual Norm Scaling = None
      Residual Norm Tolerance = 1.0e-15
    End
{endif}
```

```
  BEGIN FINITE ELEMENT MODEL cube
     database name = cube_contact_h{N}_tet10.e
     coordinate system is cartesian
     decomposition method = rcb

     BEGIN PARAMETERS FOR BLOCK block_1
material Kryptonite
     END PARAMETERS FOR BLOCK block_1

     BEGIN PARAMETERS FOR BLOCK block_2
material Kryptonite
     END PARAMETERS FOR BLOCK block_2

  END FINITE ELEMENT MODEL cube

  Begin User Function exact_soln
    Load From File ./exact_transient.so Using Function registerExactSoln
  End

  Begin User Function exact_soln_dot
    Load From File ./exact_transient.so Using Function registerExactSolnDot
  End

  Begin User Function exact_src
    Load From File ./exact_transient.so Using Function registerExactSrc
  End

  Begin User Function flux_surface_3
    Load From File ./exact_transient.so Using Function registerFlux_Surface_3
  End

  Begin User Function flux_surface_5
    Load From File ./exact_transient.so Using Function registerFlux_Surface_5
  End

  Begin User Function flux_surface_1
    Load From File ./exact_transient.so Using Function registerFlux_Surface_1
  End

  Begin User Function flux_surface_2
    Load From File ./exact_transient.so Using Function registerFlux_Surface_2
  End

  Begin Norm Postprocessor l2
    Use Function exact_soln
    Subtract Function nonlinear_solution->TEMPERATURE
    Compute Norms L2
  End

  Begin Norm Postprocessor l2_dot
    Use Function exact_soln_dot
    Subtract Function time_derivative_at_time->TEMPERATURE
    Compute Norms L2
  End

  Begin Norm Postprocessor h1
    Use Function exact_soln
    Subtract Function nonlinear_solution->TEMPERATURE
    Compute Norms H1
  End

  Begin Norm Postprocessor linf
    Use Function exact_soln
    Subtract Function nonlinear_solution->TEMPERATURE
    Compute Norms LInfinity
  End

  Begin Postprocessor Output Control pp_out
```

```
    Comment Character Is %
    Write To File errors_h{N}.dat
    Floating Point Precision Is 3
    Floating Point Format Is Scientific
  End

  BEGIN PROCEDURE myAriaProcedure

     Begin Solution Control Description
Use System Main
Begin System Main
   Begin Transient The_Time_Block
      Advance myRegion
   End
      Simulation Start Time = 0
   Simulation Termination Time = 3
End
Begin Parameters For Transient The_Time_Block
   Begin Parameters For Aria Region myRegion
     Initial Time Step Size = {0.5/2**N}
     Time Integration Method = Second_Order
     Time Step Variation = fixed
  End
End
     End

     BEGIN ARIA REGION myRegion

Nonlinear Solution Strategy = Newton
        Maximum Nonlinear Iterations = 10
        Nonlinear Residual Tolerance = 1.0e-12
        Nonlinear Correction Tolerance = 1.0e-12
        Nonlinear Relaxation Factor  = 1.0
        use dof averaged nonlinear residual

use finite element model cube
        Use Linear Solver Iterative_Solver #Direct_Solver

EQ ENERGY for TEMPERATURE on block_1 using Q2 with MASS DIFF SRC
EQ ENERGY for TEMPERATURE on block_2 using Q2 with MASS DIFF SRC

        IC const on block_1 temperature = 1.0
        IC const on block_2 temperature = 1.0

# surface_4: x=0
# surface_6: x=1

# surface_3: y=0
# surface_5: y=1

# surface_1: z=1
# surface_2: z=0

# const Temp BC (x)
        BC const dirichlet at surface_4 Temperature = 1.0
        BC const dirichlet at surface_6 Temperature = 1.0

# const flux BC (y)
BC FLUX for Energy on surface_3  = constant flux = 3
BC FLUX for Energy on surface_5  = constant flux = 5

BC FLUX for Energy on surface_3  = Encore_Function Name=flux_surface_3
BC FLUX for Energy on surface_5  = Encore_Function Name=flux_surface_5

# convective flux BC with const Temp and H (z)
        BC Flux for Energy on surface_1 = Nat_Conv T_Ref=1 H=1
        BC Flux for Energy on surface_2 = Nat_Conv T_Ref=2 H=2
```

```
 BC FLUX for Energy on surface_1  = Encore_Function Name=flux_surface_1
 BC FLUX for Energy on surface_2  = Encore_Function Name=flux_surface_2

 #  const source term
 Source For ENERGY on block_1 = Constant value=1
 Source For ENERGY on block_2 = Constant value=1

 Source For ENERGY on block_1 = Encore_Function Name=exact_src
 Source For ENERGY on block_2 = Encore_Function Name=exact_src

         begin contact definition mpc1
           contact surface surf_1 contains surface_7
           contact surface surf_2 contains surface_8

           begin interaction inter_1
             surfaces = surf_1 surf_2
           end
           begin enforcement enf_1
             Enforcement for Energy = Tied_Temperature
           end
         end

    Output Number of Nodes

 Evaluate Postprocessor l2
 Evaluate Postprocessor l2_dot
 Evaluate Postprocessor h1
 Evaluate Postprocessor linf

 BEGIN RESULTS OUTPUT LABEL diffusion output
    database Name = thermal_transient_tet10_tied_contact_h{N}.e
    at step 0, increment = {2**N}
    title Aria cube test
    nodal variables = solution->TEMPERATURE as T
    nodal variables = time_derivative_at_time->TEMPERATURE as TDOT
 END RESULTS OUTPUT LABEL diffusion output

      END ARIA REGION myRegion

   END PROCEDURE myAriaProcedure

END SIERRA myJob
```

12.4. ELEMENT DEATH

12.4.1. CDFEM Element Death (Heat Flux)

12.4.1.1. Tri3

```
BEGIN SIERRA Aria

Title \$
1-d standard conduction problem, Carslaw and Jaeger P. 292\$

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  SOLVE_TEMPERATURE
      BEGIN CG SOLVER
        BEGIN JACOBI PRECONDITIONER
        END
        MAXIMUM ITERATIONS = 10000
        RESIDUAL SCALING = R0
        CONVERGENCE TOLERANCE = 1.000000e-14
      END
    END TPETRA EQUATION SOLVER
{else}
    BEGIN Aztec EQUATION SOLVER solve_temperature
      Solution Method = cg
      Preconditioning Method = JACOBI
      Maximum Iterations = 10000
      Residual Norm Tolerance = 1e-14
      Residual norm scaling = R0
    END
{endif}

Begin Global Constants
     Stefan Boltzmann Constant = 5.67e-8  # W/m^2-K^4
     Ideal Gas Constant = 8.314           # J/mol-K
End

BEGIN ARIA MATERIAL solid
  DENSITY = constant rho = 1.
  Thermal Conductivity = constant k = 1.
  Specific Heat = Constant cp = 1.0
  Heat Conduction             = basic
END ARIA MATERIAL solid

BEGIN FINITE ELEMENT MODEL VERIFY_DEATH
  DATABASE NAME = input{N}_tri3.e
  decomposition method = rcb
  COORDINATE SYSTEM = CARTESIAN
  DATABASE TYPE = EXODUSII
  USE MATERIAL solid FOR block_1
  USE MATERIAL solid FOR block_1_dead
END FINITE ELEMENT MODEL VERIFY_DEATH

Begin String Function exact_soln
  Value Is "ln(sqrt(x*x+y*y))*(1/ln(2-t))"
  Gradient Is "(x/(x*x+y*y))*(1/ln(2-t))" "(y/(x*x+y*y))*(1/ln(2-t))"
End

Begin String Function exact_src
  Value Is "ln(sqrt(x*x+y*y))*(-1/(ln(2-t)*ln(2-t)))*(1/(2-t))*(-1)"
End

# exact flux computed at interface (r=2-t)
Begin String Function exact_flux
  Value Is "-1/((2-t)*ln(2-t))"
End
```

```
# exact interface position (radial)
Begin String Function exact_interface
  Value Is "2-t"
End

# radius function - evaluate r(x,y)
Begin String Function radius
  Value Is "sqrt(x*x+y*y)"
End

Begin Norm Postprocessor l2
  Volumes block_1
  Use Function exact_soln
  Subtract Function solution->TEMPERATURE
  Compute Norms L2
  Store In l2_err
End

Begin Norm Postprocessor h1
  Volumes block_1
  Use Function exact_soln
  Subtract Function solution->TEMPERATURE
  Compute Norms H1
  Store In h1_err
End

Begin Norm Postprocessor linf
  Volumes block_1
  Use Function exact_soln
  Subtract Function solution->TEMPERATURE
  Compute Norms LInfinity
  Store In linf_err
End

Begin Norm Postprocessor l2_interface
  Surfaces surface_1 surface_block_1_death_by_temp
  Use Function exact_interface
  Subtract Function radius
  Compute Norms L2
End

Begin Norm Postprocessor linf_interface
  Surfaces surface_1 surface_block_1_death_by_temp
  Use Function exact_interface
  Subtract Function radius
  Compute Norms Nodal LInfinity
  Store In linf_interface_err
End

Begin Postprocessor Output Control pp_out
  Comment Character Is %
  Write To File errors{N}.dat
  Floating Point Precision Is 6
  Floating Point Format Is Fixed
End

Begin Procedure myProcedure

  Begin Solution Control Description
     Use System Main
     Begin System Main
       Simulation Start Time            = 0.0
       Simulation Termination Time      = 0.9
       Begin transient MySolveBlock
           Advance myRegion
        End
     End
      begin parameters for transient MySolveBlock
```

```
      start time = 0.0
      begin parameters for aria region myRegion
        initial time step size = {0.1*(0.5**(N-1))}
        Predictor-Corrector Tolerance = {0.05*(0.5**(N-1))}
        Maximum Time Step Size = {0.2*(0.5**(N-1))}
        Time Integration Method = bdf2
        time step variation = adaptive
      end
    end
  End

  Begin Aria Region myRegion

    Use Finite Element Model VERIFY_DEATH

    Begin CDFEM Death death_by_temp
      add volume block_1
      Criterion is solution->Temperature > 1.0
    End

    Use Linear Solver solve_temperature

    nonlinear solution strategy = newton
    maximum nonlinear iterations = 2
    nonlinear correction tolerance = 1.0e-12
    nonlinear residual tolerance = 1.0e-12
    nonlinear relaxation factor  = 1.0

    use dof averaged nonlinear residual

    eq energy for temperature on all_blocks using q1 with lumped_mass diff src

    IC Encore function on block_1 Temperature = exact_soln

    BC Dirichlet for Temperature on surface_2 = encore_function name=exact_soln

    SOURCE for Energy on block_1 = encore_function name=exact_src

    BC Flux for Energy on surface_1 = encore_function name=exact_flux
    BC Flux for Energy on surface_block_1_death_by_temp = encore_function name=exact_flux

    Output Number of Nodes

    Evaluate Postprocessor l2
    Evaluate Postprocessor h1
    Evaluate Postprocessor linf

    Evaluate Postprocessor l2_interface
    Evaluate Postprocessor linf_interface

    Begin Results Output Label diffusion output
      database name = output{N}.e
      at Step 0, Interval = {2**N}
      Nodal Variables = solution->temperature as TEMP
      Nodal Variables = linf_interface_err
      Element Variables  = l2_err h1_err linf_err
    End Results Output Label diffusion output

  End Aria Region myRegion

End Procedure myProcedure

END SIERRA ARIA
```

12.4.1.2. Tet4

```
BEGIN SIERRA Aria

Title \$
1-d standard conduction problem, Carslaw and Jaeger P. 292\$

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  SOLVE_TEMPERATURE
      BEGIN CG SOLVER
        BEGIN JACOBI PRECONDITIONER
        END
        MAXIMUM ITERATIONS = 10000
        RESIDUAL SCALING = R0
        CONVERGENCE TOLERANCE = 1.000000e-14
      END
    END TPETRA EQUATION SOLVER
{else}
    BEGIN Aztec EQUATION SOLVER solve_temperature
      Solution Method = cg
      Preconditioning Method = JACOBI
      Maximum Iterations = 10000
      Residual Norm Tolerance = 1e-14
      Residual norm scaling = R0
    END
{endif}

Begin Global Constants
     Stefan Boltzmann Constant = 5.67e-8  # W/m^2-K^4
     Ideal Gas Constant = 8.314           # J/mol-K
End

BEGIN ARIA MATERIAL solid
  DENSITY = constant rho = 1.
  Thermal Conductivity = constant k = 1.
  Specific Heat = Constant cp = 1.0
  Heat Conduction             = basic
END ARIA MATERIAL solid

BEGIN FINITE ELEMENT MODEL VERIFY_DEATH
  DATABASE NAME = input{N}_tet4.e
  decomposition method = rcb
  COORDINATE SYSTEM = CARTESIAN
  DATABASE TYPE = EXODUSII
  USE MATERIAL solid FOR block_1
  USE MATERIAL solid FOR block_1_dead
END FINITE ELEMENT MODEL VERIFY_DEATH

Begin String Function exact_soln
  Value Is "(1+t)/sqrt(x*x+y*y+z*z)"
  Gradient Is "(1+t)*(-1/(x*x+y*y+z*z))*(x/sqrt(x*x+y*y+z*z))" "(1+t)*(-1/(x*x+y*y+z*z))*(y/sqrt(x*x+y*y+z*z))" "(1+t)*(-1/(x*x+
End

Begin String Function exact_src
  Value Is "1/sqrt(x*x+y*y+z*z)"
End

# exact flux computed at interface (r=2-t)
Begin String Function exact_flux
  Value Is "-1/(1+t)"
  ###Value Is "-(1+t)" ### for verification of case with no element death
End

# exact interface position (radial)
Begin String Function exact_interface
  Value Is "1+t"
End
```

```
# radius function - evaluate r(x,y)
Begin String Function radius
  Value Is "sqrt(x*x+y*y+z*z)"
End

Begin Norm Postprocessor l2
  Volumes block_1
  Use Function exact_soln
  Subtract Function solution->TEMPERATURE
  Compute Norms L2
  Store In l2_err
End

Begin Norm Postprocessor h1
  Volumes block_1
  Use Function exact_soln
  Subtract Function solution->TEMPERATURE
  Compute Norms H1
  Store In h1_err
End

Begin Norm Postprocessor linf
  Volumes block_1
  Use Function exact_soln
  Subtract Function solution->TEMPERATURE
  Compute Norms LInfinity
  Store In linf_err
End

Begin Norm Postprocessor l2_interface
  Surfaces surface_1 surface_block_1_death_by_temp
  Use Function exact_interface
  Subtract Function radius
  Compute Norms L2
End

Begin Norm Postprocessor linf_interface
  Surfaces surface_1 surface_block_1_death_by_temp
  Use Function exact_interface
  Subtract Function radius
  Compute Norms Nodal LInfinity
  Store In linf_interface_err
End

Begin Postprocessor Output Control pp_out
  Comment Character Is %
  Write To File errors{N}.dat
  Floating Point Precision Is 6
  Floating Point Format Is Fixed
End

Begin Procedure myProcedure

  Begin Solution Control Description
     Use System Main
     Begin System Main
       Simulation Start Time            = 0.0
       Simulation Termination Time      = 0.75
       Begin transient MySolveBlock
           Advance myRegion
        End
     End
      begin parameters for transient MySolveBlock
        start time = 0.0
        begin parameters for aria region myRegion
          initial time step size = {0.1*(0.5**(N-1))}
          Predictor-Corrector Tolerance = {0.05*(0.5**(N-1))}
```

```
        Maximum Time Step Size = {0.2*(0.5**(N-1))}
        Time Integration Method = bdf2
        time step variation = adaptive
      end
    end
  End

  Begin Aria Region myRegion

    Use Finite Element Model VERIFY_DEATH

    Begin CDFEM Death death_by_temp
      add volume block_1
      Criterion is solution->Temperature > 1.0
    End

    Use Linear Solver solve_temperature

    nonlinear solution strategy = newton
    maximum nonlinear iterations = 2
    nonlinear correction tolerance = 1.0e-12
    nonlinear residual tolerance = 1.0e-12
    nonlinear relaxation factor  = 1.0

    use dof averaged nonlinear residual

    eq energy for temperature on all_blocks using q1 with lumped_mass diff src

    IC Encore function on block_1 Temperature = exact_soln

    BC Dirichlet for Temperature on surface_2 = encore_function name=exact_soln

    SOURCE for Energy on block_1 = encore_function name=exact_src

    BC Flux for Energy on surface_1 = encore_function name=exact_flux
    BC Flux for Energy on surface_block_1_death_by_temp = encore_function name=exact_flux

    Output Number of Nodes

    Evaluate Postprocessor l2
    Evaluate Postprocessor h1
    Evaluate Postprocessor linf

    Evaluate Postprocessor l2_interface
    Evaluate Postprocessor linf_interface

    Begin Results Output Label diffusion output
      database name = output{N}.e
      at Step 0, Interval = {2**N}
      Nodal Variables = solution->temperature as TEMP
      Nodal Variables = linf_interface_err
      Element Variables  = l2_err h1_err linf_err
    End Results Output Label diffusion output

  End Aria Region myRegion

End Procedure myProcedure

END SIERRA ARIA
```

12.4.2. 3D Spherical Shell Enclosure

12.5. TIME INTEGRATION

12.5.1. Adaptive Time Integration

12.5.1.1. *First Order Fixed*

```
BEGIN SIERRA myJob

   BEGIN ARIA MATERIAL Kryptonite
     Density              = Polynomial Variable=Temperature Order=1 C0=1 C1=0.1
     Thermal Conductivity = Polynomial Variable=Temperature Order=1 C0=1 C1=0.1
     Specific Heat        = Constant cp=1
     heat conduction      = basic
   END ARIA MATERIAL Kryptonite

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  DIRECT_SOLVER
      BEGIN SUPERLU SOLVER
      END
    END TPETRA EQUATION SOLVER
{else}
    Begin Trilinos Equation Solver Direct_Solver
      Solution Method = amesos-superlu
    End
{endif}

   BEGIN FINITE ELEMENT MODEL cube
      database name = square_h{N}_tri3.e
      coordinate system is cartesian

      BEGIN PARAMETERS FOR BLOCK block_1
 material Kryptonite
      END PARAMETERS FOR BLOCK block_1

   END FINITE ELEMENT MODEL cube

   Begin User Function exact_soln
     Load From File ./somefunc.so Using Function registerExactSoln
   End

   Begin User Function exact_soln_dot
     Load From File ./somefunc.so Using Function registerExactSolnDot
   End

   Begin User Function exact_src
     Load From File ./somefunc.so Using Function registerExactSrc
   End

   Begin Norm Postprocessor l2
     Use Function exact_soln
     Subtract Function nonlinear_solution->TEMPERATURE
     Compute Norms L2
   End

   Begin Norm Postprocessor l2_dot
     Use Function exact_soln_dot
     Subtract Function time_derivative_at_time->TEMPERATURE
     Compute Norms L2
   End

   Begin Norm Postprocessor h1
     Use Function exact_soln
     Subtract Function nonlinear_solution->TEMPERATURE
     Compute Norms H1
   End
```

```
  Begin Norm Postprocessor linf
    Use Function exact_soln
    Subtract Function nonlinear_solution->TEMPERATURE
    Compute Norms LInfinity
  End

  Begin Postprocessor Output Control pp_out
    Comment Character Is %
    Write To File errors_1st_ord_fixed_h{N}.dat
    Floating Point Precision Is 4
    Floating Point Format Is Scientific
  End

  BEGIN PROCEDURE myAriaProcedure

     Begin Solution Control Description
 Use System Main
 Begin System Main
    Begin Transient The_Time_Block
       Advance myRegion
    End
       Simulation Start Time = 0
    Simulation Termination Time = 1
 End
Begin Parameters For Transient The_Time_Block
   Begin Parameters For Aria Region myRegion
      Initial Time Step Size = {0.1/2**N}
      Time Integration Method = First_Order
      Time Step Variation = fixed
   End
End
      End

      BEGIN ARIA REGION myRegion

 Nonlinear Solution Strategy = Newton
        Maximum Nonlinear Iterations = 10
        Nonlinear Residual Tolerance = 1.0e-12
        Nonlinear Correction Tolerance = 1.0e-12
        Nonlinear Relaxation Factor  = 1.0
        use dof averaged nonlinear residual

 use finite element model cube
        Use Linear Solver Direct_Solver

        IC Encore Function on block_1 temperature = exact_soln

        BC dirichlet for Temperature at surface_1 = Encore_Function Name=exact_soln
        BC dirichlet for Temperature at surface_2 = Encore_Function Name=exact_soln
        BC dirichlet for Temperature at surface_3 = Encore_Function Name=exact_soln
        BC dirichlet for Temperature at surface_4 = Encore_Function Name=exact_soln

 EQ ENERGY for TEMPERATURE on block_1 using Q1 with MASS DIFF SRC

 Source For ENERGY on block_1 = Encore_Scalar_Function Name=exact_src

    Output Number of TimeSteps

 Evaluate Postprocessor l2
 Evaluate Postprocessor l2_dot
 Evaluate Postprocessor h1
 Evaluate Postprocessor linf

 BEGIN RESULTS OUTPUT LABEL diffusion output
    database Name = aria_1st_ord_fixed_h{N}.e
    at step 0, increment = 1
    # time interval is 1.0
    title Aria cube test
```

```
    nodal variables = nonlinear_solution->TEMPERATURE as T
    nodal variables = time_derivative_at_time->TEMPERATURE as TDOT
 END RESULTS OUTPUT LABEL diffusion output

      END ARIA REGION myRegion

   END PROCEDURE myAriaProcedure

END SIERRA myJob
```

12.5.1.2. First Order Adaptive

```
BEGIN SIERRA myJob

   BEGIN ARIA MATERIAL Kryptonite
     Density              = Polynomial Variable=Temperature Order=1 C0=1 C1=0.1
     Thermal Conductivity = Polynomial Variable=Temperature Order=1 C0=1 C1=0.1
     Specific Heat        = Constant cp=1
     heat conduction      = basic
   END ARIA MATERIAL Kryptonite

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  DIRECT_SOLVER
      BEGIN SUPERLU SOLVER
      END
    END TPETRA EQUATION SOLVER
{else}
    Begin Trilinos Equation Solver Direct_Solver
      Solution Method = amesos-superlu
    End
{endif}

   BEGIN FINITE ELEMENT MODEL cube
      database name = square_h{N}_tri3.e
      coordinate system is cartesian

      BEGIN PARAMETERS FOR BLOCK block_1
 material Kryptonite
      END PARAMETERS FOR BLOCK block_1

   END FINITE ELEMENT MODEL cube

   Begin User Function exact_soln
     Load From File ./somefunc.so Using Function registerExactSoln
   End

   Begin User Function exact_soln_dot
     Load From File ./somefunc.so Using Function registerExactSolnDot
   End

   Begin User Function exact_src
     Load From File ./somefunc.so Using Function registerExactSrc
   End

   Begin Norm Postprocessor l2
     Use Function exact_soln
     Subtract Function nonlinear_solution->TEMPERATURE
     Compute Norms L2
   End

   Begin Norm Postprocessor l2_dot
     Use Function exact_soln_dot
     Subtract Function time_derivative_at_time->TEMPERATURE
     Compute Norms L2
   End

   Begin Norm Postprocessor h1
```

```
    Use Function exact_soln
    Subtract Function nonlinear_solution->TEMPERATURE
    Compute Norms H1
  End

  Begin Norm Postprocessor linf
    Use Function exact_soln
    Subtract Function nonlinear_solution->TEMPERATURE
    Compute Norms LInfinity
  End

  Begin Postprocessor Output Control pp_out
    Comment Character Is %
    Write To File errors_1st_ord_adapt_h{N}.dat
    Floating Point Precision Is 4
    Floating Point Format Is Scientific
  End

  BEGIN PROCEDURE myAriaProcedure

     Begin Solution Control Description
 Use System Main
 Begin System Main
    Begin Transient The_Time_Block
       Advance myRegion
    End
       Simulation Start Time = 0
    Simulation Termination Time = 1
 End
Begin Parameters For Transient The_Time_Block
  Begin Parameters For Aria Region myRegion
     Initial Time Step Size = {0.1/2**N}
             Predictor-Corrector Tolerance = {1e-1/4**N}
             Maximum Time Step Size = {0.5/2**N}
     Time Integration Method = First_Order
     Time Step Variation = adaptive
  End
End
     End

     BEGIN ARIA REGION myRegion

 Nonlinear Solution Strategy = Newton
        Maximum Nonlinear Iterations = 10
        Nonlinear Residual Tolerance = 1.0e-12
        Nonlinear Correction Tolerance = 1.0e-12
        Nonlinear Relaxation Factor  = 1.0
        use dof averaged nonlinear residual

 use finite element model cube
        Use Linear Solver Direct_Solver

        IC Encore Function on block_1 temperature = exact_soln

        BC dirichlet for Temperature at surface_1 = Encore_Function Name=exact_soln
        BC dirichlet for Temperature at surface_2 = Encore_Function Name=exact_soln
        BC dirichlet for Temperature at surface_3 = Encore_Function Name=exact_soln
        BC dirichlet for Temperature at surface_4 = Encore_Function Name=exact_soln

 EQ ENERGY for TEMPERATURE on block_1 using Q1 with MASS DIFF SRC

 Source For ENERGY on block_1 = Encore_Scalar_Function Name=exact_src

    Output Number of TimeSteps

 Evaluate Postprocessor l2
 Evaluate Postprocessor l2_dot
 Evaluate Postprocessor h1
```

```
 Evaluate Postprocessor linf

 BEGIN RESULTS OUTPUT LABEL diffusion output
    database Name = aria_1st_ord_adapt_h{N}.e
    at step 0, increment = 1
    # time interval is 1.0
    title Aria cube test
    nodal variables = nonlinear_solution->TEMPERATURE as T
    nodal variables = time_derivative_at_time->TEMPERATURE as TDOT
 END RESULTS OUTPUT LABEL diffusion output

      END ARIA REGION myRegion

   END PROCEDURE myAriaProcedure

END SIERRA myJob
```

12.5.1.3. Second Order Fixed

```
BEGIN SIERRA myJob

   BEGIN ARIA MATERIAL Kryptonite
     Density              = Polynomial Variable=Temperature Order=1 C0=1 C1=0.1
     Thermal Conductivity = Polynomial Variable=Temperature Order=1 C0=1 C1=0.1
     Specific Heat        = Constant cp=1
     heat conduction      = basic
   END ARIA MATERIAL Kryptonite

   load user plugin file ./somefunc.so

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  DIRECT_SOLVER
      BEGIN SUPERLU SOLVER
      END
    END TPETRA EQUATION SOLVER
{else}
    Begin Trilinos Equation Solver Direct_Solver
      Solution Method = amesos-superlu
    End
{endif}

   BEGIN FINITE ELEMENT MODEL cube
      database name = square_h{N}_tri3.e
      coordinate system is cartesian

      BEGIN PARAMETERS FOR BLOCK block_1
 material Kryptonite
      END PARAMETERS FOR BLOCK block_1

   END FINITE ELEMENT MODEL cube

   Begin User Function exact_soln
     Load From File ./somefunc.so Using Function registerExactSoln
   End

   Begin User Function exact_soln_dot
     Load From File ./somefunc.so Using Function registerExactSolnDot
   End

   Begin User Function exact_src
     Load From File ./somefunc.so Using Function registerExactSrc
   End

   Begin Norm Postprocessor l2
     Use Function exact_soln
     Subtract Function nonlinear_solution->TEMPERATURE
     Compute Norms L2
```

```
  End

  Begin Norm Postprocessor l2_dot
    Use Function exact_soln_dot
    Subtract Function time_derivative_at_time->TEMPERATURE
    Compute Norms L2
  End

  Begin Norm Postprocessor h1
    Use Function exact_soln
    Subtract Function nonlinear_solution->TEMPERATURE
    Compute Norms H1
  End

  Begin Norm Postprocessor linf
    Use Function exact_soln
    Subtract Function nonlinear_solution->TEMPERATURE
    Compute Norms LInfinity
  End

  Begin Postprocessor Output Control pp_out
    Comment Character Is %
    Write To File errors_2nd_ord_fixed_h{N}.dat
    Floating Point Precision Is 4
    Floating Point Format Is Scientific
  End

  BEGIN PROCEDURE myAriaProcedure

     Begin Solution Control Description
 Use System Main
 Begin System Main
    Begin Transient The_Time_Block
       Advance myRegion
    End
       Simulation Start Time = 0
    Simulation Termination Time = 1
 End
Begin Parameters For Transient The_Time_Block
   Begin Parameters For Aria Region myRegion
      Initial Time Step Size = {0.1/2**N}
      Time Integration Method = Second_Order
      Time Step Variation = fixed
   End
End
      End

      BEGIN ARIA REGION myRegion

 Nonlinear Solution Strategy = Newton
         Maximum Nonlinear Iterations = 10
         Nonlinear Residual Tolerance = 1.0e-12
         Nonlinear Correction Tolerance = 1.0e-12
         Nonlinear Relaxation Factor  = 1.0
         use dof averaged nonlinear residual

 use finite element model cube
         Use Linear Solver Direct_Solver

         IC Encore Function on block_1 temperature = exact_soln

         BC dirichlet for Temperature at surface_1 = Encore_Function Name=exact_soln
         BC dirichlet for Temperature at surface_2 = Encore_Function Name=exact_soln
         BC dirichlet for Temperature at surface_3 = Encore_Function Name=exact_soln
         BC dirichlet for Temperature at surface_4 = Encore_Function Name=exact_soln

 EQ ENERGY for TEMPERATURE on block_1 using Q1 with MASS DIFF SRC
```

```
 Source For ENERGY on block_1 = Encore_Scalar_Function Name=exact_src

    Output Number of TimeSteps

 Evaluate Postprocessor l2
 Evaluate Postprocessor l2_dot
 Evaluate Postprocessor h1
 Evaluate Postprocessor linf

 BEGIN RESULTS OUTPUT LABEL diffusion output
    database Name = aria_2nd_ord_fixed_h{N}.e
    at step 0, increment = 1
    # time interval is 1.0
    title Aria cube test
    nodal variables = nonlinear_solution->TEMPERATURE as T
    nodal variables = time_derivative_at_time->TEMPERATURE as TDOT
 END RESULTS OUTPUT LABEL diffusion output

      END ARIA REGION myRegion

   END PROCEDURE myAriaProcedure

END SIERRA myJob
```

12.5.1.4. Second Order Adaptive

```
BEGIN SIERRA myJob

   BEGIN ARIA MATERIAL Kryptonite
     Density              = Polynomial Variable=Temperature Order=1 C0=1 C1=0.1
     Thermal Conductivity = Polynomial Variable=Temperature Order=1 C0=1 C1=0.1
     Specific Heat        = Constant cp=1
     heat conduction      = basic
   END ARIA MATERIAL Kryptonite

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  DIRECT_SOLVER
      BEGIN SUPERLU SOLVER
      END
    END TPETRA EQUATION SOLVER
{else}
    Begin Trilinos Equation Solver Direct_Solver
      Solution Method = amesos-superlu
    End
{endif}

   BEGIN FINITE ELEMENT MODEL cube
      database name = square_h{N}_tri3.e
      coordinate system is cartesian

      BEGIN PARAMETERS FOR BLOCK block_1
 material Kryptonite
      END PARAMETERS FOR BLOCK block_1

   END FINITE ELEMENT MODEL cube

   Begin User Function exact_soln
     Load From File ./somefunc.so Using Function registerExactSoln
   End

   Begin User Function exact_soln_dot
     Load From File ./somefunc.so Using Function registerExactSolnDot
   End

   Begin User Function exact_src
     Load From File ./somefunc.so Using Function registerExactSrc
   End
```

```
  Begin Norm Postprocessor l2
    Use Function exact_soln
    Subtract Function nonlinear_solution->TEMPERATURE
    Compute Norms L2
  End

  Begin Norm Postprocessor l2_dot
    Use Function exact_soln_dot
    Subtract Function time_derivative_at_time->TEMPERATURE
    Compute Norms L2
  End

  Begin Norm Postprocessor h1
    Use Function exact_soln
    Subtract Function nonlinear_solution->TEMPERATURE
    Compute Norms H1
  End

  Begin Norm Postprocessor linf
    Use Function exact_soln
    Subtract Function nonlinear_solution->TEMPERATURE
    Compute Norms LInfinity
  End

  Begin Postprocessor Output Control pp_out
    Comment Character Is %
    Write To File errors_2nd_ord_adapt_h{N}.dat
    Floating Point Precision Is 4
    Floating Point Format Is Scientific
  End

  BEGIN PROCEDURE myAriaProcedure

     Begin Solution Control Description
 Use System Main
 Begin System Main
    Begin Transient The_Time_Block
       Advance myRegion
    End
       Simulation Start Time = 0
    Simulation Termination Time = 1
 End
Begin Parameters For Transient The_Time_Block
  Begin Parameters For Aria Region myRegion
     Initial Time Step Size = {0.1/2**N}
             Predictor-Corrector Tolerance = {1e-1/4**N}
             Maximum Time Step Size = {0.5/2**N}
     Time Integration Method = Second_Order
     Time Step Variation = adaptive
  End
End
     End

     BEGIN ARIA REGION myRegion

 Nonlinear Solution Strategy = Newton
        Maximum Nonlinear Iterations = 10
        Nonlinear Residual Tolerance = 1.0e-12
        Nonlinear Correction Tolerance = 1.0e-12
        Nonlinear Relaxation Factor  = 1.0
        use dof averaged nonlinear residual

 use finite element model cube
        Use Linear Solver Direct_Solver

        IC Encore Function on block_1 temperature = exact_soln
```

```
        BC dirichlet for Temperature at surface_1 = Encore_Function Name=exact_soln
        BC dirichlet for Temperature at surface_2 = Encore_Function Name=exact_soln
        BC dirichlet for Temperature at surface_3 = Encore_Function Name=exact_soln
        BC dirichlet for Temperature at surface_4 = Encore_Function Name=exact_soln

 EQ ENERGY for TEMPERATURE on block_1 using Q1 with MASS DIFF SRC

 Source For ENERGY on block_1 = Encore_Scalar_Function Name=exact_src

    Output Number of TimeSteps

 Evaluate Postprocessor l2
 Evaluate Postprocessor l2_dot
 Evaluate Postprocessor h1
 Evaluate Postprocessor linf

 BEGIN RESULTS OUTPUT LABEL diffusion output
    database Name = aria_2nd_ord_adapt_h{N}.e
    at step 0, increment = 1
    # time interval is 1.0
    title Aria cube test
    nodal variables = nonlinear_solution->TEMPERATURE as T
    nodal variables = time_derivative_at_time->TEMPERATURE as TDOT
 END RESULTS OUTPUT LABEL diffusion output

      END ARIA REGION myRegion

   END PROCEDURE myAriaProcedure

END SIERRA myJob
```

12.5.1.5. BDF2 Fixed

```
BEGIN SIERRA myJob

   BEGIN ARIA MATERIAL Kryptonite
     Density              = Polynomial Variable=Temperature Order=1 C0=1 C1=0.1
     Thermal Conductivity = Polynomial Variable=Temperature Order=1 C0=1 C1=0.1
     Specific Heat        = Constant cp=1
     heat conduction      = basic
   END ARIA MATERIAL Kryptonite

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  DIRECT_SOLVER
      BEGIN SUPERLU SOLVER
      END
    END TPETRA EQUATION SOLVER
{else}
    Begin Trilinos Equation Solver Direct_Solver
      Solution Method = amesos-superlu
    End
{endif}

   BEGIN FINITE ELEMENT MODEL cube
      database name = square_h{N}_tri3.e
      coordinate system is cartesian

      BEGIN PARAMETERS FOR BLOCK block_1
 material Kryptonite
      END PARAMETERS FOR BLOCK block_1

   END FINITE ELEMENT MODEL cube

   Begin User Function exact_soln
     Load From File ./somefunc.so Using Function registerExactSoln
   End
```

```
  Begin User Function exact_soln_dot
    Load From File ./somefunc.so Using Function registerExactSolnDot
  End

  Begin User Function exact_src
    Load From File ./somefunc.so Using Function registerExactSrc
  End

  Begin Norm Postprocessor l2
    Use Function exact_soln
    Subtract Function nonlinear_solution->TEMPERATURE
    Compute Norms L2
  End

  Begin Norm Postprocessor l2_dot
    Use Function exact_soln_dot
    Subtract Function time_derivative_at_time->TEMPERATURE
    Compute Norms L2
  End

  Begin Norm Postprocessor h1
    Use Function exact_soln
    Subtract Function nonlinear_solution->TEMPERATURE
    Compute Norms H1
  End

  Begin Norm Postprocessor linf
    Use Function exact_soln
    Subtract Function nonlinear_solution->TEMPERATURE
    Compute Norms LInfinity
  End

  Begin Postprocessor Output Control pp_out
    Comment Character Is %
    Write To File errors_bdf2_fixed_h{N}.dat
    Floating Point Precision Is 4
    Floating Point Format Is Scientific
  End

  BEGIN PROCEDURE myAriaProcedure

     Begin Solution Control Description
 Use System Main
 Begin System Main
    Begin Transient The_Time_Block
       Advance myRegion
    End
       Simulation Start Time = 0
    Simulation Termination Time = 1
 End
Begin Parameters For Transient The_Time_Block
  Begin Parameters For Aria Region myRegion
     Initial Time Step Size = {0.1/2**N}
     Time Integration Method = BDF2
     Time Step Variation = fixed
  End
End
     End

     BEGIN ARIA REGION myRegion

 Nonlinear Solution Strategy = Newton
        Maximum Nonlinear Iterations = 10
        Nonlinear Residual Tolerance = 1.0e-12
        Nonlinear Correction Tolerance = 1.0e-12
        Nonlinear Relaxation Factor  = 1.0
        use dof averaged nonlinear residual
```

```
 use finite element model cube
         Use Linear Solver Direct_Solver

         IC Encore Function on block_1 temperature = exact_soln

         BC dirichlet for Temperature at surface_1 = Encore_Function Name=exact_soln
         BC dirichlet for Temperature at surface_2 = Encore_Function Name=exact_soln
         BC dirichlet for Temperature at surface_3 = Encore_Function Name=exact_soln
         BC dirichlet for Temperature at surface_4 = Encore_Function Name=exact_soln

 EQ ENERGY for TEMPERATURE on block_1 using Q1 with MASS DIFF SRC

 Source For ENERGY on block_1 = Encore_Scalar_Function Name=exact_src

    Output Number of TimeSteps

 Evaluate Postprocessor l2
 Evaluate Postprocessor l2_dot
 Evaluate Postprocessor h1
 Evaluate Postprocessor linf

 BEGIN RESULTS OUTPUT LABEL diffusion output
    database Name = aria_bdf2_fixed_h{N}.e
    at step 0, increment = 1
    # time interval is 1.0
    title Aria cube test
    nodal variables = nonlinear_solution->TEMPERATURE as T
    nodal variables = time_derivative_at_time->TEMPERATURE as TDOT
 END RESULTS OUTPUT LABEL diffusion output

      END ARIA REGION myRegion

   END PROCEDURE myAriaProcedure

END SIERRA myJob
```

12.5.1.6. BDF2 Adaptive

```
BEGIN SIERRA myJob

   BEGIN ARIA MATERIAL Kryptonite
     Density              = Polynomial Variable=Temperature Order=1 C0=1 C1=0.1
     Thermal Conductivity = Polynomial Variable=Temperature Order=1 C0=1 C1=0.1
     Specific Heat        = Constant cp=1
     heat conduction      = basic
   END ARIA MATERIAL Kryptonite

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  DIRECT_SOLVER
      BEGIN SUPERLU SOLVER
      END
    END TPETRA EQUATION SOLVER
{else}
    Begin Trilinos Equation Solver Direct_Solver
      Solution Method = amesos-superlu
    End
{endif}

   BEGIN FINITE ELEMENT MODEL cube
      database name = square_h{N}_tri3.e
      coordinate system is cartesian

      BEGIN PARAMETERS FOR BLOCK block_1
 material Kryptonite
      END PARAMETERS FOR BLOCK block_1

   END FINITE ELEMENT MODEL cube
```

```
  Begin User Function exact_soln
    Load From File ./somefunc.so Using Function registerExactSoln
  End

  Begin User Function exact_soln_dot
    Load From File ./somefunc.so Using Function registerExactSolnDot
  End

  Begin User Function exact_src
    Load From File ./somefunc.so Using Function registerExactSrc
  End

  Begin Norm Postprocessor l2
    Use Function exact_soln
    Subtract Function nonlinear_solution->TEMPERATURE
    Compute Norms L2
  End

  Begin Norm Postprocessor l2_dot
    Use Function exact_soln_dot
    Subtract Function time_derivative_at_time->TEMPERATURE
    Compute Norms L2
  End

  Begin Norm Postprocessor h1
    Use Function exact_soln
    Subtract Function nonlinear_solution->TEMPERATURE
    Compute Norms H1
  End

  Begin Norm Postprocessor linf
    Use Function exact_soln
    Subtract Function nonlinear_solution->TEMPERATURE
    Compute Norms LInfinity
  End

  Begin Postprocessor Output Control pp_out
    Comment Character Is %
    Write To File errors_bdf2_adapt_h{N}.dat
    Floating Point Precision Is 4
    Floating Point Format Is Scientific
  End

  BEGIN PROCEDURE myAriaProcedure

     Begin Solution Control Description
 Use System Main
 Begin System Main
    Begin Transient The_Time_Block
       Advance myRegion
    End
       Simulation Start Time = 0
    Simulation Termination Time = 1
 End
Begin Parameters For Transient The_Time_Block
   Begin Parameters For Aria Region myRegion
      Initial Time Step Size = {0.1/2**N}
              Predictor-Corrector Tolerance = {1e-1/4**N}
              Maximum Time Step Size = {0.5/2**N}
      Time Integration Method = BDF2
      Time Step Variation = adaptive
   End
End
     End

     BEGIN ARIA REGION myRegion
```

```
 Nonlinear Solution Strategy = Newton
        Maximum Nonlinear Iterations = 10
        Nonlinear Residual Tolerance = 1.0e-12
        Nonlinear Correction Tolerance = 1.0e-12
        Nonlinear Relaxation Factor  = 1.0
        use dof averaged nonlinear residual

 use finite element model cube
        Use Linear Solver Direct_Solver

        IC Encore Function on block_1 temperature = exact_soln

        BC dirichlet for Temperature at surface_1 = Encore_Function Name=exact_soln
        BC dirichlet for Temperature at surface_2 = Encore_Function Name=exact_soln
        BC dirichlet for Temperature at surface_3 = Encore_Function Name=exact_soln
        BC dirichlet for Temperature at surface_4 = Encore_Function Name=exact_soln

 EQ ENERGY for TEMPERATURE on block_1 using Q1 with MASS DIFF SRC

 Source For ENERGY on block_1 = Encore_Scalar_Function Name=exact_src

    Output Number of TimeSteps

 Evaluate Postprocessor l2
 Evaluate Postprocessor l2_dot
 Evaluate Postprocessor h1
 Evaluate Postprocessor linf

 BEGIN RESULTS OUTPUT LABEL diffusion output
    database Name = aria_bdf2_adapt_h{N}.e
    at step 0, increment = 1
    # time interval is 1.0
    title Aria cube test
    nodal variables = nonlinear_solution->TEMPERATURE as T
    nodal variables = time_derivative_at_time->TEMPERATURE as TDOT
 END RESULTS OUTPUT LABEL diffusion output

      END ARIA REGION myRegion

   END PROCEDURE myAriaProcedure

END SIERRA myJob
```

12.6. ENCLOSURE RADIATION

12.6.1. 2D Cylindrical Shell Enclosure

```
BEGIN SIERRA Aria

Title Verification for two concentric spheres with radiation gap between them

Begin Global Constants
  Stefan Boltzmann constant = 5.6704E-8
End Global Constants

Begin Aria Material inner
       Heat conduction = Basic
       Density = constant rho = 1.0
       Specific heat = constant cp = 1.0
       Thermal conductivity = constant k = 2.0
End Aria Material inner

Begin Aria Material outer
       Heat conduction = Basic
       Density = constant rho = 1.0
       Specific heat = constant cp = 1.0
       Thermal conductivity = constant k = 0.35
End Aria Material outer

   Begin User Function exact_soln
     Load From File ./exact.so Using Function registerExactSoln
   End

   Begin Norm Postprocessor l2
     Use Function exact_soln
     Subtract Function nonlinear_solution->TEMPERATURE
     Compute Norms L2
   End

   Begin Norm Postprocessor h1
     Use Function exact_soln
     Subtract Function nonlinear_solution->TEMPERATURE
     Compute Norms H1
   End

   Begin Norm Postprocessor linf
     Use Function exact_soln
     Subtract Function nonlinear_solution->TEMPERATURE
     Compute Norms LInfinity
   End

   Begin Postprocessor Output Control pp_out
     Comment Character Is %
     Write To File errors{N}.dat
     Floating Point Precision Is 3
     Floating Point Format Is Scientific
   End

Begin Finite Element Model VERIFY_RAD_GAP
  Database name = input{N}.g
  Coordinate System = Cartesian
  Database Type = EXODUSII
  Begin Parameters for Block block_1
     Material inner
  End
  Begin Parameters for Block block_2
     Material outer
  End
End Finite Element Model VERIFY_RAD_GAP
```

```
{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  SOLVE_TEMPERATURE
      BEGIN CG SOLVER
        BEGIN JACOBI PRECONDITIONER
        END
        MAXIMUM ITERATIONS = 1000
        RESIDUAL SCALING = RHS
        CONVERGENCE TOLERANCE = 1.000000e-14
      END
    END TPETRA EQUATION SOLVER
{else}
    BEGIN Aztec Equation Solver solve_temperature
      Solution Method = cg
      Preconditioning Method = jacobi
      Maximum Iterations = 1000
      Residual Norm Tolerance = 1.0e-14
      Residual Norm Scaling = RHS
    END
{endif}

Begin Procedure myProcedure

  Begin Solution Control Description
    Use System Main
    Begin System Main
      Begin Sequential Steady
          Advance myRegion
      End
    End
  End

  Begin Aria Region myRegion

    Use Finite Element Model VERIFY_RAD_GAP
    Use Linear Solver solve_temperature

    Nonlinear Solution Strategy = Newton
    maximum nonlinear iterations = 1000
    nonlinear residual tolerance = 1.0e-10
    nonlinear relaxation factor = 1.0

    EQ energy for Temperature for all_volumes using Q1 with Diff
    IC const for all_volumes Temperature = 300.0
    BC const Dirichlet at surface_1 Temperature = 300.0
    BC const Dirichlet at surface_4 Temperature = 1300.0

    Output Number of Nodes
    Evaluate Postprocessor l2
    Evaluate Postprocessor linf
    Evaluate Postprocessor h1

    begin enclosure definition sph_shell
      add surface surface_2
      add surface surface_3
      blocking surfaces
      use viewfactor calculation vf_calc
      use viewfactor smoothing vf_smooth
      use radiosity solver rad_solver
#      enclosure id           = 1
      emissivity = 0.50 on surface_2
      emissivity = 0.80 on surface_3
    end enclosure definition sph_shell

    begin viewfactor calculation vf_calc
      bsp tree max depth = 0 and min list length = 25
      compute rule                = hemicube
      geometric tolerance         = 1.0E-6
```

```
      hemicube max subdivides     = 5
      hemicube min separation     = 5.0
      hemicube resolution         = 500
#      check rowsum with tolerance = .001
      output rule                 = verbose
    end viewfactor calculation vf_calc

    begin viewfactor smoothing vf_smooth
      convergence tolerance = 1.0E-10
      method                = least-squares
      weight power          = 2
      maximum iterations    = 150
      reciprocity rule      = average
      output rule           = verbose
    end viewfactor smoothing vf_smooth

    begin radiosity solver rad_solver
      coupling              = mason
      solver                = chaparral gmres
      convergence tolerance = 1.0E-8
      maximum iterations    = 800
      output rule           = verbose
    end radiosity solver rad_solver

    Begin Results Output Label diffusion output
      database name = output{N}.e
      at Step 0, increment = 1
      Nodal Variables = solution->temperature as TEMP
    End Results Output Label diffusion output

  End Aria Region myRegion

End Procedure myProcedure

END SIERRA Aria
```

12.6.2. 2D Annular Enclosure

```
BEGIN SIERRA Aria

Title Verification for two concentric spheres with radiation gap between them

Begin Global Constants
  Stefan Boltzmann constant = 5.6704E-8
End Global Constants

Begin Aria Material inner
  Heat conduction = Basic
  Thermal conductivity = constant k = 1.0
End Aria Material inner

Begin User Function exact_soln
  Load From File ./exact.so Using Function registerExactSoln
End

Begin User Function exact_src
  Load From File ./exact.so Using Function registerExactSrc
End

Begin User Function flux_surface_1
  Load From File ./exact.so Using Function registerExactFlux
End

Begin User Function exact_radiosity
  Load From File ./exact.so Using Function registerExactRadiosity
End
```

```
Begin User Function exact_irradiance
  Load From File ./exact.so Using Function registerExactIrradiance
End

Begin Field Function radiosity
  Use Edge Field radiosity As Value
End

Begin Field Function irradiance
  Use Edge Field irradiance As Value
End

Begin Field Function rad_flux
  Use Edge Field rad_flux As Value
End

Begin Norm Postprocessor l2
  Use Function exact_soln
  Subtract Function nonlinear_solution->TEMPERATURE
  Compute Norms L2
  Store In l2_err
End

Begin Norm Postprocessor h1
  Use Function exact_soln
  Subtract Function nonlinear_solution->TEMPERATURE
  Compute Norms H1
  Store In h1_err
End

Begin Norm Postprocessor linf
  Use Function exact_soln
  Subtract Function nonlinear_solution->TEMPERATURE
  Compute Norms LInfinity
  Store In linf_err
End

Begin Norm Postprocessor l2_radiosity
  Surfaces surface_1
  Use Function exact_radiosity
  Subtract Function radiosity
  Compute Norms L2
  Store In l2_radiosity_err
End

Begin Norm Postprocessor l2_irradiance
  Surfaces surface_1
  Use Function exact_irradiance
  Subtract Function irradiance
  Compute Norms L2
  Store In l2_irradiance_err
End

Begin Norm Postprocessor l2_heatflux
  Surfaces surface_1
  Use Function flux_surface_1
  Subtract Function rad_flux
  Compute Norms L2
  Store In l2_heatflux_err
End

Begin Postprocessor Output Control pp_out
  Comment Character Is %
  Write To File errors{N}.dat
  Floating Point Precision Is 3
  Floating Point Format Is Scientific
End
```

```
Begin Finite Element Model VERIFY_RAD_GAP
  Database name = annulus_crack_h{N}_tri3.e
  Coordinate System = Cartesian
  decomposition method = rcb
  Database Type = EXODUSII
  Begin Parameters for Block block_1
     Material inner
  End
End Finite Element Model VERIFY_RAD_GAP

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  SOLVE_TEMPERATURE
      BEGIN BICGSTAB SOLVER
        BEGIN JACOBI PRECONDITIONER
        END
        MAXIMUM ITERATIONS = 1000
        RESIDUAL SCALING = RHS
        CONVERGENCE TOLERANCE = 1.000000e-14
      END
    END TPETRA EQUATION SOLVER
{else}
    BEGIN Aztec Equation Solver solve_temperature
      Solution Method = bicgstab
      Preconditioning Method = jacobi
      Maximum Iterations = 1000
      Residual Norm Tolerance = 1.0e-14
      Residual Norm Scaling = RHS
    END
{endif}

Begin Procedure myProcedure

  Begin Solution Control Description
    Use System Main
    Begin System Main
      Begin Sequential Steady
          Advance myRegion
      End
    End
  End

  Begin Aria Region myRegion

    Use Finite Element Model VERIFY_RAD_GAP
    Use Linear Solver solve_temperature

    Nonlinear Solution Strategy = Newton
    maximum nonlinear iterations = 1000
    nonlinear residual tolerance = 1.0e-10
    nonlinear correction tolerance = 1.0e-10
    nonlinear relaxation factor = 1.0

    EQ energy for Temperature for all_volumes using Q1 with Diff Src
    IC const for all_volumes Temperature = 600.0

    Source For ENERGY on block_1 = Encore_Function Name=exact_src

    BC dirichlet for Temperature at surface_2 = Encore_Function Name=exact_soln
    BC dirichlet for Temperature at surface_3 = Encore_Function Name=exact_soln
    BC dirichlet for Temperature at surface_4 = Encore_Function Name=exact_soln

    Output Number of Nodes

    Evaluate Postprocessor l2
    Evaluate Postprocessor h1
    Evaluate Postprocessor linf
```

```
    Evaluate Postprocessor l2_radiosity
    Evaluate Postprocessor l2_irradiance
    #Evaluate Postprocessor l2_heatflux

    Interpolate Function Value of exact_soln Into Nodal Field Tex
    Interpolate Function Value of exact_src  Into Nodal Field Src

    Begin Results Output Label diffusion output
      database name = output{N}.e
      at Step 1, increment = 1
      Nodal Variables = solution->temperature as TEMP
      Nodal Variables = Tex linf_err Src
      Element Variables = l2_err h1_err TGrad linf_err
      edge variables = radiosity as J
      edge variables = rad_flux as q
      edge variables = irradiance as I
      edge variables = l2_radiosity_err
      edge variables = l2_irradiance_err
      edge variables = l2_heatflux_err
    End Results Output Label diffusion output

# TODO: remove this boundary condition
#    # DEBUG
#    BC dirichlet for Temperature at surface_1 = Encore_Function Name=exact_soln

# TODO: remove this boundary condition
#    # DEBUG
#     BC FLUX for Energy on surface_1  = Encore_Function Name=flux_surface_1


# TODO: un-comment the enclosure BC
    begin enclosure definition sph_shell
      add surface surface_1
      nonblocking surfaces
      use viewfactor calculation vf_calc_pairwise #vf_calc_hemicube #
      use viewfactor smoothing vf_smooth
      use radiosity solver rad_solver
      emissivity = 0.9 on surface_1
      Database Name is enc{N}.vf in pnetcdf format
      disable parallel redistribution
    end

    begin viewfactor calculation vf_calc_hemicube
      compute rule                = hemicube
      geometric tolerance         = {0.5*0.5**N}
      hemicube max subdivides     = {2*(2**N)}
      hemicube min separation     = 5.0
      hemicube resolution         = {100*(2**N)}
      output rule                 = verbose
    end

    begin viewfactor calculation vf_calc_pairwise
      compute rule                = pairwise
      geometric tolerance         = {0.5*0.5**N}
      output rule                 = verbose
      Pairwise Monte Carlo Sample Rule = Halton
      Pairwise Monte Carlo Tol1 = 1e-5
      Pairwise Monte Carlo Tol2 = 1e-5
      Pairwise Number Of Visibility Samples = 1
      Pairwise Visibility Sample Rule = Uniform
    end

    begin viewfactor smoothing vf_smooth
      convergence tolerance = 1.0E-10
      method                = least-squares
      weight power          = 2
      maximum iterations    = {150*(2**N)}
      reciprocity rule      = average
```

```
      output rule           = verbose
    end viewfactor smoothing vf_smooth

    begin radiosity solver rad_solver
      coupling              = mason
      solver                = chaparral gmres
      convergence tolerance = 1.0E-11
      maximum iterations    = {150*(2**N)}
      output rule           = none
    end radiosity solver rad_solver

  End Aria Region myRegion

End Procedure myProcedure

END SIERRA Aria
```

12.6.3. 3D Spherical Shell Enclosure

12.6.4. 3D Spherical Shell Partial Enclosure

```
BEGIN SIERRA Aria

Title Verification for two concentric spheres with radiation gap between them

load user plugin file ./exact.so

Begin Global Constants
  Stefan Boltzmann constant = 5.6704E-8
End Global Constants

Begin Aria Material inner
       Heat conduction = Basic
       Density = constant rho = 1.0
       Specific heat = constant cp = 1.0
       Thermal conductivity = constant k = 2.0
       emissivity = constant e = 0.50
End Aria Material inner

Begin Aria Material outer
       Heat conduction = Basic
       Density = constant rho = 1.0
       Specific heat = constant cp = 1.0
       Thermal conductivity = constant k = 0.35
       emissivity = constant e = 0.80
End Aria Material outer

   Begin User Function exact_soln
     Load From File ./exact.so Using Function registerExactSoln
   End

   Begin Norm Postprocessor l2
     Use Function exact_soln
     Volumes block_1 block_2
     Subtract Function nonlinear_solution->TEMPERATURE
     Compute Norms L2
     Store In l2_err
   End

   Begin Norm Postprocessor h1
     Use Function exact_soln
     Volumes block_1 block_2
     Subtract Function nonlinear_solution->TEMPERATURE
     Compute Norms H1
```

```
      Store In h1_err
    End

    Begin Norm Postprocessor linf
      Use Function exact_soln
      Volumes block_1 block_2
      Subtract Function nonlinear_solution->TEMPERATURE
      Compute Norms LInfinity
      Store In linf_err
    End

    Begin Postprocessor Output Control pp_out
      Comment Character Is %
      Write To File errors{N}.dat
      Floating Point Precision Is 3
      Floating Point Format Is Scientific
    End

  BEGIN Field Function numerical_solution
    USE NODAL FIELD solution->TEMPERATURE
  END Field Function numerical_solution

  BEGIN Difference Function temp_error
    Difference is exact_soln - numerical_solution
  END Difference Function temp_error

Begin Finite Element Model VERIFY_RAD_GAP
  Database name = sphere_cutout_h{N}.g
  Coordinate System = Cartesian
  Database Type = EXODUSII
  Begin Parameters for Block block_1
     Material inner
  End
  Begin Parameters for Block block_2
     Material outer
  End
End Finite Element Model VERIFY_RAD_GAP

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  SOLVE_TEMPERATURE
      BEGIN CG SOLVER
        BEGIN JACOBI PRECONDITIONER
        END
        MAXIMUM ITERATIONS = 1000
        RESIDUAL SCALING = RHS
        CONVERGENCE TOLERANCE = 1.000000e-10
      END
    END TPETRA EQUATION SOLVER
{else}
    BEGIN Aztec Equation Solver solve_temperature
      Solution Method = cg
      Preconditioning Method = jacobi
      Maximum Iterations = 1000
      Residual Norm Tolerance = 1.0e-10
      Residual Norm Scaling = RHS
    END
{endif}

Begin Procedure myProcedure

  Begin Solution Control Description
    Use System Main
    Begin System Main
      Begin Sequential Steady
          Advance myRegion
      End
    End
  End
```

```
  Begin Aria Region myRegion

    Use Finite Element Model VERIFY_RAD_GAP
    Use Linear Solver solve_temperature

    Nonlinear Solution Strategy = Newton
    maximum nonlinear iterations = 1000
    nonlinear residual tolerance = 1.0e-8
    nonlinear correction tolerance = 1.0e-8
    nonlinear relaxation factor = 1.0

    EQ energy for Temperature for all_volumes using Q1 with Diff
    IC const for all_volumes Temperature = 300.0
    BC const Dirichlet at surface_1 Temperature = 300.0
    BC const Dirichlet at surface_4 Temperature = 1300.0
    BC Dirichlet for Temperature on surface_5 = encore_function name=exact_soln

    Output Number of Nodes

    Evaluate Postprocessor l2
    Evaluate Postprocessor linf
    Evaluate Postprocessor h1

    interpolate function value of exact_soln into nodal field analytic_temp on volumes block_1 block_2
    Interpolate Function Value of temp_error into nodal field temp_error on volumes block_1 block_2

    begin enclosure definition sph_shell
      add surface surface_2
      add surface surface_3
      blocking surfaces
      use viewfactor calculation vf_calc
      use viewfactor smoothing vf_smooth
      use radiosity solver rad_solver
      emissivity = 0.50 on surface_2
      emissivity = 0.80 on surface_3
      Partial Enclosure Emissivity = 0.8
      Partial Enclosure Area = {2.0*PI*0.03*(0.03-0.025)}
      Partial Enclosure Temperature = 1035.02
    end enclosure definition sph_shell

    begin viewfactor calculation vf_calc
      bsp tree max depth = 0 and min list length = 25
      compute rule                = hemicube
      geometric tolerance         = 1.0E-10
      hemicube max subdivides     = 5
      hemicube min separation     = 5.0
      hemicube resolution         = 500
#      check rowsum with tolerance = .001
      output rule                 = verbose
    end viewfactor calculation vf_calc

    begin viewfactor smoothing vf_smooth
      method                = none
    end viewfactor smoothing vf_smooth

    begin radiosity solver rad_solver
      coupling              = mason
      solver                = chaparral gmres
      convergence tolerance = 1.0E-9
      maximum iterations    = 80
      output rule           = summary
    end radiosity solver rad_solver

    Begin Results Output Label diffusion output
      database name = output{N}.e
      at Step 0, increment = 1
      Nodal Variables = solution->temperature as T
```

```
      nodal variables = analytic_temp
      nodal variables = temp_error
      element variables = h1_err l2_err linf_err
    End Results Output Label diffusion output

  End Aria Region myRegion

End Procedure myProcedure

END SIERRA Aria
```

12.6.5. Fully 2D Enclosure Radiation

```
BEGIN SIERRA Aria

Title Verification for two concentric spheres with radiation gap between them

Begin Global Constants
  Stefan Boltzmann constant = 5.6704E-8
End Global Constants

Begin Aria Material inner
  Heat conduction = Basic
  Thermal conductivity = constant k = 1.0
End Aria Material inner

Begin User Function exact_soln
  Load From File ./exact.so Using Function registerExactSoln
End

Begin User Function exact_src
  Load From File ./exact.so Using Function registerExactSrc
End

Begin User Function flux_surface_1
  Load From File ./exact.so Using Function registerExactFlux
End

Begin User Function exact_radiosity
  Load From File ./exact.so Using Function registerExactRadiosity
End

Begin User Function exact_irradiance
  Load From File ./exact.so Using Function registerExactIrradiance
End

Begin Field Function radiosity
  Use Edge Field radiosity As Value
End

Begin Field Function irradiance
  Use Edge Field irradiance As Value
End

Begin Field Function rad_flux
  Use Edge Field rad_flux As Value
End

Begin Norm Postprocessor l2
  Use Function exact_soln
  Subtract Function nonlinear_solution->TEMPERATURE
  Compute Norms L2
  Store In l2_err
End

Begin Norm Postprocessor h1
```

```
  Use Function exact_soln
  Subtract Function nonlinear_solution->TEMPERATURE
  Compute Norms H1
  Store In h1_err
End

Begin Norm Postprocessor linf
  Use Function exact_soln
  Subtract Function nonlinear_solution->TEMPERATURE
  Compute Norms LInfinity
  Store In linf_err
End

Begin Norm Postprocessor l2_radiosity
  Surfaces surface_1
  Use Function exact_radiosity
  Subtract Function radiosity
  Compute Norms L2
  Store In l2_radiosity_err
End

Begin Norm Postprocessor l2_irradiance
  Surfaces surface_1
  Use Function exact_irradiance
  Subtract Function irradiance
  Compute Norms L2
  Store In l2_irradiance_err
End

Begin Norm Postprocessor l2_heatflux
  Surfaces surface_1
  Use Function flux_surface_1
  Subtract Function rad_flux
  Compute Norms L2
  Store In l2_heatflux_err
End

Begin Postprocessor Output Control pp_out
  Comment Character Is %
  Write To File errors{N}.dat
  Floating Point Precision Is 3
  Floating Point Format Is Scientific
End

Begin Finite Element Model VERIFY_RAD_GAP
  Database name = annulus_crack_h{N}_tri3.e
  Coordinate System = Cartesian
  decomposition method = rcb
  Database Type = EXODUSII
  Begin Parameters for Block block_1
     Material inner
  End
End Finite Element Model VERIFY_RAD_GAP

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  SOLVE_TEMPERATURE
      BEGIN BICGSTAB SOLVER
        BEGIN JACOBI PRECONDITIONER
        END
        MAXIMUM ITERATIONS = 1000
        RESIDUAL SCALING = RHS
        CONVERGENCE TOLERANCE = 1.000000e-14
      END
    END TPETRA EQUATION SOLVER
{else}
    BEGIN Aztec Equation Solver solve_temperature
      Solution Method = bicgstab
      Preconditioning Method = jacobi
```

```
      Maximum Iterations = 1000
      Residual Norm Tolerance = 1.0e-14
      Residual Norm Scaling = RHS
    END
{endif}

Begin Procedure myProcedure

  Begin Solution Control Description
    Use System Main
    Begin System Main
      Begin Sequential Steady
          Advance myRegion
      End
    End
  End

  Begin Aria Region myRegion

    Use Finite Element Model VERIFY_RAD_GAP
    Use Linear Solver solve_temperature

    Nonlinear Solution Strategy = Newton
    maximum nonlinear iterations = 1000
    nonlinear residual tolerance = 1.0e-10
    nonlinear correction tolerance = 1.0e-10
    nonlinear relaxation factor = 1.0

    EQ energy for Temperature for all_volumes using Q1 with Diff Src
    IC const for all_volumes Temperature = 600.0

    Source For ENERGY on block_1 = Encore_Function Name=exact_src

    BC dirichlet for Temperature at surface_2 = Encore_Function Name=exact_soln
    BC dirichlet for Temperature at surface_3 = Encore_Function Name=exact_soln
    BC dirichlet for Temperature at surface_4 = Encore_Function Name=exact_soln

    Output Number of Nodes

    Evaluate Postprocessor l2
    Evaluate Postprocessor h1
    Evaluate Postprocessor linf

    Evaluate Postprocessor l2_radiosity
    Evaluate Postprocessor l2_irradiance
    #Evaluate Postprocessor l2_heatflux

    Interpolate Function Value of exact_soln Into Nodal Field Tex
    Interpolate Function Value of exact_src  Into Nodal Field Src

    Begin Results Output Label diffusion output
      database name = output{N}.e
      at Step 1, increment = 1
      Nodal Variables = solution->temperature as TEMP
      Nodal Variables = Tex linf_err Src
      Element Variables = l2_err h1_err TGrad linf_err
      edge variables = radiosity as J
      edge variables = rad_flux as q
      edge variables = irradiance as I
      edge variables = l2_radiosity_err
      edge variables = l2_irradiance_err
      edge variables = l2_heatflux_err
    End Results Output Label diffusion output

# TODO: remove this boundary condition
#    # DEBUG
#    BC dirichlet for Temperature at surface_1 = Encore_Function Name=exact_soln
```

```
# TODO: remove this boundary condition
#    # DEBUG
#     BC FLUX for Energy on surface_1  = Encore_Function Name=flux_surface_1


# TODO: un-comment the enclosure BC
    begin enclosure definition sph_shell
      add surface surface_1
      nonblocking surfaces
      use viewfactor calculation vf_calc_pairwise #vf_calc_hemicube #
      use viewfactor smoothing vf_smooth
      use radiosity solver rad_solver
      emissivity = 0.9 on surface_1
      Database Name is enc{N}.vf in pnetcdf format
      disable parallel redistribution
    end

    begin viewfactor calculation vf_calc_hemicube
      compute rule               = hemicube
      geometric tolerance        = {0.5*0.5**N}
      hemicube max subdivides    = {2*(2**N)}
      hemicube min separation    = 5.0
      hemicube resolution        = {100*(2**N)}
      output rule                = verbose
    end

    begin viewfactor calculation vf_calc_pairwise
      compute rule               = pairwise
      geometric tolerance        = {0.5*0.5**N}
      output rule                = verbose
      Pairwise Monte Carlo Sample Rule = Halton
      Pairwise Monte Carlo Tol1 = 1e-5
      Pairwise Monte Carlo Tol2 = 1e-5
      Pairwise Number Of Visibility Samples = 1
      Pairwise Visibility Sample Rule = Uniform
    end

    begin viewfactor smoothing vf_smooth
      convergence tolerance = 1.0E-10
      method                = least-squares
      weight power          = 2
      maximum iterations    = {150*(2**N)}
      reciprocity rule      = average
      output rule           = verbose
    end viewfactor smoothing vf_smooth

    begin radiosity solver rad_solver
      coupling              = mason
      solver                = chaparral gmres
      convergence tolerance = 1.0E-11
      maximum iterations    = {150*(2**N)}
      output rule           = none
    end radiosity solver rad_solver

  End Aria Region myRegion

End Procedure myProcedure

END SIERRA Aria
```

12.7. CHEMISTRY

12.7.1. First Order Reaction (Uniform Temperature)

12.7.2. First Order Reaction (Spatially Varying Temperature)

```
BEGIN SIERRA Aria

  Title Verification Problem for Coupled Chemistry Diffusion

  load user plugin file ./Exact_solution.so

  Begin Field Function species
     Use Quadrature Field species
     Integration Order Is 2
     Dimension Is 2
  End

  Begin User Function ufuncAB
     Load From File ./Exact_solution.so Using Function registerExactSolnAB
  End

  Begin User Function ufuncT
     Load From File ./Exact_solution.so Using Function registerExactSolnT
  End

  Begin User Function exact_src
     Load From File ./Exact_solution.so Using Function registerExactSrc
  End

  Begin Postprocessor Output Control pp_out
    Comment Character is %
    Write To File errors{N}.dat
  End

  BEGIN Aria MATERIAL hmx
    density = constant  rho = 1
    specific heat = constant  cp = 1
    heat conduction = basic
    thermal conductivity = constant  k = 1
    begin parameters for chemeq model hmx

      number of reactions = 1

      species names are A B
      species phases are Condensed GAS

      Condensed Fraction = 0.0
      Steric Coefficients are 0.0
      Log Preexponential Factors are 5
      Activation Energies are 1000.0
      Energy Releases are 0 # insure temperature stays const

      Concentration Exponents for A are 1.0
      Concentration Exponents for B are 0.0


      Stoichiometric coefficients for A are -1.0
      Stoichiometric coefficients for B are 1.0

    end parameters for chemeq model hmx

  end Aria MATERIAL hmx

  BEGIN GLOBAL CONSTANTS
```

```
    Ideal Gas Constant = 1.9872 #CGS_cal
  END GLOBAL CONSTANTS

  BEGIN FINITE ELEMENT MODEL block
    Database Name = input{N}.g
    decomposition method = rcb
    Use material hmx for block_1
  END FINITE ELEMENT MODEL block

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  SOLVE_TEMPERATURE
      BEGIN CG SOLVER
        BEGIN JACOBI PRECONDITIONER
        END
        MAXIMUM ITERATIONS = 1000
        RESIDUAL SCALING = NONE
        CONVERGENCE TOLERANCE = 1.000000e-12
      END
    END TPETRA EQUATION SOLVER
{else}
    BEGIN AZTEC EQUATION SOLVER solve_temperature
      solution method = cg
      preconditioning method = jacobi
      maximum iterations = 1000
      residual norm scaling = NONE
      residual norm tolerance = 1.0E-12
    END AZTEC EQUATION SOLVER solve_temperature
{endif}


  BEGIN procedure myProcedure

  begin solution control description
    Use System Main
    Begin System Main
      Simulation Start Time       = 0.0
      Simulation Termination Time = 0.04
      Begin Transient time_block
        advance myregion
      End Transient time_block
    End System Main

      BEGIN parameters for transient time_block
        start time = 0.0
        termination time = 0.04

        BEGIN PARAMETERS FOR Aria REGION myRegion
          time step variation = fixed
          time integration method = second_order
          initial time step size = {0.01*0.5**(N-1)}
        END PARAMETERS FOR Aria REGION myRegion

     END parameters for transient time_block

  end solution control description

    begin aria region myRegion

    Output Number Of Nodes
    Compute Difference L2        Of ufuncAB species
    Compute Difference L2        Of ufuncT solution->temperature

    Interpolate Function Value of ufuncAB Into Element Field AEX

    EQ energy for temperature on all_blocks using Q1 with diff mass src

    Source for Energy on block_1 = chemeq_heating MODEL = hmx
    Source For ENERGY on block_1 = Encore_Function Name=exact_src
```

```
    BC const dirichlet at surface_1 Temperature = 400.0

    IC Encore Function on block_1 temperature = ufuncT

    maximum nonlinear iterations = 10
    nonlinear residual tolerance = 1.0E-10
    nonlinear correction tolerance = 1.0E-10
    Nonlinear Relaxation Factor = 1.

    BEGIN CHEMEQ SOLVER FOR hmx
      ODE SOLVER = CVODE ADAMS 12 FUNCTIONAL
      Absolute Tolerance = 1e-14
      Relative Tolerance = 1e-10
      Chemistry step multiplier = 100 # default
      Epsilon Min = 0.0001 # default
      Epsilon Max = 10.0 # default
      Minimum Chemistry Timestep = 1.0E-15 # default
      Percentage Asymptotics = 0.0 # default
      Asymptotic tolerance = 100.0 # default
      Minimum Concentration for A = 1.0E-12 # default
      Activation Temperature = 100.0
      Deactivation Temperature = 500.0 Continue
      species A = 1.0
      species B = 0.0
   END CHEMEQ SOLVER FOR hmx

     BEGIN RESULTS OUTPUT LABEL diffusion output
       database Name = output{N}.e
       At Step 0, Increment = {2**(N)}
       Timestep Adjustment Interval = 1
       Title Aria Chem/Diffusion Verification
       Nodal Variables = solution->temperature as T
       Element Variables = A B AEX species
     END RESULTS OUTPUT LABEL diffusion output

     USE FINITE ELEMENT MODEL block
     usE LINEAR SOLVER solve_temperature

    END Aria REGION myRegion

  END procedure myProcedure

END SIERRA Aria
```

12.7.3. First Order Reaction

```
BEGIN SIERRA Aria

  Title Verification Problem for Coupled Chemistry Diffusion

  load user plugin file ./Exact_solution.so

  Begin Field Function species
     Use Quadrature Field species
     Integration Order Is 2
     Dimension Is 2
  End

  Begin User Function ufuncAB
     Load From File ./Exact_solution.so Using Function registerExactSolnAB
  End

  Begin User Function ufuncT
     Load From File ./Exact_solution.so Using Function registerExactSolnT
  End
```

```
Begin User Function energySrc
   Load From File ./Exact_solution.so Using Function registerEnergySrc
End

Begin Norm Postprocessor L2_AB
   Use Function ufuncAB
   Subtract Function species
   Compute Norms L2
End

Begin Norm Postprocessor L2_T
   Use Function ufuncT
   Subtract Function solution->temperature
   Compute Norms L2
End

Begin Norm Postprocessor LInf_T
   Use Function ufuncT
   Subtract Function solution->temperature
   Compute Norms LInfinity
End

Begin Norm Postprocessor H1_T
   Use Function ufuncT
   Subtract Function solution->temperature
   Compute Norms H1
End

Begin Postprocessor Output Control pp_out
  Comment Character is %
  Write To File error{N}.txt
End

BEGIN Aria MATERIAL hmx
  density = constant  rho = 1
  specific heat = constant  cp = 1
  heat conduction = basic
  thermal conductivity = constant  k = 1
  begin parameters for chemeq model hmx

    number of reactions = 1

    species names are A B
    species phases are Condensed GAS

    Condensed Fraction = 0.0
    Steric Coefficients are 0.0
    Log Preexponential Factors are 5
    Activation Energies are 1000.0
    Energy Releases are -20.0

    Concentration Exponents for A are 1.0
    Concentration Exponents for B are 0.0


    Stoichiometric coefficients for A are -1.0
    Stoichiometric coefficients for B are 1.0

  end parameters for chemeq model hmx

end Aria MATERIAL hmx

BEGIN GLOBAL CONSTANTS
  Ideal Gas Constant = 1.9872 #CGS_cal
END GLOBAL CONSTANTS

BEGIN FINITE ELEMENT MODEL block
```

```
    Database Name = grid{N}x.exo $ exodusii
    decomposition method = rib

    Use material hmx for block_1
  END FINITE ELEMENT MODEL block

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  SOLVE_TEMPERATURE
      BEGIN CG SOLVER
        BEGIN JACOBI PRECONDITIONER
        END
        MAXIMUM ITERATIONS = 1000
        RESIDUAL SCALING = NONE
        CONVERGENCE TOLERANCE = 1.000000e-06
      END
    END TPETRA EQUATION SOLVER
{else}
    BEGIN AZTEC EQUATION SOLVER solve_temperature
      solution method = cg
      preconditioning method = jacobi
      maximum iterations = 1000
      residual norm scaling = NONE
      residual norm tolerance = 1.0E-6
    END AZTEC EQUATION SOLVER solve_temperature
{endif}

  BEGIN procedure myProcedure

  begin solution control description
    Use System Main
    Begin System Main
      Simulation Start Time       = 0.0
      Simulation Termination Time = 0.04
      Begin Transient time_block
        advance myregion
      End Transient time_block
    End System Main

      BEGIN parameters for transient time_block
        start time = 0.0
        termination time = 0.04

        BEGIN PARAMETERS FOR Aria REGION myRegion
          time step variation = fixed
          time integration method = second_order
          initial time step size = {0.001*0.5**(N-1)}
        END PARAMETERS FOR Aria REGION myRegion

     END parameters for transient time_block

  end solution control description

    begin aria region myRegion

    Output Number Of Elements

    Evaluate Postprocessor L2_AB
    Evaluate Postprocessor L2_T
    Evaluate Postprocessor LInf_T
    Evaluate Postprocessor H1_T

    EQ energy for temperature on all_blocks using Q1 with diff mass src

    Source for Energy on all_blocks = chemeq_heating MODEL = hmx

    use data block region_data

    maximum nonlinear iterations = 10
```

```
    nonlinear residual tolerance = 1.0E-10
    nonlinear correction tolerance = 1.0E-10
    Nonlinear Relaxation Factor = 1.

    BEGIN CHEMEQ SOLVER FOR hmx
#       Chemistry step multiplier = 10.0
#       Epsilon Min =  0.0001
#       Epsilon Max =  10.0
#       Minimum Chemistry Timestep = 1.0E-15
#       Percentage Asymptotics = 0.0
#       Asymptotic tolerance = 100.0
      ODE SOLVER = CVODE ADAMS 12 FUNCTIONAL
      Absolute Tolerance = 1e-12
      Relative Tolerance = 1e-9
      Minimum Concentration for A = 1.0E-08
      Activation Temperature = 0.0
       species A = 1.0
       species B = 0.0
    END CHEMEQ SOLVER FOR hmx

    BEGIN RESULTS OUTPUT LABEL diffusion output
       database Name = output{N}.e
       At Step 0, Increment = {2**(N-1)}
       Timestep Adjustment Interval = 1
       Title Aria Chem/Diffusion Verification
       Nodal Variables = solution->temperature as T
       Element Variables = A B species
    END RESULTS OUTPUT LABEL diffusion output

    IC Encore Function on block_1 temperature = ufuncT

    BC dirichlet for Temperature at surface_1 = Encore_Function Name=ufuncT

    Source For ENERGY on block_1 = Encore_Function Name=energySrc

    USE FINITE ELEMENT MODEL block
    usE LINEAR SOLVER solve_temperature

    END Aria REGION myRegion

  END procedure myProcedure

END SIERRA Aria
```

12.7.4. DAE and Pressure Test

```
BEGIN SIERRA Aria

  Title Verification Problem for Coupled Chemistry Diffusion

  load user plugin file ./Exact_solution.so

  Begin Field Function species
     Use Quadrature Field species
     Integration Order Is 2
     Dimension Is 1
  End

  Begin User Function ufuncA
     Load From File ./Exact_solution.so Using Function registerExactSolnA
  End

  Begin Norm Postprocessor L2_A
     Use Function ufuncA
     Subtract Function species
     Compute Norms L2
```

```
  End

  Begin Postprocessor Output Control pp_out
    Comment Character is %
    Write To File error.txt
  End

  BEGIN Aria MATERIAL hmx
    density = constant  rho = 1
    specific heat = constant  cp = 1
    heat conduction = basic
    thermal conductivity = constant  k = 1
    pressure = constant value=3

    begin parameters for chemeq model hmx
      number of reactions = 1

      species names are A
      species phases are Condensed

      Condensed Fraction = 0.0
      Steric Coefficients are 0.0
      Log Preexponential Factors are {log(5)}
      Activation Energies are 10.0
      Energy Releases are 0.0

      Concentration Exponents for A are 0.0

      Stoichiometric coefficients for A are -1.0

      # Pressure dependence
      Reference pressure = 2.
      Pressure exponents are 2.
      Pressure = From_Material_Definition

      #Distributed activation energy
      Activation energy st devs are 1.
      extent of reaction based on A

    end parameters for chemeq model hmx

  end Aria MATERIAL hmx

  BEGIN GLOBAL CONSTANTS
    Ideal Gas Constant = 1.
  END GLOBAL CONSTANTS

  BEGIN FINITE ELEMENT MODEL block
    Database Name = 1block.g
    decomposition method = rib

    Use material hmx for block_1
  END FINITE ELEMENT MODEL block

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  SOLVE_TEMPERATURE
      BEGIN CG SOLVER
        BEGIN JACOBI PRECONDITIONER
        END
        MAXIMUM ITERATIONS = 1000
        RESIDUAL SCALING = NONE
        CONVERGENCE TOLERANCE = 1.000000e-12
      END
    END TPETRA EQUATION SOLVER
{else}
    BEGIN AZTEC EQUATION SOLVER solve_temperature
      solution method = cg
      preconditioning method = jacobi
```

```
      maximum iterations = 1000
      residual norm scaling = NONE
      residual norm tolerance = 1.0E-12
    END AZTEC EQUATION SOLVER solve_temperature
{endif}

  BEGIN procedure myProcedure

  begin solution control description
    Use System Main
    Begin System Main
      Simulation Start Time       = 0.0
      Simulation Termination Time = 2.0
      Begin Transient time_block
        advance myregion
      End Transient time_block
    End System Main

      BEGIN parameters for transient time_block
        start time = 0.0
        termination time = 2.0

        BEGIN PARAMETERS FOR Aria REGION myRegion
          time step variation = fixed
          time integration method = second_order
          initial time step size = {0.01*0.5}
        END PARAMETERS FOR Aria REGION myRegion

     END parameters for transient time_block

  end solution control description

    begin aria region myRegion

    Evaluate Postprocessor L2_A

    EQ energy for temperature on all_blocks using Q1 with diff mass src
    Source for Energy on all_blocks = chemeq_heating MODEL = hmx
    IC for temperature on all_blocks = constant value=3

    maximum nonlinear iterations = 10
    nonlinear residual tolerance = 1.0E-10
    nonlinear correction tolerance = 1.0E-10
    Nonlinear Relaxation Factor = 1.

    BEGIN CHEMEQ SOLVER FOR hmx
      ODE SOLVER = CVODE ADAMS 12 FUNCTIONAL
      Absolute Tolerance = 1e-12
      Relative Tolerance = 1e-10
      Activation Temperature = 0.0
      species A = 1.0
    END CHEMEQ SOLVER FOR hmx

    Begin Postprocessor Group exact_soln
      Interpolate function value of ufuncA into nodal field exact_A
    End

    BEGIN RESULTS OUTPUT LABEL diffusion output
       database Name = output.e
       At Step 0, Increment = 1
       Timestep Adjustment Interval = 1
       Title Aria Chem/Diffusion Verification
       Nodal Variables = solution->temperature as T
       Nodal Variables = exact_A
       Element Variables = A
    END RESULTS OUTPUT LABEL diffusion output

    USE FINITE ELEMENT MODEL block
```

```
    usE LINEAR SOLVER solve_temperature

    END Aria REGION myRegion

  END procedure myProcedure

END SIERRA Aria
```

12.7.5. PMDI Plugin Test

```
{ECHO(OFF)}
{include("params_nom")}
{ECHO(OFF)}
{include("params")}

BEGIN SIERRA aria
Title PMDI_Plugin_Verification
load user plugin file pmdi_multspecies.so

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  SOLVE_TEMPERATURE
      BEGIN CG SOLVER
        BEGIN JACOBI PRECONDITIONER
        END
        MAXIMUM ITERATIONS = 10000
        RESIDUAL SCALING = NONE
        CONVERGENCE TOLERANCE = 1.000000e-08
      END
    END TPETRA EQUATION SOLVER
{else}
    BEGIN TRILINOS EQUATION SOLVER solve_temperature
      solution method = CG
      preconditioning method = jacobi
      maximum iterations = 10000
      residual norm tolerance = 1e-08
      residual norm scaling = NONE
    END TRILINOS EQUATION SOLVER solve_temperature
{endif}

  BEGIN GLOBAL CONSTANTS
    Stefan Boltzmann Constant = 5.67e-8 # W/m^2-K^4
    ideal gas constant = 8314.          # J/kgmol-K
  END GLOBAL CONSTANTS

    begin data block pmdi_data
    real data_real = (\# Variable  definition, units
      {to}           \# to        Initial gas temperature, K- necessary to calculate pressure for first timestep
      {vexOTvex}     \# vex/Tvex  Excess volume/temp excess volume, m^3/K
      {po}           \# po        Initial pressure, PA
      {rbo*uden_pmdi} \# rbo      Initial bulk density, kg/m^3
      {rco}          \# rco       Initial condensed density, kg/m^3
      {kb_1}         \# kb,       effectve cond. for Keff, W/mK (for20lb: 0.0486 0.706) radiation coefficient- 16/3/(a +sig s)
      {kb_2}         \# kb,       W/mK
      {t_1}          \# t,        K
      {t_2}          \# t,        K
      {rad_coef}     \#
      {ukb}          \#
      {ukrad}        \#
      {ukeff_pmdi}   \#
      {upress} )
    end data block pmdi_data

  BEGIN ARIA MATERIAL pmdifoam
    use data block pmdi_data
    Emissivity = constant e = {0.8*uemis_pmdi}
    density = constant rho = {rbo*uden_pmdi} #
```

```
  specific heat = constant cp = 1
  tensor thermal conductivity = calore_user_sub name = ktdirpu type = element_tensor # W/m-K

  Heat Conduction = generalized

  BEGIN PARAMETERS FOR CHEMEQ MODEL reaction_model
    number of reactions is 3
    species names are FOAMA FOAMB FOAMC CHAR CO2 LMWO HMWO
    species phases are Condensed Condensed Condensed Condensed Gas Condensed Condensed
    condensed fraction is 0.                       # Not used
    steric coefficients are 0. 0.  0.                 # Not used
    log preexponential factors are 0. 0. 0.  # Set these to 0 to prevent any reactions for the purpose of verification
    activation energies are {179441062.*uE1_pmdi} {179441062.*uE1_pmdi} {179441062.*uE1_pmdi} # J/kmol (e/R=21583 KENDATA)
    energy release units are per unit mass
    energy releases are 0 0  0     # J/Kg  no energy for first cut

    # Rxn-->1  2  # Mechanism
    concentration exponents for FOAMA ARE  1. 0. 0. # A -> CO2 --> 0.45 PMDIRPU -> 0.252 CO2 + 0.198 LMWO
    concentration exponents for FOAMB ARE  0. 1. 0. # B-> HMWO --> 0.15 PMDIRPU -> 0.15 HMWO
    concentration exponents for FOAMC ARE  0. 0. 1. # C-> HMWO --> 0.4  PMDIRPU -> 0.2 HMWO+0.2 char
    concentration exponents for CHAR ARE   0. 0. 0. # 20% CHAR FORMATION
    concentration exponents for CO2 ARE    0. 0. 0. #
    concentration exponents for LMWO ARE   0. 0. 0. #
    concentration exponents for HMWO ARE   0. 0. 0.

    stoichiometric coefficients for FOAMA ARE -1.0    0.0    0.0   # dA/dt = r1
    stoichiometric coefficients for FOAMB ARE  0.0   -1.0    0.0
    stoichiometric coefficients for FOAMC ARE  0.0    0.0   -1.0
    stoichiometric coefficients for CHAR ARE   0.0    0.0    0.5
    stoichiometric coefficients for CO2 ARE   +0.56    0.0    0.0 # dB/dt = 0.252/0.45 r1
    stoichiometric coefficients for LMWO ARE  +0.44    0.0    0.0 # dC/dt = 0.198/0.45 r1
    stoichiometric coefficients for HMWO ARE  +0.0   +1.0   +0.5 # dD/dt =  r2 + r3

    aux variable names are sf, phi, keff, frxn, krad   #, p, krad, kbulk
    aux variable subroutine is calcauxvar
  END PARAMETERS FOR CHEMEQ MODEL reaction_model
END ARIA MATERIAL pmdifoam

BEGIN FINITE ELEMENT MODEL FoamInCan
  database name is 1block.g
  Use Material pmdifoam for block_1
END FINITE ELEMENT MODEL FoamInCan

BEGIN PROCEDURE myProcedure

begin solution control description
  use system main
  begin system main
    simulation start time = 0.0
    simulation termination time = 1.0

    begin transient solution_block_1
      advance myRegion
    end transient solution_block_1
  end system main

  begin parameters for transient solution_block_1
    start time = 0.0
    begin parameters for aria region myRegion
      time step variation = fixed
      initial time step size = 0.1
    end parameters for aria region myRegion
  end
end solution control description

BEGIN ARIA REGION myRegion
  use finite element model FoamInCan Model Coordinates are model_coordinates
  use linear solver solve_temperature
```

```
    nonlinear solution strategy = newton
    maximum nonlinear iterations = 10
    nonlinear residual tolerance = 1.0e-8
    nonlinear relaxation factor  = 1.0
    use dof averaged nonlinear residual

    BEGIN CHEMEQ SOLVER FOR reaction_model
      ODE SOLVER = CVODE ADAMS 12 FUNCTIONAL
      absolute tolerance = 1e-12
      relative tolerance = 1e-9
#      aux variable names are sf, phi, rbulk, keff
      aux variable sf    = 1.0    # initial solid fraction value
      aux variable phi   = {phi}  # initial gas volume fraction
      aux variable keff  = 0. # initial effective thermal conductivity
      aux variable frxn = 1.0 # initial bulk density
      aux variable krad  = 0.0 # radcond
      species FOAMA = {1./7.}
      species FOAMB = {1./7.}
      species FOAMC = {1./7.}
      species CHAR  = {1./7.}
      species CO2   = {1./7.}
      species LMWO  = {1./7.}
      species HMWO  = {1./7.}
      minimum concentration for FOAMA = 1e-12
      minimum concentration for FOAMB = 1e-12
      minimum concentration for FOAMC = 1e-12
      chemistry step multiplier = 1E5
    END CHEMEQ SOLVER FOR reaction_model

    EQ ENERGY for TEMPERATURE on block_1 using Q1 with mass src
    Source for energy on block_1 = chemeq_heating model=reaction_model
    IC for temperature on block_1 = constant value={2*to}

#---------------------------------------
# User variable definition
#---------------------------------------
    Define Global Scalar gmasco2 as real operation sum initial value 0.0
    Define Global Scalar gmasn2 as real operation sum initial value 0.0
    Define Global Scalar gmaslowmw as real operation sum initial value 0.0
    Define Global Scalar gmashighmw as real operation sum initial value 0.0

    Define Global Scalar itv as real operation sum initial value 0.0
    Define Global Scalar gvtot as real operation sum initial value 0
    Define Global Scalar p as real operation min initial value 101325.0
    Define Global Scalar psig as real operation min initial value 0.0
    Define Global Scalar padmix as real operation min initial value 101325.0
    Define Global Scalar psigadmix as real operation min initial value 0.0
    Define Global Scalar mcvT as real operation sum initial value 0.0
    Define Global Scalar mcv as real operation min initial value 0.0
    Define Global Scalar gvol as real operation sum initial value 0.0

    Define Global Scalar psig1 as real operation min initial value 0.0
    Define Global Scalar psigadmix1 as real operation min initial value 0.0
    Define Global Scalar poc as real operation max initial value 0.0
    Define Global Scalar count as int  operation min initial value 0

    Define Global Scalar psigxuncert as real operation min initial value 0.0
    Define Global Scalar pxuncertsig as real operation min initial value 0.0

    Define Global Scalar molesn2 as real operation min initial value 0.0
    Define Global Scalar molesco2 as real operation min initial value 0.0

    Define Global Scalar moleslowmw as real operation min initial value 0.0
    Define Global Scalar moleshighmw as real operation min initial value 0.0
    Define Global Scalar molesofv as real operation min initial value 0.0
    Define Global Scalar molestotal as real operation min initial value 0.0
```

```
    BEGIN RESULTS OUTPUT output_1
      Database Name is %B.e
      Database Type is EXODUSII
      at step 0, increment is 1
      nodal variables = solution->temperature as temp
      nodal variables = solution->temperatureDot as TDOT
      element variables = Density as RHO
      element variables = FOAMA FOAMB FOAM C CO2 CHAR LMWO HMWO
      element variables = sf, phi, keff, frxn, krad
      global variables = p
      global variables = psig
    END RESULTS OUTPUT output_1

    END ARIA REGION myRegion
   END PROCEDURE myProcedure
END SIERRA aria
```

12.8. MISCELLANEOUS

12.8.1. Thermal Postprocessing

```
BEGIN SIERRA myJob

   BEGIN ARIA MATERIAL Kryptonite
      Density    = CONSTANT rho = 1
      Thermal Conductivity = Constant k   = 1
      Specific Heat    = Constant cp  = 1
      heat conduction     = basic
   END

   BEGIN ARIA MATERIAL Mathite
      Density    = CONSTANT rho = 1
      Thermal Conductivity = Constant k   = 1
      Specific Heat    = Constant cp  = 1
      heat conduction     = basic
   END

   Begin Global Constants
      Stefan Boltzmann Constant = 5.67e-8
   End

   Begin Aria Material surf_2_models
      BC Reference Temperature  = encore_function name = cf_Tref
      Heat Transfer Coefficient = constant h=10.0
   End

   Begin Aria Material surf_3_models
      BC Rad Reference Temperature = encore_function name = rf_Tref
      Emissivity                  = Constant E=0.6
      Radiation form factor        = Constant F=1.0
   End

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  SOLVE_TEMPERATURE
      BEGIN CG SOLVER
        BEGIN JACOBI PRECONDITIONER
        END
        MAXIMUM ITERATIONS = 1000
        RESIDUAL SCALING = R0
        CONVERGENCE TOLERANCE = 1.000000e-14
      END
    END TPETRA EQUATION SOLVER
{else}
    BEGIN AZTEC EQUATION SOLVER solve_temperature
      solution method = cg
      preconditioning method = jacobi
      maximum iterations = 1000
      residual norm scaling = r0
      residual norm tolerance = 1.0e-14
    END AZTEC EQUATION SOLVER solve_temperature
{endif}

   BEGIN FINITE ELEMENT MODEL cube
      database name = cube_two_blocks_hex8_h{N}.g
      coordinate system is cartesian

      # [0,1] x [-0.5,0.5] x [-0.5,0.5]
      BEGIN PARAMETERS FOR BLOCK block_1
 material Kryptonite
      END

      # [-1,0] x [-0.5,0.5] x [-0.5,0.5]
      BEGIN PARAMETERS FOR BLOCK block_2
```

```
material Mathite
     END

     Use Material surf_2_models for surface_2
     Use Material surf_3_models for surface_3

  END FINITE ELEMENT MODEL cube

  # specify text output for Encore PPs
  Begin Postprocessor Output Control pp_out
     Write to File encoreinfo{N}.txt
     Enable Small Output Rounding To Zero
     Floating Point Precision Is 10
  End

  Begin Global Function Parameters gfp
     Parameter T0 = 400 # [K]
     Parameter C0 = 2.0
     Parameter C1 = 3.0
     Parameter C2 = 4.0
     Parameter C3 = 0.4
     Parameter h = 10.0
     Parameter eps = 0.6
     Parameter sigma = 5.67e-8
  End

  Begin Field Function ffunc
     Use Nodal Field nonlinear_solution->TEMPERATURE
  End

  # exact solution
  Begin User Function ufunc
     Load From File ./somefunc.so Using Function registerExactSoln
  End

  Begin Difference Function dfunc
     Difference Is ufunc - ffunc
  End

  Begin User Function src
     Integration Order Is 4
     Load From File ./somefunc.so Using Function registerSrc
  End

  Begin User Function cf_Tref
     Integration Order Is 4
     Load From File ./somefunc.so Using Function registerConvHeatFlux_Tref
  End

  # exact convective flux
  Begin User Function cf_bc_exact
     Integration Order Is 4
     Load From File ./somefunc.so Using Function registerExactConvHeatFlux
  End

  Begin User Function rf_Tref
     Load From File ./somefunc.so Using Function registerRadFlux_Tref
  End

  # exact radiative flux
  Begin User Function rf_bc_exact
     Integration Order Is 4
     Load From File ./somefunc.so Using Function registerExactRadFlux
  End

  Begin Norm Postprocessor l2_error
    Use Function ufunc
    Subtract Function ffunc
```

```
  Compute Norm L2
End

Begin Integrate Function Postprocessor cf_bc_ipo_ex
   Use Function cf_bc_exact
   Surfaces surface_2
   Disable Output
End

Begin Integrate Function Postprocessor rf_bc_ipo_ex
   Use Function rf_bc_exact
   Surfaces surface_3
   Disable Output
End

Begin Average Value Postprocessor cf_bc_ifo_ex
   Use Function cf_bc_exact
   Surfaces surface_2
   Disable Output
End

Begin Average Value Postprocessor rf_bc_ifo_ex
   Use Function rf_bc_exact
   Surfaces surface_3
   Disable Output
End

Begin Integrate Function Postprocessor src_ipo_ex
   Use Function src
   Volumes block_1 block_2
   Disable Output
End

Begin Evaluate Function Postprocessor eval_b1
  Use Function ffunc
  Evaluate Value
  # random interior point in block_2
  Location  -0.151720462393008   0.146935733548329  -0.393641401879319
  parametric search tolerance 1.0e-10
End

Begin Evaluate Function Postprocessor eval_b1_ex
  Use Function ufunc
  Evaluate Value
  # random interior point in block_2
  Location  -0.151720462393008   0.146935733548329  -0.393641401879319
  Disable Output
End

Begin Evaluate Function Postprocessor eval_b1b2
  Use Function ffunc
  Evaluate Value
  # random interior point on block interface (x=0)
  Location  0 0.162595269728099  -0.377464159584852
  parametric search tolerance 1.0e-10
End

Begin Evaluate Function Postprocessor eval_b1b2_ex
  Use Function ufunc
  Evaluate Value
  # random interior point on block interface (x=0)
  Location  0 0.162595269728099  -0.377464159584852
  Disable Output
End

Begin Evaluate Function Postprocessor eval_s2
  Use Function ffunc
  Evaluate Value
```

```
    # random interior point on sideset 2 (z=0.5)
    Location -0.855758209426849 0.159603369582751 0.5
  End

  Begin Evaluate Function Postprocessor eval_s2_ex
    Use Function ufunc
    Evaluate Value
    # random interior point on sideset 2 (z=0.5)
    Location -0.855758209426849 0.159603369582751 0.5
    Disable Output
  End

  Begin Difference Postprocessor cf_bc_ipo_err
     Difference is cf_bc_ipo_ex - cf_bc_ipo
  End

  Begin Difference Postprocessor rf_bc_ipo_err
     Difference is rf_bc_ipo_ex - rf_bc_ipo
  End

  Begin Difference Postprocessor cf_bc_ifo_err
     Difference is cf_bc_ifo_ex - cf_bc_ifo
  End

  Begin Difference Postprocessor rf_bc_ifo_err
     Difference is rf_bc_ifo_ex - rf_bc_ifo
  End

  Begin Difference Postprocessor src_ipo_err
     Difference is src_ipo_ex - src_ipo
  End

  Begin Difference Postprocessor eval_b1_err
     Difference is eval_b1_ex - eval_b1
  End

  Begin Difference Postprocessor eval_b1b2_err
     Difference is eval_b1b2_ex - eval_b1b2
  End

  Begin Difference Postprocessor eval_s2_err
     Difference is eval_s2_ex - eval_s2
  End

  Begin Tabular Function Output Postprocessor tfo_sset2
     Use Functions model_coordinates ffunc ufunc dfunc
     Surfaces surface_2
     Write To File values_sset2_{N}.dat
  End

  BEGIN PROCEDURE myAriaProcedure

     Begin Solution Control Description
Use System Main
Begin System Main
      Begin Transient MySolveBlock
      Advance myRegion
           End
   Simulation Max Global Iterations = 1
   Simulation Start Time = 0
   Simulation Termination Time = 1
End
        Begin Parameters for Transient MySolveBlock
        End
     End

     BEGIN ARIA REGION myRegion
```

```
 use finite element model cube
 use linear solver solve_temperature

 nonlinear solution strategy = newton

 maximum nonlinear iterations = 10
 nonlinear residual tolerance = 1.0e-16
 nonlinear correction tolerance = 1.0e-12
 nonlinear relaxation factor  = 1.0
        use dof averaged nonlinear residual

 EQ ENERGY for TEMPERATURE on all_blocks using Q1 with DIFF SRC

        MESH GROUP Dirichlet_Surface = surface_4 surface_5 surface_6 surface_7
 BC Dirichlet for Temperature on Dirichlet_Surface = encore_function name=ufunc

        BC Flux for Energy on surface_2 = Generalized_Nat_Conv Power_Output=cf_bc_ipo Flux_Output=cf_bc_ifo

        BC Flux for Energy on surface_3 = Generalized_Rad Power_Output=rf_bc_ipo Flux_Output=rf_bc_ifo

        SOURCE for ENERGY on all_blocks = encore_function name=src Power_Output=src_ipo

        Evaluate Postprocessor eval_b1
        Evaluate Postprocessor eval_b1b2
        Evaluate Postprocessor eval_s2

        Evaluate Postprocessor tfo_sset2

        Begin Postprocessor Group zzz
          Output Number of Nodes

          Evaluate Postprocessor l2_error

          Evaluate Postprocessor cf_bc_ipo_ex
          Evaluate Postprocessor cf_bc_ipo_err

          Evaluate Postprocessor rf_bc_ipo_ex
          Evaluate Postprocessor rf_bc_ipo_err

          Evaluate Postprocessor cf_bc_ifo_ex
          Evaluate Postprocessor cf_bc_ifo_err

          Evaluate Postprocessor rf_bc_ifo_ex
          Evaluate Postprocessor rf_bc_ifo_err

          Evaluate Postprocessor src_ipo_ex
          Evaluate Postprocessor src_ipo_err

          Evaluate Postprocessor eval_b1_ex
          Evaluate Postprocessor eval_b1_err

          Evaluate Postprocessor eval_b1b2_ex
          Evaluate Postprocessor eval_b1b2_err

          Evaluate Postprocessor eval_s2_ex
          Evaluate Postprocessor eval_s2_err
        End

     END ARIA REGION myRegion

   END PROCEDURE myAriaProcedure

END SIERRA myJob
```

12.8.2. Postprocess Min/Max

```
BEGIN SIERRA myJob

   BEGIN ARIA MATERIAL Kryptonite
     Density              = constant rho=1
     Thermal Conductivity = constant k=1
     Specific Heat        = Constant cp=1
     heat conduction      = basic
   END ARIA MATERIAL Kryptonite

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  DIRECT_SOLVER
      BEGIN SUPERLU SOLVER
      END
    END TPETRA EQUATION SOLVER
{else}
    Begin Trilinos Equation Solver Direct_Solver
      Solution Method = amesos-superlu
    End
{endif}

   BEGIN FINITE ELEMENT MODEL cube
      database name = square_h{N}.e
      coordinate system is cartesian
      decomposition method = rib

      BEGIN PARAMETERS FOR BLOCK block_1
 material Kryptonite
      END PARAMETERS FOR BLOCK block_1

   END FINITE ELEMENT MODEL cube

   Begin String Function exact_soln
     Value Is "sin(7*x) * sin(8*y)"
     Gradient Is "7 * cos(7*x) * sin(8*y)" "8 * sin(7*x) * cos(8*y)"
   End

   Begin String Function exact_src
     Value Is "(49 + 64) * sin(7*x) * sin(8*y)"
   End

   Begin Field Function ffunc
      Use Nodal Field nonlinear_solution->TEMPERATURE
   End

   Begin Norm Postprocessor l2
     Use Function exact_soln
     Subtract Function ffunc
     Compute Norms L2
   End

   Begin Norm Postprocessor h1
     Use Function exact_soln
     Subtract Function ffunc
     Compute Norms H1
   End

   Begin Norm Postprocessor linf
     Use Function exact_soln
     Subtract Function ffunc
     Compute Norms LInfinity
   End

   Begin Min Max Postprocessor max_node_b1
     Use Function ffunc
     Compute Max
```

```
  Volumes block_1
End

Begin Min Max Postprocessor min_node_b1
  Use Function ffunc
  Compute Min
  Volumes block_1
End

Begin Min Max Postprocessor max_node_s2
  Use Function ffunc
  Compute Max
  Surfaces surface_2 # x=1
End

Begin Min Max Postprocessor min_node_s2
  Use Function ffunc
  Compute Min
  Surfaces surface_2 # x=1
End

# code used to compute exact errors in Min Max PP
Begin String Function sfunc_max_node_b1_ex
   Value Is "1.0"
End

Begin String Function sfunc_min_node_b1_ex
   Value Is "-1.0"
End

Begin String Function sfunc_max_node_s2_ex
   Value Is "sin(7)"
End

Begin String Function sfunc_min_node_s2_ex
   Value Is "-sin(7)"
End

Begin Evaluate Function Postprocessor max_node_b1_ex
  Use Function sfunc_max_node_b1_ex
  Location 0 0 0
End

Begin Evaluate Function Postprocessor min_node_b1_ex
  Use Function sfunc_min_node_b1_ex
  Location 0 0 0
End

Begin Evaluate Function Postprocessor max_node_s2_ex
  Use Function sfunc_max_node_s2_ex
  Location 0 0 0
End

Begin Evaluate Function Postprocessor min_node_s2_ex
  Use Function sfunc_min_node_s2_ex
  Location 0 0 0
End

Begin Difference Postprocessor max_node_b1_err
   Difference is max_node_b1_ex - max_node_b1
End

Begin Difference Postprocessor min_node_b1_err
   Difference is min_node_b1 - min_node_b1_ex
End

Begin Difference Postprocessor max_node_s2_err
   Difference is max_node_s2_ex - max_node_s2
```

```
    End

    Begin Difference Postprocessor min_node_s2_err
       Difference is min_node_s2 - min_node_s2_ex
    End
    # end code used to compute exact errors in Min Max PP

    Begin Postprocessor Output Control pp_out
      Comment Character Is %
      Write To File errors_h{N}.dat
      Floating Point Precision Is 8
      Floating Point Format Is Scientific
    End

    BEGIN PROCEDURE myAriaProcedure

       Begin Solution Control Description
  Use System Main
  Begin System Main
     Begin Sequential The_Time_Block
        Advance myRegion
     End
        Simulation Start Time = 0
     Simulation Termination Time = 1
  End
 Begin Parameters For Transient The_Time_Block
 End
       End

       BEGIN ARIA REGION myRegion

  Nonlinear Solution Strategy = Newton
          Maximum Nonlinear Iterations = 10
          Nonlinear Residual Tolerance = 1.0e-12
          Nonlinear Correction Tolerance = 1.0e-12
          Nonlinear Relaxation Factor  = 1.0
          use dof averaged nonlinear residual

  use finite element model cube
          Use Linear Solver Direct_Solver

          BC dirichlet for Temperature at surface_1 = Encore_Function Name=exact_soln
          BC dirichlet for Temperature at surface_2 = Encore_Function Name=exact_soln
          BC dirichlet for Temperature at surface_3 = Encore_Function Name=exact_soln
          BC dirichlet for Temperature at surface_4 = Encore_Function Name=exact_soln

  EQ ENERGY for TEMPERATURE on block_1 using Q1 with DIFF SRC

  Source For ENERGY on block_1 = Encore_Scalar_Function Name=exact_src

          Evaluate Postprocessor max_node_b1
          Evaluate Postprocessor min_node_b1

          Evaluate Postprocessor max_node_s2
          Evaluate Postprocessor min_node_s2

          Begin Postprocessor Group zzz
            Output Number of Nodes

    Evaluate Postprocessor l2
    Evaluate Postprocessor h1
        Evaluate Postprocessor linf

            Evaluate Postprocessor max_node_b1_err
            Evaluate Postprocessor min_node_b1_err
            Evaluate Postprocessor max_node_s2_err
            Evaluate Postprocessor min_node_s2_err
          End
```

```
        Begin Solution Options
  post process normalized temperature on surface_2 as t_s2
  post process normalized temperature on block_1 as t_b1
        End

 BEGIN RESULTS OUTPUT LABEL diffusion output
   database Name = aria_h{N}.e
   at step 0, increment = 1
   # time interval is 1.0
   title Aria cube test
   nodal variables = nonlinear_solution->TEMPERATURE as T
           global variables = t_s2 t_b1
 END RESULTS OUTPUT LABEL diffusion output

        Begin History Output blah
          database Name = aria_h{N}.hist
  at time 1 interval is 1
          Variable = global t_s2
          Variable = global t_b1
        End

     END ARIA REGION myRegion

  END PROCEDURE myAriaProcedure

END SIERRA myJob
```

12.8.3. Local Coordinates: Cartesian

```
# Aria input file heat condution in local
# coodinate system

BEGIN SIERRA MyProblem

  Begin User Function ufunc
    Load From File ./cartesian.so Using Function registerExactSolution
  End

  Begin Postprocessor Output Control pp_out
     Comment Character Is %
     Write To File errors{N}.dat
     Floating Point Precision Is 3
     Floating Point Format Is Scientific
  End

  load user plugin file ./cartesian.so
  load user plugin file ./cartesian.so
  load user plugin file ./cartesian.so

  begin data block region_data
#                  T0    T1    Kxx  Kyy Kzz  Lx  Ly  Lz theta1 theta2
    Real r_data = 400.0 100.0 10.0 1.0 1.0 1.0 1.0 1.0  45.0   22.5
  end data block region_data

  BEGIN LOCAL COORDINATE SYSTEM CS_Block
      TYPE   = Cartesian
      ORIGIN =  0.000000          0.000000          0.00000
      POINT  =  0.707106781186548 0.653281482438188 0.270598050073098
      VECTOR =  0                -0.382683432365090 0.923879532511287
  END

  BEGIN ARIA MATERIAL M_Block
    DENSITY = CONSTANT rho = 0.1
    TENSOR THERMAL CONDUCTIVITY = CONSTANT  XX=10.0 YY=1.0 ZZ=1.0
    SPECIFIC HEAT   = CONSTANT  CP = 0.5
```

```
    Heat Conduction             = Generalized
  END ARIA MATERIAL M_Block

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  LINEARSOLVER
      BEGIN GMRES SOLVER
        BEGIN JACOBI PRECONDITIONER
        END
        MAXIMUM ITERATIONS = 1000
        RESIDUAL SCALING = R0
        CONVERGENCE TOLERANCE = 1.000000e-12
      END
    END TPETRA EQUATION SOLVER
{else}
    BEGIN AZTEC EQUATION SOLVER LinearSolver
      SOLUTION METHOD = gmres
      PRECONDITIONING METHOD = jacobi
      MAXIMUM ITERATIONS = 1000
      RESIDUAL NORM TOLERANCE = 1.0e-12
      RESIDUAL NORM SCALING = r0
    END AZTEC EQUATION SOLVER LinearSolver
{endif}

  BEGIN FINITE ELEMENT MODEL FE_Block
    DATABASE NAME = cartesian{N}.g
    coordinate system is cartesian
    decomposition method = rcb

    BEGIN PARAMETERS FOR BLOCK block_1
      MATERIAL M_Block
      LOCAL COORDINATE SYSTEM = CS_Block
    END PARAMETERS FOR BLOCK block_1
  END

  BEGIN PROCEDURE MyProcedure

     Begin Solution Control Description
Use System Main
Begin System Main
   Begin Sequential MyBlock
      Advance Region_Block
   End
End
     End

    BEGIN ARIA REGION Region_Block
      nonlinear solution strategy    = newton
      use data block region_data

      Output Number of Nodes
      Compute Difference L2        Of ufunc solution->temperature Store In l2_error_norm2
      Compute Difference LInfinity Of ufunc solution->temperature Store In linf_error_norm

      NONLINEAR RESIDUAL TOLERANCE   = 1.0e-10
      NONLINEAR CORRECTION TOLERANCE = 1.0e-10
      MAXIMUM NONLINEAR ITERATIONS   = 10
      NONLINEAR RELAXATION FACTOR    = 1.0

      IC for temperature on block_1 = calore_user_sub name = localCoord_ic type=node

      BC dirichlet for temperature on surface_1 = calore_user_sub name = localCoord_bc type=node
      BC dirichlet for temperature on surface_2 = calore_user_sub name = localCoord_bc type=node
      BC dirichlet for temperature on surface_3 = calore_user_sub name = localCoord_bc type=node
      BC dirichlet for temperature on surface_4 = calore_user_sub name = localCoord_bc type=node
      BC dirichlet for temperature on surface_5 = calore_user_sub name = localCoord_bc type=node
      BC dirichlet for temperature on surface_6 = calore_user_sub name = localCoord_bc type=node

#      IC CONST ON block_1 Temperature = 0.0
```

```
#      # along z
#      BC Const Dirichlet on surface_1 Temperature = 100.0
#      BC Const Dirichlet on surface_2 Temperature = 0.0
#      # along y
#      BC Linear Dirichlet on surface_3 Temperature Coeff = 50. 0. -38.37 92.39
#      BC Linear Dirichlet on surface_5 Temperature Coeff = 50. 0. -38.37 92.39
#      # along x
#      BC Linear Dirichlet on surface_4 Temperature Coeff = 50. 0. -38.37 92.39
#      BC Linear Dirichlet on surface_6 Temperature Coeff = 50. 0. -38.37 92.39

      EQ ENERGY FOR TEMPERATURE ON block_1 USING Q1 WITH DIFF #SRC
      #SOURCE for Temperature on block_1 =

      Begin Volume Heating juan
        add volume block_1
        element subroutine = localCoord_vhs
      End

      USE FINITE ELEMENT MODEL FE_Block

      BEGIN RESULTS OUTPUT TemperatureOutput
        DATABASE NAME = output{N}.e
        AT STEP 1, INCREMENT = 1
        TITLE Aria Temperature in Local Coordinate System Verification Problem
        NODAL VARIABLES = solution->TEMPERATURE AS T
        Element Variables = l2_error_norm2 as l2error
        Element Variables = linf_error_norm as linf
      END RESULTS OUTPUT TemperatureOutput

      USE LINEAR SOLVER LinearSolver
    END

  END
END SIERRA MyProblem
```

12.8.4. Local Coordinates: Cylindrical

```
# Aria input file heat condution in local
# coodinate system

BEGIN SIERRA MyProblem

  Begin Field Function ffunc
    Use Nodal Field solution->temperature
  End

  Begin User Function ufunc
    Load From File ./cylindrical.so Using Function registerExactSolution
  End

  Begin Definition for Function krr
    Type is piecewise linear
    Begin Values
     0   1.0
     400 1.0
    End Values
    Scale by 10.0
  End

  Begin Definition for Function ktt
    Type is piecewise linear
    Begin Values
     0   1.0
     400 1.0
    End Values
    Scale by 1.0
```

```
  End

  Begin Definition for Function kzz
    Type is piecewise linear
    Begin Values
     0   1.0
     400 1.0
    End Values
  End

  Begin Postprocessor Output Control pp_out
     Comment Character Is %
     Write To File errors{N}.dat
     Floating Point Precision Is 6
     Floating Point Format Is Scientific
  End

  load user plugin file ./cylindrical.so

  begin data block region_data
#                  T0    T1   Krr  Ktt Kzz Lx  Lz  theta1 theta2
    Real r_data = 400.0 100.0 10.0 1.0 1.0 1.0 1.0 45.0   22.5
  end data block region_data

  BEGIN LOCAL COORDINATE SYSTEM CS_Block
      TYPE   = Cylindrical
      ORIGIN =  0.000000          0.000000          0.00000
      POINT  =  0.707106781186548 0.653281482438188 0.270598050073098
      VECTOR =  0                -0.382683432365090 0.923879532511287
  END

  BEGIN ARIA MATERIAL M_Block
    DENSITY = CONSTANT rho = 0.1
    #tensor thermal conductivity = user_function X=Temperature Name_XX=krr Name_YY=ktt Name_ZZ=kzz
    TENSOR THERMAL CONDUCTIVITY = CONSTANT  XX=10.0 YY=1.0 ZZ=1.0
    SPECIFIC HEAT   = CONSTANT  CP = 0.5
    Heat Conduction             = Generalized
  END ARIA MATERIAL M_Block

{if(useTpetra)}
    BEGIN TPETRA EQUATION SOLVER  LINEARSOLVER
      BEGIN GMRES SOLVER
        BEGIN JACOBI PRECONDITIONER
        END
        MAXIMUM ITERATIONS = 1000
        RESIDUAL SCALING = R0
        CONVERGENCE TOLERANCE = 1.000000e-12
      END
    END TPETRA EQUATION SOLVER
{else}
    BEGIN AZTEC EQUATION SOLVER LinearSolver
      SOLUTION METHOD = gmres
      PRECONDITIONING METHOD = jacobi
      MAXIMUM ITERATIONS = 1000
      RESIDUAL NORM TOLERANCE = 1.0e-12
      RESIDUAL NORM SCALING = r0
    END AZTEC EQUATION SOLVER LinearSolver
{endif}

  BEGIN FINITE ELEMENT MODEL FE_Block
    DATABASE NAME = cylindrical{N}.g
    coordinate system is cartesian
    decomposition method = rcb

    BEGIN PARAMETERS FOR BLOCK block_1
      MATERIAL M_Block
      LOCAL COORDINATE SYSTEM = CS_Block
    END PARAMETERS FOR BLOCK block_1
```

```
  END

  BEGIN PROCEDURE MyProcedure

     Begin Solution Control Description
Use System Main
Begin System Main
   Begin Sequential MyBlock
      Advance Region_Block
   End
End
     End

    BEGIN ARIA REGION Region_Block
      nonlinear solution strategy    = newton
      use data block region_data

      Output Number of Nodes
      Compute Difference L2        Of ufunc ffunc Store In l2_error_norm2
      Compute Difference LInfinity Of ufunc ffunc Store In linf_error_norm

      NONLINEAR RESIDUAL TOLERANCE   = 1.0e-10
      NONLINEAR CORRECTION TOLERANCE = 1.0e-10
      MAXIMUM NONLINEAR ITERATIONS   = 10
      NONLINEAR RELAXATION FACTOR    = 1.0

      BC dirichlet for temperature on surface_1 = calore_user_sub name = localCoord_bc type=node
      BC dirichlet for temperature on surface_2 = calore_user_sub name = localCoord_bc type=node
      BC dirichlet for temperature on surface_3 = calore_user_sub name = localCoord_bc type=node

      EQ ENERGY FOR TEMPERATURE ON block_1 USING Q1 WITH DIFF SRC

      Begin Volume Heating juan
        add volume block_1
        element subroutine = localCoord_vhs
      End

      Begin Initial Condition BlockName
        All Volumes
        Temperature = 400.0
      End

      USE FINITE ELEMENT MODEL FE_Block

      Interpolate Function Value of ufunc Into Nodal Field Tex

      BEGIN RESULTS OUTPUT TemperatureOutput
        DATABASE NAME = output{N}.e
        AT STEP 1, INCREMENT = 1
        TITLE Aria Temperature in Local Coordinate System Verification Problem
        NODAL VARIABLES = solution->TEMPERATURE AS T
        NODAL VARIABLES = Tex
        Element Variables = l2_error_norm2 as l2error
        Element Variables = linf_error_norm as linf
      END RESULTS OUTPUT TemperatureOutput

      USE LINEAR SOLVER LinearSolver
    END

  END
END SIERRA MyProblem
```

Appendices

DISTRIBUTION

Email—Internal[redacted]

Name	Org.	Sandia Email Address
Technical Library	01177	libref@sandia.gov