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Sierra/Aria 4.48 Verification Manual

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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

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Chapter 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

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

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.

Chapter 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.

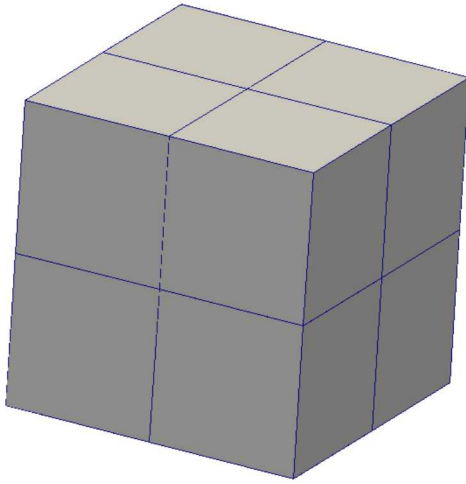
2.1.4 Verification of Solution

A manufactured solution is chosen as

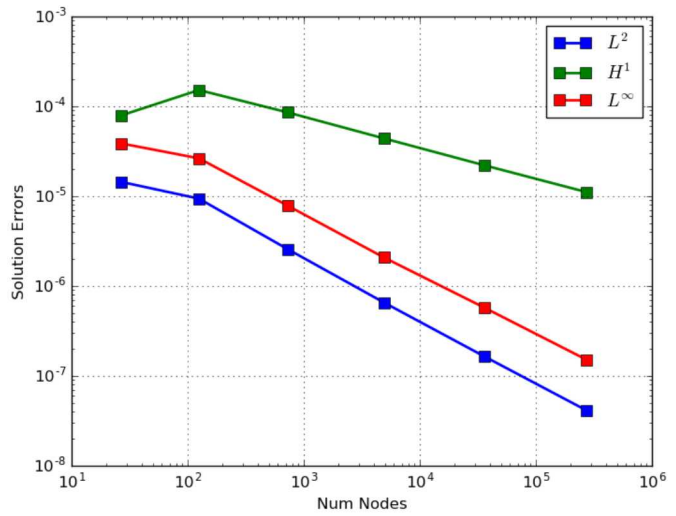
$$T(x, y, z) = 1 + (x - x^2)^2(y - y^2)^2(z - z^2)^2.$$

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. Steady Heat Conduction: Hex8 Meshes

Table 2.1. 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).

For input decks see [Appendix 12.1.2](#).

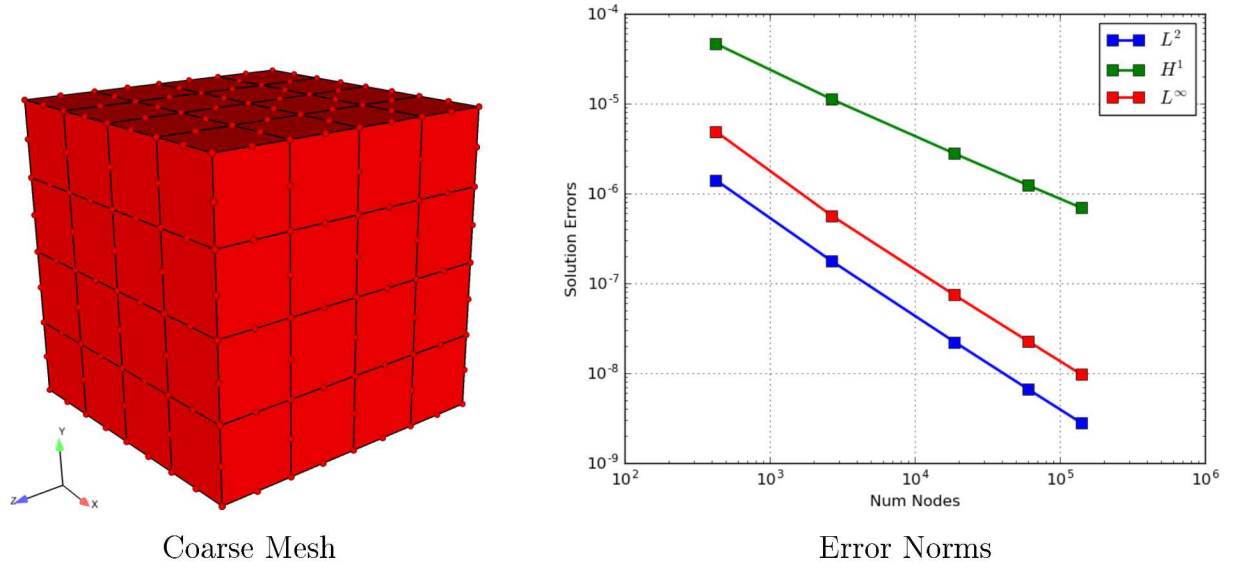


Figure 2.2. Steady Heat Conduction: Hex20 Meshes

Table 2.2. 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

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.

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).

Table 2.3. 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](#).

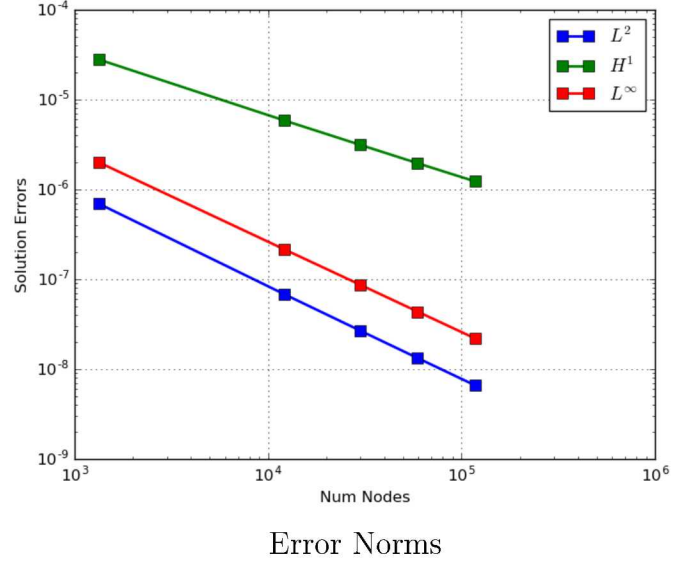
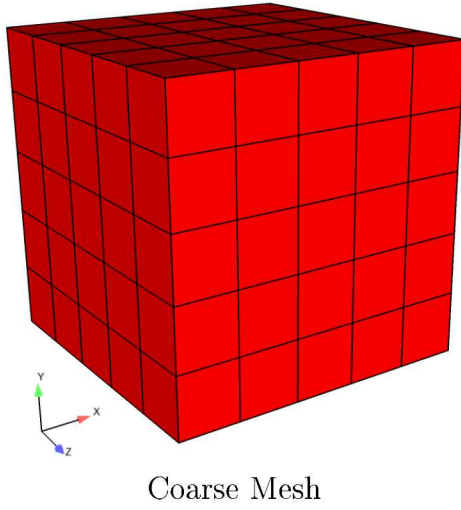


Figure 2.3. Steady Heat Conduction: Hex27 Meshes

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.

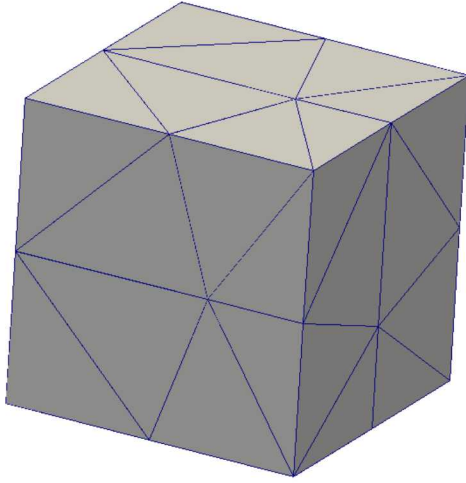
2.4.3 Material Parameters

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

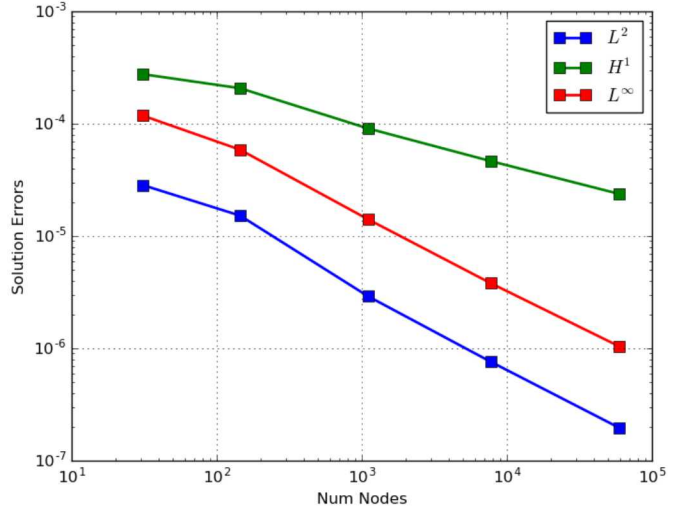
2.4.4 Verification of Solution

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.



Coarse Mesh



Error Norms

Figure 2.4. Steady Heat Conduction: Tet4 Meshes

Table 2.4. 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.

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.

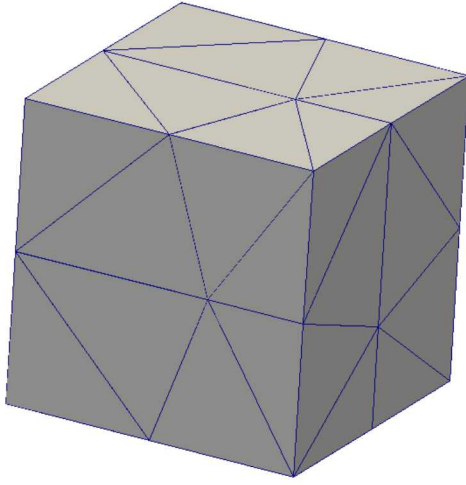
Table 2.5. Steady Heat Conduction: Convergence Rates
for Tet4Tet10 Meshes

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

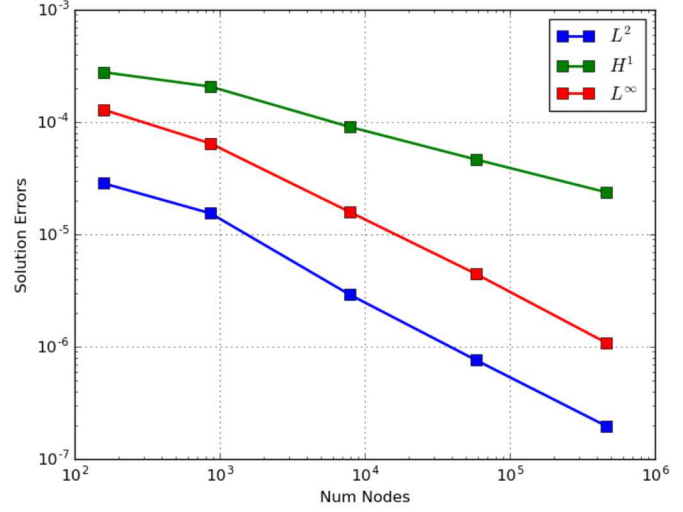
For input decks see Appendix 12.1.5.

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.



Coarse Mesh



Error Norms

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

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 conver-

gence 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.

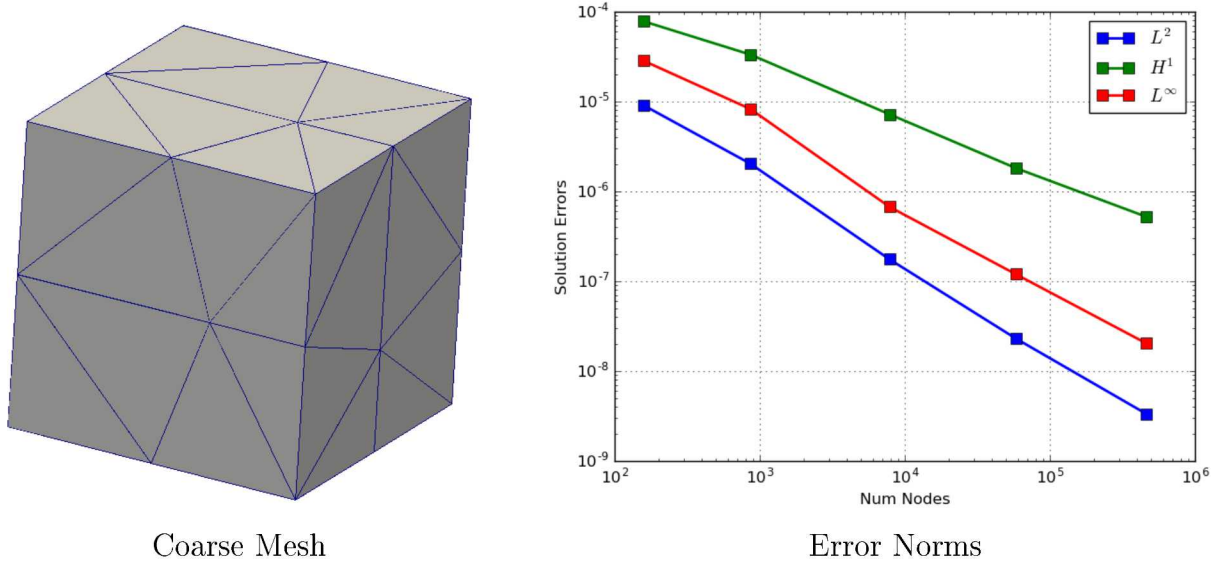


Figure 2.6. Steady Heat Conduction: Tet10 Meshes

Table 2.6. 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

For input decks see Appendix [12.1.6](#).

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

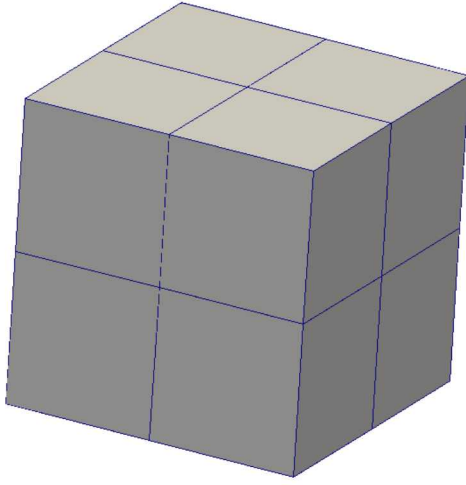
A manufactured solution is chosen as

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

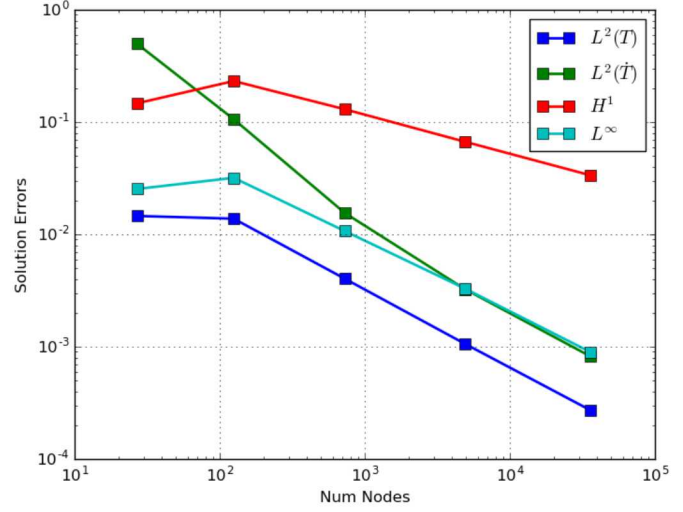
The source and heat flux user subroutines are chosen so that the solution satisfies the heat equation with the correct boundary conditions.

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).

For input decks see Appendix [12.1.7](#).



Coarse Mesh



Error Norms

Figure 2.7. Transient Heat Conduction: Hex8 Meshes

Table 2.7. 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

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.

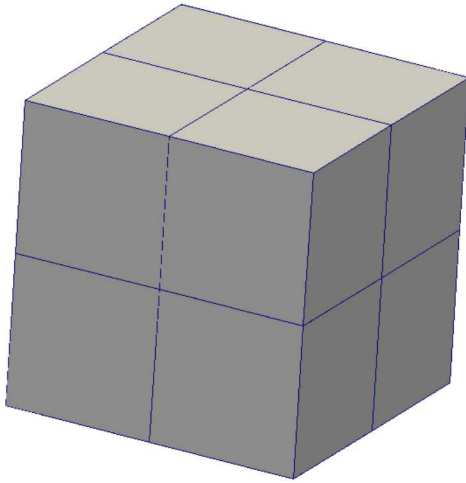
2.8.3 Material Parameters

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

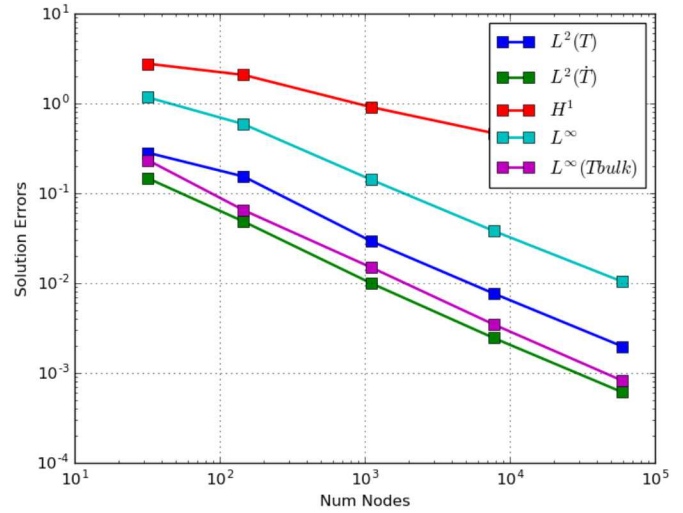
2.8.4 Verification of Solution

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. Transient Heat Conduction: Tet4 Meshes

For input decks see Appendix 12.1.8.

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

Num Dofs	$L^2(T)$	$L^2(\dot{T})$	H^1	L^∞	$L^\infty(T_{bulk})$
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

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

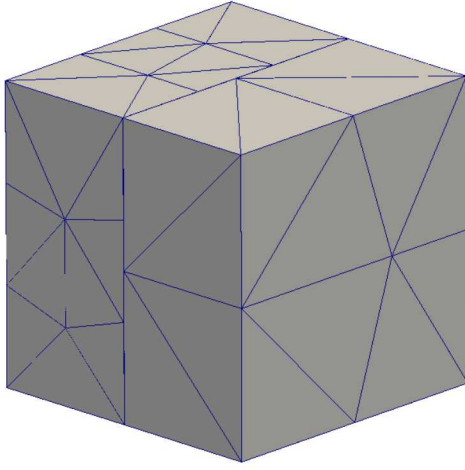
The values of density, thermal conductivity, and specific heat are all constant, equal to one in both blocks.

2.9.4 Verification of Solution

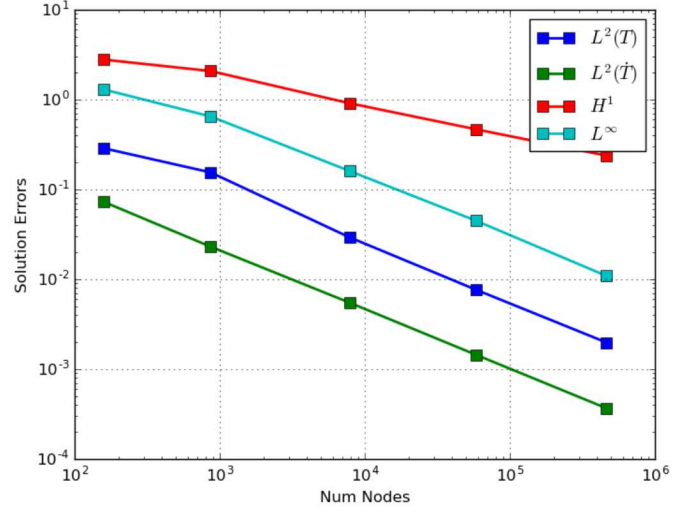
A manufactured solution is chosen as in Section 2.8.

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.

For input decks see Appendix 12.1.9.



Coarse Mesh



Error Norms

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

Table 2.9. 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

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

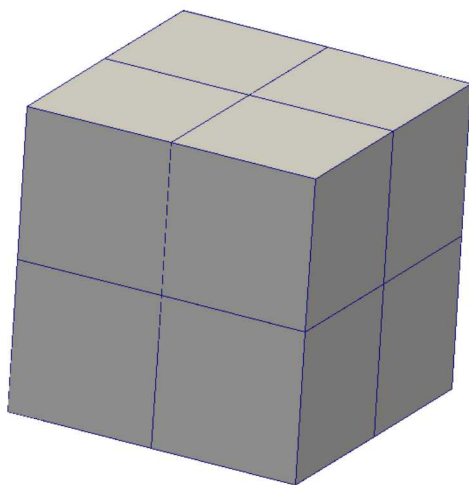
2.10.3 Material Parameters

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

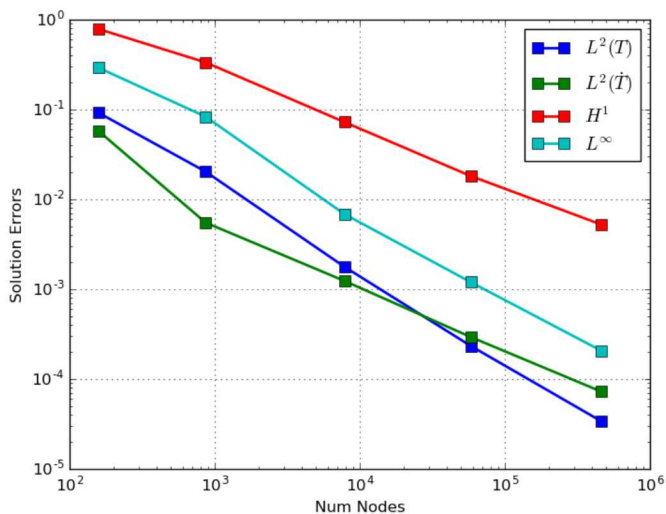
2.10.4 Verification of Solution

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. Transient Heat Conduction: Tet10 Meshes

For input decks see Appendix 12.1.10.

Documentation for the following tests is in progress:

```
1 nlin_verify1/1dnonlin_verify1.test|np8
2 o_2d/aniso_2d.test|np8
```

Table 2.10. 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

```

3 o_3d/aniso_3d.test|np8
4 shell_2d/cyl_shell_2d.test|np8
5 shell_3d/cyl_shell_3d.test|np8
6 in_C_fi/nonlin_C_fi.test|np1
7 in_C_trap/nonlin_C_trap.test|np1
8 process_minmax/postprocess_minmax.test|np8
9 ce_parab/source_parab.test|np1
10 ce_parab_2d/source_parab_2d.test|np1
11 shell_axi/sph_shell_axi.test|np1
12 rical_shell/spherical_shell.test|np4
13 mal_steady_hex8_adapt/thermal_steady_hex8_adapt.test|np1
14 11_nonlin/x11b11_nonlin.test|np1

```


Chapter 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 temperature 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).

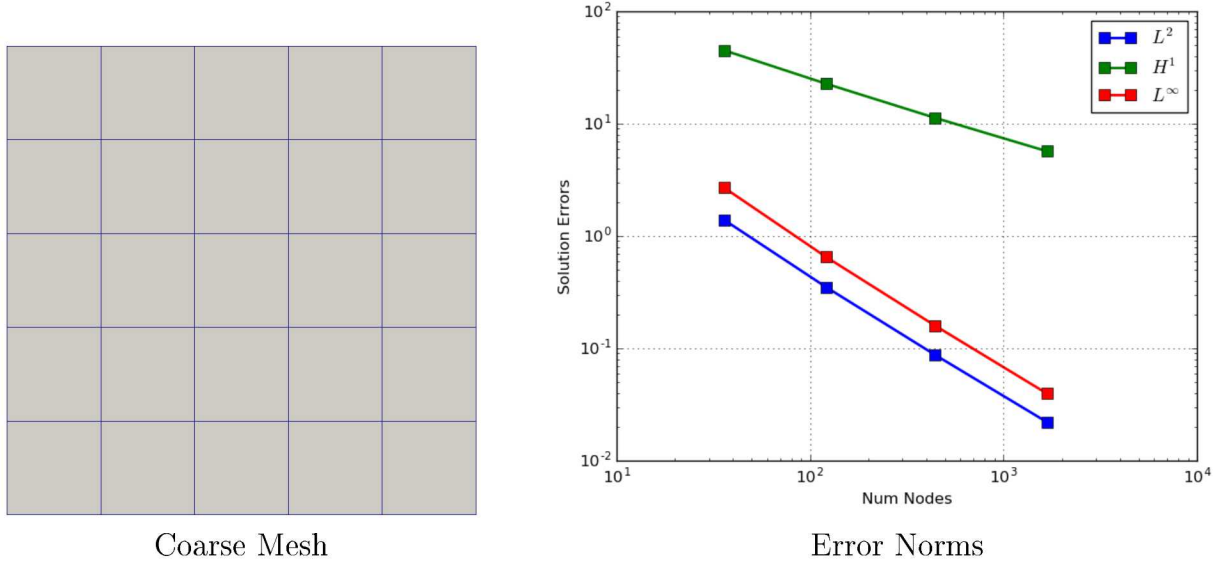


Figure 3.1. Radiative Heat Flux

Table 3.1. 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

For input decks see Appendix [12.2.1](#).

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).

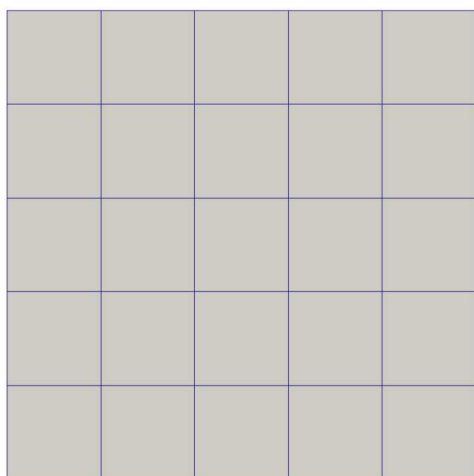
Table 3.2. Convective Heat Flux: Convergence Rates for Hex8 Meshes

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

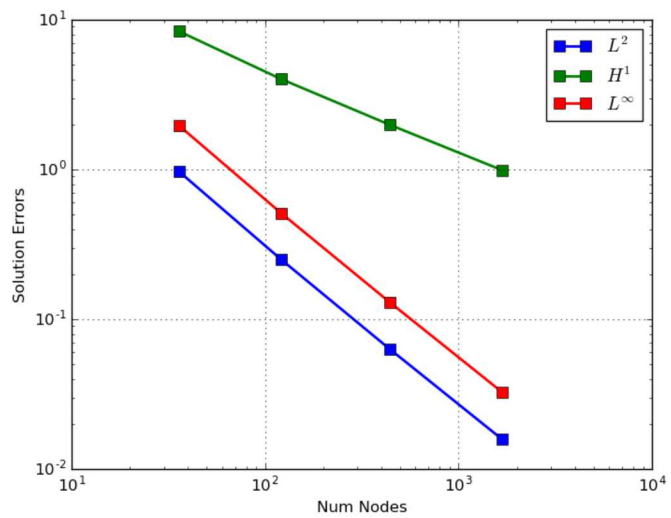
For input decks see Appendix [12.2.3](#).

Documentation for the following tests is in progress:

```
1 mal_rad_flux_test1/thermal_rad_flux_test1.test|np3
2 mal_rad_flux_test2/thermal_rad_flux_test2.test|np3
3 mal_rad_flux_test3/thermal_rad_flux_test3.test|np3
4 mal_conv_flux_test1/thermal_conv_flux_test1.test|np3
5 mal_conv_flux_test2/thermal_conv_flux_test2.test|np3
6 mal_heat_flux_test1/thermal_heat_flux_test1.test|np3
7 mal_heat_flux_test2/thermal_heat_flux_test2.test|np3
```



Coarse Mesh



Error Norms

Figure 3.2. Convective Heat Flux

```
mal_heat_flux_test3/thermal_heat_flux_test3.test|np3
mal_heat_flux_test4/thermal_heat_flux_test4.test|np3
```


Chapter 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

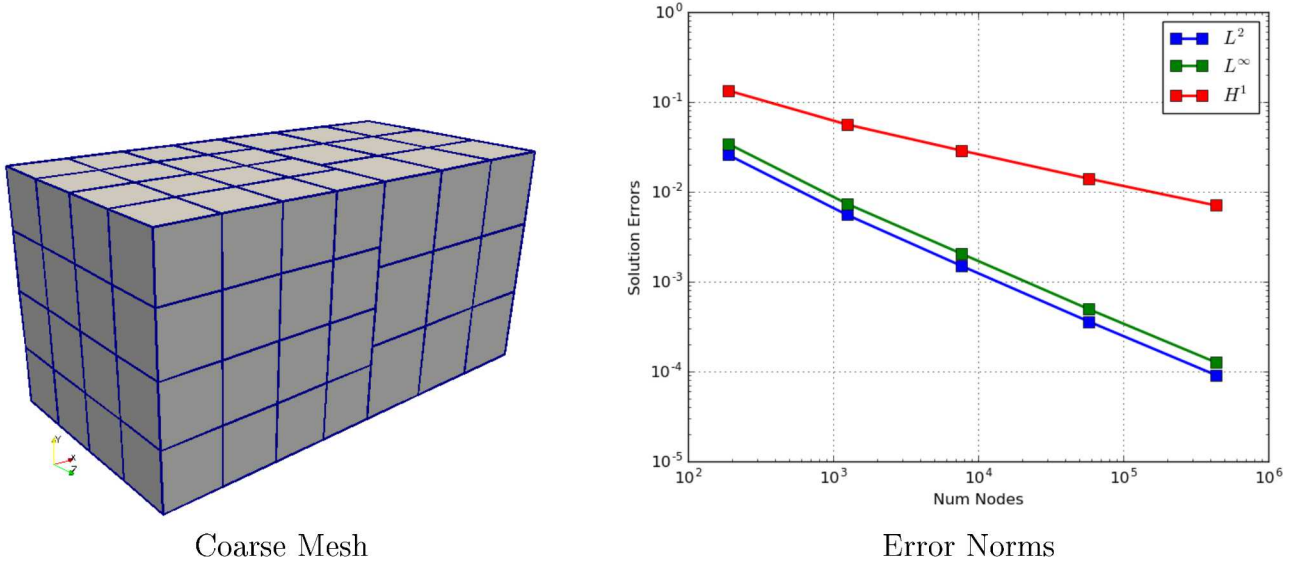
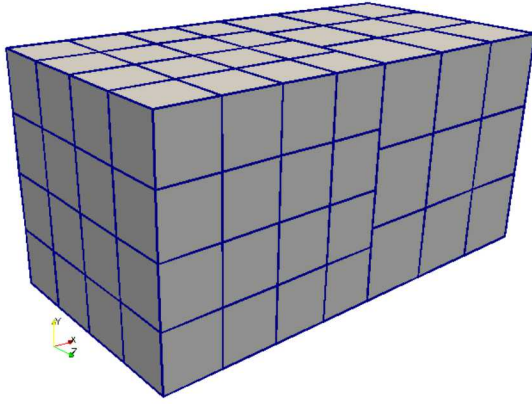


Figure 4.1. 1D Flat Contact: Hex8 Tied

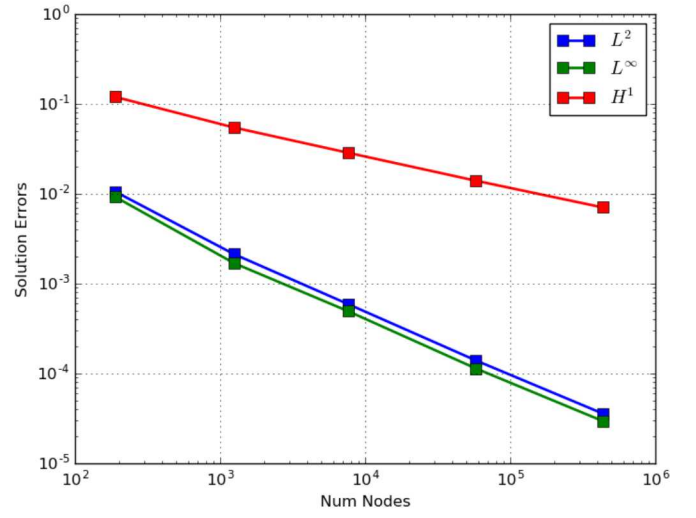
Table 4.1. 1D Flat Contact: Convergence Rates for Hex8
Tied

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

4.1.6 Results: Hex8 Resistance



Coarse Mesh



Error Norms

Figure 4.2. 1D Flat Contact: Hex8 Resistance

Table 4.2. 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

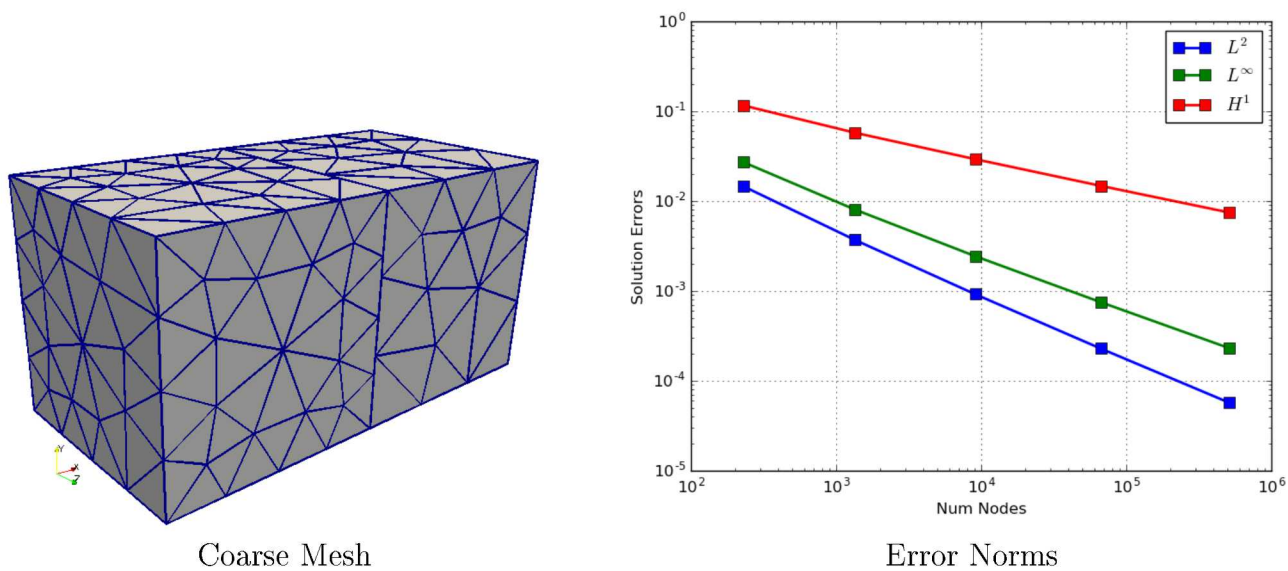
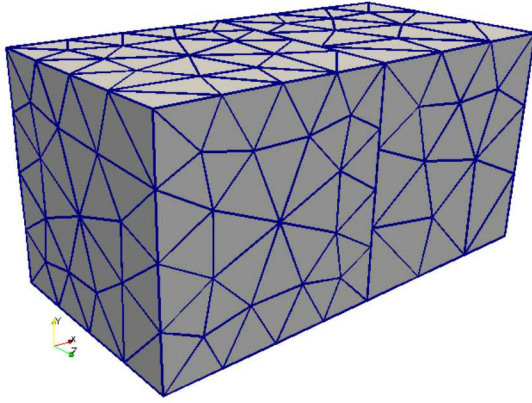


Figure 4.3. 1D Flat Contact: Tet4 Tied

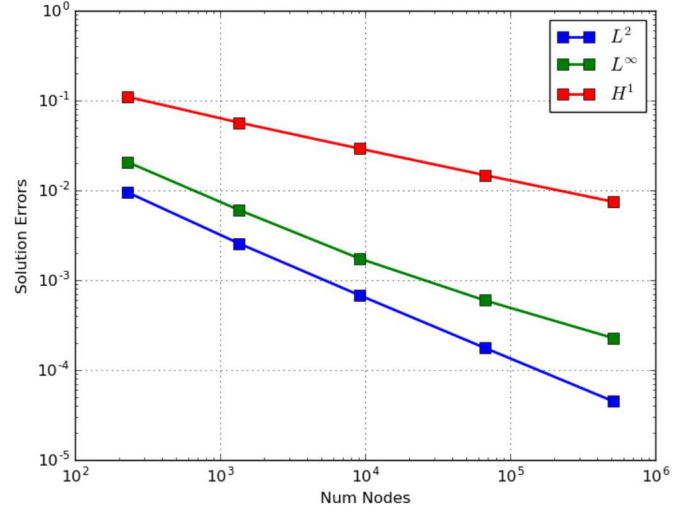
Table 4.3. 1D Flat Contact: Convergence Rates for Tet4 Tied

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 4.4. 1D Flat Contact: Tet4 Resistance

Table 4.4. 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

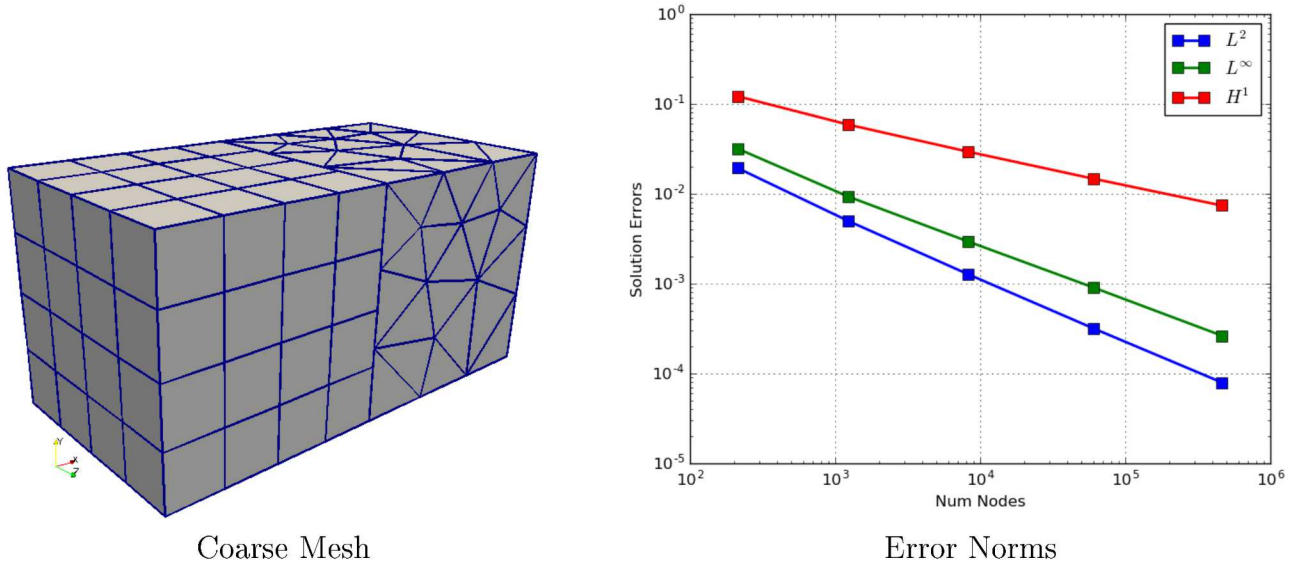


Figure 4.5. 1D Flat Contact: Hex8-Tet4 Tied

Table 4.5. 1D Flat Contact: Convergence Rates for Hex8-Tet4 Tied

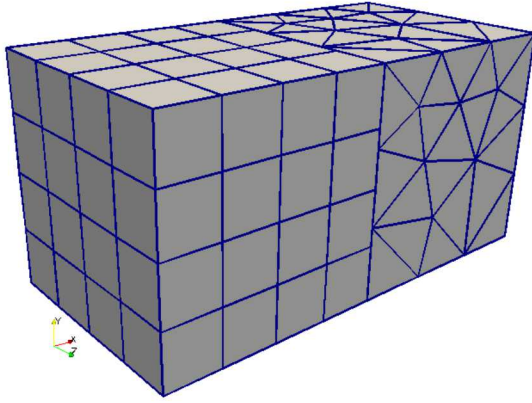
Num Dofs	L^2	L^∞	H^1
1231	2.32	2.10	1.24
8284	2.16	1.82	1.09
60570	2.09	1.78	1.04
462800	2.04	1.82	1.02

4.1.10 Results: Hex8-Tet4 Resistance

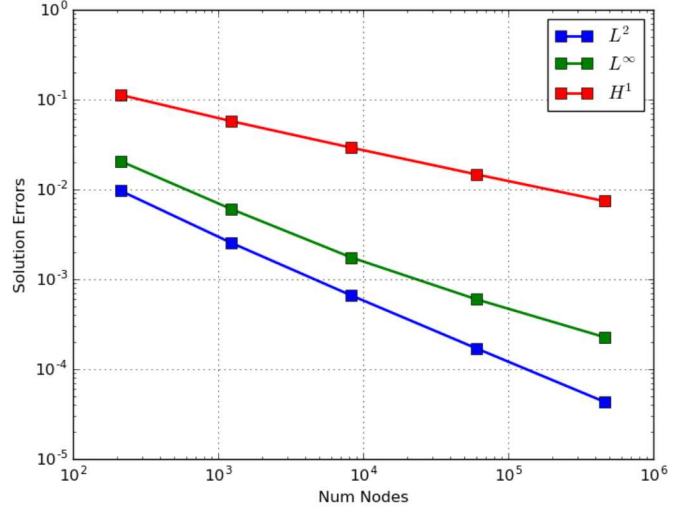
4.2 3D Curved Contact

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.



Coarse Mesh



Error Norms

Figure 4.6. 1D Flat Contact: Hex8-Tet4 Resistance

Table 4.6. 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

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.

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

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

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).

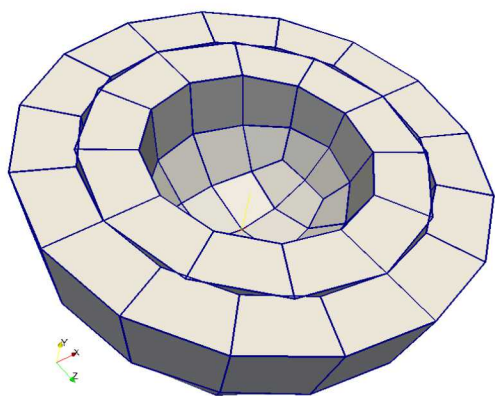
These rates are observed for the hex-hex case; however, both of the cases involving tet meshes exhibit a reduced order of convergence in the L^∞ norms (convergence rate about 1.7).

For input decks see [Appendix 12.3.2](#).

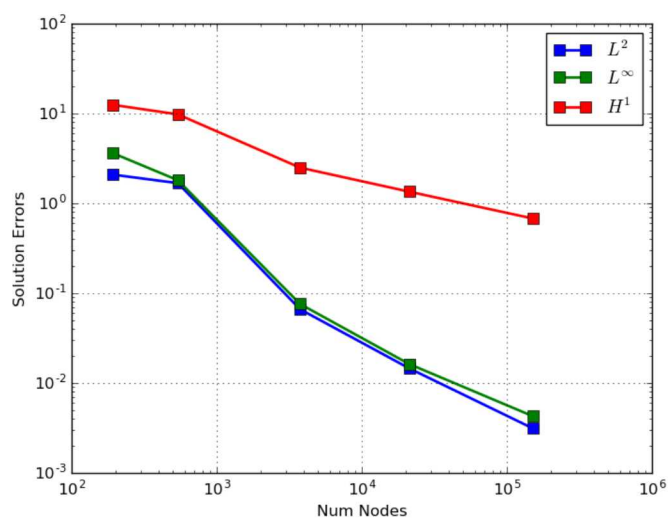
4.2.5 Results: Hex8-Hex8 Contact

Table 4.7. 3D Curved Contact: Convergence Rates for Hex8-Hex8

Num Dofs	L^2	L^∞	H^1
540	0.64	2.01	0.70
3752	5.00	4.91	2.11
21220	2.62	2.66	1.07
150700	2.35	2.05	1.06



Coarse Mesh



Error Norms

Figure 4.7. 3D Curved Contact: Hex8-Hex8 Case

4.2.6 Results: Tet4-Tet4 Contact

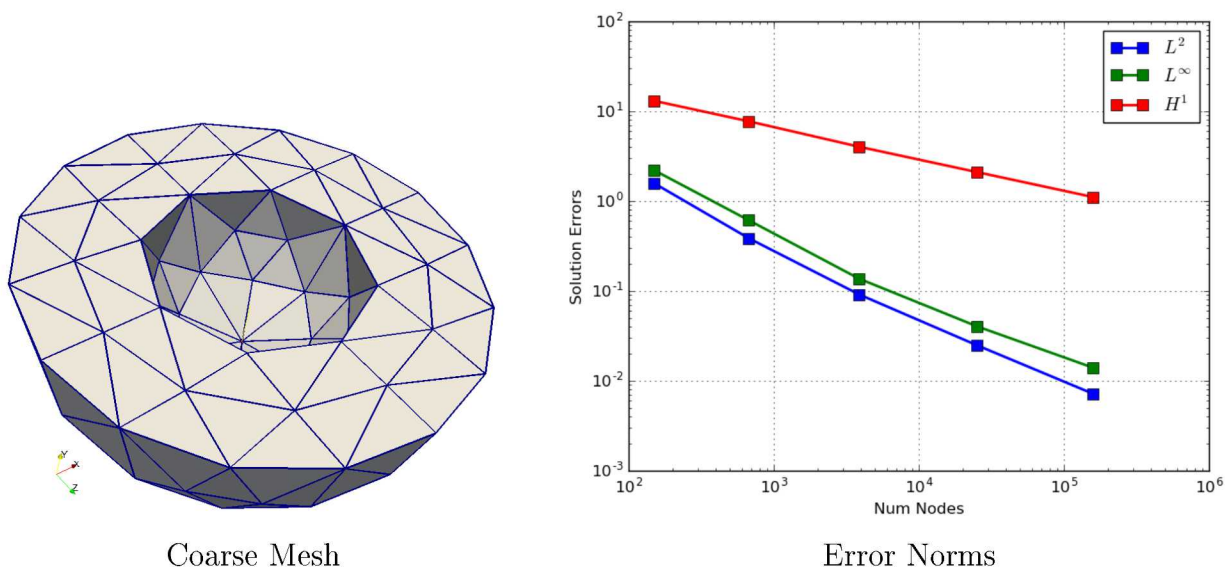


Figure 4.8. 3D Curved Contact: Tet4-Tet4 Case

Table 4.8. 3D Curved Contact: Convergence Rates for Tet4-Tet4

Num Dofs	L^2	L^∞	H^1
674	2.82	2.56	1.05
3881	2.47	2.57	1.12
25010	2.09	1.96	1.04
159100	2.02	1.73	1.04

4.2.7 Results: Hex8-Tet4 Contact

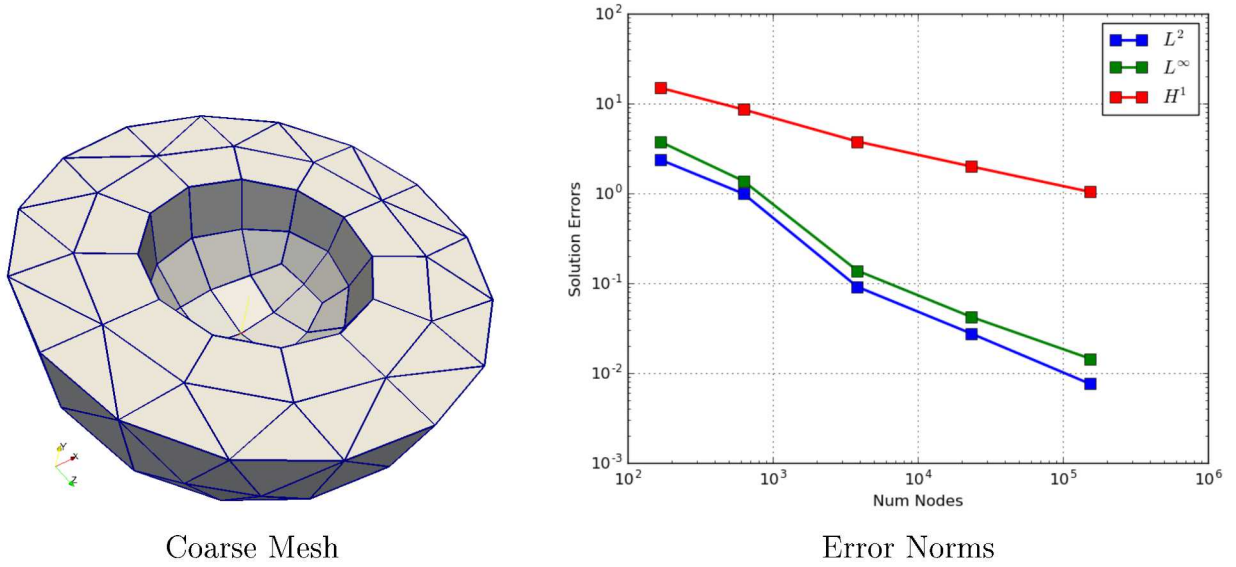


Figure 4.9. 3D Curved Contact: Hex8-Tet4 Case

Table 4.9. 3D Curved Contact: Convergence Rates for Hex8-Tet4

Num Dofs	L^2	L^∞	H^1
630	1.98	2.29	1.26
3830	3.96	3.82	1.36
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 4.10. 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](#).

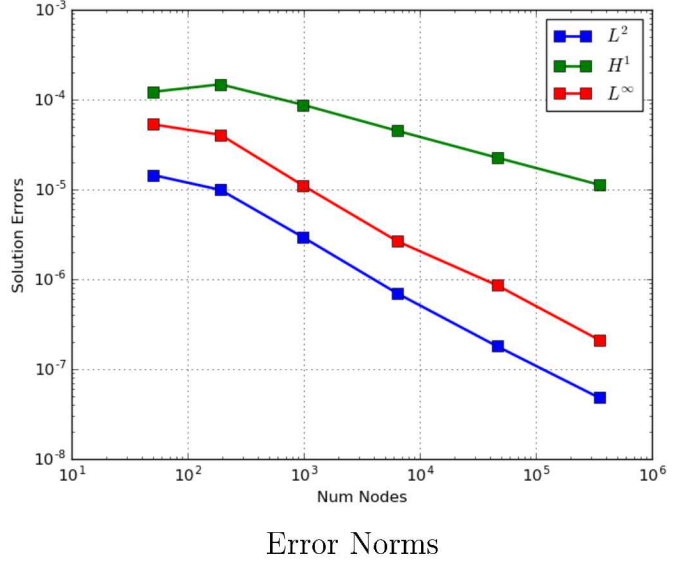
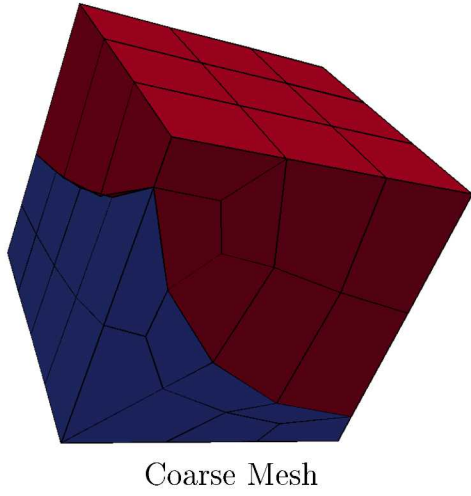


Figure 4.10. Steady Tied Contact: Hex8 Meshes

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.

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).

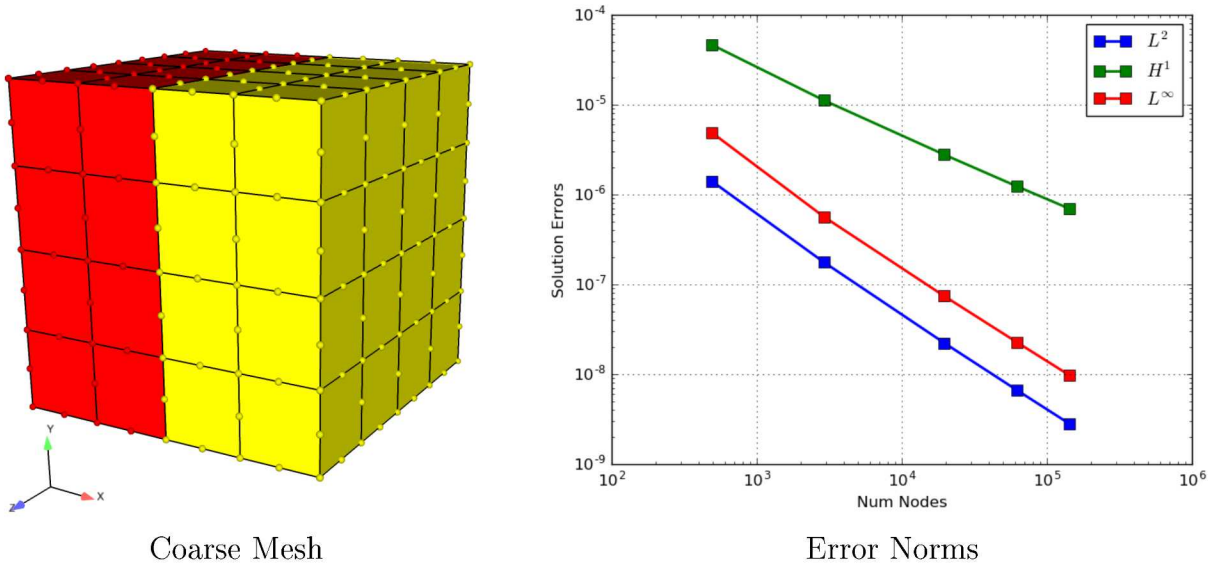


Figure 4.11. Steady Heat Conduction: Hex20 Meshes

For input decks see Appendix [12.3.4](#).

Table 4.11. 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

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).

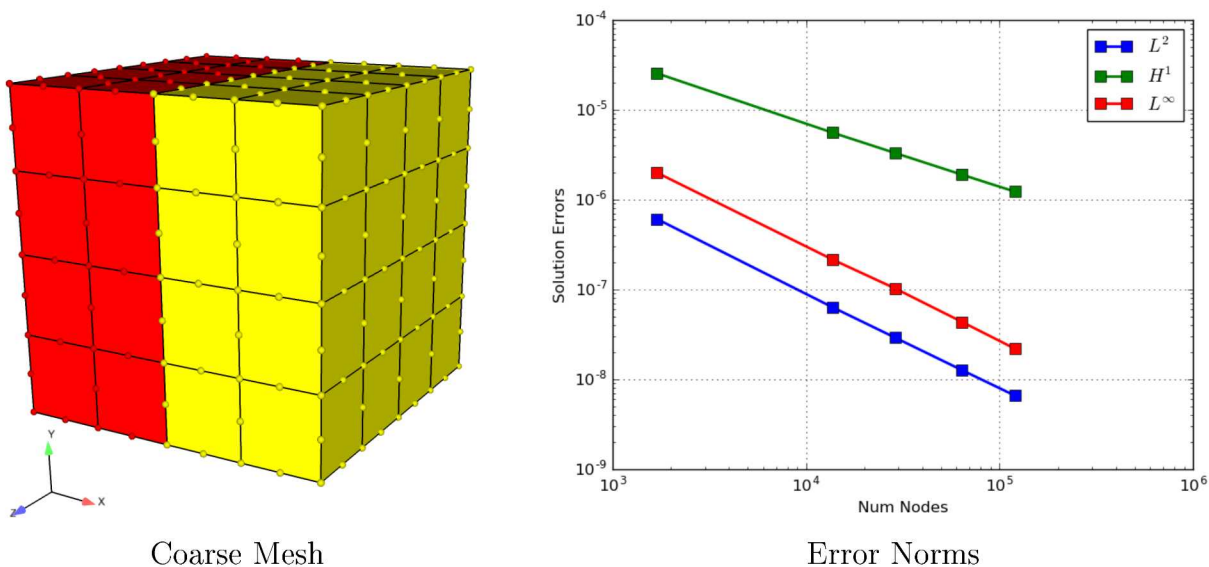


Figure 4.12. Steady Heat Conduction: Hex27 Meshes

Table 4.12. 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

For input decks see Appendix [12.3.5](#).

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.

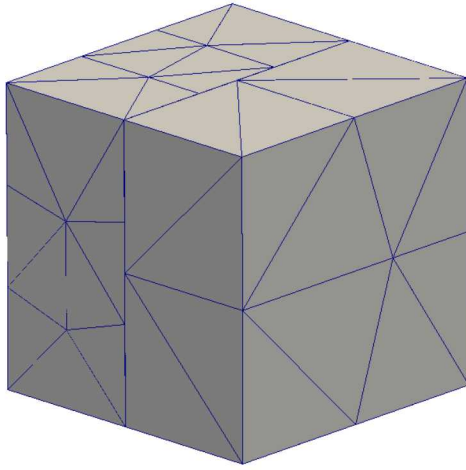
4.6.4 Verification of Solution

Same as in Section 2.1.

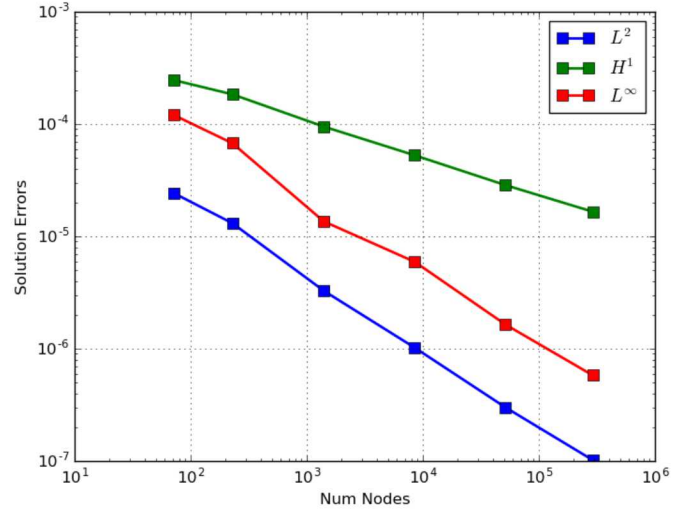
Table 4.13. Steady Tied Contact: Convergence Rates for Tet4 Meshes

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.



Coarse Mesh



Error Norms

Figure 4.13. Steady Tied Contact: Tet4 Meshes

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

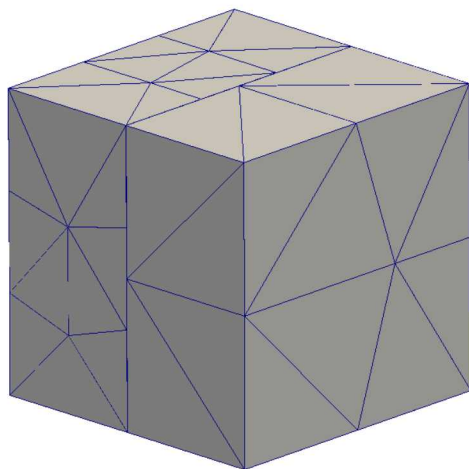
Same as in Section 2.1.

4.7.3 Material Parameters

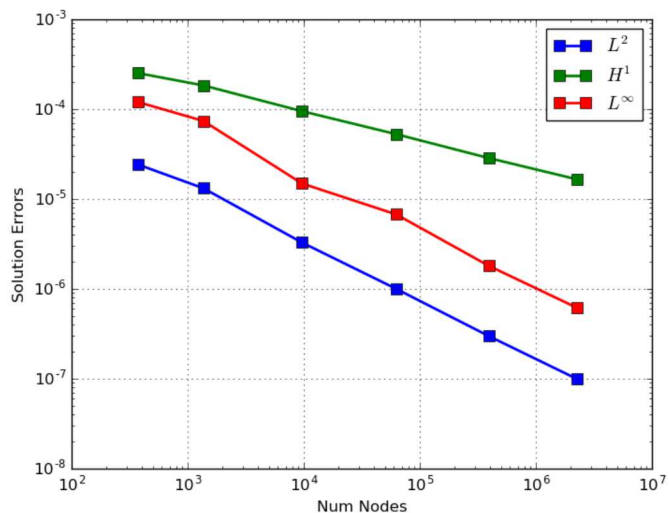
The values of density, thermal conductivity, and specific heat are all constant, equal to one in both blocks.

4.7.4 Verification of Solution

Same as in Section 2.1.



Coarse Mesh



Error Norms

Figure 4.14. Steady Tied Contact: Tet4 Meshes

Table 4.14. Steady Tied Contact: Convergence Rates for Tet4 Meshes

Num Dofs	L^2	H^1	L^∞
1364	1.40	0.72	1.12
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

For input decks see Appendix 12.3.7.

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

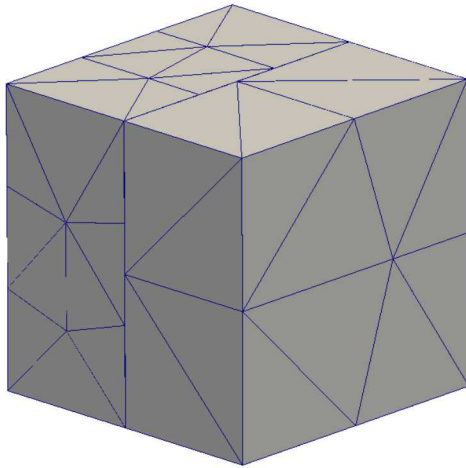
Same as in Section 2.1.

4.8.3 Material Parameters

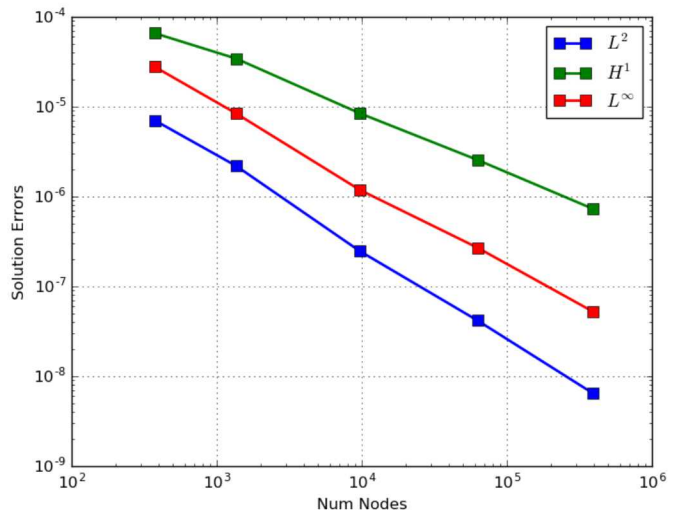
The values of density, thermal conductivity, and specific heat are all constant, equal to one in both blocks.

4.8.4 Verification of Solution

Same as in Section 2.1.



Coarse Mesh



Error Norms

Figure 4.15. Steady Tied Contact: Tet10 Meshes

For input decks see Appendix 12.3.8.

Table 4.15. 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

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.

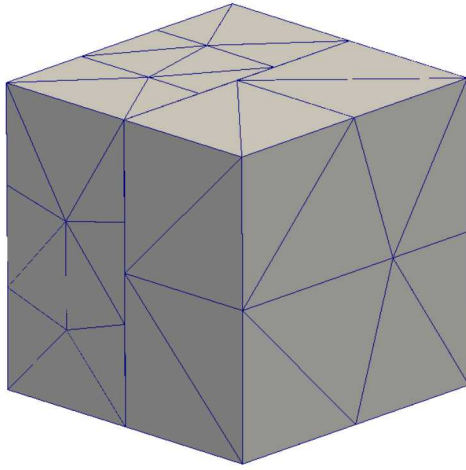
4.9.3 Material Parameters

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

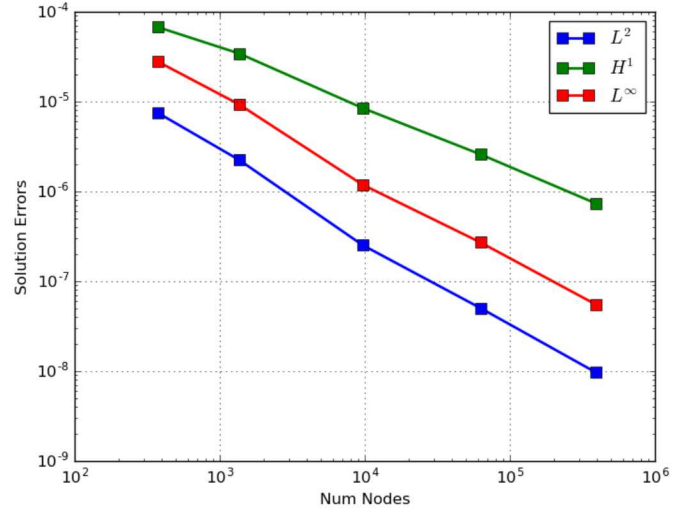
4.9.4 Verification of Solution

Same as in Section 2.1.

For input decks see Appendix 12.3.9.



Coarse Mesh



Error Norms

Figure 4.16. Steady Tied Dash Contact: Tet10 Meshes

Table 4.16. 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

4.10 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

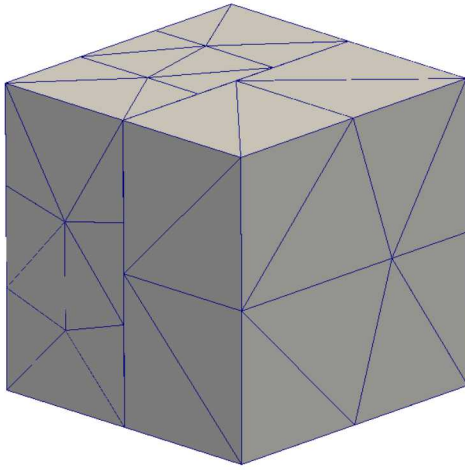
The values of density, thermal conductivity, and specific heat are all constant, equal to one in both blocks.

4.10.4 Verification of Solution

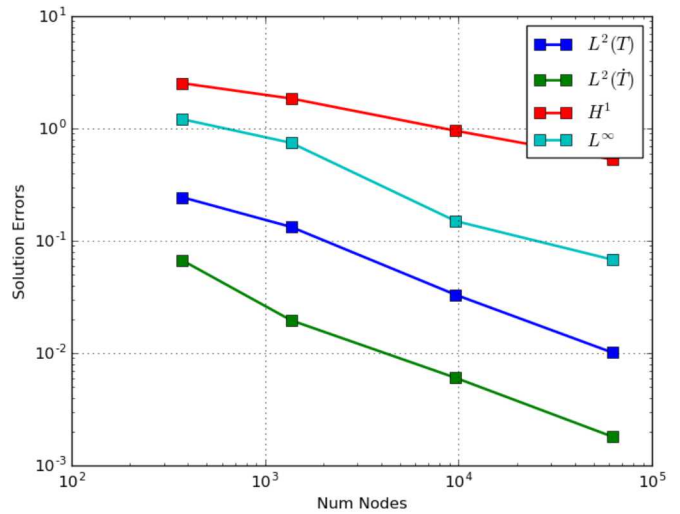
A manufactured solution is chosen as

$$T(x, y, z, t) = (x - x^2)^2 (y - y^2)^2 (z - z^2)^2 m(t) + 1,$$
$$m(t) = 10^4 [1. - \exp(-t) + t * \exp(-(t - 1.0) * (t - 1.0))];$$

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 4.17. Transient Tied Contact: Tet10 Meshes

For input decks see Appendix [12.3.10](#).

Table 4.17. Transient Tied Contact: Convergence Rates
for Tet10 Meshes

Num Dofs	$L^2(T)$	$L^2(\dot{T})$	H^1	L^∞
1364	1.40	2.84	0.72	1.12
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.

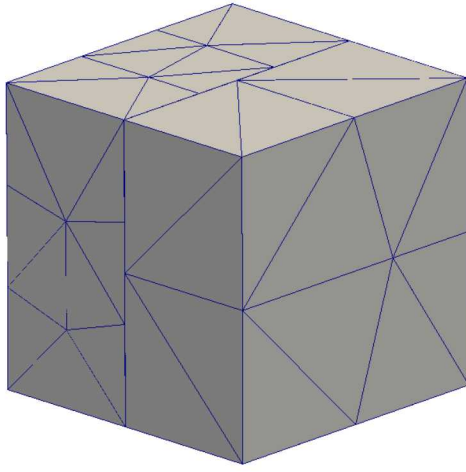
4.11.4 Verification of Solution

A manufactured solution is chosen as

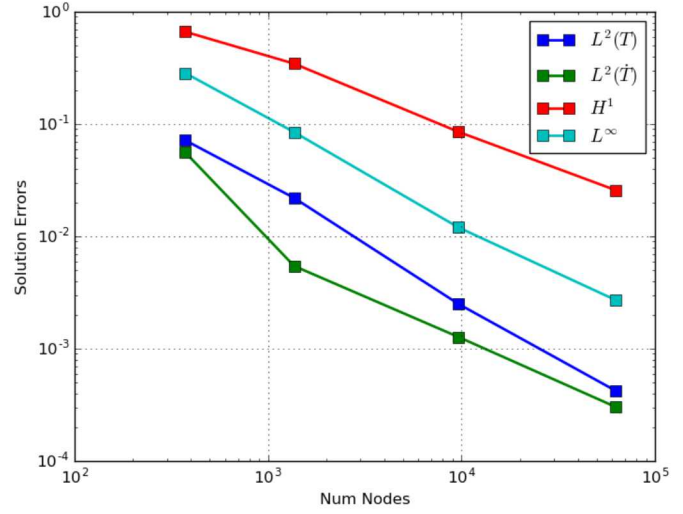
$$T(x, y, z, t) = (x - x^2)^2 (y - y^2)^2 (z - z^2)^2 m(t) + 1,$$

$$m(t) = 10^4 [1. - \exp(-t) + t * \exp(-(t - 1.0) * (t - 1.0))];$$

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 4.18. Transient Tied Contact: Tet10 Meshes

Table 4.18. 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

For input decks see Appendix [12.3.11](#).

Documentation for the following tests is in progress:

```

1 mal_transient_hex8_tied_contact/thermal_transient_hex8_tied_contact.test|np8
2 mal_transient_tet4_tied_contact/thermal_transient_tet4_tied_contact.test|np8

```

Chapter 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

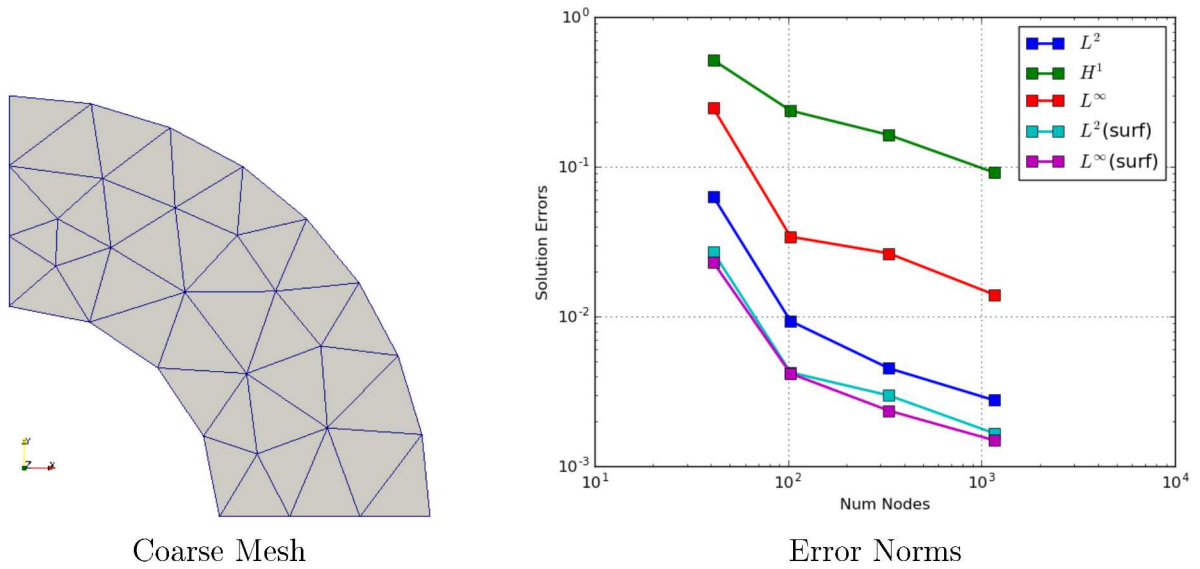


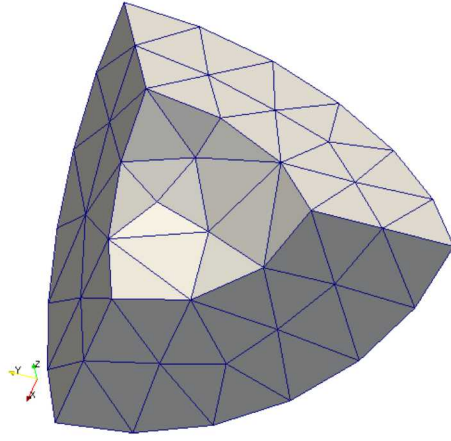
Figure 5.1. CDFEM Element Death (Heat Flux): Tri3

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

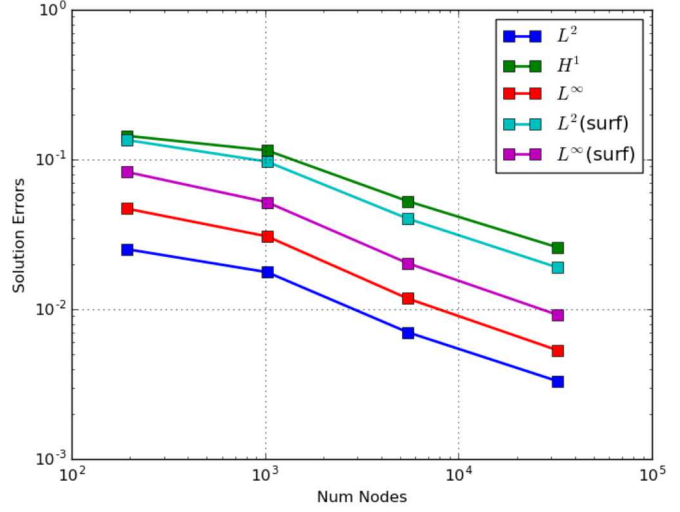
Num Dofs	L^2	H^1	L^∞	$L^2(\text{surf})$	$L^\infty(\text{surf})$
103	4.16	1.69	4.30	4.03	3.73
332	1.24	0.64	0.44	0.60	0.98
1163	0.78	0.93	1.01	0.93	0.73

5.1.6 Results: Tet4

For input decks see Appendix 12.4.1.



Coarse Mesh



Error Norms

Figure 5.2. CDFEM Element Death (Heat Flux): Tet4

Table 5.2. CDFEM Element Death (Heat Flux): Convergence Rates for Tet4

Num Dofs	L^2	H^1	L^∞	$L^2(\text{surf})$	$L^\infty(\text{surf})$
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

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 5.3.

Table 5.3. 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 5.4.

Table 5.4. 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:

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

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

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 5.3; 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

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

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

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

$$q_2 = -\kappa_2 \frac{\partial T_i}{\partial r} \Big|_{r=r_2} = \kappa_2 \frac{T_c - T_1}{r_1^2 (1/r_2 - 1/r_1)} \quad (5.5)$$

$$q_3 = -\kappa_3 \frac{\partial T_o}{\partial r} \Big|_{r=r_3} = \kappa_3 \frac{T_4 - C_o}{r_3^2 (1/r_4 - 1/r_3)} \quad (5.6)$$

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

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

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 5.3.

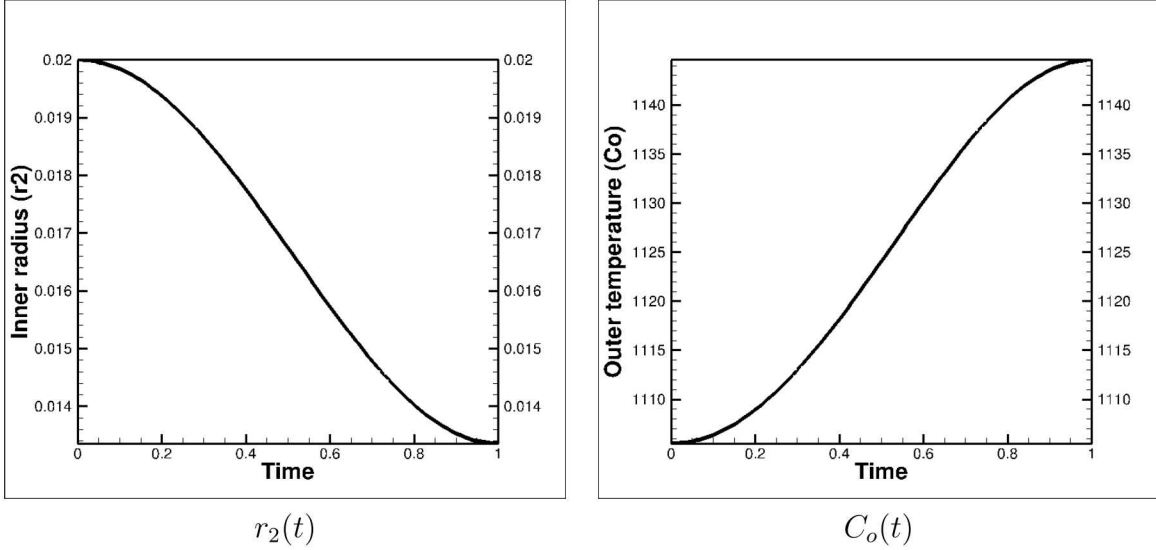


Figure 5.3. Evolution of parameters r_2 and C_o .

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

$$\partial_t T_i \equiv \dot{T}_1 + (T_c - \dot{T}_1) \frac{1/r - 1/r_1}{1/r_2 - 1/r_1} + (T_c - T_1) \frac{\dot{r}_2(1/r - 1/r_1)}{r_2^2(1/r_2 - 1/r_1)^2}, \quad r_1 \leq r \leq r_2, \quad (5.7)$$

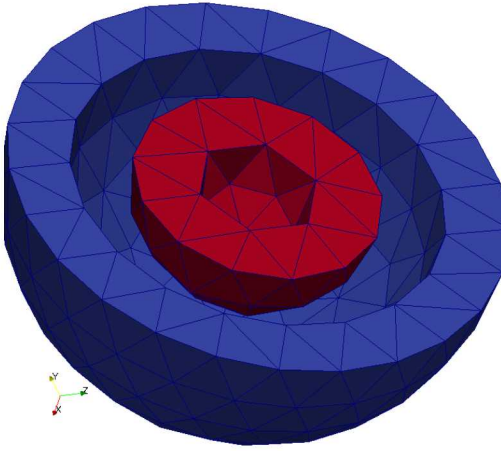
$$\partial_t T_o \equiv \dot{C}_o \left(1 - \frac{1/r - 1/r_3}{1/r_4 - 1/r_3}\right), \quad r_3 \leq r \leq r_4 \quad (5.8)$$

5.2.6 Results

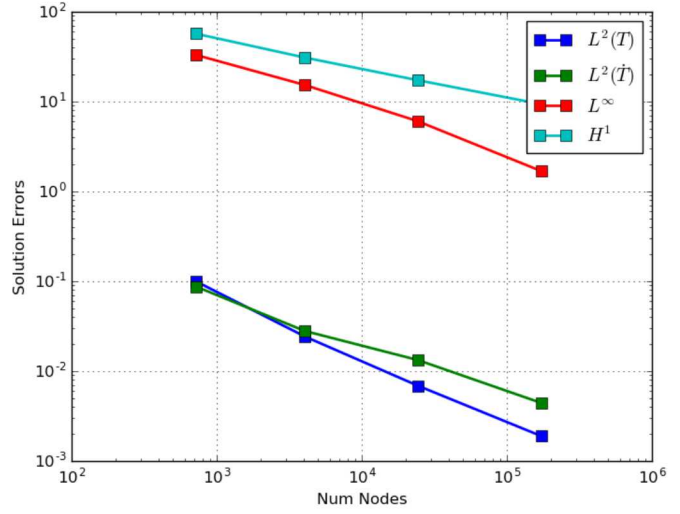
Results are presented running the problem on three meshes up to time $t = 0.9$.

For input decks see Appendix 12.4.2.

Documentation for the following tests is in progress:



Coarse Mesh



Error Norms ($t = 0.9$)

Table 5.5. Convergence Rates at $t = 0.9$

Num Dofs	$L^2(T)$	$L^2(\dot{T})$	L^∞	H^1
4056	2.45	1.98	1.34	1.06
24370	2.11	1.25	1.55	0.97
173600	1.98	1.68	1.96	0.94

```

1 mal_eddeath_1d_heatflux/thermal_eddeath_1d_heatflux.test |
  thermal_eddeath_1d_heatflux_hex8
2 mal_eddeath_1d_heatflux/thermal_eddeath_1d_heatflux.test |
  thermal_eddeath_1d_heatflux_quad4
3 mal_eddeath_1d_heatflux/thermal_eddeath_1d_heatflux.test |
  thermal_eddeath_1d_heatflux_tet4
4 mal_eddeath_1d_heatflux/thermal_eddeath_1d_heatflux.test |
  thermal_eddeath_1d_heatflux_tri3
5 mal_eddeath_2d_heatflux/thermal_eddeath_2d_heatflux.test |
  thermal_eddeath_2d_heatflux_quad4
6 mal_eddeath_2d_heatflux/thermal_eddeath_2d_heatflux.test |
  thermal_eddeath_2d_heatflux_quad4_unstruct
7 mal_eddeath_2d_heatflux/thermal_eddeath_2d_heatflux.test |
  thermal_eddeath_2d_heatflux_tri3
8 mal_eddeath_3d_heatflux/thermal_eddeath_3d_heatflux.test |
  thermal_eddeath_3d_heatflux_hex8
9 mal_eddeath_3d_heatflux/thermal_eddeath_3d_heatflux.test |
  thermal_eddeath_3d_heatflux_tet4

```


Chapter 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

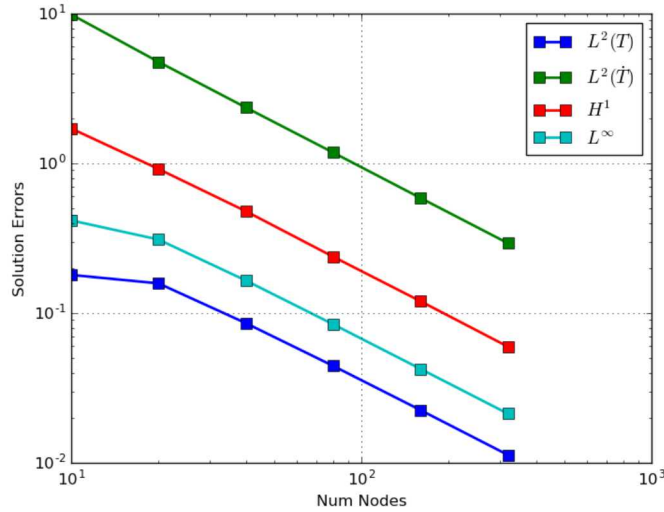


Figure 6.1. Adaptive Time Integration: Errors for First Order Fixed

6.1.6 Results: First Order Adaptive

Table 6.1. 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

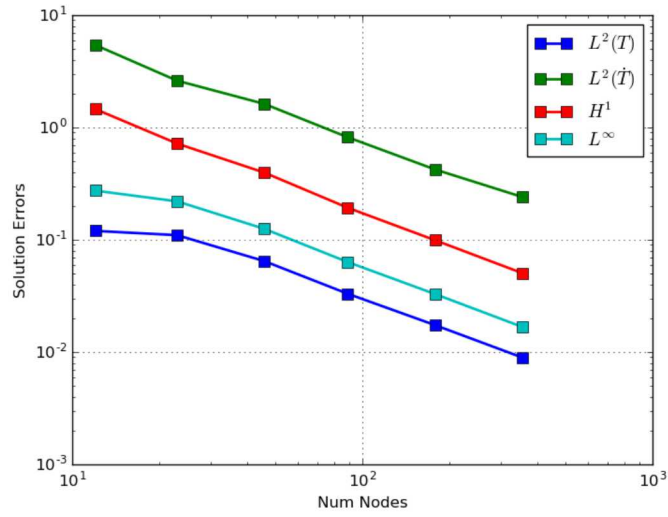


Figure 6.2. Adaptive Time Integration: Errors for First Order Adaptive

Table 6.2. 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

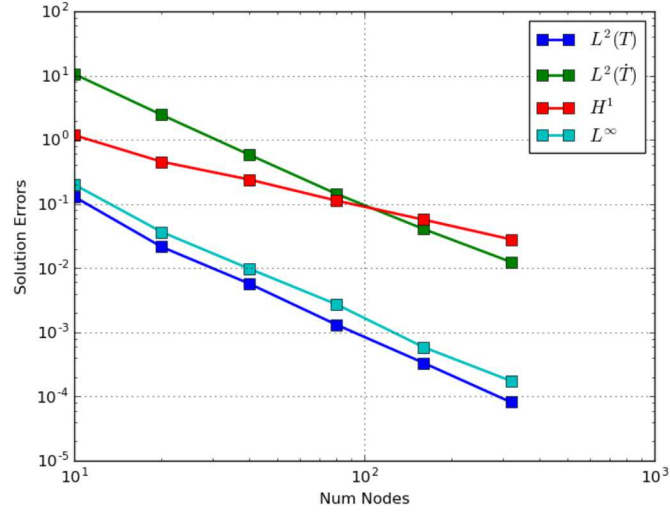


Figure 6.3. Adaptive Time Integration: Errors for Second Order Fixed

Table 6.3. 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

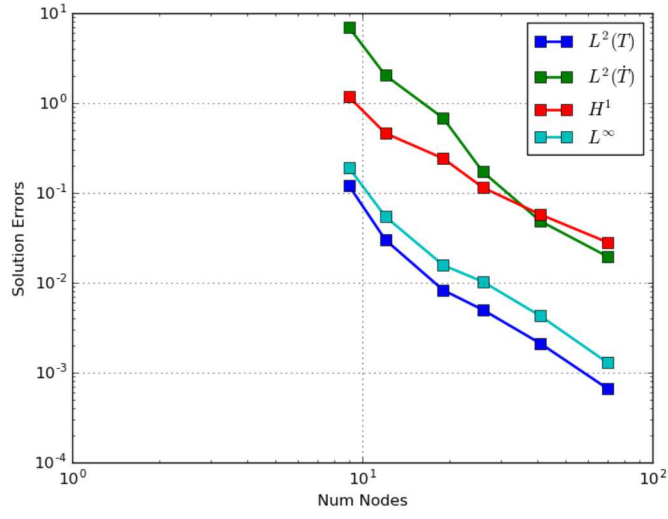


Figure 6.4. Adaptive Time Integration: Errors for Second Order Adaptive

Table 6.4. 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

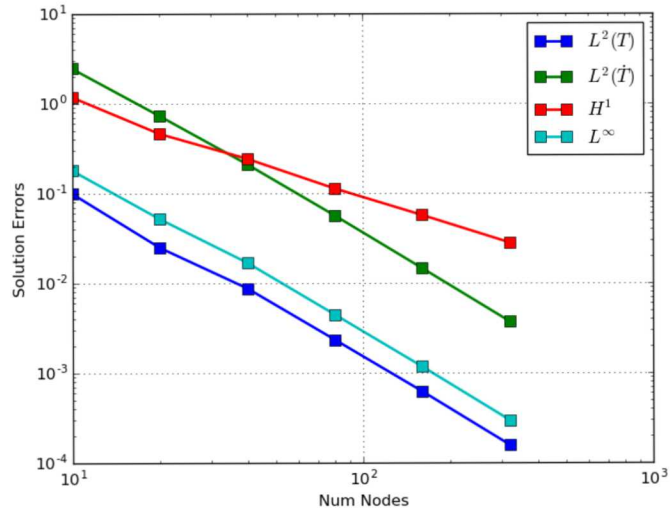


Figure 6.5. Adaptive Time Integration: Errors for BDF2 Fixed

Table 6.5. 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

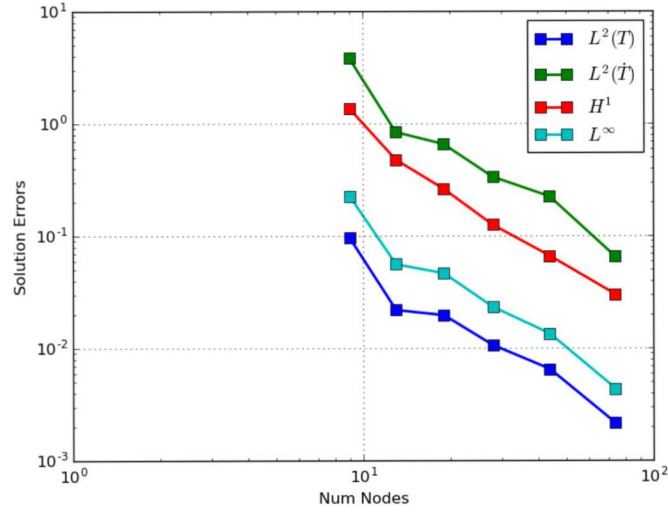


Figure 6.6. Adaptive Time Integration: Errors for BDF2 Adaptive

Table 6.6. 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

Chapter 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.

Table 7.1. 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 7.2.

Table 7.2. 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 $r_i, i = 1, \dots, 4$ 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

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

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

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.

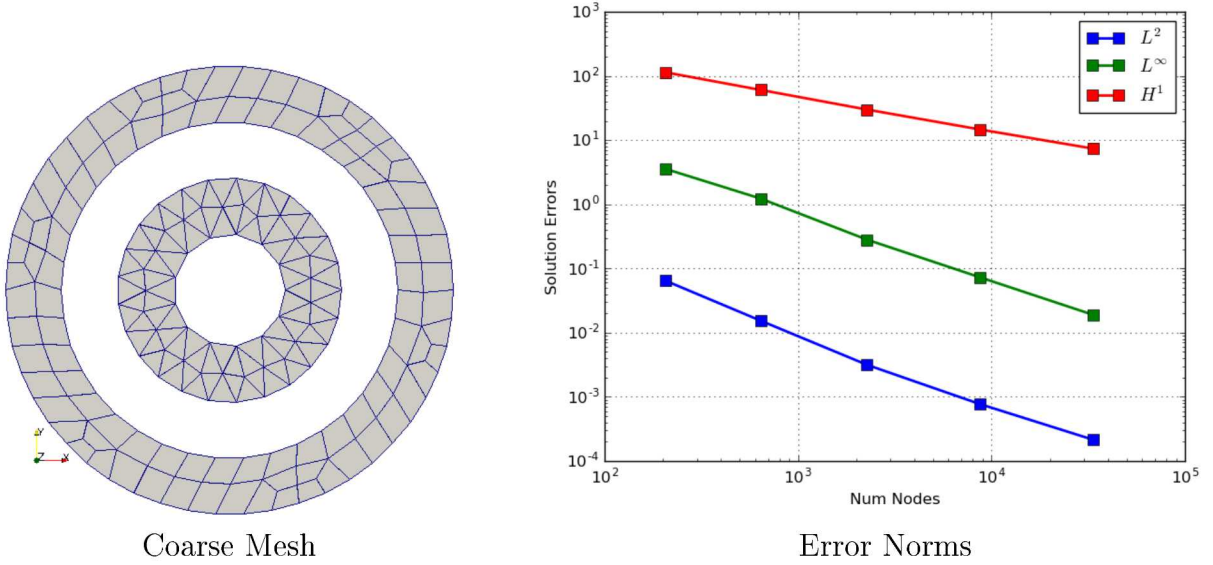


Figure 7.1. Enclosure Radiation 2D

Table 7.3. 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

For input decks see Appendix [12.6.1](#).

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

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

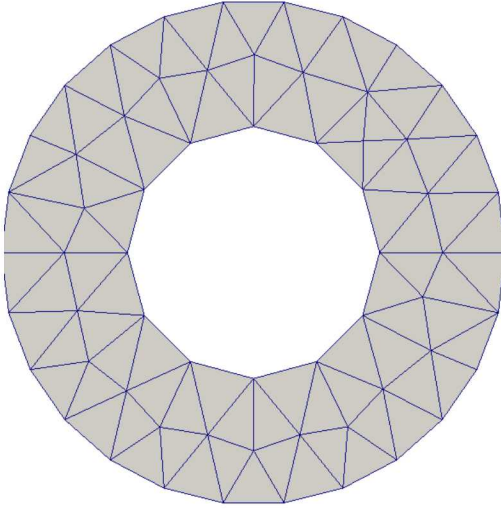
where J is the radiosity, H is the irradiance, q is the flux, and

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

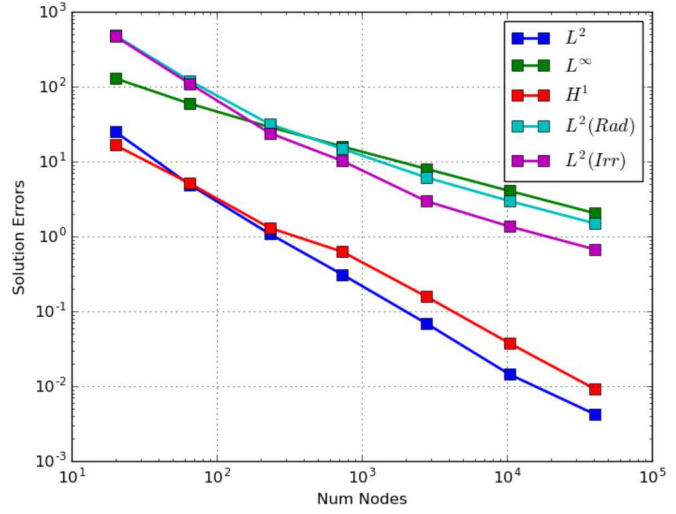
For each mesh, the errors in the temperature solution are computed in the L^2 , L^∞ and H^1 norms. The test passes, only if the observed rates of convergence in these norms are

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.



Coarse Mesh



Error Norms

Figure 7.2. 2D Full Enclosure Radiation

Table 7.4. 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

For input decks see Appendix [12.6.2](#).

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 7.5.

Table 7.5. 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 7.6.

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

Table 7.6. 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

be

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

for arbitrary constants C_1 and C_2 . We will use $r_i, i = 1, \dots, 4$ 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

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

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

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 $T_3 = T_{outer}(r_3)$:

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

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

The fluxes at the surfaces between the two hollow spheres are

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

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

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

$$J_2 = \epsilon_2 \sigma T_2^4 + (1 - \epsilon_2)[F_{22} J_2 + F_{23} J_3]$$

$$J_3 = \epsilon_3 \sigma T_3^4 + (1 - \epsilon_3)[F_{32} J_2 + F_{33} J_3]$$

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.

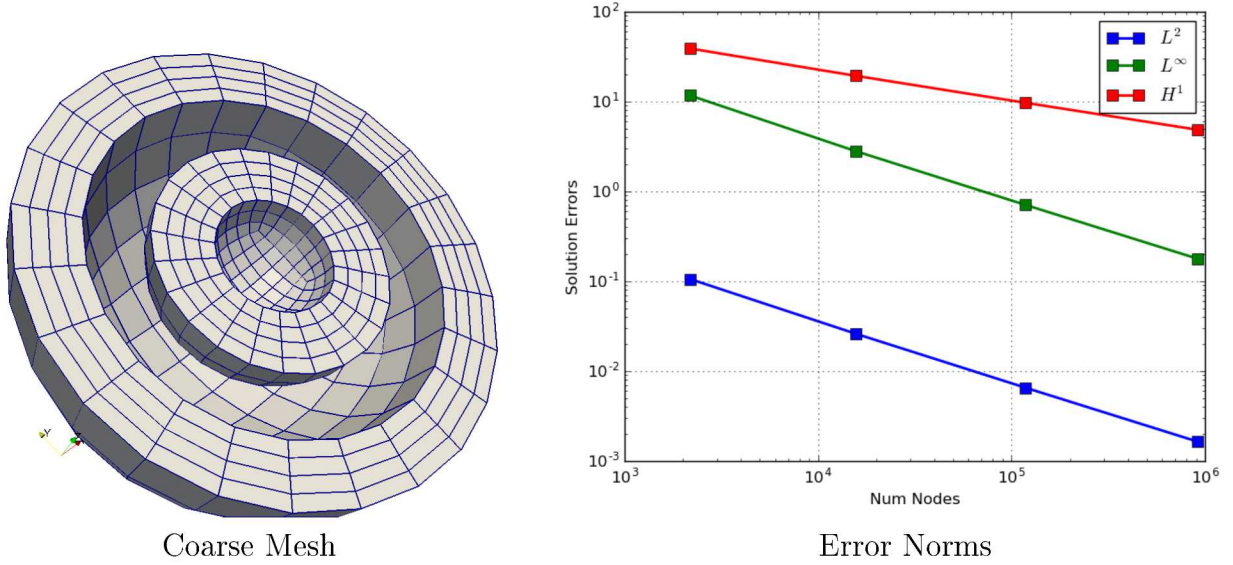


Figure 7.3. Enclosure Radiation

Table 7.7. 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](#).

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.

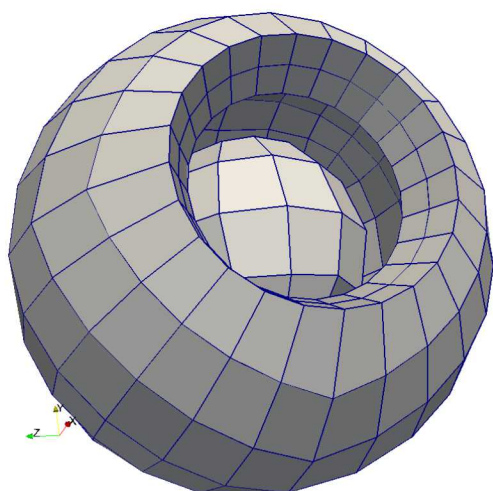
For each mesh, the errors in the temperature solution are computed in the L^2 , L^∞ and H^1 norms. The test passes, only if the observed rates of convergence in these norms are 2, 2, and 1, respectively (within a tolerance).

These optimal rates are observed in this test.

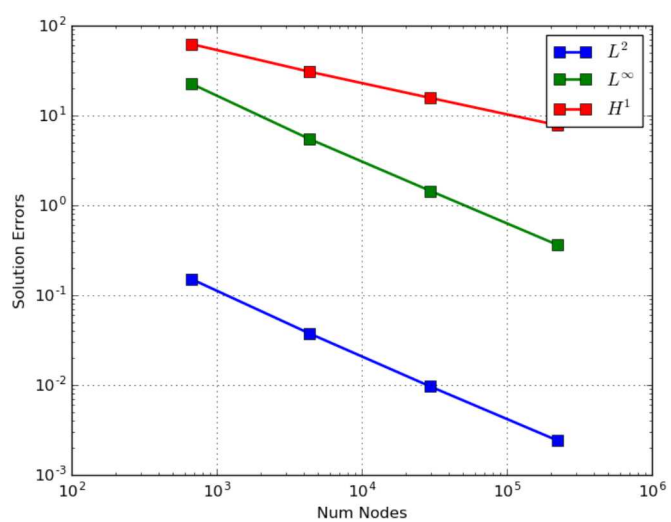
Table 7.8. Partial Enclosure Radiation: Convergence Rates

Num Dofs	L^2	L^∞	H^1
4338	2.23	2.27	1.13
29690	2.12	2.07	1.06
223200	2.06	2.06	1.03

For input decks see Appendix 12.6.4.



Coarse Mesh



Error Norms

Figure 7.4. Partial Enclosure Radiation

Chapter 8

Chemistry

8.1 First Order Reaction (Uniform Temperature)

This problem tests the interface to the CHEMEQ solver under the assumption that the temperature remains constant in space and time. The geometry consists of a unit cube meshed with a single Hex8 element.

8.1.1 Features Tested

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

8.1.2 Boundary Conditions

No boundary conditions are applied. This enables the temperature at all nodes to remain uniform in space and time. The initial temperature is constant 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

$$\begin{aligned} T(x) &= 400, \\ A(t) &= \exp(-\exp(5) \exp(-1000/(RT)) t), \\ B(t) &= 1 - A(t) \end{aligned}$$

where $R = 1.9872$ is the ideal gas constant.

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

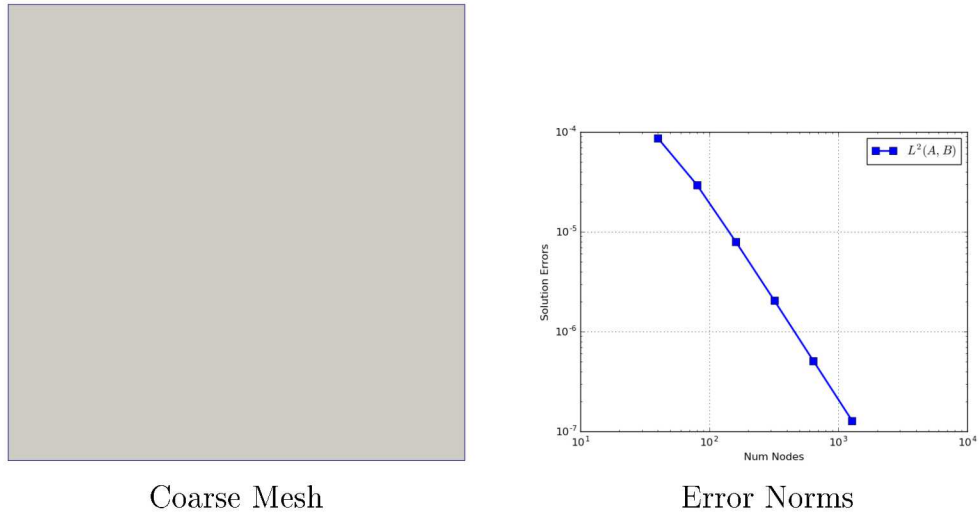


Figure 8.1. First Order Reaction (Uniform Temperature)

Table 8.1. First Order Reaction (Uniform Temperature):
Convergence Rates for Hex8 Meshes

Num Dofs	$L^2(A, B)$
80	1.54
160	1.89
320	1.97
640	2.00
1280	2.00

For input decks see Appendix [12.7.1](#).

8.2 First Order Reaction (Spatially Varying Temperature)

This problem tests the interface to the CHEMEQ solver under the assumption that the temperature remains 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).

8.2.1 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.

8.2.2 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 $B = 0$.

8.2.3 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.

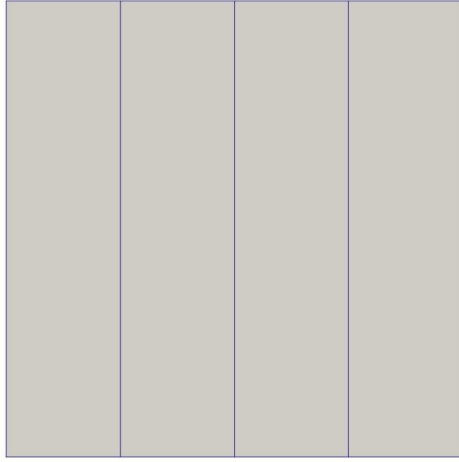
8.2.4 Verification of Solution

A manufactured solution is chosen as

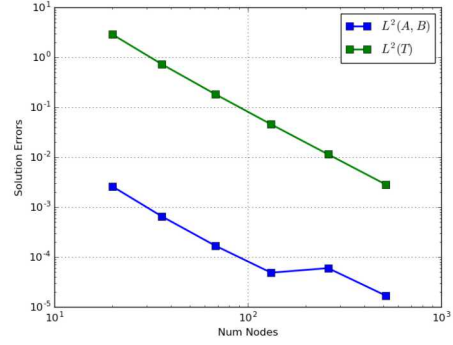
$$\begin{aligned} T(x) &= 400 (1 + 0.2 \cos(\pi x)), \\ A(x, t) &= \exp \left\{ -\exp(5) \exp\left(-\frac{1000}{RT(x)}\right) t \right\}, \\ B(x, t) &= 1 - A(x, t) \end{aligned}$$

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 8.2. First Order Reaction (Spatially Varying Temperature)

Table 8.2. First Order Reaction (Spatially Varying Temperature): Convergence Rates for Hex8 Meshes

Num Dofs	$L^2(A, B)$	$L^2(T)$
36	2.35	2.34
68	2.12	2.18
132	1.88	2.09
260	-0.31	2.04
516	1.85	2.02

For input decks see Appendix [12.7.2](#).

8.3 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.

8.3.1 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.

8.3.2 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 $B = 0$.

8.3.3 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.

8.3.4 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

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

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](#).

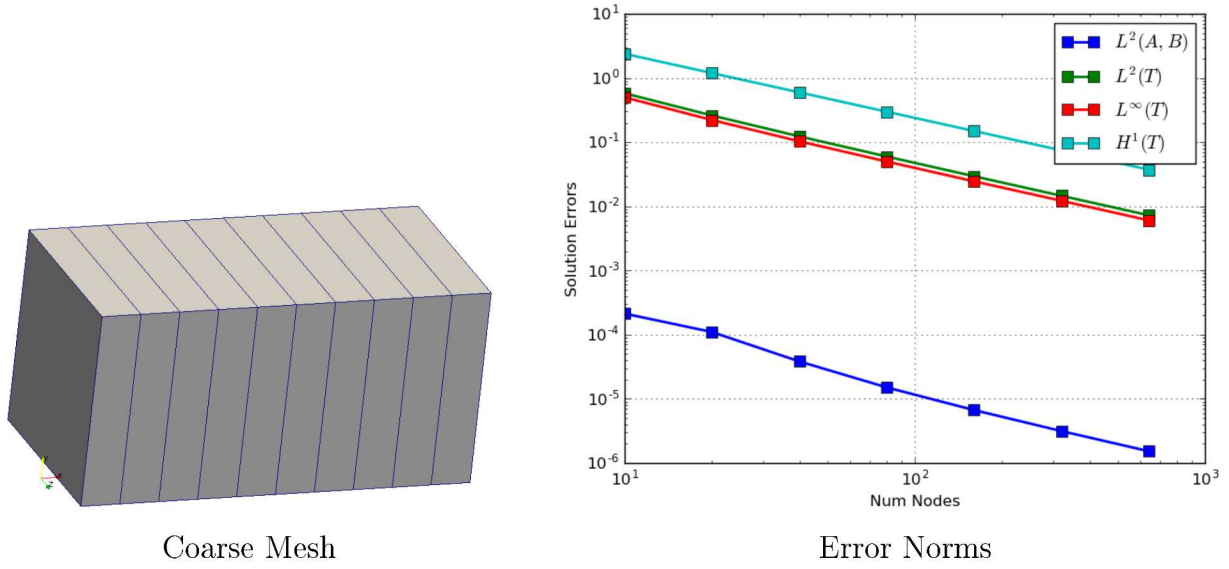


Figure 8.3. First Order Reaction

Table 8.3. First Order Reaction: Convergence Rates for Hex8 Meshes

Num Dofs	$L^2(A, B)$	$L^2(T)$	$L^\infty(T)$	$H^1(T)$
20	0.96	1.15	1.18	1.00
40	1.52	1.08	1.09	1.00
80	1.34	1.04	1.05	1.00
160	1.18	1.02	1.02	1.00
320	1.09	1.01	1.01	1.00
640	1.04	1.01	1.01	1.00

8.4 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.

8.4.1 Features Tested

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

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, thermal conductivity, and specific heat are all constant.

8.4.4 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

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

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](#).

8.5 PMDI Plugin Test

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

8.5.1 Features Tested

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

8.5.2 Boundary Conditions

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

8.5.3 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.

8.5.4 Verification of Solution

The initial conditions are specified as follows: The test includes a Mathematica notebook file

Table 8.4. 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	

(ExpectedSolution.nb) for calculation of expected pressure which is 1.15125e7 Pa or 1669.75 psi.

For input decks see Appendix [12.7.5](#).

Chapter 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

$$T_0 + \exp(C_0(x^2 - 1) + C_1(y^2 - 0.25) + C_2(z^2 - 0.25) + C_3t).$$

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.

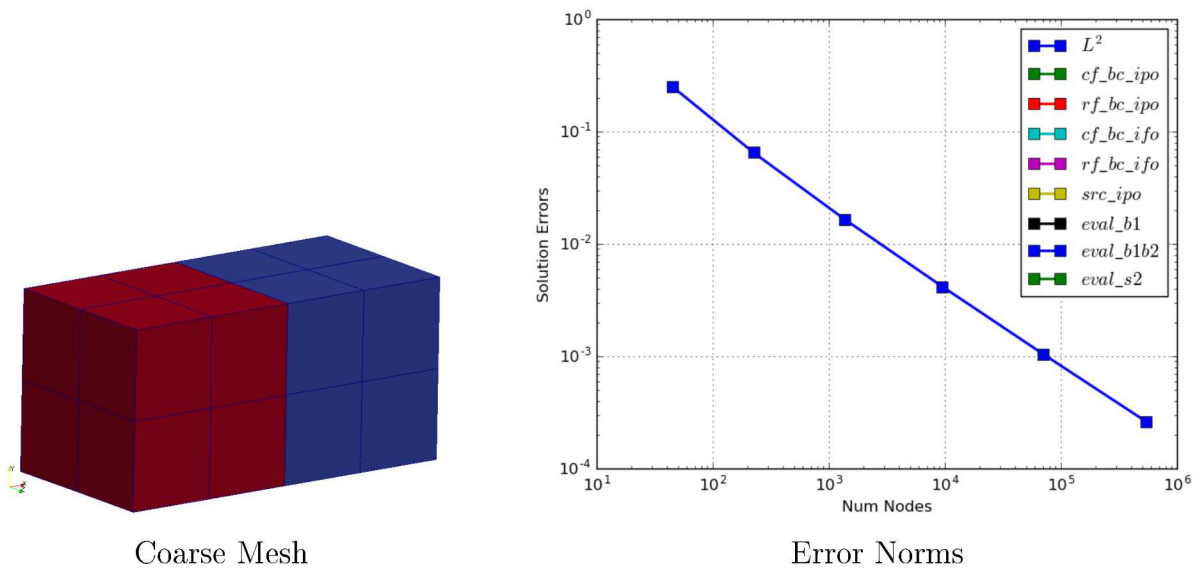


Figure 9.1. Thermal Postprocess

Table 9.1. 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

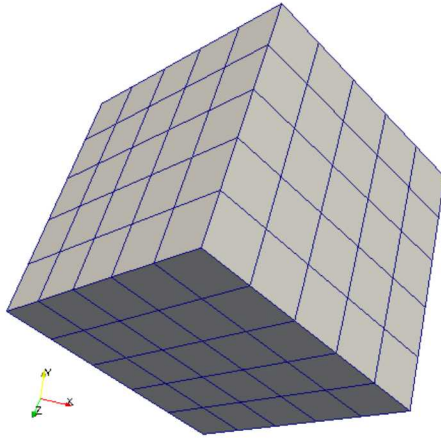
A manufactured solution is chosen as

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

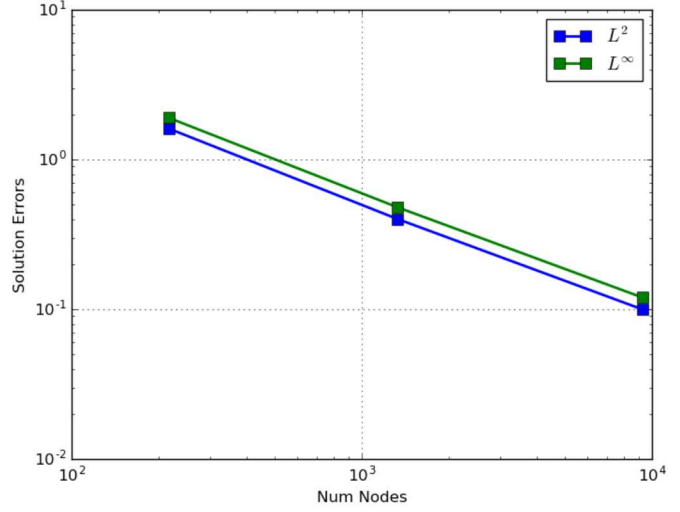
where (X, Y, Z) are the local material coordinates, which are related to the Cartesian coordinates (x, y, z) by a rotation matrix consisting of a product of rotations (22.5 deg around the z -axis and 45 deg around the x -axis).

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).

For input decks see [Appendix 12.8.3](#).



Coarse Mesh



Error Norms

Figure 9.2. Local Cartesian Coordinate System

Table 9.2. Local Cartesian Coordinate System: Convergence Rates

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

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.

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).

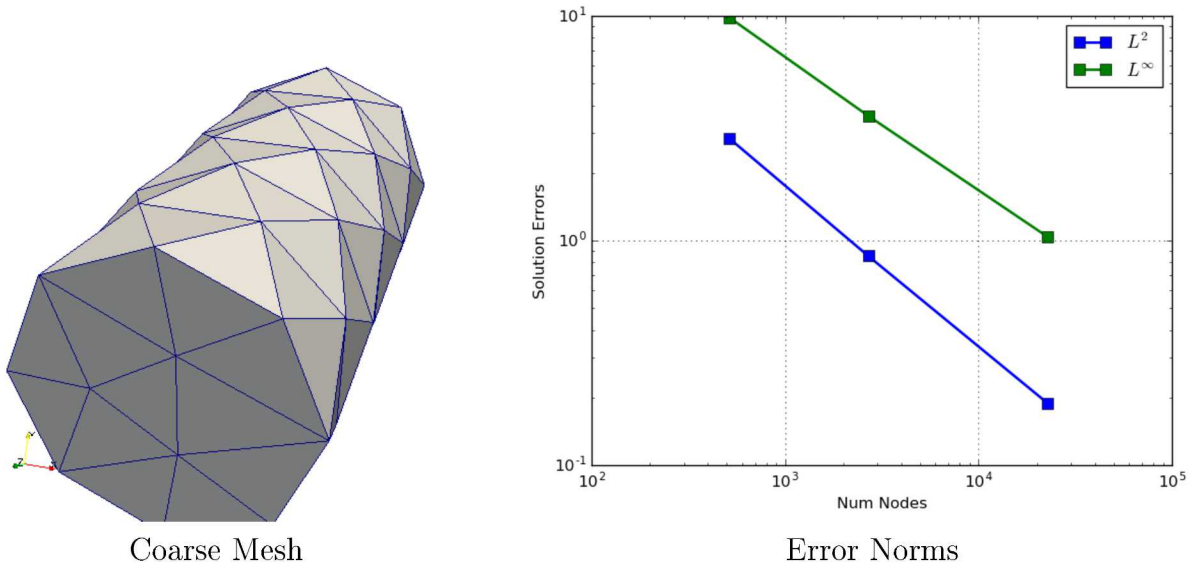


Figure 9.3. Local Cylindrical Coordinate System

For input decks see Appendix 12.8.4.

Documentation for the following tests is in progress:

```
1 nic_material_decomposition/organic_material_decomposition.test|np4
2 tion_verification/solution_verification.test|np8
```

Table 9.3. Local Cylindrical Coordinate System: Convergence Rates

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

Chapter 10

Low-Mach Fluid Flow

Documentation for the following tests is in progress:

```
1 _rtest/aria/cvfemConvTaylorVortex/cvfemConvTaylorVortex.test|np4
2 _rtest/aria/gfemConvTaylorVortex/gfemConvTaylorVortex.test|np4
3 _rtest/aria/hfemConvTaylorVortex/hfemConvTaylorVortex.test|np4
4 mConvTaylorVortex/cvfemConvTaylorVortex.test|np8
5 mSteadyTaylorVortex/cvfemSteadyTaylorVortex.test|np8
6 mSteadyTaylorVortexKeps/cvfemSteadyTaylorVortexKeps.test|np8
7 m_couette_flow/cdfem_couette_flow.test|cdfem_couette_flow_tri3
8 m_couette_flow/cdfem_couette_flow.test|cdfem_couette_flow_tri6
9 ConvTaylorVortex/gfemConvTaylorVortex.test|np8
10 SteadyTaylorVortex/gfemSteadyTaylorVortex.test|np8
```


Chapter 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.

Chapter 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

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

```

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

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

  Begin Trilinos Equation Solver Direct_Solver
    Solution Method = amesos-superlu
  End

  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

```



```

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

  Begin Trilinos Equation Solver Direct_Solver
    Solution Method = amesos-superlu
  End

  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

  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

  Begin Trilinos Equation Solver Direct_Solver
    Solution Method = amesos-superlu
  End

  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

  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

    Begin Trilinos Equation Solver Direct_Solver
        Solution Method = amesos-superlu
    End

    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

    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

  Begin Trilinos Equation Solver Direct_Solver
    Solution Method = amesos-superlu
  End

  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

  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

  Begin Trilinos Equation Solver Direct_Solver
    Solution Method = amesos-superlu
  End

  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

  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 vhl
        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

    Begin Trilinos Equation Solver Direct_Solver
        Solution Method = amesos-superlu
    End

    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

    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

  Begin Trilinos Equation Solver Direct_Solver
    Solution Method = amesos-superlu
  End

  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

  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

Begin Trilinos Equation Solver Direct_Solver
  Solution Method = amesos-superlu
End

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

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
```

```

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

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

#####

Begin TRILINOS Equation Solver trilinos_solve #instead of AZTEC
#Solution Method = cg
Solution Method = GMRES #use GMRES with contact
#Solution Method = BICGSTAB

Preconditioning Method = DD-ILUT #jacobi
#Preconditioning Method = jacobi

Maximum Iterations = 1000
Matrix Scaling = row-sum
Residual Norm Tolerance = 1.0e-12
Residual Norm Scaling = R0 #NONE

Restart Iterations is 100 #use with GMRES
preconditioning steps is 1 #use with GMRES
Param-Real AZ_ilut_fill value 5.0

polynomial order = 300 #<=== needed for convergence
ilu threshold = 1.0e-6 #<=== needed for convergence

End TRILINOS Equation Solver trilinos_solve

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 transfer 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

#
# xA xB azimuthal section 1 -dphi/2 ~ +theta
# A | AB | B axial (x axis) regions 0-theta y| y| V
# ===== surfaces | _ > 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

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

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
    End System Main
  End

  Begin Transient Time_Block
  advance myRegion
  End

  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](#)

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

    begin trilinos equation solver direct_solver
        solution method = amesos-umfpack
    end trilinos equation solver direct_solver

    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

    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
  end
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
    normal tolerance = 0.
    tangential tolerance = 0.
  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

```

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

```

```

End Finite Element Model bar

begin trilinos equation solver direct_solver
  solution method = amesos-umfpack
end trilinos equation solver direct_solver

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

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
    normal tolerance = 0.
    tangential tolerance = 0.
  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

```

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

    begin trilinos equation solver direct_solver
        solution method = amesos-umfpack
    end trilinos equation solver direct_solver

    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

    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

```

```

        normal tolerance = 0.
        tangential tolerance = 0.
    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

```

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

    begin trilinos equation solver direct_solver
        solution method = amesos-umfpack
    end trilinos equation solver direct_solver

```

```

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

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
  end
end

```

```

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
    normal tolerance = 0.
    tangential tolerance = 0.
  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

```

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

begin trilinos equation solver direct_solver
  solution method = amesos-umfpack
end trilinos equation solver direct_solver

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

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
                normal tolerance = 0.
                tangential tolerance = 0.
            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

```

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

    begin trilinos equation solver direct_solver
        solution method = amesos-umfpack
    end trilinos equation solver direct_solver

    Begin Trilinos Equation Solver Iterative_Solver
        Solution Method      = GMRES
        Preconditioning Method = Jacobi
        Maximum Iterations   = 20000
        Residual Norm Scaling = R0
    End

```

```

    Residual Norm Tolerance = 1.0e-12
End

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
        normal tolerance = 0.
        tangential tolerance = 0.
    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

Hex8-Hex8 Case

Tet4-Tet4 Case

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

  Begin Trilinos Equation Solver Direct_Solver
    Solution Method = amesos-superlu
  End

  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

  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
    tangential tolerance = 0.0
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

  Begin Trilinos Equation Solver Direct_Solver
    Solution Method = amesos-superlu
  End

  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

  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
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 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
      normal tolerance = 0.0
      tangential tolerance = 0.0
    end
    begin enforcement enf_1
      Enforcement for Energy = Tied_Temperature
    end
  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

  Begin Trilinos Equation Solver Direct_Solver

```



```

    Solution Method = amesos-superlu
End

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

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
    normal tolerance = 0.0
    tangential tolerance = 0.0
  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

  Begin Trilinos Equation Solver Direct_Solver
    Solution Method = amesos-superlu
  End

  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

  BEGIN FINITE ELEMENT MODEL cube
    database name = cube_contact_h{N}_tet4.e
    coordinate system is cartesian
  END

```

```

        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

```

```

        normal tolerance = 0.0
        tangential tolerance = 0.0
    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

    Begin Trilinos Equation Solver Direct_Solver
        Solution Method = amesos-superlu
    End

    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

    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
END SIERRA myJob

```

```

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
    normal tolerance = 0.0
    tangential tolerance = 0.0
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

  Begin Trilinos Equation Solver Direct_Solver
    Solution Method = amesos-superlu
  End

  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

  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
    normal tolerance = 0.0
    tangential tolerance = 0.0
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

    Begin Trilinos Equation Solver Direct_Solver
        Solution Method = amesos-superlu
    End

    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

    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

  Begin Trilinos Equation Solver Direct_Solver
    Solution Method = amesos-superlu
  End

  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

  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

```

```

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
    normal tolerance = 0.0
    tangential tolerance = 0.0
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

    Begin Trilinos Equation Solver Direct_Solver
        Solution Method = amesos-superlu
    End

    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

    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

```

```

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
    normal tolerance = 0.0
    tangential tolerance = 0.0
  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)

Tri3

```
BEGIN SIERRA Aria

Title \$
1-d standard conduction problem, Carslaw and Jaeger P. 292\$

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

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
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

```

Tet4

```

BEGIN SIERRA Aria

Title \$
1-d standard conduction problem, Carslaw and Jaeger P. 292\$

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

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+y*y+z*z))*(z/sqrt(x*x+y*y+z*z))"
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
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

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

  Begin Trilinos Equation Solver Direct_Solver
    Solution Method = amesos-superlu
  End

  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

```

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

  Begin Trilinos Equation Solver Direct_Solver
    Solution Method = amesos-superlu
  End

  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

  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

```

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

    Begin Trilinos Equation Solver Direct_Solver
        Solution Method = amesos-superlu
    End

    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

```

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

    Begin Trilinos Equation Solver Direct_Solver
        Solution Method = amesos-superlu
    End

    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

```

```

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

```

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

  Begin Trilinos Equation Solver Direct_Solver
    Solution Method = amesos-superlu
  End

  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

```

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

    Begin Trilinos Equation Solver Direct_Solver
        Solution Method = amesos-superlu
    End

    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

```

```

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

    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

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

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

```

```

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

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

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

Begin Procedure myProcedure

    Begin Solution Control Description
        Use System Main
        Begin System Main
            Begin Sequential Steady
                Advance myRegion
            End
        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
    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-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

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

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)

```
BEGIN SIERRA Aria

  Title Verification Problem for Coupled Chemistry Diffusion

  Begin Field Function species
    Use Quadrature Field species
    Integration Order Is 2
    Dimension Is 2
  End

  load user plugin file ./Exact_solution.so

  Begin User Function ufuncAB
    Load From File ./Exact_solution.so Using Function registerExactSolnAB
  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 = cube_one_hex8.g
    Use material hmx for block_1
  END FINITE ELEMENT MODEL block

  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

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 = {0.001/2** (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 TimeSteps
  Compute Difference L2      Of ufuncAB species
  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 all_blocks = chemeq_heating MODEL = hmx

  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 = 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)}
    Title Aria Chem/Diffusion Verification
    Nodal Variables = solution->temperature as T
    Element Variables = A B AEX

```

```

END RESULTS OUTPUT LABEL diffusion output

IC const on block_1 temperature = 400.0

USE FINITE ELEMENT MODEL block
use LINEAR SOLVER solve_temperature

END Aria REGION myRegion

END procedure myProcedure

END SIERRA Aria

```

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

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

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
  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}.exo $ exodusii
  decomposition method = rib

  Use material hmx for block_1
END FINITE ELEMENT MODEL block

```

```

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

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
  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

    begin parameters for chemeq model hmx
      number of reactions = 1

      species names are A
      species phases are Condensed
    end
  end

```

```

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 = constant value=3

#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

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

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
  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_multispecies.so

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

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
{vex0Tvex}    \# 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,         effective 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 iblock.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
#       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 gvcl 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

  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

  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

      Begin Trilinos Equation Solver Direct_Solver

```

```

        Solution Method = amesos-superlu
    End

    BEGIN FINITE ELEMENT MODEL cube
        database name = square_h{N}_tri3.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 conduction in local
# coordinate 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
#       TO      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 0.000000
        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

    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

    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 conduction in local
# coordinate 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 0.000000
    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

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

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

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1 MS 0899 Technical Library, 9536 (electronic copy)

