ALBANY EXAMPLE: Transient heat problem

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Note: To complete this tutorial you must have access to Simmetrix Inc. products.

Find the temperature in a long bar with constant cross section and homogeneous material, which is oriented along the x-axis and is perfectly insulated laterally, so the heat flows in the x-direction only.

Material properties	Geometric properties	Loading
$k = 1$ $\rho c_p = 1$	$L = 1$	$T(x,0) = 1$ $T(0,t) = 0$ $T(L,t) = 0$

Analysis assumption and modeling notes

The problem is solved in 3D using an unstructured mesh. The temperature solution is governed by the one-dimensional heat equation:

$$\frac{\partial T}{\partial t} = \frac{k}{\rho c_p}\frac{\partial^2 T}{\partial x^2}$$

The boundary conditions are as follows:

$$T(0,t) = 0 \quad T(L,t) = 0 \quad for\ all\ t\ \geq 0$$

Furthermore the initial temperature in the bar at t =0 must satisfy

$$T(x,0) = T_i$$

The analytical solution is given in terms of a Fourier series:

$$T(x,t) = \sum_{n=1}^{\infty} B_n \sin\frac{n\pi x}{L} e^{-k\lambda_n^2 t}$$

Where

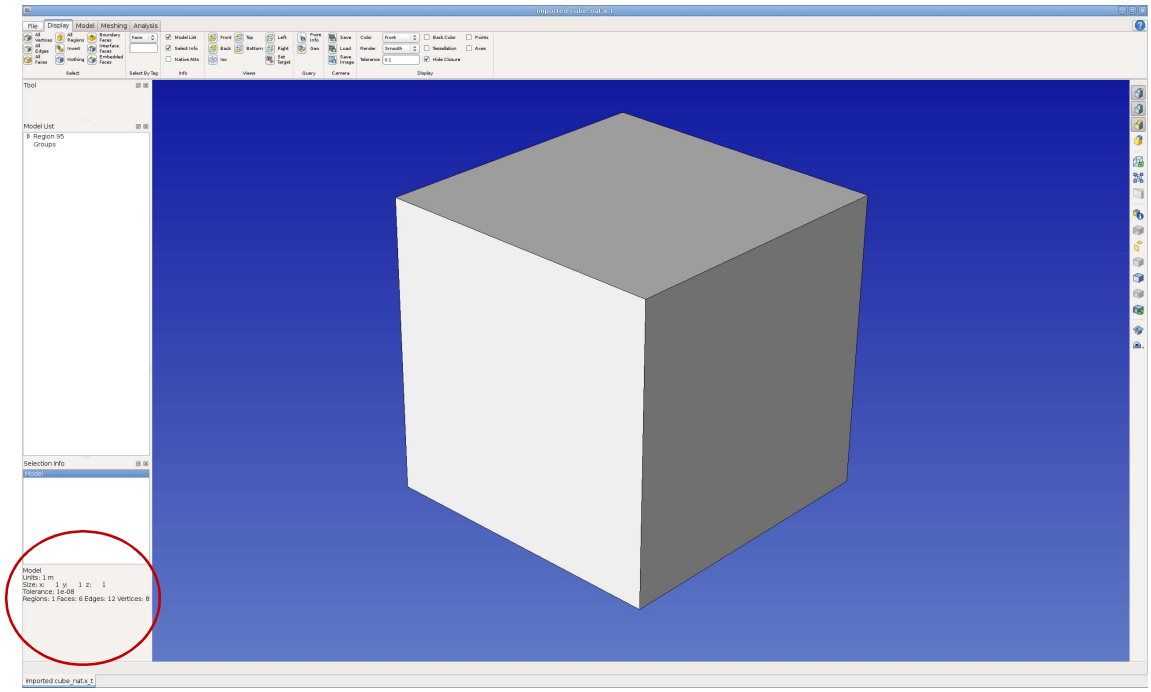
$$B_n = \frac{2}{L}\int_0^L T_i \sin\frac{n\pi x}{L}\, dx$$

And

$$\lambda_n = \frac{n\pi}{L}$$

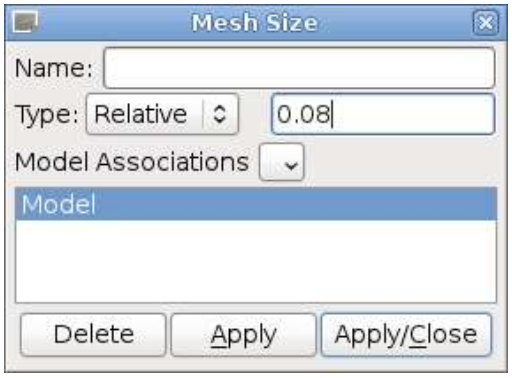
Step by step instructions:

- Make a directory that will store your files (i.e. HeatTransfer/). You may also want to put the meshes and models in a different folder (i.e. HeatTransfer/mesh/)
- Using a CAD system (i.e. NX), create a cube with length L = 1 m (or 1000 mm). Save the model as a parasolid model (i.e. cube_nat.x_t).
- Open simmoder -> File -> Import Geometry …
  Choose the model *cube_nat.x_t* that you generated in the previous step.

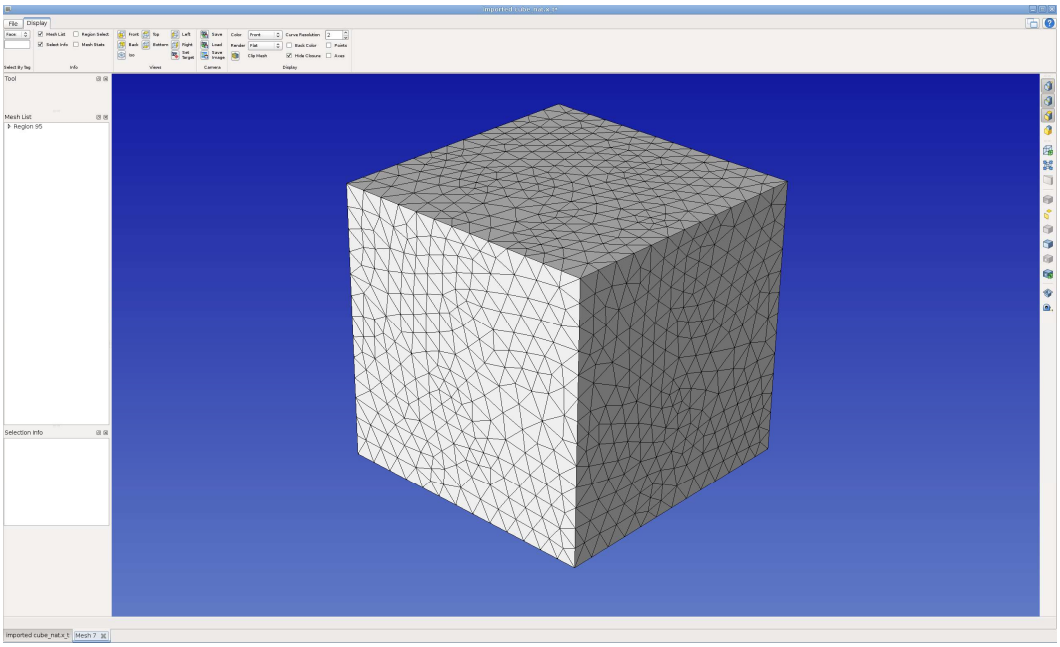


Verify that units in 'm' and x: 1, y: 1 and z: 1.

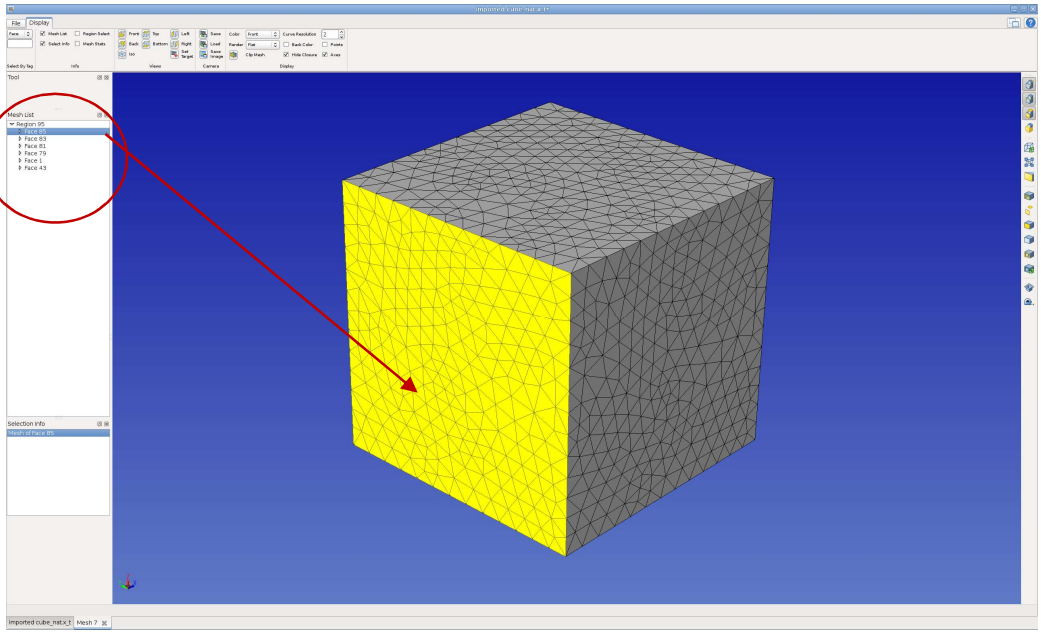
- Meshing -> Mesh Attributes -> Mesh Size -> Relative
  Specify 0.08 -> Apply / Close



Generate Mesh -> Start -> Show Mesh



File -> Save Mesh… (i.e. cube.sms). Save the model too (i.e. cube.smd)



Take note of the name of the region (Region 95) and the name of the faces (if you click on the face it will highlight the name, for this case Face 85.), you will need this information to construct the Albany input deck.

- Close simmodeler
- Cases are setup in Albany by editing input decks. Users should select an editor of choice with which to do this, such as emacs, vi, gedit, kate, nedit, etc. Copy, for example, the input decks

from “Albany/examples/LCM/HeatTransient/inputT.xml” and “Albany/examples/LCM/HeatTransient/materials.xml”.

- Open inputT.xml using emacs.

```
<ParameterList>
    <ParameterList name="Problem">
        <Parameter name="Name" type="string" value="Mechanics 3D"/>
        <Parameter name="Solution Method" type="string" value="Transient"/>
        <Parameter name="MaterialDB Filename" type="string" value="materials.xml"/>
        <Parameter name="Second Order" type="string" value="Trapezoid Rule"/>
        <ParameterList name="Temperature">
            <Parameter name="Variable Type" type="string" value="DOF"/>
        </ParameterList>
        <ParameterList name="Displacement">
            <Parameter name="Variable Type" type="string" value="None" />
        </ParameterList>
        <ParameterList name="Dirichlet BCs">
            <Parameter name="DBC on NS xmin for DOF T" type="double" value="0.0" />
            <Parameter name="DBC on NS xmax for DOF T" type="double" value="0.0" />
        </ParameterList>

        <ParameterList name="Initial Condition">
            <Parameter name="Function" type="string" value="Constant" />
            <Parameter name="Function Data" type="Array(double)" value="{1.0}" />
        </ParameterList>
        <ParameterList name="Initial Condition Dot">
            <Parameter name="Function" type="string" value="Constant"/>
            <Parameter name="Function Data" type="Array(double)" value="{0.0}"/>
        </ParameterList>

        <ParameterList name="Parameters">
            <Parameter name="Number" type="int" value="1"/>
            <Parameter name="Parameter 0" type="string" value="Time"/>
        </ParameterList>

        <ParameterList name="Response Functions">
            <Parameter name="Number" type="int" value="1"/>
            <Parameter name="Response 0" type="string" value="Solution Average"/>
        </ParameterList>


    </ParameterList>
```

The box highlighted above are the main parts that you would like to change. The first block correspond to the location and name of the material file. The second block specify where are the Dirichlet boundary conditions. For this particular case we are applying DBC (Dirichlet Boundary Conitions) on NS (nodal set) xmin and xmax for DOF (Degree of Freedom) T (Temperature). Xmin and xmax are defined in the discretization section as shown below. The third block is used to specify the initial conditions. In this example we are using a predictor/corrector algorithm (based on the trapezoidal rule) to integrate the heat equation in time.

```
</ParameterList>

<ParameterList name="Discretization">
    <Parameter name="Method" type="string" value="Sim" />
    <Parameter name="Workset Size" type="int" value="50" />
    <Parameter name="Sim Model Input File Name" type="string" value="mesh/cube.smd" />
    <Parameter name="Sim Input File Name" type="string" value="mesh/cube.sms" />
    <Parameter name="Sim Output File Name" type="string" value="out.vtk" />
    <Parameter name="Element Block Associations" type="TwoDArray(string)" value="2x1:{95,cube}" />
    <Parameter name="Node Set Associations" type="TwoDArray(string)" value="2x2:{85,81,xmin,xmax}" />
    <Parameter name="Cubature Degree" type="int" value="1" />
    <Parameter name="Separate Evaluators by Element Block" type="bool" value="false" />
    <Parameter name="QP Temperature from Nodes" type="bool" value="false"/>
    <!-- Have both velocity and acceleration -->
    <Parameter name="Number Of Time Derivatives" type="int" value="2"/>
</ParameterList>
```

This is the discretization section. The first box specify the location and names of the simmetrix model and mesh. The second block specify that we have one block, identified with ID 95 (corresponding to Region 95) and we want to assign the name “cube” to it. The next line associate a node set with the model. We are specifying that xmin correspond to ID 85 (Face 85) and xmax to ID 81 (Face 81). *Keep Number of Time Derivatives equal to 2.*

```
<ParameterList name="Piro">
    <ParameterList name="Trapezoid Rule">
        <Parameter name="Num Time Steps" type="int" value="100"/>
        <Parameter name="Final Time" type="double" value="0.05"/>
        <Parameter name="Initial Time" type="double" value="0.0"/>
        <ParameterList name="NOX">
            <ParameterList name="Printing">
                <ParameterList name="Output Information">
                    <Parameter name="Error" type="bool" value="true" />
                    <Parameter name="Warning" type="bool" value="true" />
                    <Parameter name="Outer Iteration" type="bool" value="true" />
                    <Parameter name="Parameters" type="bool" value="false" />
                    <Parameter name="Details" type="bool" value="false" />
                    <Parameter name="Linear Solver Details" type="bool" value="true" />
                    <Parameter name="Stepper Iteration" type="bool" value="true" />
                    <Parameter name="Stepper Details" type="bool" value="true" />
                    <Parameter name="Stepper Parameters" type="bool" value="false" />
                </ParameterList>
                <Parameter name="Output Precision" type="int" value="3" />
                <Parameter name="Output Processor" type="int" value="0" />
            </ParameterList>
        </ParameterList>
    </ParameterList>
```

The time step is defined by: (Final Time – Initial Time) / Number of Time Steps.

```
<ParameterList name="NOX">
    <ParameterList name="Direction">
        <Parameter name="Method" type="string" value="Newton"/>
        <ParameterList name="Newton">
            <ParameterList name="Linear Solver">
                <Parameter name="Tolerance" type="double" value="1e-6"/>
            </ParameterList>
            <Parameter name="Forcing Term Method" type="string" value="Constant"/>
            <Parameter name="Rescue Bad Newton Solve" type="bool" value="1"/>
            <ParameterList name="Stratimikos Linear Solver">
                <ParameterList name="NOX Stratimikos Options">
                </ParameterList>
                <ParameterList name="Stratimikos">
                    <Parameter name="Linear Solver Type" type="string" value="Belos"/>
                    <ParameterList name="Linear Solver Types">
                        <ParameterList name="Belos">
                            <Parameter name="Solver Type" type="string" value="Block GMRES"/>
                            <ParameterList name="Solver Types">
                                <ParameterList name="Block GMRES">
                                    <Parameter name="Convergence Tolerance" type="double" value="1e-12"/>
                                    <Parameter name="Output Frequency" type="int" value="10"/>
                                    <Parameter name="Output Style" type="int" value="1"/>
                                    <Parameter name="Verbosity" type="int" value="33"/>
                                    <Parameter name="Maximum Iterations" type="int" value="400"/>
                                    <Parameter name="Num Blocks" type="int" value="200"/>
                                    <Parameter name="Flexible Gmres" type="bool" value="true" />
                                </ParameterList>
                            </ParameterList>
                        </ParameterList>
                    </ParameterList>
                    <Parameter name="Preconditioner Type" type="string" value="Ifpack2"/>
                    <ParameterList name="Preconditioner Types">
                        <ParameterList name="Ifpack2">
                            <Parameter name="Overlap" type="int" value="2" />
                            <Parameter name="Prec Type" type="string" value="RILUK" />
                            <ParameterList name="Ifpack2 Settings">
                                <Parameter name="fact: drop tolerance"     type="double" value="0.0" />
                                <Parameter name="fact: ilut level-of-fill" type="double" value="1" />
                                <Parameter name="fact: level-of-fill"      type="int"    value="1" />
                            </ParameterList>
```

In this block you specify the type of linear solver and preconditioner that you want to use. For this is example is block GMRES with RILUK preconditioner.

```
            <ParameterList name="Line Search">
                <ParameterList name="Full Step">
                    <Parameter name="Full Step" type="double" value="1"/>
                </ParameterList>
            </ParameterList>
            <Parameter name="Nonlinear Solver" type="string" value="Line Search Based"/>
            <ParameterList name="Status Tests">
                <Parameter name="Test Type" type="string" value="Combo"/>
                <Parameter name="Combo Type" type="string" value="OR"/>
                <Parameter name="Number of Tests" type="int" value="2"/>
                <ParameterList name="Test 0">
                    <Parameter name="Test Type" type="string" value="NormF"/>
                    <Parameter name="Norm Type" type="string" value="Two Norm"/>
                    <Parameter name="Scale Type" type="string" value="Scaled"/>
                    <Parameter name="Tolerance" type="double" value="1e-3"/>
                </ParameterList>
                <ParameterList name="Test 1">
                    <Parameter name="Test Type" type="string" value="MaxIters"/>
                    <Parameter name="Maximum Iterations" type="int" value="20"/>
                </ParameterList>
            </ParameterList>
        </ParameterList>
    </ParameterList>
</ParameterList>
```

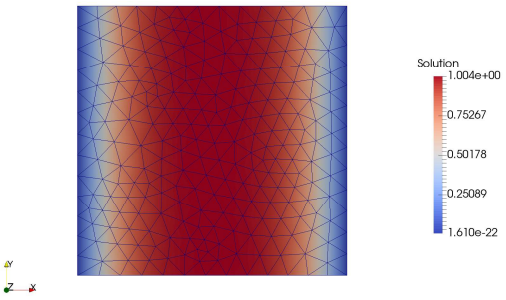
This section specify the termination criteria for the nonlinear step. We are specifying 2 termination criteria. Whatever is reach first the nonlinear iteration will stop.

Now we look at the material file:

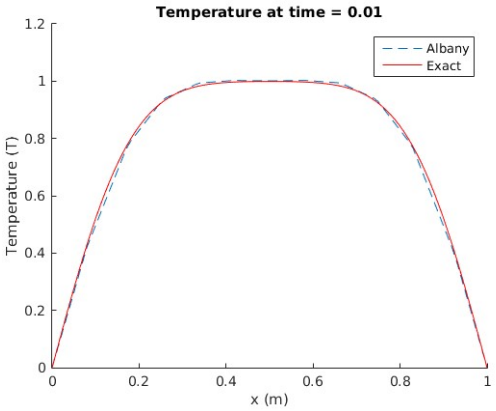
```
<ParameterList>
    <!-- <Parameter name="Reference Material" type="string" value="Metal"/> -->

    <ParameterList name="ElementBlocks">

       <ParameterList name="cube">
            <Parameter name="material" type="string" value="Iron" />
       </ParameterList>
    </ParameterList>

    <ParameterList name="Materials">

        <ParameterList name="Iron">
            <ParameterList name="Material Model">
                <Parameter name="Model Name" type="string" value="Elastic"/>
            </ParameterList>
            <ParameterList name="Elastic Modulus">
                <Parameter name="Elastic Modulus Type" type="string" value="Constant"/>
                <Parameter name="Value" type="double" value="1.0"/>
            </ParameterList>
            <ParameterList name="Poissons Ratio">
                <Parameter name="Poissons Ratio Type" type="string" value="Constant"/>
                <Parameter name="Value" type="double" value="0.0"/>
            </ParameterList>
            <ParameterList name="Thermal Conductivity">
                <Parameter name="Thermal Conductivity Type" type="string" value="Constant"/>
                <Parameter name="Value" type="double" value="1.0"/>
            </ParameterList>
            <Parameter name="Reference Temperature" type="double" value="0.0"/>
            <Parameter name="Initial Temperature" type="double" value="1.0"/>
            <Parameter name="Thermal Transient Coefficient" type="double" value="1.0"/>
            <Parameter name="Thermal Expansion Coefficient" type="double" value="0.0"/>
            <Parameter name="Density" type="double" value="1.0"/>
            <Parameter name="Heat Capacity" type="double" value="1.0"/>
        </ParameterList>

    </ParameterList>

</ParameterList>
```

The first box specify were this material will be applied. In this case the region ID name “cube” (assigned in the discretization). Then we specify a name to this material, “Iron”. The next block specify the properties of the material named “Iron”. The only properties affecting this model correspond to the last two box highlighted. The other properties are not used at all.

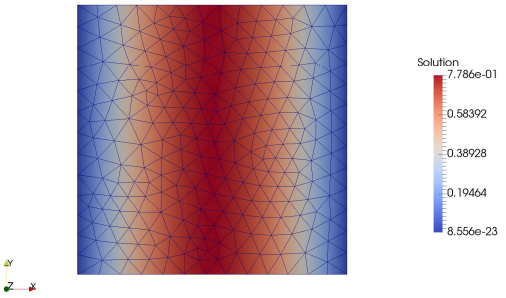
- Running Albany in serial: AlbanyT inputT.xml. Where “AlbanyT” is the executable.
- Use paraview to post-process the output files.



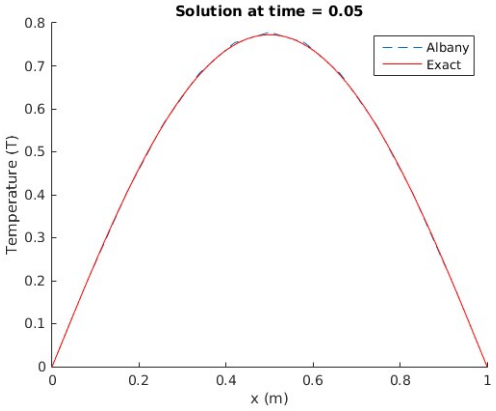
(a)



(b)



(c)



(d)

Figure 1. Temperature distribution. (a) Temperature at time t = 0.01. (b) Temperature profile comparing Albany with exact solution for time t = 0.01. (c) Temperature at time t = 0.05. (d) Temperature profile comparing Albany with exact solution for time t = 0.05.