TriComp 5.0

TDiff

Finite-element Thermal Transport
with Temperature-dependent Materials

Field Precision
Copyright 2002

PO Box 13595
Albuquerque, New Mexico 87192 U.S.A.
Telephone: 505-220-3975
FAX: 505-294-0222
E Mail: techinfo@fieldp.com
Internet: http://www.fieldp.com
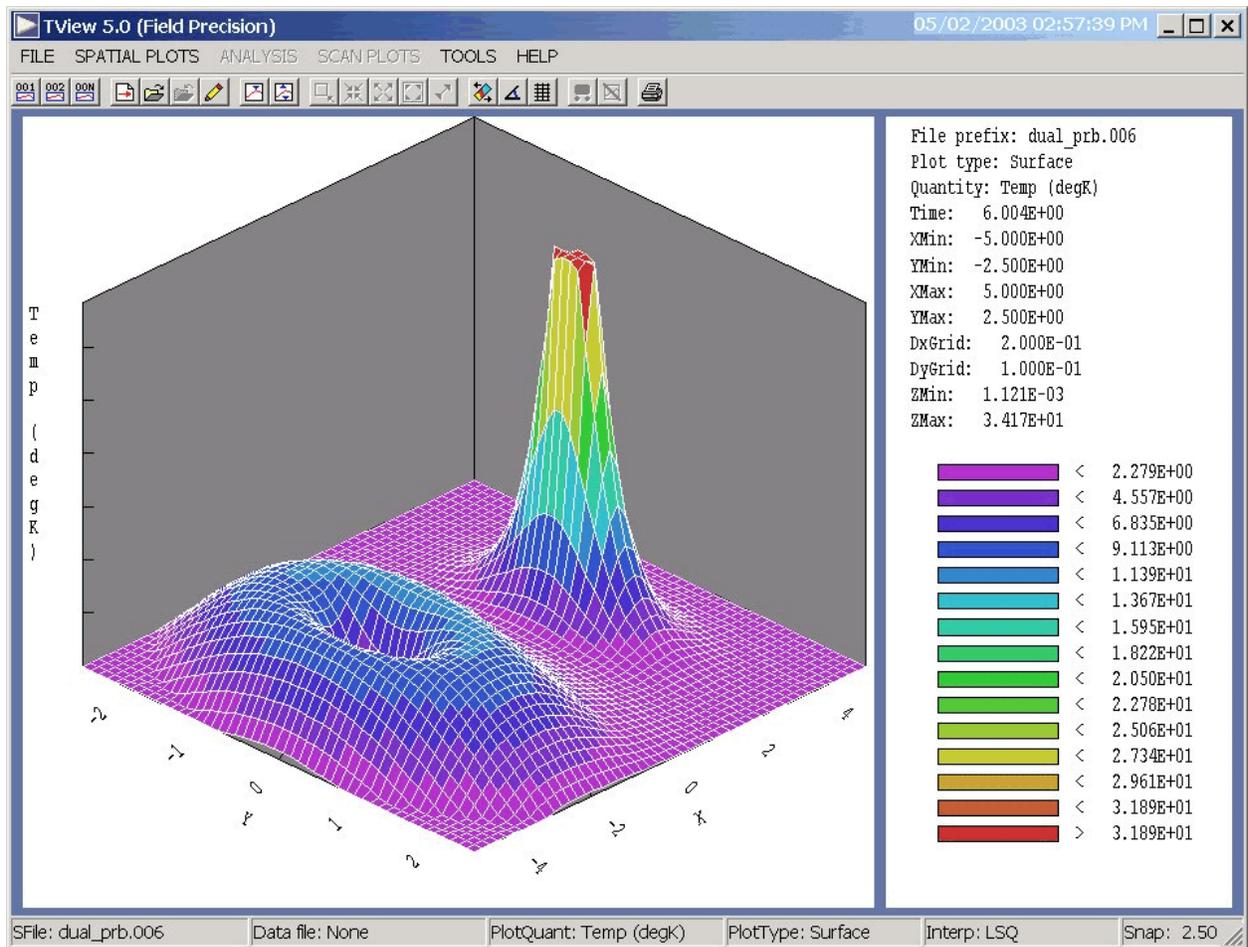
Figure 1. **TView** post-processor work environment

1. Program function

The **TDiff** package handles a wide variety of thermal transport problems in solids or gels. The program solves the two-dimensional thermal diffusion equation in cylindrical and rectangular geometries by finite-element methods . **TDiff** can determine steady-state as well as dynamic solutions. In time-dependent solutions you can define multiple sources with arbitrary temperature histories using a flexible system of tabular function input. There is also the option to define temperature-dependent thermal conductivity and specific heat. In dynamic runs the program produces multiple data files at specified times and a history file of temperature at given locations. Data files can be analyzed with **TView**, an interactive graphical post-processor. The package also contains the standard Field Precision utility **Probe** for inspecting history files.

The walkthrough example in the following section gives an overview of the solution process. Section 3 summarizes units and conversion factors used in **TDiff** solutions. Section 4 outlines typical steps in run while Section 5 covers the structure of the command script that controls the program. Sections 6 and 7 describe script commands to set control parameters and material properties for steady-state solutions. Sections 8 through 11 cover script commands for dynamic solutions. Section 12 reviews special correction features in **Mesh** to avoid numerical instabilities in dynamic simulations. Section 13 discusses the interpretation of boundary conditions in thermal solution. Section 14 covers operation of **TDiff** as an interactive Windows program that you can run from the **TC** program launcher. Section 15 explains how to run **TDiff** in the background from the Command Prompt or under the control of the **GCon** utility for extended data runs. Sections 16 through 20 address operation of the **TView** post-processor used to create plots and to perform quantitative analysis. Finally, Section 21 documents the format of the **TView** output file.

2. Walkthrough example

You can test your installation with the following example that illustrates the steps of a **TDiff** solution. In the discussion we assume that the programs are installed in the directory `\TRICOMP` and that input and output files will be stored in the directory `\TRICOMP\BUFFER`. In preparation move the files `WALKTHROUGH.MIN`, `WALKTHROUGH.TIN`, `WALKTHROUGH.TMP` and `WALKTHROUGH.CND` to `\TRICOMP\BUFFER`. Run **TC** and use the commands at the bottom of the menu to make sure that the program directory is set to `\TRICOMP` and the data directory to `\TRICOMP\BUFFER`.

The simulation illustrates a dynamic calculation with time-dependent applied temperature and temperature-dependent thermal conductivity. Although the example does not represent a specific application, similar setups may be encountered in simulations of medical procedures. Figure 2 shows the geometry. A cylindrical metal probe penetrates a spherical volume of material with a relatively high value of non-linear thermal conductivity k. This material is surrounded by a infinite region of poor conductor at ambient temperature (37 °C). The procedure is to raise the temperature of the probe to 95 °C and to determine the range of heated material after a treatment time of 1000 seconds.

3
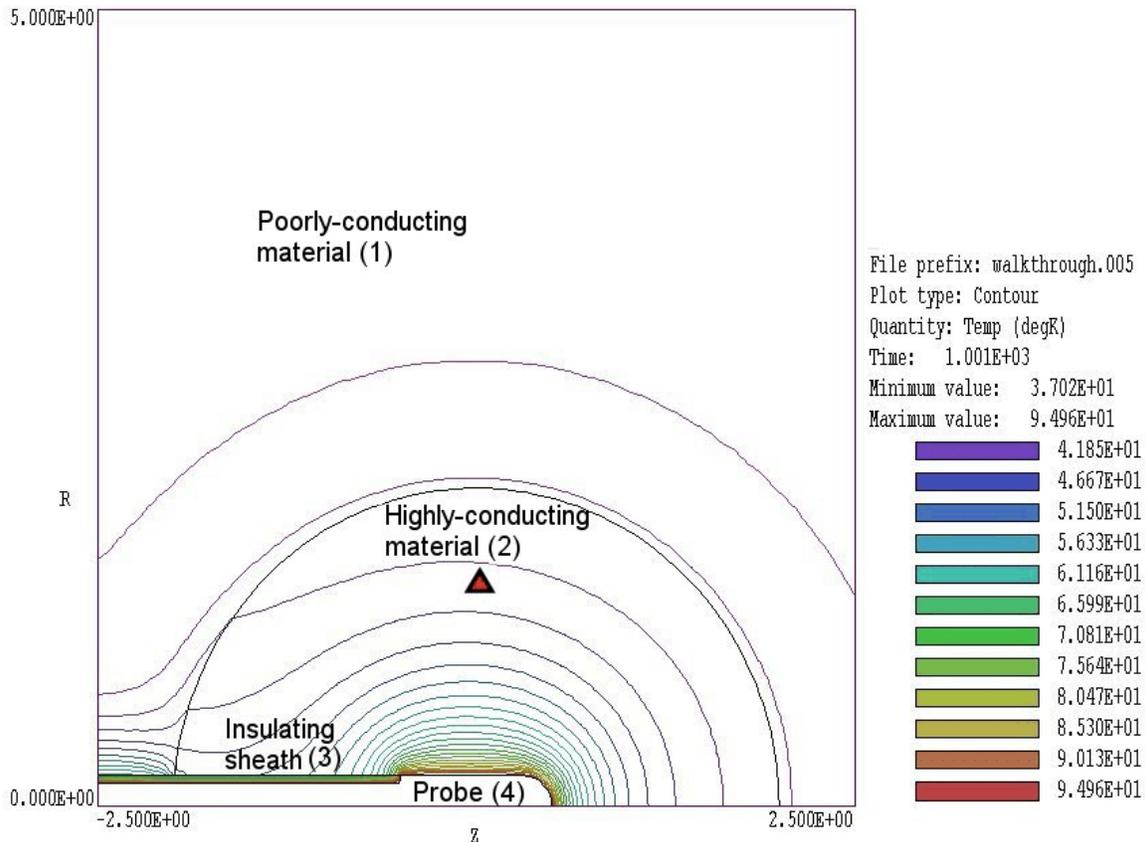
Figure 2. Geometry for the WALKTHROUGH example, showing region numbers and the location of the probe (close-up view).

From **TC** run **Mesh** then process and save the mesh following the instructions in the **Mesh** manual. The program creates the files WALKTHROUGH.MLS and WALKTHROUGH.MOU. The first file is a listing of run information that you can usually ignore if there are no problems. The second file describes the mesh – it is a listing of node coordinates and region numbers associated with nodes and elements. Like all **TriComp** files, WALKTHROUGH.MOU is in ASCII format so you can inspect it with a text editor or transfer the information to your own programs. Before leaving the program, check out the mesh using the plot functions of **Mesh**. The file illustrates good use of variable resolution to achieve high accuracy. It is not possible to simulate an infinite system in a finite-element calculation, but we can come close. Note that there is an extended region of surrounding material modeled at low resolution and that the outer boundary is set to the ambient temperature value of 37 °C.
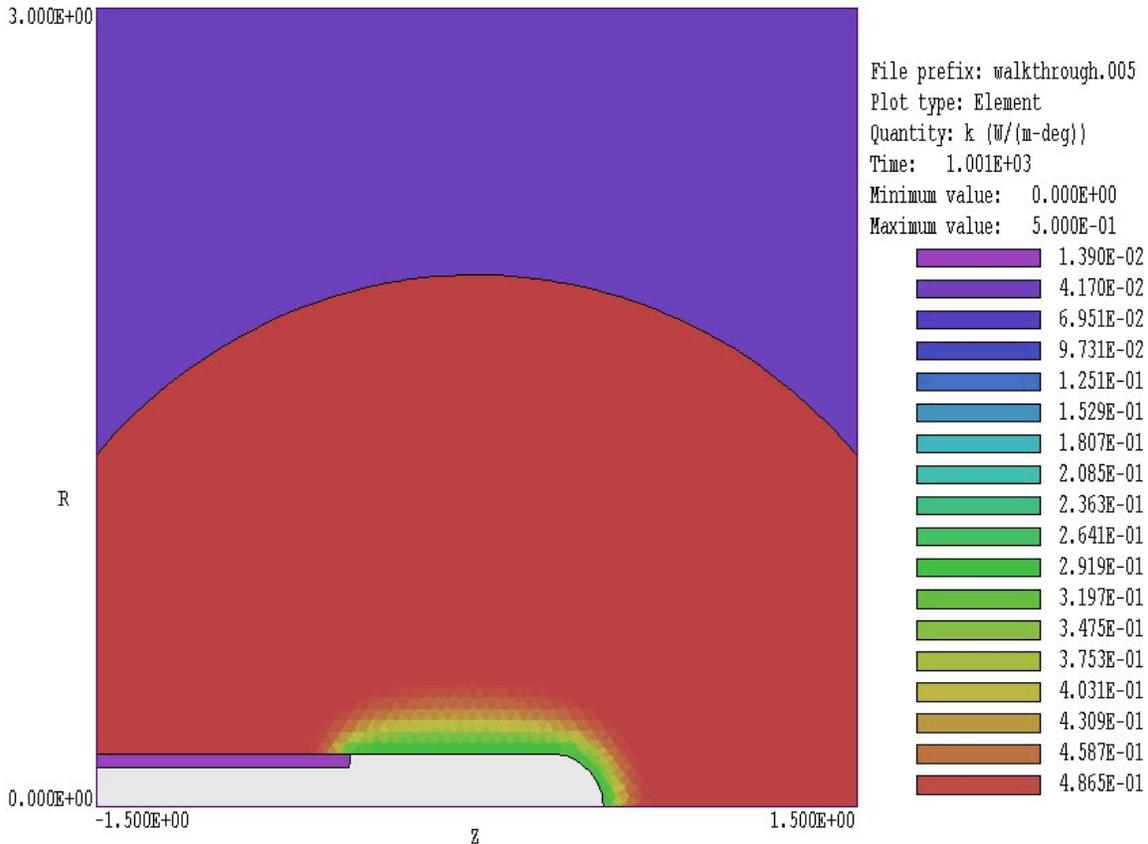
Figure 3. Color-coded element plot of thermal conductivity, WALKTHROUGH example.

Next run **TDiff** from **TC**. Pick *START RUN* in the *RUN* menu and choose the script file WALKTHROUGH.TIN that will control program operation. **TDiff** takes less than 20 seconds to complete the run, creating the following files:

WALKTHROUGH.TLS (Listing of run information for diagnostics)
WALKTHROUGH.001 (Snapshot of the simulation at 200 s)
WALKTHROUGH.002 (Snapshot of the simulation at 400 s)
WALKTHROUGH.003 (Snapshot of the simulation at 600 s)
WALKTHROUGH.004 (Snapshot of the simulation at 800 s)
WALKTHROUGH.005 (Snapshot of the simulation at 1000 s)
WALKTHROUGH.P01 (Time variations of thermal quantities at the position $z = 0.0$ cm, $r = 1.5$ cm.

The solution is complete. Before proceeding to analyses we shall take a look at some components of the simulation. In the *FILE* menu pick *EDIT FILE* and load WALKTHROUGH.CND. The contents of this file (shown in

Table 1) define a temperature-dependent conductivity. The value of k is 0.5 W/°C-m at low temperatures and drops to 0.3 W/°C-m in the range 60 °C to 90 °C. In a biological application the difference could represent chemical changes in tissue at increasing temperature. Next, click on *EDIT INPUT FILES* in the *FILE* menu and pick *WALKTHROUGH.TIN*. The contents are illustrated in Table 2 with added line numbers. At this point, we will not try to understand all the commands in detail but simply point out some features of the script.

Table 1. Definition of temperature-dependent conductivity – contents of the file WALKTHROUGH.CND

```
* Walkthrough example, decreasing thermal
conductivity
   0.0000    0.5000
  20.0000    0.5000
  40.0000    0.5000
  59.0000    0.5000
  60.0000    0.5000
  62.0000    0.4978
  64.0000    0.4914
  66.0000    0.4809
  68.0000    0.4669
  70.0000    0.4500
  72.0000    0.4309
  74.0000    0.4105
  76.0000    0.3895
  78.0000    0.3691
  80.0000    0.3500
  82.0000    0.3331
  84.0000    0.3191
  86.0000    0.3086
  88.0000    0.3022
  90.0000    0.3000
  92.0000    0.3000
  95.0000    0.3000
 100.0000    0.3000
ENDFILE
```

Table 2. Control script WALKTHROUGH.TIN

```
01: SET MODE TVar

02: SET DUNIT 100.0
03: SET GEOMETRY Cylin
04: SET SAFETY 5.0
05: SET NCHECK 20
06: SET TMAX 1001.0
07: SET DTMAX 0.50
08: SET DTMIN 0.01

09: REGION(1) COND = 0.05
10: REGION(1) DENS = 1100.0
11: REGION(1) CP = 5000.0
12: REGION(1) INIT = 37.0
13: REGION(2) COND TABLE WALKTHROUGH.CND
14: REGION(2) DENS = 1100.0
15: REGION(2) CP = 5000.0
16: REGION(2) INIT = 37.0
17: REGION(3) COND = 0.010
18: REGION(3) DENS = 800.0
19: REGION(3) CP = 2500.0
20: REGION(3) INIT = 0.0
21: REGION(4) FIXED TABLE WALKTHROUGH.TMP
22: REGION(5) FIXED 37.0

23: DIAG DTIME 200.0
24: DIAG HISTORY 0.0 1.5

25: ENDFILE
```

Line 01 is required input. In this case it specifies that the run addresses a dynamic solution. Lines 02 through 08 are control commands. Line 02 indicates that coordinates in the **Mesh** MOU file are in centimeters while Line 03 specifies that the solution has cylindrical symmetry. The commands of Lines 04 through 08 control the adjustable time step (Section 9). Lines 09 through 22 set material properties for regions of the solution space (thermal conductivity, mass density, specific heat and initial temperature) . Figure 2 shows the numbers associated with regions. Line 13 states that the thermal conductivity of the spherical region (Region 2) should be determined from the tabular file WALKTHROUGH.CND. Line 21 states that the time-dependent temperature of the probe (Region 4) should be determined from the file WALKTHROUGH.TMP.The final two commands control code diagnostics.

The command of Line 23 specifies data dumps of complete spatial information at intervals of 200 seconds. Line 24 sets a temperature probe at the position $z = 0.0$ cm, $r = 1.5$ cm.

Next run **TView** and click on *LOAD FIRST SOLUTION FILE* in the *FILE* menu. Pick the file `WALKTHROUGH.001.` The program loads the first data dump (created at 200 seconds) and displays a contour plot of temperature. To see the final temperature distribution at 1000 seconds, click on *LOAD SOLUTION FILE NUMBER* and enter 5 in the dialog. You can use the *ZOOM WINDOW* command in the *SPATIAL PLOTS* menu top reconstruct the plot of Fig. 2. Next, pick *PLOT TYPE* in the *SPATIAL PLOTS* menu and specify *ELEMENT*. In this plot the temperature is displayed through color-coded elements. Pick *PLOT QUANTITY* in the *SPATIAL PLOTS* menu and specify *k* (thermal conductivity). You should see the plot of Fig. 3. Note that a sheath of low conductivity has formed around the probe inhibiting thermal conduction.

In addition to plots, **TView** can perform several quantitative calculations. In the *FILE* menu click on *OPEN DATA LISTING FILE* and accept the default file prefix `WALKTHROUGH`. The results of all subsequent operations will be recorded in the ASCII file..Next, click on *REGION PROPERTIES* in the *ANALYSIS* menu. Move the mouse to a point inside the probe and left-click. **TView** performs an analysis of the probe volume and surface. Complete information is recorded in the data file and a summary given on the screen. After closing the data file with the *CLOSE DATA LISTING FILE* command, you can inspect it with the *EDIT DATA FILE* command. The entry for the region analysis is:

```
   --- Region Information ---
  Region No:    4
  Volume:    5.059E-07 m3
  AvgT:    9.500E+01 deg
  PeakT:    9.500E+01 deg
  ZPeak:    0.000E+00
  RPeak:    0.000E+00
  Flux:    1.356E+00 W
```

The quantity *Flux* is the integral of $k\nabla_n T$ over the region surface. An analysis of Region 2 (the surrounding sphere) gives *Flux* = 0.21391 W, a net influx of energy. In the steady state this figure should be close to zero because the power entering from the probe surface should equal the power lost through the boundary with Region 1. Therefore, Region 2 is still heating at $t = 1000$ seconds. To confirm this conclusion, we can look at
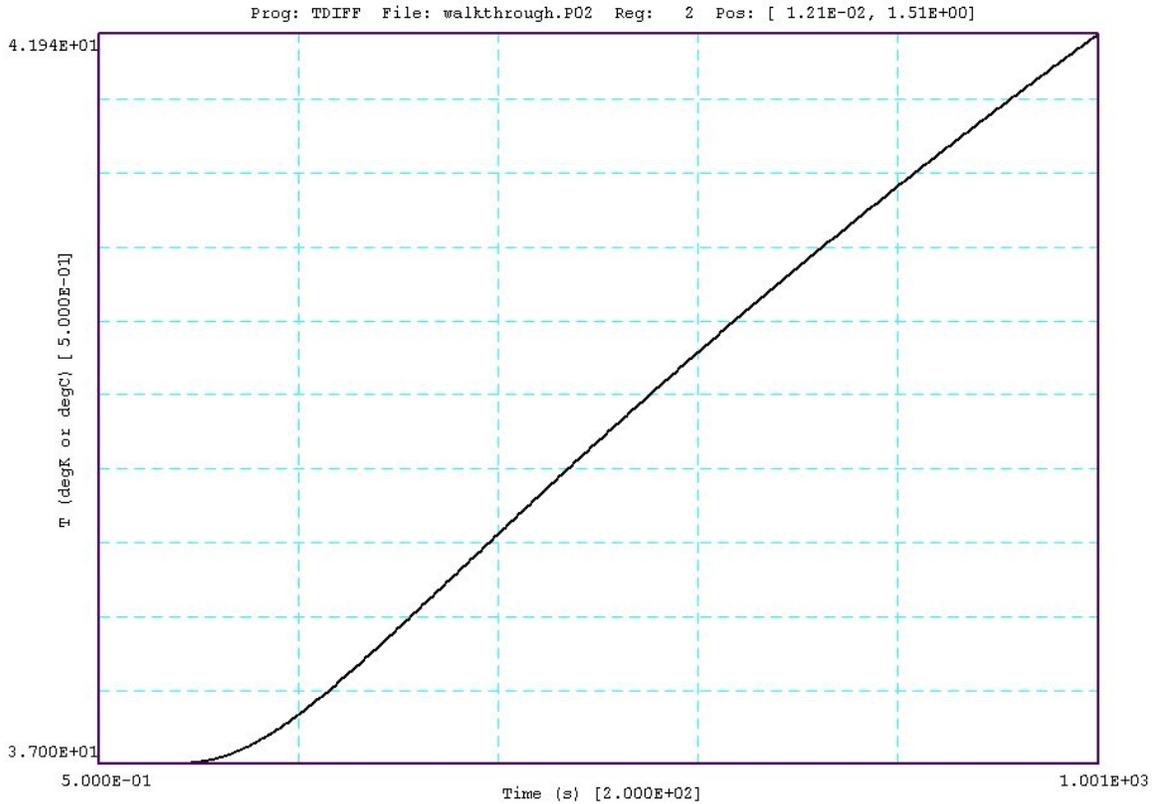
Figure 4. Plot of the time-variation of temperature at the probe position created by the **Probe** program.

the record of the probe at the position shown in Fig. 2 (colored triangle). From **TC** run **Probe**, click on *LOAD PROBE FILE* and choose WALKTHROUGH.P01. You should see the plot of Fig. 4. The temperature in the outer portion of Region 2 is still rising at t = 1000 seconds and will take several thousand seconds to approach an equilibrium.