Module 3: OOF2 Walkthrough

Stresses on a Bimetallic Strip

In this example, we shall use `OOF2` to use the finite element method to analyze the physical behavior of a bimetallic strip. The strip is comprised of two sheets of metal bonded together at an interface, as indicated below. The properties and geometry of the strip in the dimension coming out of the plane of the paper are assumed to be quasi-infinite uniform, allowing a two-dimensional treatment of this system. In this system, the upper (red) layer is copper, bonded to a lower (blue) layer of carbon steel.

Figure 1: *Bimetallic strip*

The differential thermal expansion of the two metals upon heating or cooling causes structural deformation of the strip, and is exploited in thermostatic feedback loops in domestic ovens and other appliances to maintain fixed chamber temperatures.

We shall analyze the physical and mechanical behavior of the strip upon heating. Of particular interest is the interfacial stress, which—if it becomes too large—can lead to delamination of the two metals, causing the bimetallic strip to fail and compromising the thermostatic feedback loop.

This guide is neither exhaustive nor comprehensive. To see the full range of `OOF2` features, and explore the details of the features exhibited within this guide, please see the OOF2 Manual. Hovering your cursor over the options in the OOF2 GUI will also provide on-demand information about the various options. Alternatively, you can run any of the interactive tutorials. The necessary example input files are installed in `/class/mse404ela/OOF2/examples` (which is an automount directory; you will need to access the directory first in order to read the files).

We will access `OOF2` using the local EWS installation; please load

```
module load OOF2
```

to proceed. Alternatively, you can use `OOF2` via the web implementation at nanoHUB.org. This requires an active nanoHUB account (free), and note that you must use the "Upload/Download" dialog to upload an image file.

N.B. As we have seen, `OOF2` has no predefined units, and we may use any consistent units of our choosing. Throughout this guide we will employ the SI convention (m, kg, Pa, J, N, etc.).

References

- OOF2:
  - OOF2: www.ctcms.nist.gov/oof/oof2/
  - OOF2 tutorial: www.ctcms.nist.gov/~rlua/redblue/
- nanoHUB:
  - Nanohub: nanohub.org
- Finite Element Method:

- Olek C Zienkiewicz, Robert L Taylor, J.Z. Zhu, *The Finite Element Method: Its Basis and Fundamentals*, Butterworth-Heinemann (2005).
- Reid *et al.* "Modelling Microstructures with OOF2" *Int. J. Materials and Product Technology* **35**, 361 (2009).

Step-by-step simulation guide

1. **Prepare files, load module.** First, load `OOF2` with `module load OOF2`. Next create your own local directory for your work, including today's walkthrough. From `/class/mse404ela/OOF2/Walkthrough`, copy the file `bimetallic.png` into your local directory.

2. **Start OOF2.** After changing into your local directory, run `oof2`.

   It is instructive to spend a moment reading the text in the `OOF2` welcome pane describing the basic `OOF2` workflow. **N.B.** You can save your work as a Python log using `File | Save`. It is strongly recommended that you save frequently to a Python log file to checkpoint your work.

3. **Create microstructure.** Change to the `Microstructure` task in the main `OOF2` window. Click "New from Image File" in the resulting window.

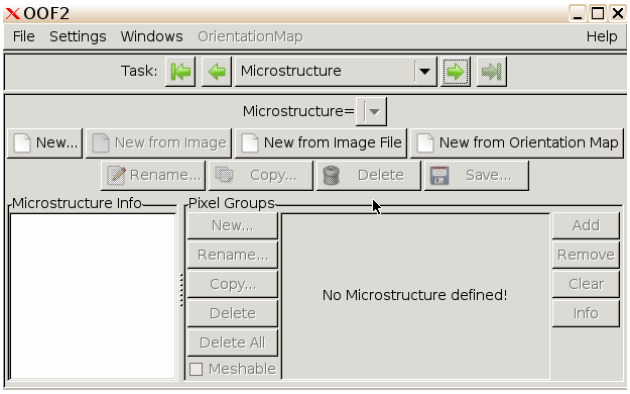


Figure 2: *Microstructure task*

   Select `bimetallic.png` and set the height to 0.01 m.

   Click OK, and the microstructure window will now contain your uploaded image data.

   From the dropdown `Windows` menu, select `Graphics` and click `New` to see your uploaded image.

4. **Build Pixel Groups.** We shall now inform `OOF2` that we have two separate materials, by forming "Pixel Groups".

   From the `Toolbox` menu, select `Pixel Selection`, and in the Method menu select `Color`.

   Click on the upper red layer. A value will appear in the Selection Size variable box defining the size of the selected layer.

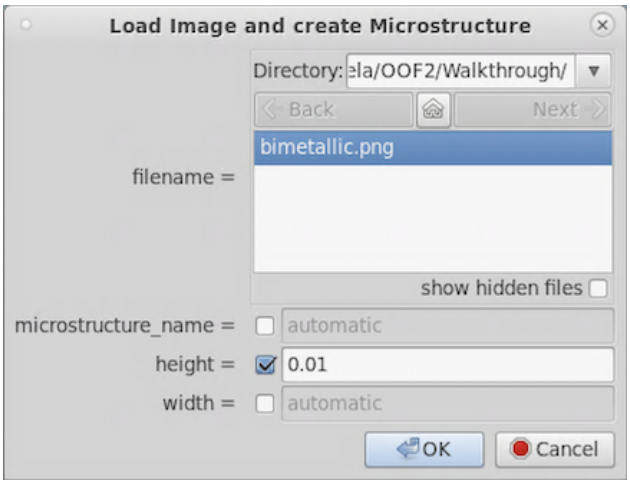


Figure 3: *Load image*

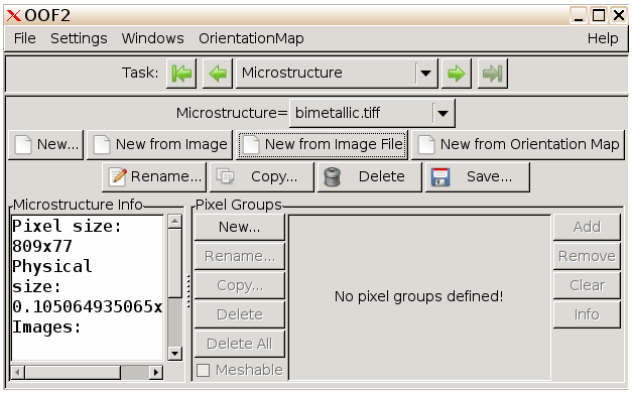


Figure 4: *Uploaded microstructure*

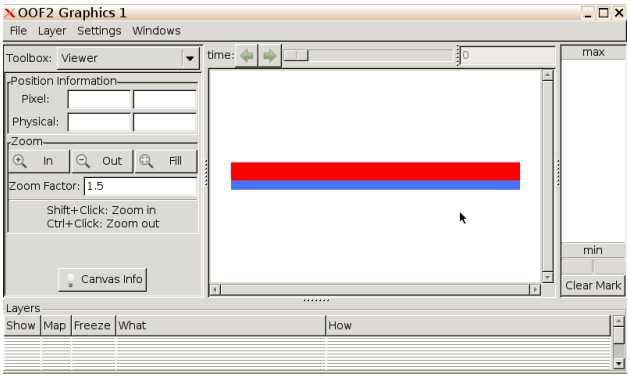


Figure 5: *Graphics window*

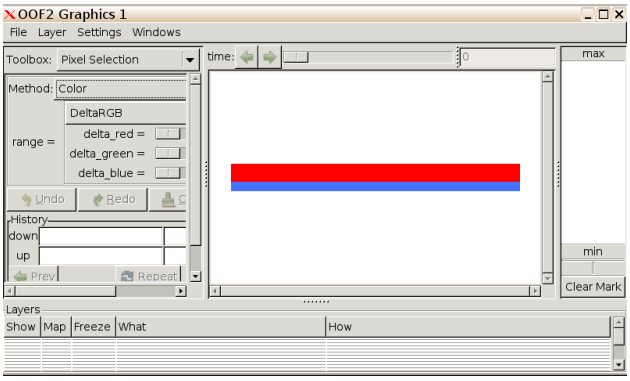


Figure 6: *Pixel selection*

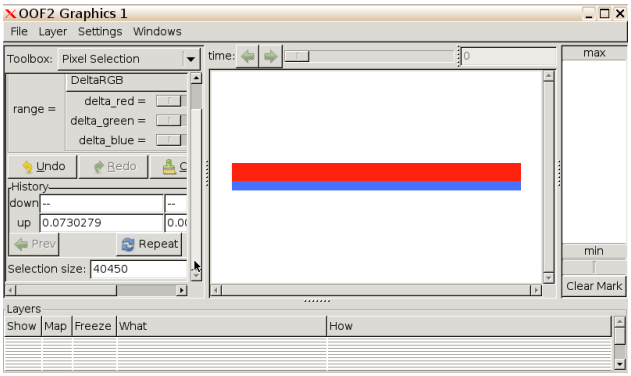


Figure 7: *Pixel selection with selection size*

Drag the “Graphics 1” window out of the way and return to the main `OOF2` window. Click on `New...` under `Pixel Groups` and name the selected group “upper”. Click OK.

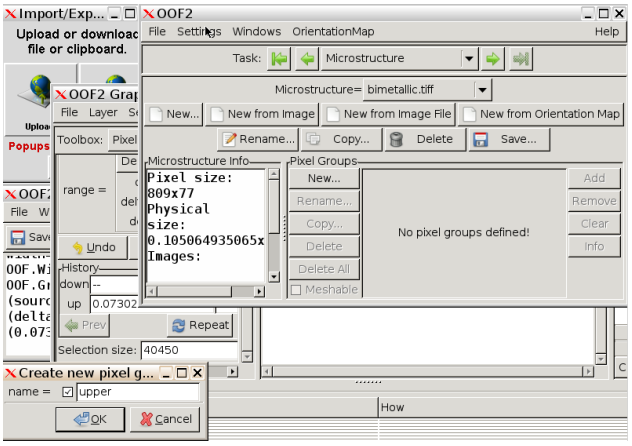


Figure 8: *Defining a pixel group*

You will see that we have established a new Pixel Group.

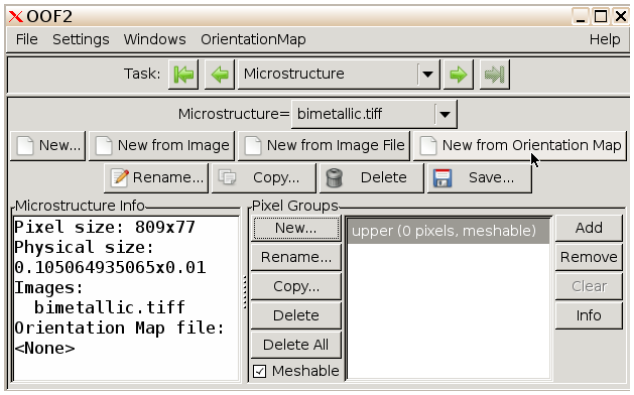


Figure 9: *New pixel group info in main OOF2 window*

Click the `Add` button to the right of the window to add our selected pixels to this group.

Repeat this process for the bottom layer, to generate a pixel group named “lower”.

5. **Build material properties.** We shall now input the physical properties for each layer in the strip—copper (upper), and carbon steel (lower). In the main `OOF2` window, use the `Task` dropdown to navigate to the `Materials` pane.

   Click `New...` to add a new material. Name the materials “copper” and “steel”, and leave their specification as bulk.

   We shall now assign the following properties to the two materials:

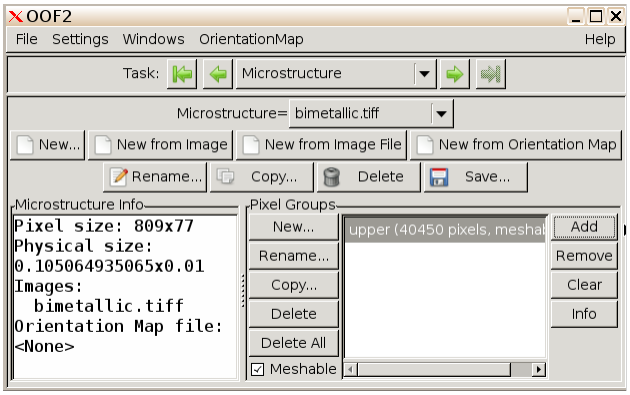


Figure 10: *Pixel group added*

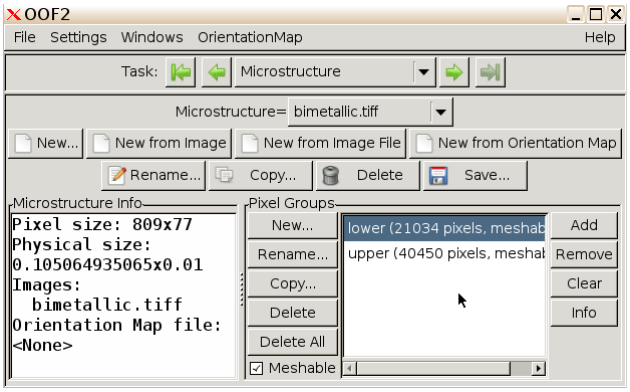


Figure 11: *After adding "lower"*

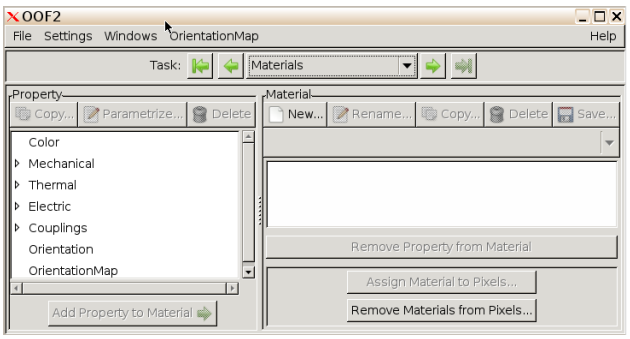


Figure 12: *Materials pane*

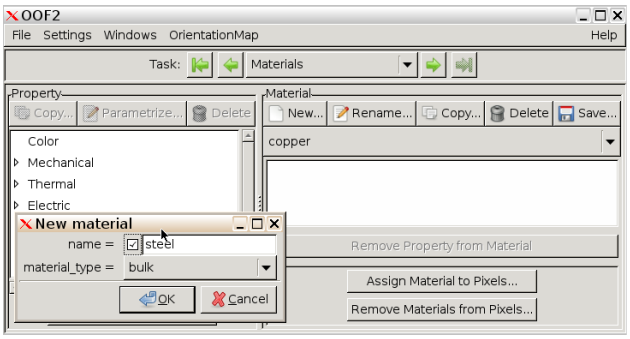


Figure 13: *Naming new materials*

Property	Copper	Steel
Young's modulus E [*GPa*]	117	200
Poisson's ratio ν	0.33	0.27
Thermal conductivity k [*W/m°C*]	390	41
Thermal expansion coefficient α_T at $T_0 = 0$°C [K^{-1}]	51×10^{-6}	36×10^{-6}
Color [*R,G,B*]	[1,0,0]	[0,0,1]

Let's first consider copper.

To specify the Young's modulus, in the `Property` window on the left click the triangle to the left of `Mechanical`, followed by the triangle to the left of `Elasticity`, then highlight the word `Isotropic`. At the top of the `Property` window, click `Copy...`, name the property "Young_copper" and click OK.

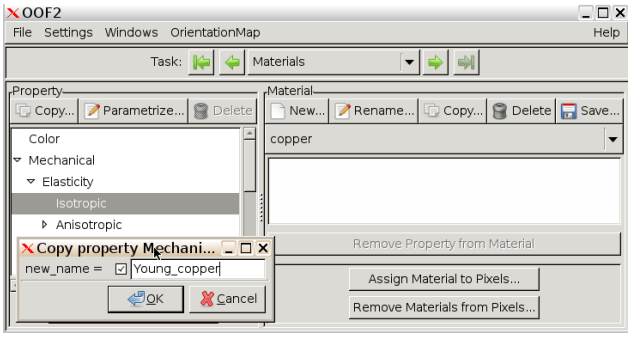
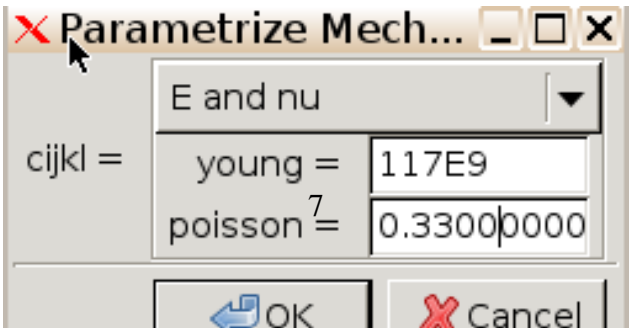


Figure 14: *Isotropic elasticity*

Select `Young_copper` and click `Parametrize...` and in the drop down menu, select `E and nu`. Input the values for Young's modulus and Poisson's ratio (ν) from the table above and click OK.



Property	Selection
Thermal conductivity, k	Thermal -> Conductivity -> Isotropic
Thermal expansion coefficient, α_T at $T_0 = 0°C$	Couplings -> Thermal Expansion -> Isotropic
Color	Color

6. **Attach materials properties.** Select copper in the `Material` column on the right hand side of the main `OOF2` window. Select each of the four materials properties we assigned in turn (Young + Poisson, k, alpha, color) in the `Property` column on the left side and click `Add Property to Material`.

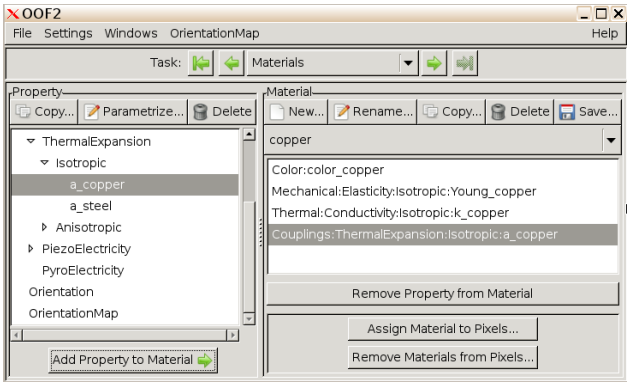


Figure 16: *Adding properties to material*

Repeat for steel.

7. **Assign materials to pixel groups.** Select copper in the Material column and click `Assign Material to Pixels...`. Choose upper to make the upper layer of the bimetallic strip copper.

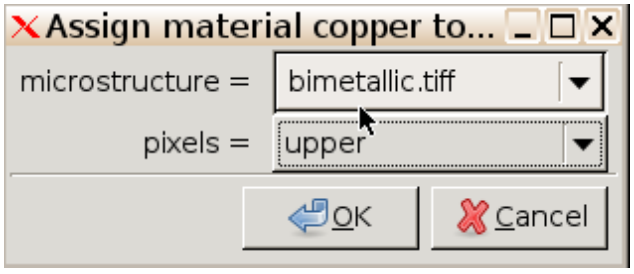


Figure 17: *Assigning material to pixels*

Follow an analogous process to make the lower layer steel.

8. **Generate skeleton.** In `OOF2`, we first create a "skeleton" of finite elements that we subsequently use to create the mesh. The skeleton is purely geometric, whereas the mesh contains element properties and basis functions.

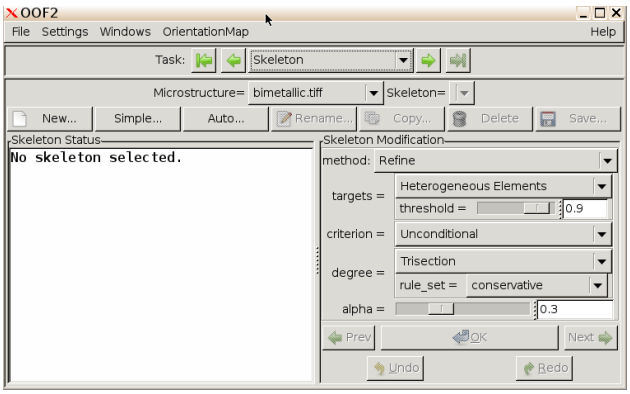


Figure 18: *Skeleton pane*

In the main `OOF2` window, use the `Task` dropdown to navigate to the `Skeleton` pane.

Click `New...` to specify a new skeleton, and set the number of x elements to 50, the number of y elements to 11, the mesh type to TriSkeleton, and the arrangement to Liberal. Click OK.

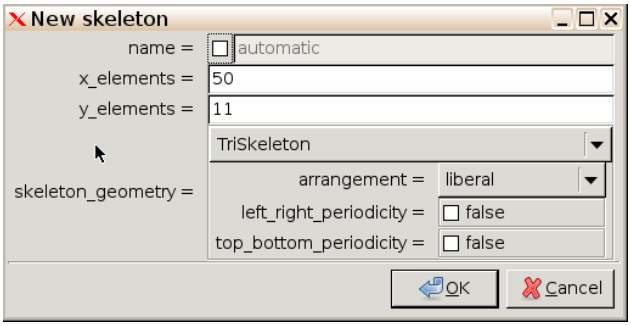


Figure 19: *New skeleton*

The Graphics window will now display your initial skeleton over your microstructure.

Careful inspection of the skeleton reveals that there are some "heterogeneous elements" containing both copper and steel within their area, and there are too few elements near the interface where we expect large variation in properties.

We shall perform a number of rounds of skeleton refinement to generate more reasonable domain decomposition using the `Skeleton Modification` tools in the right hand column of the main `OOF2` window.

These tools attempt to minimize the skeleton energy, where the energy is defined as a linear combination of a homogeneity and a shape term:

$$E = \alpha E_{\text{homogeneous}} + (1-\alpha) E_{\text{shape}}$$

Heterogeneous elements and those with high aspect ratios have high energies. The parameter α (not to be confused with thermal expansion!) controls the trade-off between these contributions.

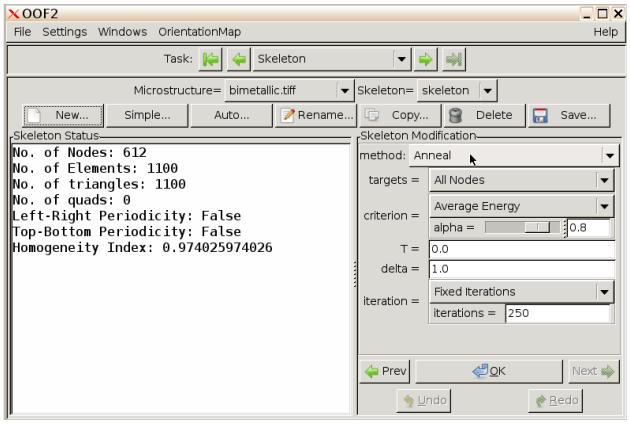


Figure 20: *End result of making skeleton*

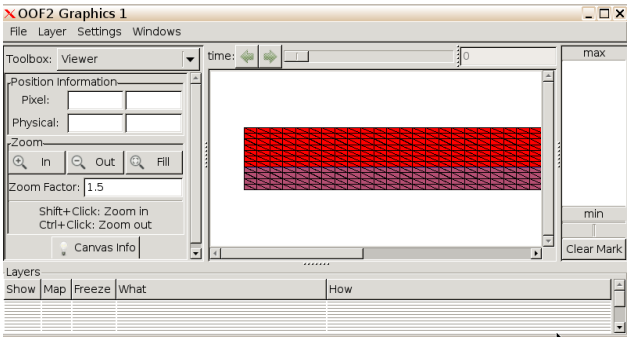


Figure 21: *Skeleton in graphics window*

(i) From the method menu, select `Anneal`. This process attempts to make the elements more homogenous using a random skeleton refinement protocol similar to simulated annealing. Use as a criterion "Average Energy" with alpha = 0.9 and specify 100 iterations. T is the effective temperature, with T=0 permitting only downhill moves in energy.

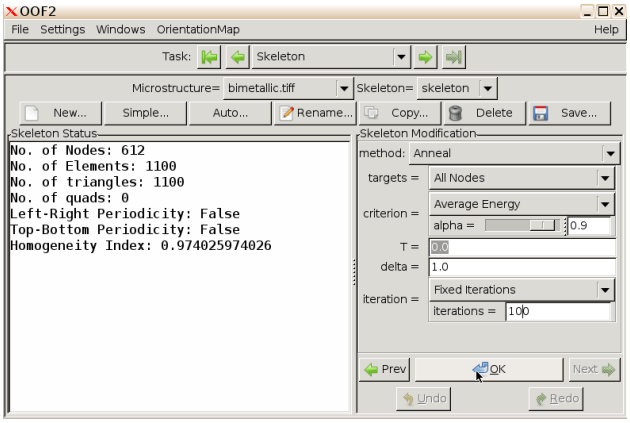


Figure 22: *Skeleton anneal*

Click OK to perform the annealing procedure. You can watch the skeleton evolve in the Graphics window, and the numerical convergence in the Messages and Activity window.

In the Graphics window, we can access Zoom options via the dropdown Settings menu. Zooming in on the skeleton shows that we have improved alignment of the mesh with the phase boundaries.

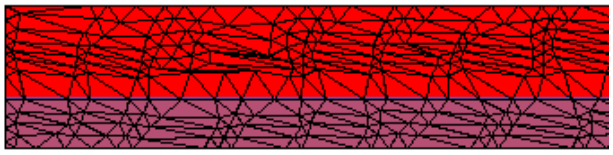


Figure 23: *Annealed skeleton*

(ii) From the method menu, select `Swap Edges` to perform a random flipping of element edges in an effort to achieve better phase boundary alignment. Use alpha = 0.8. Click OK.

(iii) From the method menu, select "Smooth" to adjust node locations. Use alpha = 0.8 and specify 50 iterations with T=0. Click OK.

The skeleton is well aligned with the phase boundary, and the homogeneity index is 0.99 indicating excellent alignment with phase boundaries.

(*N.B.* We will not do this here to save computational time, but we can use the "Refine" method to increase the number of elements. Set the targets to "All Elements", criterion to

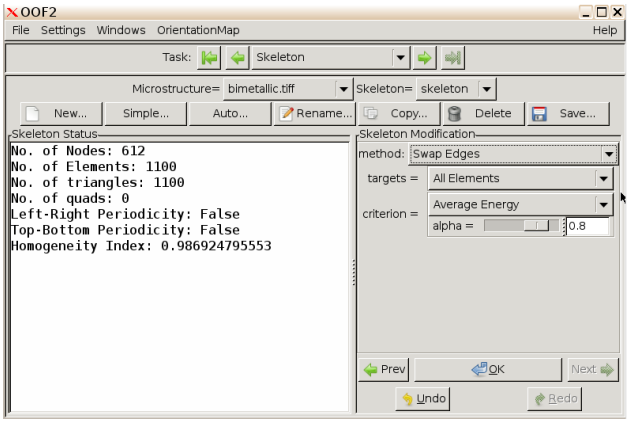


Figure 24: *Swapping edges*

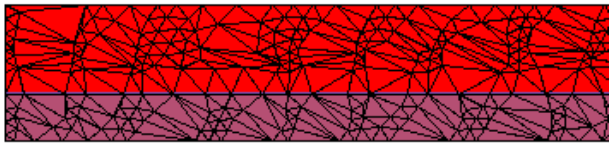


Figure 25: *Swapped edges skeleton*

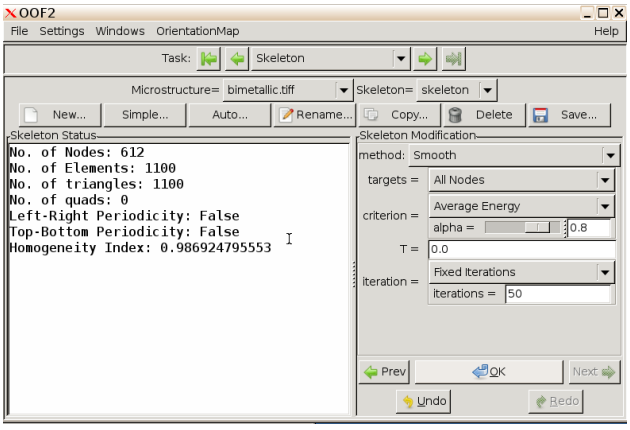


Figure 26: *Smoothing*

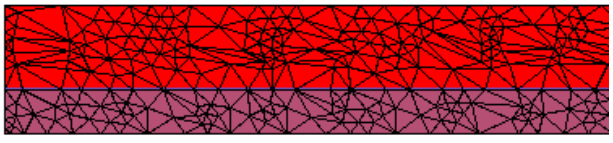


Figure 27: *Smoothed skeleton*

"Unconditional", degree to "Bisection", rule set to "Liberal" and alpha to 0.8. Click OK.){ width=50% }

9. **Generate mesh.** In the main `OOF2` window, use the Task dropdown to navigate to the `FE Mesh` pane.

   Click `New...` to generate a mesh based on our skeleton. Leave mapping order and interpolation order as 1. (For higher accuracy—at the expense of longer computation times—we may wish to select 2.) Click OK.

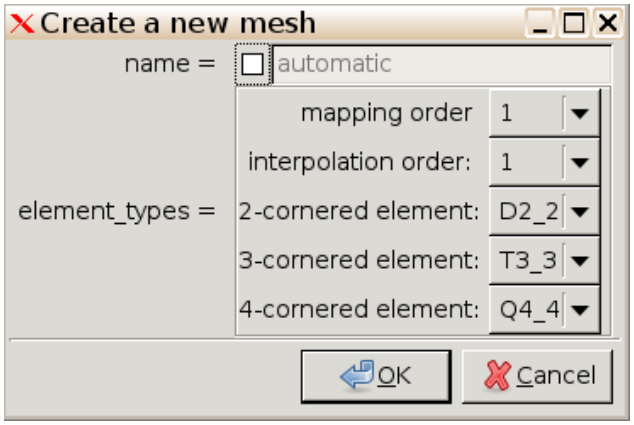


Figure 28: *New mesh*

We now have a mesh with properties listed in the left column of the FE Mesh window.

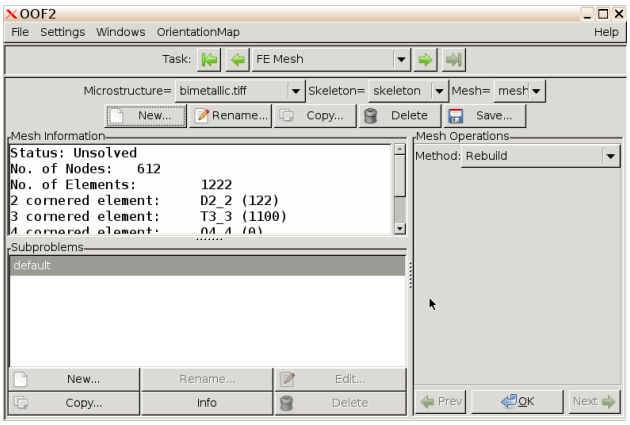


Figure 29: *Mesh properties*

10. **Specify equations.** In the main `OOF2` window, use the Task dropdown to navigate to the `Fields and Equations` pane.

    In the `Fields` column on the left, tick all three boxes (`defined`, `active`, `in-plane`) in the rows for `Temperature` and `Displacement`.

    In the `Equations` column on the right, tick the boxes next to `Heat Eqn` and `Force Balance`.

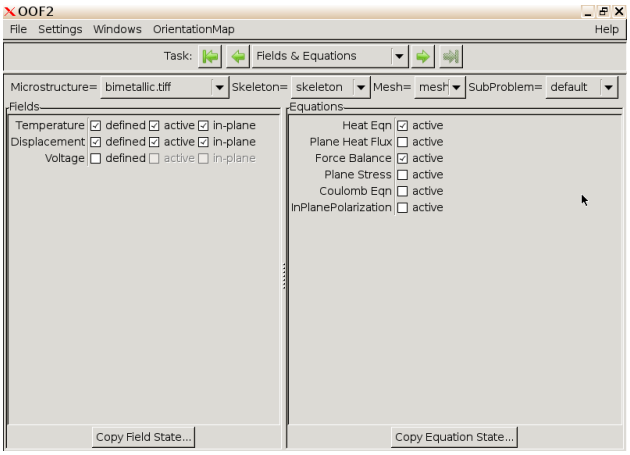


Figure 30: *Equations selections*

11. **Specify boundary conditions.** In the main `OOF2` window, use the Task dropdown to navigate to the `Boundary Conditions` pane.

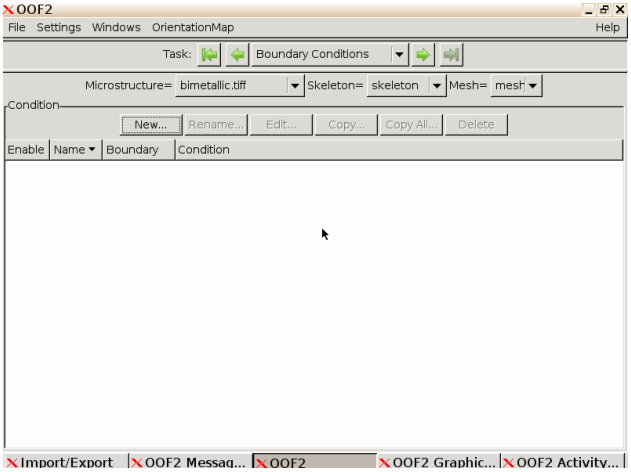


Figure 31: *Boundary conditions pane*

Click `New...`. Using Dirichlet boundary conditions for the temperature field, specify the right boundary to $450°$C.

Following the same protocol, specify the left boundary to be $0°$C.

Following a similar protocol, fix the right boundary y-displacement to zero.

Following a similar protocol, fix the right boundary x-displacement to zero.

We can see the specified BCs in the main `OOF2` window.

12. **Solving.** In the main `OOF2` window, use the Task dropdown to navigate to the `Solver` pane.

    Select the first line in the Solver pane and click "Set..." to specify the solver options. Select "Advanced", choose BiCGStab (stabilized biconjugate gradient solver) and set tolerance to

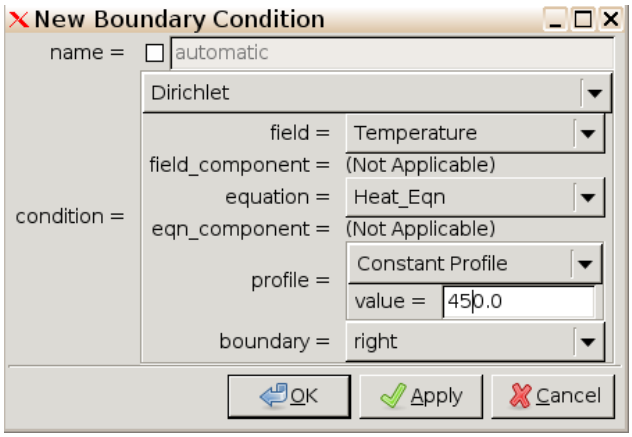


Figure 32: *New boundary condition*

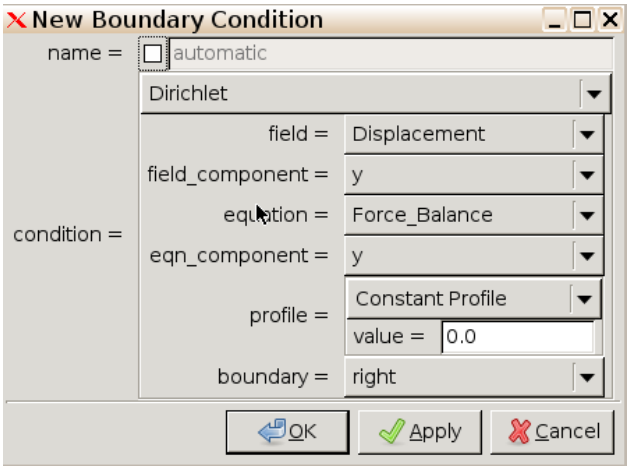


Figure 33: *y displacement boundary*

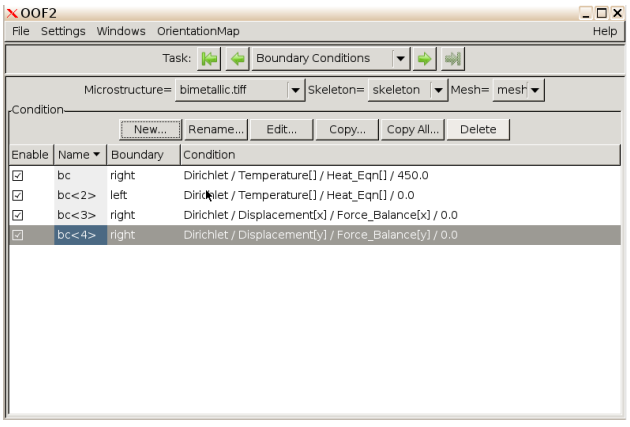


Figure 34: *Boundary condition summary*

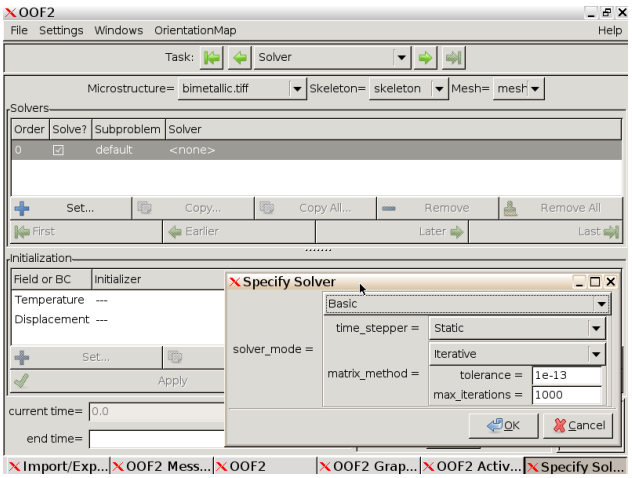


Figure 35: *Solver pane*

1e-9, max_iterations to 100,000 and click OK.

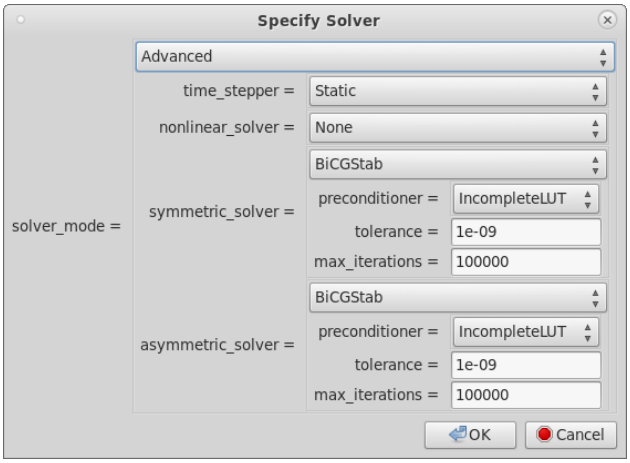


Figure 36: *Solver options*

Back in the main pane, click `Solve` in the bottom right hand corner to solve the FEM problem. This may take seconds to minutes. We can watch the progress in the `Messages` and `Activity` windows.

13. **Visualize result.** Switch over to the `Graphics` window. You will see three layers—the micrograph, the initial skeleton, and the final mesh.

    To better visualize the final mesh, uncheck the skeleton in the Layers menu at the bottom of the window.

    As we may have anticipated, the larger thermal expansion coefficient of the copper relative to the steel has caused the strip to bend downwards under the applied thermal gradient. Depending on the details of your skeleton and mesh, your bimetallic strip may or may not bend as much as this. (In a more detailed study, we should, of course, check how hpr-refinement affects our results.)

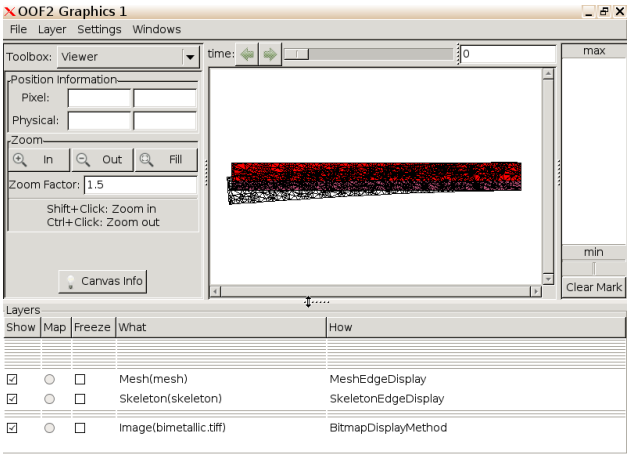


Figure 37: *Graphics window with multiple layers*

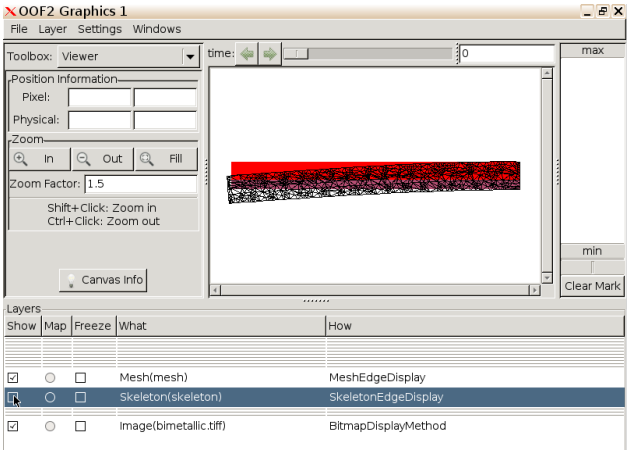


Figure 38: *Graphics window without skeleton*

We shall now visualize the temperature gradient over the final mesh. From the Layer dropdown menu, select `New...`. In the Displayed Object column on the left, select category `Mesh`.

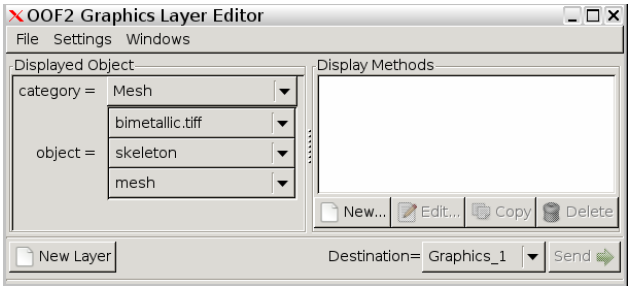


Figure 39: *Graphics layer editor*

In the Display Methods column on the right, click `New...` and select `Filled Contour`. Specify field to be `Temperature`, and where to be `actual`. Click OK.

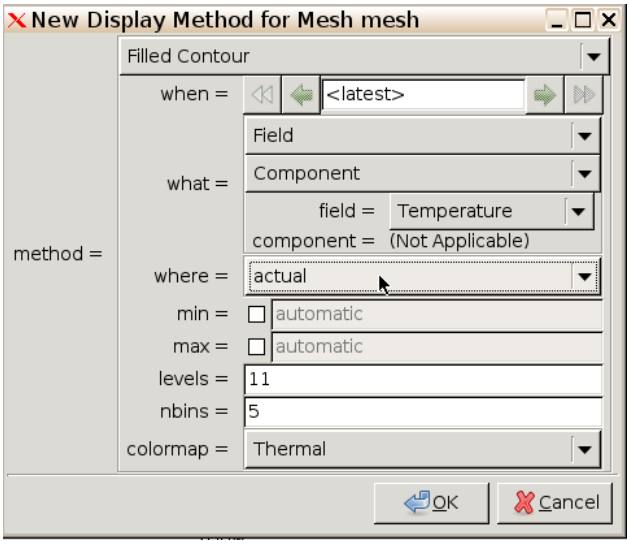


Figure 40: *Filled contour*

Back in the Graphics window, we now have the terminal temperature gradient overlaid on our final deformed mesh.

14. **Analysis.** We will now proceed to extract some numerical results. In the main `OOF2` window, use the Task dropdown to navigate to the `Analysis` pane.

    (i) First we shall look at the temperature profile in the final structure.

    Specify in the `Output` menu, field to be `Temperature`, in the `Sampling` menu, x_points = 10 and y_points = 10, and in the Destination menu the Message Window for output. (Alternatively, we can write to file by clicking `New...` and download the file to our local machine using the Upload/Download window.) Click `Go`.

    The temperature over a grid is output to the `Message` window.

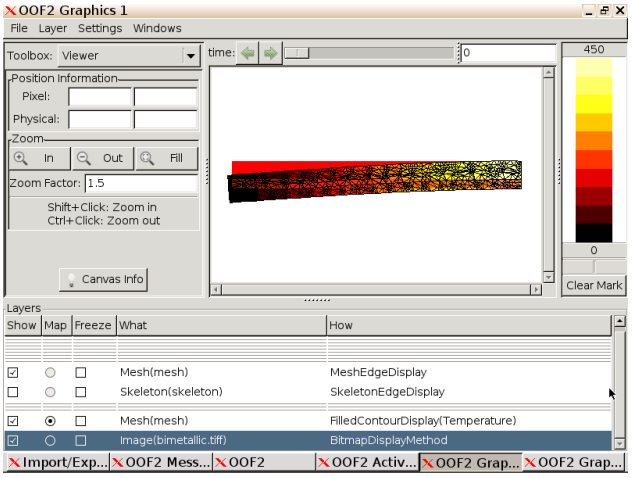


Figure 41: *Graphics layer with temperature gradient*

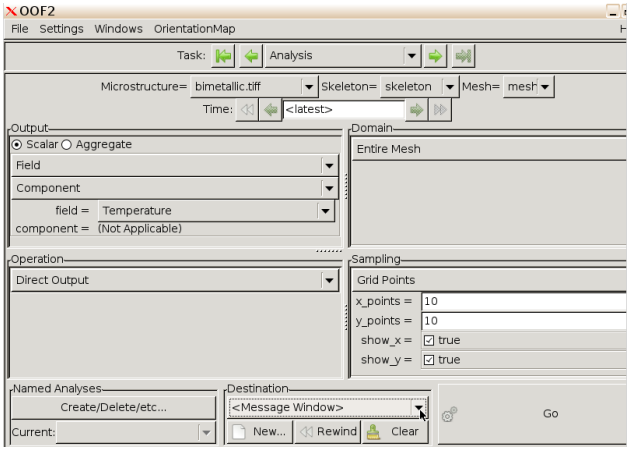


Figure 42: *Analysis pane*

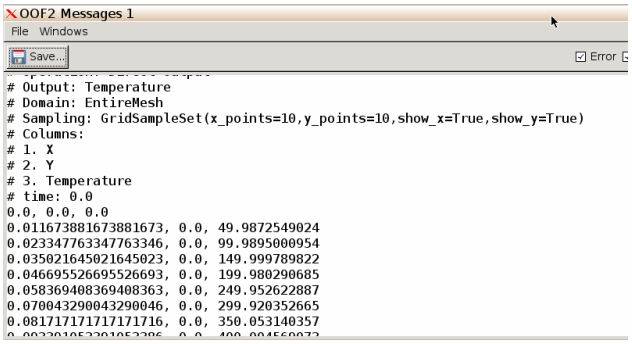


Figure 43: *Message window with temperature*

(ii) We can also look at properties along a cross section of the final structure.

First create a new layer in the same manner as before. In the Displayed Object column on the left, select category `Mesh`. In the Display Methods column, click `New...` and select `Material Color`. Click OK.

Back in the Graphics window, deselect all Layers except the MeshMaterialDisplay that we just created. From the Toolbox menu in the top left, select `Mesh Cross Section` and then using your pointer, draw a cross section over the deformed strip. Leave n_points as 50. We will now analyze the temperature at 50 uniformly spaced points along this line.

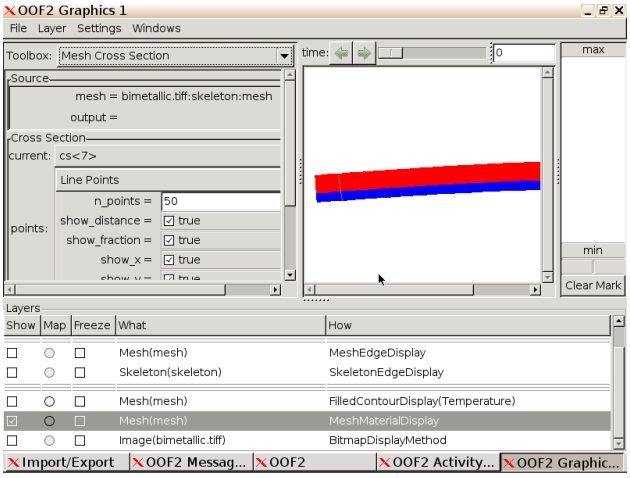


Figure 44: *50 evenly spaced points*

Switch back to the `Analysis` window. Set field to temperature, and Domain to Cross Section. Deselect `show_distance` and `show_fraction` since these are unimportant to us, and leave the Destination as the Message Window. Click Go.

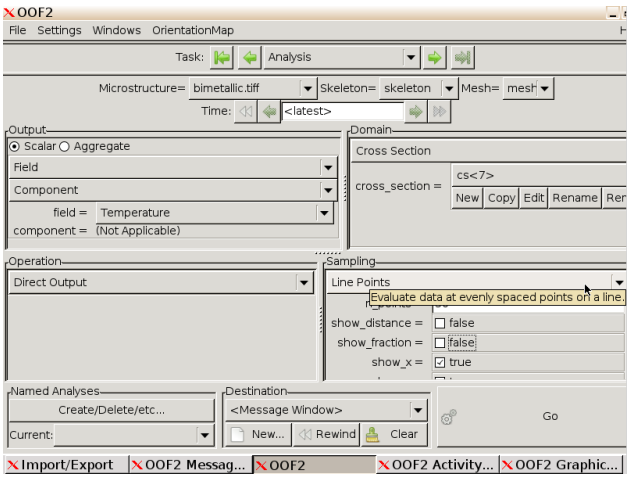


Figure 45: *Analysis pane*

Checking back in the Message window, we find our results.

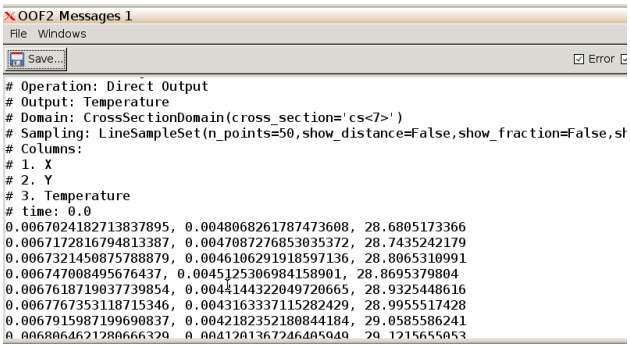


Figure 46: *Message window with temperature cross-sections*