MODULE 3:
FINITE ELEMENT METHOD

Practice: OOF2

I. What is OOF2?

OOF2

OOF: Finite Element Analysis of Microstructures

NIST National Institute of Standards and Technology • U.S. Department of Commerce

http://www.ctcms.nist.gov/oof/oof2/

OOF2

- Object Oriented Finite Element Analysis Tool

- Originally developed in the late 90's at NIST by Craig Carter, Ed Fuller, Andy Roosen, and Steve Langer

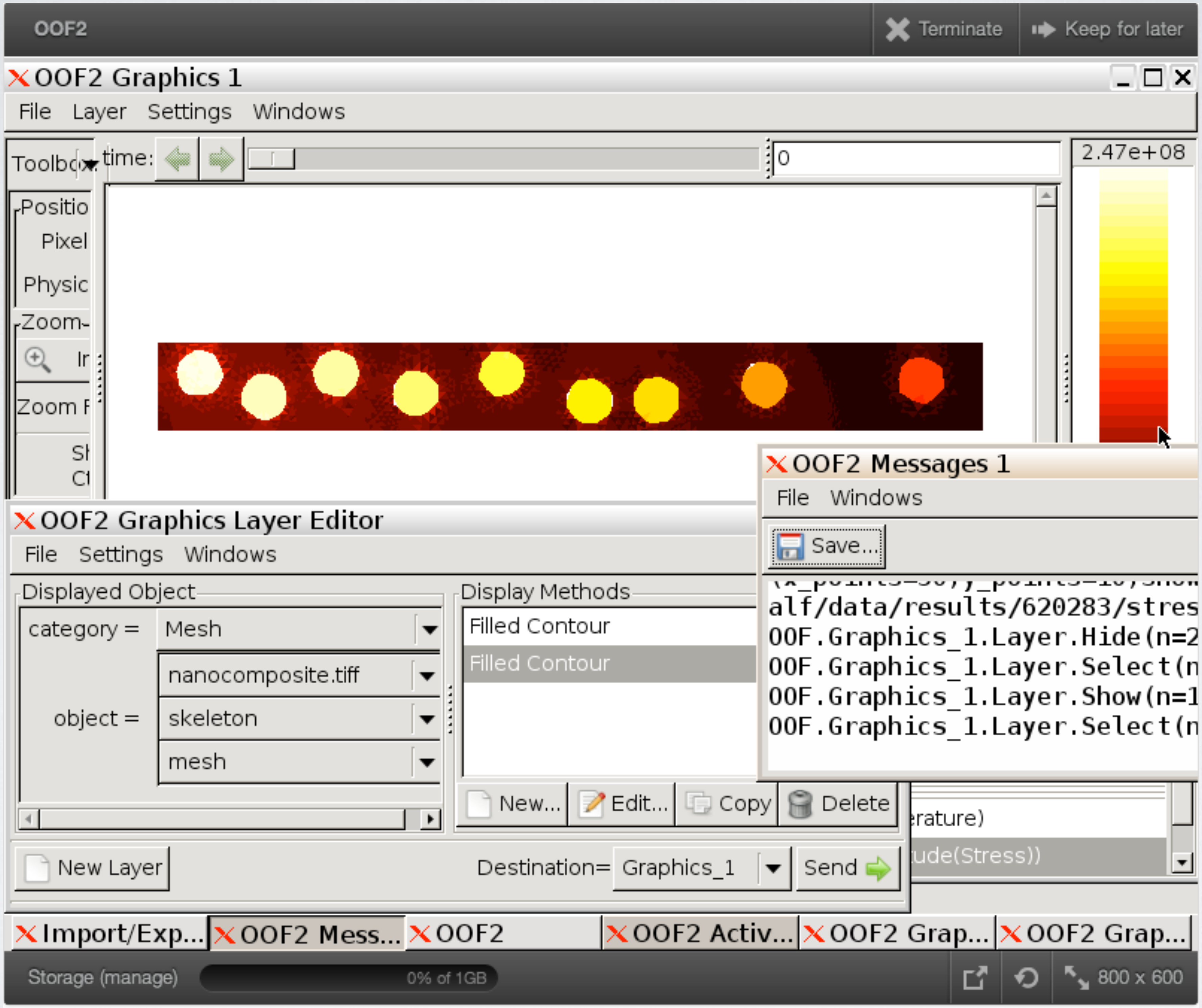
- Fundamentally a **two-dimensional** FEM tool

OOF2 is public domain software created at the National Institute of Standards and Technology (NIST) to investigate the properties of microstructures. The microstructure of a material is the (usually) complex ensemble of polycrystalline grains, second phases, cracks, pores, and other features occurring on length scales large compared to atomic sizes.

At the simplest level, **OOF2** is designed to answer questions like, "I know what this material looks like and what it's made of, but I wonder what would happen if I pull on it in different ways?", or "I have a picture of this stuff and I know that different parts expand more than others as the temperature increases -- I wonder where the stresses are greatest?"

OOF2

- Very user-friendly GUI



- CLI also available

$$$

- **FREE** to the end user!

Useability

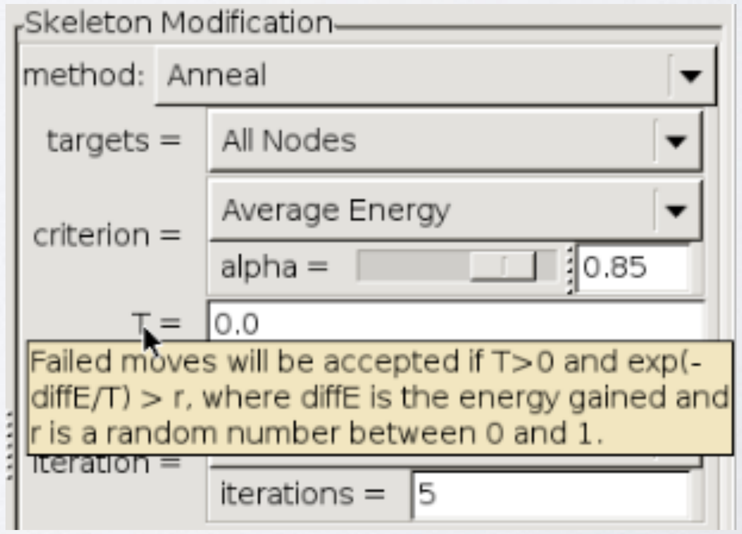
- Very well documented

  http://www.ctcms.nist.gov/~langer/oof2man/

- Many tutorials and guides available

  http://www.ctcms.nist.gov/~rlua
  www.ctcms.nist.gov/oof/talks/workshop06/SteveLanger/example.pdf
  http://nanohub.org/resources/4732

- Rollover help within the GUI



Availability

- Free download of source code from

  http://www.ctcms.nist.gov/oof/oof2/#download

- Supported by Linux and Mac OS X, but many pre-reqs

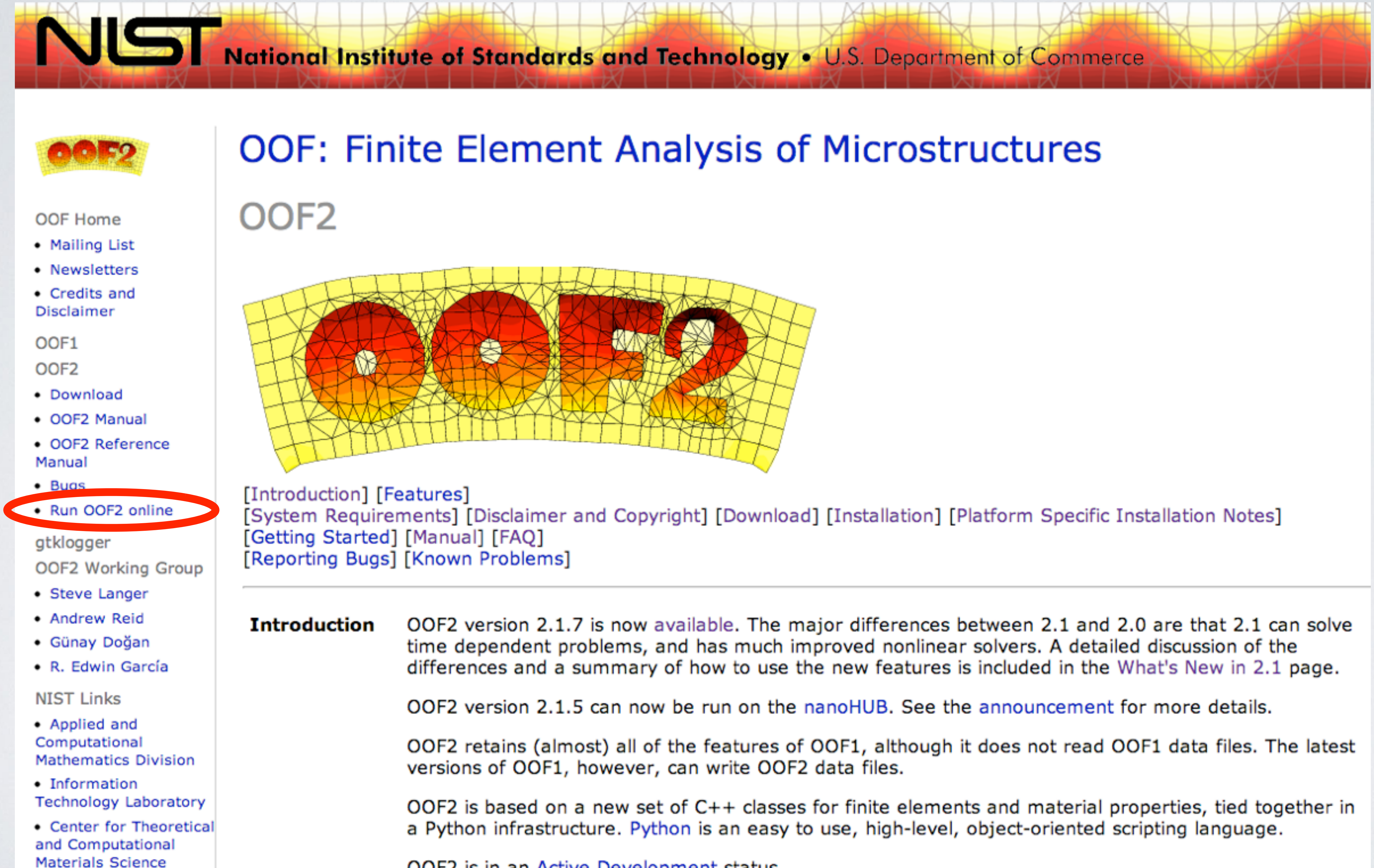
  http://www.ctcms.nist.gov/oof/oof2/prerequisites.html

```
Python (2.4 through 2.7)    http://www.python.org
Magick++                    http://www.imagemagick.org/www/Magick++/index.html
gtk+-2.0 (2.6 or later)     http://www.gtk.org/download/
libgnomecanvas2             http://directory.fsf.org/graphics/misc/libgnomecanvas.html
pygtk2 (2.6 or later)       http://www.pygtk.org
swig 1.1 build 883          http://www.swig.org/download.html
```

- Local installation can be tricky
- **EWS:** `module load OOF2`

Availability

- But...



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OOF Home
- Mailing List
- Newsletters
- Credits and Disclaimer

OOF1
OOF2
- Download
- OOF2 Manual
- OOF2 Reference Manual
- Bugs
- Run OOF2 online

gtklogger
OOF2 Working Group
- Steve Langer
- Andrew Reid
- Günay Doğan
- R. Edwin García

NIST Links
- Applied and Computational Mathematics Division
- Information Technology Laboratory
- Center for Theoretical and Computational Materials Science

OOF: Finite Element Analysis of Microstructures

OOF2

[Introduction] [Features]
[System Requirements] [Disclaimer and Copyright] [Download] [Installation] [Platform Specific Installation Notes]
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Introduction

OOF2 version 2.1.7 is now available. The major differences between 2.1 and 2.0 are that 2.1 can solve time dependent problems, and has much improved nonlinear solvers. A detailed discussion of the differences and a summary of how to use the new features is included in the What's New in 2.1 page.

OOF2 version 2.1.5 can now be run on the nanoHUB. See the announcement for more details.

OOF2 retains (almost) all of the features of OOF1, although it does not read OOF1 data files. The latest versions of OOF1, however, can write OOF2 data files.

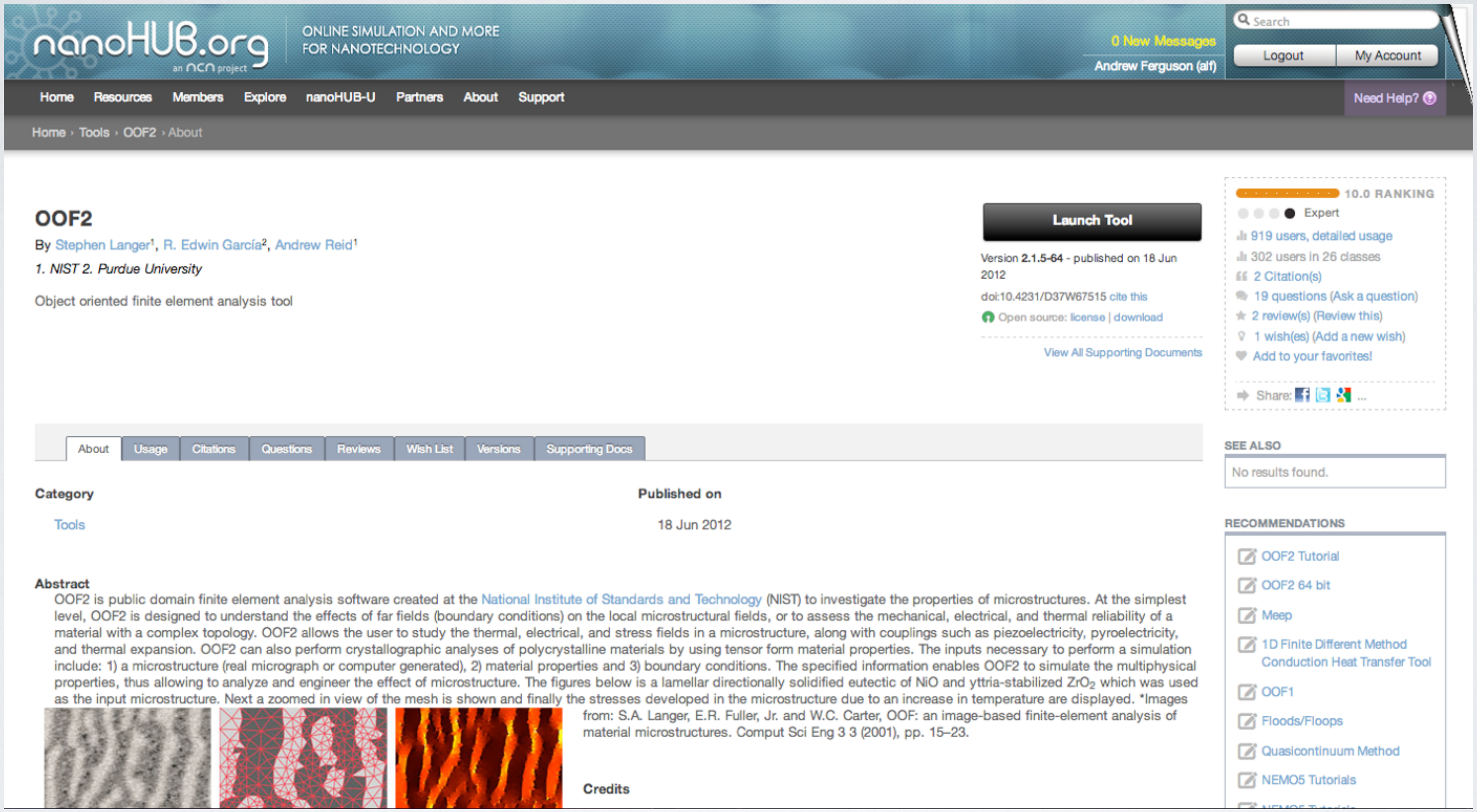
OOF2 is based on a new set of C++ classes for finite elements and material properties, tied together in a Python infrastructure. Python is an easy to use, high-level, object-oriented scripting language.

OOF2 is in an Active Development status.

Availability

- Online webtool available at nanoHUB

https://nanohub.org/tools/oof2/

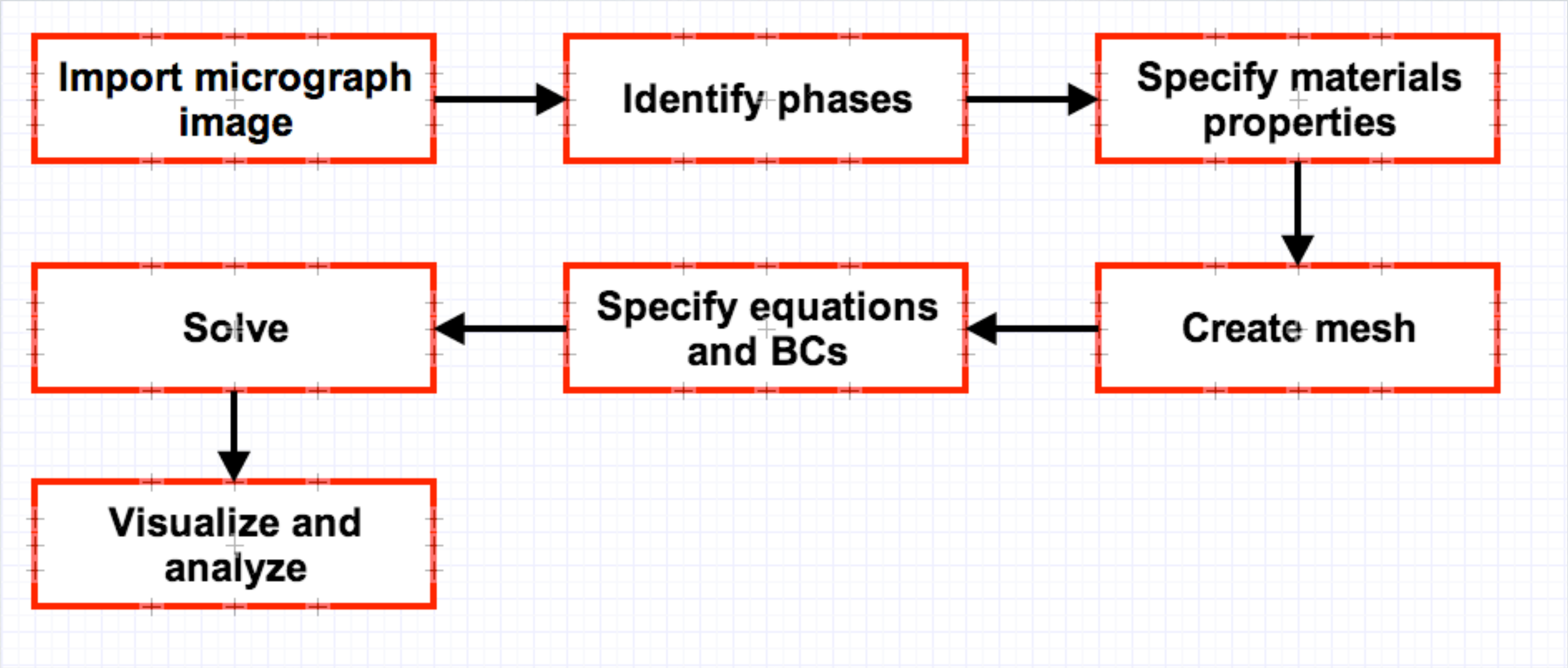


- Requires a **free** nanoHUB account for access

(Please register for nanoHUB, Facebook/Google sign-ins can be buggy.)

II. OOF2 basics

Workflow



- All tasks performed in seamlessly and in sequence using OOF2 integrated GUI
- Windows based environment

https://www.gliffy.com

Units

- **OOF2 has no units!**

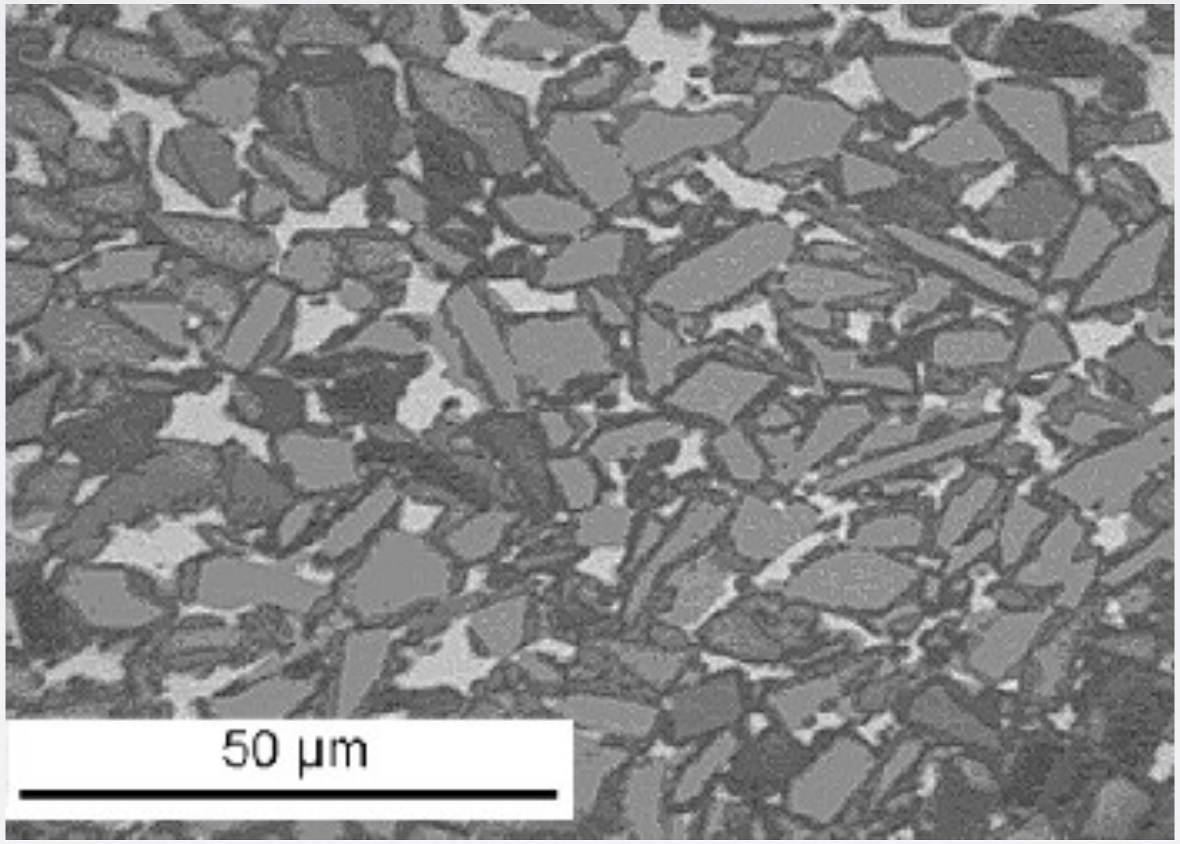
Use most convenient units
No conversions required

No error/consistency checking
GIGO
One error multiplies...

Microstructures

- Fundamental ethos of OOF2 is to process and simulate FEM systems based on experimental microstructures

- Establish microstructure in OOF2 by **image upload**



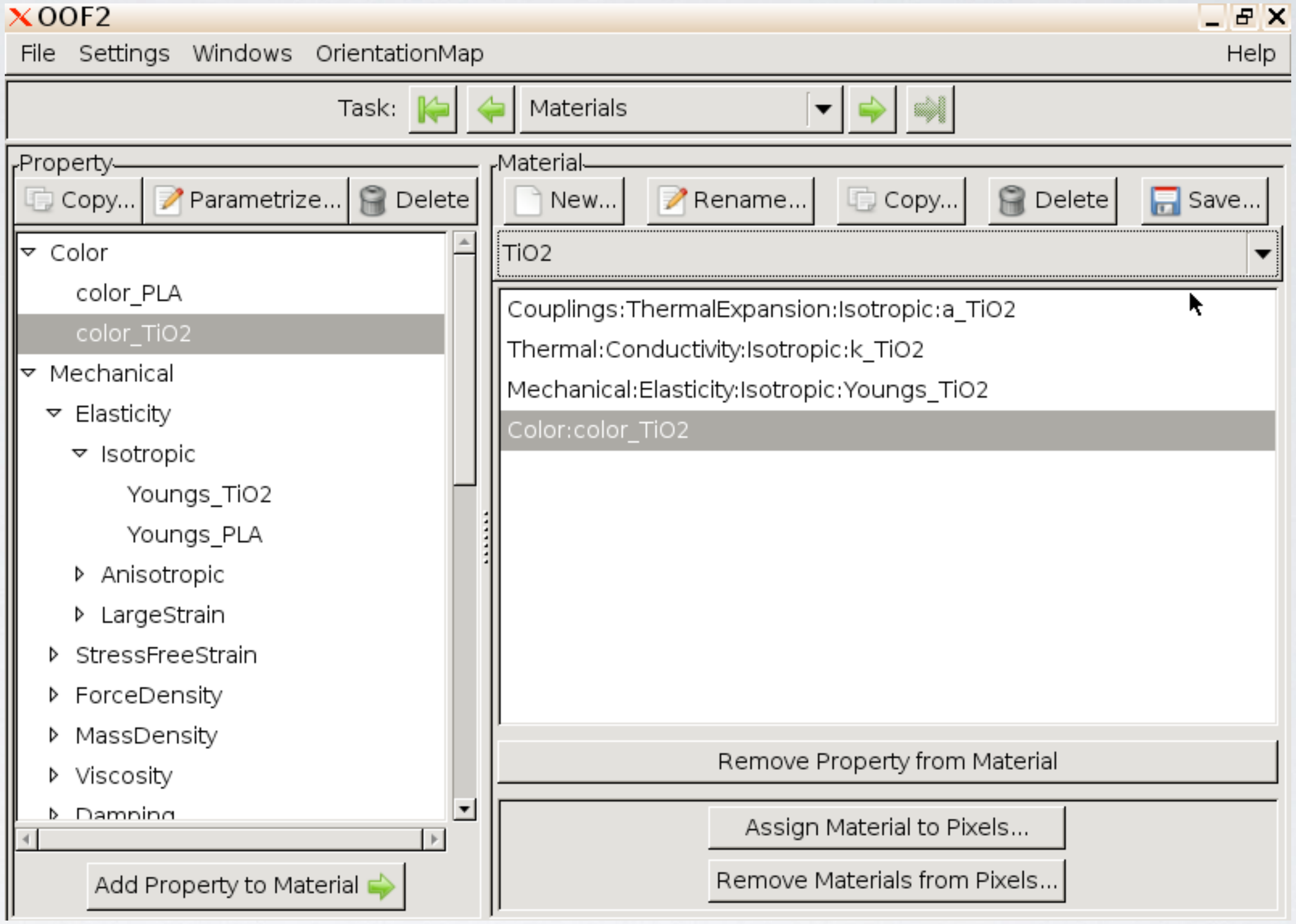
silicon carbide micrograph

- Different phases / materials identified by groups of pixels

http://pwatlas.mt.umist.ac.uk/internetmicroscope/micrographs/microstructures/silicon-carbide.html

Materials

- Materials with defined properties created and assigned to pixel groups



- Isotropic or anisotropic properties supported

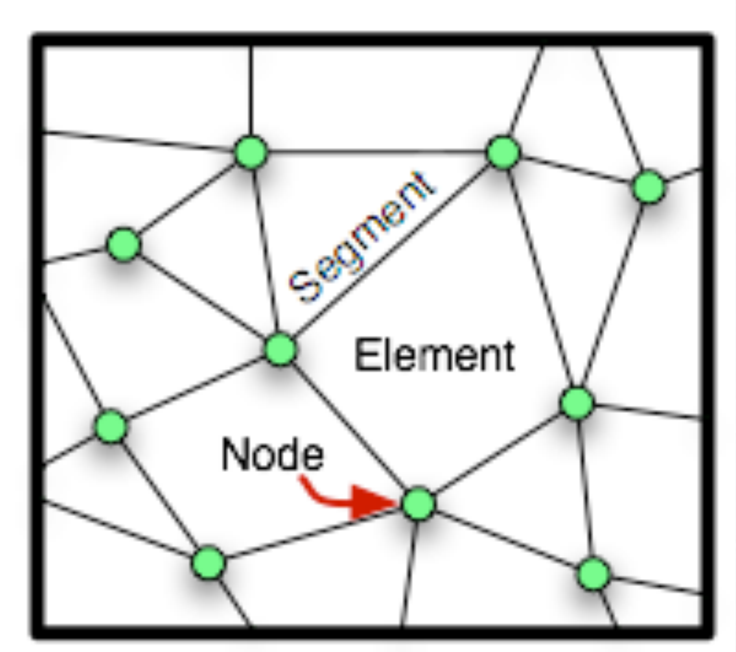
- Materials properties: Young's modulus Poisson's ratio thermal conductivity coefficient of thermal expansion dielectric permittivity viscosity density color ...

Skeletons

- A **skeleton** is a partitioning of the micrograph into finite elements, it contains only geometric information

- A **mesh** is derived from the skeleton, containing geometry + equations, fields and boundary conditions

- Modifying the boundary conditions, material properties, or equations to be solved requires rebuilding of the mesh but <u>not</u> the skeleton

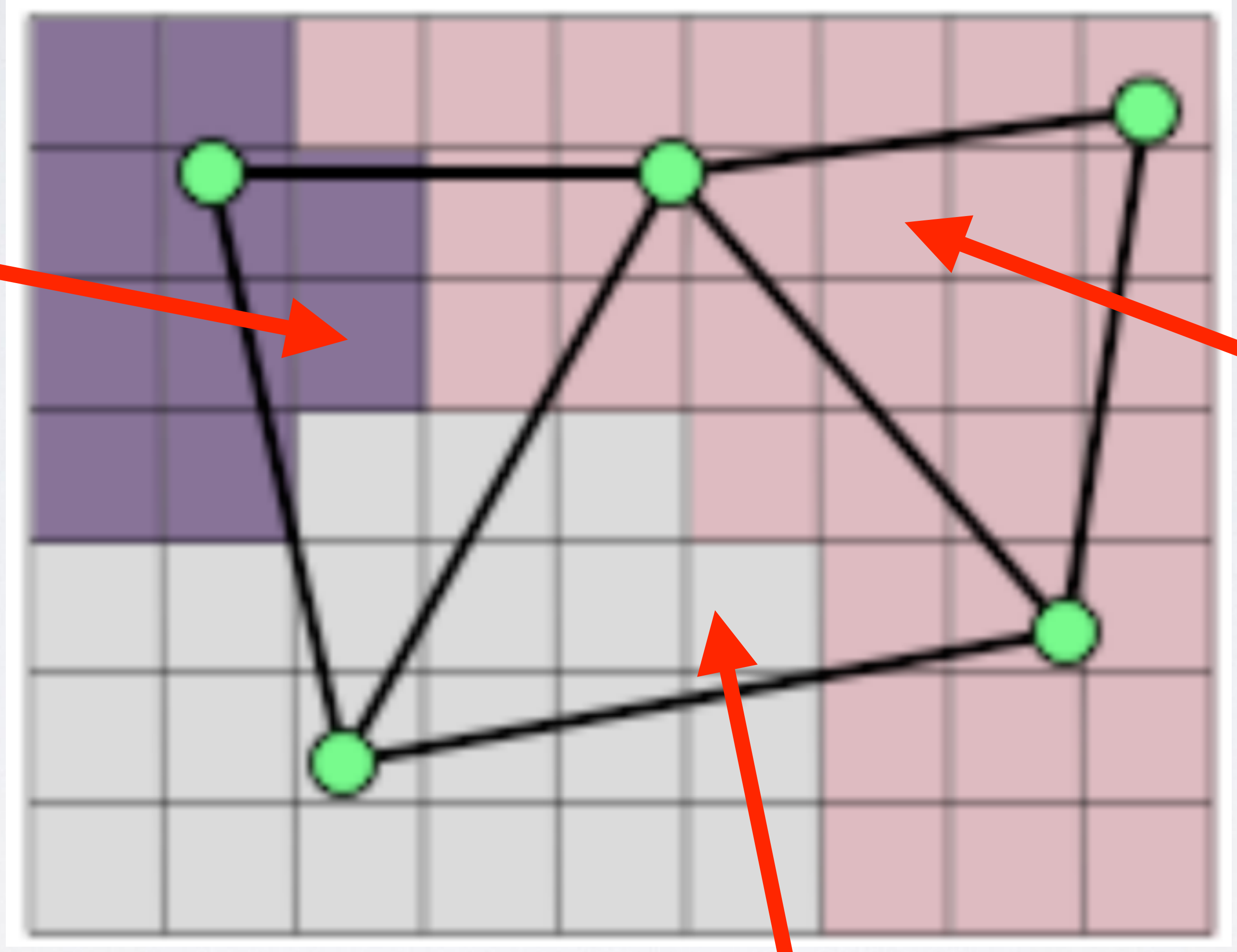


http://www.ctcms.nist.gov/~langer/oof2man/Section-Concepts-Skeleton.html

Element homogeneity

- A good skeleton is highly **homogeneous** (homogeneity index ~0.99) - each element contains a single phase

heterogeneous
(HI ~ 0.3)



homogeneous
(HI = 1.0)

heterogeneous
(HI ~ 0.5)

http://www.ctcms.nist.gov/~langer/oof2man/Section-Concepts-Skeleton.html

Skeleton refinement

- A good skeleton also contains very few high-aspect ratio elements, yielding better FEM numerical solutions

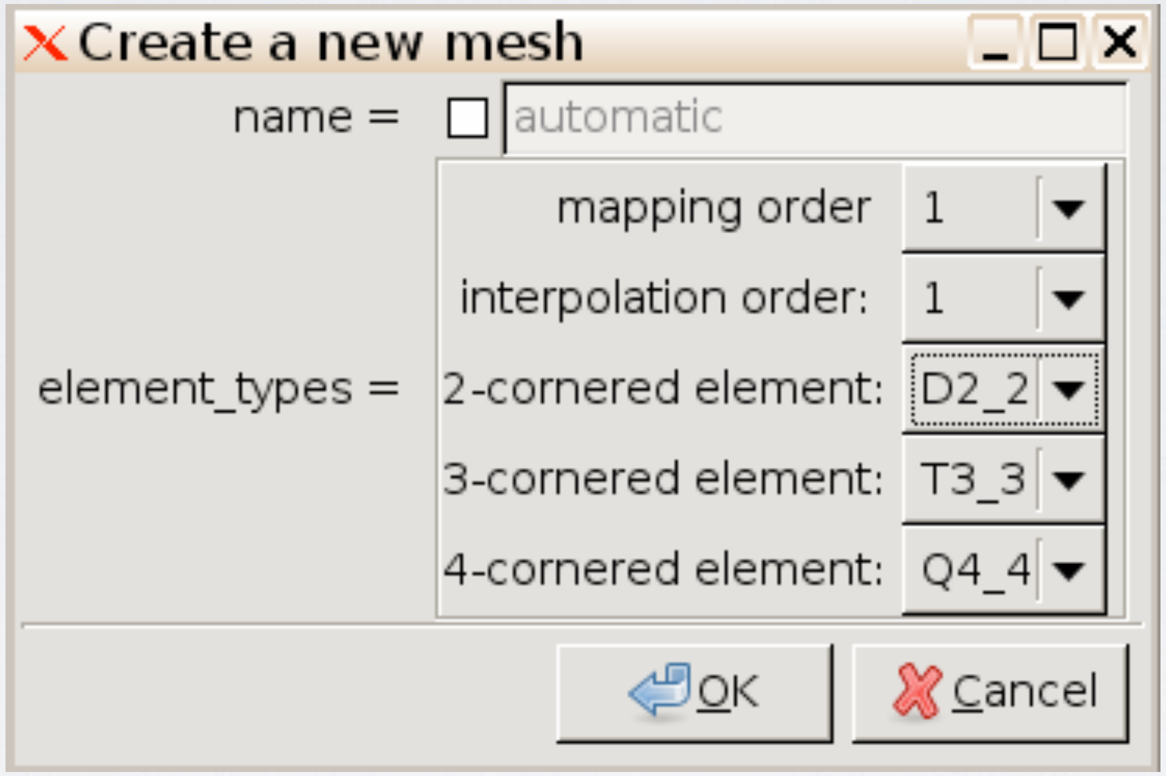
- A number of skeleton refinement tools exist to minimize the **effective energy**

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

- annealing
- edge swapping
- smoothing
- refinement (element partitioning)

Meshing

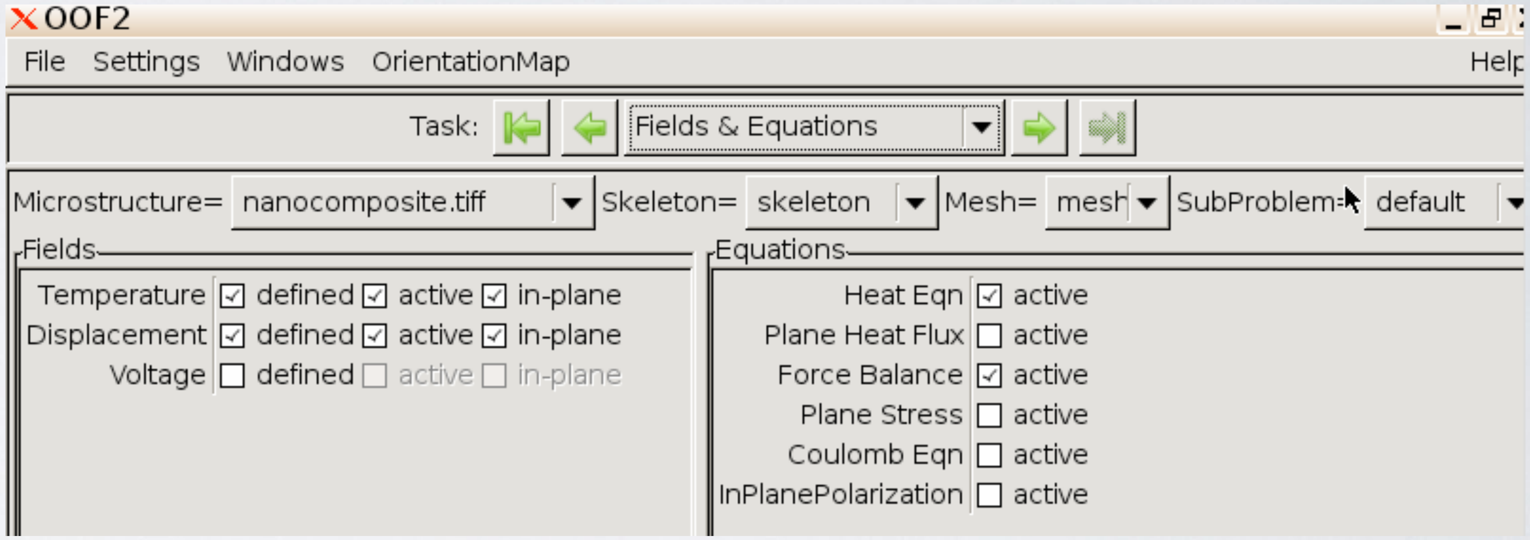
- The **mesh** is constructed from the **skeleton**
- The mesh elements in OOF2 support linear and quadratic interpolation functions



- These functions interpolate values from the mesh nodes to the element interiors

Equations

- OOF2 supports solution of the following equations:
  - heat equation
  - force balance
  - Coulomb equation
  - plane stress
  - in-plane polarization
  - plane heat flux



- Complex boundary conditions supported (Dirichlet, Neumann, periodic, generalized force)

- Complex fields possible (T, displacement, voltage)

Solvers

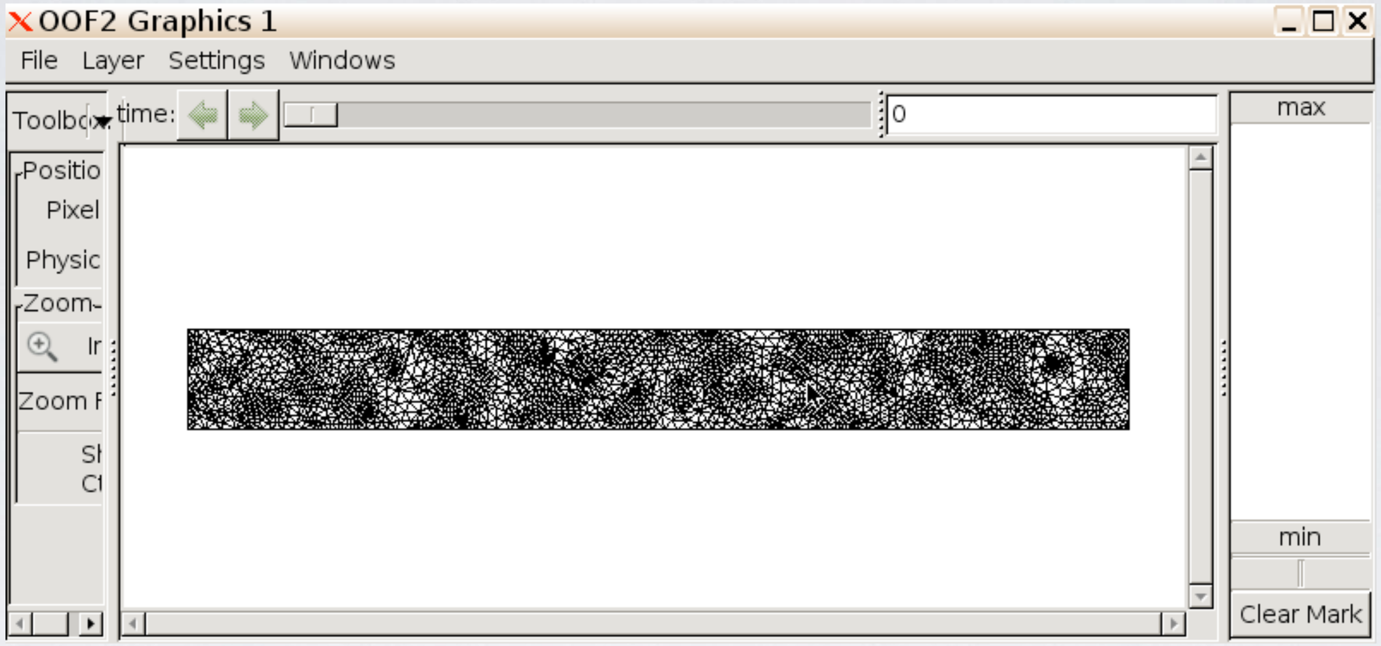
- A number of advanced numerical solvers are available
- User-specified tolerance and maximum iterations
- Problems are typically **large** and **sparse**

direct: slow
high accuracy
unsuitable for large problems (hi RAM rqmts)

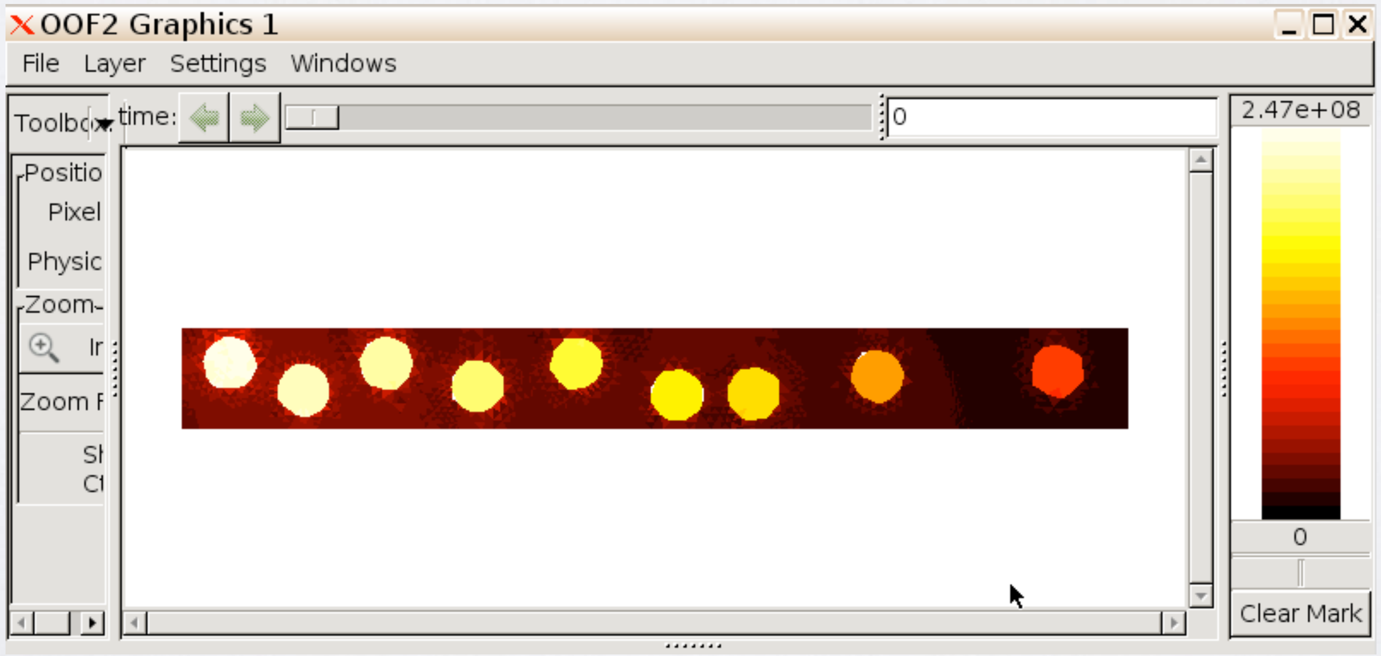
iterative: fast
lower accuracy
only choice for large problems

Visualization

- Micrograph, skeleton, and mesh visualized in Graphics pane

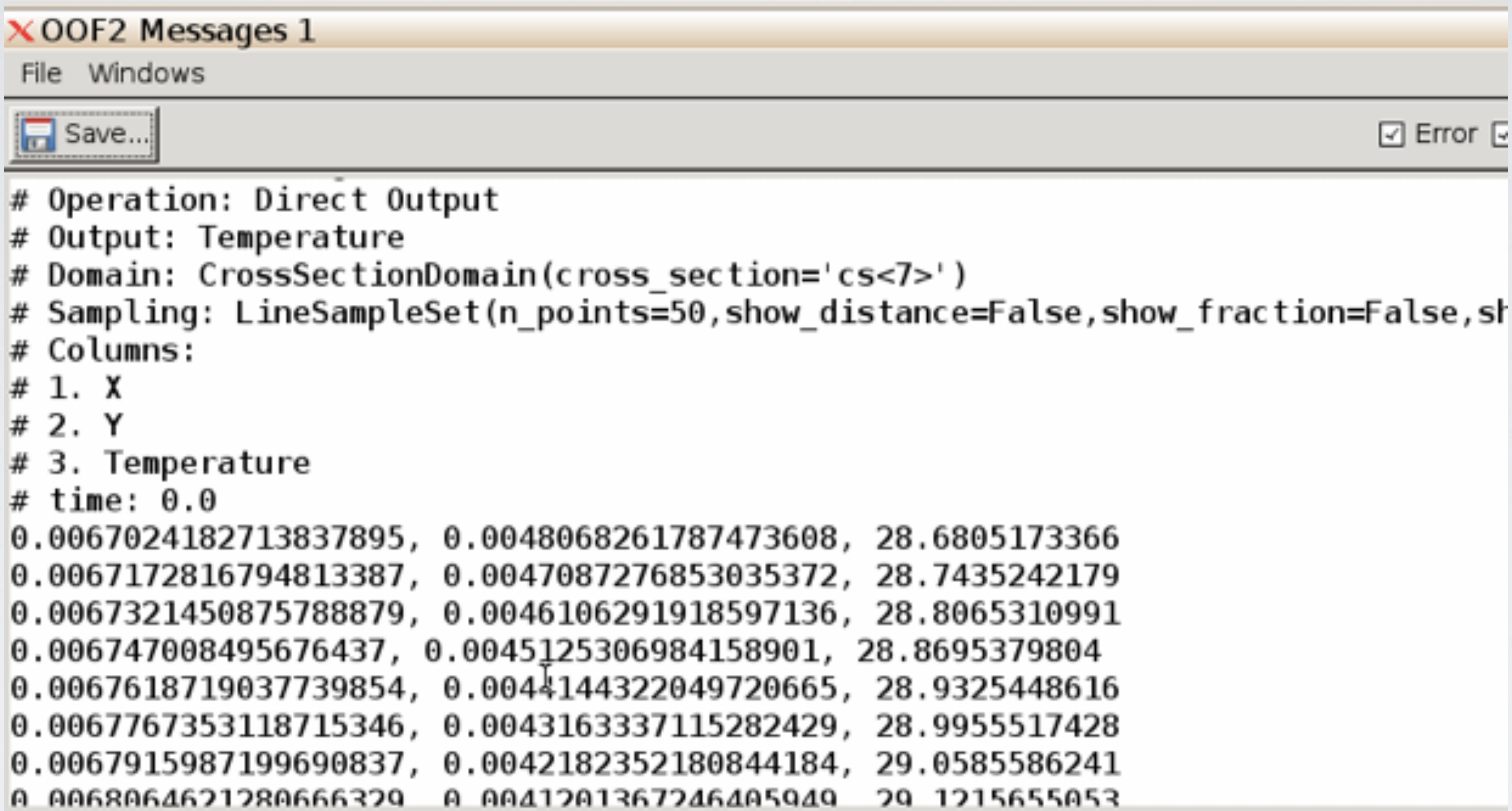


- Also used to visualize solutions (stresses, temperature) computed over the terminal mesh



Analysis

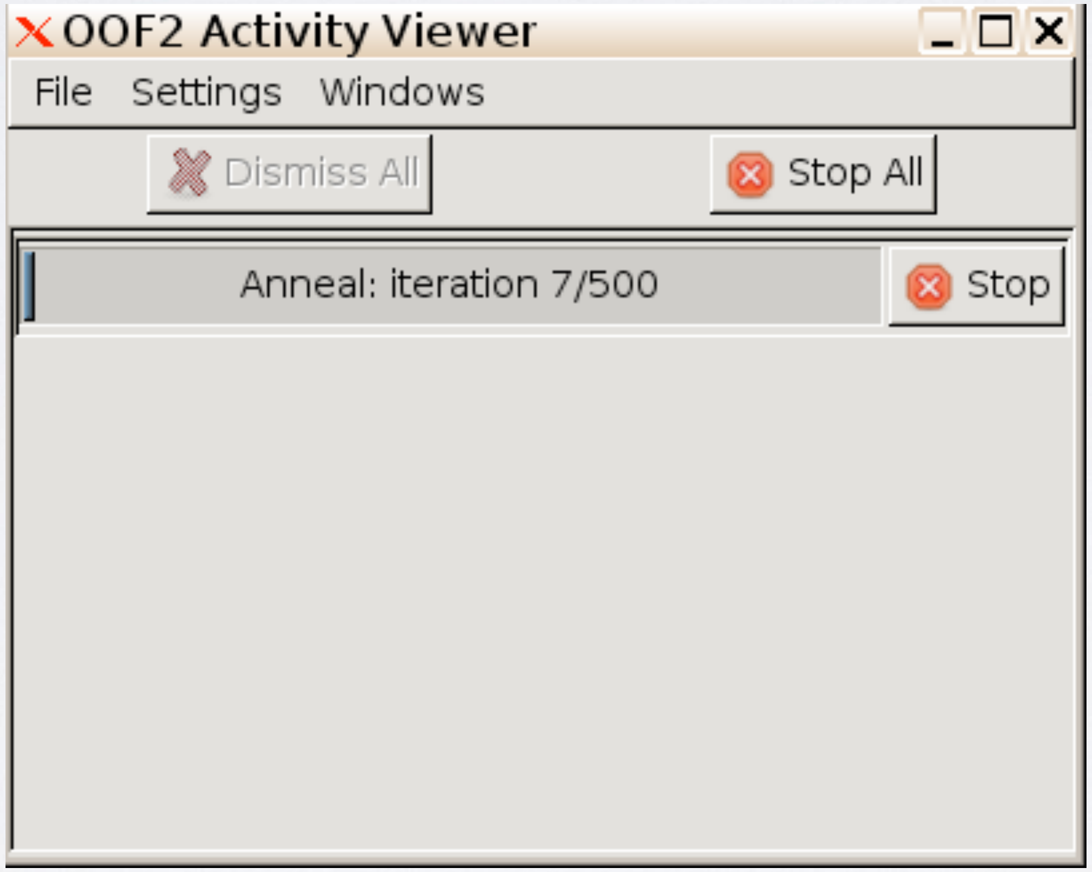
- The solution of scalar and vector fields over the terminal mesh can be outputted using the Analysis pane



- Data can be dumped to file for offline analysis

Activity viewer

- The Activity window indicates the current tasks occupying OOF2
- Very useful for monitoring long processes (solving, skeleton refinement, visualization)



Messages

- The Messages window provides detailed task information, and communications to the user