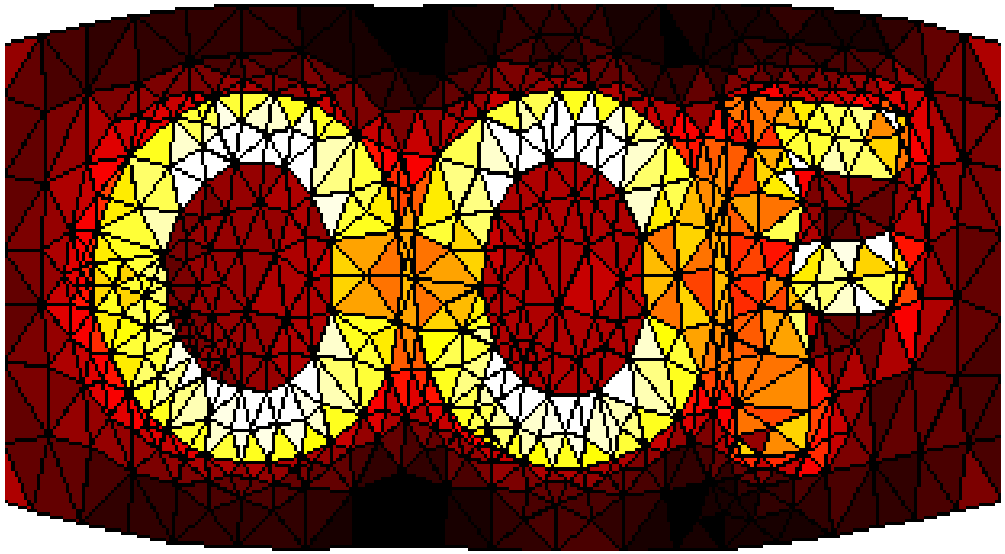
Object Oriented Finite Element Analysis of Material Microstructure



NIST

National Institute of Standards and Technology

Technology Administration, U.S. Department of Commerce

Information Technology Laboratory

and

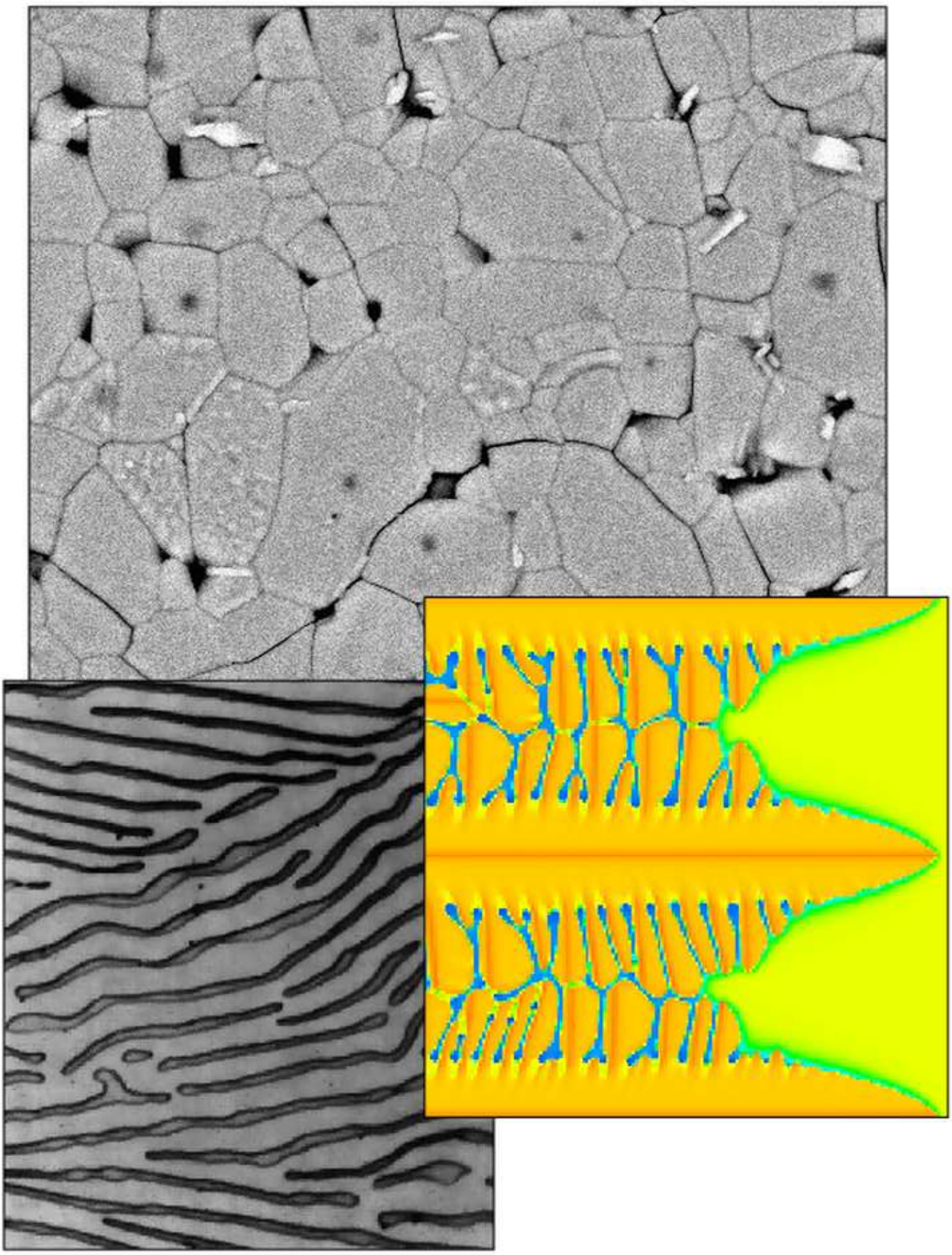
Center for Theoretical and Computational Materials Science

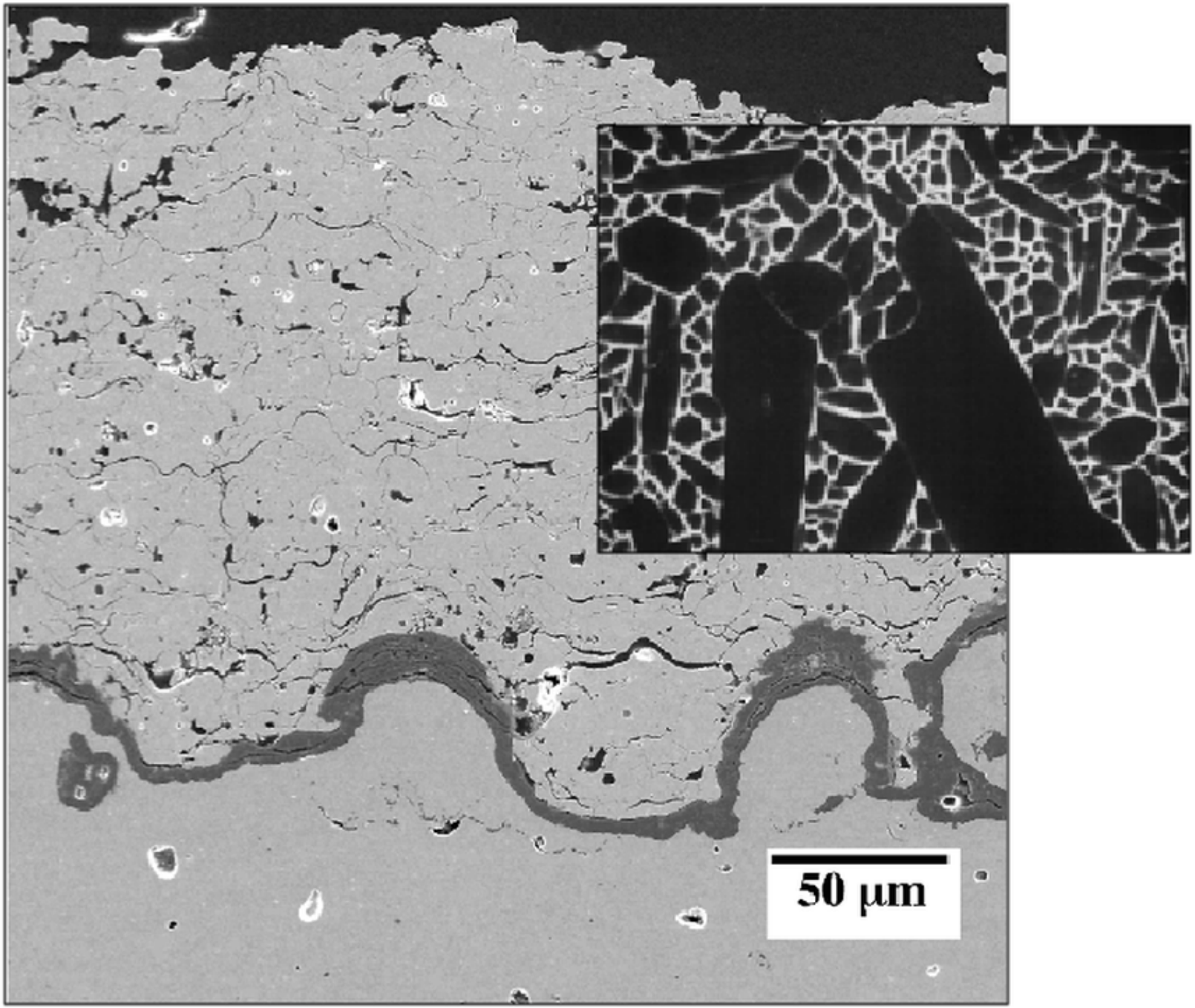
INDUSTRY WEEK IW

1999
Technology
of the year.

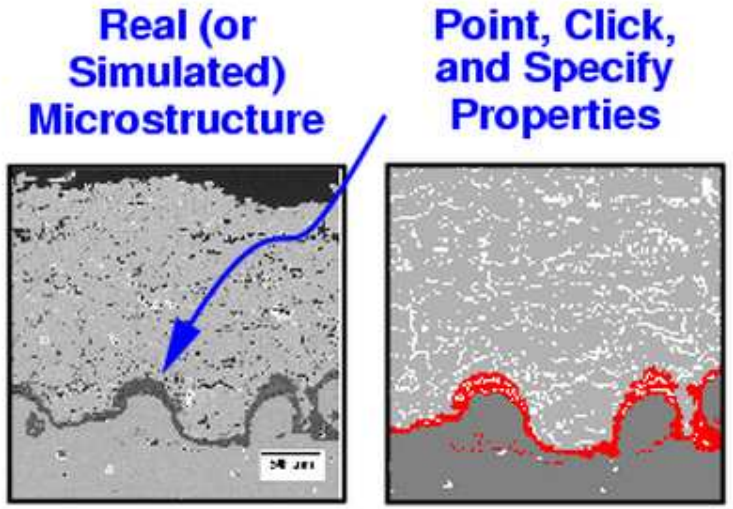
Current participants

- Developers
  - Steve Langer — NIST ITL staff — full time
  - Andrew Reid — MIT/NIST CTCMS post-doc — full time
  - Seung-Ill Haan — UMBC post-doc — part time
  - Andrew Roosen — NIST MSEL staff — mostly sysadmin
  - Edwin Garcia — MIT grad student — OOF1 mods/thesis
  - Kevin Chang — MBHS — summer project
- Advisors
  - Ed Fuller — NIST MSEL
  - Panos Charalambides — UMBC Mech Eng.
  - Craig Carter — MIT MSE

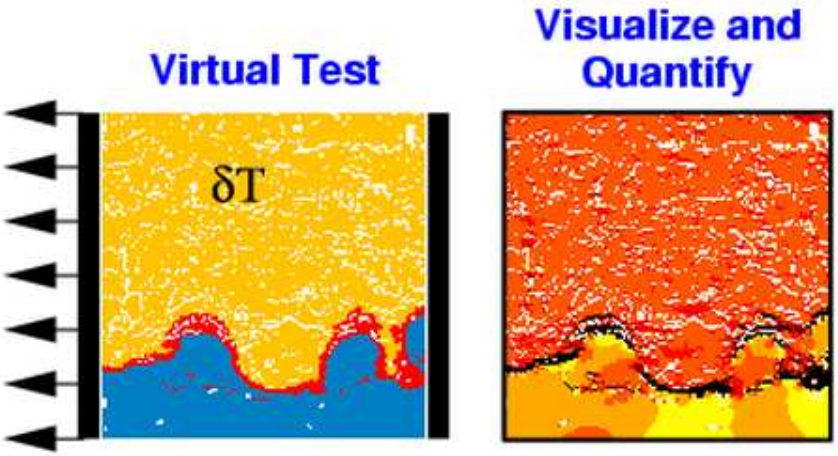


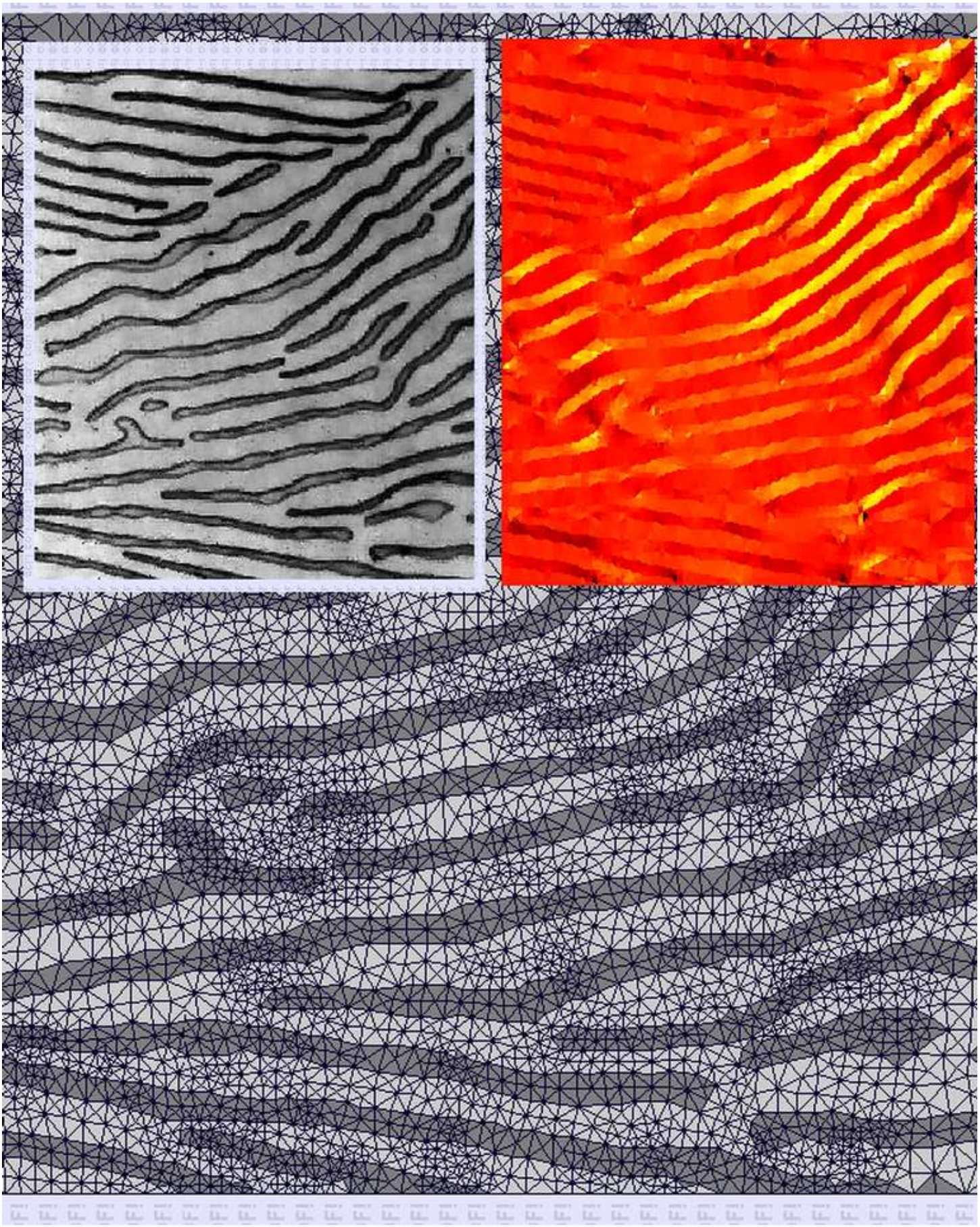

50 µm

ppm2oof: **a tool to convert an image or a micrograph of a heterogeneous, multi–component material into a finite element mesh with constitutive properties specified by the user.**



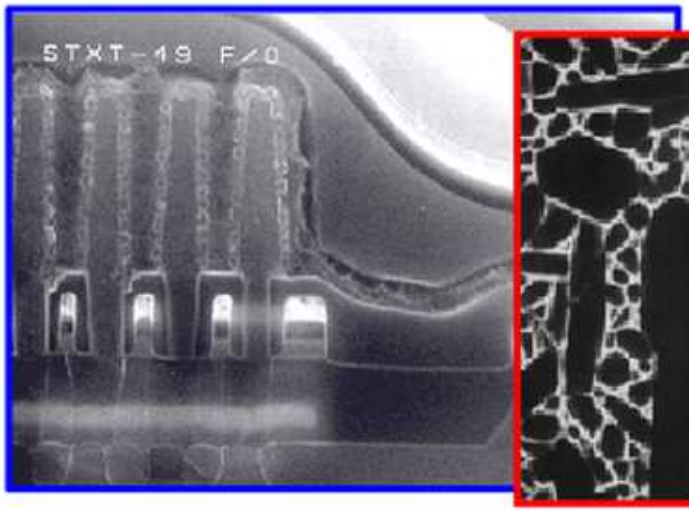
oof: **a tool to test physical properties and to investigate the influence of microstructure on macroscopic behavior, via finite element analysis.**

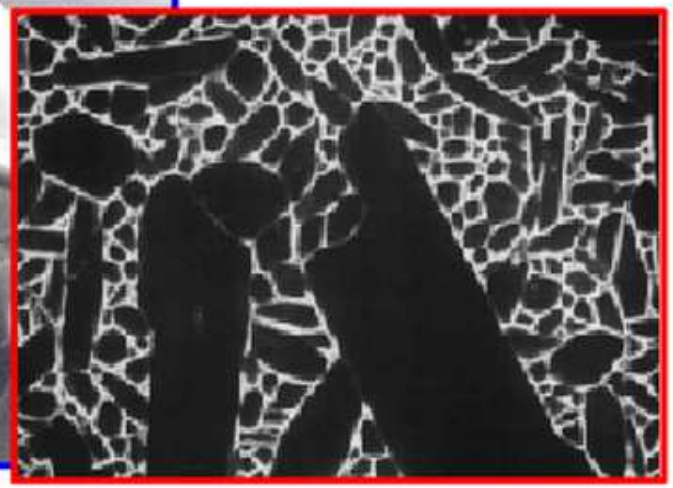




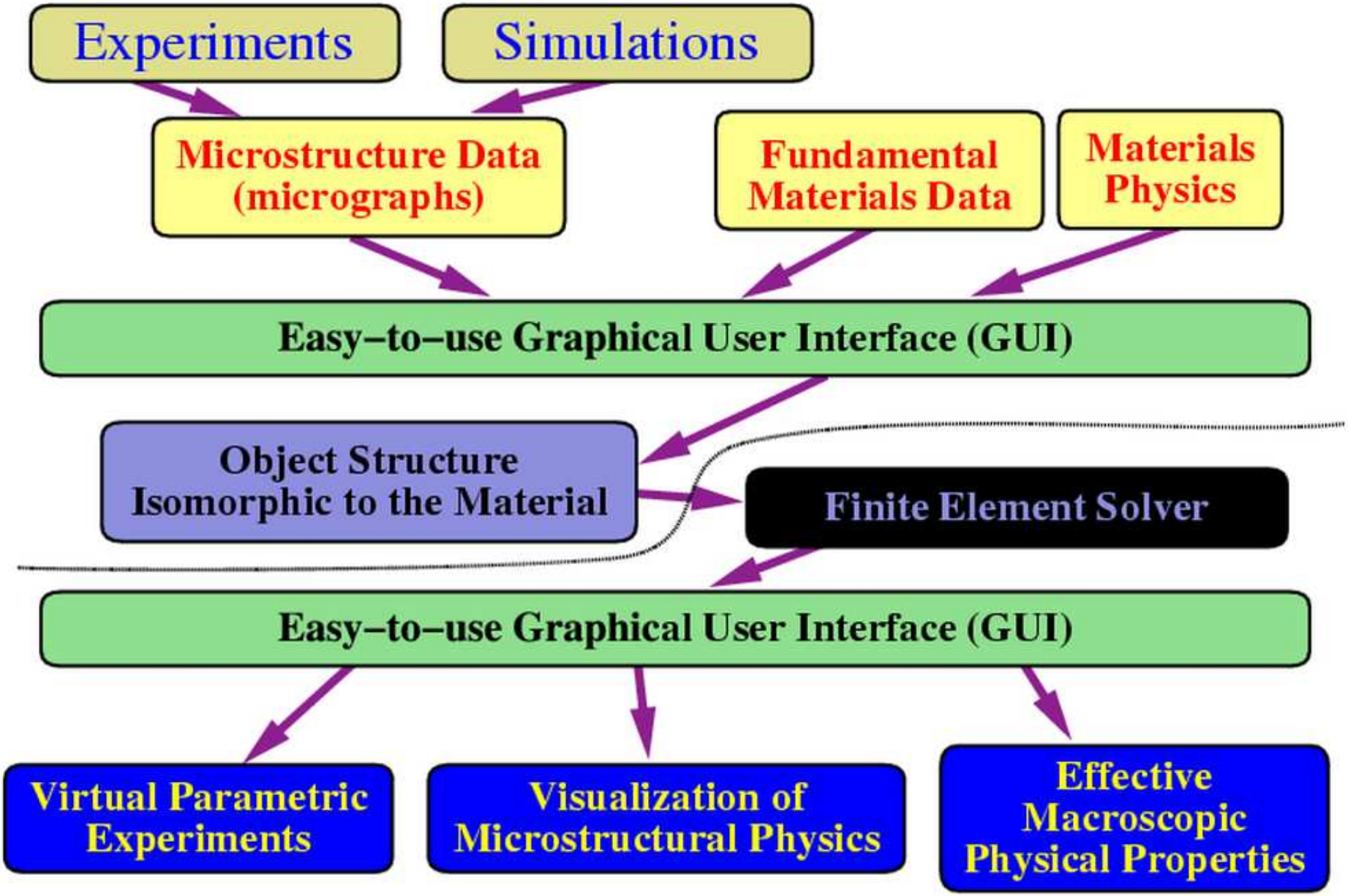
Why OOF?

- Commercial finite element packages work best for large–scale systems with regularly shaped components.
- Materials systems are small–scale and disordered.
- OOF is designed to answer the questions that materials scientists want to ask.
- OOF is easy to use.





Building a Microstructural Model



Current Capabilities

- Unstructured 2 dimensional triangular mesh fit to material boundaries.
- Linear elasticity with thermal expansion.
  - isotropic
  - hexagonal
  - ***etc***.
  - New crystal symmetries added easily
- Thermal Diffusion

Current Capabilities

- Plane stress or plane strain.
- Boundary conditions:
  - Fixed displacement, temperature.
  - Free.
  - Constrained motion.
  - Any combination of the above.
- Distortions:
  - Applied displacement, temperature
  - Applied force, heat flux

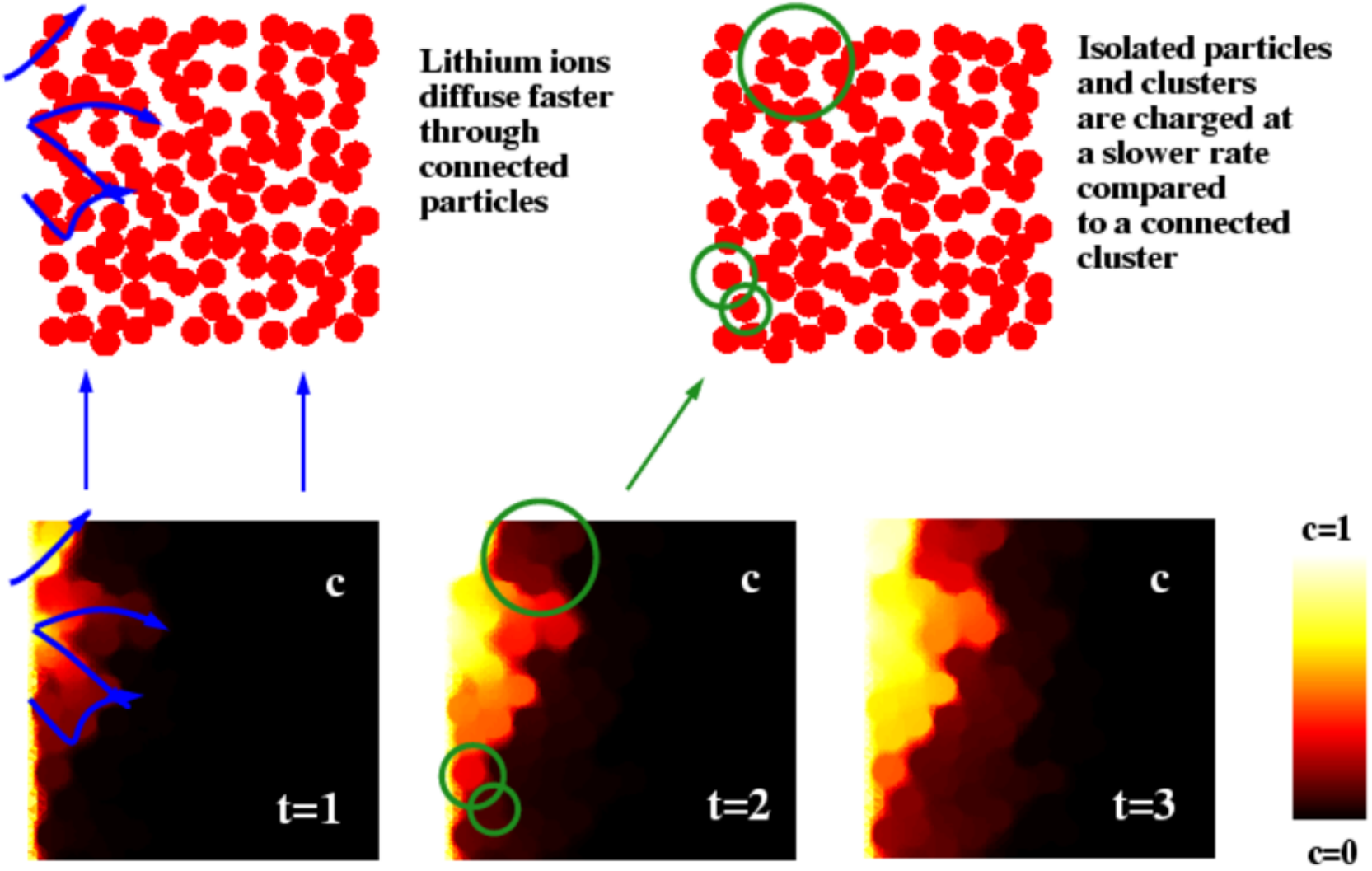
Current Capabilities

- Simple models of fracture.
- Designer elements.
- Controlled from graphical user interface or script.
  - Menu driven.
  - Commands in tree of submenus.
- Runs on SGI, Sun, Intel/Linux and Alpha/Linux.
- OOF2ABAQUS converts OOF meshes to Abaqus format.

Extensions to OOF1 by Edwin Garcia

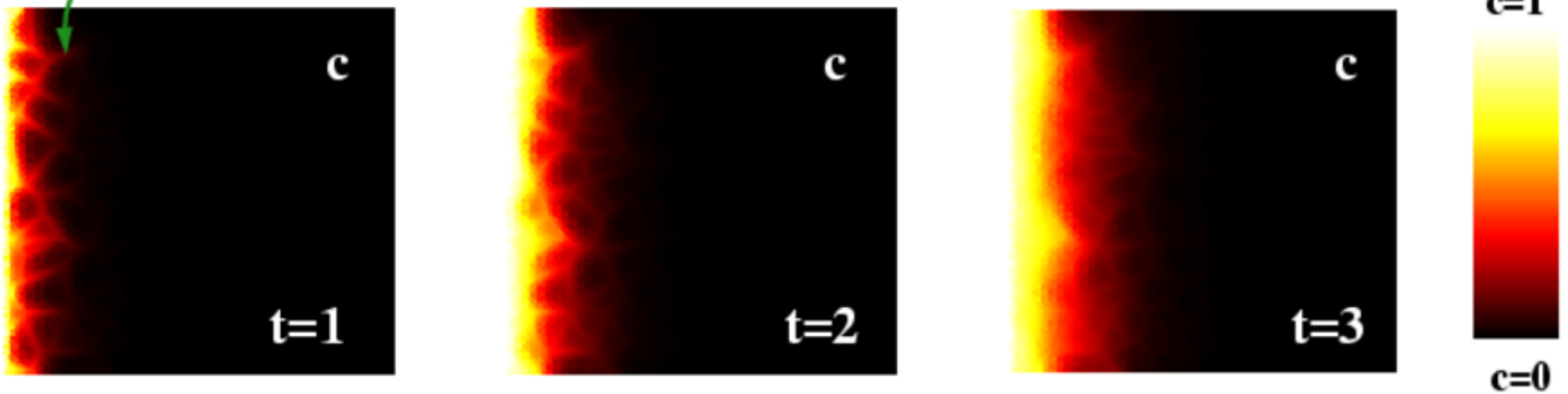
- Poisson's equation
- Piezoelectricity & Ferroelectricity
- Thermal conductivity
- Time dependent diffusion
- Viscoplasticity (with Rajesh Raghavan)

- Modifications did not fit easily into the OOF1 framework.
  - Inconsistent GUI, not suitable for distribution to the public.
    - New OOF2 framework required.

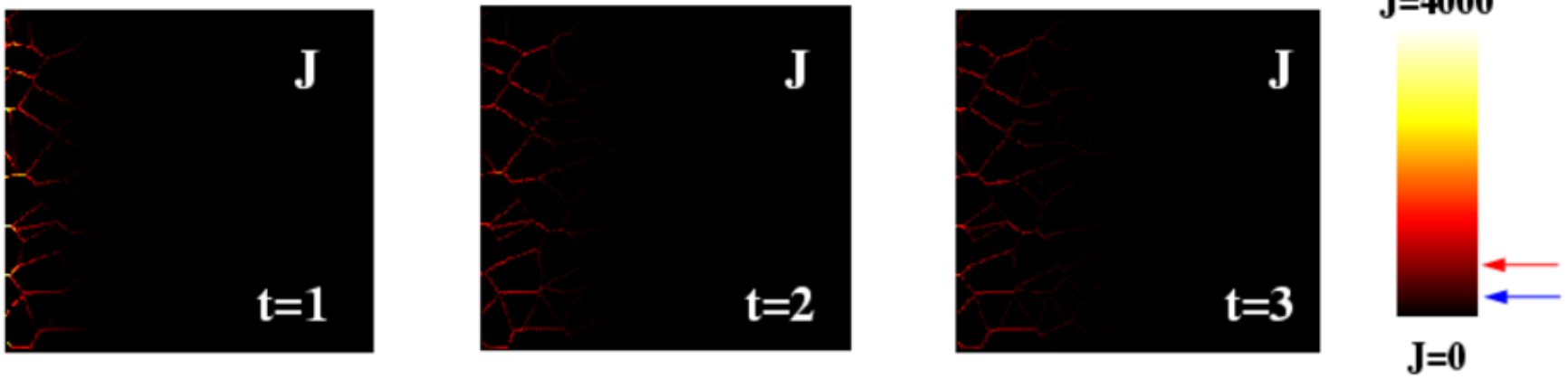


http://gargery.mit.edu/~edwin/portfolio.html

Grain boundary diffusion dominates initially → Large ‘‘Vegard–Type’’ stresses



Grain boundaries constitutes dominating transport path



← **steady state value for grain boundaries**

← **steady state value for bulk**

http://gargery.mit.edu/~edwin/portfolio.html

OOF2

more powerful and flexible

- Easily extendable to a wide variety of problems:
  - Elasticity, plasticity, thermal conductivity, mass diffusion, electrical polarization, piezoelectricity, ferroelasticity, ferroelectricity, Darcy's Law fluid flow, ***etc.***

OOF2

more powerful and flexible

- Designed for simple addition of new fields (u), properties (k), fluxes (σ), forces (f), and couplings between fields.
- Materials constructed by choosing & combining Properties.
- Easy addition of new types of finite elements.
  - different shapes, different orders, special properties.
  - Element order & type is independent of Material.
- Generalized plane-flux (plane-stress) relations.

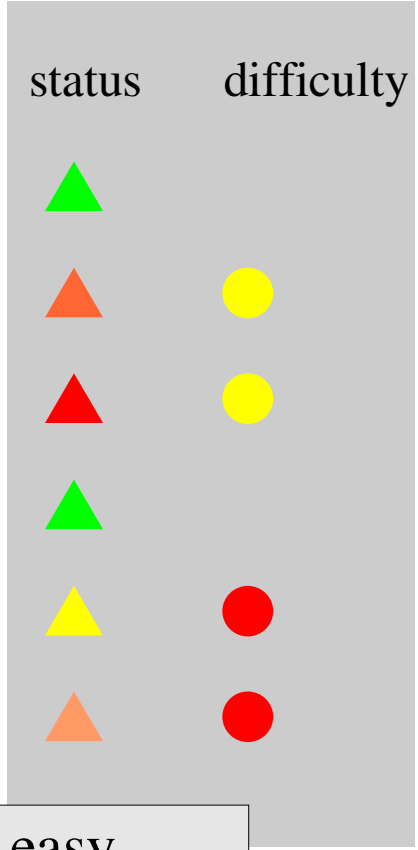
OOF2

more powerful and flexible

- Will solve linear, nonlinear and time dependent problems.
  - ***eg***, plasticity
- Error control through automatic mesh refinement.
- Better image analysis tools.
  - Automatic detection of grain boundaries, etc.
- OOF2 will form the basis for OOF3D
  - UMBC collaboration on adapting mesh generation techniques to 3D

OOF2 Status

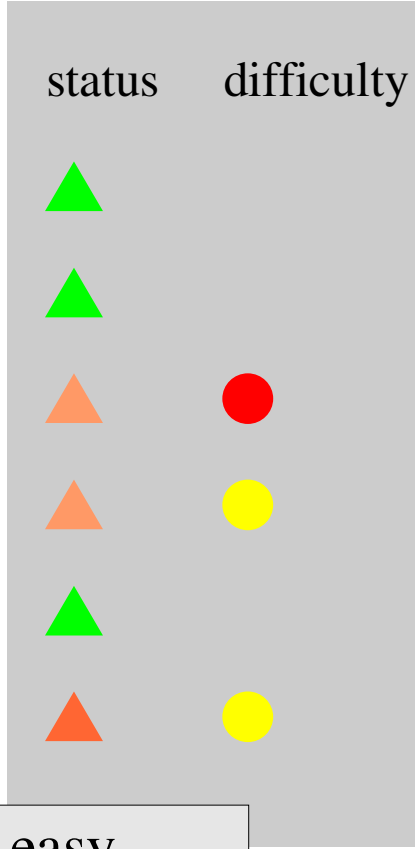
- Core Finite Element Classes
  - General purpose 2D elements
  - Line elements
  - Specialized elements
  - Linear solver
  - Nonlinear solvers
  - Adaptive meshing while solving



▲ done
▲ current/soon
▲ later
● easy
● moderate
● difficult

OOF2 Status

- Equations
  - Divergence equations
  - Plane flux equations
  - Helmholtz equation
  - Time dependence
  - Nonperiodic boundary conds.
  - Periodic boundary conditions

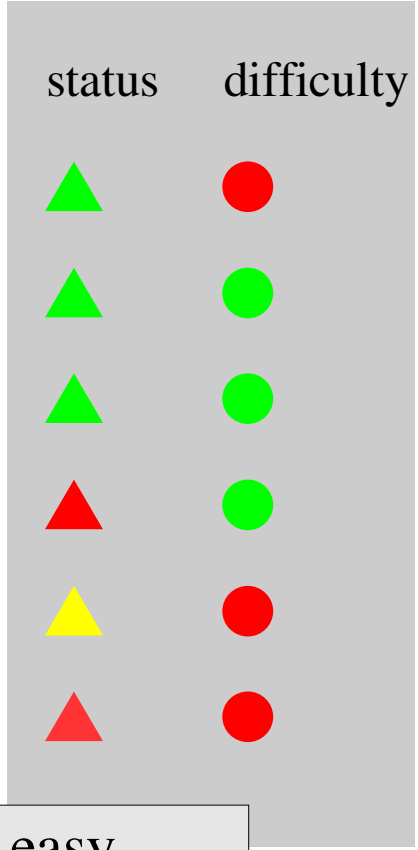


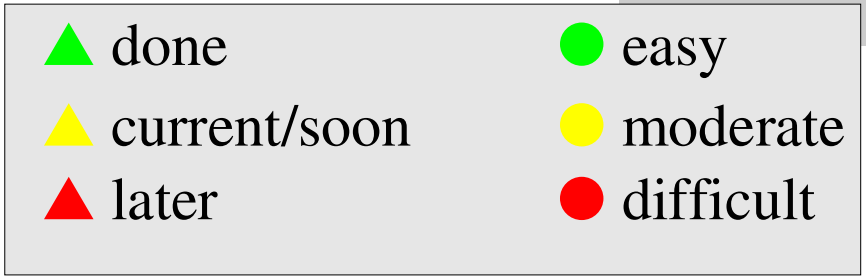
▲ done
▲ current/soon
▲ later

● easy
● moderate
● difficult

OOF2 Status

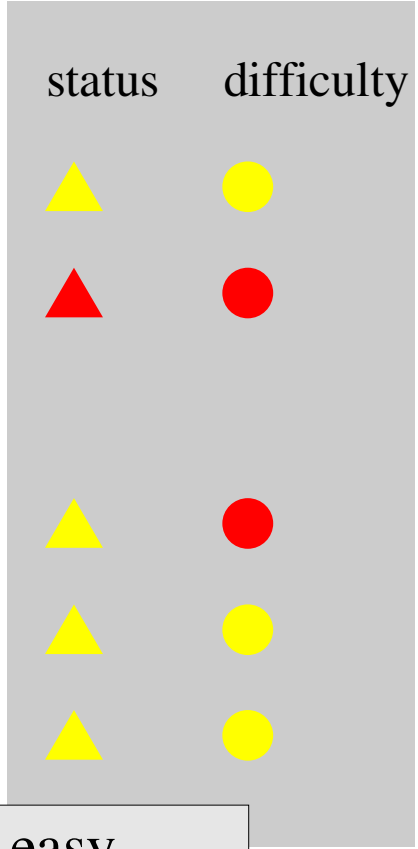
- Material Properties
  - Infrastructure
  - Elasticity
  - Thermal Conductivity
  - Other linear properties
  - Plasticity
  - Other non-linear properties

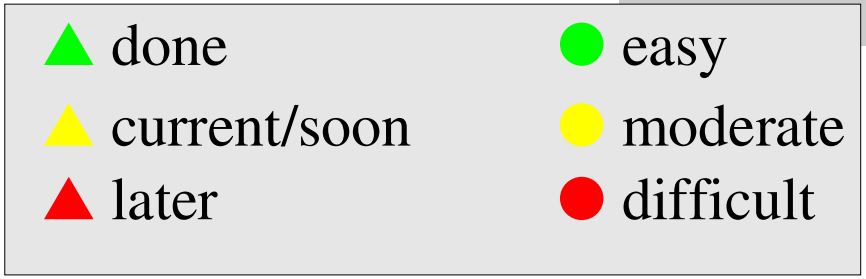




OOF2 Status

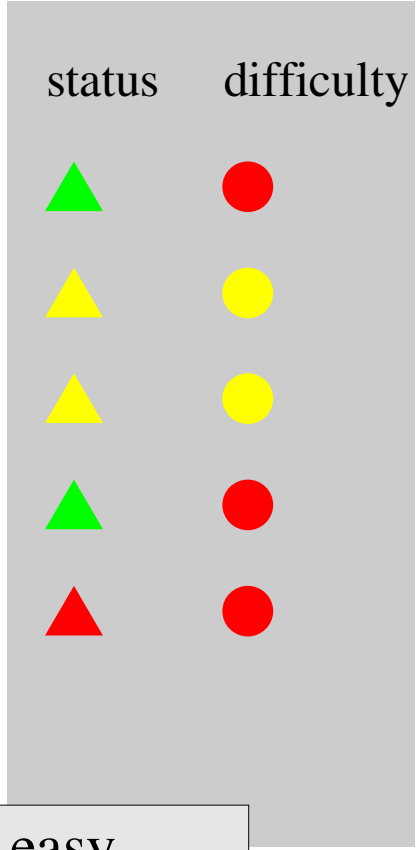
- Image Processing Tools
  - Port tools from OOF1
  - New tools
- Mesh Generation
  - Infrastructure
  - Port tools from OOF1
  - Quad mesh refinement





OOF2 Status

- Graphical User Interface
  - Define materials and Properties
  - Construct meshes from images
  - Define problem parameters
  - Plot predefined quantities
  - Define new quantities to plot



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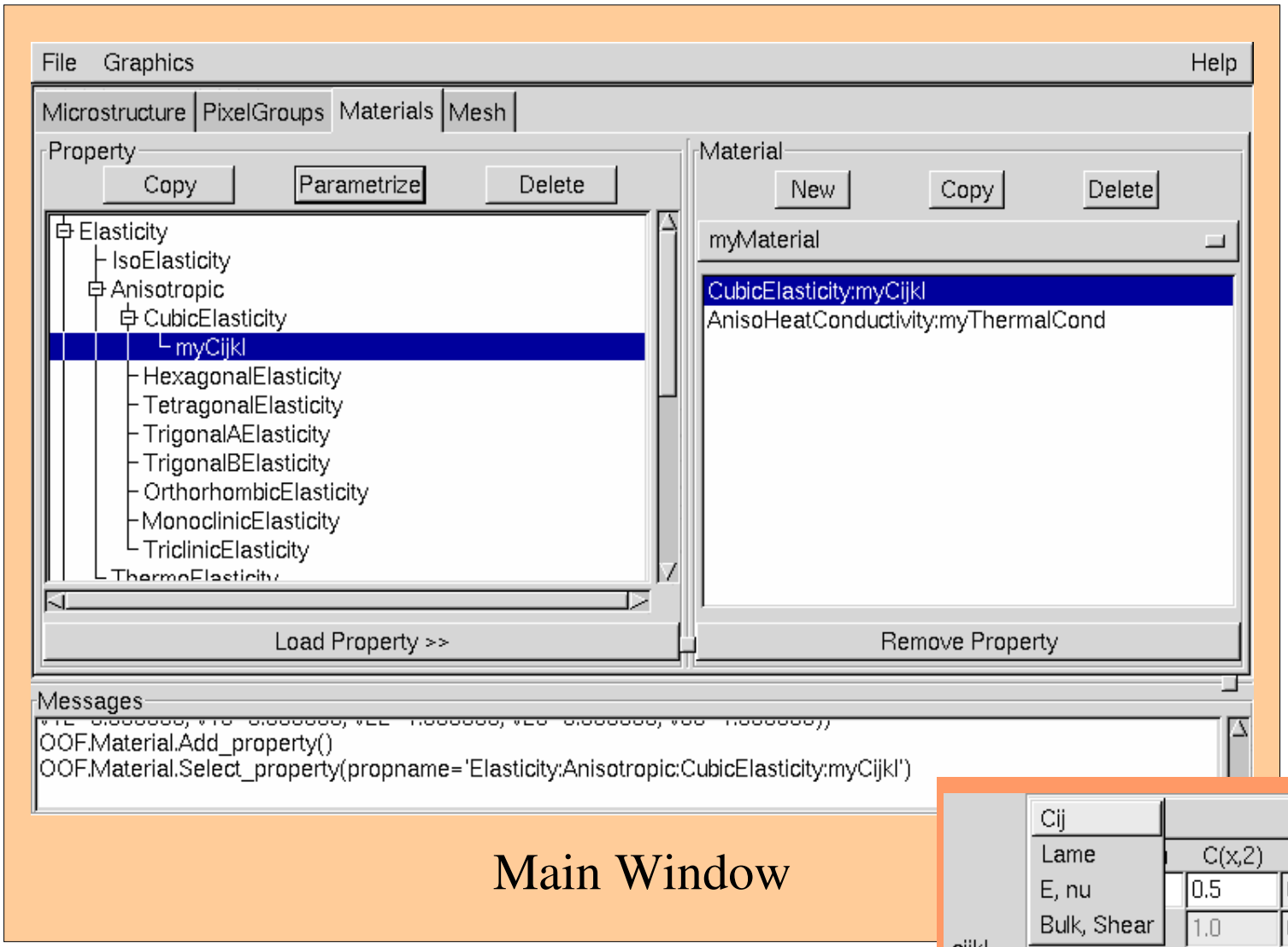
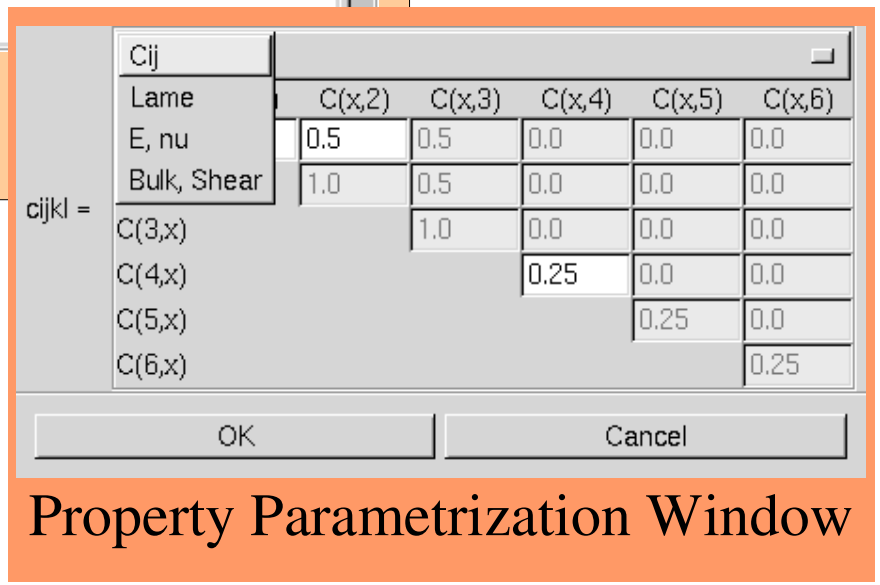
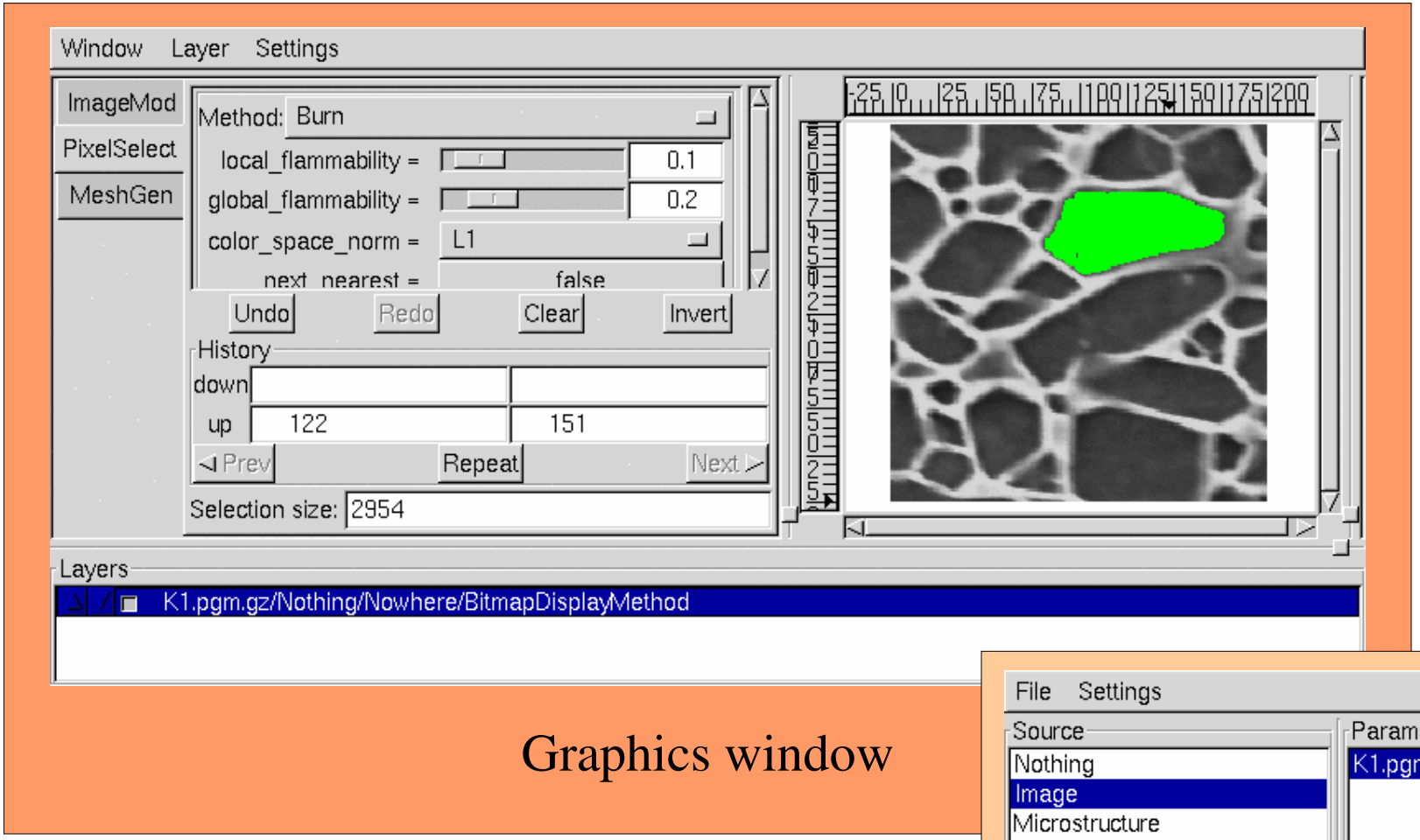


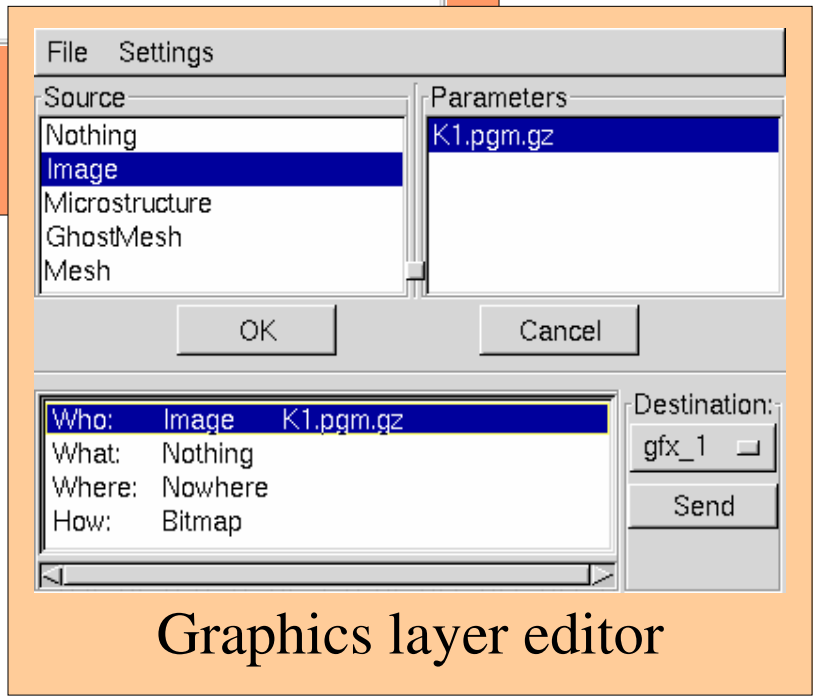
Main Window



Property Parametrization Window



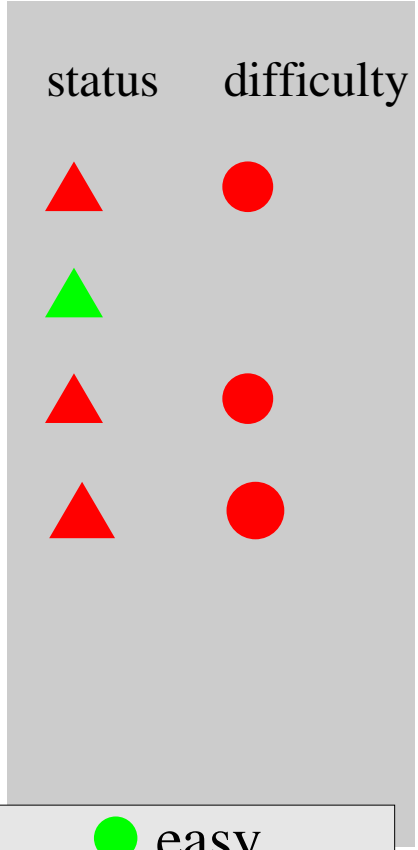
Graphics window



Graphics layer editor

OOF2 Status

- System Programming
  - Threads
  - Command logging and playback
  - Parallelization
- Three dimensions



Tentative Time Frame

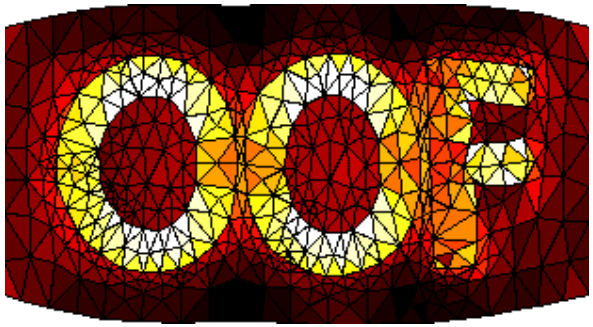
- Preliminary OOF2 release this fall:
  - All OOF1 features, plus
    - higher order & quadrilateral elements
    - more image formats
    - new mix & match properties.
- Next year:
    - Plasticity & non-linear solvers
    - More image analysis tools
- Following year:
    - 3D
    - Parallelization

Contacts:

stephen.langer@nist.gov

oof_manager@ctcms.nist.gov

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



- Download:
  - Source code
  - Binaries
    - SGI
    - Sun
    - Intel (Linux)
    - Alpha (Linux)
  - Manuals, examples, and tutorials