MSC Software
Fuel Cell Analysis

MSC Software
SIMULATING REALITY

Pacific Northwest
National Laboratory

May 12, 2004

Who is MSC?

MSC.Software is the largest* supplier of functional virtual prototyping software, systems, & services. We enable manufacturers of mechanical systems to assess the performance of their products on the computer, thus reducing their reliance on physical prototyping.

What this allows you to do:

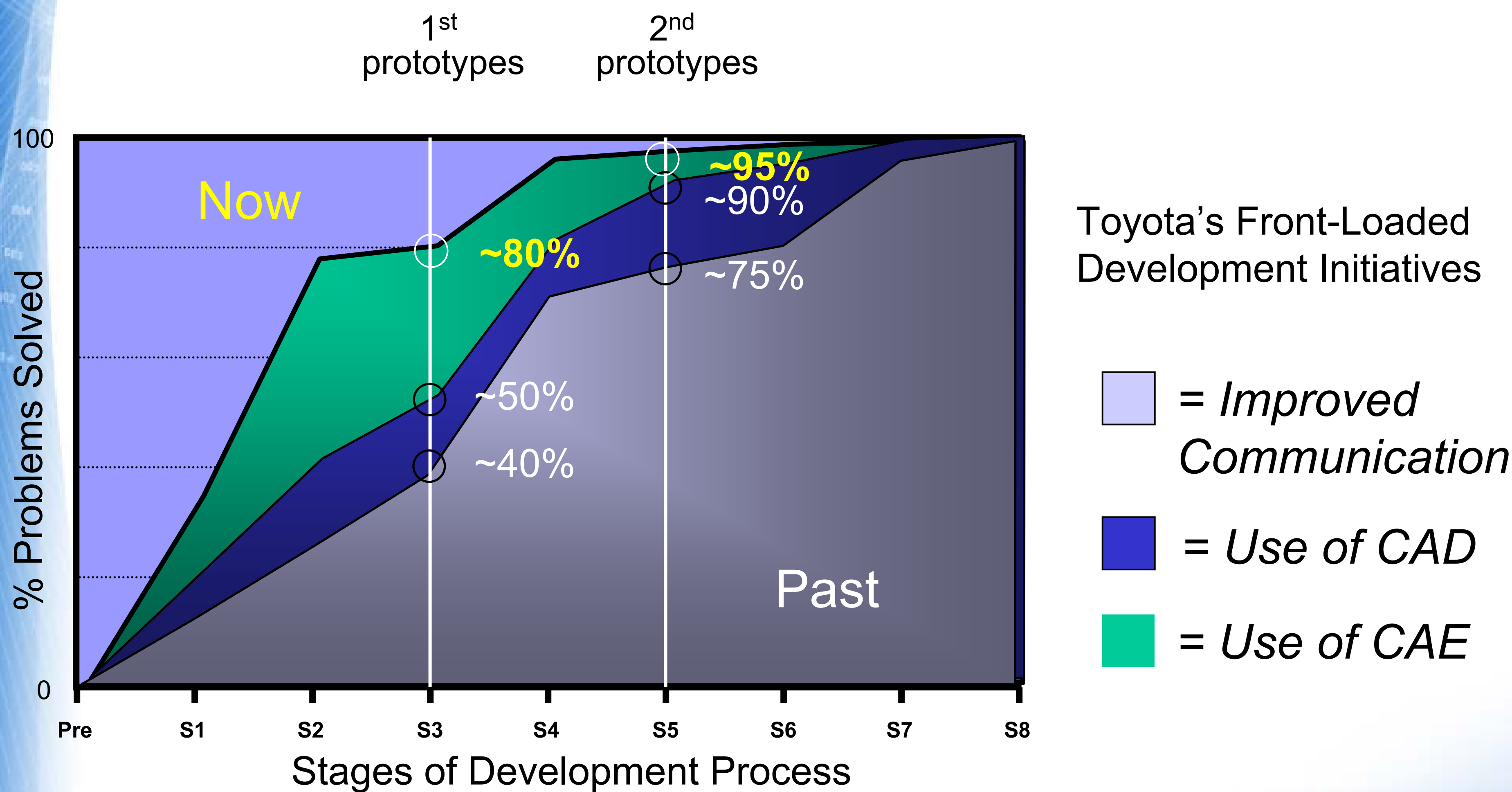
1. Manage Risk
2. [illegible]
3. Drive Collaboration

Better Information Earlier

*** Based on 2001 revenue of CAE companies. Source: Daratech**

Better Information Earlier

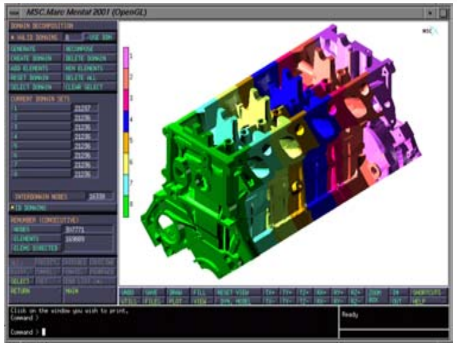
How this has helped Toyota

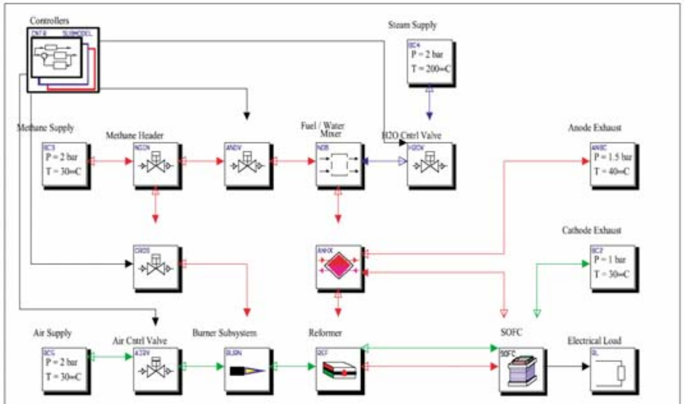


End Result: 65% fewer prototypes (!)

Fuel Cell Simulation Tools

- MSC.Software
  - MSC.Mentat – Graphical Interface
  - MSC.Marc – Mulit-Physics solver
  - Easy5 – Fuel Cell Library
- PNL Electro-Chemistry solver
  - Electrochemistry
  - Chemical Reaction
  - Heat Generation
  - Flow Solution





The MSC.EASY5 model shown here includes the SOFC fuel cell stack, the steam reformer, a system burner, heat exchangers, control valves, a resistive/inductive electrical load, and a series of logic and PID controllers.

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MSC/PNL Collaboration

MSC.Marc Solver Provides:

- Heat Transfer Solution
  - Conduction – through all solid and fluid layers
  - Convection – Boundary layer heat transfer between fluid and solids layers
- Mass Flow
  - Convective energy transfer of moving fluid streams
- Mechanical performance
  - Thermal Distortions – affect local flow
  - Thermal Stress/Strain – determines structural integrity of all fuel cell components, especially seals and PEN layers

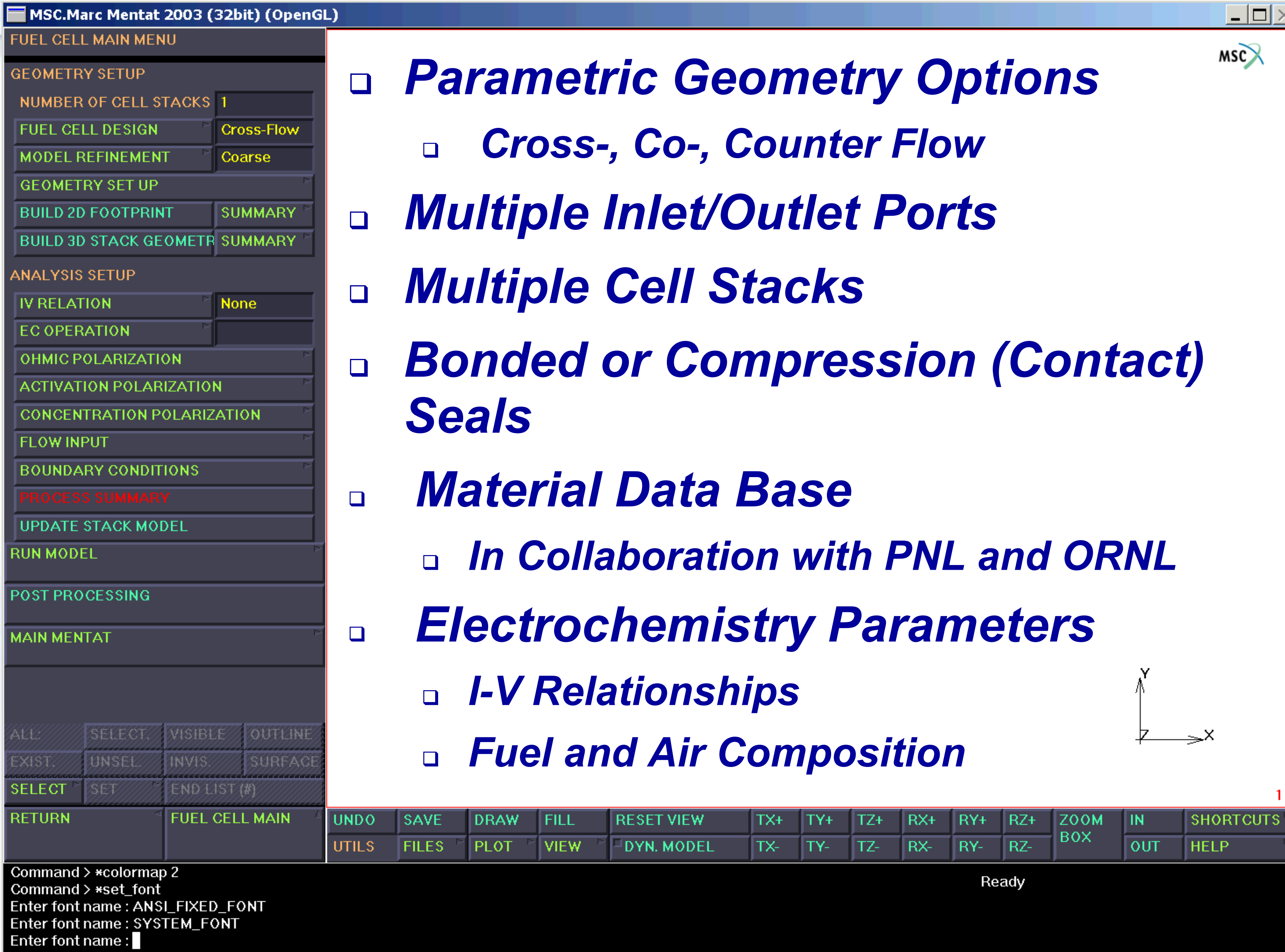
PNL Electro-Chemical performance of the PEN

- Current Density – IV performance versus fuel utilization
- Fuel Utilization – spatial distribution of species across cell
- Heat Generation – spatial distribution versus local EC

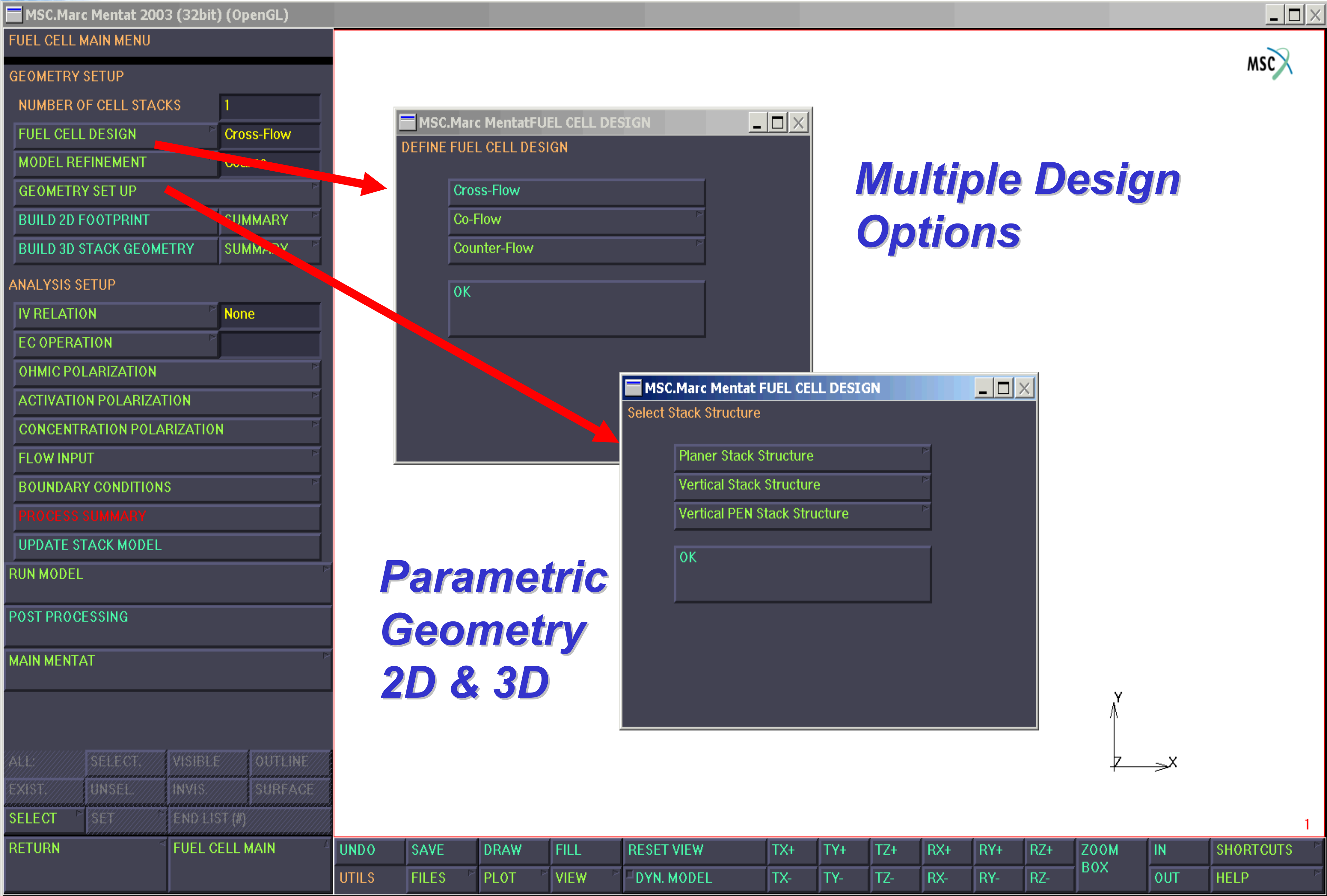
MSC.Mentat

- Tightly Integrated GUI for MSC.Marc solver
- Customized Interface for SOFC Fuel Cell modeling
  - PNNL-NETL-MSC Collaborative Development
- Automated Model Generation and Analysis
  - Full 3D multi-stack model generation < 1min.
  - Allows for simulation by non-FEA experts
  - Parametric design and performance evaluation
  - Material and flow input evaluation

SOFC Fuel Cell GUI



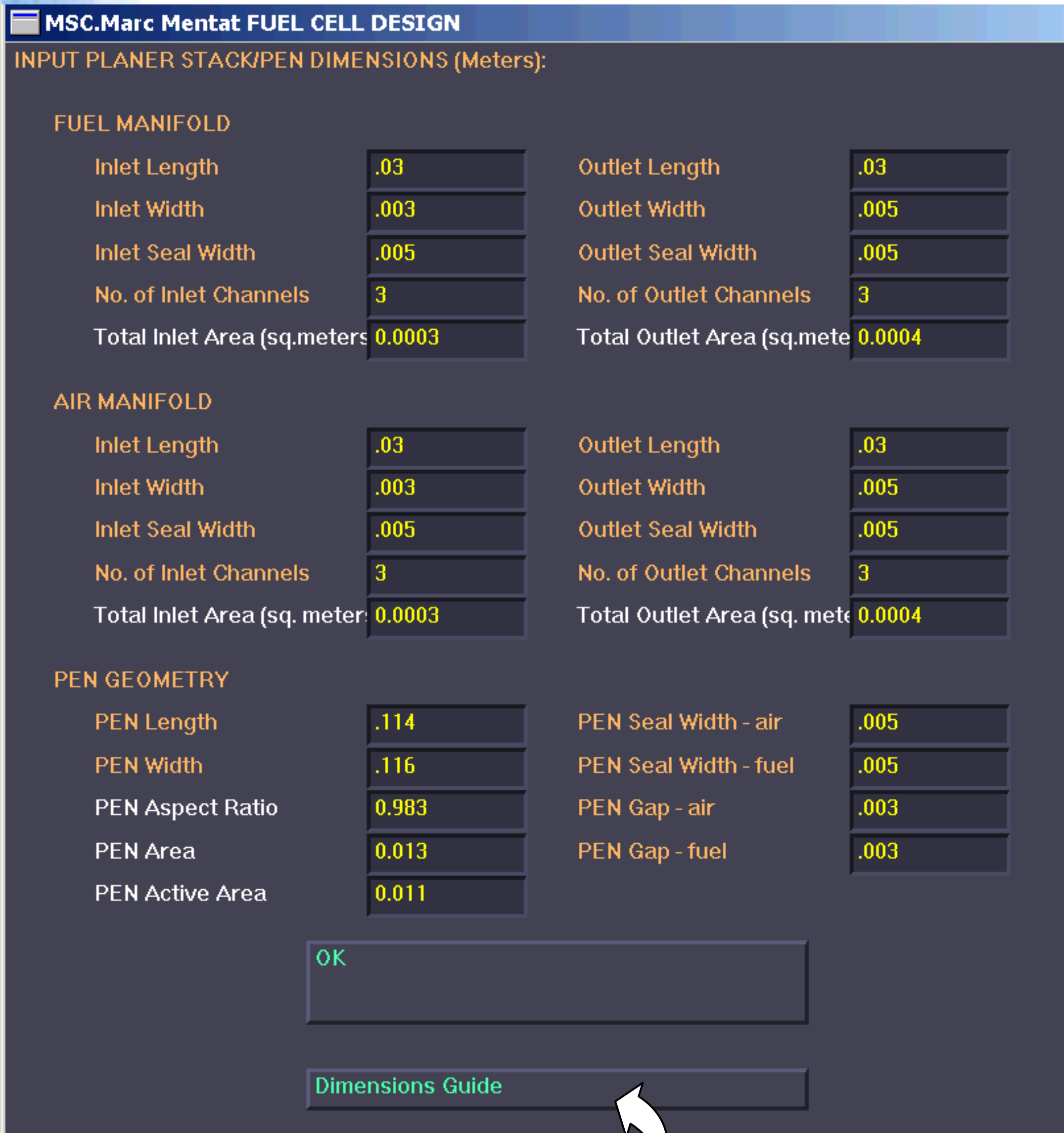
Model Creation

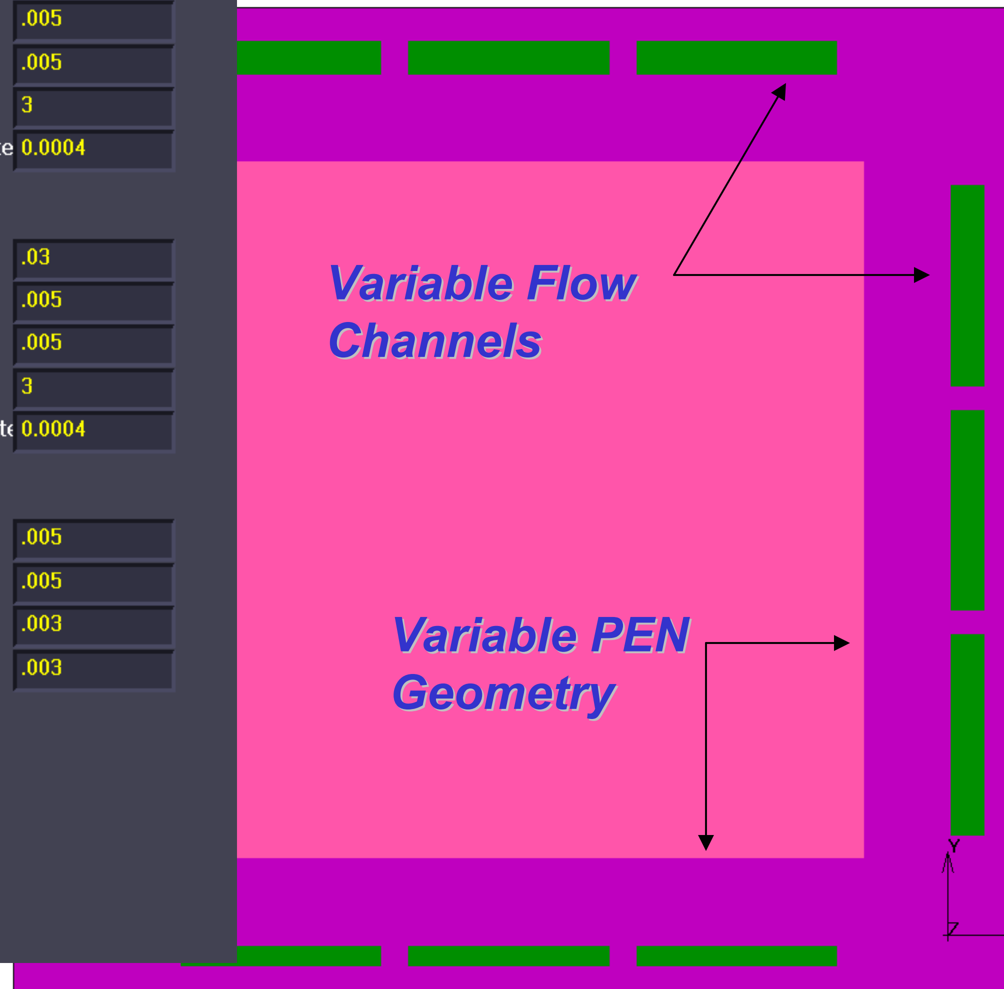


Multiple Design Options

Parametric Geometry 2D & 3D

Planar Configuration - 2D Footprint





Detailed User Guides

Multiple User Help Guides

MSC.Marc Mentat FUEL CELL DESIGN

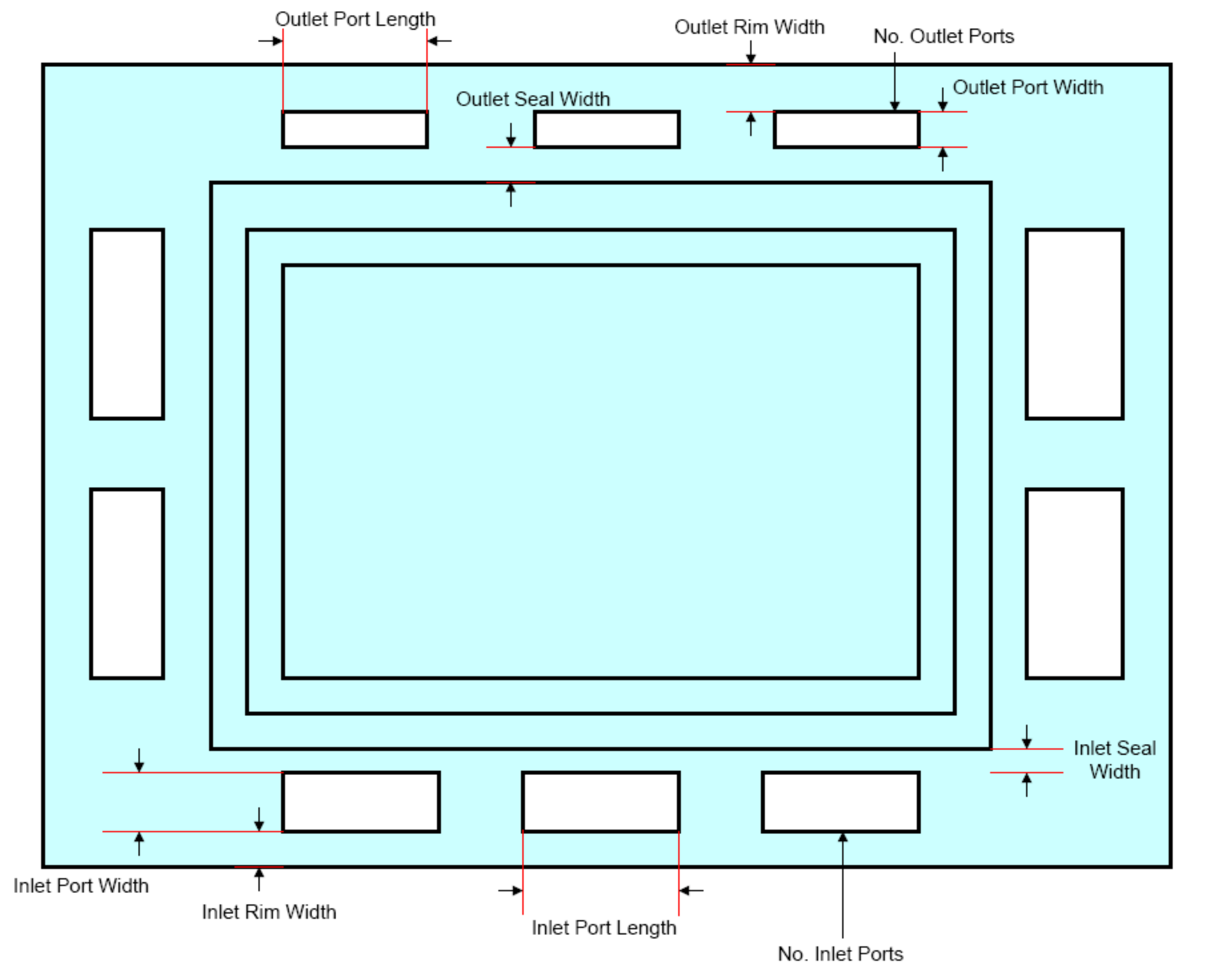
INPUT PLANER STACK/PEN DIMENSIONS (Meters):

FUEL MANIFOLD	
Inlet Length	.03
Inlet Width	.003
Inlet Seal Width	.005
No. of Inlet Channels	3
Total Inlet Area (sq.meters	0.0003
AIR MANIFOLD	
Inlet Length	.03
Inlet Width	.003
Inlet Seal Width	.005
No. of Inlet Channels	3
Total Inlet Area (sq. meter	0.0003
PEN GEOMETRY	
PEN Length	.114
PEN Width	.116
PEN Aspect Ratio	0.983
PEN Area	0.013
PEN Active Area	0.011

OK

Dimensions Guide

Dimensions – Crossflow Manifold (Fuel)



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3D – Vertical Stack
Seal and Layer Configurations

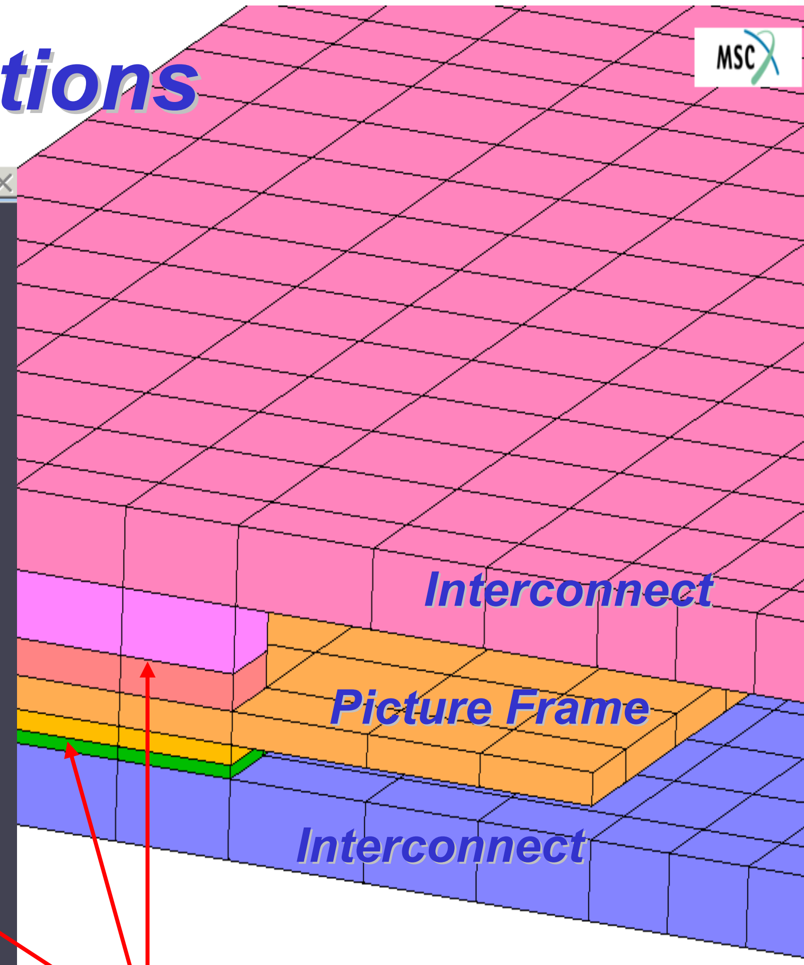
MSC.Marc Mentat FUEL CELL DESIGN

INPUT VERTICAL STACK COMPONENT DIMENSIONS (meters):

INTERCONNECT (TOP)			
Thickness	0.0012	Material	SS-430
COMPOSITE SEAL 1			
Seal Thickness	0.001	Seal Material	Glass Seal
Spacer Thickness	0.00055	Spacer Material	SS-430
PICTURE FRAME			
Thickness	0.0005	Material	SS-430
COMPOSITE SEAL 2			
Seal Thickness	0.0003	Seal Material	Glass Seal
Spacer Thickness	0.0002	Spacer Material	SS-430
INTERCONNECT (BOTTOM)			
Thickness	0.0012	Material	SS-430

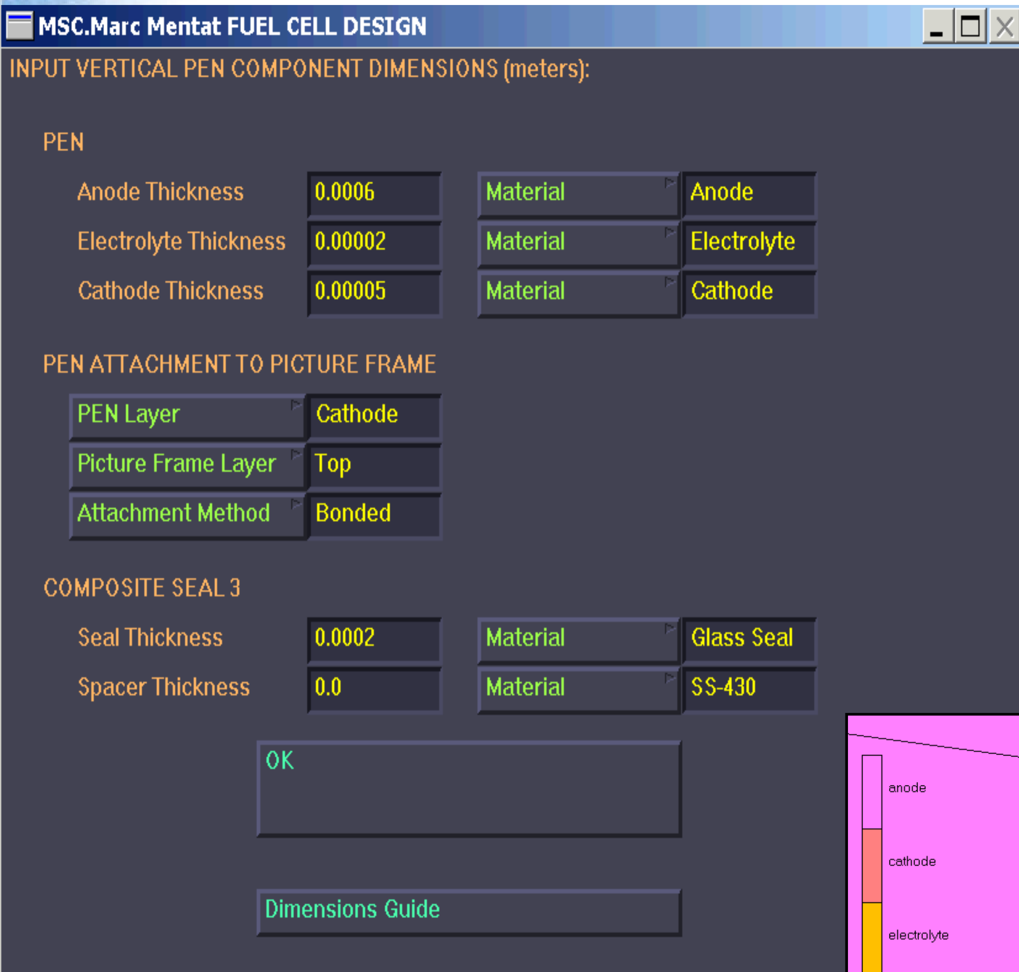
OK

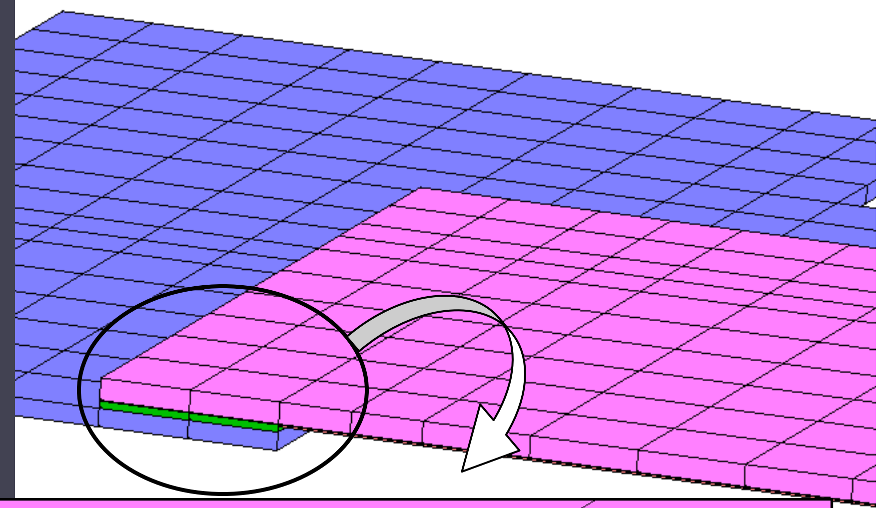
Dimensions Guide

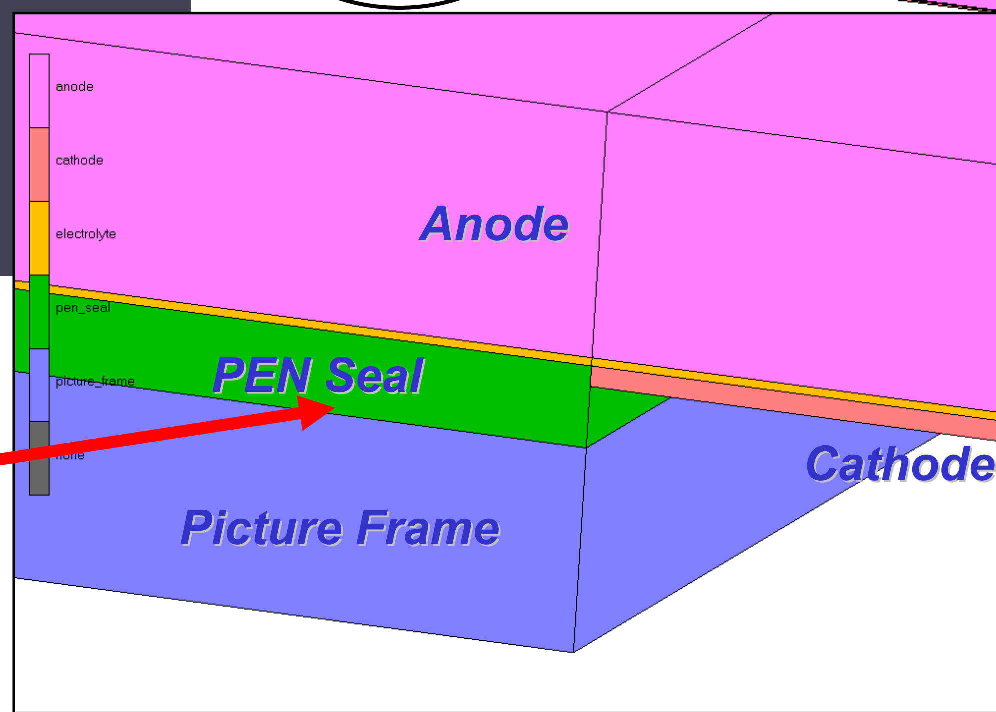


Multiple Seal/Spacer Layers/Materials

3D – Vertical Stack PEN Design Options







PEN Attachment Options

- Bonded
- Sliding

Material Database Options

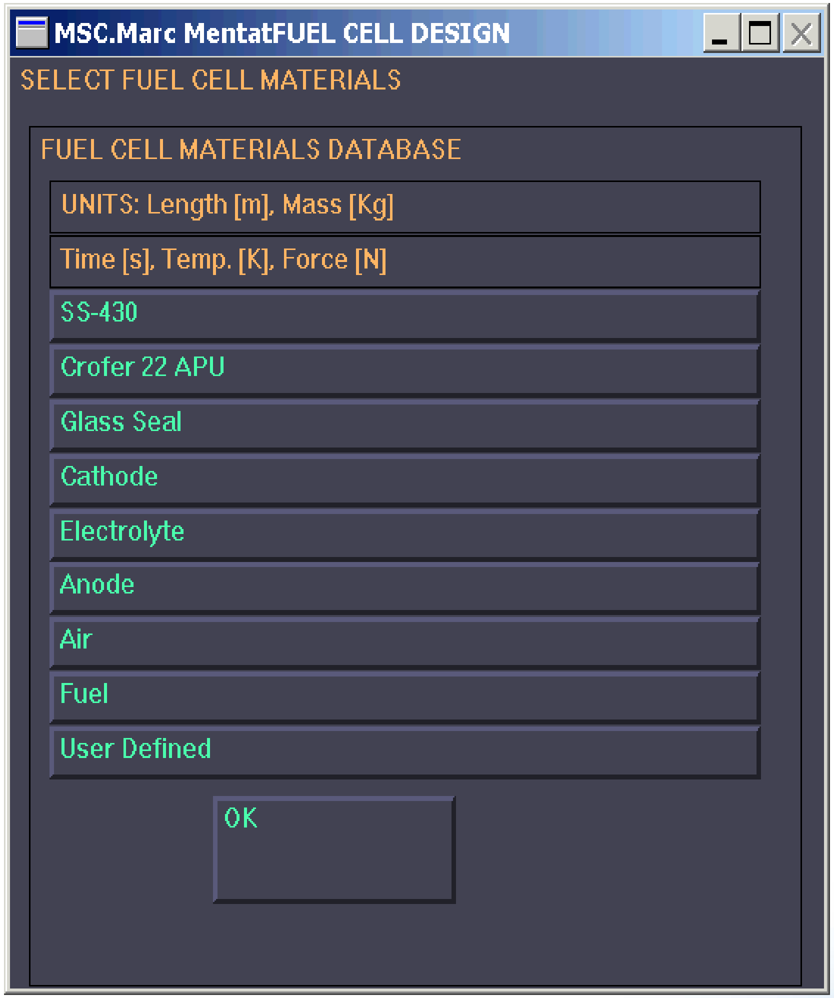
PNL/ORNL-

- Thermal
  - Temp Depend HT
- Mechanical
  - Temp Depend
- Nonlinear
  - Creep
  - Viscoelastic
  - Elastic Plastic

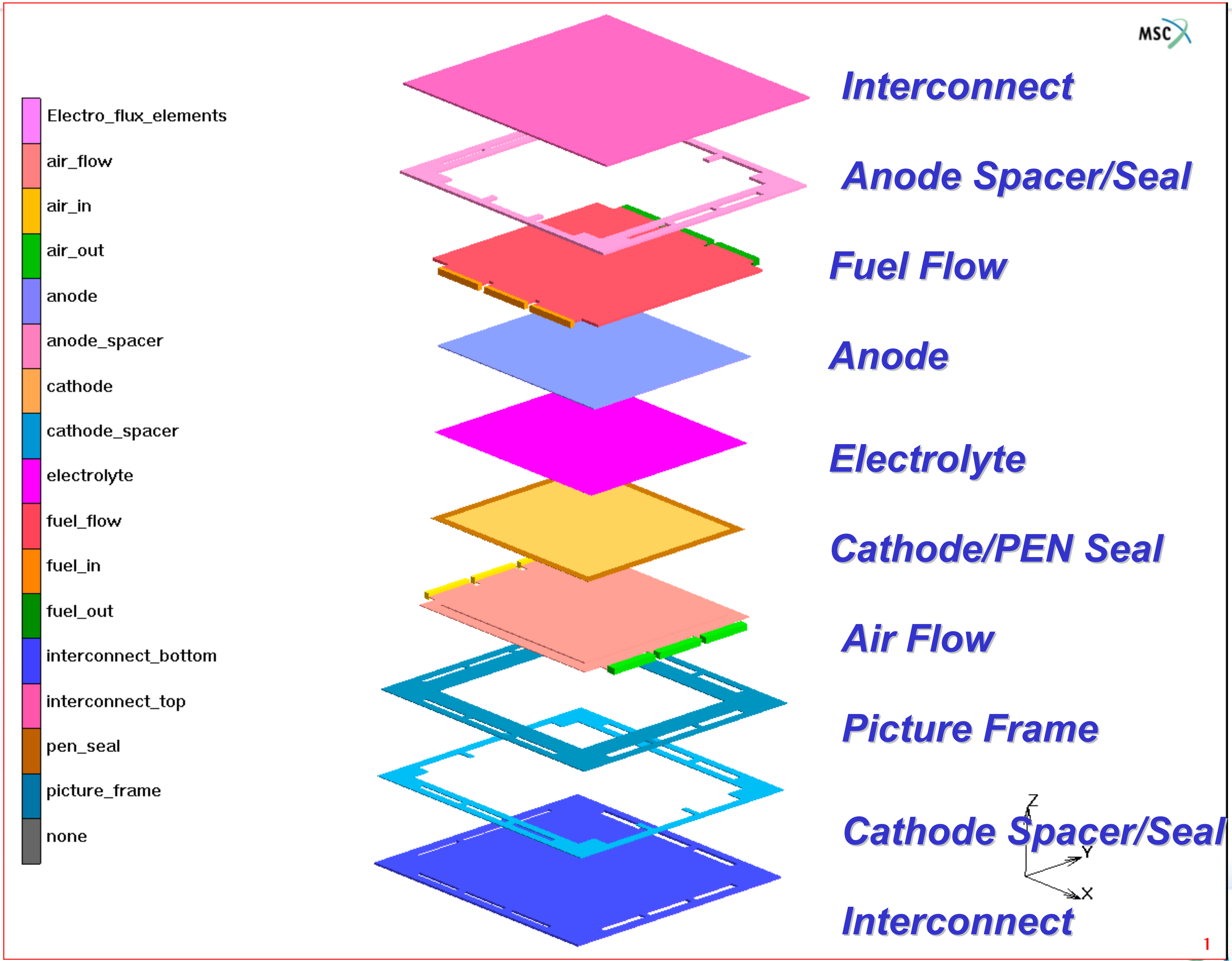
PNL –

- EC Materials

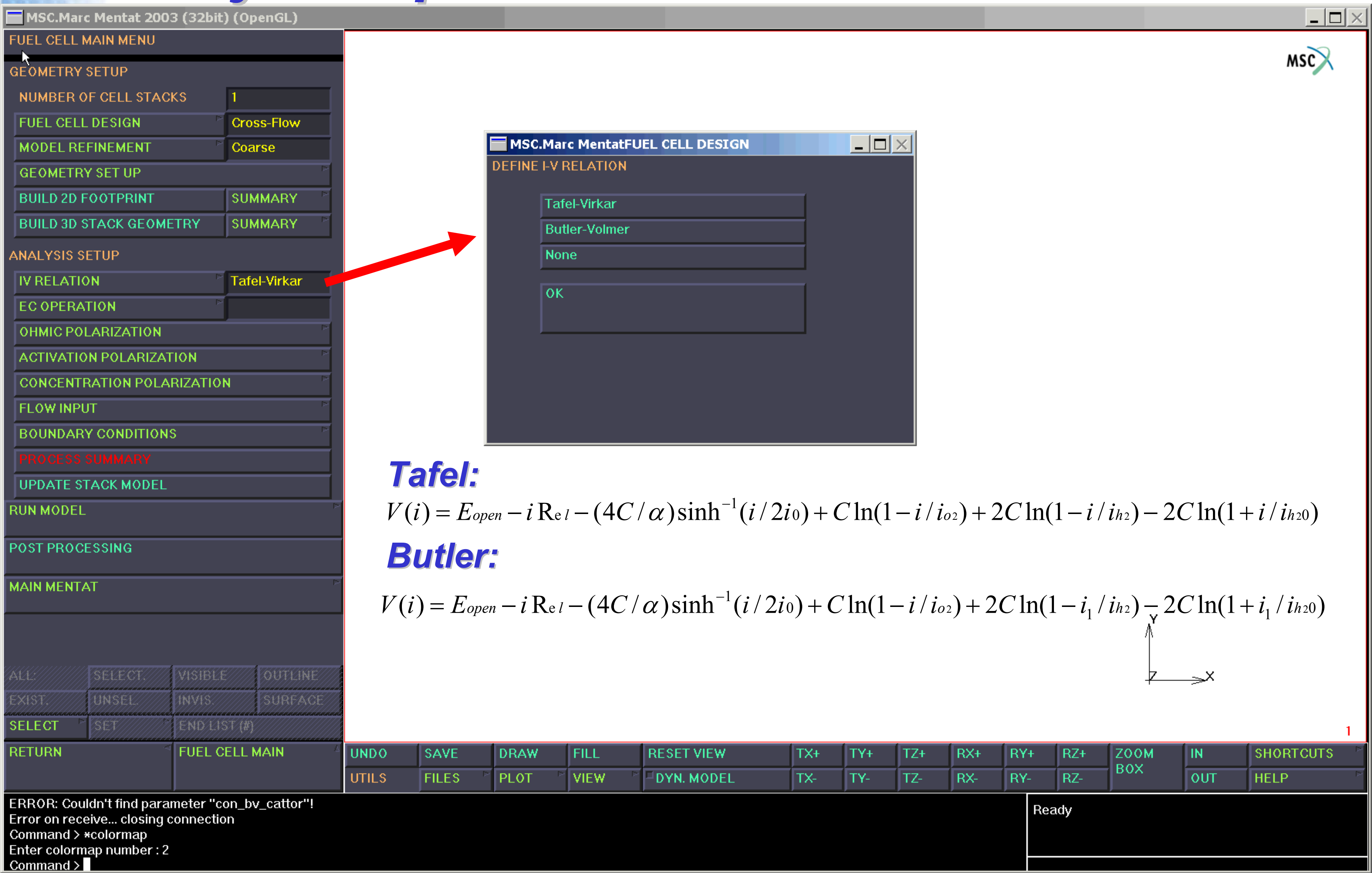
User Defined



…Final 3D SOFC Cell Model



Analysis Options - Select I-V Relations



Tafel:

$$V(i) = E_{open} - i R_{el} - (4C/\alpha)\sinh^{-1}(i/2i_0) + C\ln(1 - i/i_{o2}) + 2C\ln(1 - i/i_{h2}) - 2C\ln(1 + i/i_{h20})$$

Butler:

$$V(i) = E_{open} - i R_{el} - (4C/\alpha)\sinh^{-1}(i/2i_0) + C\ln(1 - i/i_{o2}) + 2C\ln(1 - i_1/i_{h2}) - 2C\ln(1 + i_1/i_{h20})$$

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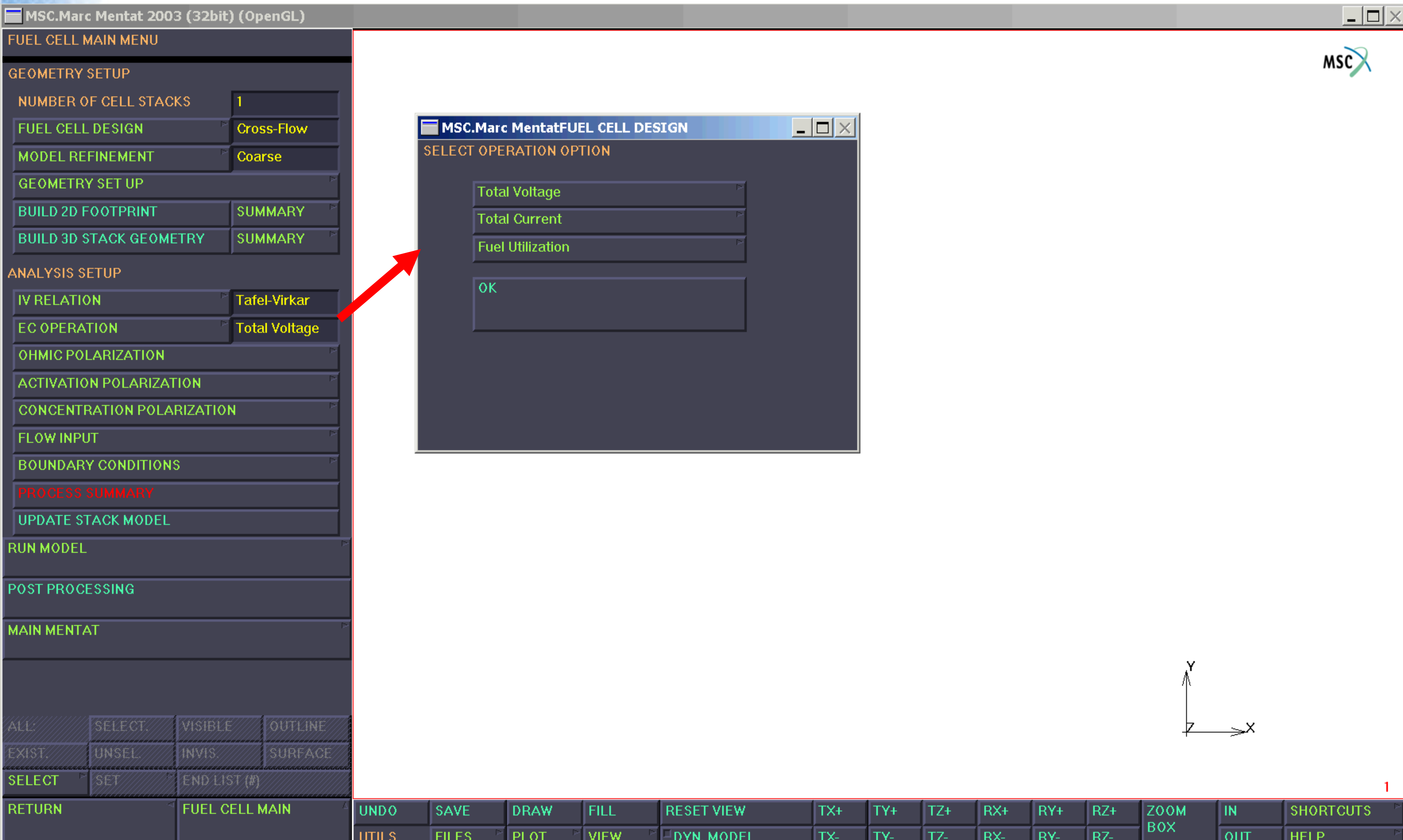
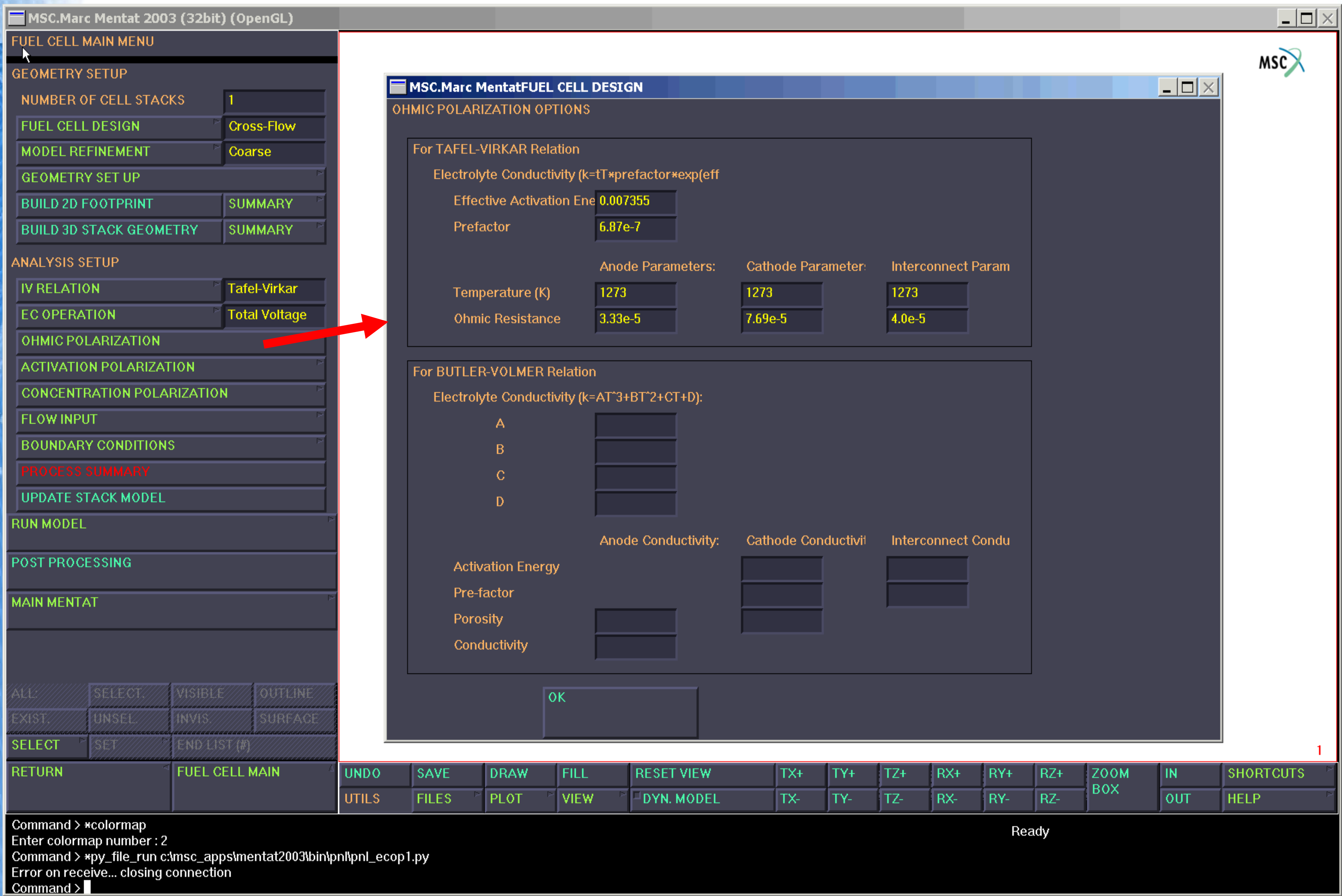
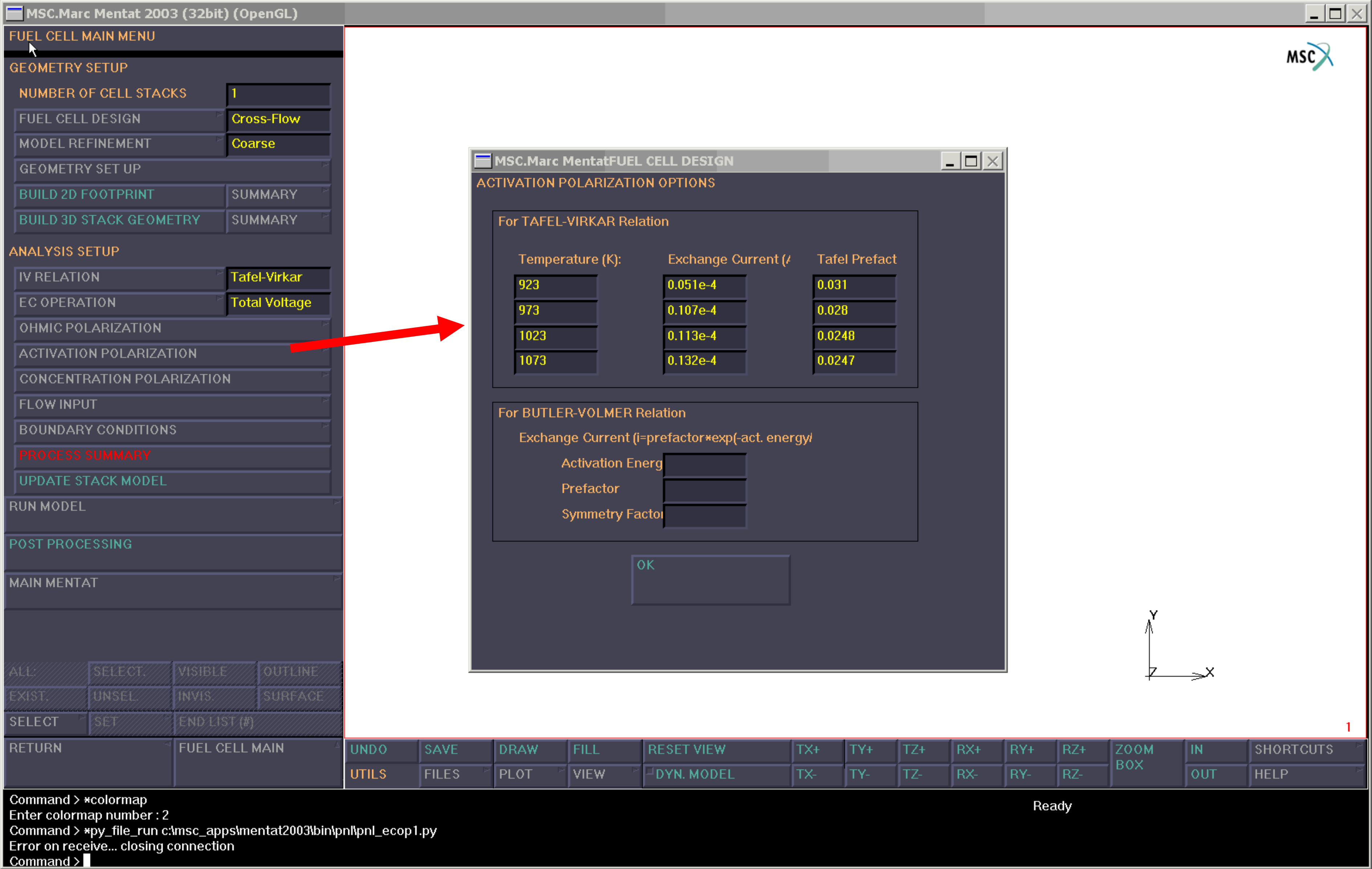
Analysis Options – EC Operation



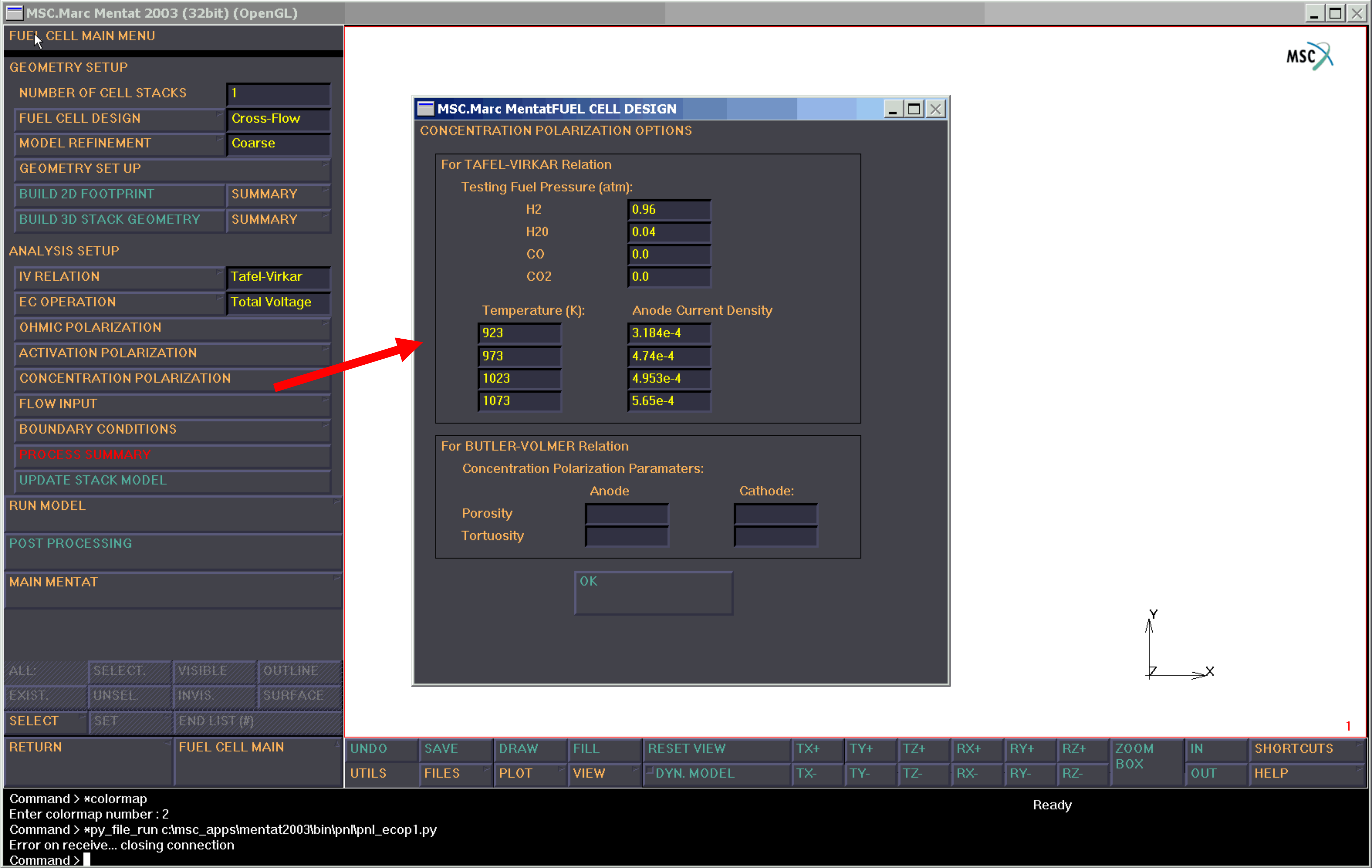
EC Parameters – Ohmic Polarization



EC Parameters - Activation Polarization



EC Parameters - Concentration Polarization



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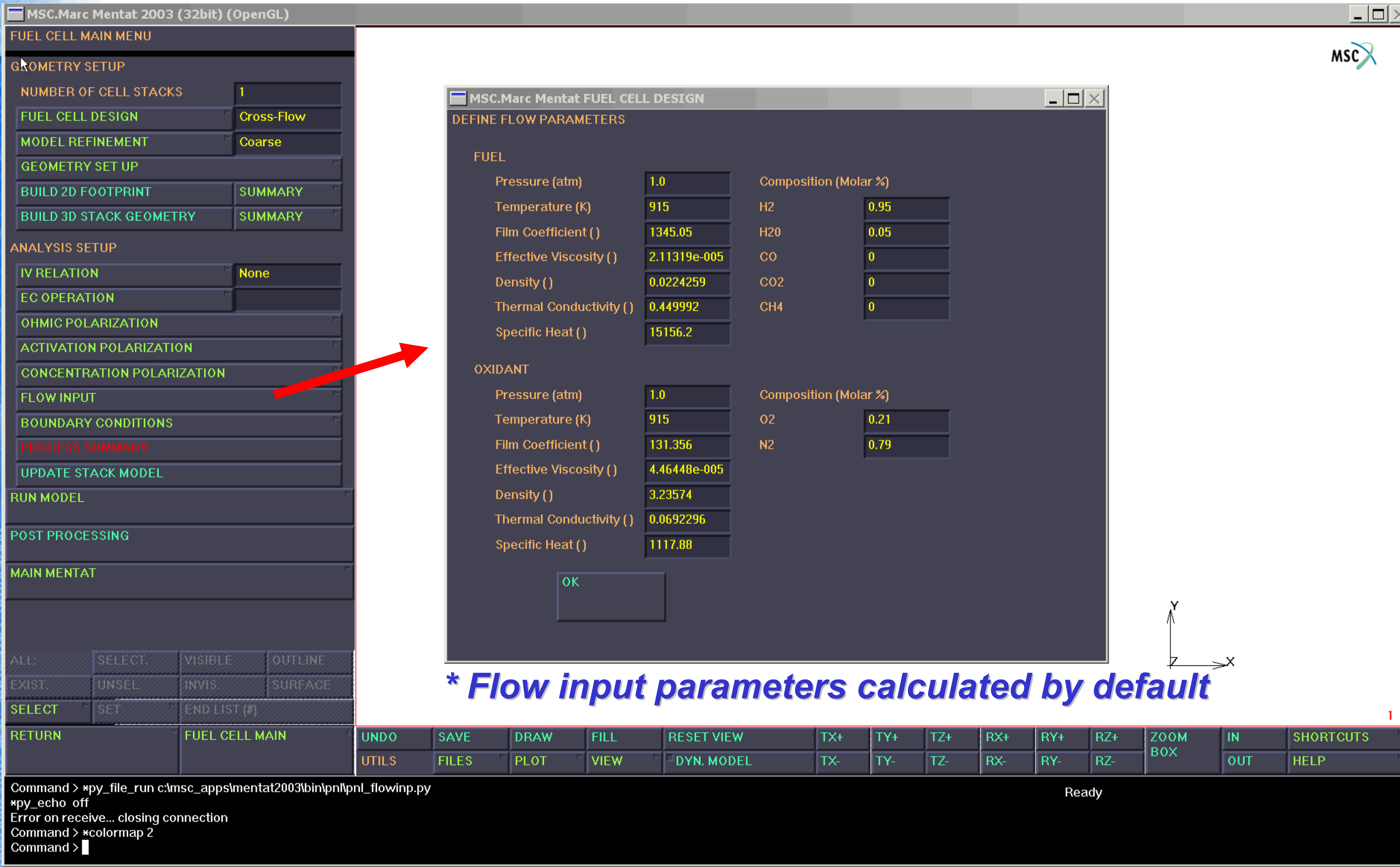
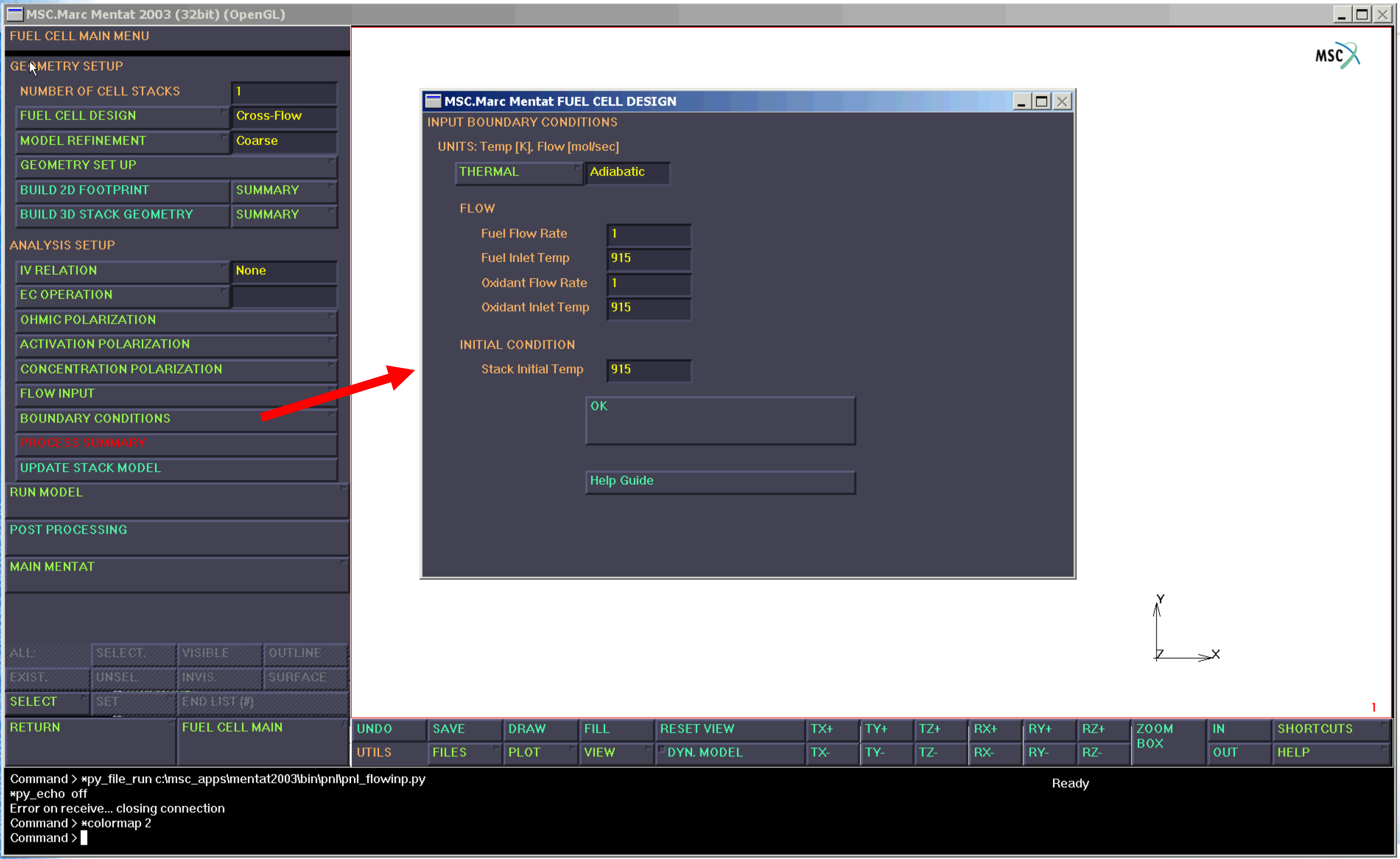
Flow Input Parameters

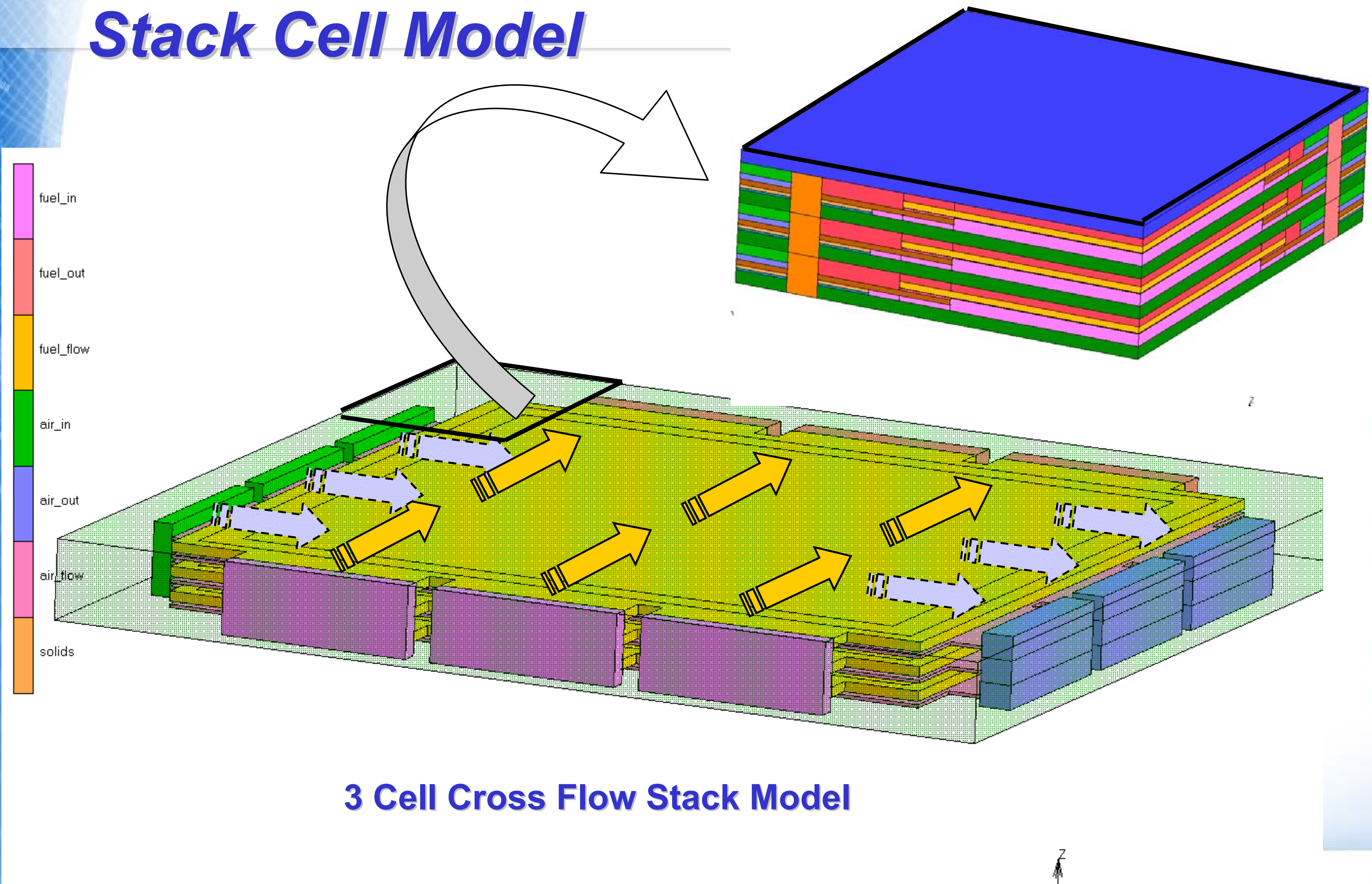


* *Flow input parameters calculated by default*

Initial Boundary Conditions

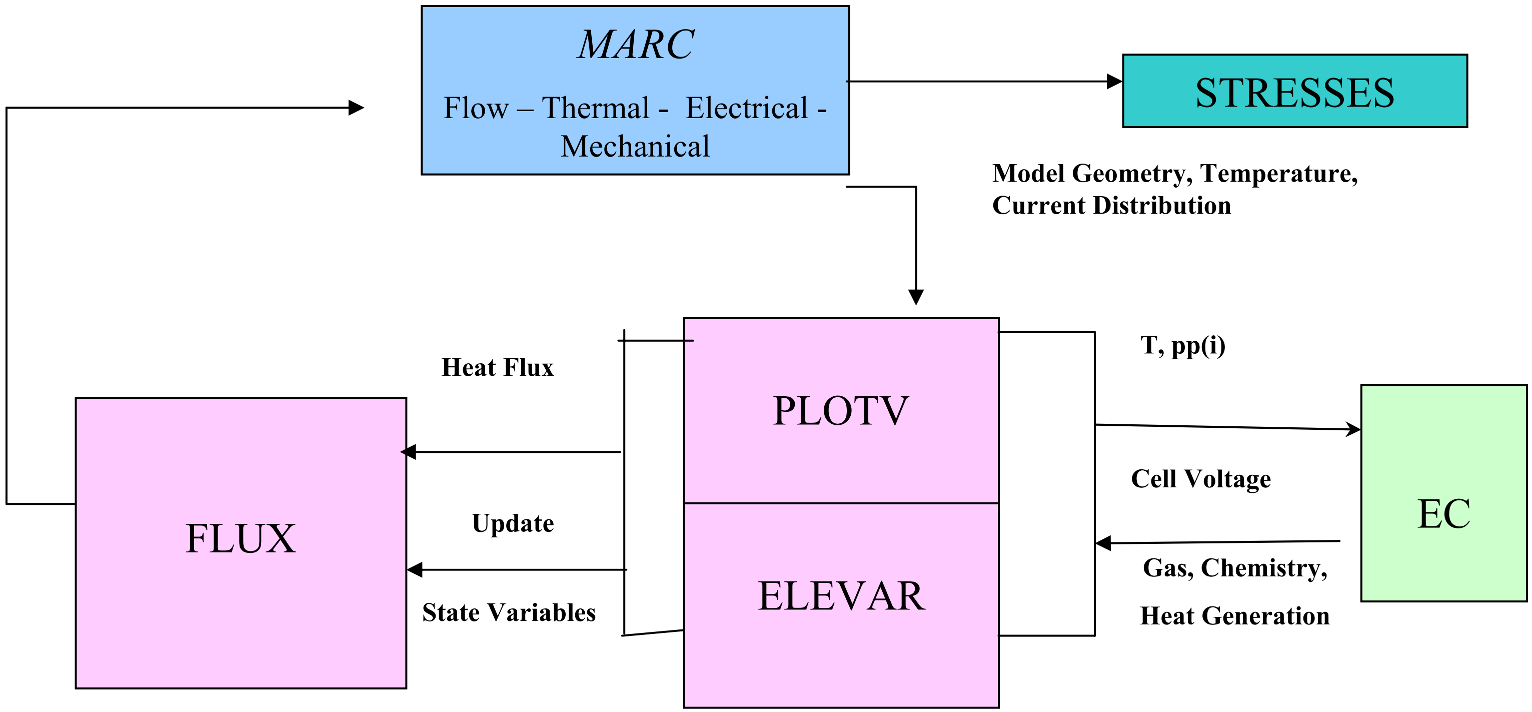


…Complete 3D Multiple Stack Cell Model



3 Cell Cross Flow Stack Model

…Ready to Run Transient Heat Transfer with Electrochemistry Solution…

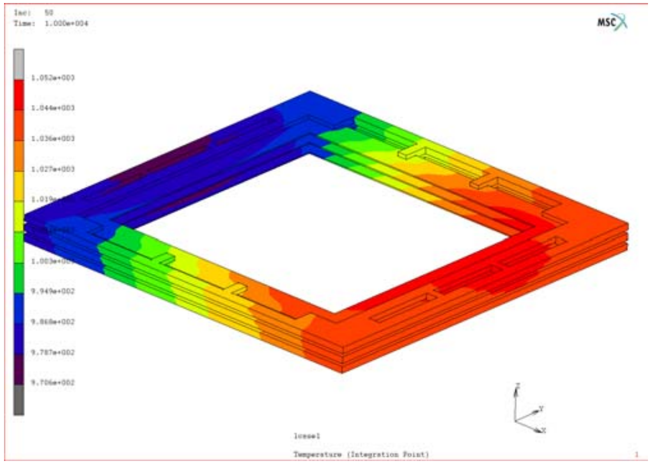


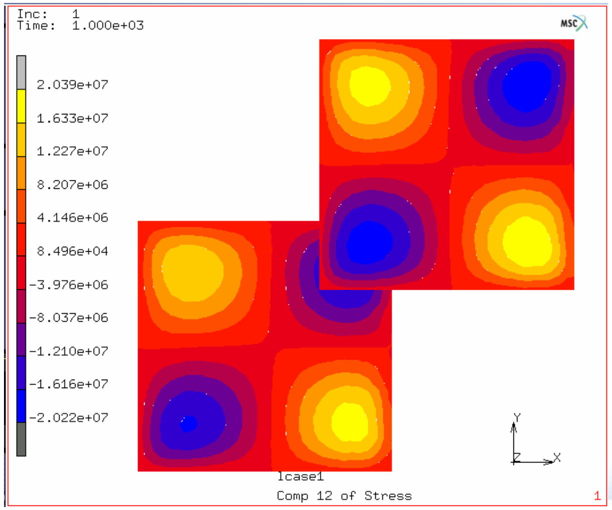
CPU Time:
1 Cell Model ≅ 45 min.
(laptop computer)

Analysis Results…

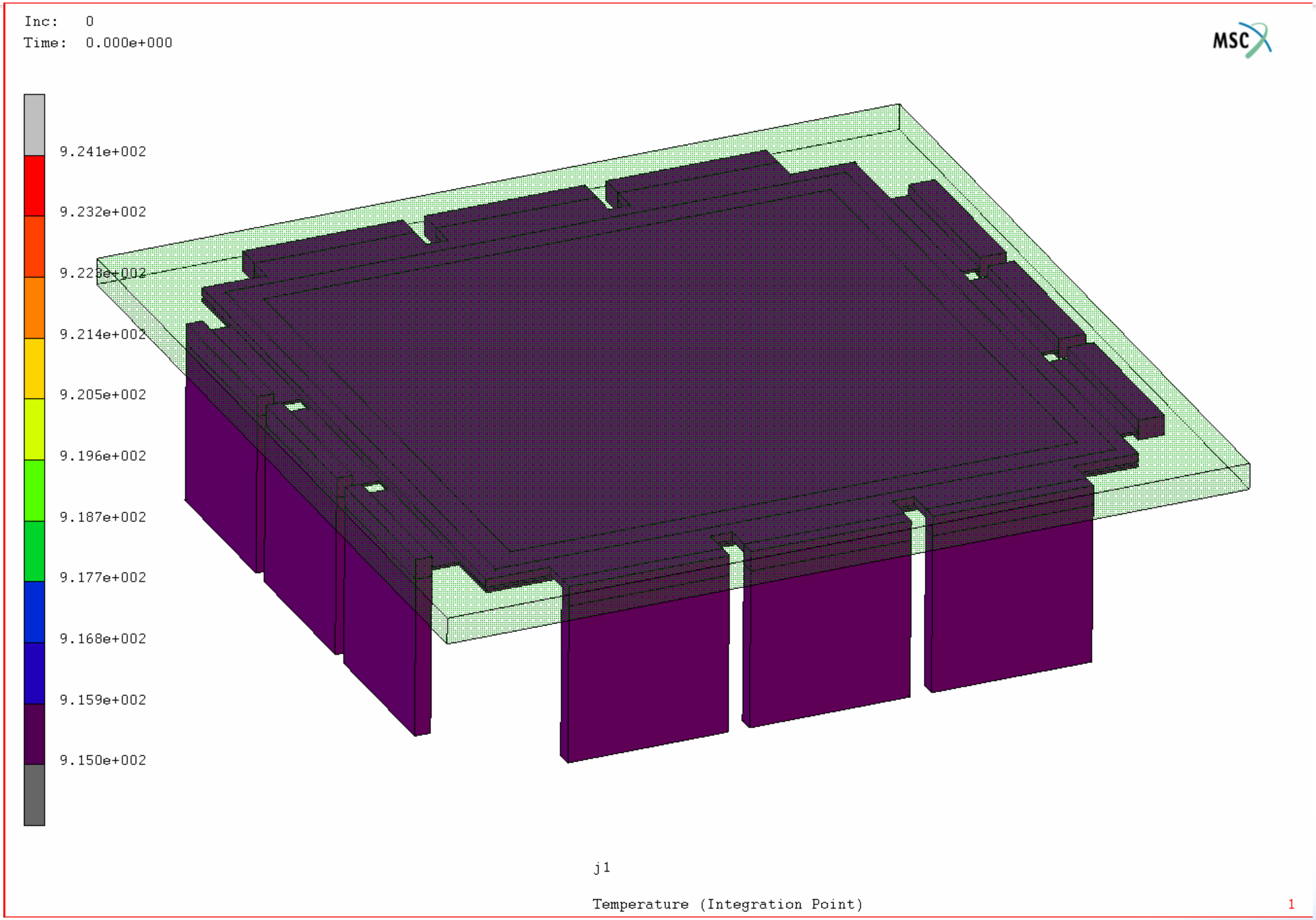
Fuel Cell Analysis Output

- Temperature Distributions
- Stress & Strain Distributions
  - Thermal
  - Mechanical
  - Compressive (contact)
- 3D Displacement Distribution
- Species Concentration
- Degradation Mechanisms
  - Fracture
  - Creep
  - Relaxation
  - Damage

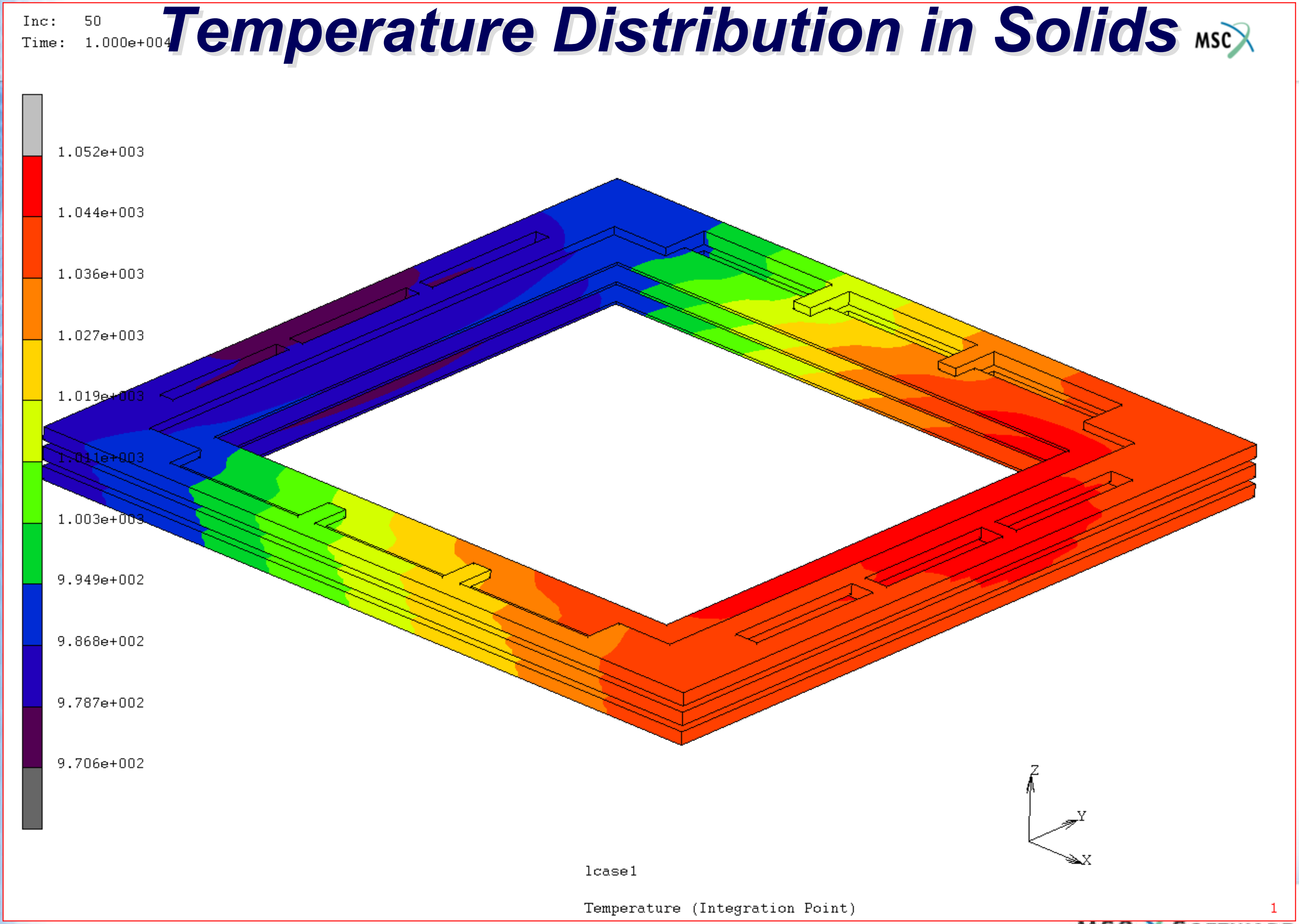




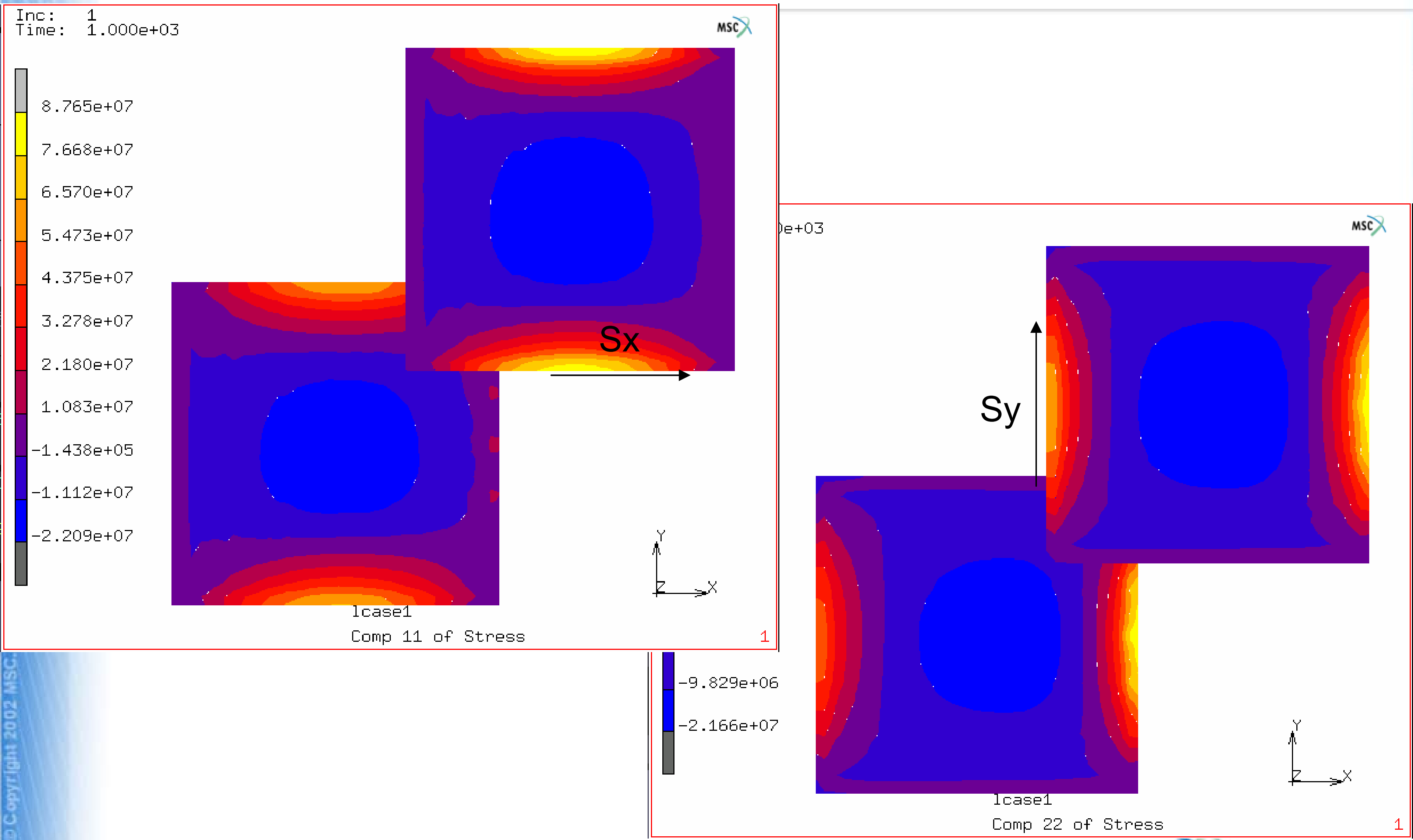
Temperature Distribution in PEN



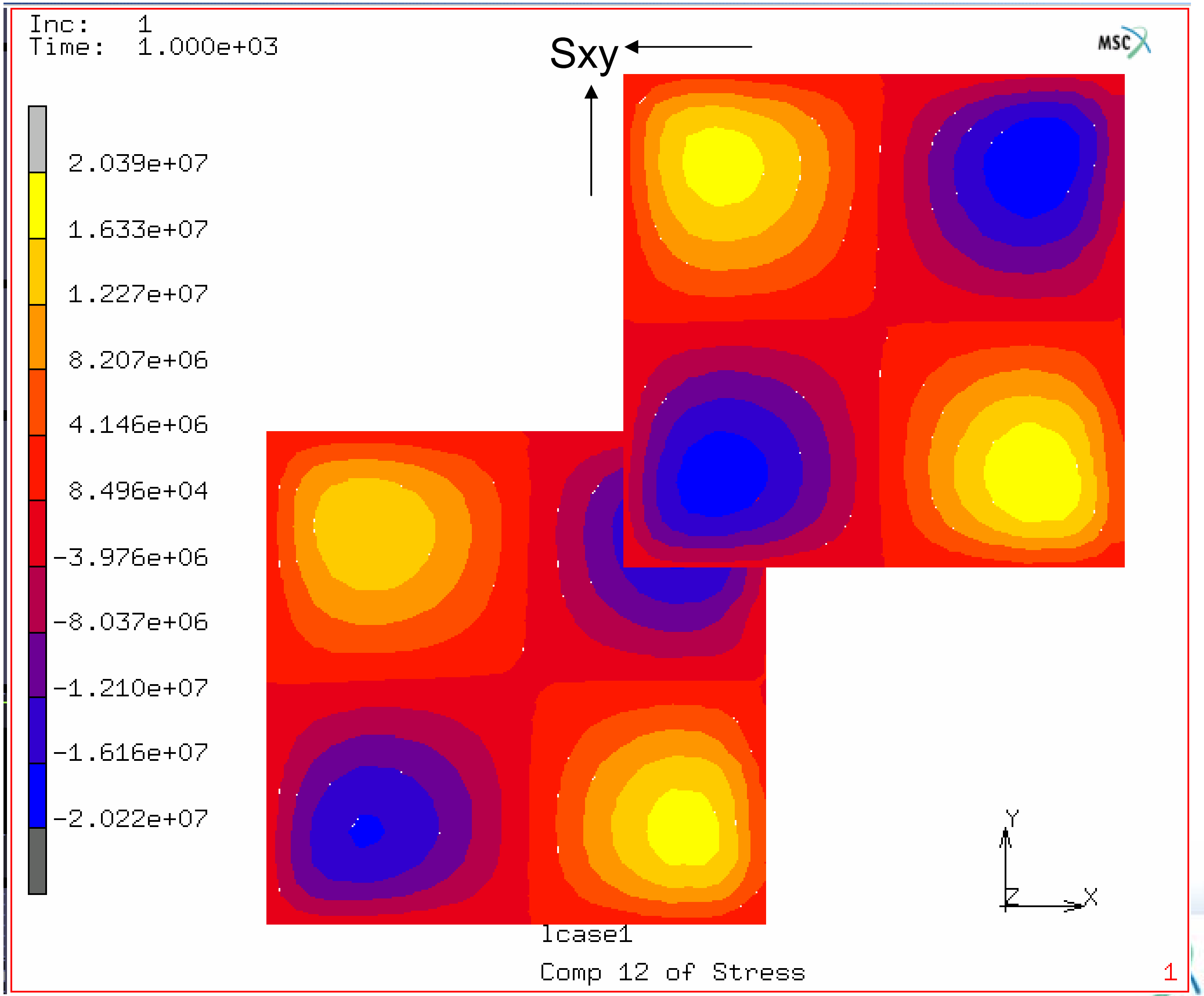
Temperature Distribution in Solids



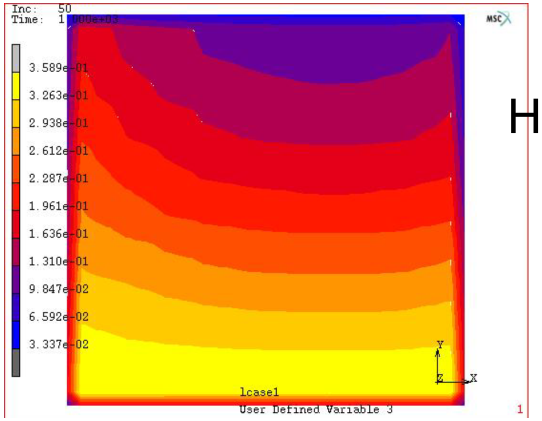
Stress in Electrolyte



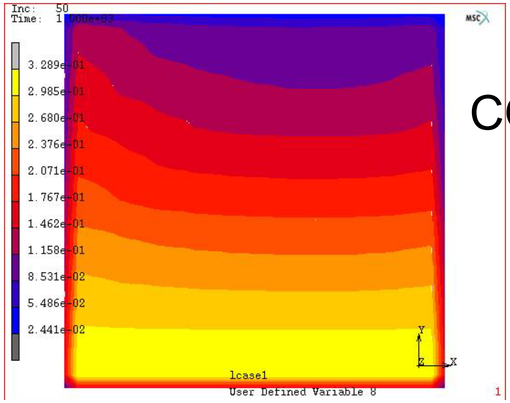
Shear stress in electrolyte



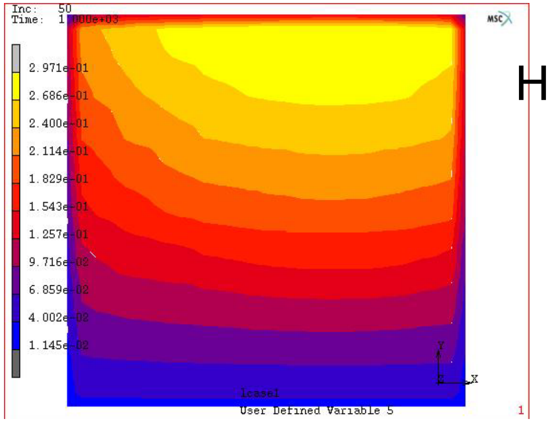
Species Concentration



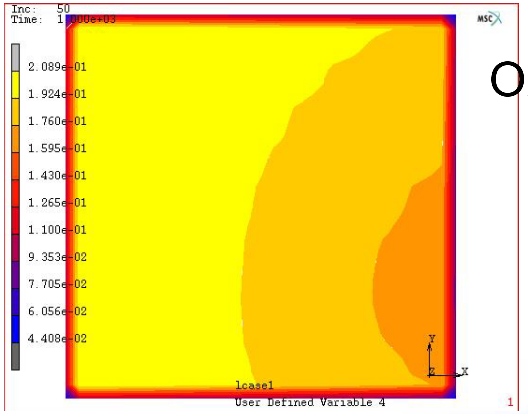
H2



CO

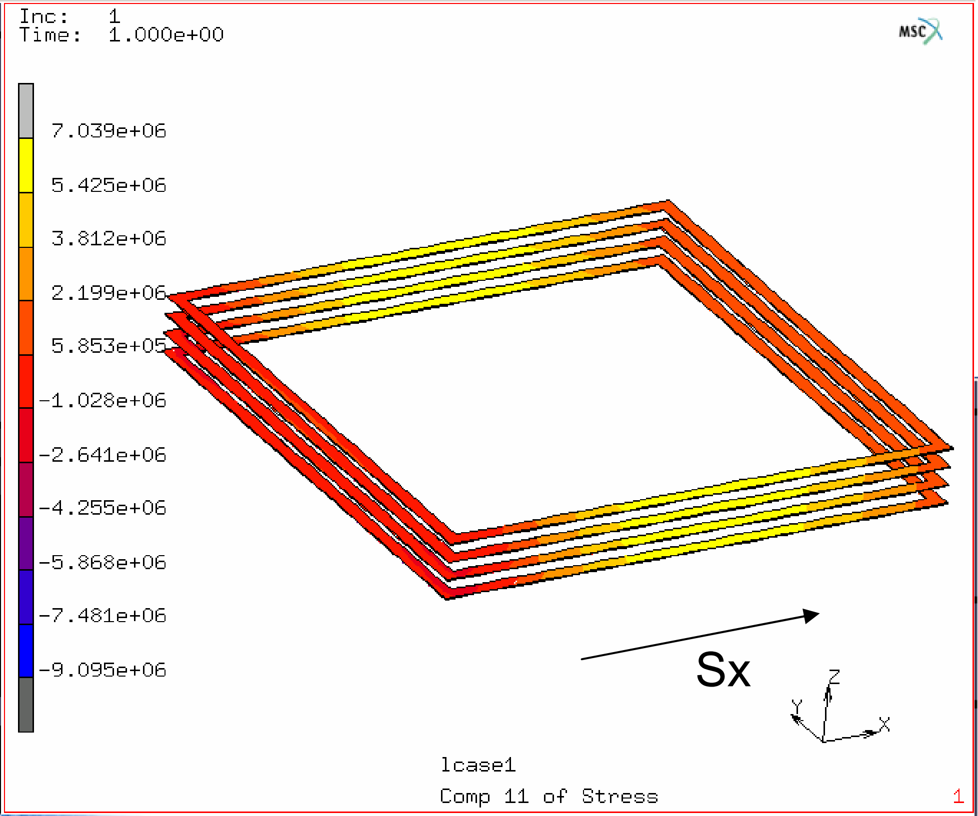


H2O



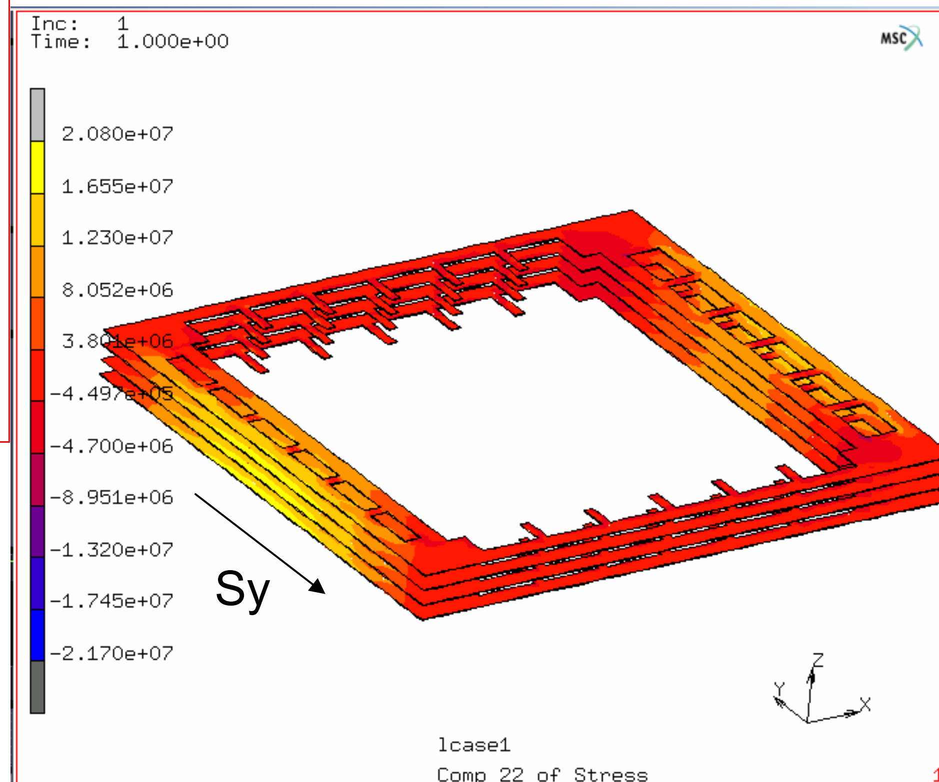
O2

Seal Stress



Seals between picture frame and cathode side of PEN

Seals between Anode Spacer and Interconnect



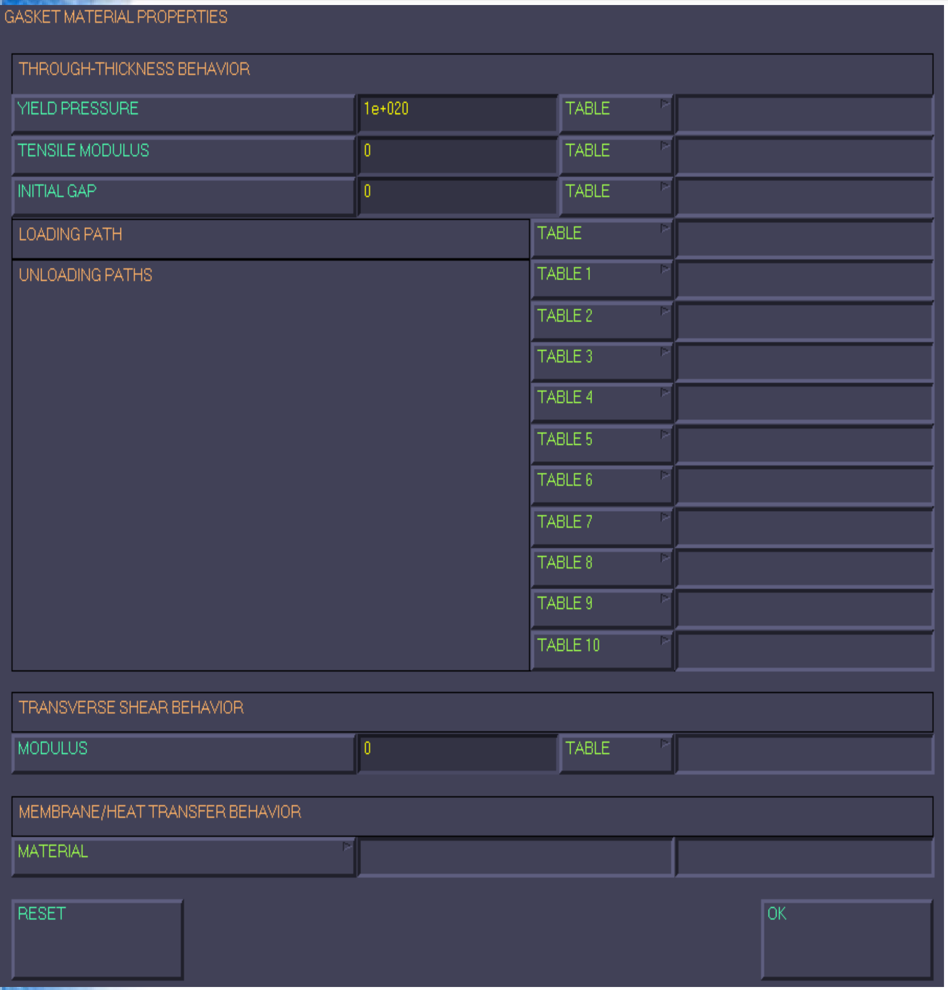
Potential SOFC Degradation Mechanisms

- Fracture
  - Electrolyte, anode, rigid seals, interfacial separations
- Thermal/mechanical loading
  - Loading includes thermal gradient, thermal shock, mechanical acceleration (mobile applications)
- Compositional changes affect mechanical response
- Thermal cycling affects mechanical response
  - Fatigue
  - Creep/relaxation
- Continuum damage
  - PEN, rigid seals

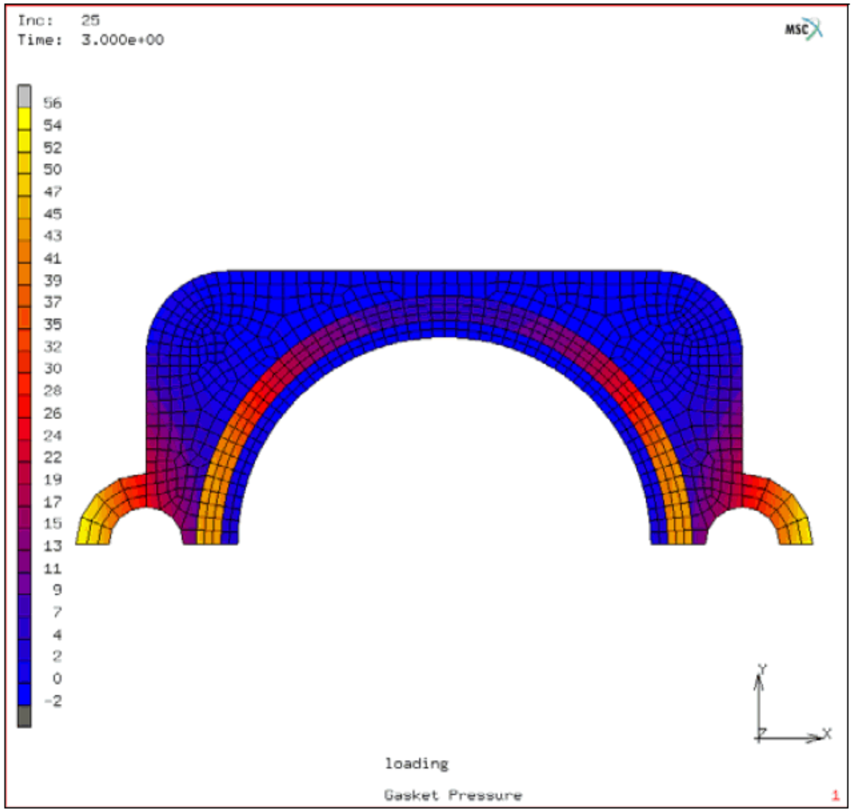
Failure Models

- Creep/Relaxation
  - Viscoelastic
  - Viscoplastic
  - User Defined - CRPLAW
- Damage
  - Gurson
  - Gasket
  - User Defined

Gasket Material Model



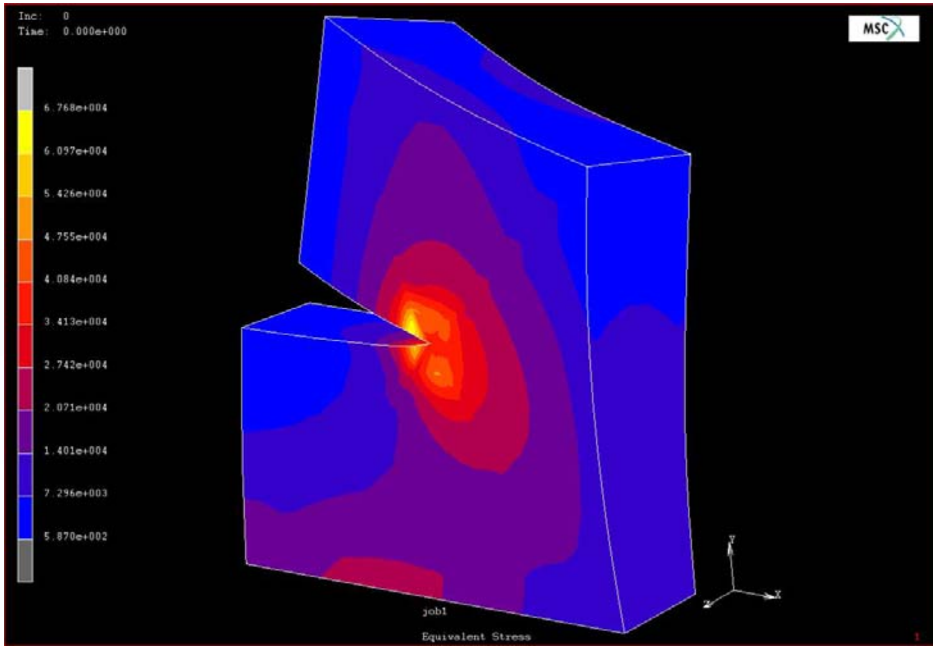
Models complex material behavior with single thickness layer



Can be used to model compression glass compression seals

Fracture Analysis

- Progressive Failure
- Cracking
- Deactivate Elements
- J-Integral
- Stress Intensity Factors
- Mode Separation



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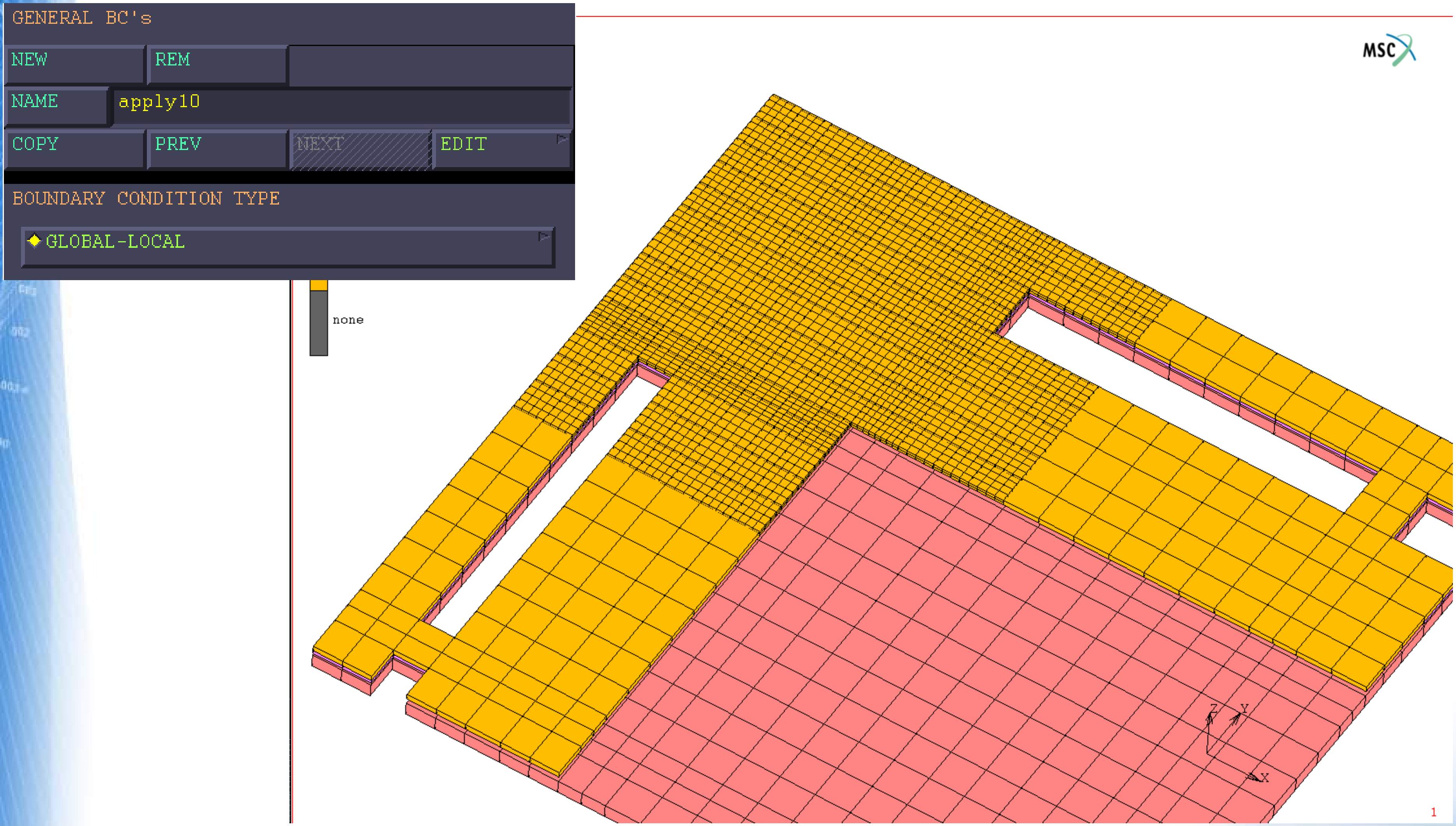
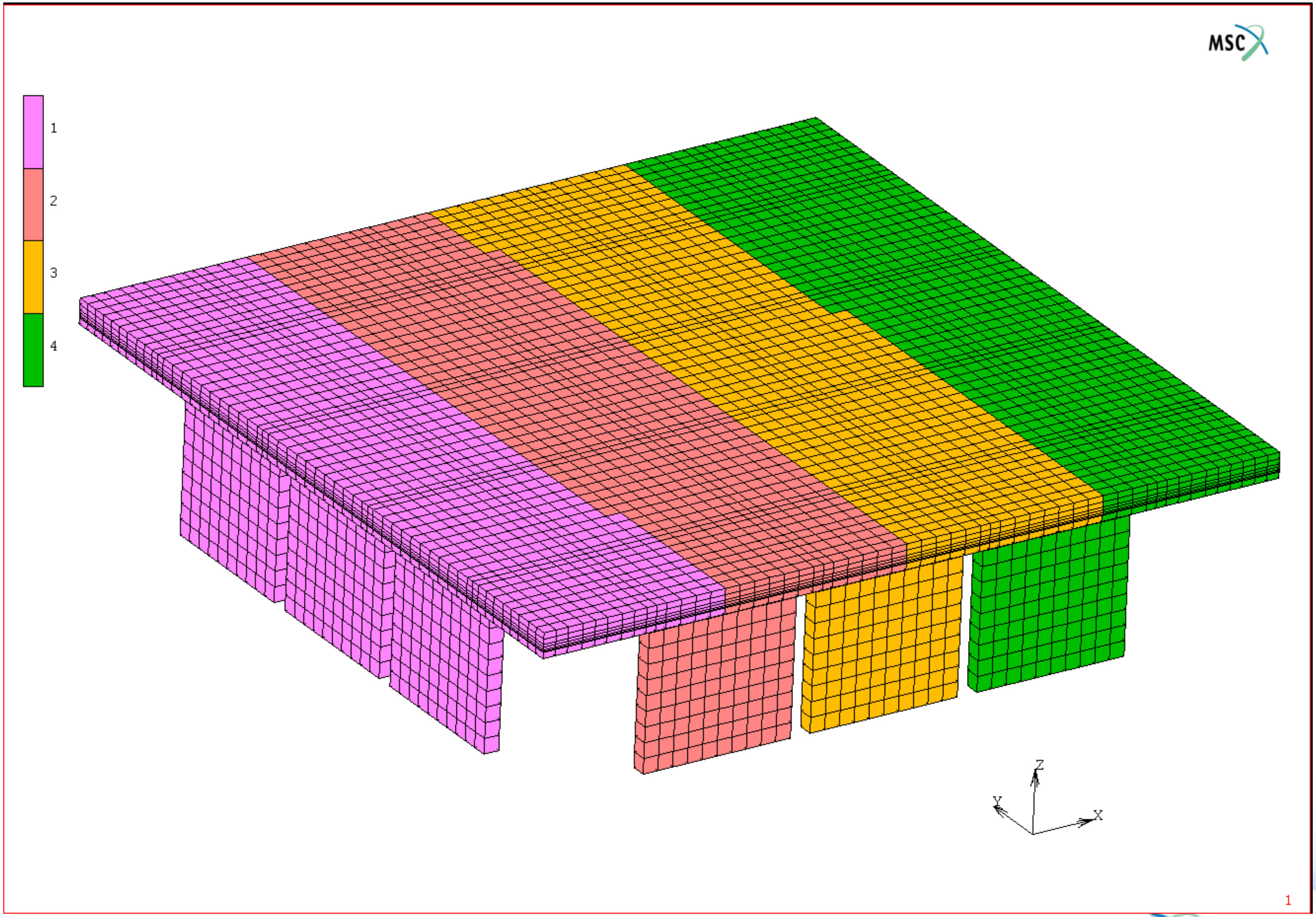
Global-Local Analysis



Parallel Processing – DDM Method



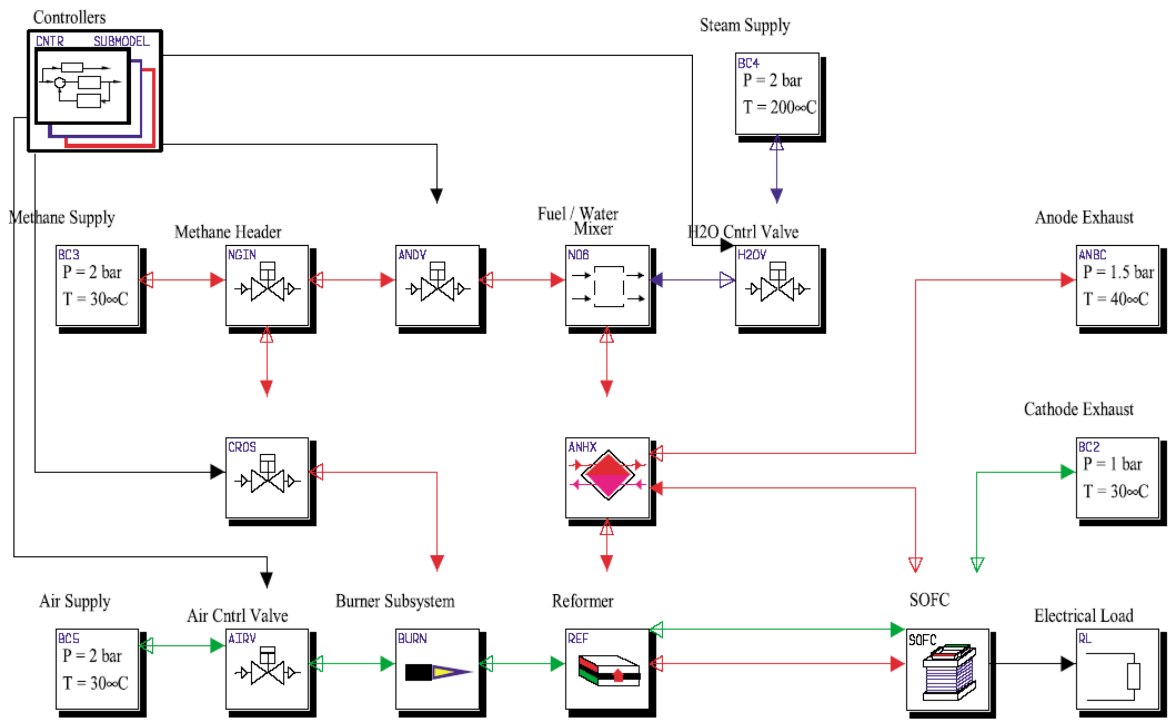
Current and Planned Work

- Finalize modeling of multi-cell stacks.
- Finalize material database.
- Further enhance routines for parallel processing of EC routings
- User solid model import capability

Estimated Release for use 30 days (possibly included in SECA software training at PNNL).

Looking into providing MSC/PNL utility on SECA computer at PNNL.

MSC.Easy 5 Simulation



The MSC.EASY5 model shown here includes the SOFC fuel cell stack, the steam reformer, a system burner, heat exchangers, control valves, a resistive/inductive electrical load, and a series of logic and PID controllers.

- Graphical Based Simulation Tool
- Open Architecture – links to many CAE software/hardware tools (Simulink, ADAMS, DADS…)
- User Defined Libraries
- Ricardo Fuel Cell Library

Thank You !

Please visit our booth for more information

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Multi-Physical Analysis with MSC

May 2004

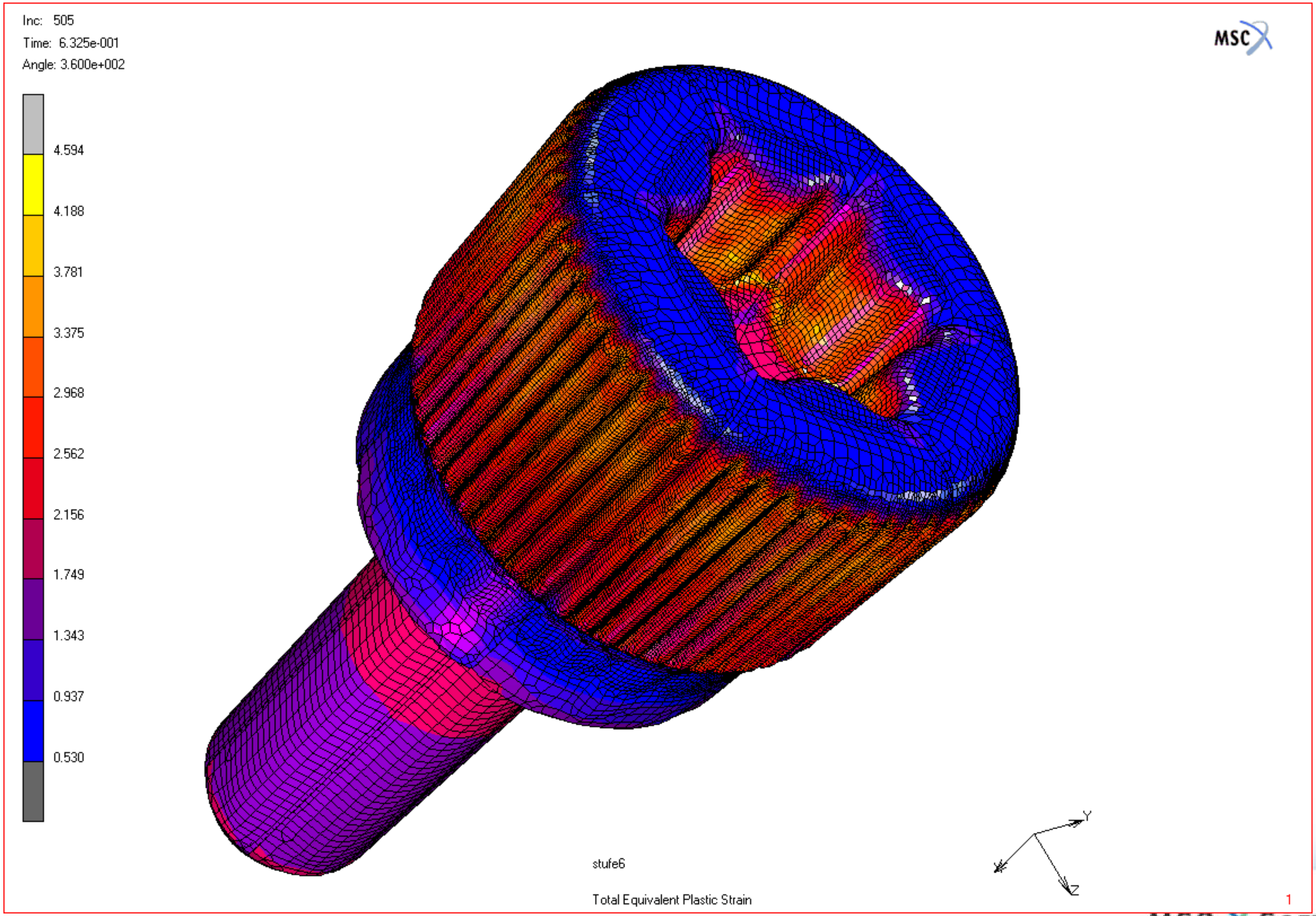
Analysis Capabilities

- Structural (Nastran, Marc, Dytran)
- Thermal (Nastran, Marc, Thermal)
- Pore-Pressure (Marc)
- Hydrodynamic bearing (Marc)
- Fluids (Nastran (added mass), Marc, Dytran)
- Acoustics (Nastran, Marc)
- Electrostatics (Marc)
- Magnetostatics (Marc)
- Electro-magnetics (Marc)

Marc Multi-Physics

- Thermal- Mechanical (loosely)
- Thermal- Electric – Joule (loosely)
- Thermal-Joule-Structural (Loosely)
- Poro-elasticity – Soil (tightly)
- Electro-Magnetic (tightly)
- Piezo-Electric (Tightly)
- Acoustic-Structural (tightly)
- Fluid-Thermal (tightly)
- Fluid-Structural (loosely)

Thermal – Mechanical Manufacturing



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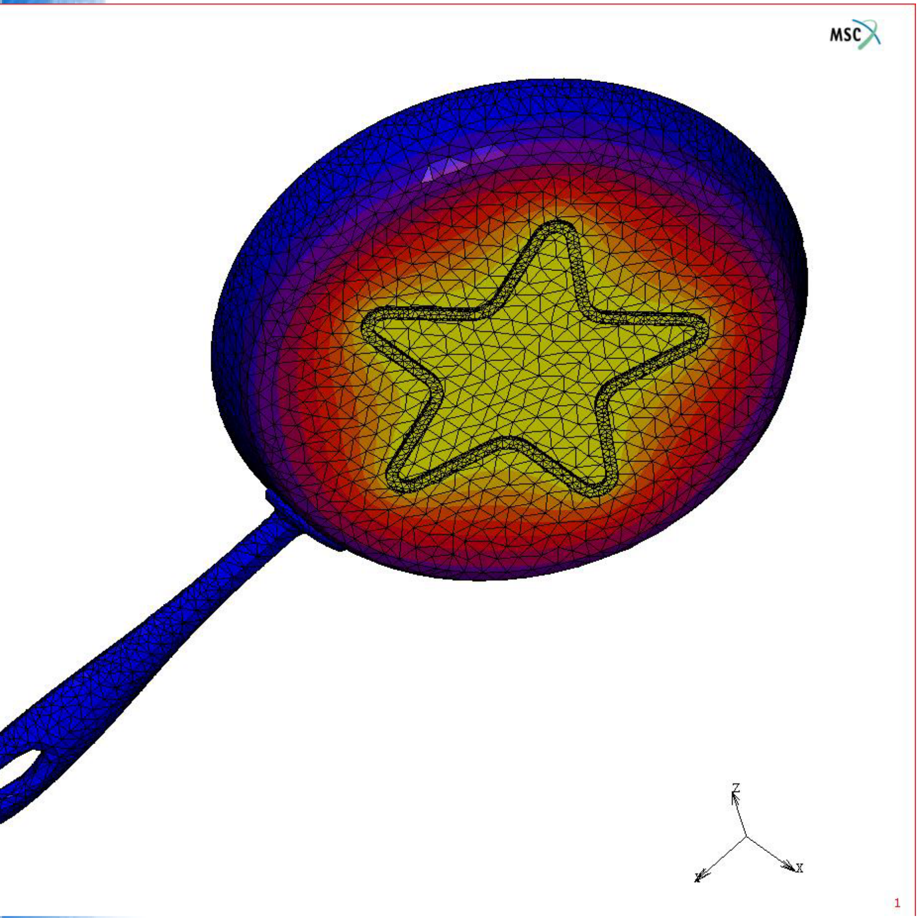
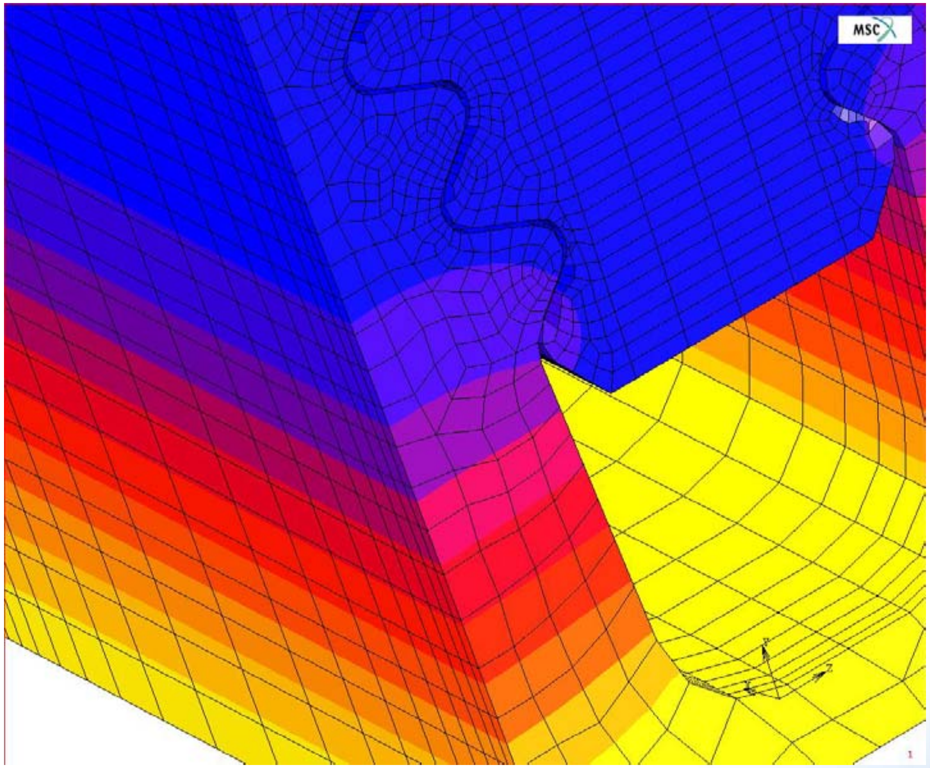
Thermal Contact Examples

Catia Assembly



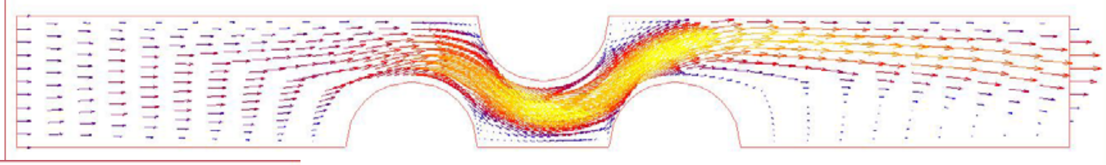
Fir tree



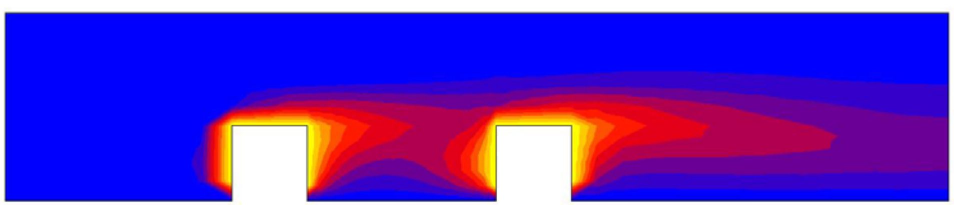
Fluid Capabilities

- 2-D, Axisymmetric , 3-D
- Navier Stokes
- Newtonian and Non-Newtonian Fluid
- Coupled Thermal-Fluid Capabilities
- Coupled Fluid-Structural

Fluid Capabilities



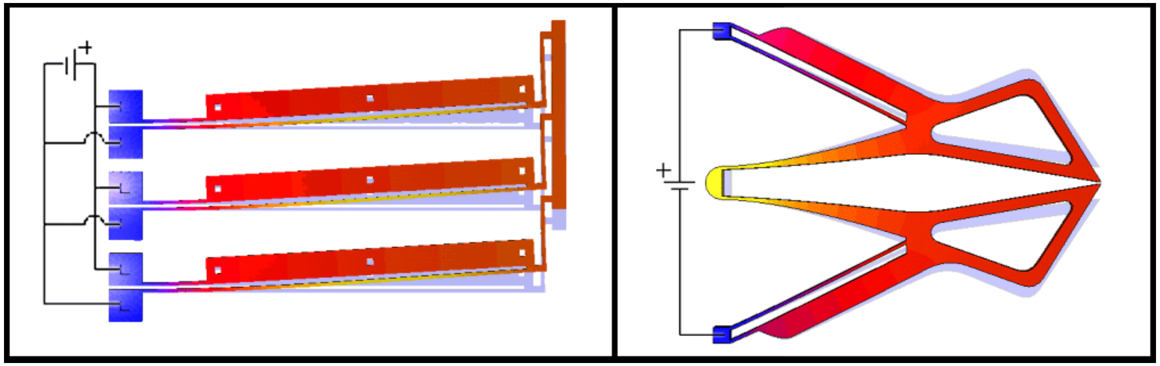
Velocity of Fluid in Heat Exchanger



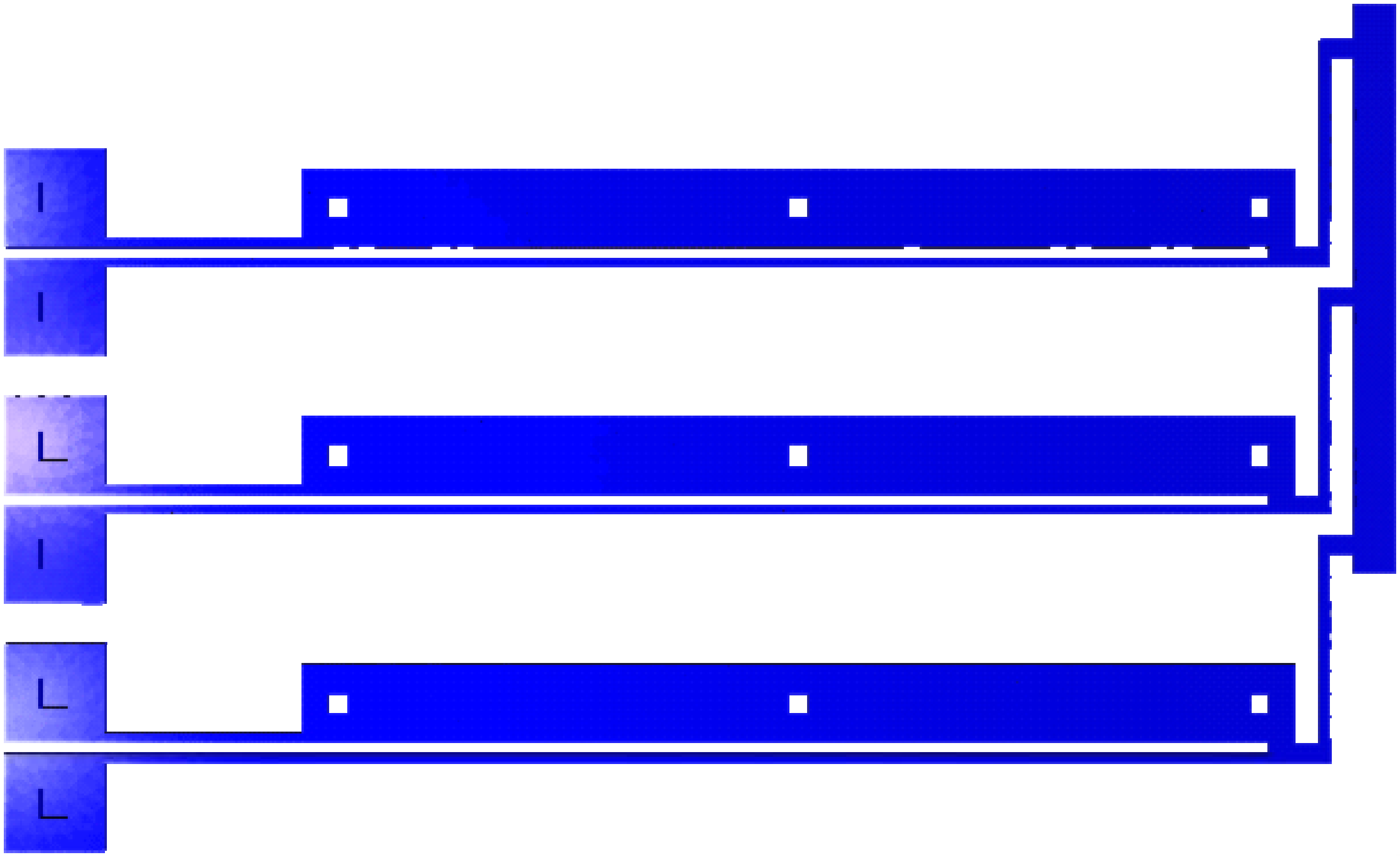
Temperature in Flow Over Chips

Coupled Electrical-Thermal-Mechanical Analysis

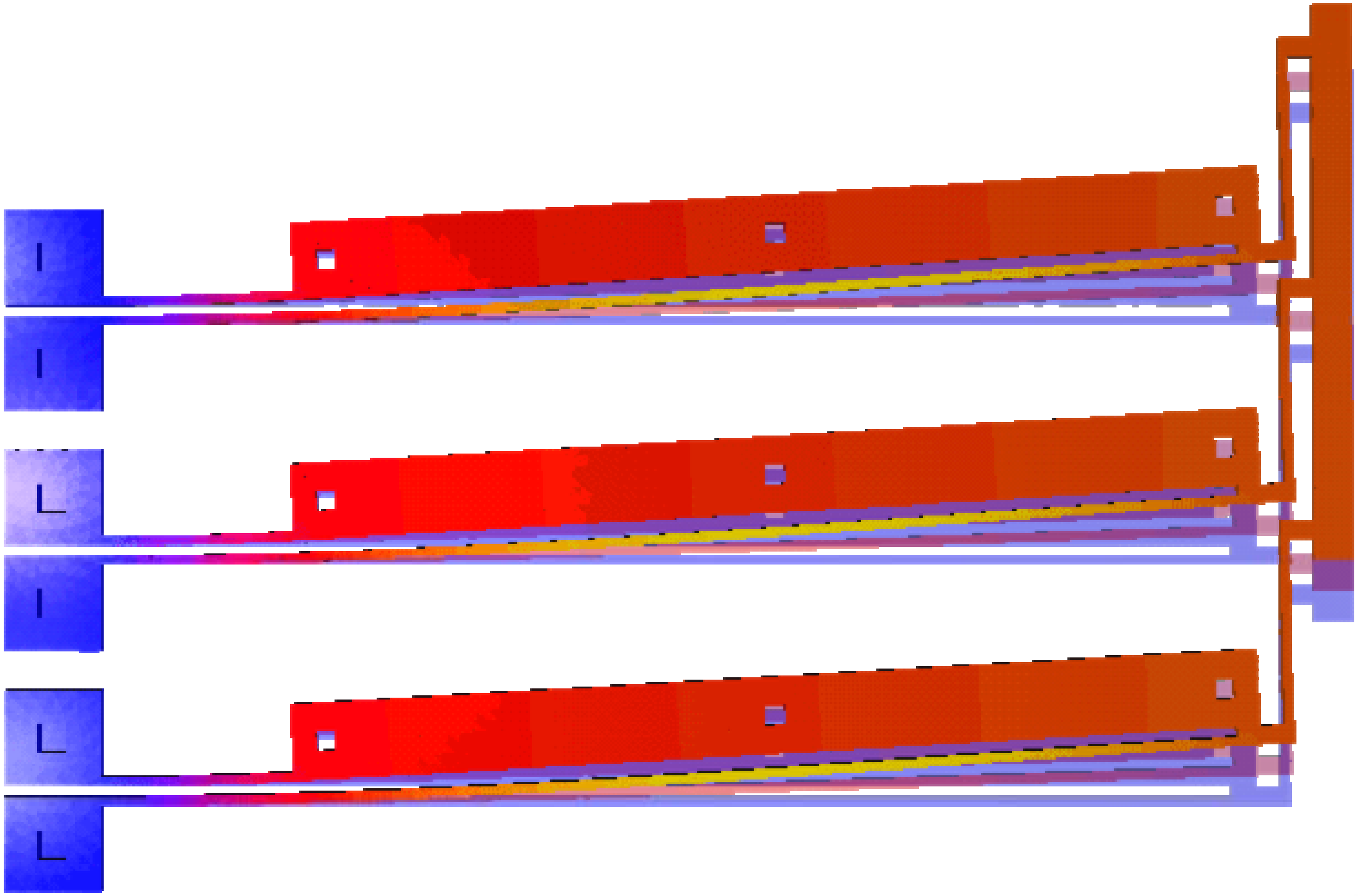
- **Multi-physics functionality couples electrical, thermal and mechanical behavior**
- **Applications:**
  - **MEMS actuators, high voltage switches and electronic circuits.**



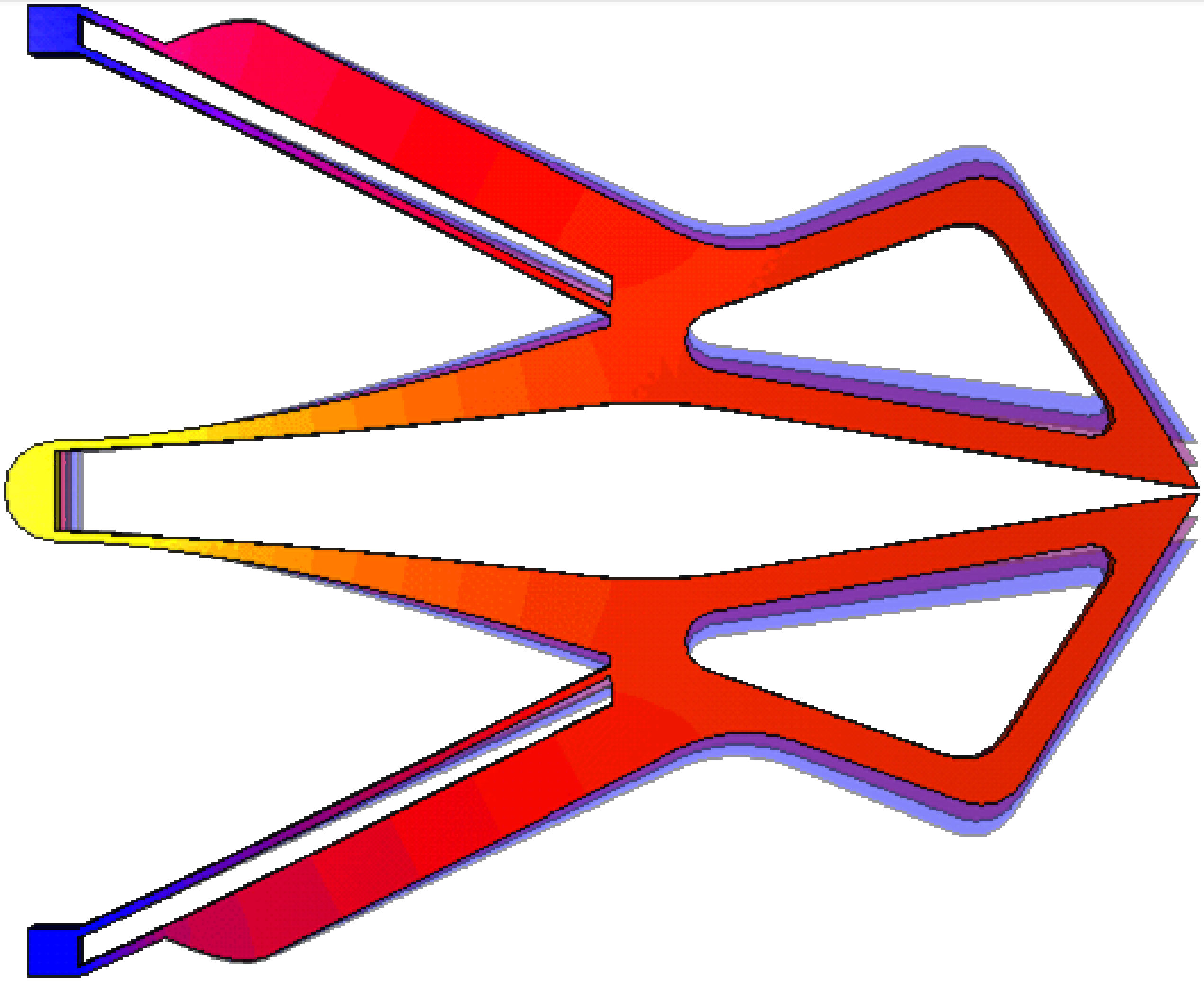
MEMS Micro-actuator



MEMS Micro-actuator

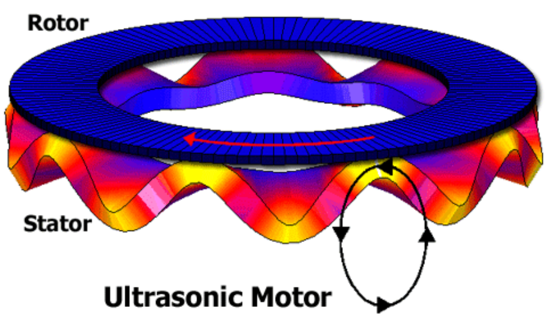


MEMS Micro-gripper



Piezoelectric Analysis

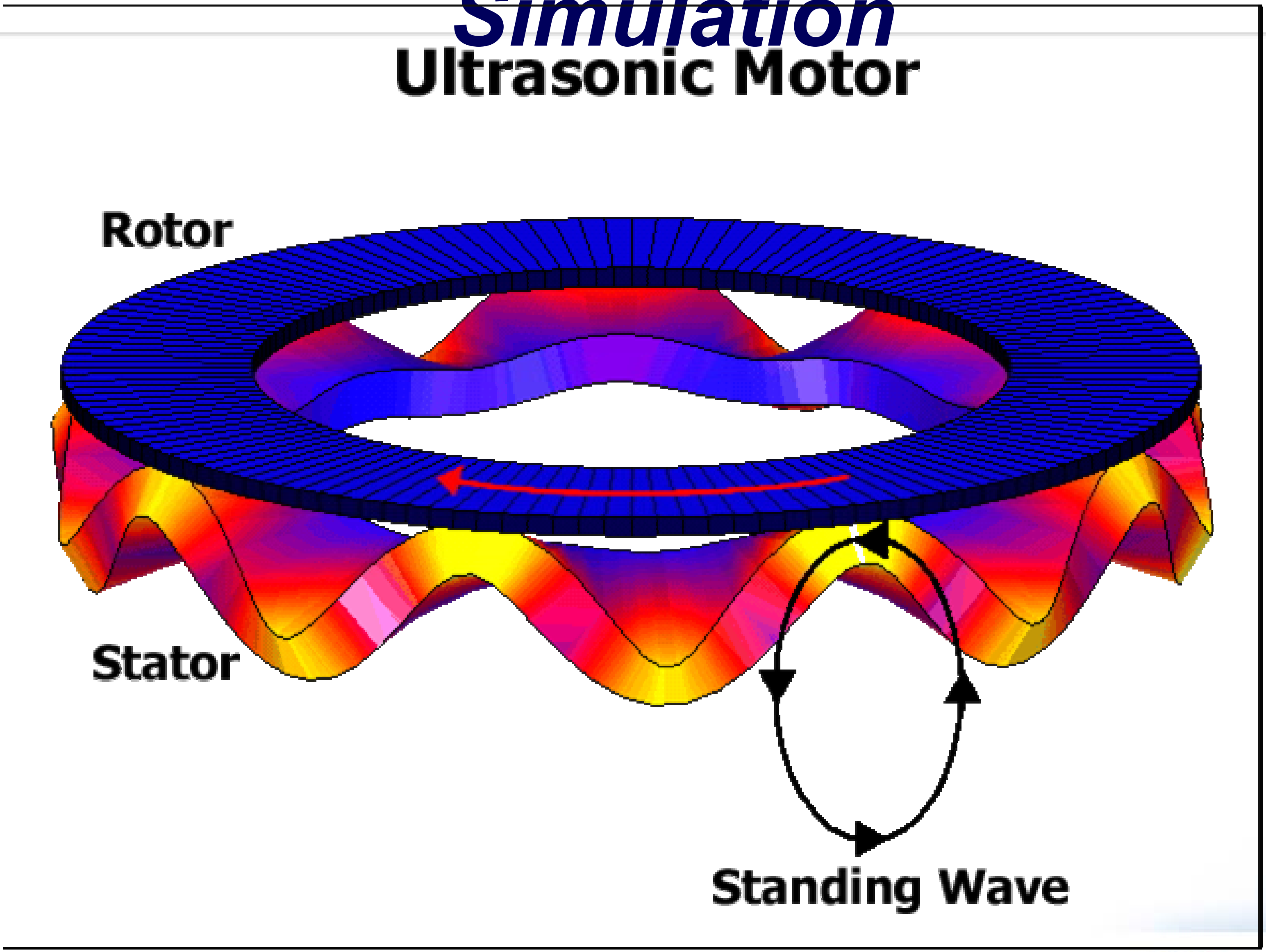
- Coupling Stress and Electric Field
- Coupling includes Contact
- Analysis Types Include:
  - static, modal, harmonic and transient dynamic



Characteristics

Coupled Displacement-Electric Potential
Piezoelectric Ceramic is Polarized
Standing Waves Generate Traveling Wave
Traveling Wave Moves Rotor
Low Rotational Speed, High Torque

Ultrasonic Motor Transient Simulation



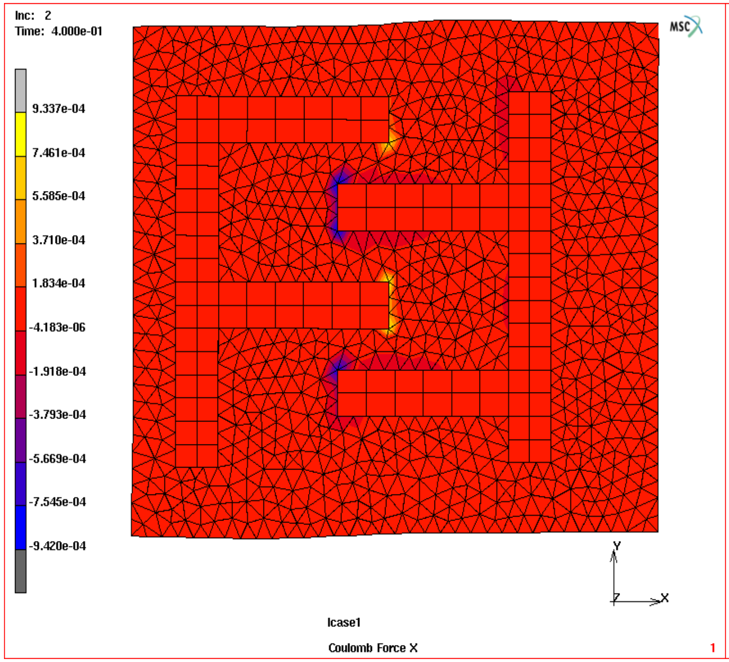
Marc 2005 Multi-Physics

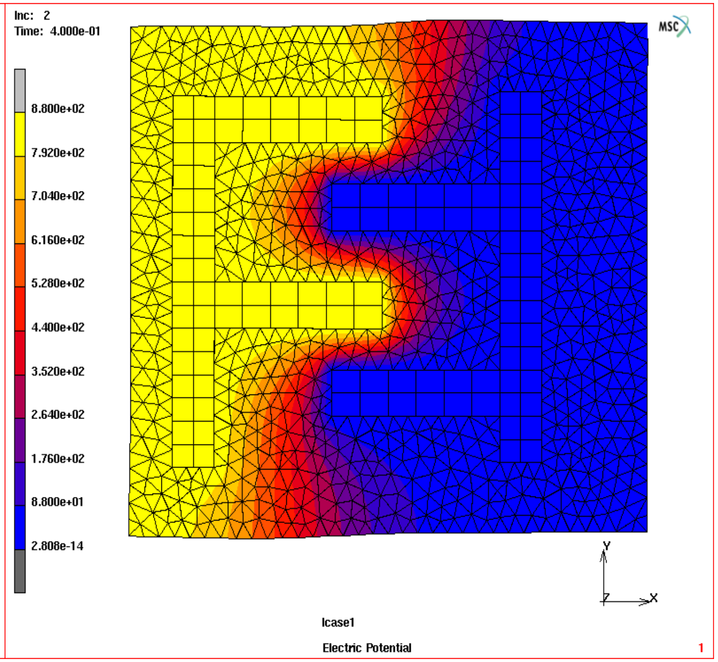
- Data Structures are rewritten so almost all physics can be used in one analysis
- Input Structure were rewritten so input file could support input of all material properties and boundary conditions simultaneously
- Control structures are rewritten so almost all physics can be used in one analysis.

Marc 2005 Multi-Physics

- **Coupled Thermal-Diffusion Analysis**
- **Coupled Electrostatic-Structural**

Coupled Electrostatic-Structural

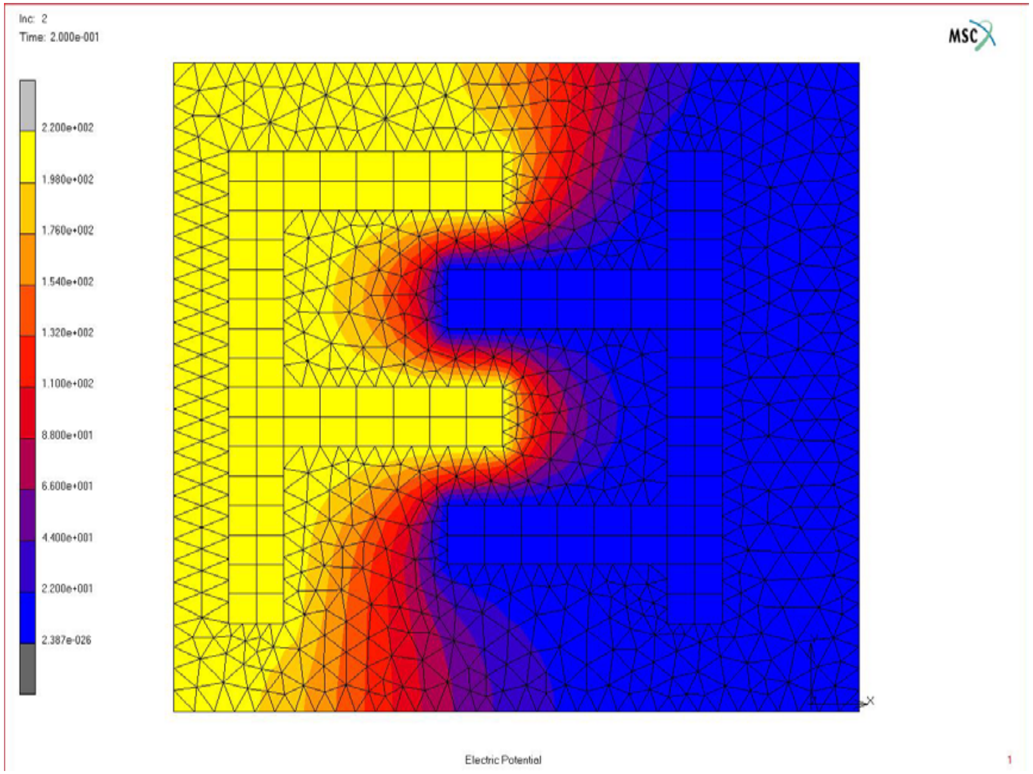




Coulomb Force

Electrical Potential

Coupled Electrostatic-Structural

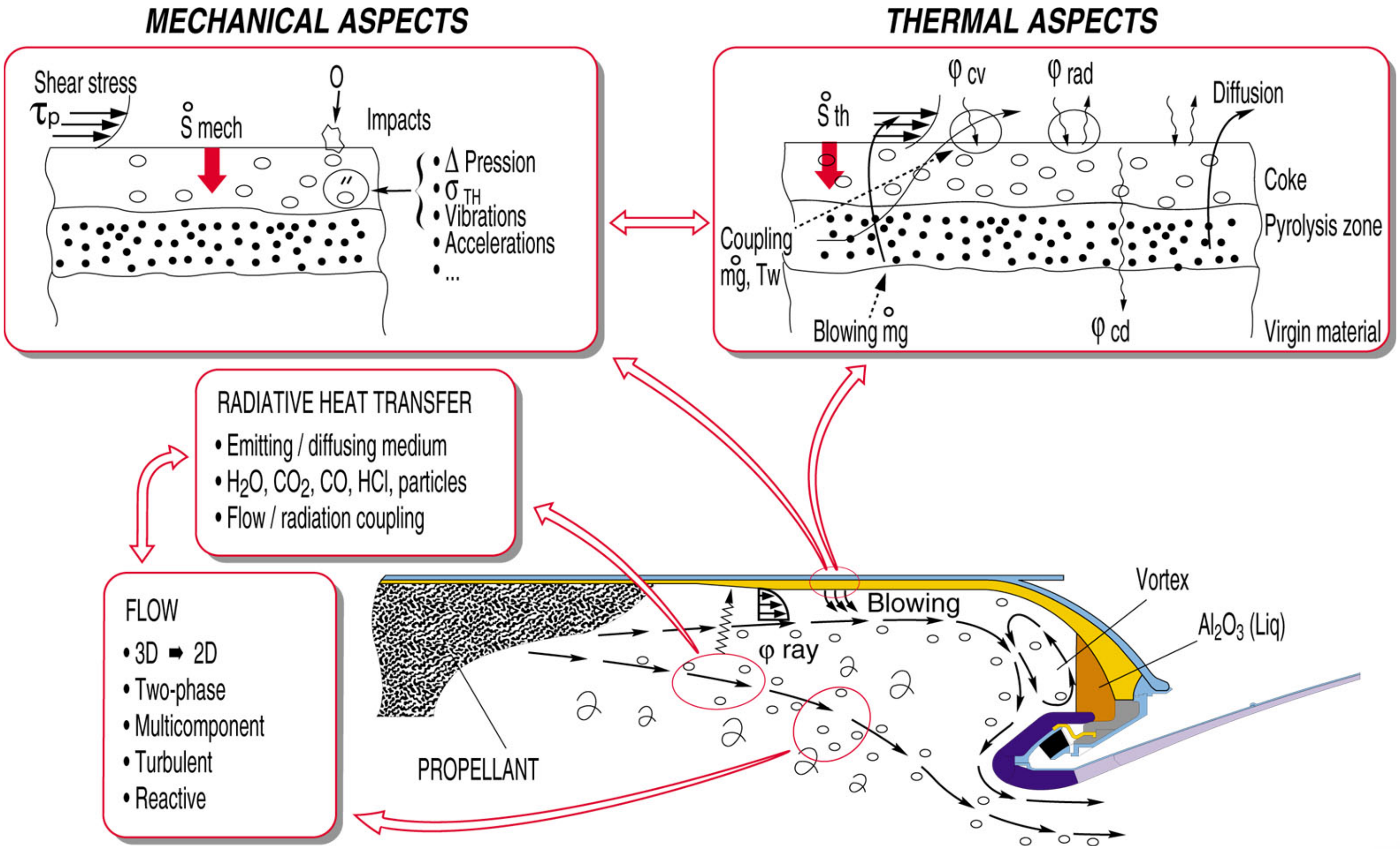


Finite Element Mesh of the Air is Remeshed Automatically During the Analysis

Multi-Physics and Thermal

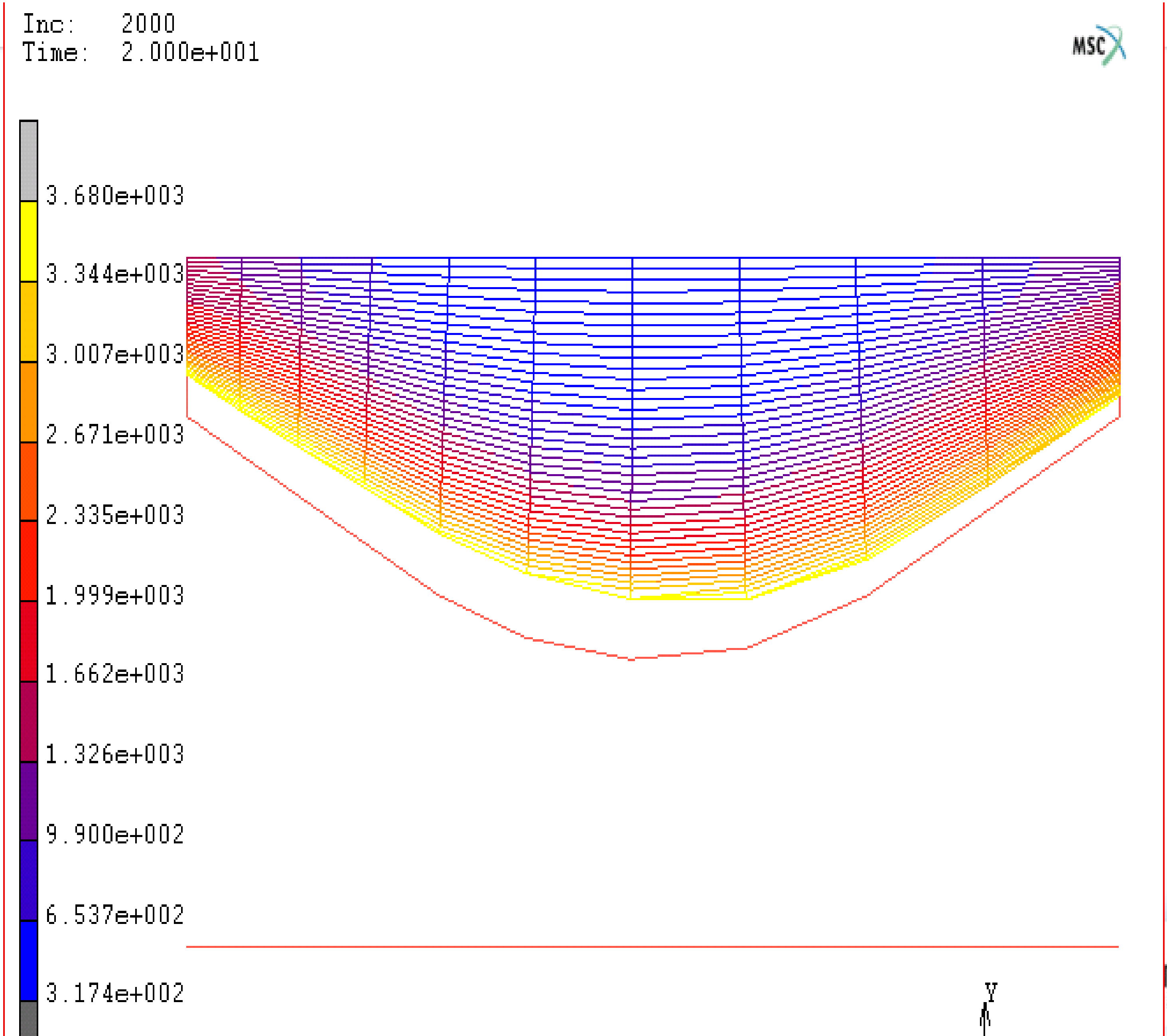
- **Advanced Thermal Analysis**
  - **Radiation**
  - **Pyrolysis**
  - **Ablation**

Physics overview



MSC SOFTWARE. SIMULATING REALITY

Ablation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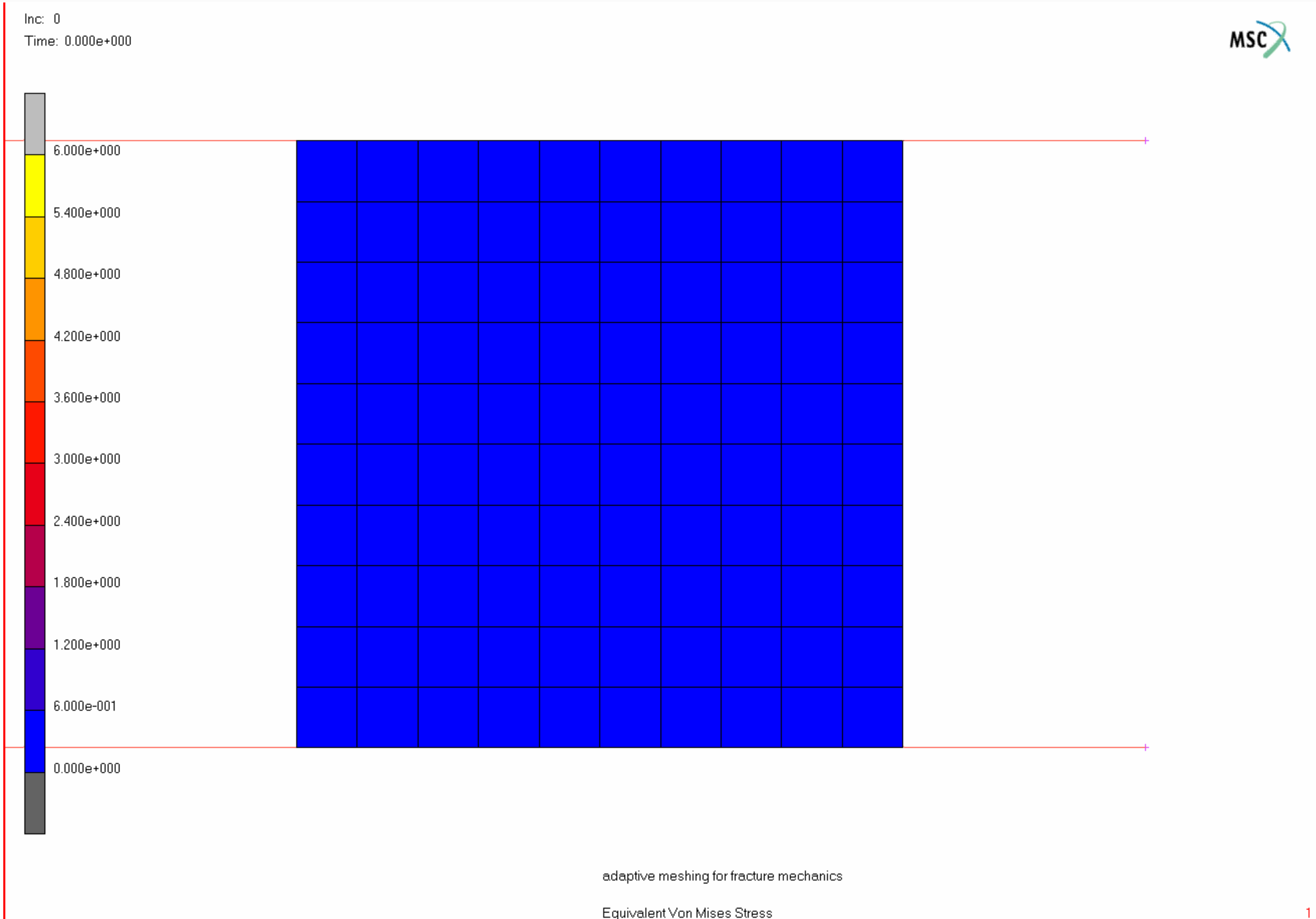
1.326e+003
9.900e+002
6.537e+002
3.174e+002
Y

Fracture Mechanics

- Progressive Failure
- Cracking
- Deactivate Elements
- Gurson Damage Model
- Lemaitre Damage Model
- Rubber Damage Models
- J-Integral
- Stress Intensity Factors
- Mode Separation

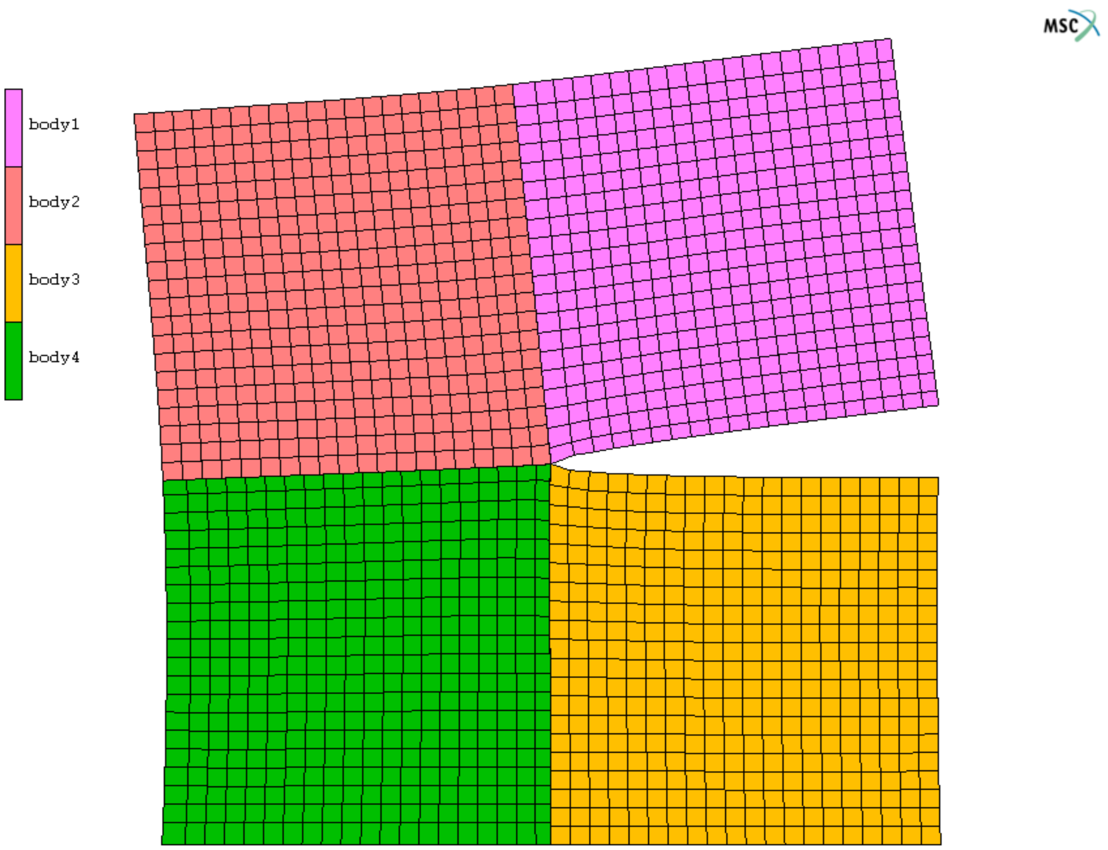
Crack Mesh Insertion



Contact on Crack Surfaces

- Crack tip closes due to (cyclic) load
- Design based upon Mode I crack may be too conservative
- Sliding along the surface results in Mode II and Mode III behavior
- Domain Integral Approach is more accurate than directly evaluating J
- The normal and friction forces due to contact contribute to J Integral
- Applicable for 2-D and 3-D

Mode I Crack – Test Contact



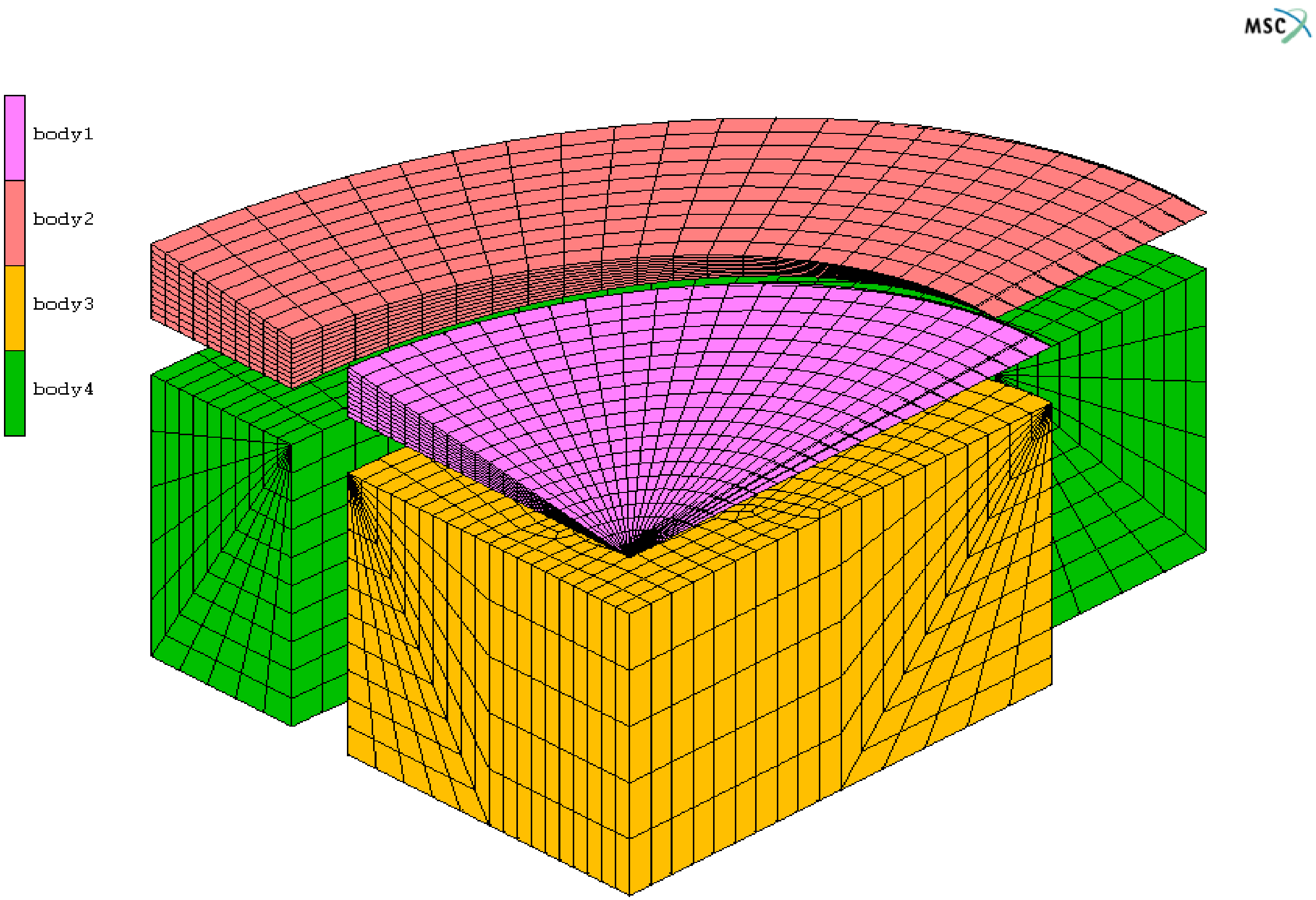
Meshing Flexibility

- Nice Hexahedral Meshes in vicinity of crack tip
- Glue Meshes near crack tip
- Glue Cracking Region in Far-Field with Tetrahedral Mesh

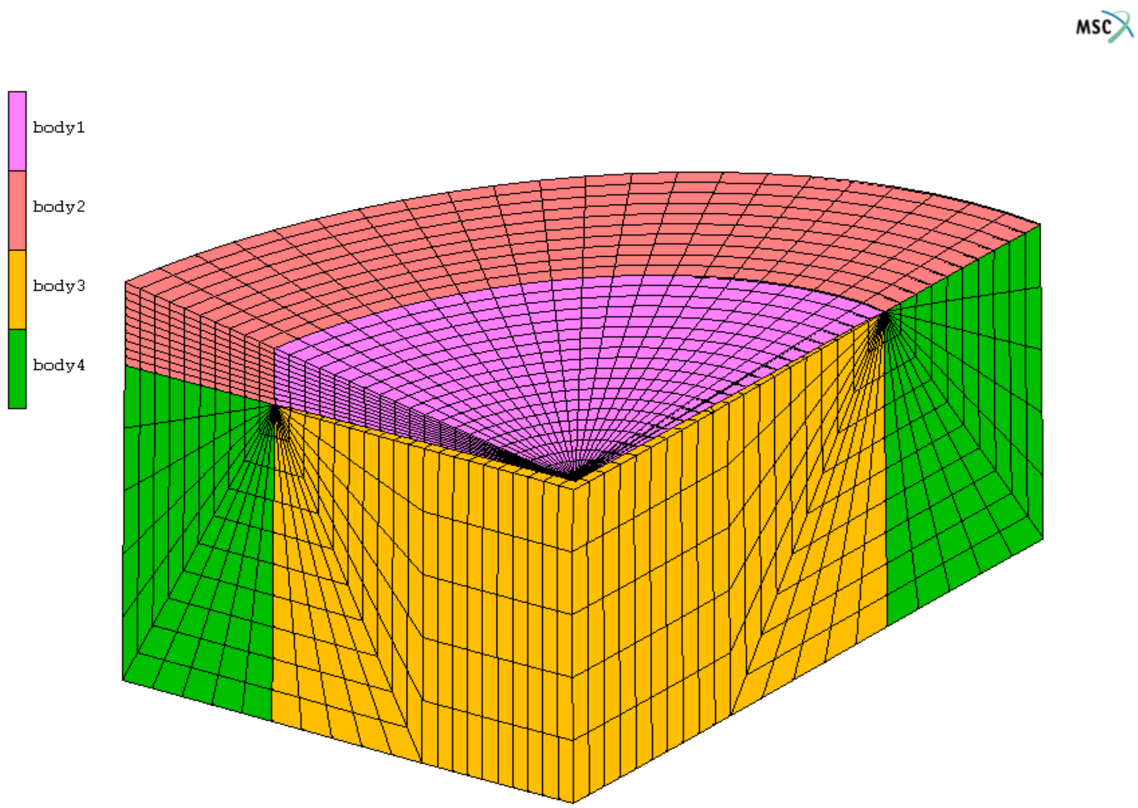
Example : Crack face between body 1 and 2

: Crack front at intersection of all bodies

Contact Bodies Used to Mesh Crack Region



Opened Crack Face



MSC SOFTWARE. SIMULATING REALITY

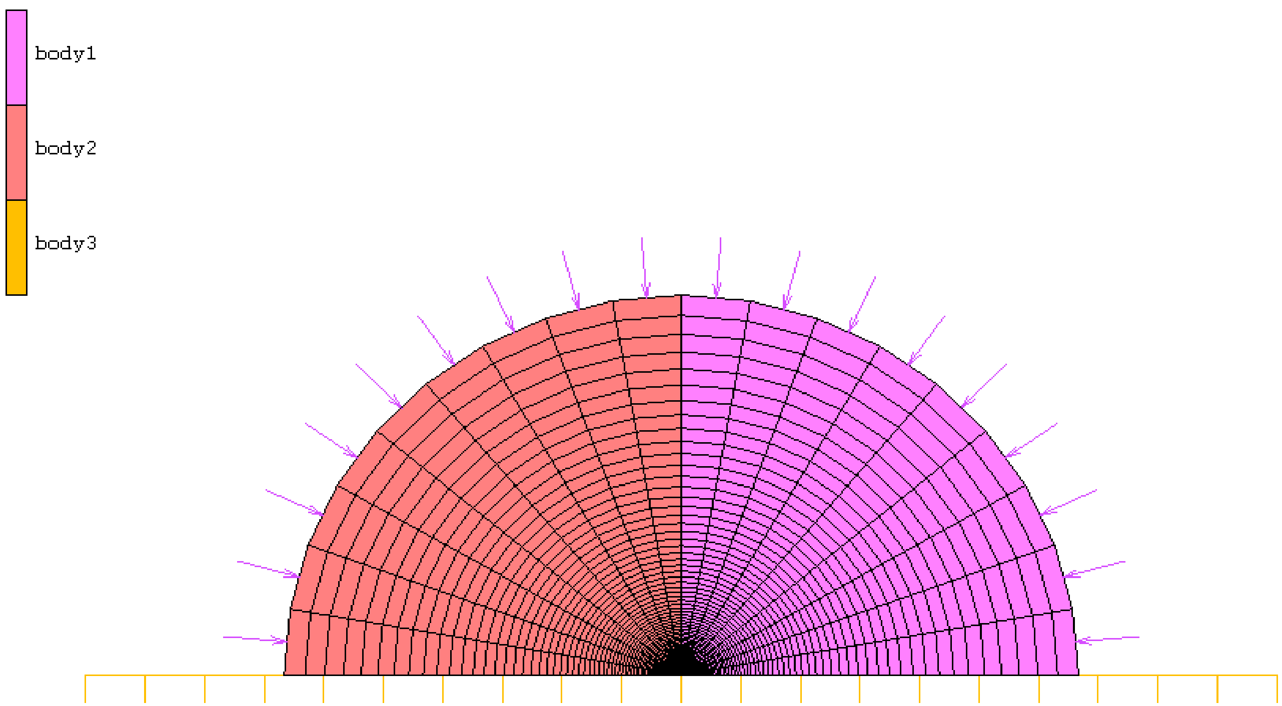
Comparison of domain integral from a homogeneous mesh and glued mesh of four bodies – Material is Neo-Hookean

Domain#	1	2	3	4	5	6	7	8
No-Glue	0.21377	0.21792	0.21872	0.21893	0.21904	0.21908	0.21911	0.21912
Glue	0.21498	0.21977	0.21914	0.21962	0.21925	0.21941	0.21916	0.21924

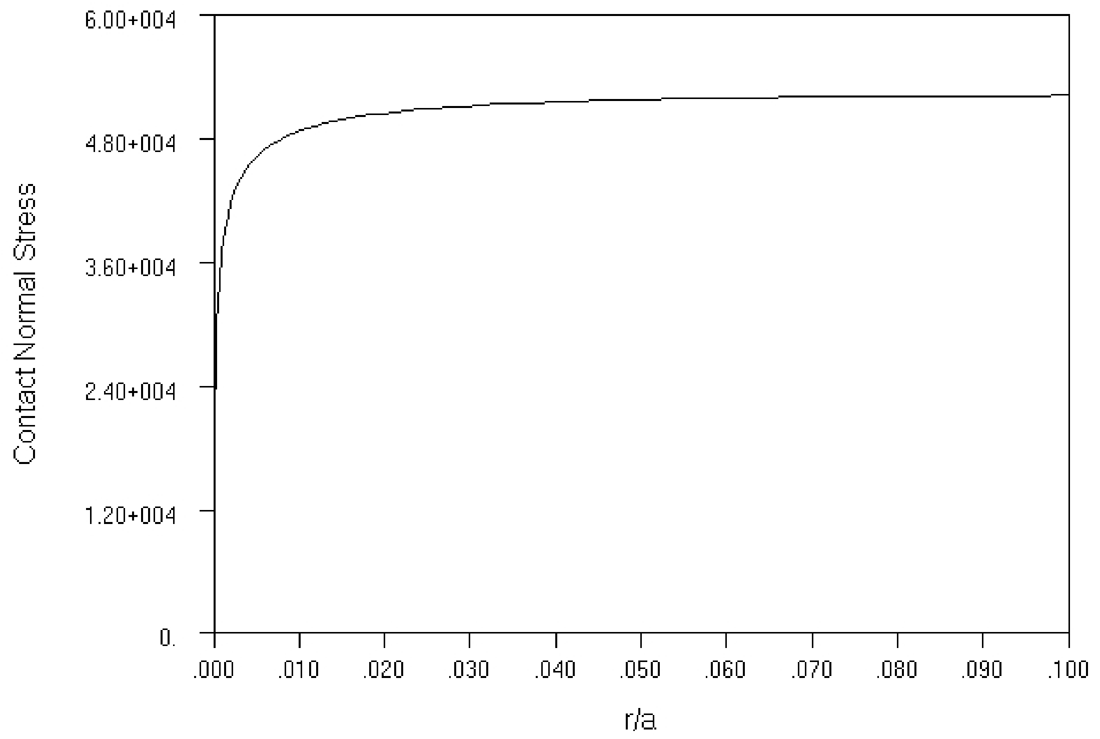
Results of two nodes from 3-d model – elastic body subjected to tensile load

Domain#	1	2	3	4	5	6	7	8
Node 1	11.591	11.713	11.453	10.313	10.294	10.278	10.270	10.279
Node 2	11.262	11.351	11.371	11.354	11.358	11.359	11.362	11.371

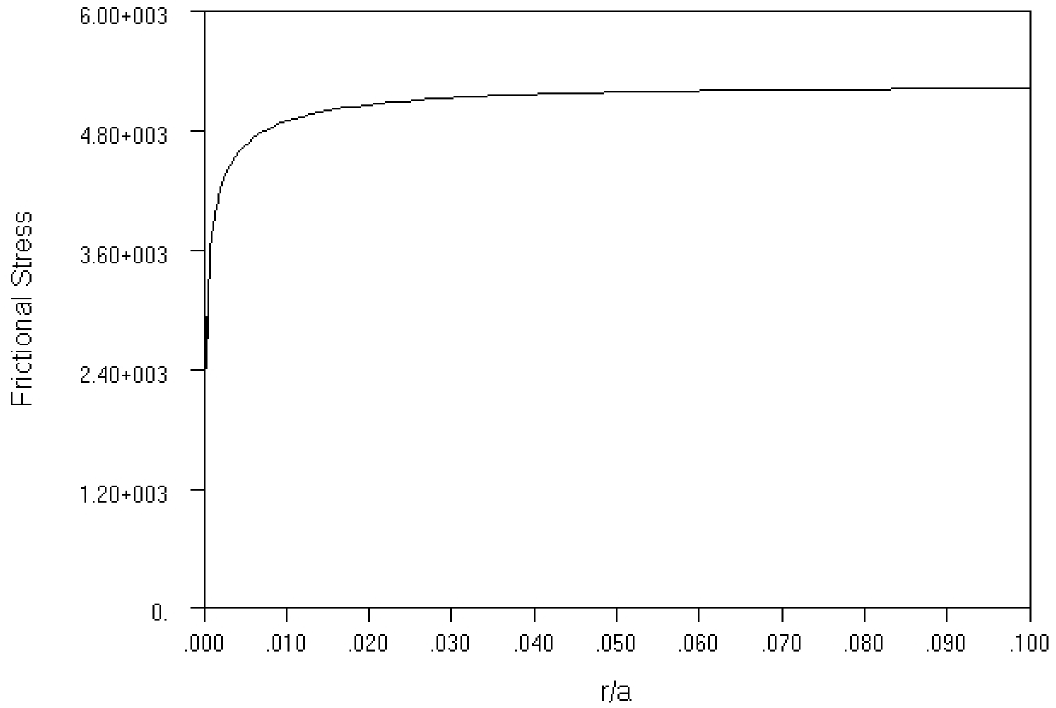
Concentric Load Driving Closure and Friction



Normal Stress on Crack Face

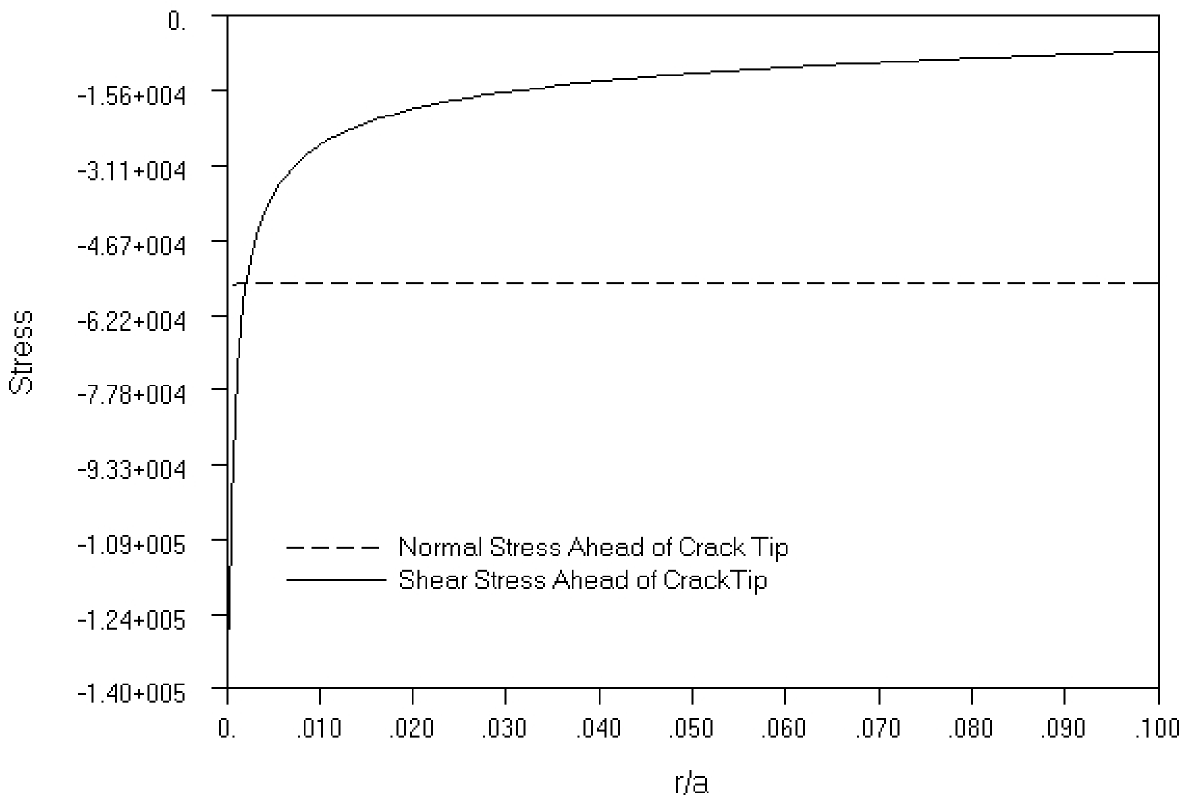


Frictional Stress on Crack Face

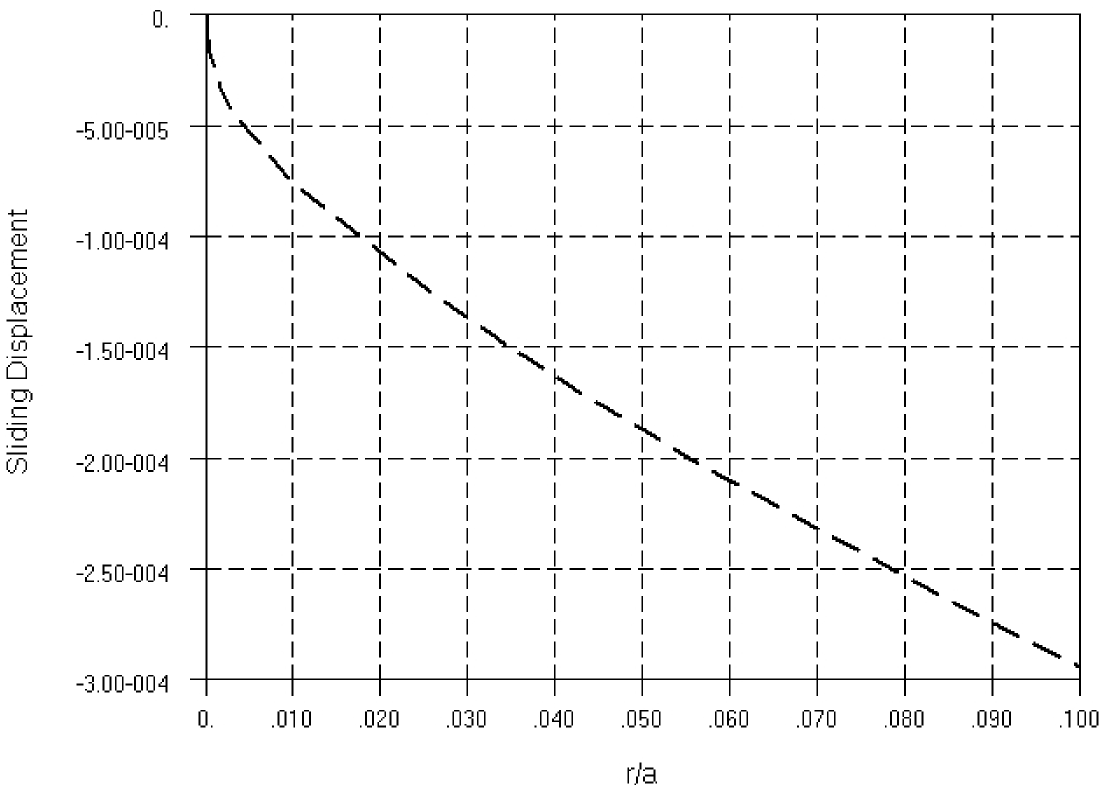


Stresses Ahead of Crack Tip

Note Shear Stress Singularity



Sliding Displacement

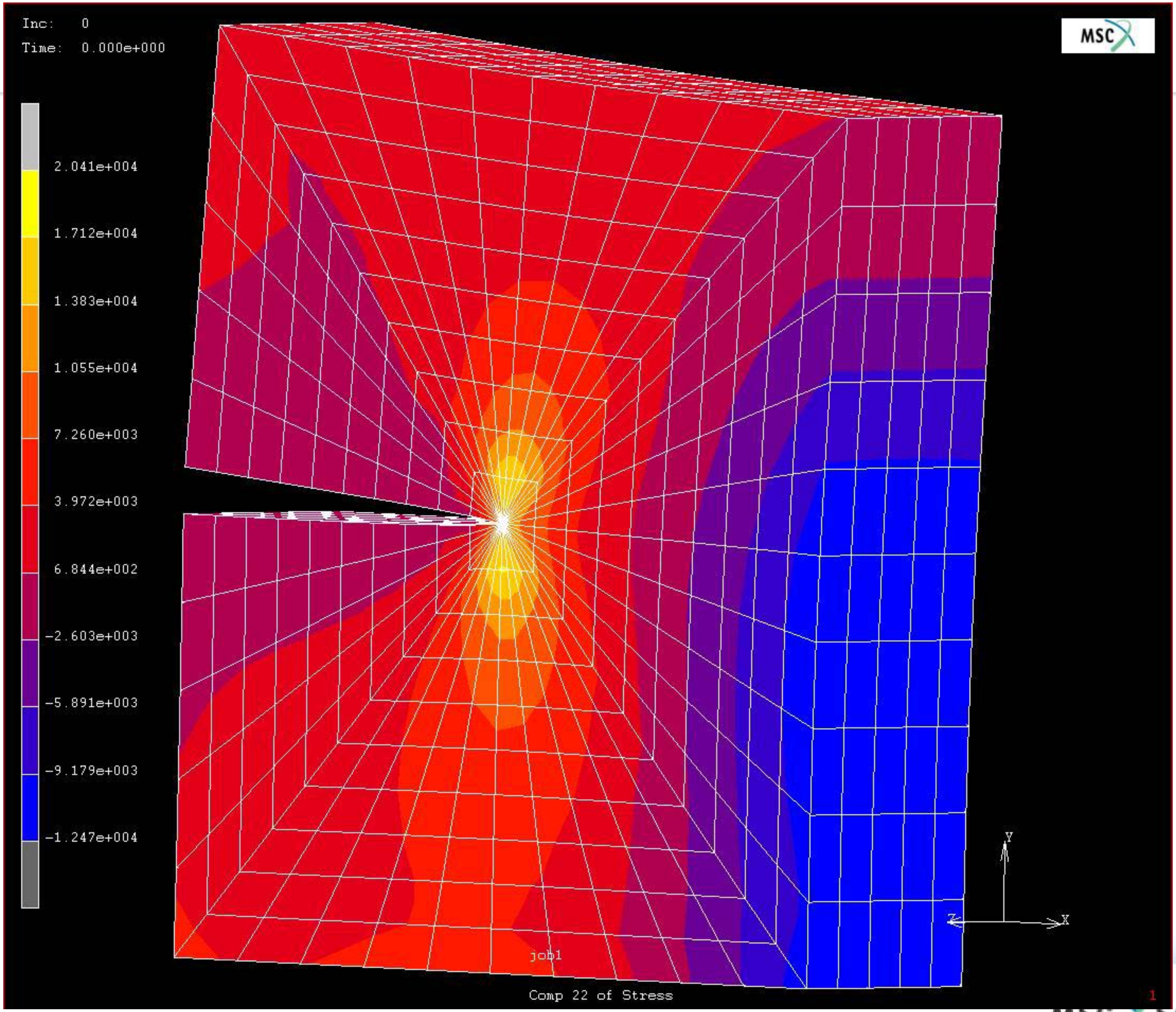


Fracture Mechanics Conclusion

- For No Closure – No Friction Case – Obtain Domain Independence
- When Closure and Friction are Present – Require a Finer Mesh at Crack Front
- Higher Order Elements (using quarter point technique) show more stable results when closure and friction is present

Mode Separation

- New Capability for 2-D and 3-D
- Currently – Elastic Isotropic Material
- Under development – Elastic Orthotropic Material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6.844e+002
-2.603e+003
-5.891e+003
-9.179e+003
-1.247e+004
job1
Comp 22 of Stress
Y
Z
X

Typical Output

j-integral estimations:

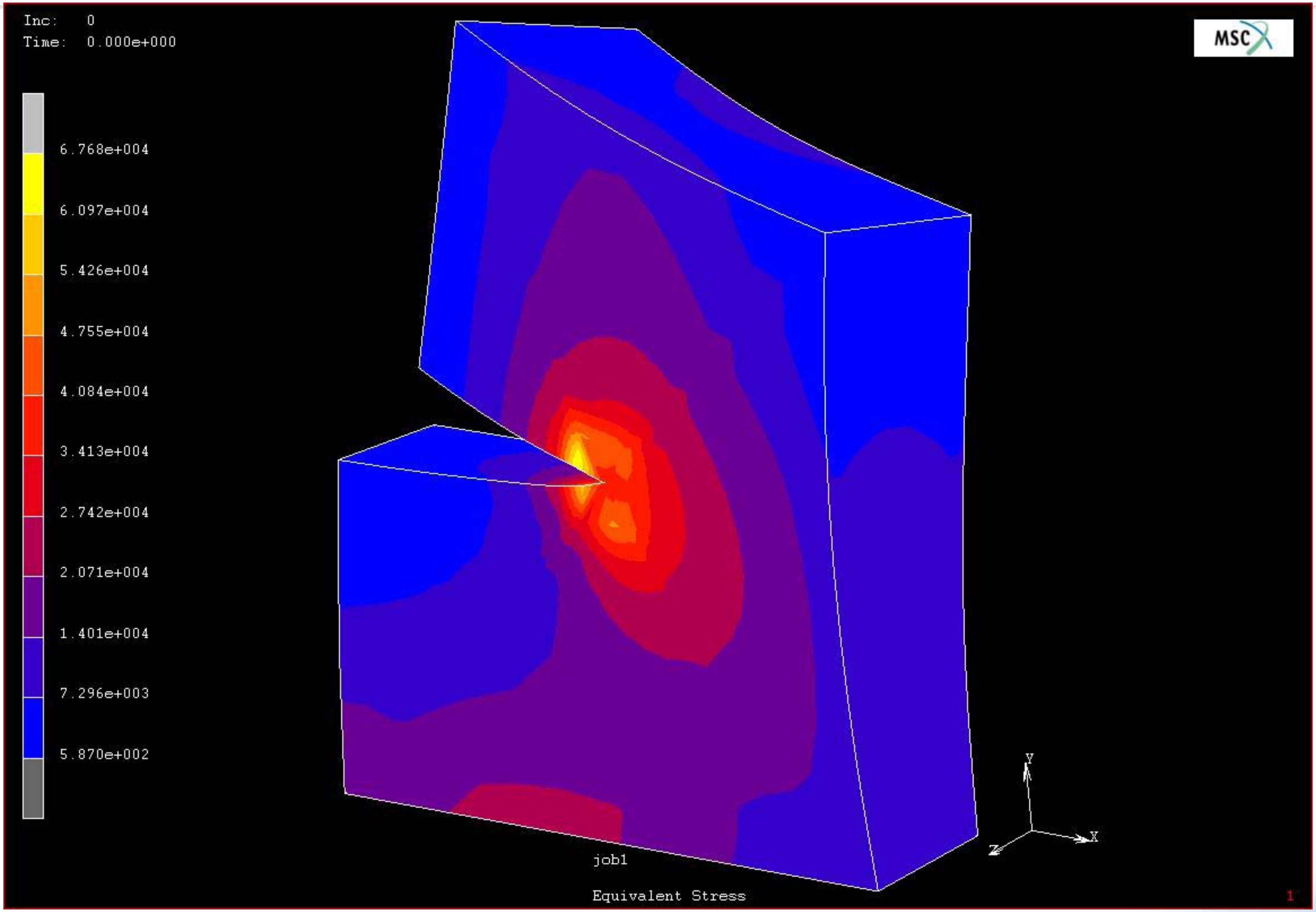
crack tip node	path radius	j-integral value
422	1.4142E-01	1.4294E+01
422	2.8284E-01	1.4596E+01
422	4.2426E-01	1.4654E+01
422	5.6569E-01	1.4677E+01
422	7.0711E-01	1.4693E+01
422	8.4853E-01	1.4709E+01
422	9.8995E-01	1.4729E+01
422	1.1314E+00	1.4760E+01

Typical Output – Mode Separation

results for mode I and II: crack1

crack tip node	path radius	stress intensity factor K_I	K_II
422	1.4142E-01	1.1669E+04	1.7884E+03
422	2.8284E-01	1.2245E+04	1.7963E+03
422	4.2426E-01	1.2891E+04	1.7614E+03
422	5.6569E-01	1.3585E+04	1.7391E+03
422	7.0711E-01	1.4308E+04	1.7396E+03
422	8.4853E-01	1.5054E+04	1.7593E+03
422	9.8995E-01	1.5820E+04	1.7892E+03
422	1.1314E+00	1.6589E+04	1.8178E+03

Combined Modes



Typical Output – Mode Separation

crack tip node	path radius	K_I	K_II	K_III
6	1.4142E-01	1.9772E+05	-2.5638E+05	-2.4568E+05
6	2.8284E-01	4.1616E+05	-4.7860E+05	-3.9508E+05
6	4.2426E-01	6.9078E+05	-7.6445E+05	-5.4648E+05
6	5.6569E-01	1.0130E+06	-1.1113E+06	-6.9291E+05
6	7.0711E-01	1.3774E+06	-1.5155E+06	-8.3125E+05
6	8.4853E-01	1.7803E+06	-1.9739E+06	-9.5891E+05
6	9.8995E-01	2.2191E+06	-2.4833E+06	-1.0726E+06
6	1.1314E+00	2.6918E+06	-3.0410E+06	-1.1669E+06