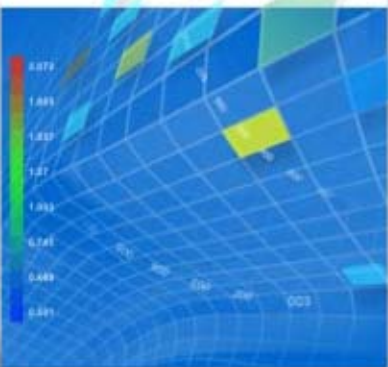


MSC SOFTWARE.
SIMULATING REALITY

MSC Software Fuel Cell Analysis



**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***

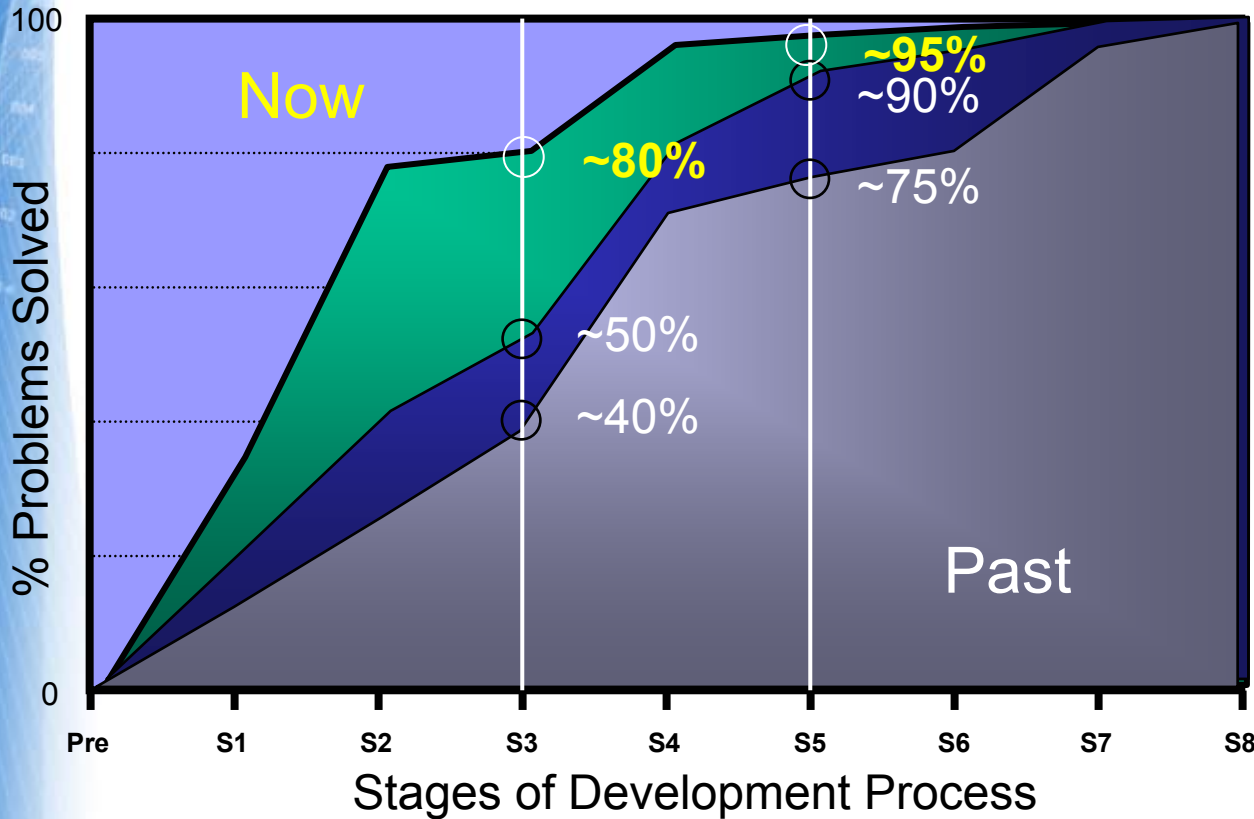
Better Information Earlier
Drive Collaboration

© Copyright 2002 MSC Software Corporation
*** Based on 2001 revenue of CAE companies. Source: Daratech**




Better Information Earlier

How this has helped Toyota

1st prototypes 2nd prototypes



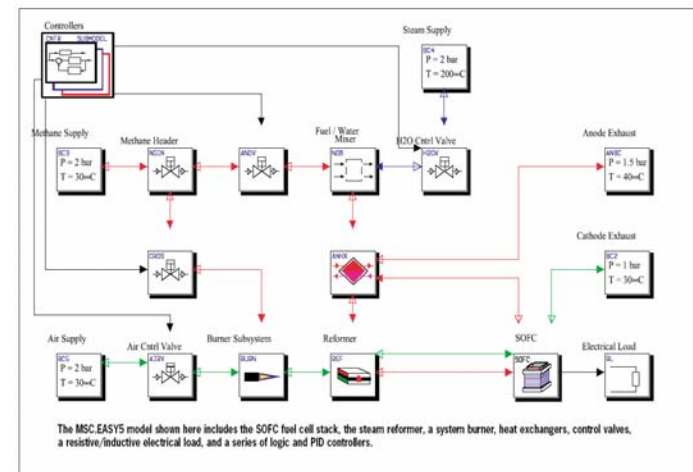
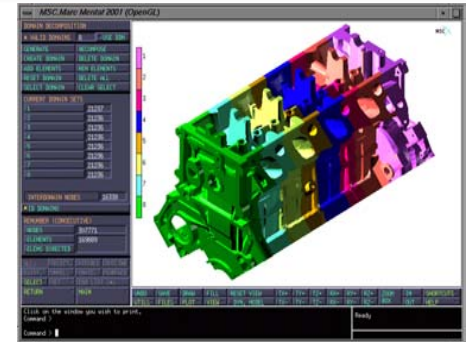
Toyota's Front-Loaded Development Initiatives

-  = Improved Communication
-  = Use of CAD
-  = Use of CAE

End Result: 65% fewer prototypes (!)

Fuel Cell Simulation Tools

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



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National Laboratory

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



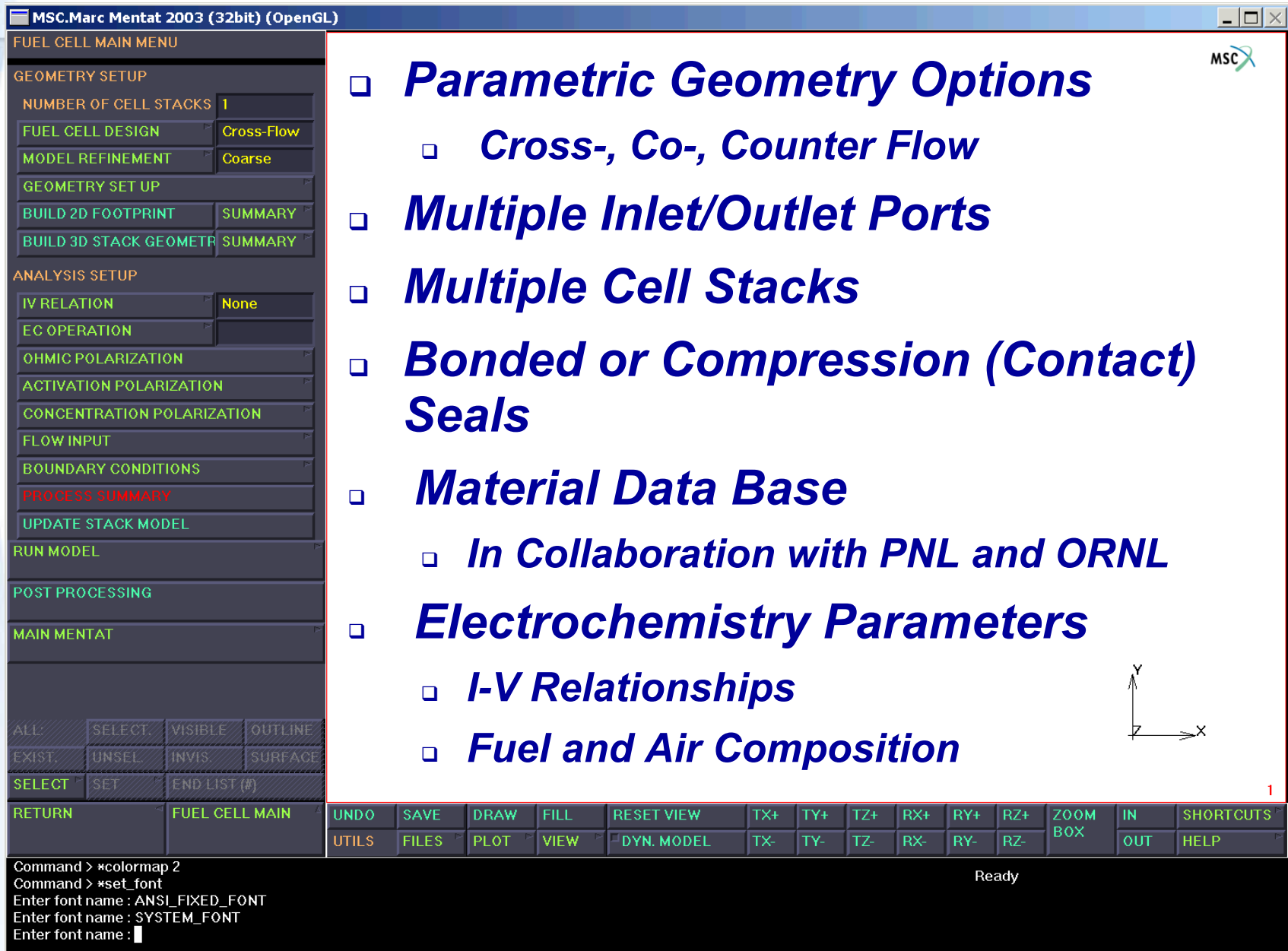
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MSC SOFTWARE.
SIMULATING REALITY

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



The screenshot displays the MSC.Marc Mentat 2003 (32bit) (OpenGL) software interface. The main window is titled "FUEL CELL MAIN MENU" and contains a sidebar menu on the left and a central workspace. The sidebar menu is organized into several sections: GEOMETRY SETUP, ANALYSIS SETUP, RUN MODEL, POST PROCESSING, and MAIN MENTAT. The GEOMETRY SETUP section includes options for NUMBER OF CELL STACKS (1), FUEL CELL DESIGN (Cross-Flow), MODEL REFINEMENT (Coarse), and BUILD 2D FOOTPRINT (SUMMARY). The ANALYSIS SETUP section includes options for IV RELATION (None), EC OPERATION, OHMIC POLARIZATION, ACTIVATION POLARIZATION, CONCENTRATION POLARIZATION, FLOW INPUT, BOUNDARY CONDITIONS, and PROCESS SUMMARY. The RUN MODEL section includes UPDATE STACK MODEL. The POST PROCESSING section includes MAIN MENTAT. The MAIN MENTAT section includes a table with columns ALL, SELECT, VISIBLE, and OUTLINE, and rows EXIST, UNSEL, INVIS, SURFACE, and SELECT. The central workspace contains a list of parametric geometry options, a 3D coordinate system (X, Y, Z), and a command line at the bottom. The command line shows the following commands: Command > *colormap 2, Command > *set_font, Enter font name : ANSL_FIXED_FONT, Enter font name : SYSTEM_FONT, and Enter font name : . The status bar at the bottom right indicates "Ready".

FUEL CELL MAIN MENU

GEOMETRY SETUP

- NUMBER OF CELL STACKS 1
- FUEL CELL DESIGN Cross-Flow
- MODEL REFINEMENT Coarse
- GEOMETRY SET UP
- BUILD 2D FOOTPRINT SUMMARY
- BUILD 3D STACK GEOMETR SUMMARY

ANALYSIS SETUP

- IV RELATION None
- EC OPERATION
- OHMIC POLARIZATION
- ACTIVATION POLARIZATION
- CONCENTRATION POLARIZATION
- FLOW INPUT
- BOUNDARY CONDITIONS
- PROCESS SUMMARY
- UPDATE STACK MODEL

RUN MODEL

- UPDATE STACK MODEL

POST PROCESSING

- MAIN MENTAT

MAIN MENTAT

ALL:	SELECT	VISIBLE	OUTLINE
EXIST.	UNSEL	INVIS	SURFACE
SELECT	SET	END LIST (#)	

- Parametric Geometry Options**
 - Cross-, Co-, Counter Flow
- Multiple Inlet/Outlet Ports**
- Multiple Cell Stacks**
- Bonded or Compression (Contact) Seals**
- Material Data Base**
 - In Collaboration with PNL and ORNL
- Electrochemistry Parameters**
 - I-V Relationships
 - Fuel and Air Composition

Command > *colormap 2
Command > *set_font
Enter font name : ANSL_FIXED_FONT
Enter font name : SYSTEM_FONT
Enter font name :

Ready

Model Creation



MSC.Marc Mentat 2003 (32bit) (OpenGL)

FUEL CELL MAIN MENU

GEOMETRY SETUP

NUMBER OF CELL STACKS: 1

FUEL CELL DESIGN: Cross-Flow

MODEL REFINEMENT: ...

GEOMETRY SET UP

BUILD 2D FOOTPRINT: SUMMARY

BUILD 3D STACK GEOMETRY: SUMMARY

ANALYSIS SETUP

IV RELATION: None

EC OPERATION

OHMIC POLARIZATION

ACTIVATION POLARIZATION

CONCENTRATION POLARIZATION

FLOW INPUT

BOUNDARY CONDITIONS

PROCESS SUMMARY

UPDATE STACK MODEL

RUN MODEL

POST PROCESSING

MAIN MENTAT

ALL:	SELECT.	VISIBLE	OUTLINE
EXIST.	UNSEL.	INVIS.	SURFACE
SELECT	SET	END LIST (#)	

RETURN FUEL CELL MAIN

MSC.Marc Mentat FUEL CELL DESIGN

DEFINE FUEL CELL DESIGN

Cross-Flow

Co-Flow

Counter-Flow

OK

Multiple Design Options

MSC.Marc Mentat FUEL CELL DESIGN

Select Stack Structure

Planer Stack Structure

Vertical Stack Structure

Vertical PEN Stack Structure

OK

Parametric Geometry 2D & 3D



UNDO	SAVE	DRAW	FILL	RESET VIEW	TX+	TY+	TZ+	RX+	RY+	RZ+	ZOOM BOX	IN	SHORTCUTS
UTILS	FILES	PLOT	VIEW	DYN. MODEL	TX-	TY-	TZ-	RX-	RY-	RZ-		OUT	HELP

Planar Configuration - 2D Footprint

MSC.Marc Mentat FUEL CELL DESIGN

INPUT PLANER STACK/PEN DIMENSIONS (Meters):

FUEL MANIFOLD

Inlet Length	.03	Outlet Length	.03
Inlet Width	.003	Outlet Width	.005
Inlet Seal Width	.005	Outlet Seal Width	.005
No. of Inlet Channels	3	No. of Outlet Channels	3
Total Inlet Area (sq.meters)	0.0003	Total Outlet Area (sq.meters)	0.0004

AIR MANIFOLD

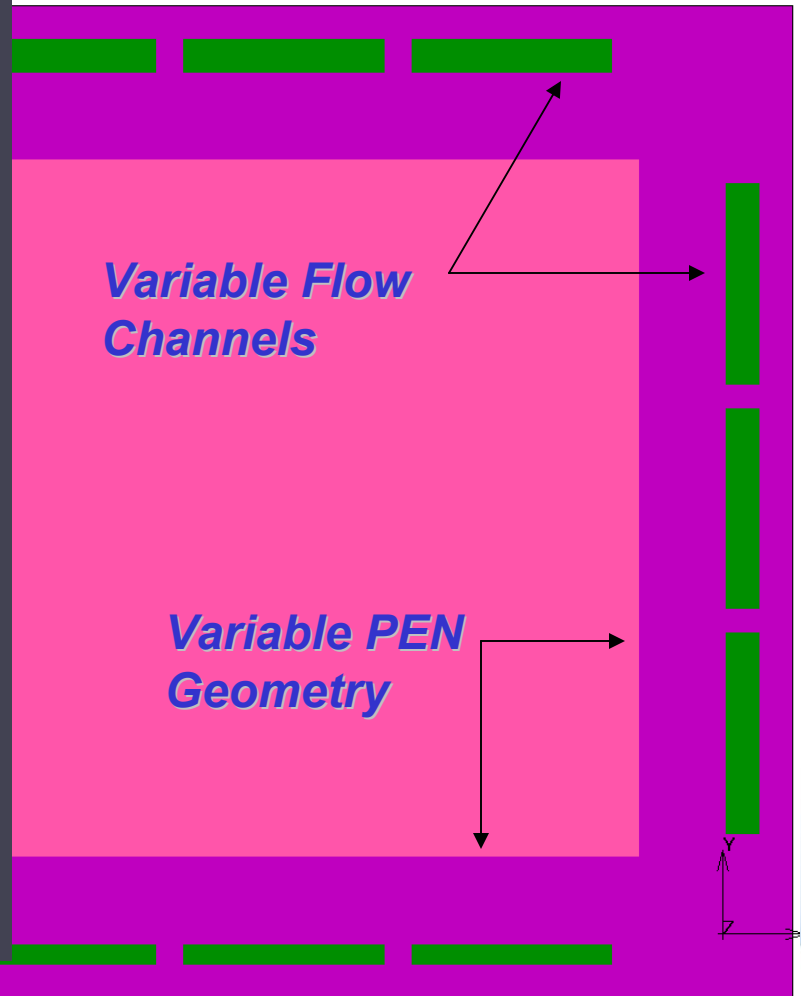
Inlet Length	.03	Outlet Length	.03
Inlet Width	.003	Outlet Width	.005
Inlet Seal Width	.005	Outlet Seal Width	.005
No. of Inlet Channels	3	No. of Outlet Channels	3
Total Inlet Area (sq. meter)	0.0003	Total Outlet Area (sq. meter)	0.0004

PEN GEOMETRY

PEN Length	.114	PEN Seal Width - air	.005
PEN Width	.116	PEN Seal Width - fuel	.005
PEN Aspect Ratio	0.983	PEN Gap - air	.003
PEN Area	0.013	PEN Gap - fuel	.003
PEN Active Area	0.011		

OK

Dimensions Guide



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

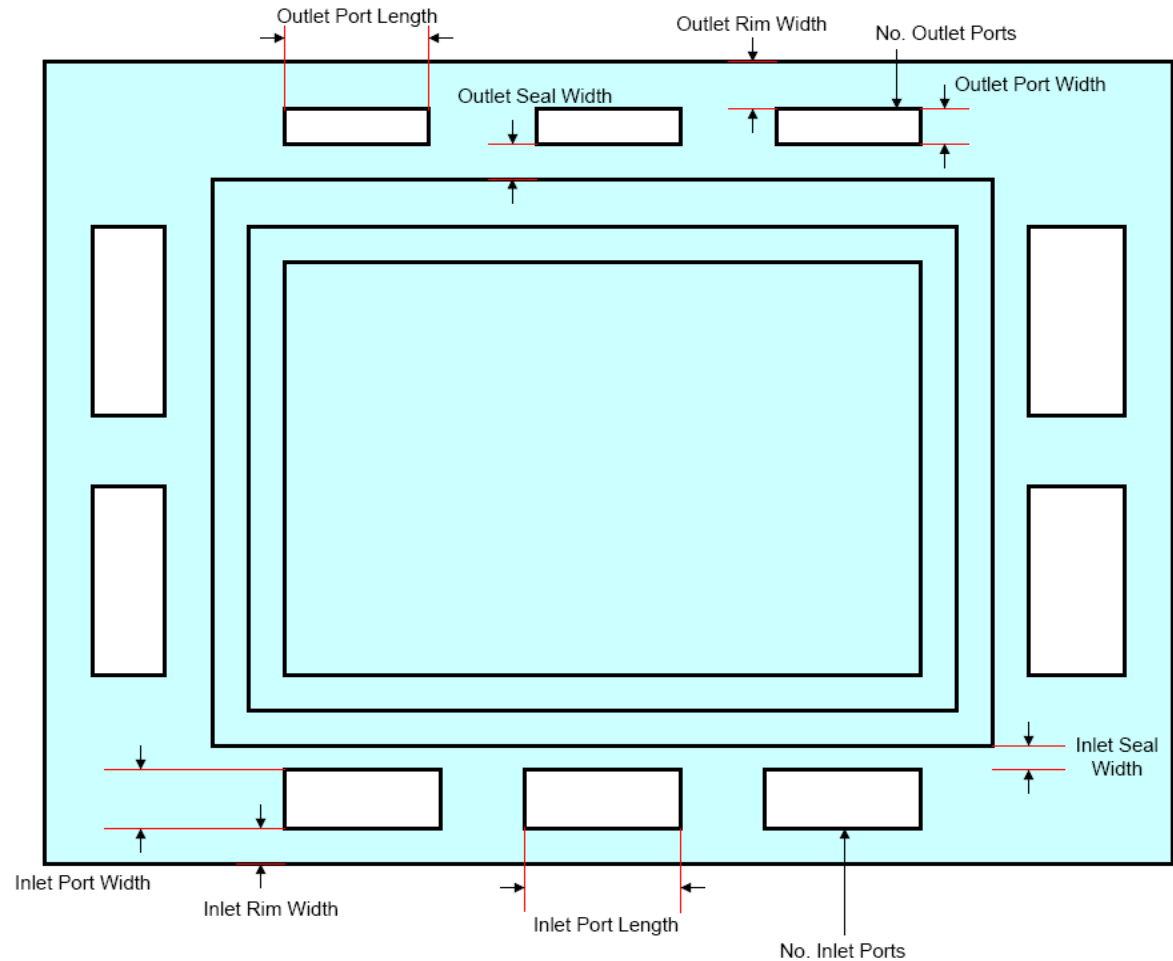
PEN GEOMETRY

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)



3D – Vertical Stack Seal and Layer Configurations



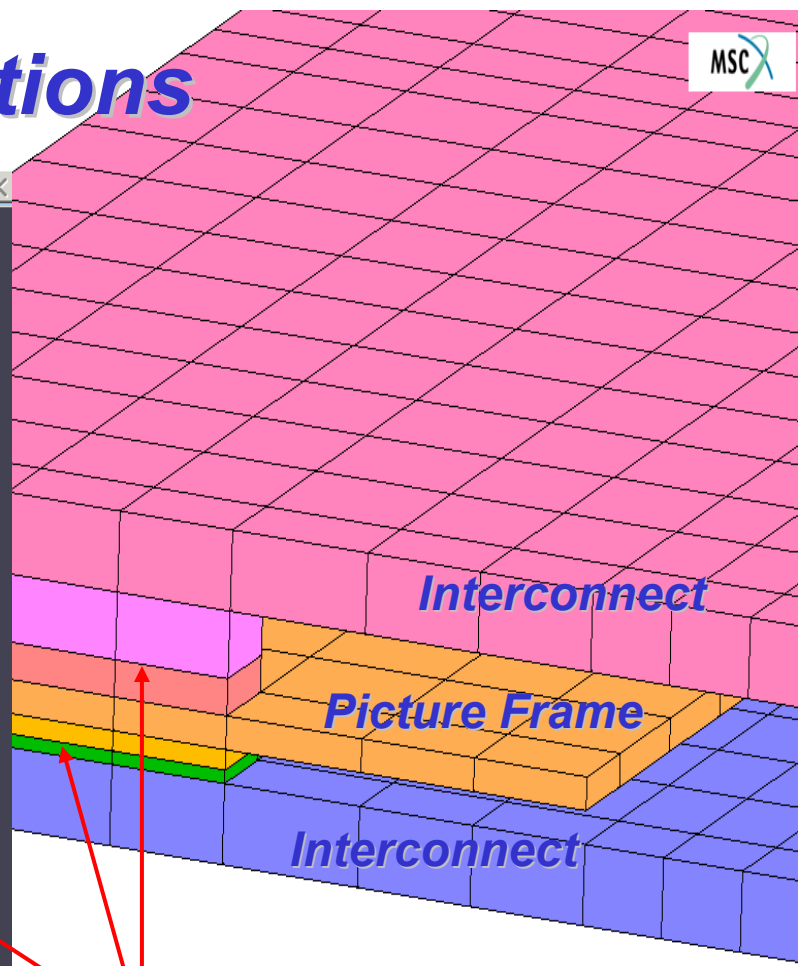
MSC.Marc Mentat FUEL CELL DESIGN

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



INPUT VERTICAL PEN COMPONENT DIMENSIONS (meters):

PEN

Anode Thickness	0.0006	Material	Anode
Electrolyte Thickness	0.00002	Material	Electrolyte
Cathode Thickness	0.00005	Material	Cathode

PEN ATTACHMENT TO PICTURE FRAME

PEN Layer	Cathode
Picture Frame Layer	Top
Attachment Method	Bonded

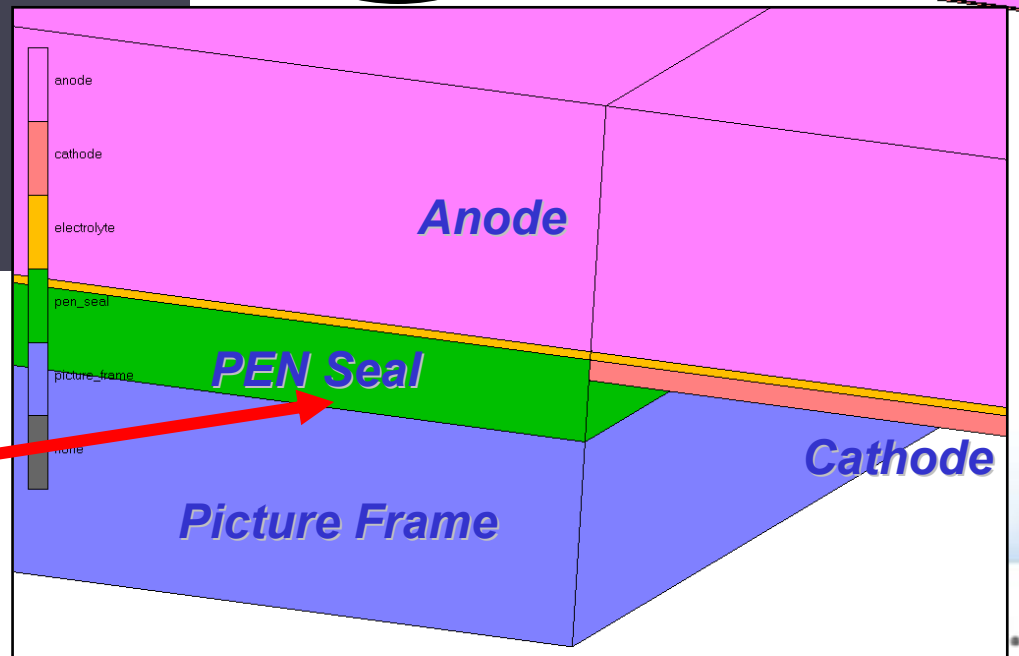
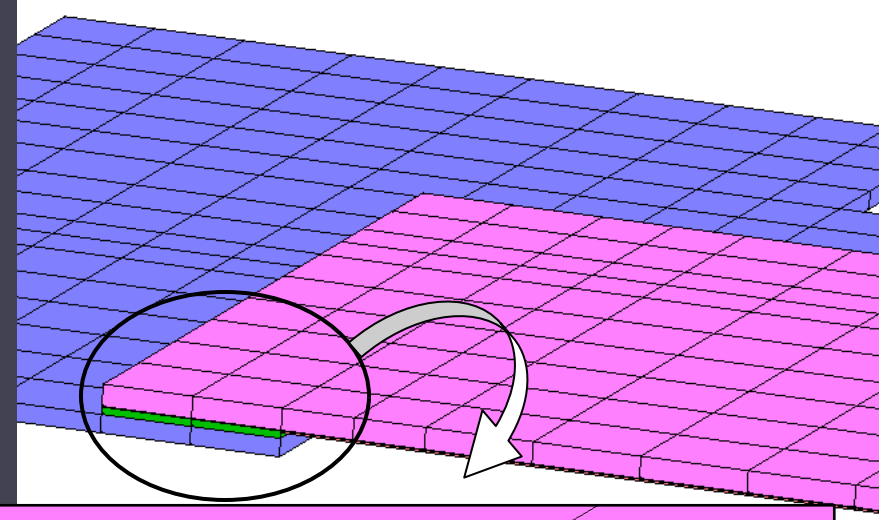
COMPOSITE SEAL 3

Seal Thickness	0.0002	Material	Glass Seal
Spacer Thickness	0.0	Material	SS-430

OK

Dimensions Guide

3D – Vertical Stack PEN Design Options



PEN Attachment Options

- **Bonded**
- **Sliding**

Material Database Options

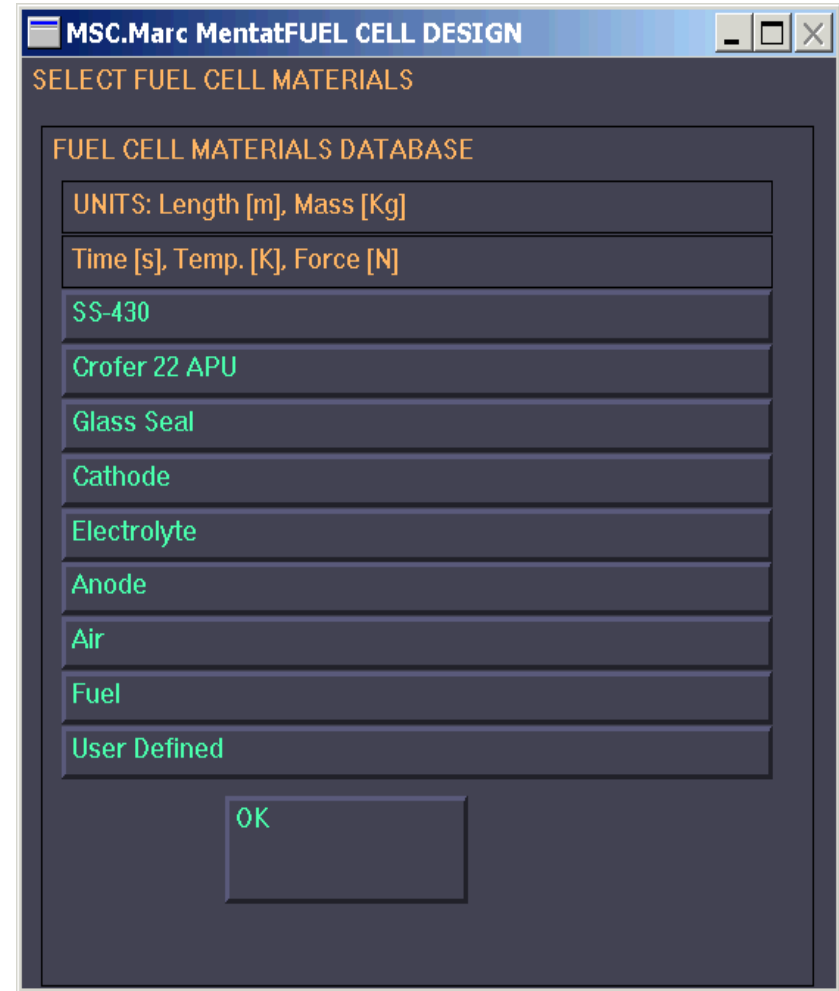
PNL/ORNL-

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

PNL –

- **EC Materials**

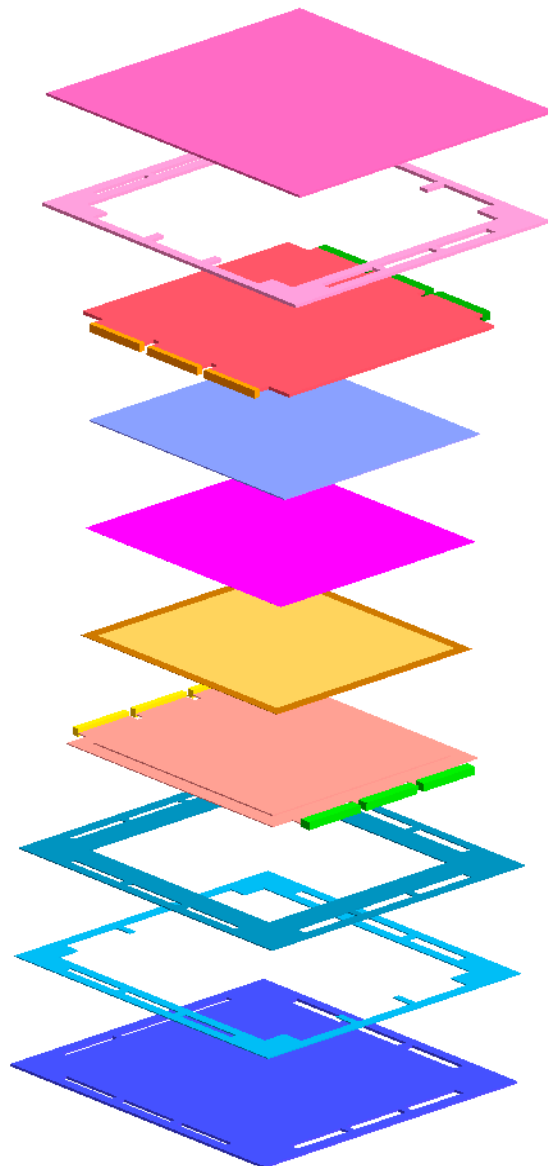
User Defined



...Final 3D SOFC Cell Model



- Electro_flux_elements
- air_flow
- air_in
- air_out
- anode
- anode_spacer
- cathode
- cathode_spacer
- electrolyte
- fuel_flow
- fuel_in
- fuel_out
- interconnect_bottom
- interconnect_top
- pen_seal
- picture_frame
- none



Interconnect

Anode Spacer/Seal

Fuel Flow

Anode

Electrolyte

Cathode/PEN Seal

Air Flow

Picture Frame

Cathode Spacer/Seal

Interconnect



Analysis Options - Select I-V Relations

MSC.Marc Mentat 2003 (32bit) (OpenGL)

FUEL CELL MAIN MENU

GEOMETRY SETUP

NUMBER OF CELL STACKS 1

FUEL CELL DESIGN Cross-Flow

MODEL REFINEMENT Coarse

GEOMETRY SET UP

BUILD 2D FOOTPRINT SUMMARY

BUILD 3D STACK GEOMETRY SUMMARY

ANALYSIS SETUP

IV RELATION Tafel-Virkar

EC OPERATION

OHMIC POLARIZATION

ACTIVATION POLARIZATION

CONCENTRATION POLARIZATION

FLOW INPUT

BOUNDARY CONDITIONS

PROCESS SUMMARY

UPDATE STACK MODEL

RUN MODEL

POST PROCESSING

MAIN MENTAT

ALL: SELECT VISIBLE OUTLINE

EXIST. UNSEL INVIS SURFACE

SELECT SET END LIST (#)

RETURN FUEL CELL MAIN

MSC.Marc Mentat FUEL CELL DESIGN

DEFINE I-V RELATION

Tafel-Virkar

Butler-Volmer

None

OK

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:

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

Y

X

UNDO SAVE DRAW FILL RESET VIEW TX+ TY+ TZ+ RX+ RY+ RZ+ ZOOM IN SHORTCUTS

UTILS FILES PLOT VIEW DYN. MODEL TX- TY- TZ- RX- RY- RZ- BOX OUT HELP

ERROR: Couldn't find parameter "con_bv_cattor"!

Error on receive... closing connection

Command > *colormap

Enter colormap number : 2

Command >

Ready

Analysis Options – EC Operation



MSC.Marc Mentat 2003 (32bit) (OpenGL)

FUEL CELL MAIN MENU

GEOMETRY SETUP

- NUMBER OF CELL STACKS: 1
- FUEL CELL DESIGN: Cross-Flow
- MODEL REFINEMENT: Coarse
- GEOMETRY SET UP
 - BUILD 2D FOOTPRINT: SUMMARY
 - BUILD 3D STACK GEOMETRY: SUMMARY

ANALYSIS SETUP

- IV RELATION: Tafel-Virkar
- EC OPERATION: Total Voltage
- OHMIC POLARIZATION
- ACTIVATION POLARIZATION
- CONCENTRATION POLARIZATION
- FLOW INPUT
- BOUNDARY CONDITIONS
- PROCESS SUMMARY
- UPDATE STACK MODEL

RUN MODEL

POST PROCESSING

MAIN MENTAT

ALL: SELECT, VISIBLE, OUTLINE
EXIST, UNSEL, INVIS, SURFACE
SELECT, SET, END LIST (#)
RETURN, FUEL CELL MAIN

MSC.Marc MentatFUEL CELL DESIGN

SELECT OPERATION OPTION

- Total Voltage
- Total Current
- Fuel Utilization
- OK

Y
X

1

UNDO SAVE DRAW FILL RESET VIEW TX+ TY+ TZ+ RX+ RY+ RZ+ ZOOM BOX IN SHORTCUTS
UTILS FILES PLOT VIEW DYN. MODEL TX- TY- TZ- RX- RY- RZ- OUT HELP

EC Parameters – Ohmic Polarization

MSC.Marc Mentat FUEL CELL DESIGN

OHMIC POLARIZATION OPTIONS

For Tafel-Virkar Relation

Electrolyte Conductivity ($k = T \cdot \text{prefactor} \cdot \exp(\text{eff})$)

Effective Activation Ene: 0.007355

Prefactor: 6.87e-7

	Anode Parameters:	Cathode Parameter:	Interconnect Param
Temperature (K)	1273	1273	1273
Ohmic Resistance	3.33e-5	7.69e-5	4.0e-5

For BUTLER-VOLMER Relation

Electrolyte Conductivity ($k = AT^3 + BT^2 + CT + D$):

A	
B	
C	
D	

	Anode Conductivity:	Cathode Conductivii	Interconnect Condu
Activation Energy			
Pre-factor			
Porosity			
Conductivity			

OK

```
Command > *colormap
Enter colormap number : 2
Command > *py_file_run c:\msc_apps\mentat2003\bin\pnl\pnl_ecop1.py
Error on receive... closing connection
Command >
```

Ready

EC Parameters - Activation Polarization

MSC.Marc Mentat 2003 (32bit) (OpenGL)

FUEL CELL MAIN MENU

GEOMETRY SETUP

NUMBER OF CELL STACKS: 1

FUEL CELL DESIGN: Cross-Flow

MODEL REFINEMENT: Coarse

GEOMETRY SET UP

BUILD 2D FOOTPRINT: SUMMARY

BUILD 3D STACK GEOMETRY: SUMMARY

ANALYSIS SETUP

IV RELATION: Tafel-Virkar

EC OPERATION: Total Voltage

OHMIC POLARIZATION

ACTIVATION POLARIZATION

CONCENTRATION POLARIZATION

FLOW INPUT

BOUNDARY CONDITIONS

PROCESS SUMMARY

UPDATE STACK MODEL

RUN MODEL

POST PROCESSING

MAIN MENTAT

ALL: SELECT, VISIBLE, OUTLINE

EXIST: UNSEL, INVIS, SURFACE

SELECT: SET, END LIST (#)

RETURN: FUEL CELL MAIN

UNDO SAVE DRAW FILL RESET VIEW TX+ TY+ TZ+ RX+ RY+ RZ+ ZOOM IN SHORTCUTS

UTILS FILES PLOT VIEW DYN. MODEL TX- TY- TZ- RX- RY- RZ- BOX OUT HELP

Command > *colormap
Enter colormap number : 2
Command > *py_file_run c:\msc_apps\mentat2003\bin\pnl\pnl_ecop1.py
Error on receive... closing connection
Command >

Ready

MSC

MSC.Marc Mentat FUEL CELL DESIGN

ACTIVATION POLARIZATION OPTIONS

For TAFEL-VIRKAR Relation

Temperature (K):	Exchange Current (i ₀)	Tafel Prefact
923	0.051e-4	0.031
973	0.107e-4	0.028
1023	0.113e-4	0.0248
1073	0.132e-4	0.0247

For BUTLER-VOLMER Relation

Exchange Current (i = prefactor * exp(-act. energy))

Activation Energy:

Prefactor:

Symmetry Factor:

OK

Y
X

1

EC Parameters - Concentration Polarization

MSC.Marc Mentat 2003 (32bit) (OpenGL)

FUEL CELL MAIN MENU

GEOMETRY SETUP

NUMBER OF CELL STACKS: 1

FUEL CELL DESIGN: Cross-Flow

MODEL REFINEMENT: Coarse

GEOMETRY SET UP

BUILD 2D FOOTPRINT: SUMMARY

BUILD 3D STACK GEOMETRY: SUMMARY

ANALYSIS SETUP

IV RELATION: Tafel-Virkar

EC OPERATION: Total Voltage

OHMIC POLARIZATION

ACTIVATION POLARIZATION

CONCENTRATION POLARIZATION

FLOW INPUT

BOUNDARY CONDITIONS

PROCESS SUMMARY

UPDATE STACK MODEL

RUN MODEL

POST PROCESSING

MAIN MENTAT

ALL: SELECT. VISIBLE OUTLINE

EXIST. UNSEL. INVIS. SURFACE

SELECT SET END LIST (#)

RETURN FUEL CELL MAIN

UNDO SAVE DRAW FILL RESET VIEW TX+ TY+ TZ+ RX+ RY+ RZ+ ZOOM IN SHORTCUTS

UTILS FILES PLOT VIEW DYN. MODEL TX- TY- TZ- RX- RY- RZ- BOX OUT HELP

Command > *colormap
 Enter colormap number : 2
 Command > *py_file_run c:\msc_apps\mentat2003\bin\pn\pnl_ecop1.py
 Error on receive... closing connection
 Command >

MSC.Marc Mentat FUEL CELL DESIGN

CONCENTRATION POLARIZATION OPTIONS

For TAFEL-VIRKAR Relation

Testing Fuel Pressure (atm):

H2	0.96
H2O	0.04
CO	0.0
CO2	0.0

Temperature (K): Anode Current Density

923	3.184e-4
973	4.74e-4
1023	4.953e-4
1073	5.65e-4

For BUTLER-VOLMER Relation

Concentration Polarization Parameters:

	Anode	Cathode:
Porosity		
Tortuosity		

OK

Y
X

Ready

MSC

1

SIMULATING REALITY

Flow Input Parameters



MSC.Marc Mentat 2003 (32bit) (OpenGL)

FUEL CELL MAIN MENU

GEOMETRY SETUP

- NUMBER OF CELL STACKS: 1
- FUEL CELL DESIGN: Cross-Flow
- MODEL REFINEMENT: Coarse
- GEOMETRY SET UP
- BUILD 2D FOOTPRINT: SUMMARY
- BUILD 3D STACK GEOMETRY: SUMMARY

ANALYSIS SETUP

- IV RELATION: None
- EC OPERATION
- OHMIC POLARIZATION
- ACTIVATION POLARIZATION
- CONCENTRATION POLARIZATION
- FLOW INPUT
- BOUNDARY CONDITIONS
- PROCESS SUMMARY
- UPDATE STACK MODEL

RUN MODEL

POST PROCESSING

MAIN MENTAT

ALL: SELECT, VISIBLE, OUTLINE

EXIST: UNSEL, INVIS, SURFACE

SELECT SET END LIST (#)

RETURN FUEL CELL MAIN

MSC.Marc Mentat FUEL CELL DESIGN

DEFINE FLOW PARAMETERS

FUEL

Pressure (atm)	1.0	Composition (Molar %)	
Temperature (K)	915	H2	0.95
Film Coefficient ()	1345.05	H2O	0.05
Effective Viscosity ()	2.11319e-005	CO	0
Density ()	0.0224259	CO2	0
Thermal Conductivity ()	0.449992	CH4	0
Specific Heat ()	15156.2		

OXIDANT

Pressure (atm)	1.0	Composition (Molar %)	
Temperature (K)	915	O2	0.21
Film Coefficient ()	131.356	N2	0.79
Effective Viscosity ()	4.46448e-005		
Density ()	3.23574		
Thermal Conductivity ()	0.0692296		
Specific Heat ()	1117.88		

OK

** Flow input parameters calculated by default*

UNDO SAVE DRAW FILL RESET VIEW TX+ TY+ TZ+ RX+ RY+ RZ+ ZOOM IN SHORTCUTS

UTILS FILES PLOT VIEW DYN. MODEL TX- TY- TZ- RX- RY- RZ- BOX OUT HELP

Ready

```
Command > *py_file_run c:\msc_apps\mentat2003\bin\pnl\pnl_flowinp.py
*py_echo off
Error on receive... closing connection
Command > *colormap 2
Command >
```


Initial Boundary Conditions



MSC.Marc Mentat 2003 (32bit) (OpenGL)

FUEL CELL MAIN MENU

GEOMETRY SETUP

- NUMBER OF CELL STACKS: 1
- FUEL CELL DESIGN: Cross-Flow
- MODEL REFINEMENT: Coarse
- GEOMETRY SET UP
- BUILD 2D FOOTPRINT: SUMMARY
- BUILD 3D STACK GEOMETRY: SUMMARY

ANALYSIS SETUP

- IV RELATION: None
- EC OPERATION
- OHMIC POLARIZATION
- ACTIVATION POLARIZATION
- CONCENTRATION POLARIZATION
- FLOW INPUT
- BOUNDARY CONDITIONS
- PROCESS SUMMARY
- UPDATE STACK MODEL

RUN MODEL

POST PROCESSING

MAIN MENTAT

ALL: SELECT, VISIBLE, OUTLINE

EXIST. UNSEL, INVIS, SURFACE

SELECT SET, END LIST (#)

RETURN FUEL CELL MAIN

UNDO SAVE DRAW FILL RESET VIEW TX+ TY+ TZ+ RX+ RY+ RZ+ ZOOM BOX IN SHORTCUTS

UTILS FILES PLOT VIEW DYN. MODEL TX- TY- TZ- RX- RY- RZ- OUT HELP

Command > *py_file_run c:\msc_apps\mentat2003\bin\pn\pn_flowinp.py
 *py_echo off
 Error on receive... closing connection
 Command > *colormap 2
 Command > █

Ready

MSC.Marc Mentat FUEL CELL DESIGN

INPUT BOUNDARY CONDITIONS

UNITS: Temp [K], Flow [mol/sec]

THERMAL: Adiabatic

FLOW

- Fuel Flow Rate: 1
- Fuel Inlet Temp: 915
- Oxidant Flow Rate: 1
- Oxidant Inlet Temp: 915

INITIAL CONDITION

- Stack Initial Temp: 915

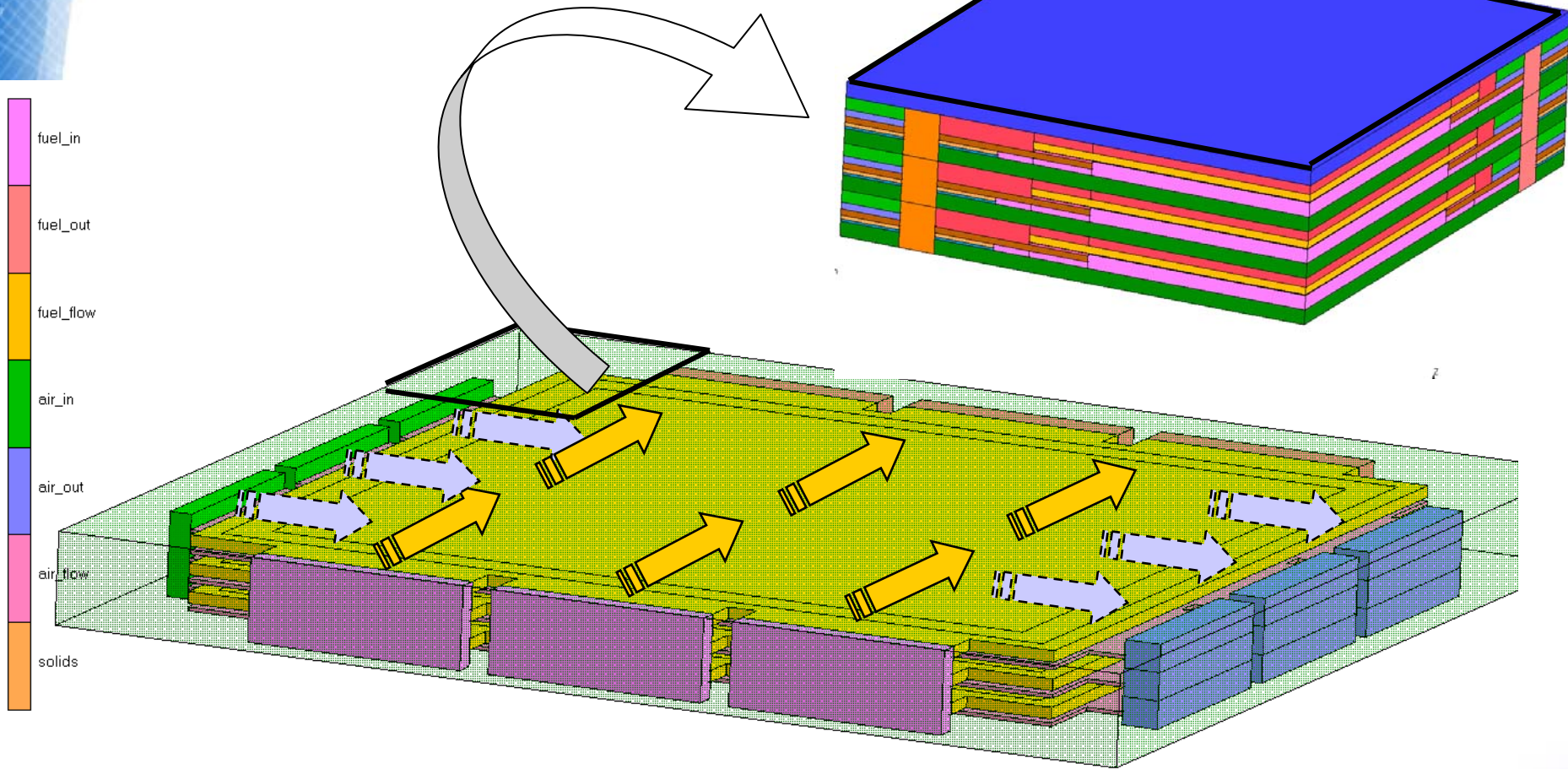
OK

Help Guide

Y

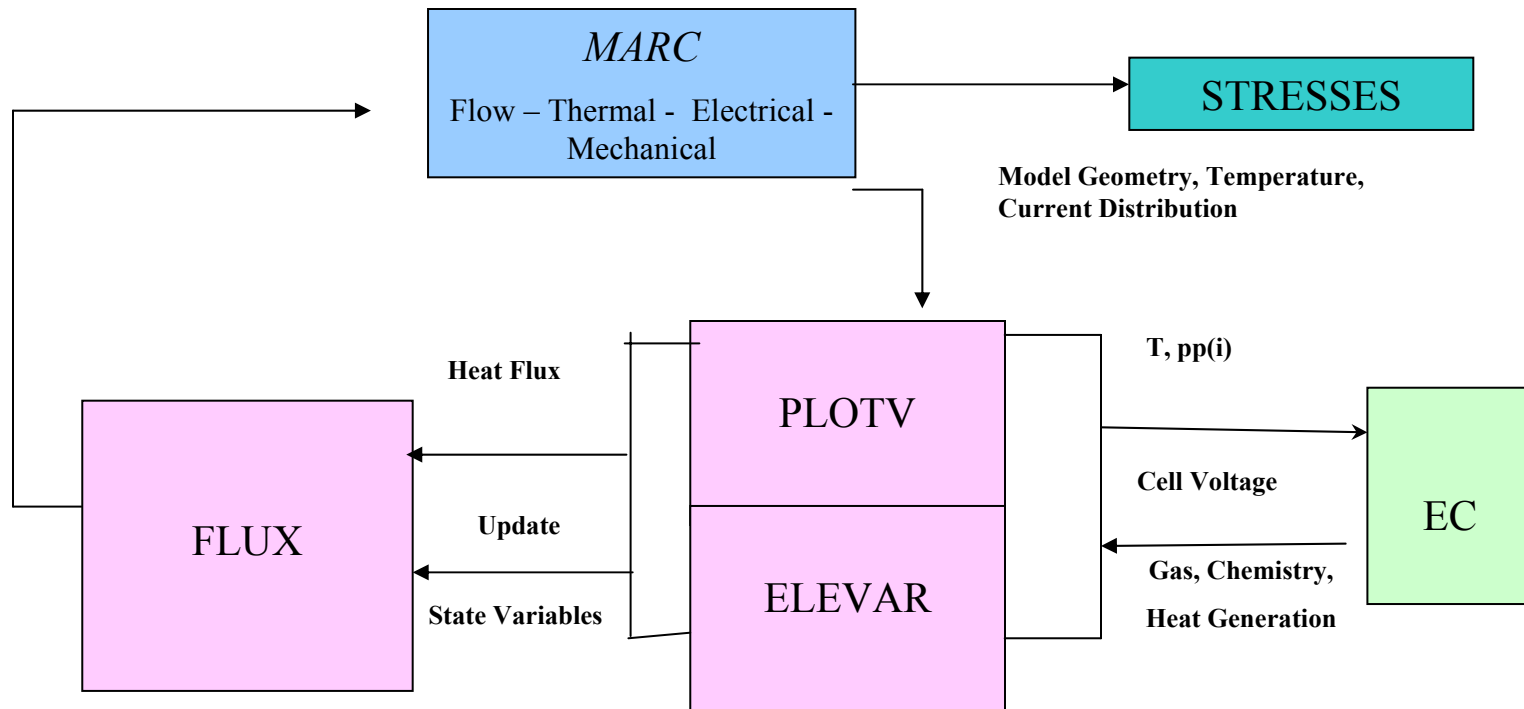
X

... Complete 3D Multiple Stack Cell Model



3 Cell Cross Flow Stack Model

...Ready to Run Transient Heat Transfer with Electrochemistry Solution...

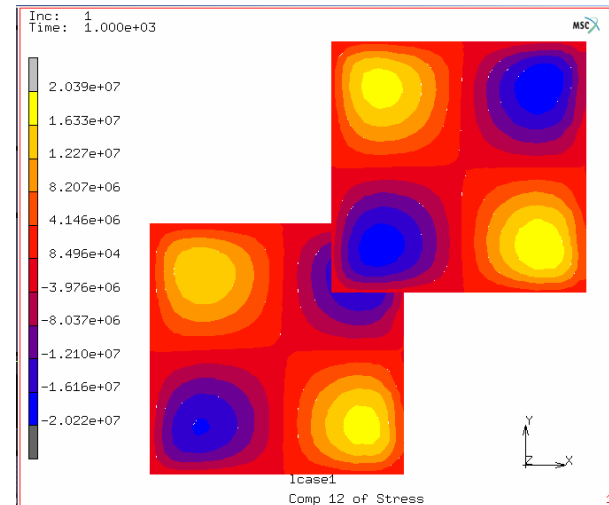
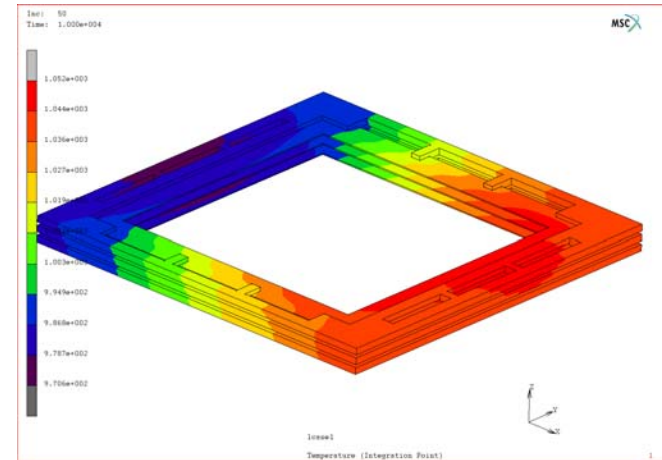


CPU Time:
1 Cell Model \cong 45 min.
(laptop computer)

Analysis Results...

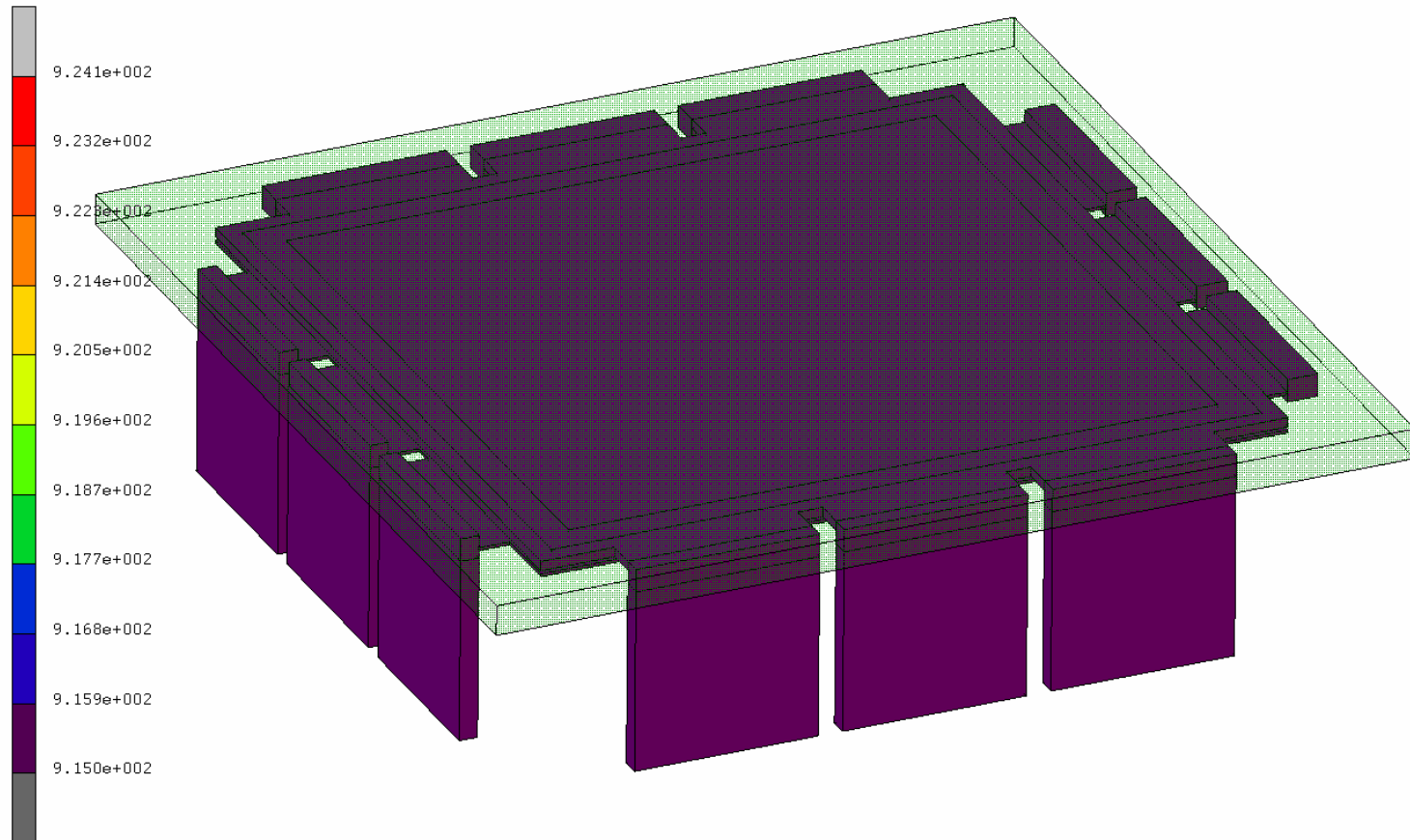
Fuel Cell Analysis Output

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



Temperature Distribution in PEN

Inc: 0
Time: 0.000e+000



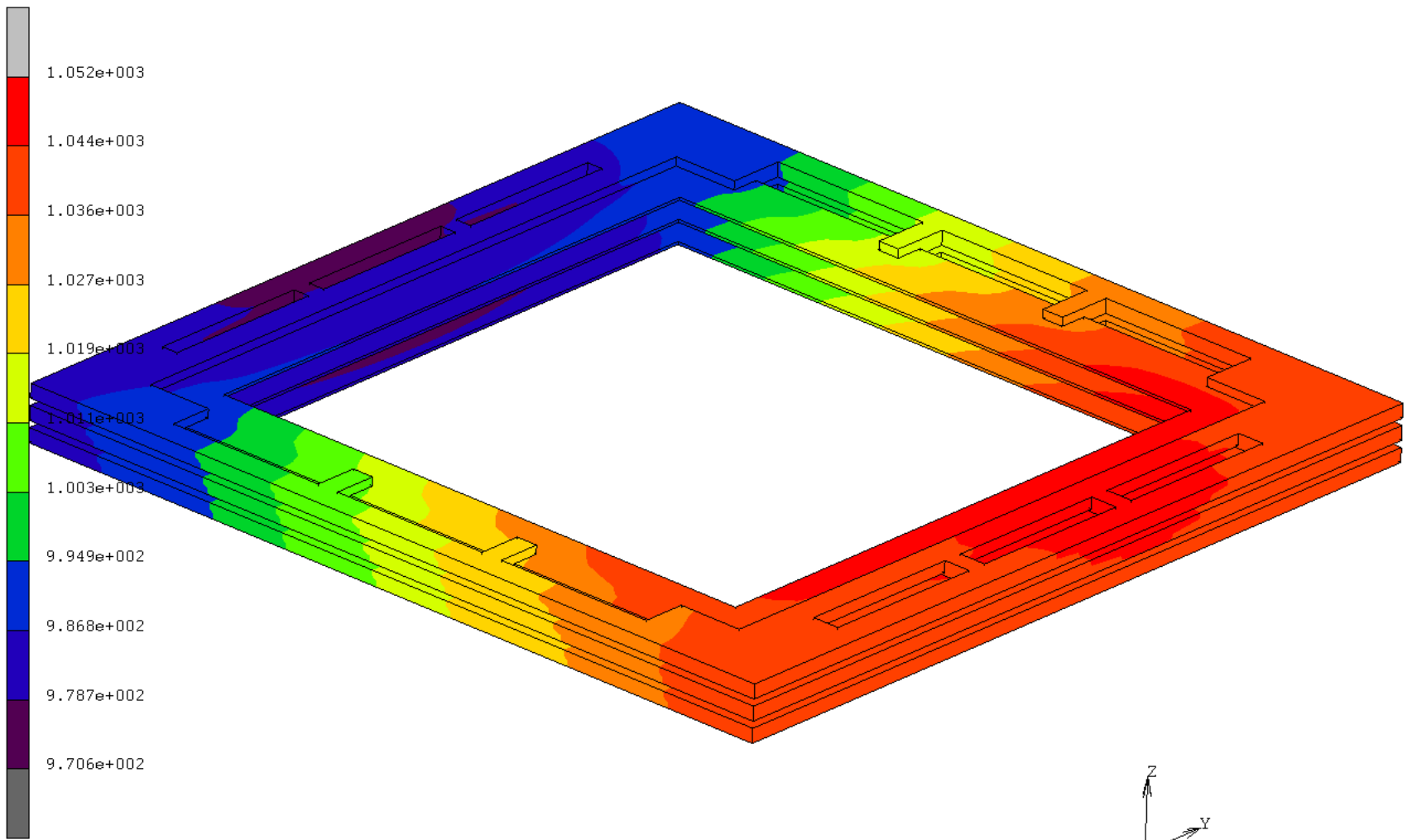
j1

Temperature (Integration Point)

1

Inc: 50
Time: 1.000e+004

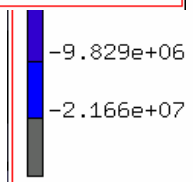
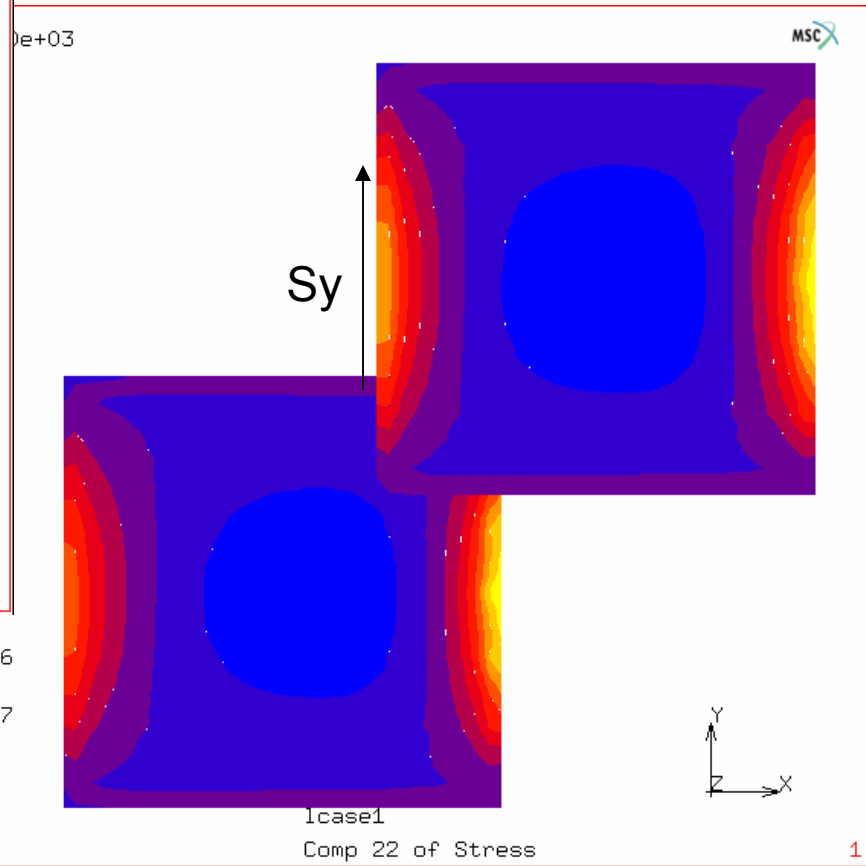
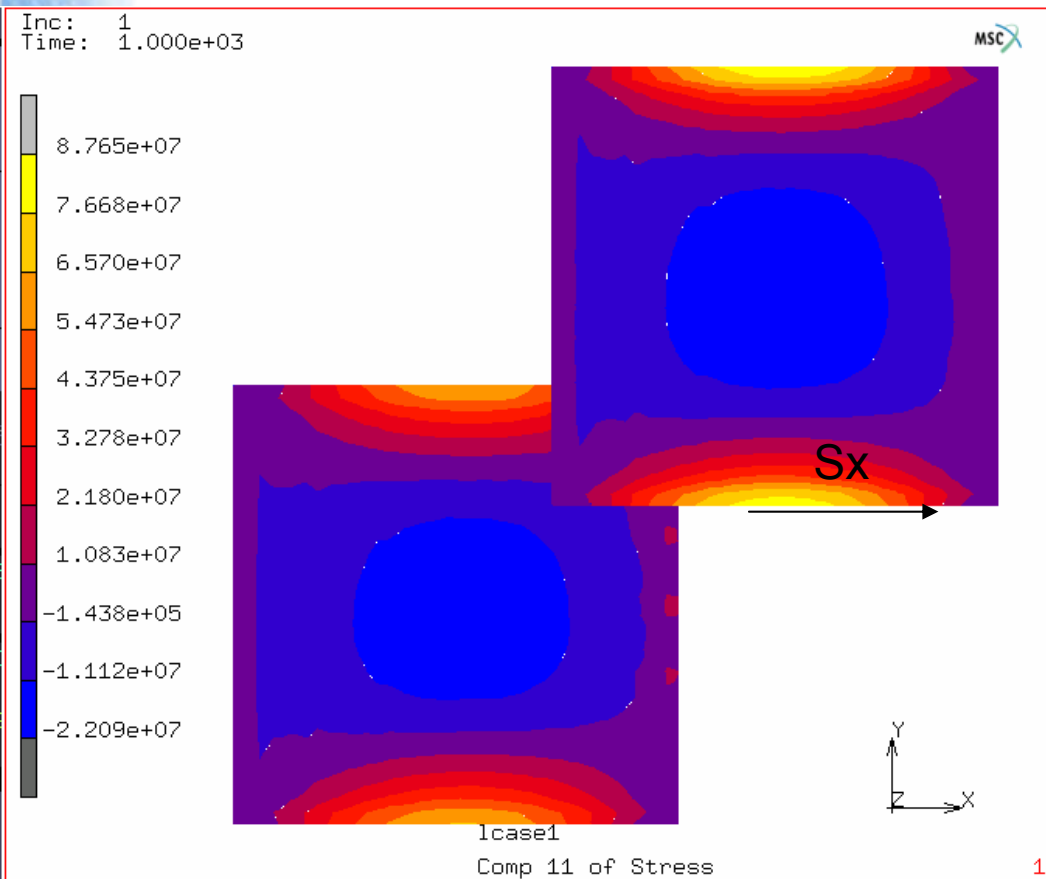
Temperature Distribution in Solids



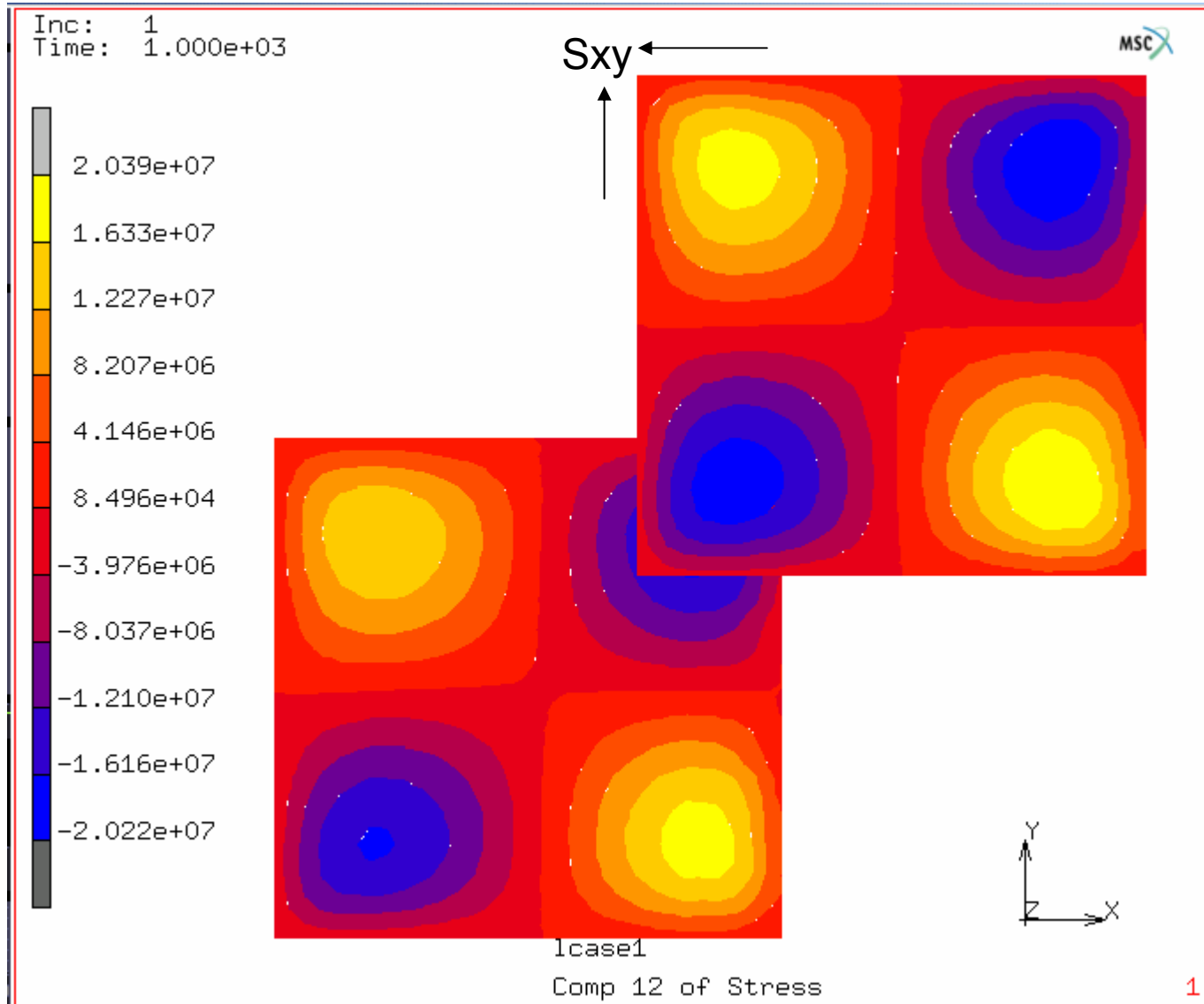
lcase1

Temperature (Integration Point)

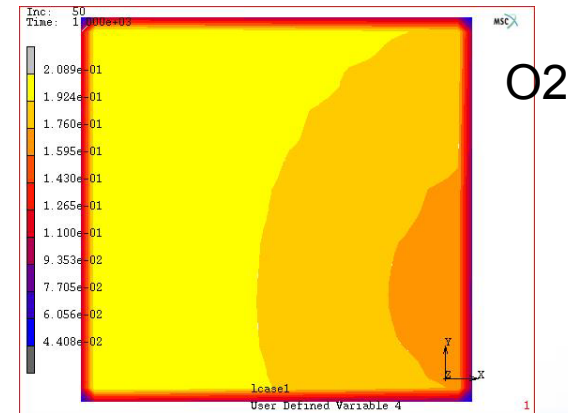
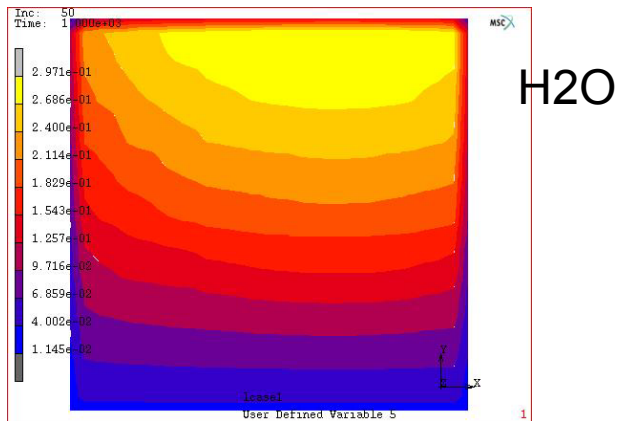
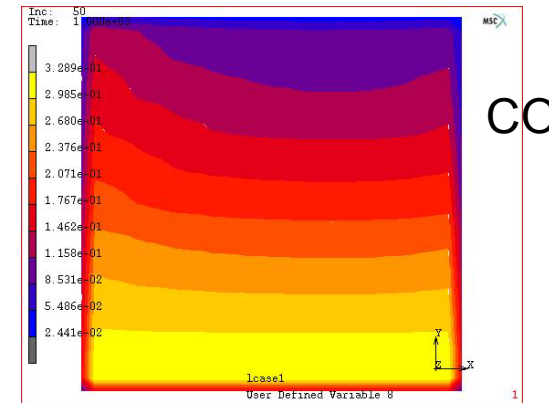
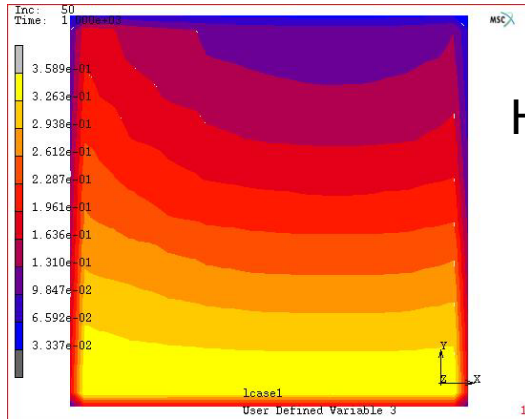
Stress in Electrolyte



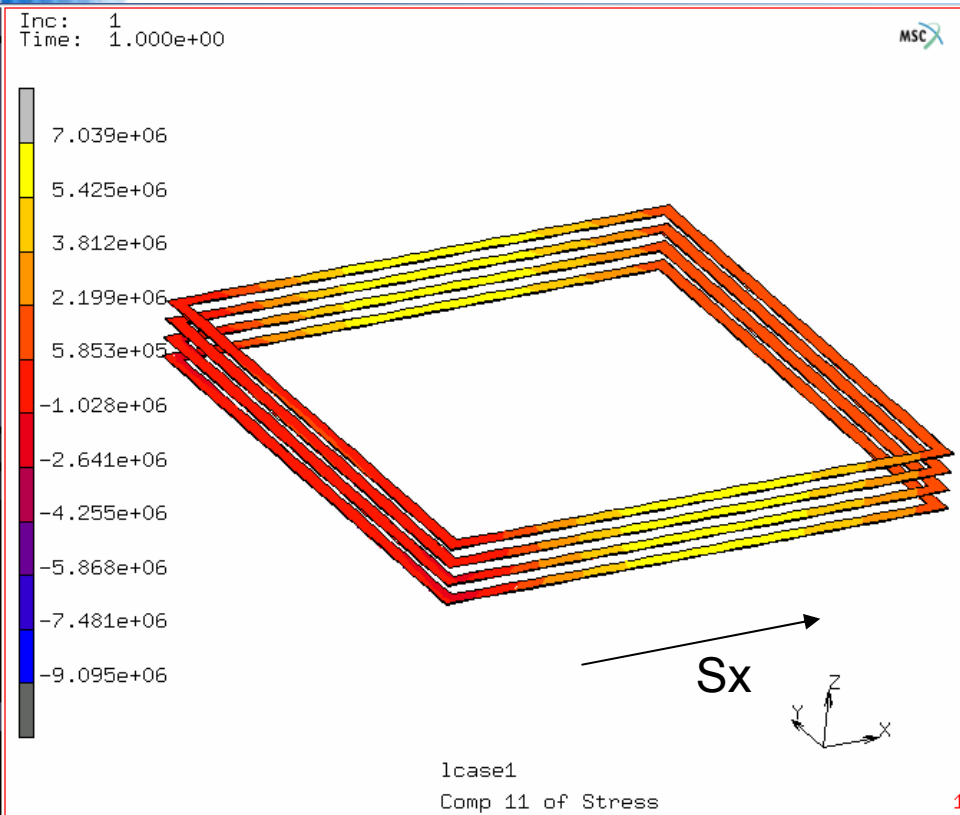
Shear stress in electrolyte



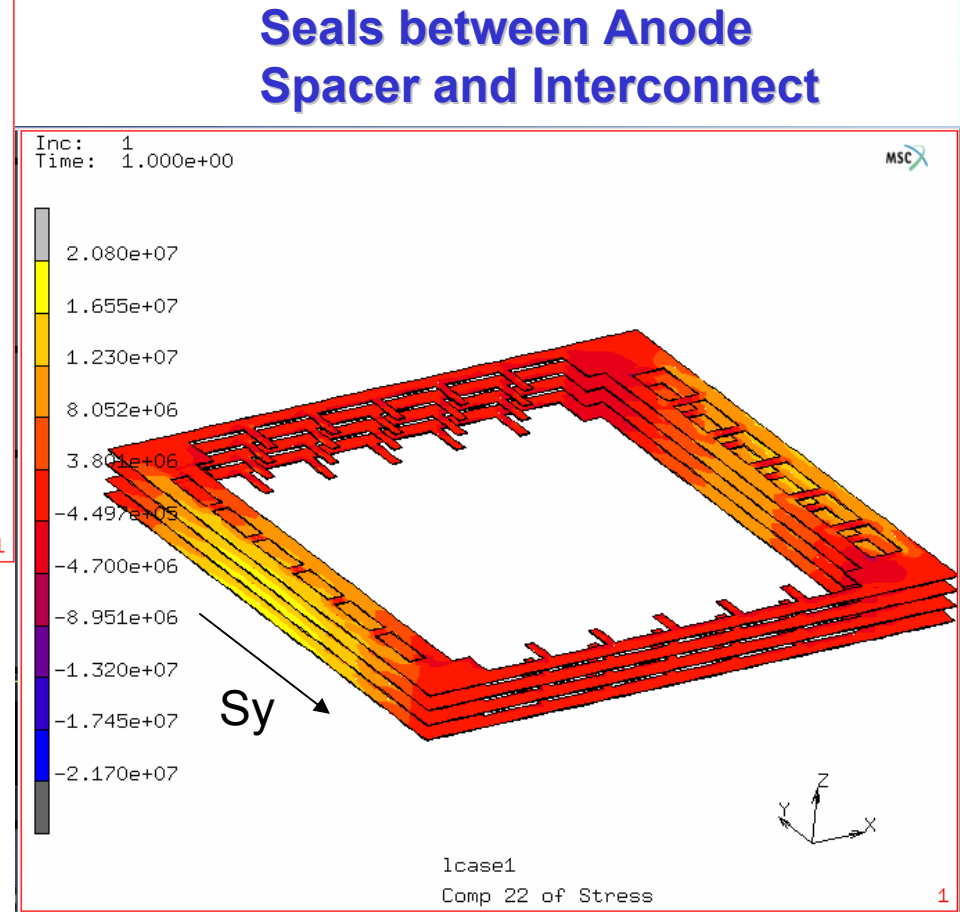
Species Concentration



Seal Stress



Seals between picture frame and cathode side of PEN



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

GASKET MATERIAL PROPERTIES

THROUGH-THICKNESS BEHAVIOR

YIELD PRESSURE	1e+020	TABLE
TENSILE MODULUS	0	TABLE
INITIAL GAP	0	TABLE
LOADING PATH	TABLE	
UNLOADING PATHS	TABLE 1	
	TABLE 2	
	TABLE 3	
	TABLE 4	
	TABLE 5	
	TABLE 6	
	TABLE 7	
	TABLE 8	
	TABLE 9	
	TABLE 10	

TRANSVERSE SHEAR BEHAVIOR

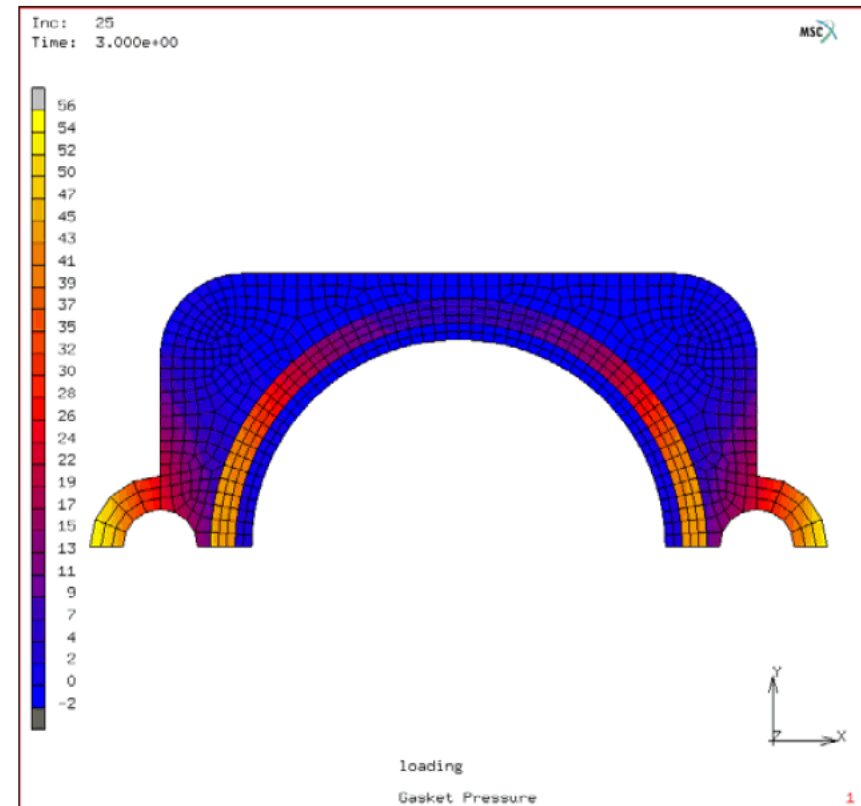
MODULUS	0	TABLE
---------	---	-------

MEMBRANE/HEAT TRANSFER BEHAVIOR

MATERIAL	
----------	--

RESET OK

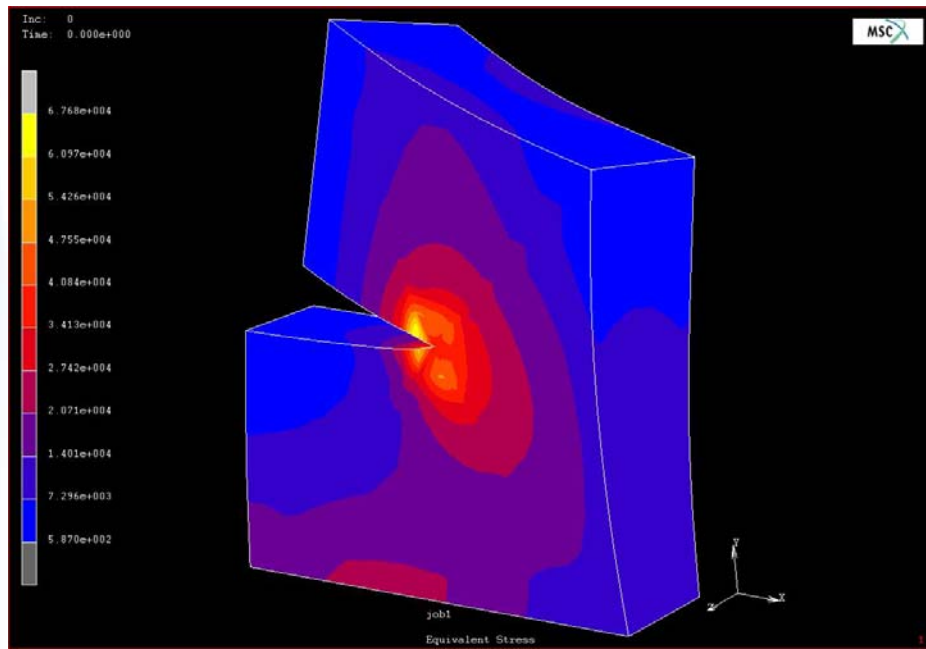
Models complex material behavior with single thickness layer



Can be used to model compression glass compression seals

Fracture Analysis

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



CRACKS (3-D)

NEW REM

NAME crack1

COPY PREV NEXT EDIT

RIGID REGION METHOD

◇ AUTOMATIC (TOPOLOGY SEARCH)
◆ AUTOMATIC (GEOMETRY SEARCH)
◇ MANUAL

RIGID REGIONS 1

1	RADIUS	0
	LENGTH	0.5
2	RADIUS	0
	LENGTH	0.5
3	RADIUS	0
	LENGTH	0.5

CRACK TIP NODE PATH

SET CLEAR

Global-Local Analysis

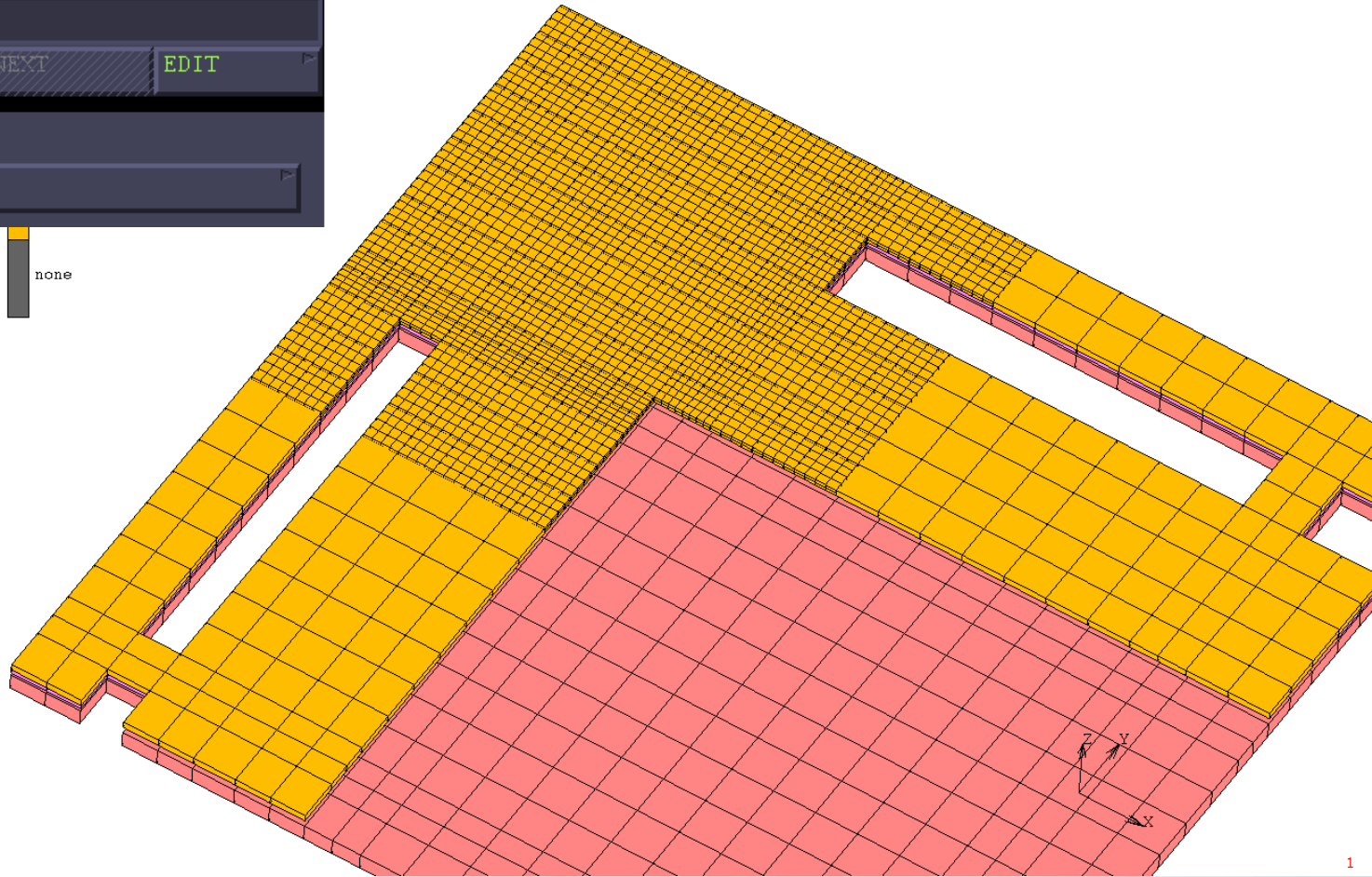


GENERAL BC's

NEW	REM	
NAME	apply10	
COPY	PREV	NEXT
EDIT		

BOUNDARY CONDITION TYPE

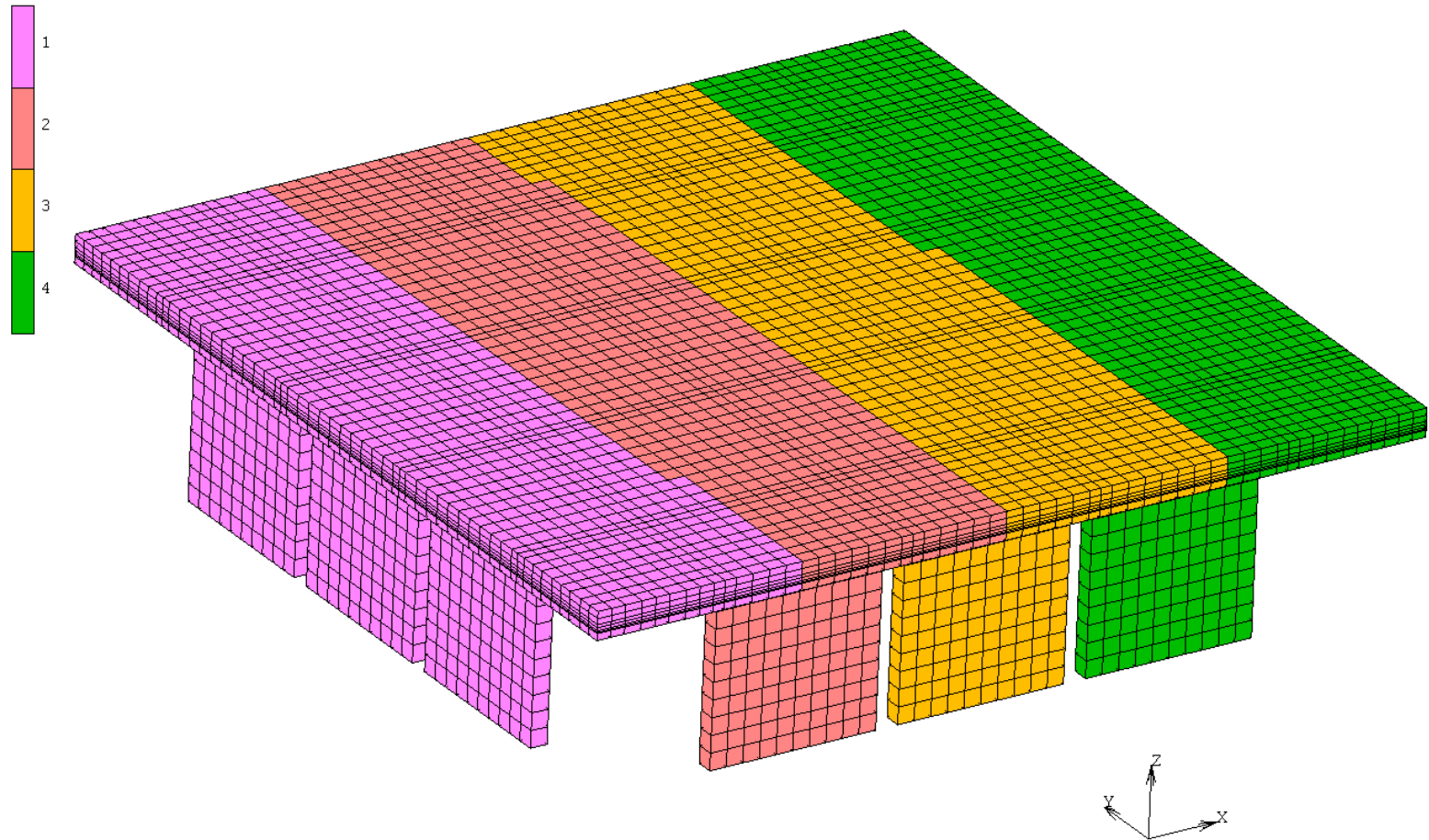
GLOBAL-LOCAL



none

Parallel Processing – DDM Method

MSC



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.

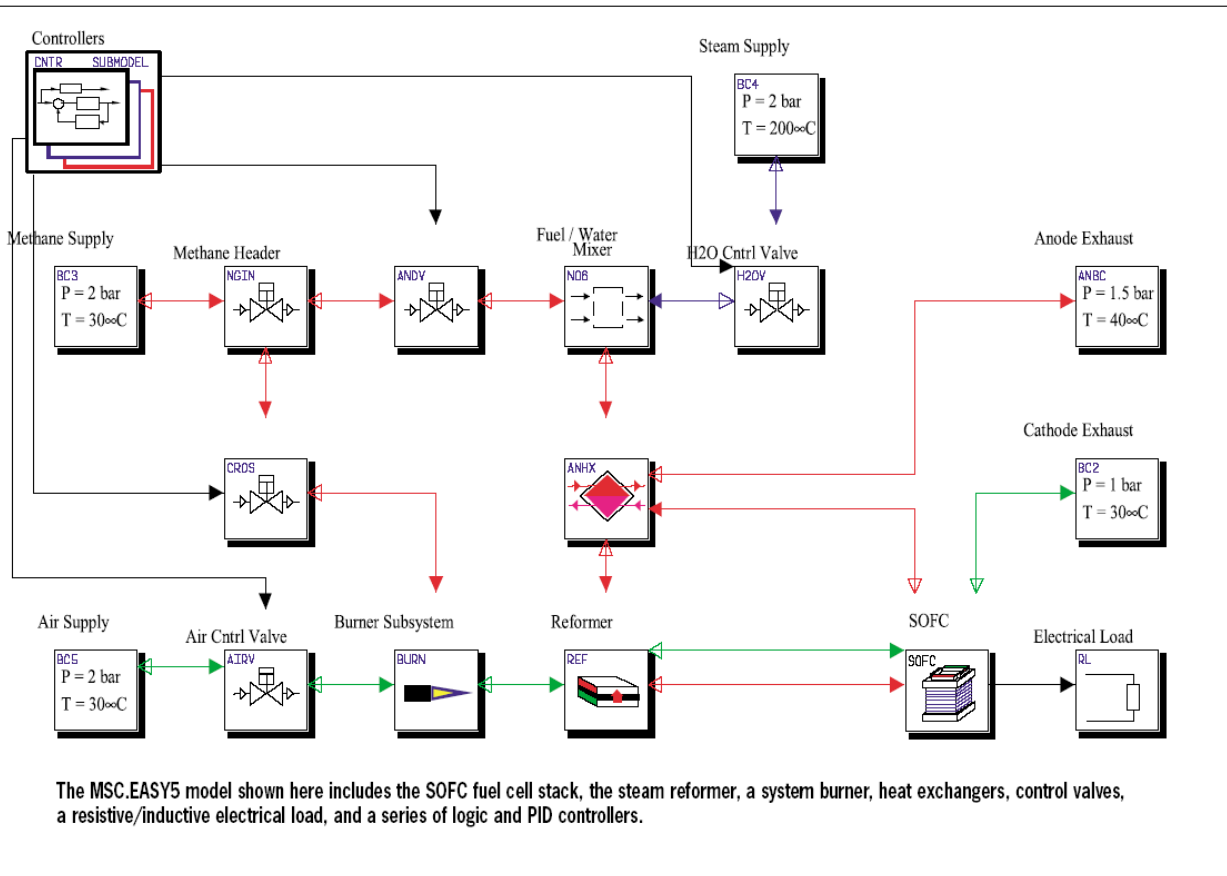
MSC.Easy 5 Simulation

- **Graphical Based Simulation Tool**

- **Open Architecture – links to many CAE software/hardware tools (Simulink, ADAMS, DADS...)**

- **User Defined Libraries**

- **Ricardo Fuel Cell Library**



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.

Thank You !

Please visit our booth for more information



**Pacific Northwest
National Laboratory**

MSC SOFTWARE.
SIMULATING REALITY

MSC SOFTWARE.
SIMULATING REALITY

Multi-Physical Analysis with MSC

May 2004

Analysis Capabilities

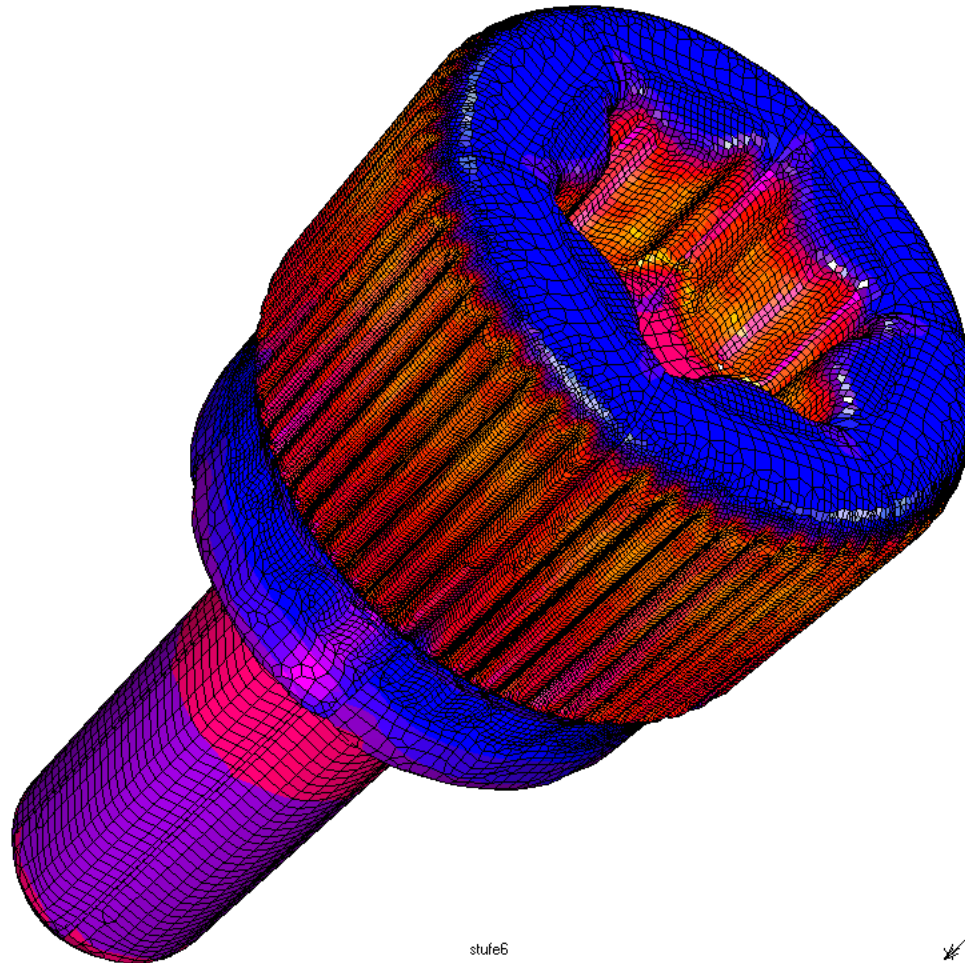
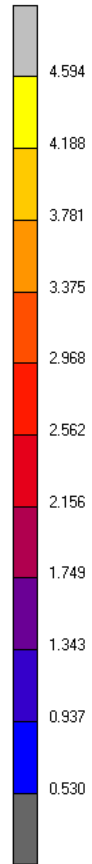
- **Structural (Nastran, Marc, Dytran)**
- **Thermal (Nastran, Marc, Thermal)**
- **Pore-Pressure (Marc)**
- **Hydrodynamic bearing (Marc)**
- **Fluids (Nastran (added mass), Marc, Dytran)**
- **Acoustics (Nastran, Marc)**
- **Electrostatics (Marc)**
- **Magnetostatics (Marc)**
- **Electro-magnetics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

Marc Multi-Physics

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

Thermal – Mechanical Manufacturing

Inc: 505
Time: 6.325e-001
Angle: 3.600e+002



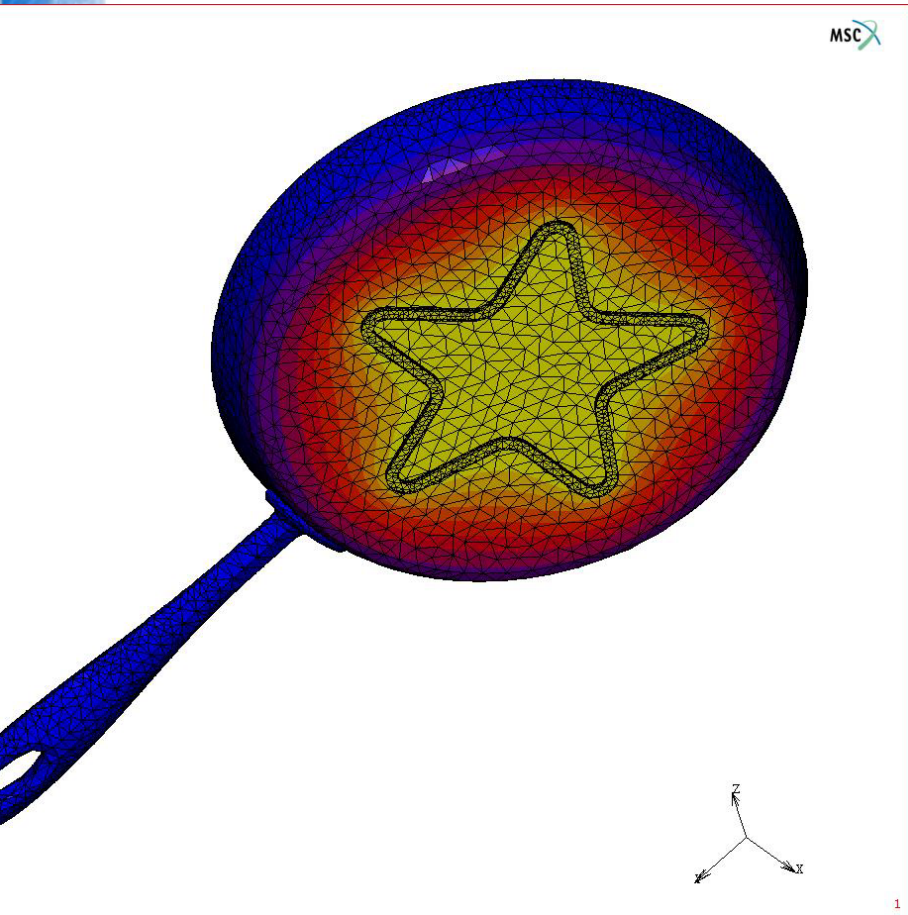
stuf6

Total Equivalent Plastic Strain

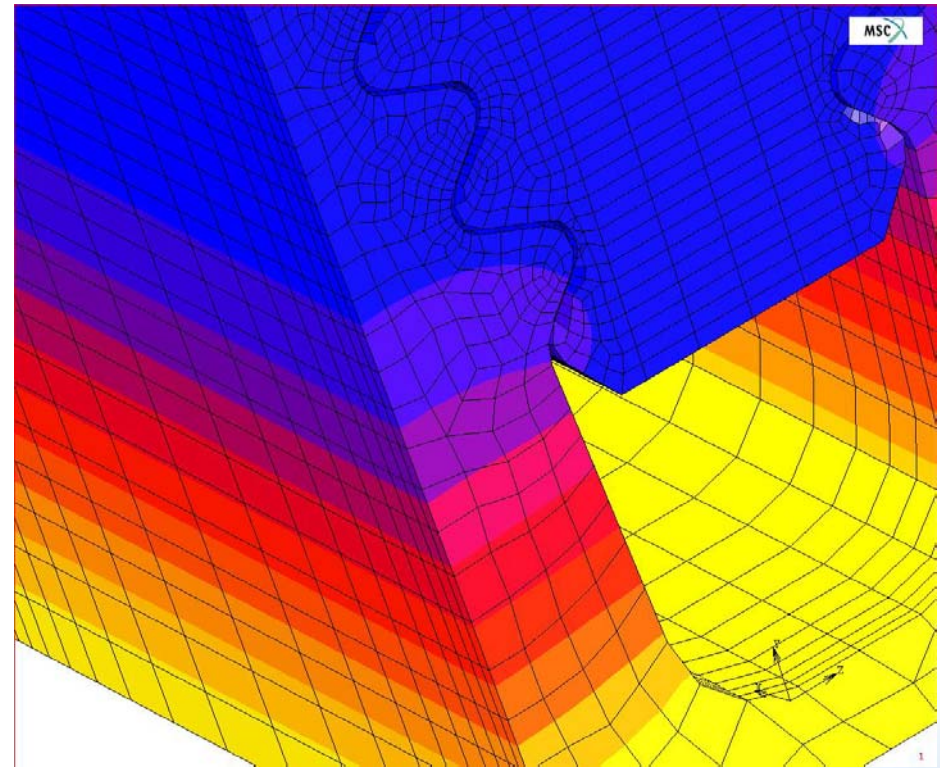


Thermal Contact Examples

Catia Assembly



Fir tree

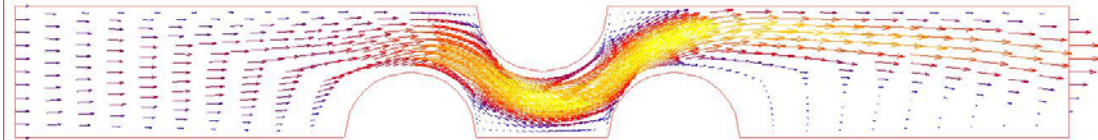


Fluid Capabilities

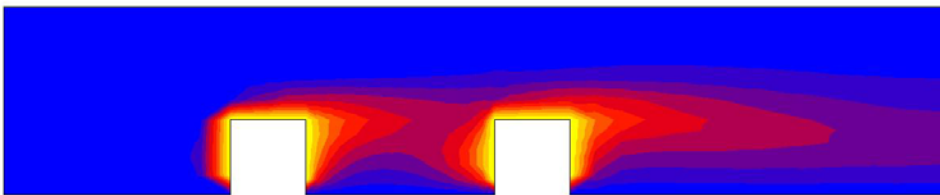
- **2-D, Axisymmetric , 3-D**
- **Navier Stokes**
- **Newtonian and Non-Newtonian Fluid**
- **Coupled Thermal-Fluid Capabilities**
- **Coupled Fluid-Structural**

Fluid Capabilities

MSC



MSC

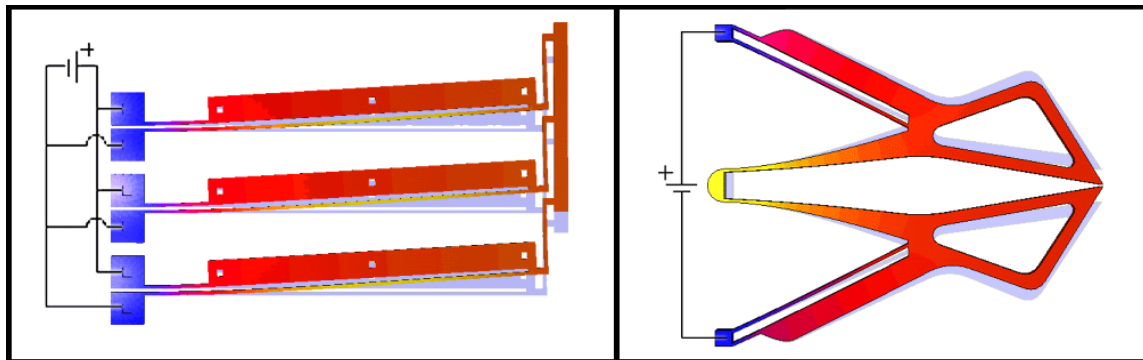


Velocity of Fluid in
Heat Exchanger

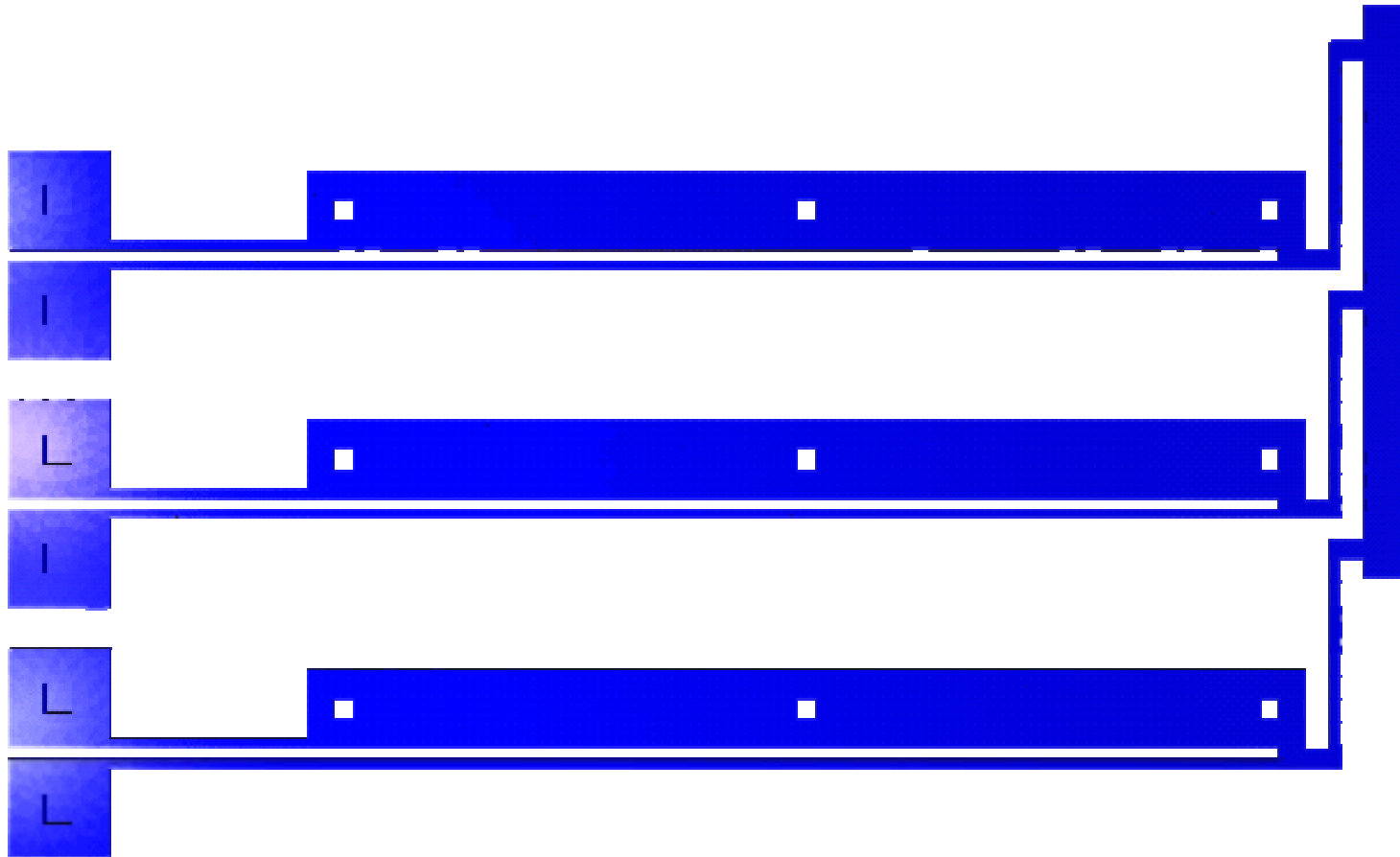
Temperature in Flow Over Chips

Coupled Electrical-Thermal-Mechanical Analysis

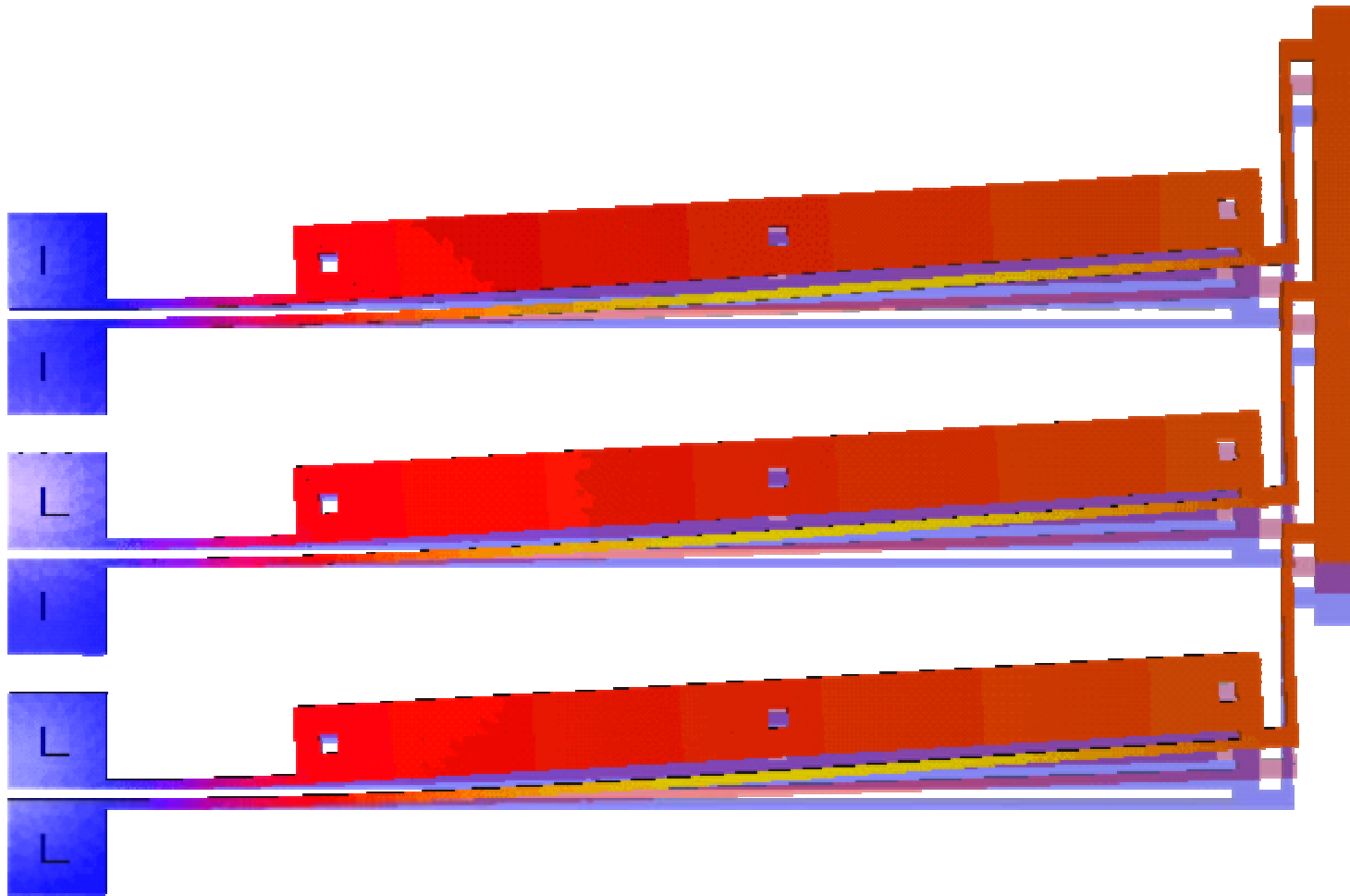
- **Multi-physics functionality couples electrical, thermal and mechanical behavior**
- **Applications:**
 - **MEMS actuators, high voltage switches and electronic circuits.**



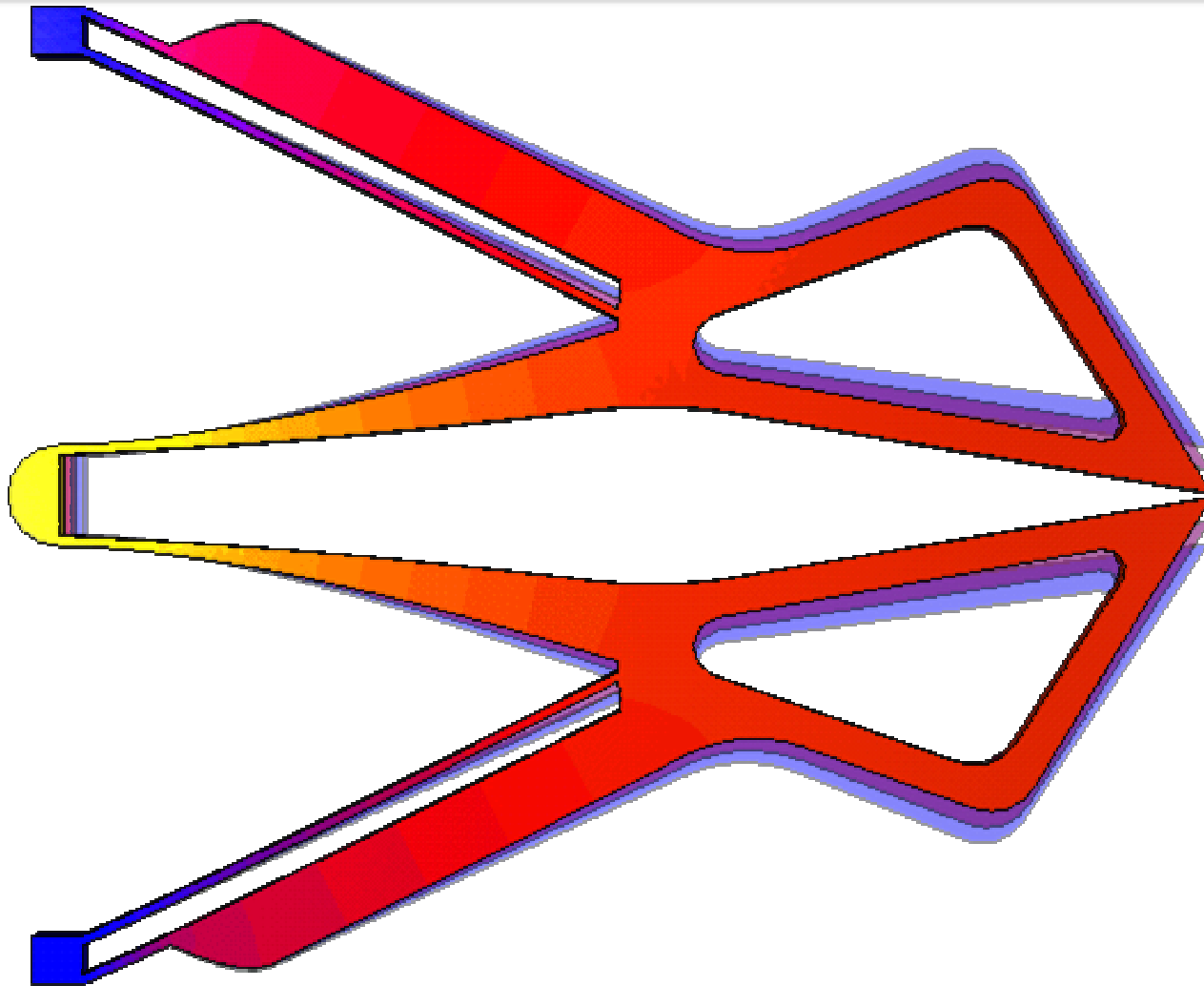
MEMS Micro-actuator



MEMS Micro-actuator

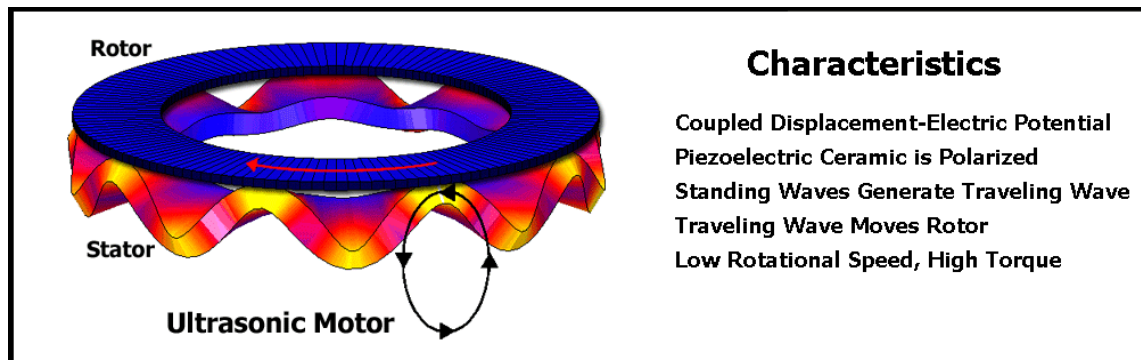


MEMS Micro-gripper



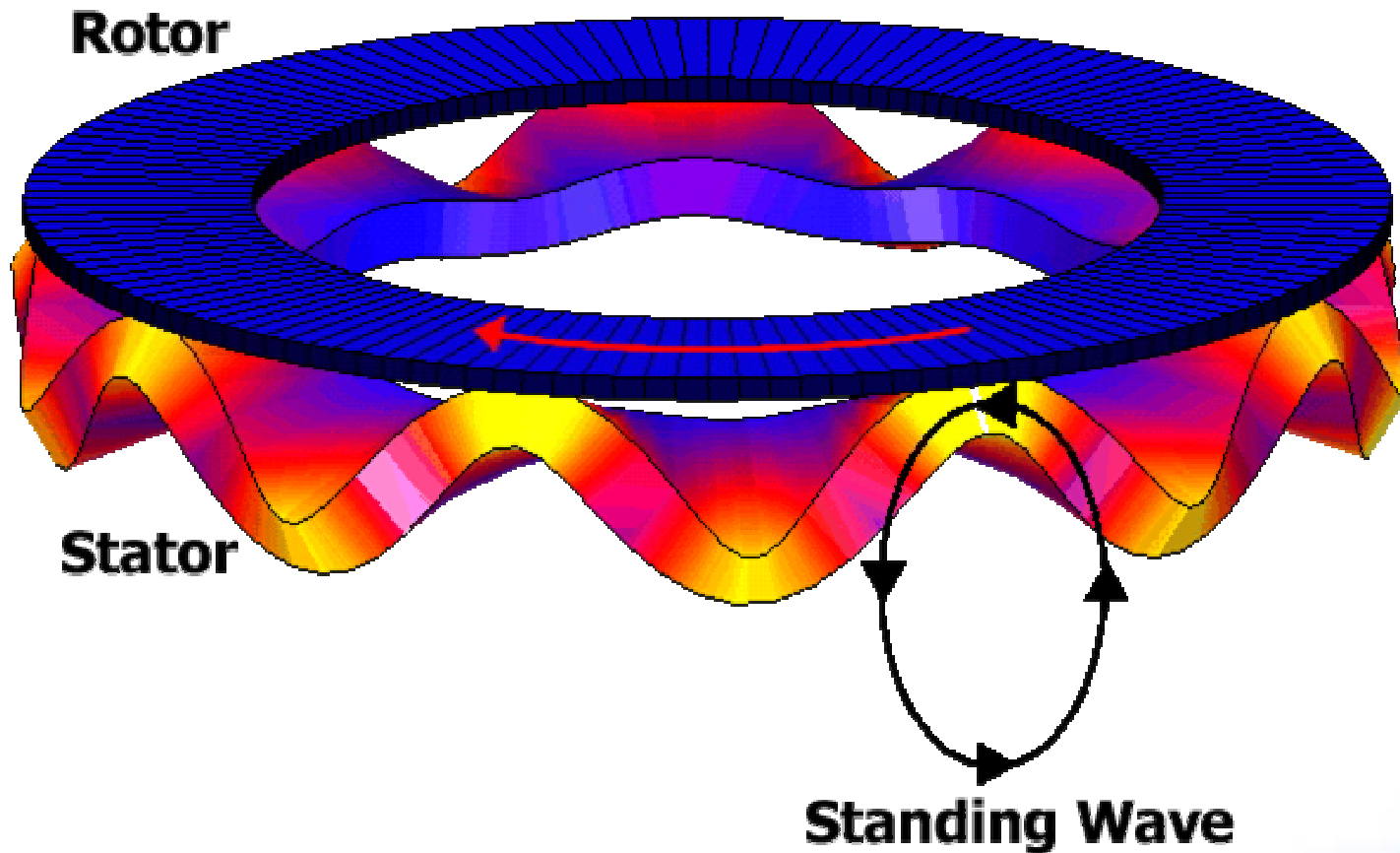
Piezoelectric Analysis

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



Ultrasonic Motor Transient

Simulation Ultrasonic Motor



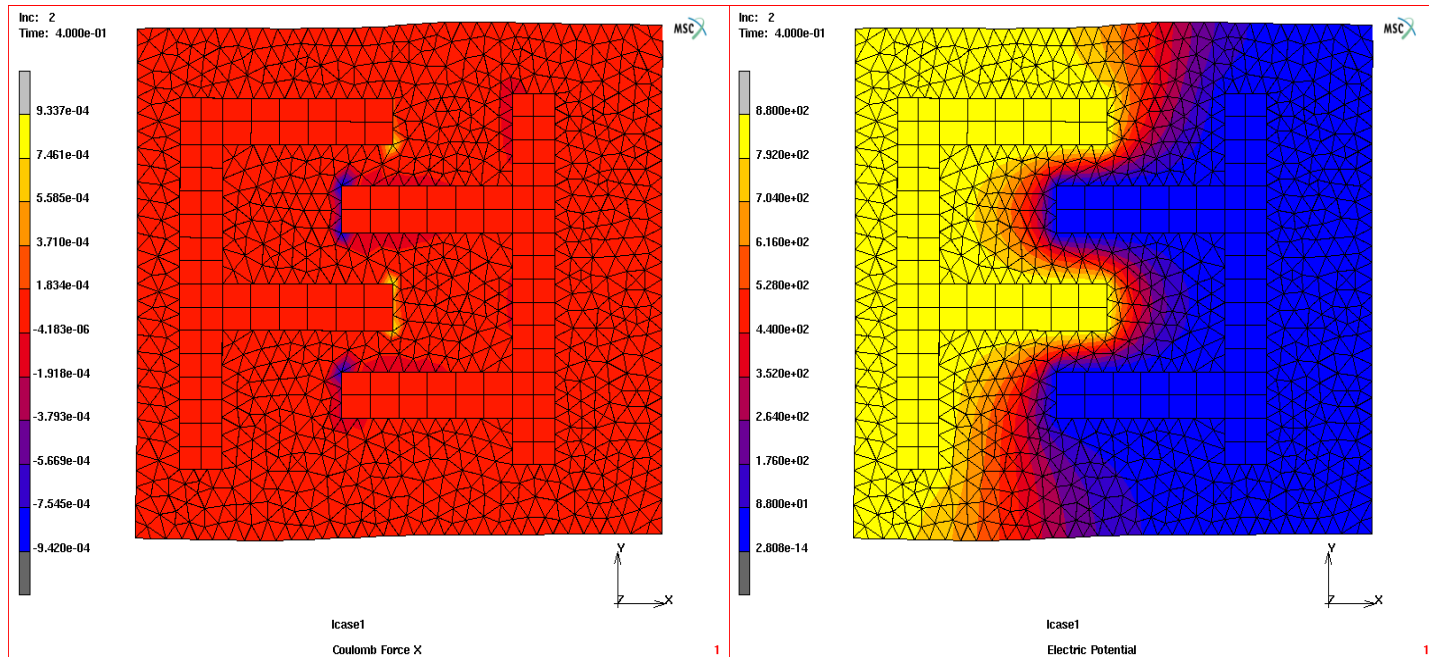
Marc 2005 Multi-Physics

- **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**

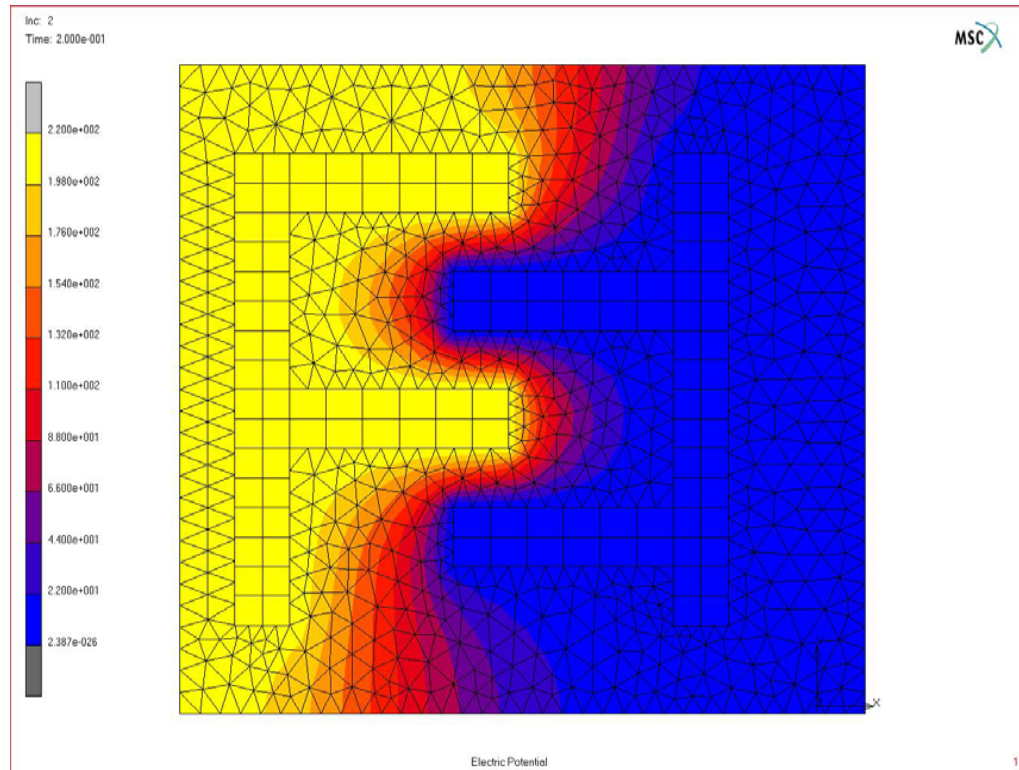
Coupled Electrostatic-Structural



Coulomb Force

Electrical Potential

Coupled Electrostatic-Structural



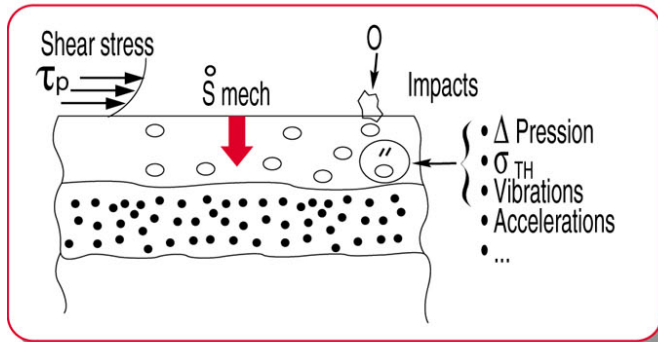
**Finite Element Mesh of the Air is Remeshed Automatically
During the Analysis**

Multi-Physics and Thermal

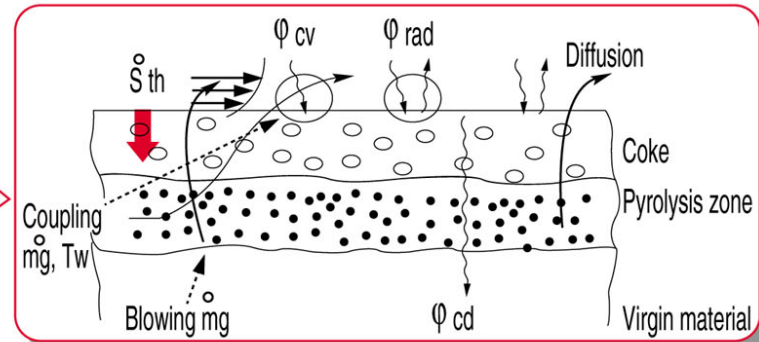
- **Advanced Thermal Analysis**
 - **Radiation**
 - **Pyrolysis**
 - **Ablation**

Physics overview

MECHANICAL ASPECTS



THERMAL ASPECTS

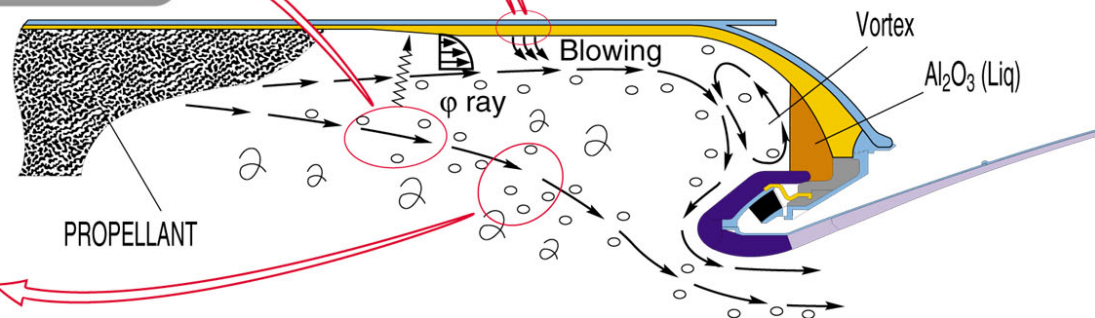


RADIATIVE HEAT TRANSFER

- Emitting / diffusing medium
- H_2O, CO_2, CO, HCl , particles
- Flow / radiation coupling

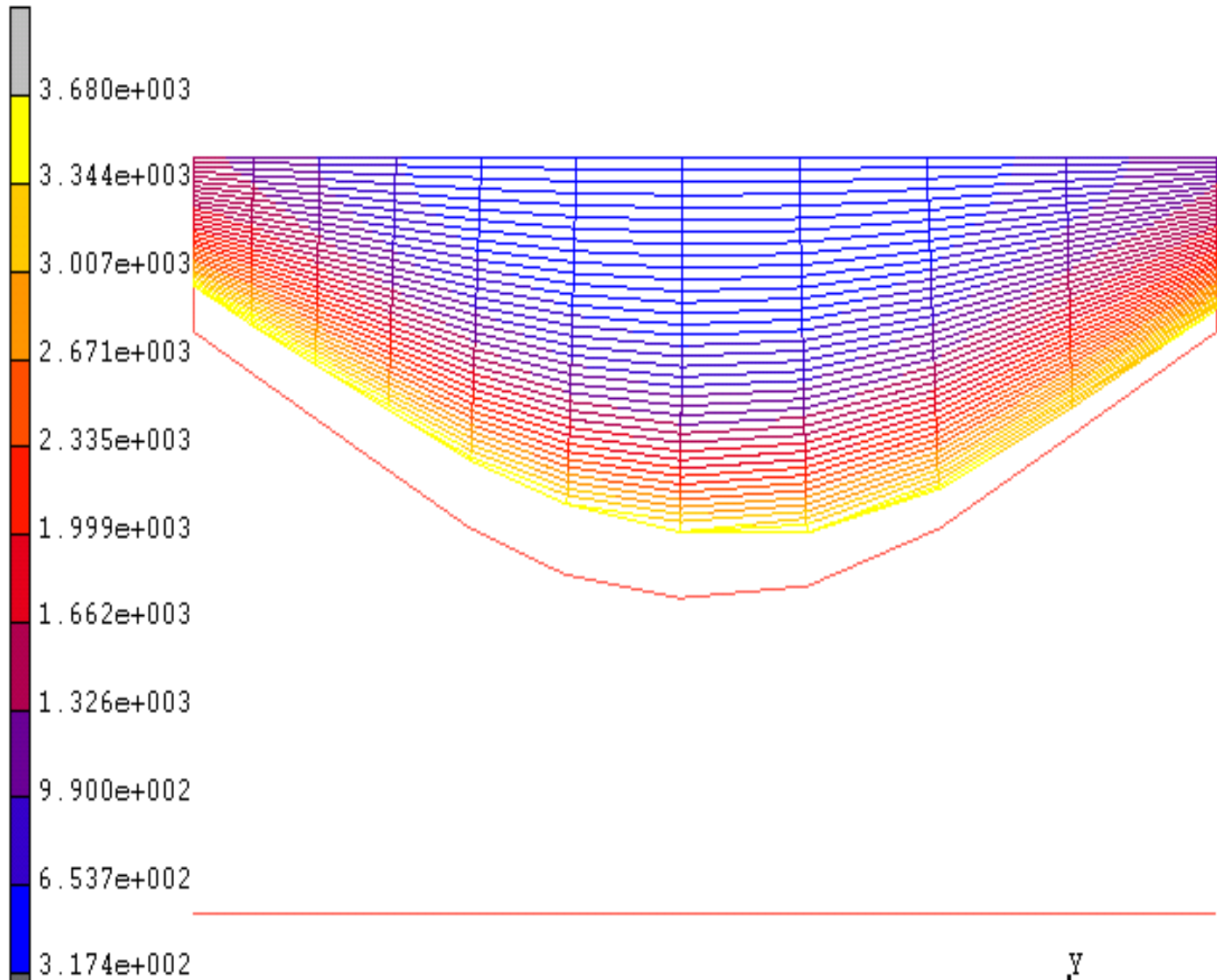
FLOW

- 3D \Rightarrow 2D
- Two-phase
- Multicomponent
- Turbulent
- Reactive



Ablation

Inc: 2000
Time: 2.000e+001



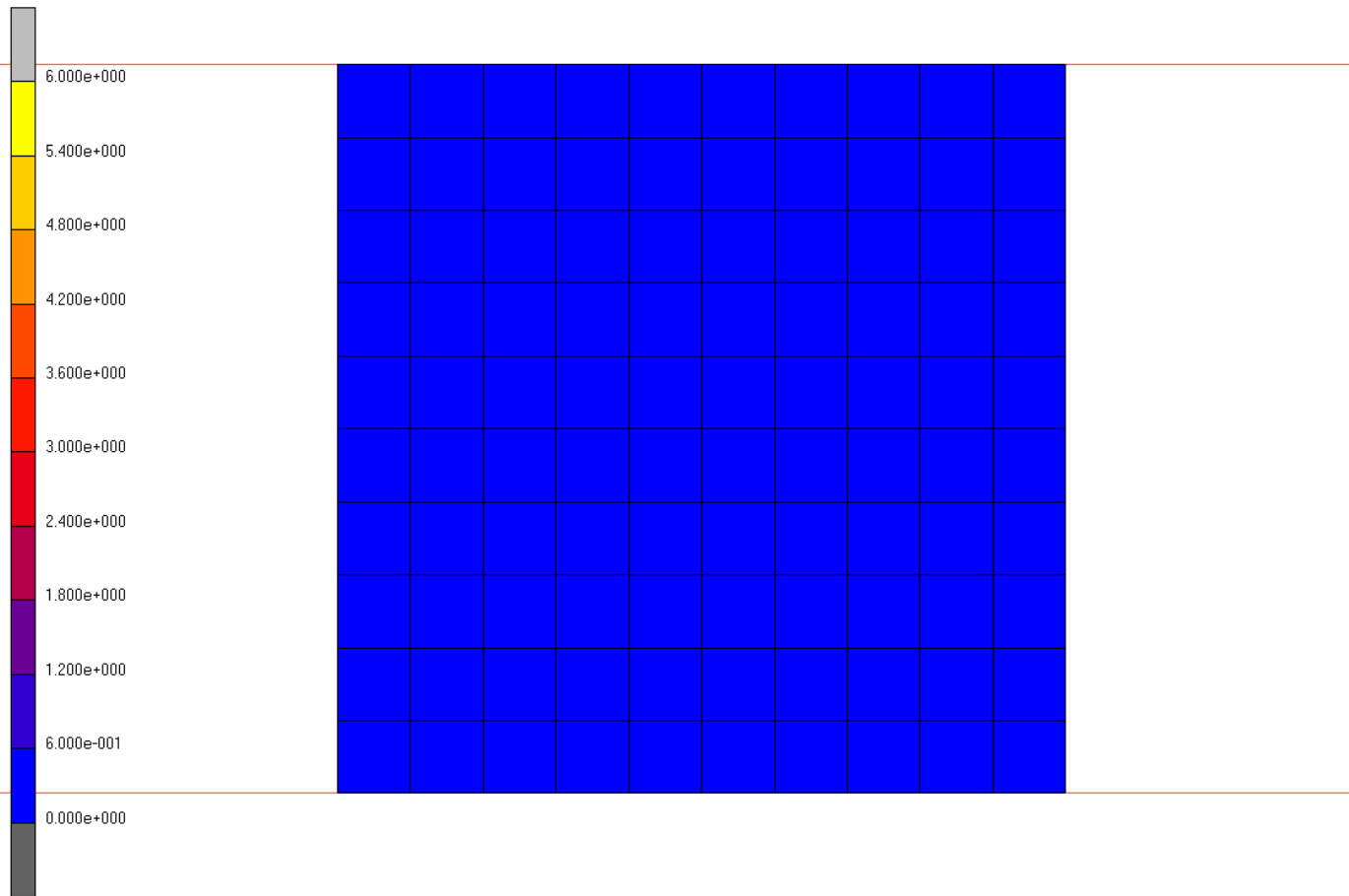
Fracture Mechanics

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

Crack Mesh Insertion



Inc: 0
Time: 0.000e+000



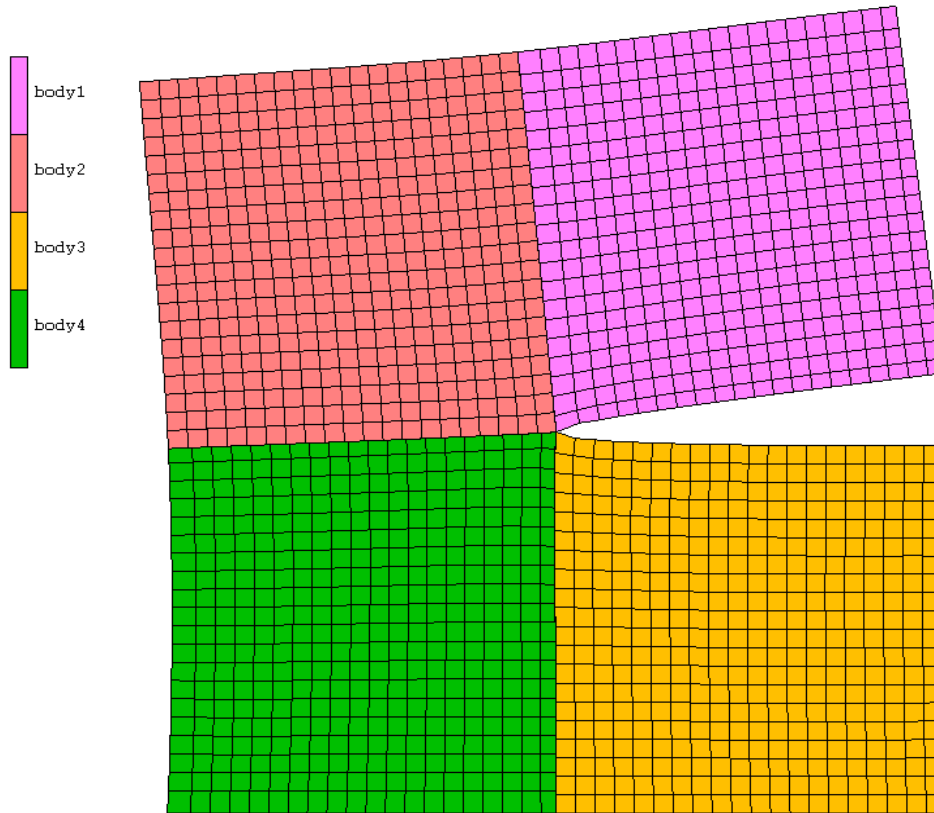
adaptive meshing for fracture mechanics

Equivalent Von Mises Stress

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

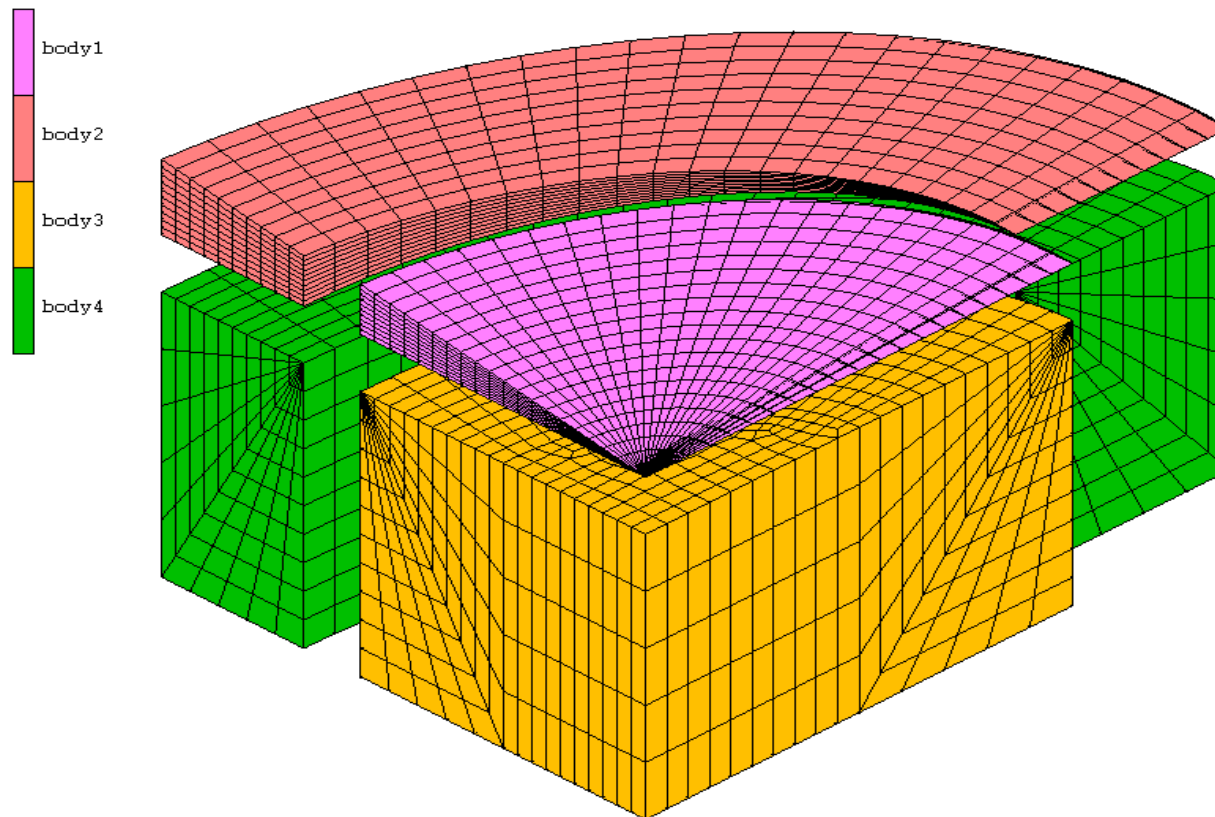


Meshing Flexibility

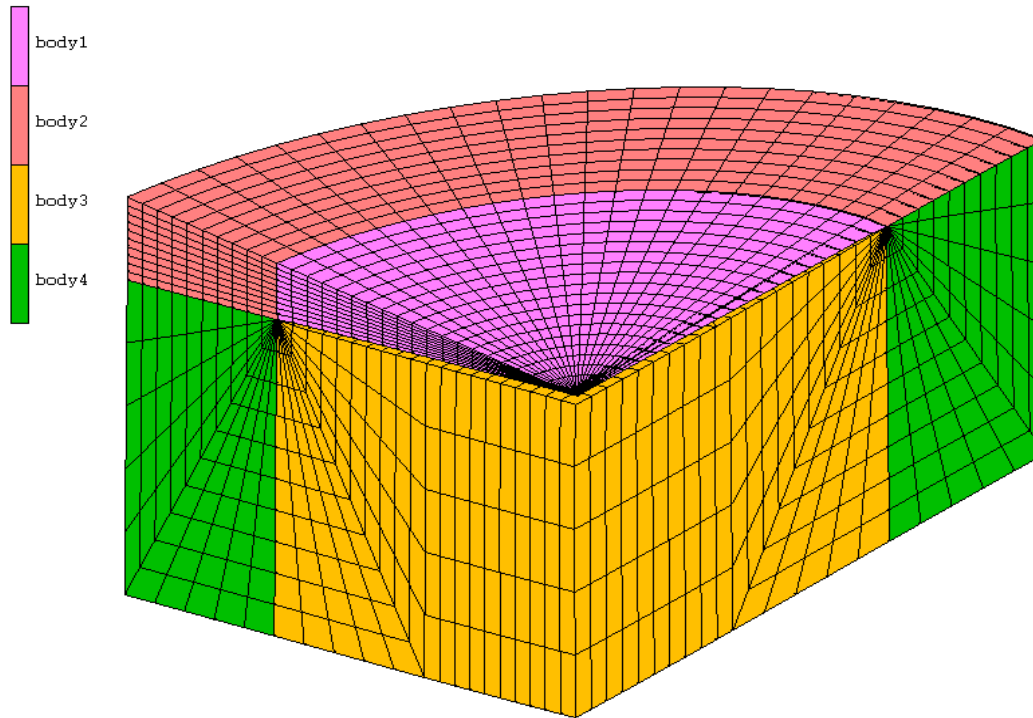
- **Nice Hexahedral Meshes in vicinity of crack tip**
- **Glue Meshes near crack tip**
- **Glue Cracking Region in Far-Field with Tetrahedral Mesh**

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



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

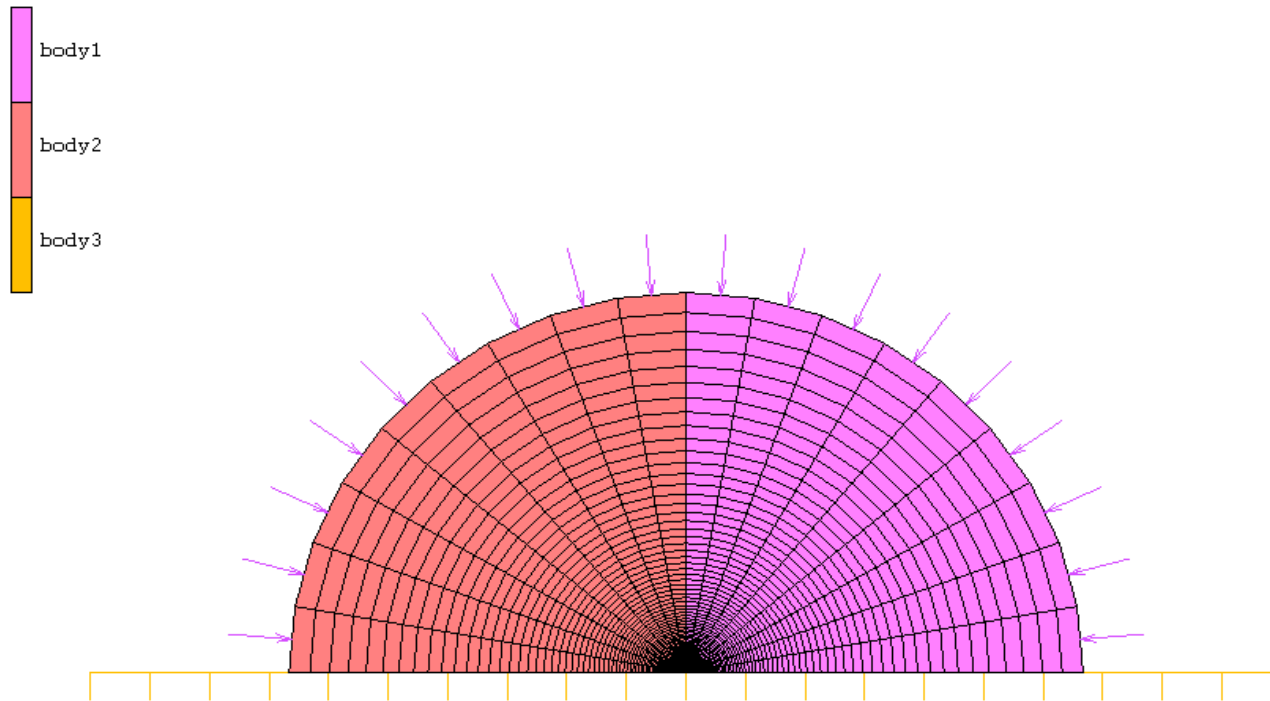
Domain#	1	2	3	4	5	6	7	8
No-Glue	0.21377	0.21792	0.21872	0.21893	0.21904	0.21908	0.21911	0.21912
Glue	0.21498	0.21977	0.21914	0.21962	0.21925	0.21941	0.21916	0.21924

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

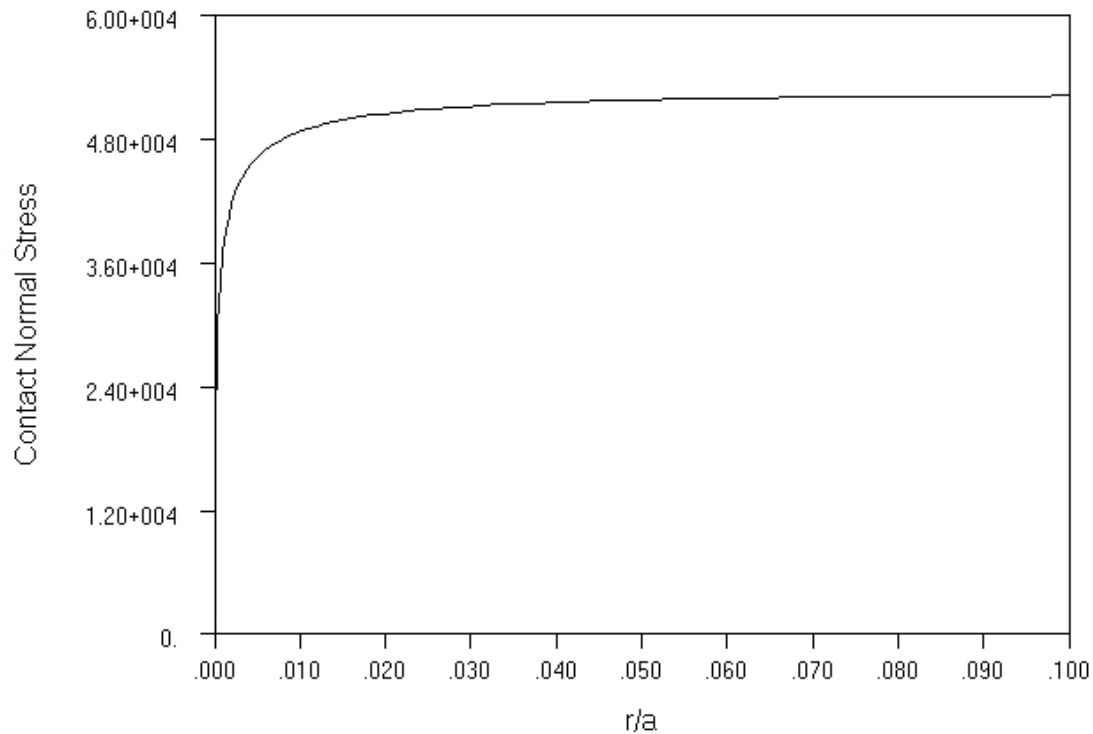
Domain#	1	2	3	4	5	6	7	8
Node 1	11.591	11.713	11.453	10.313	10.294	10.278	10.270	10.279
Node 2	11.262	11.351	11.371	11.354	11.358	11.359	11.362	11.371

Concentric Load Driving Closure and Friction

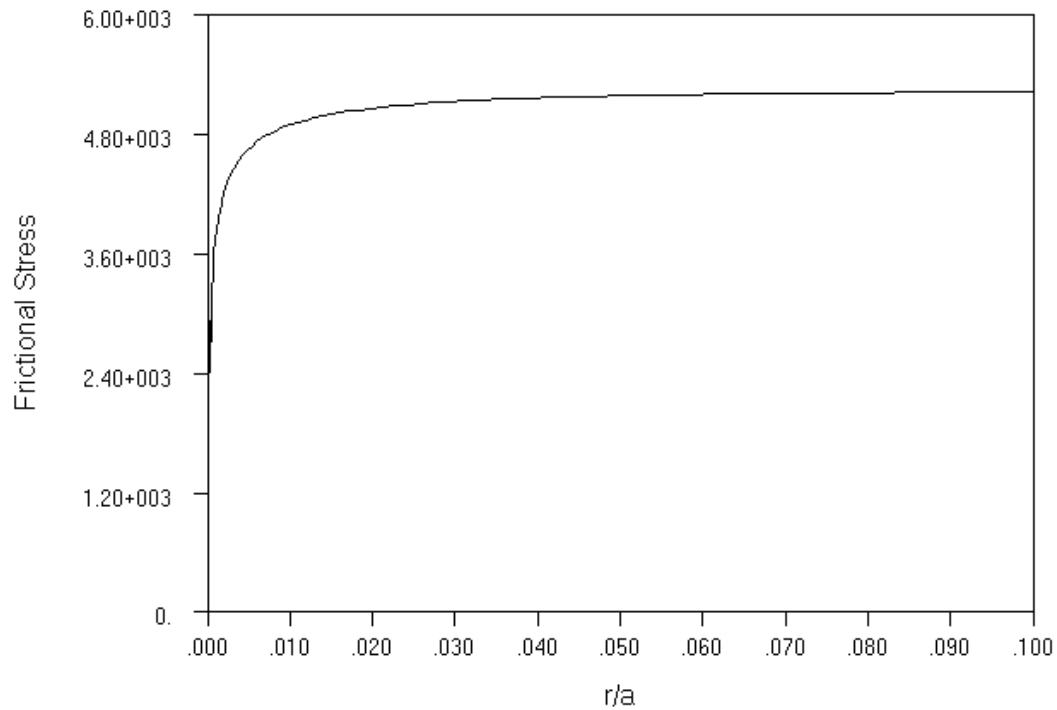
MSC



Normal Stress on Crack Face

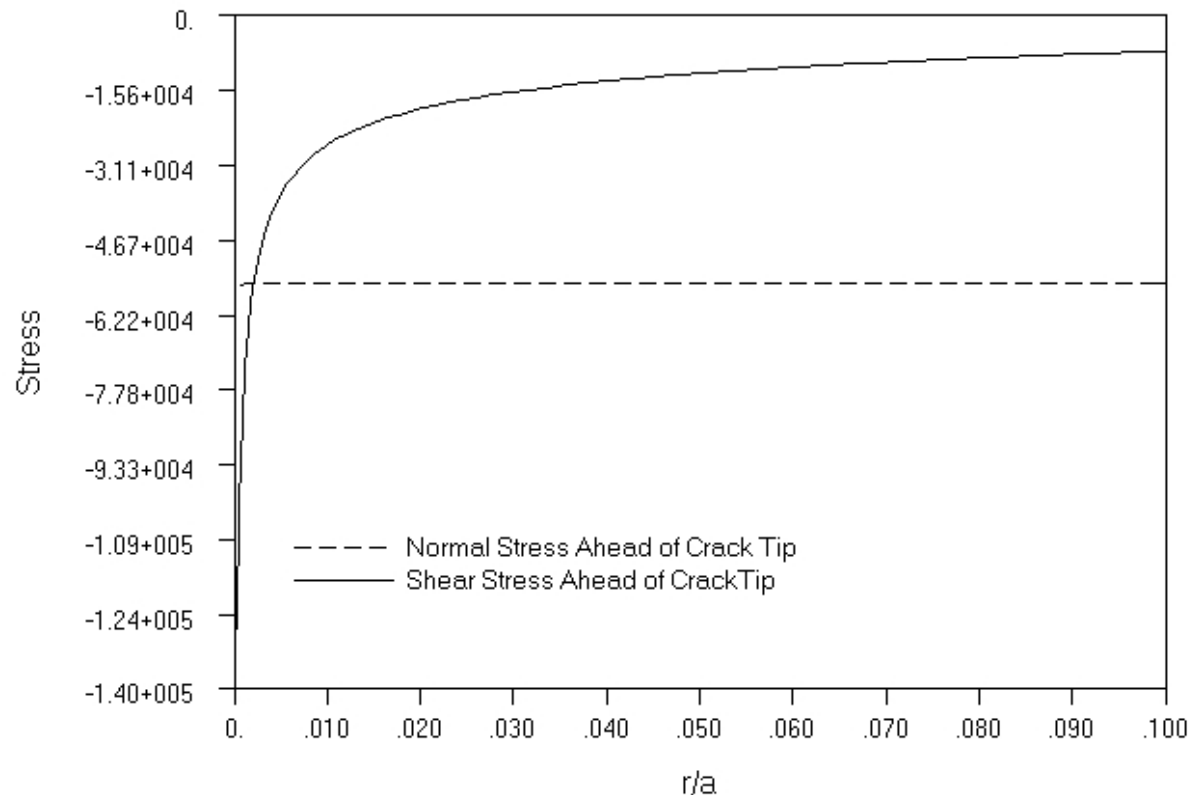


Frictional Stress on Crack Face

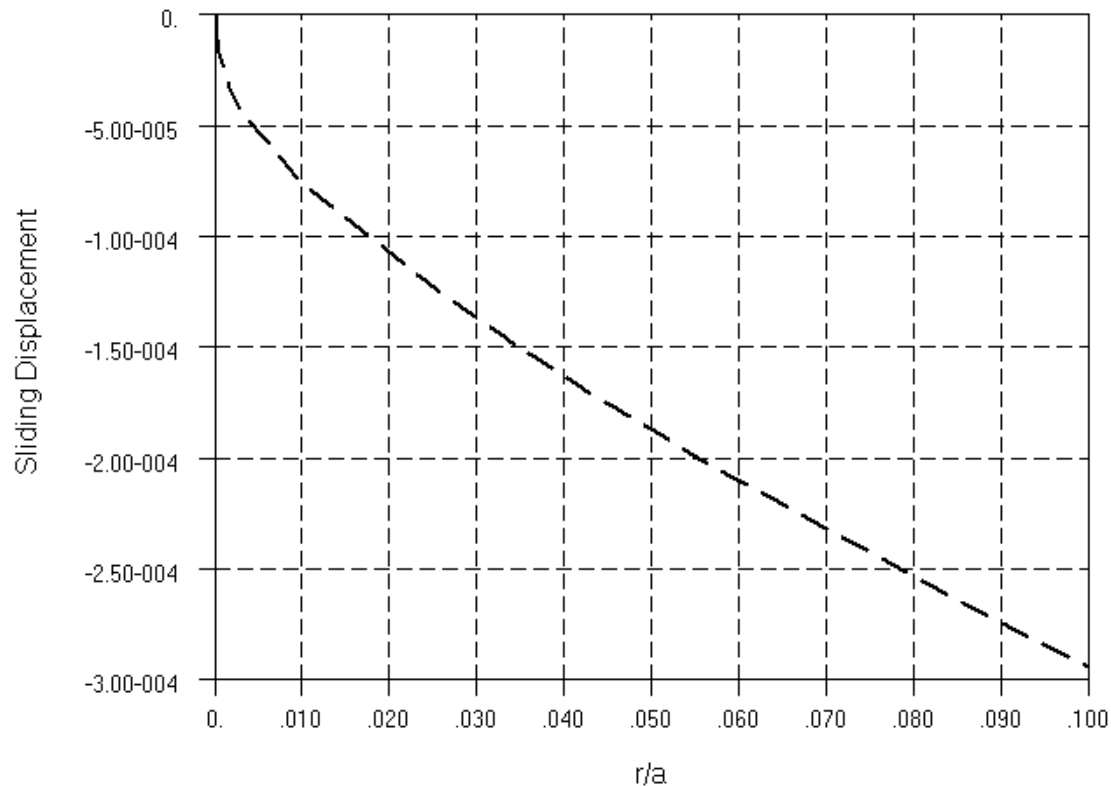


Stresses Ahead of Crack Tip

Note Shear Stress Singularity



Sliding Displacement



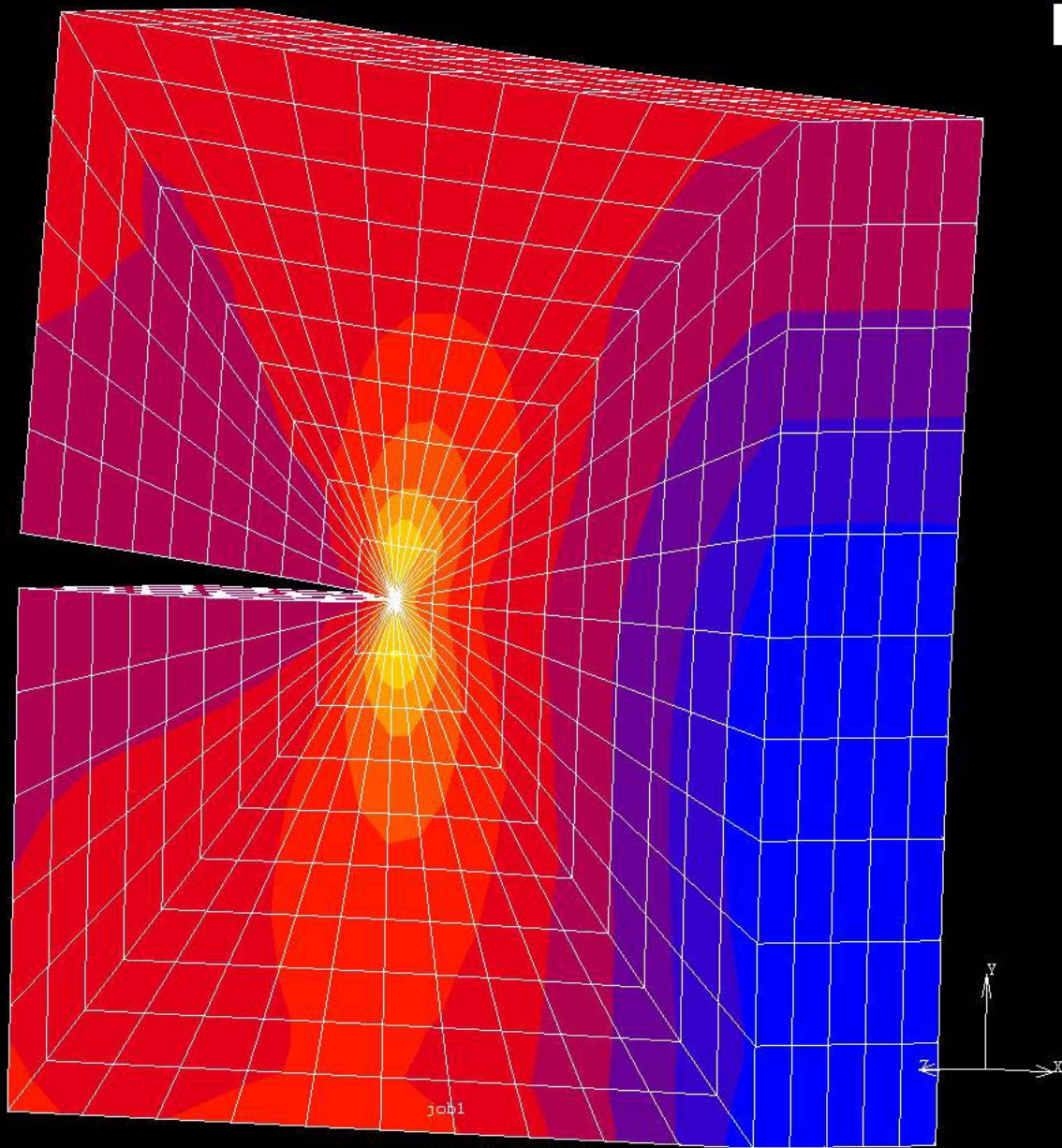
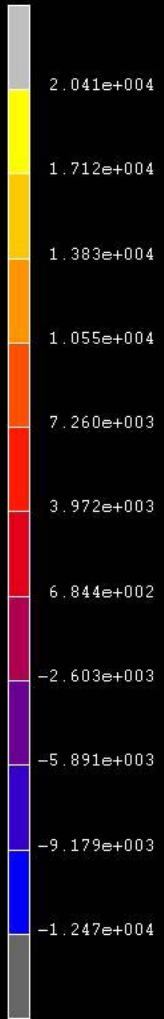
Fracture Mechanics Conclusion

- **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**

Inc: 0
Time: 0.000e+000



Comp 22 of Stress

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Typical Output

j-integral estimations:

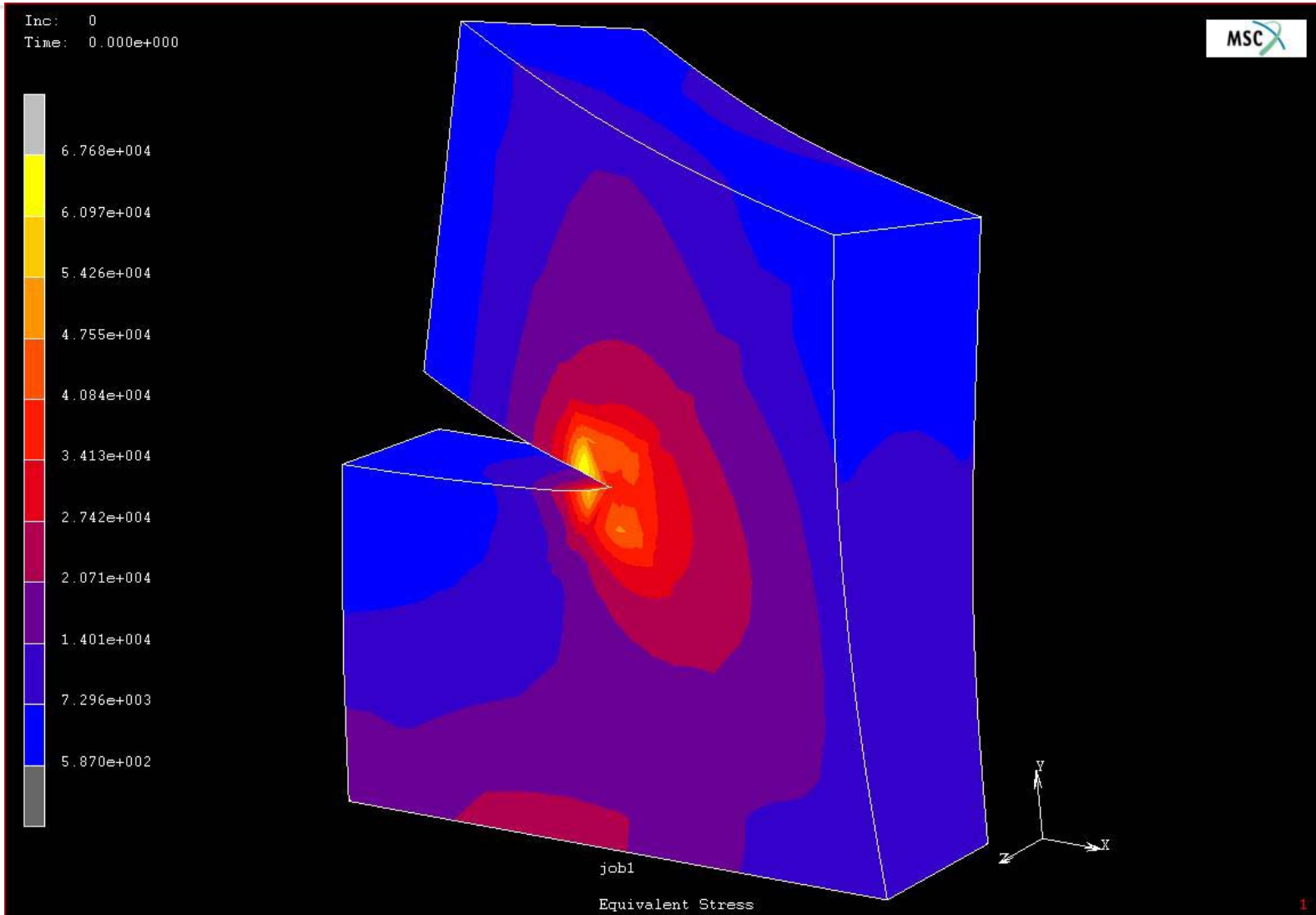
crack tip node	path radius	j-integral value
422	1.4142E-01	1.4294E+01
422	2.8284E-01	1.4596E+01
422	4.2426E-01	1.4654E+01
422	5.6569E-01	1.4677E+01
422	7.0711E-01	1.4693E+01
422	8.4853E-01	1.4709E+01
422	9.8995E-01	1.4729E+01
422	1.1314E+00	1.4760E+01

Typical Output – Mode Separation

results for mode I and II: crack1

		stress intensity factor	
crack	path radius	K_I	K_II
tip node			
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



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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