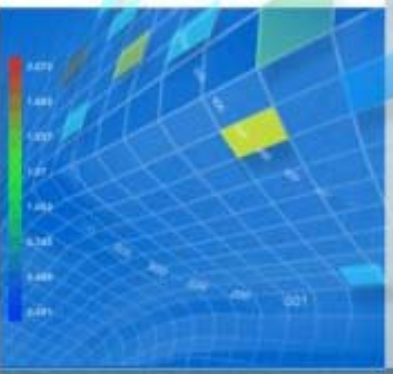

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Fuel Cell Applications

Contents

- Meshing/Remeshing
- Analysis of Composite Materials (shell/solid)
- Fracture Mechanics Capabilities
- Heat Transfer and Coupled Thermal Stresses
- Running Jobs in Parallel
- Fluids
- User Subroutines
- Future Work
- PEN Fuel Cell Modeling

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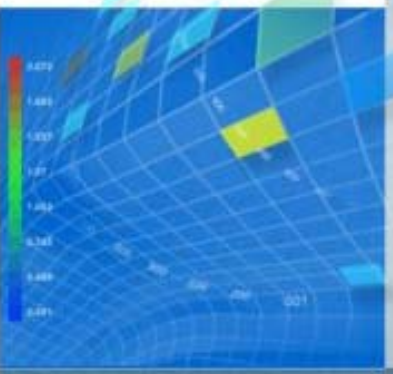
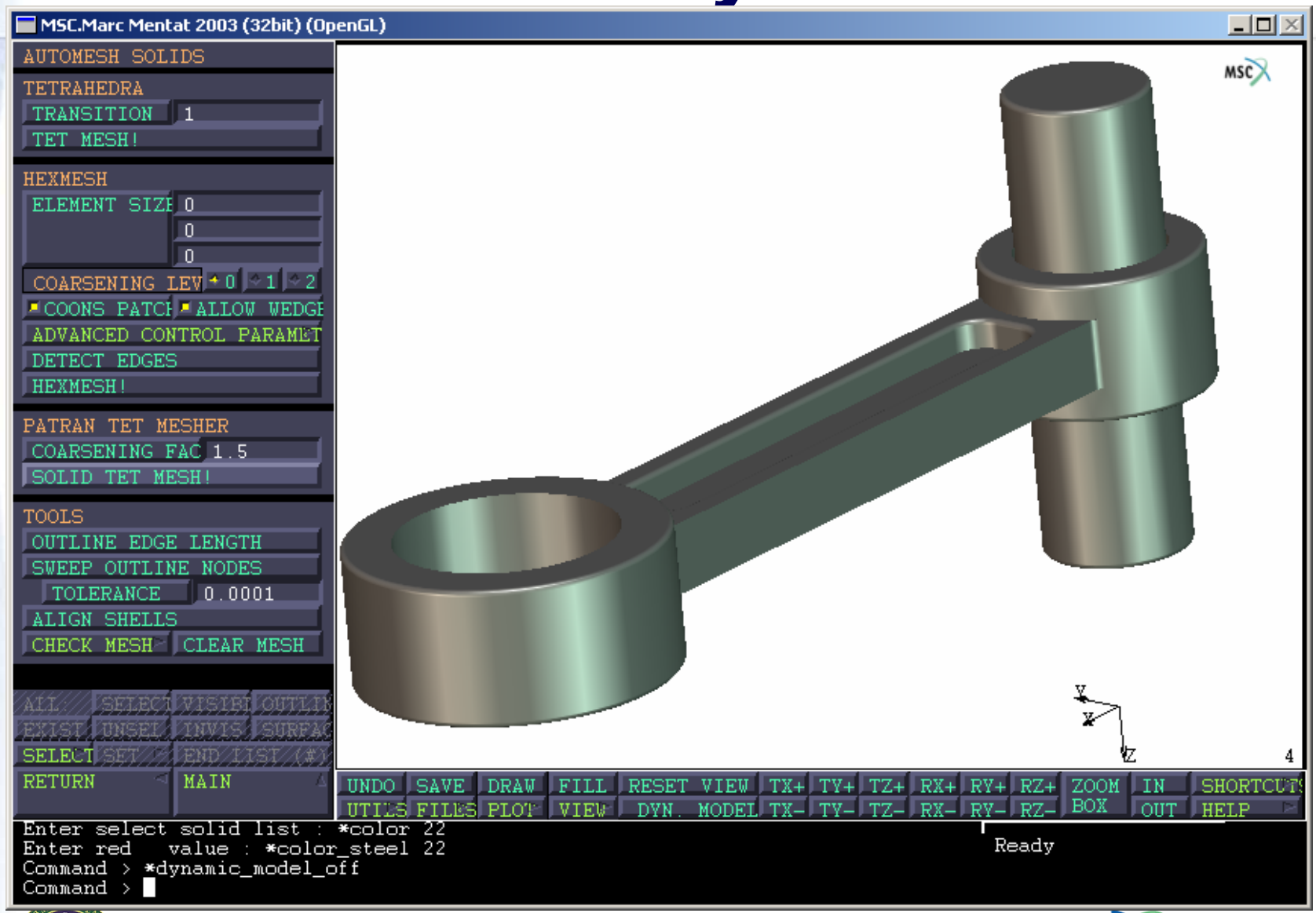
Meshing/Remeshing



CAD Connectivity: ACIS Solid



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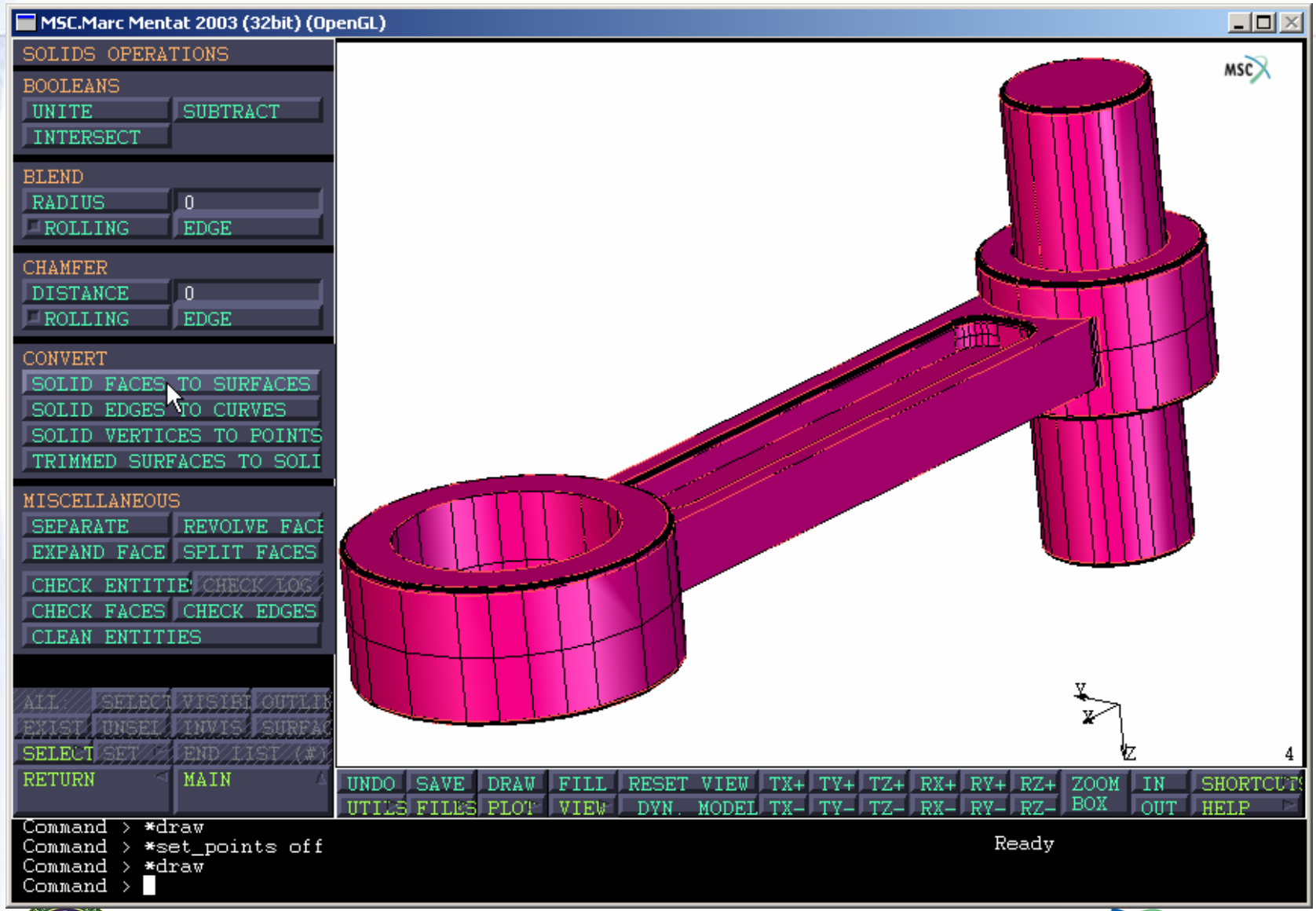
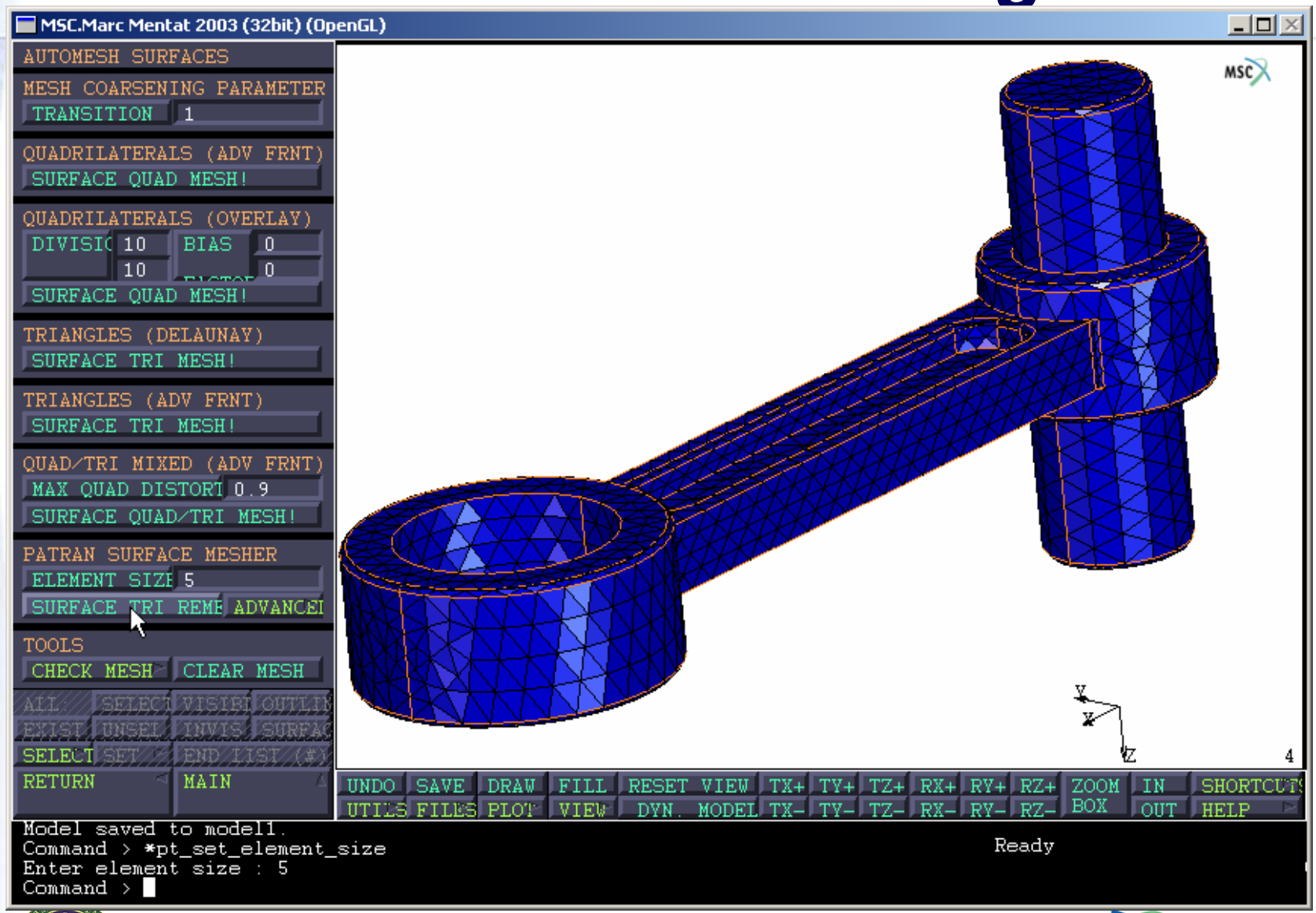
Convert to Surfaces



Automatic Meshing



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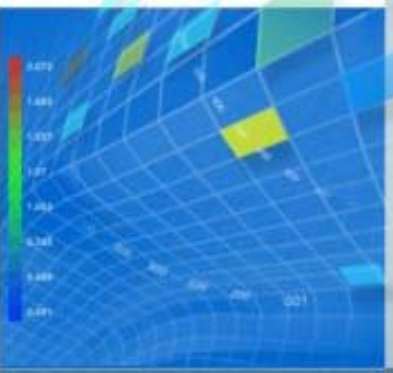
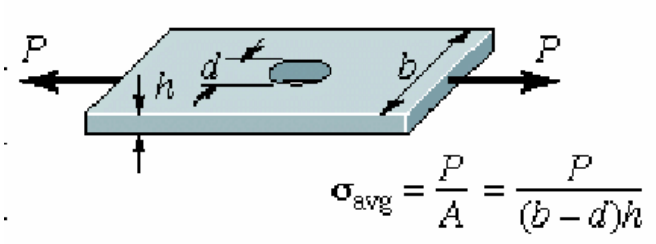
Local Remeshing



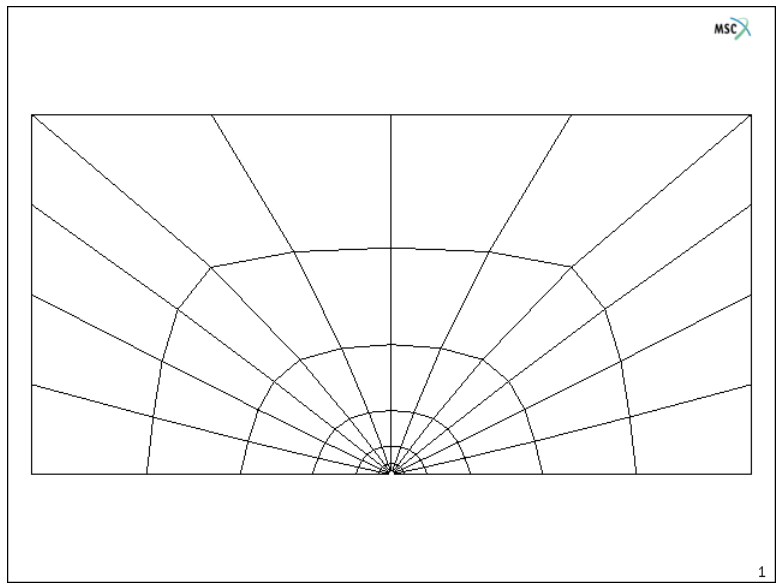
Stress Concentration – Plate with Hole

Uniform Axial Load

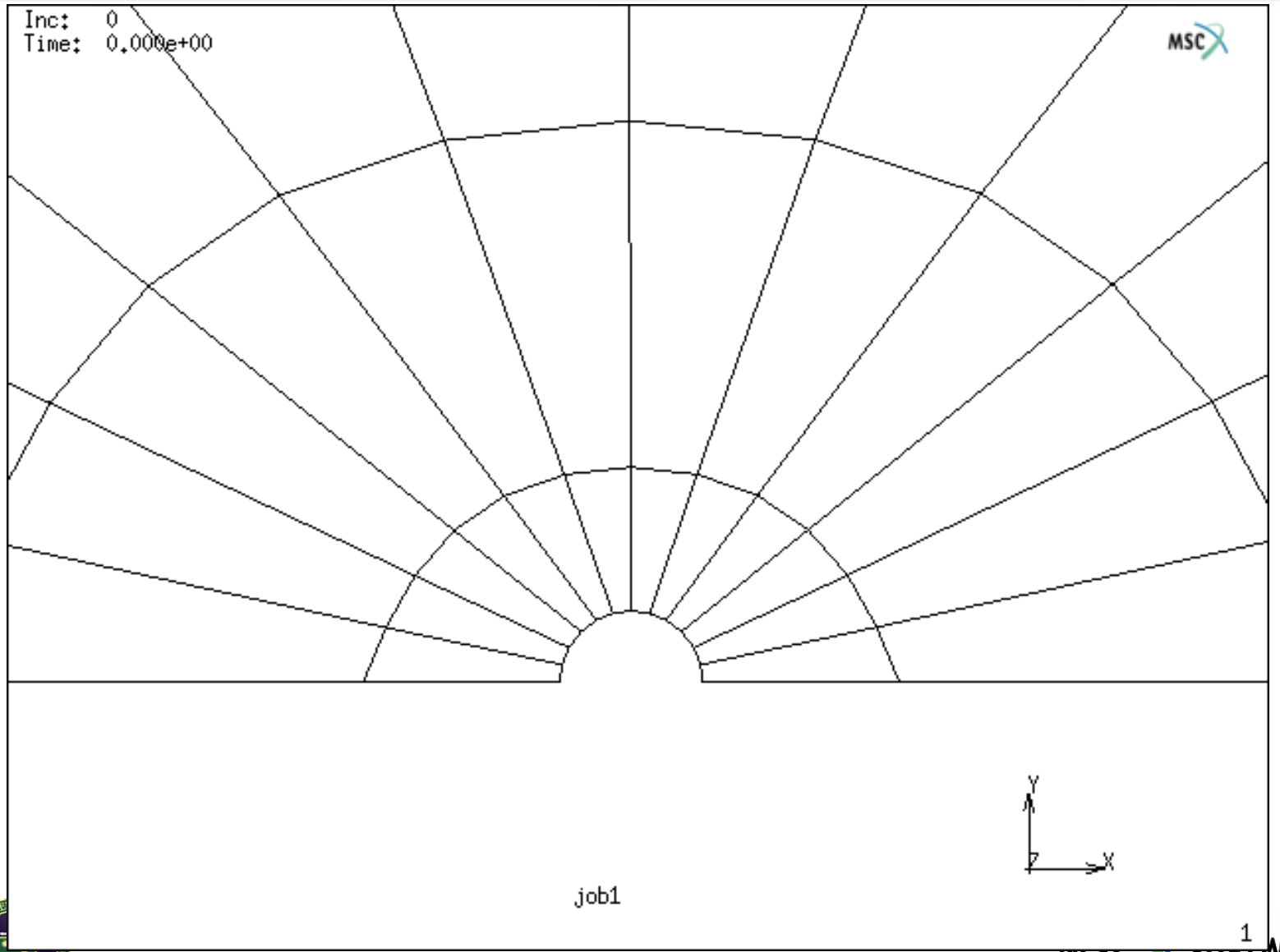


$$\sigma_{\max} = K_c \sigma_{avg}$$

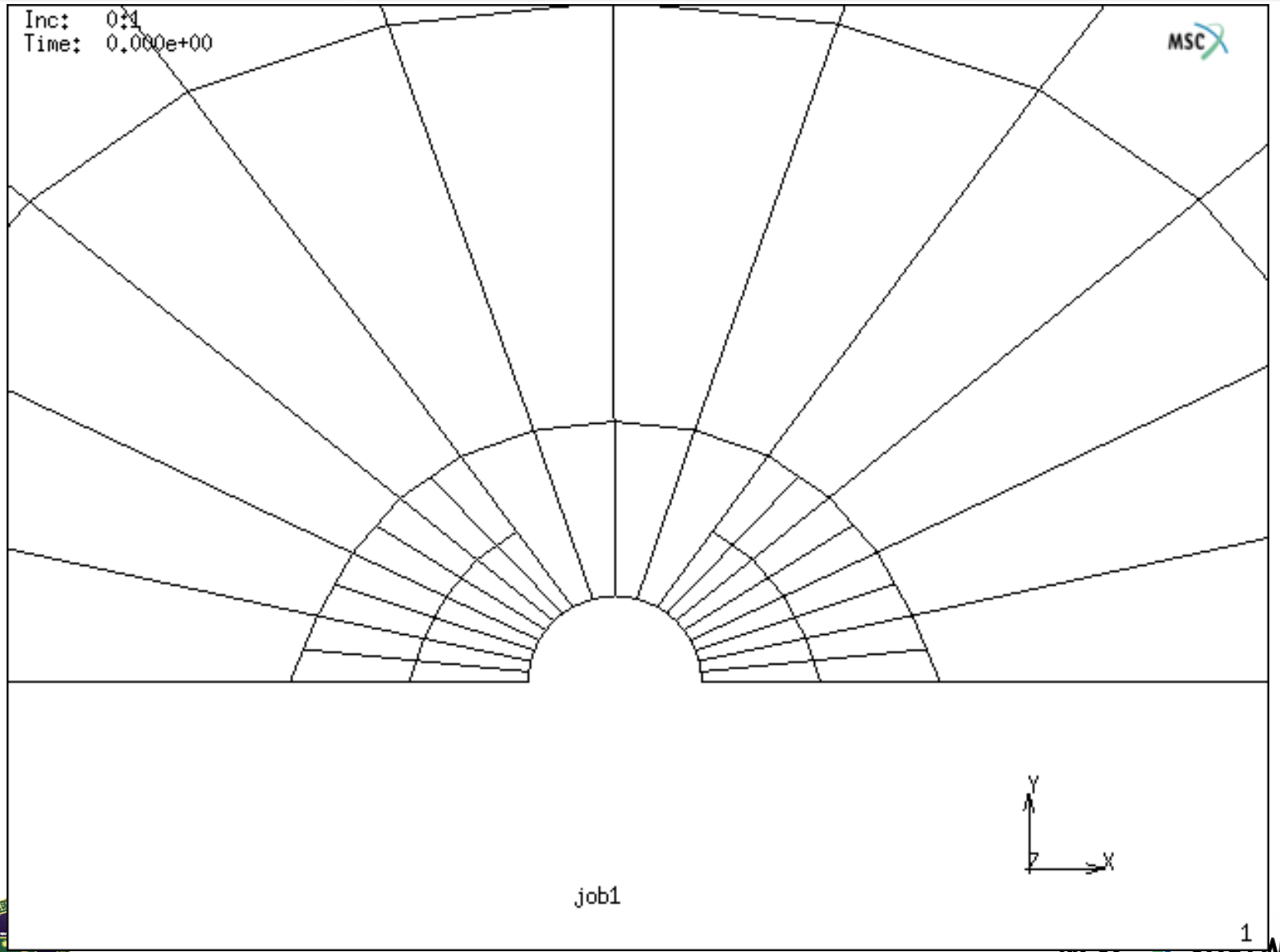
h = 1
b = 10
d = .1



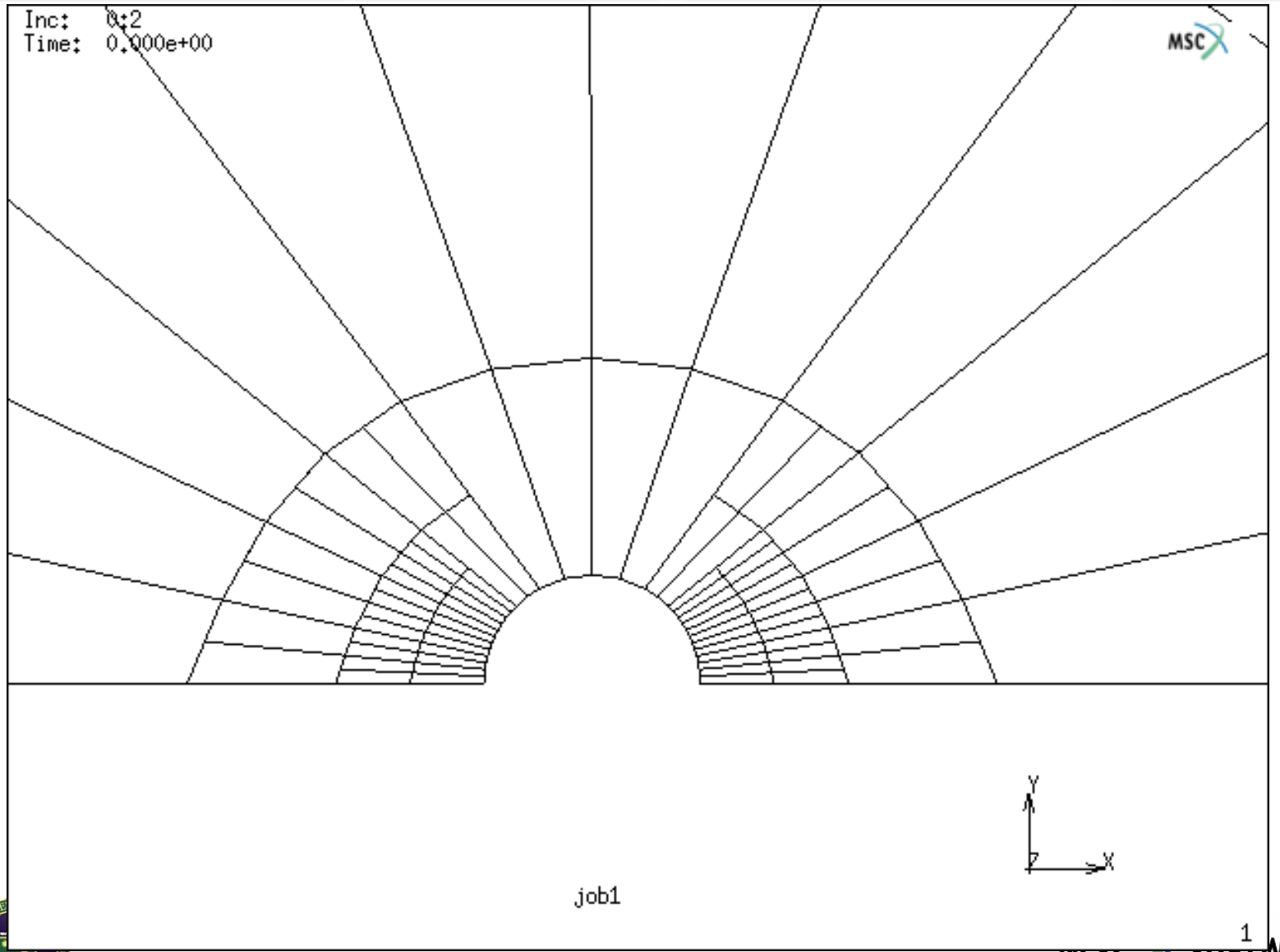
72 Elements, Kc = 1.84



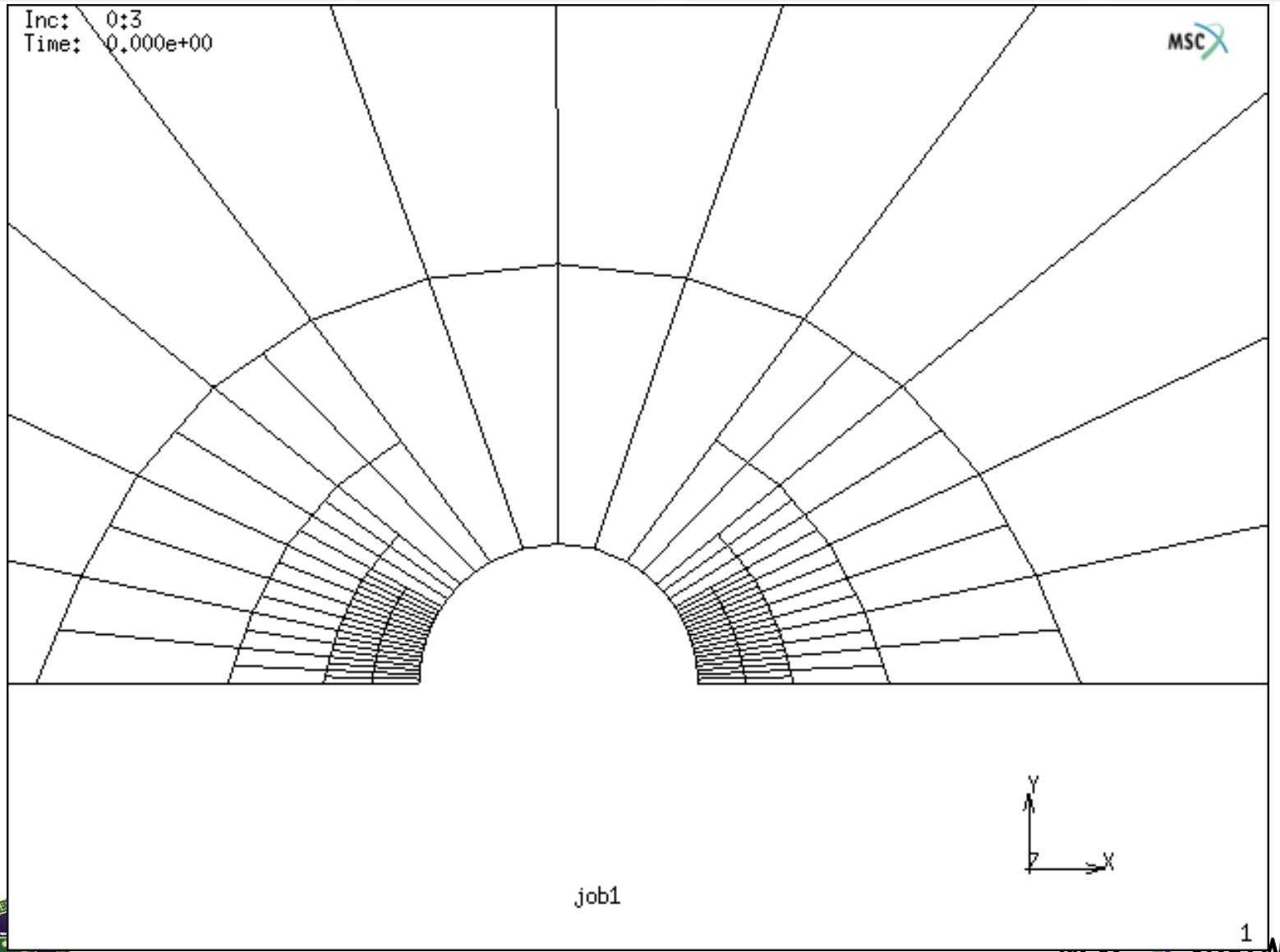
96 Elements, Kc = 2.26



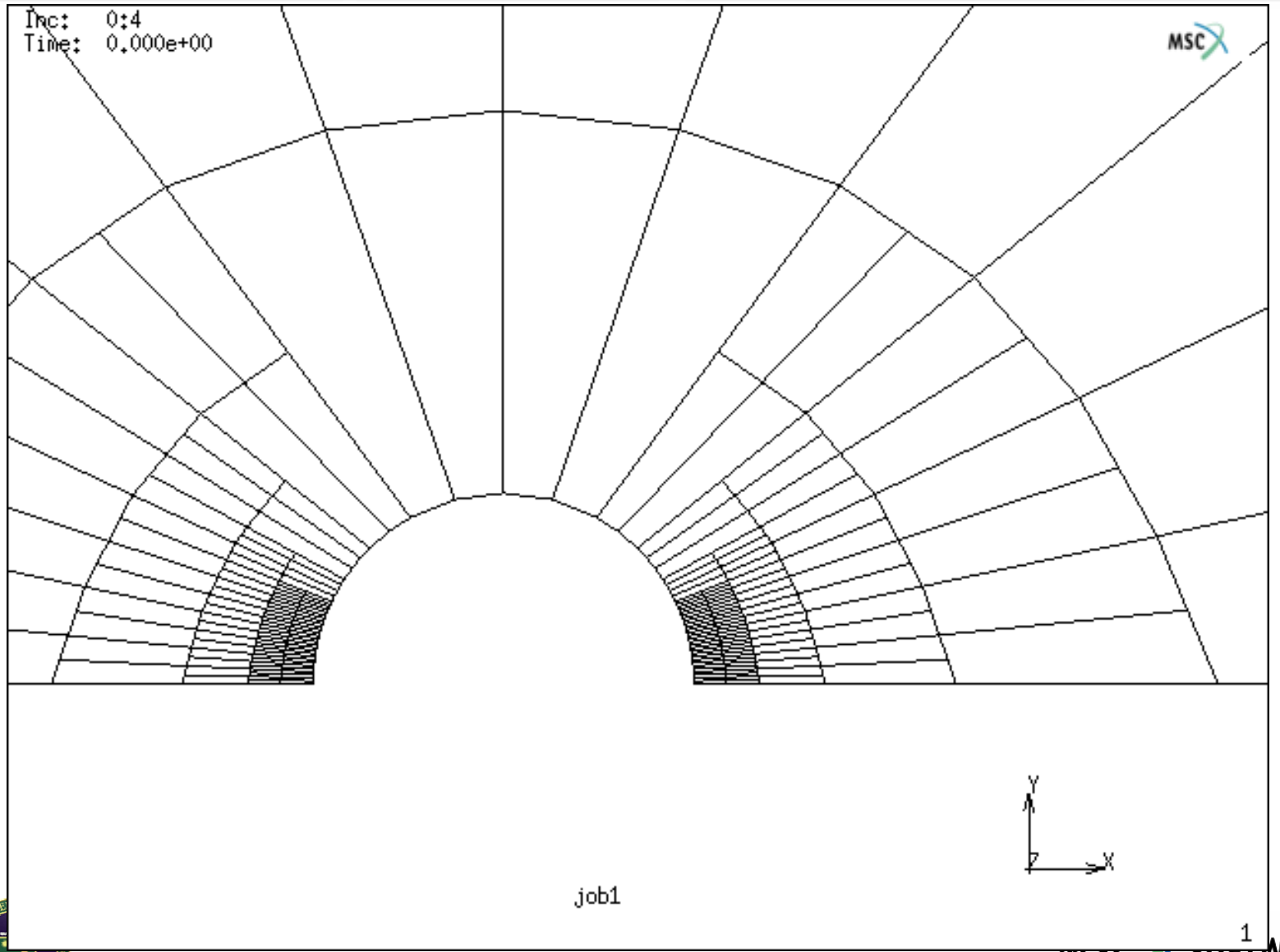
132 Elements, Kc = 2.63



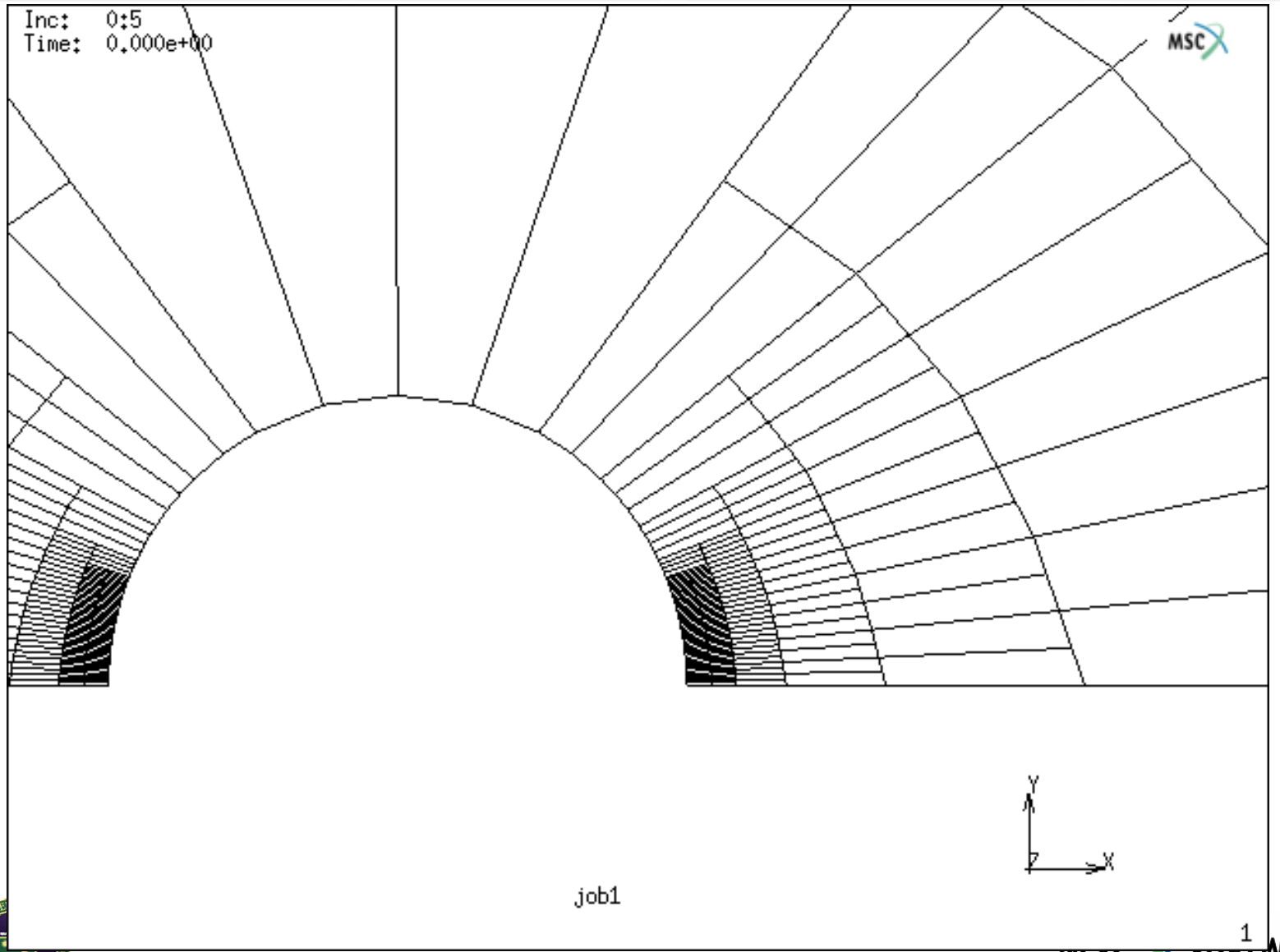
186 Elements, Kc = 2.89



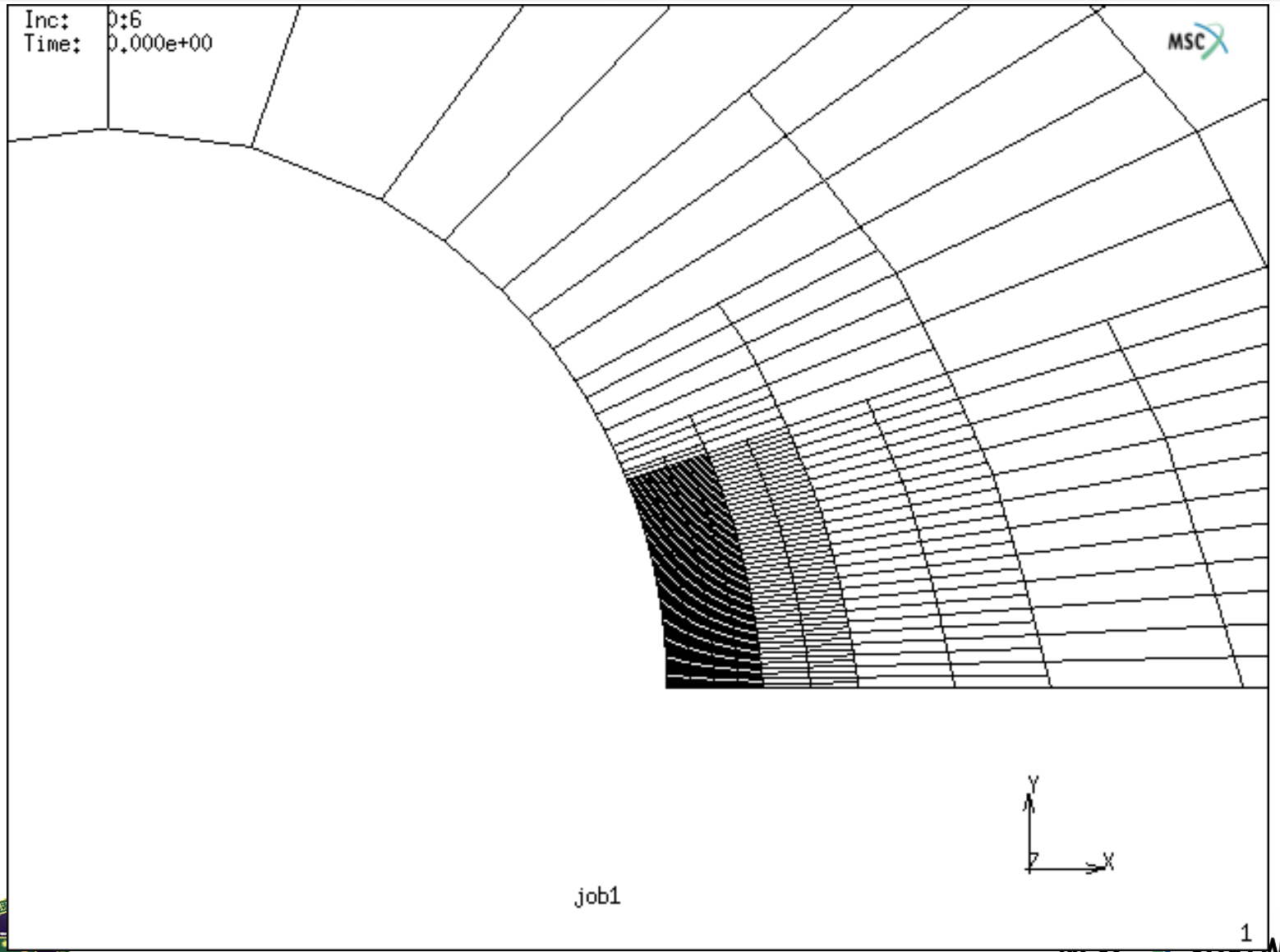
270 Elements, Kc = 3.01



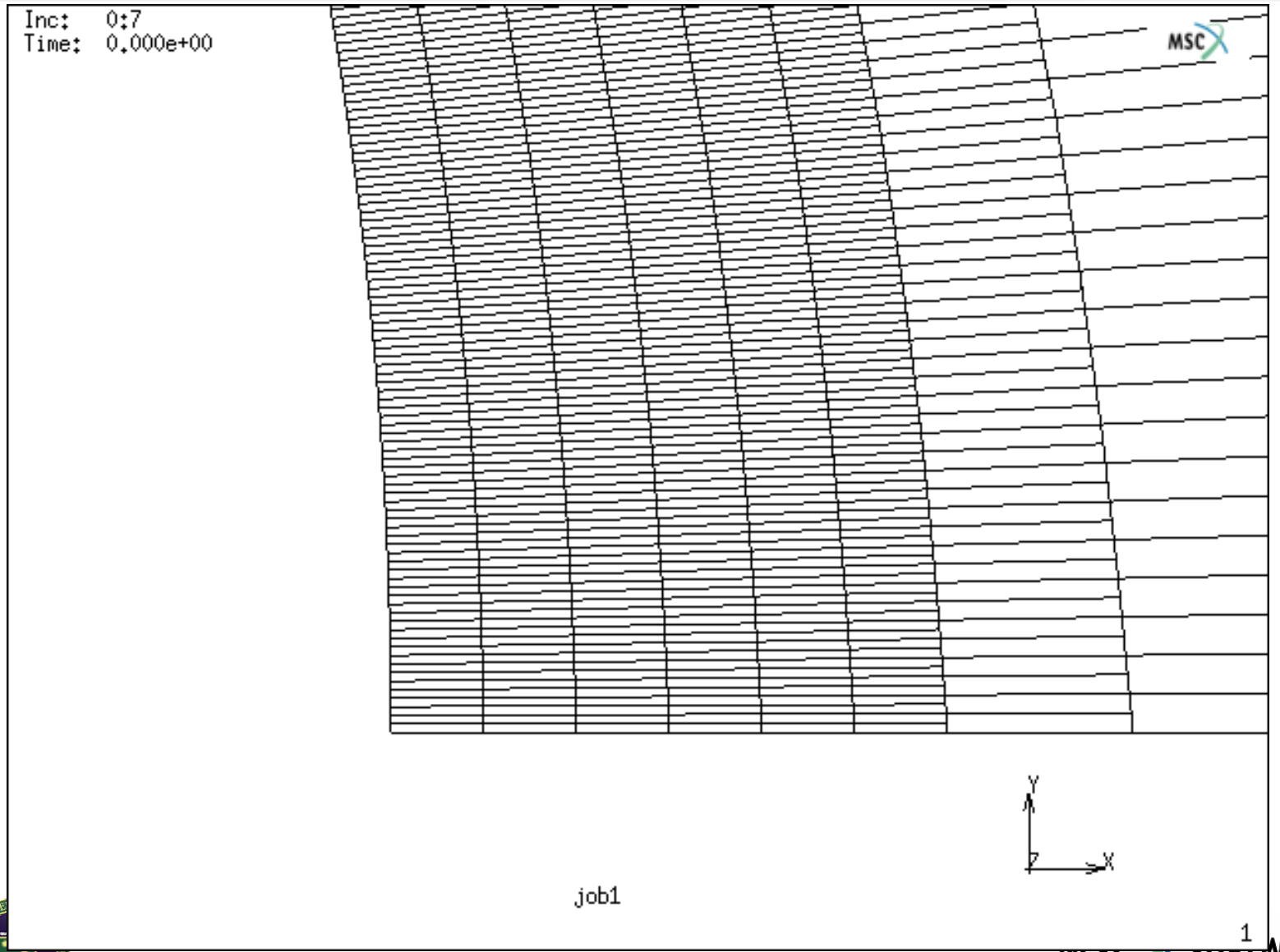
414 Elements, Kc = 3.03



1278 Elements, Kc = 3.03



2715 Elements, Kc = 3.03



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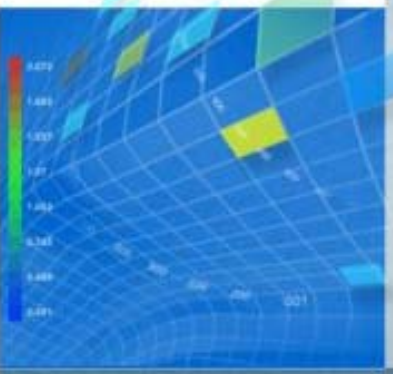
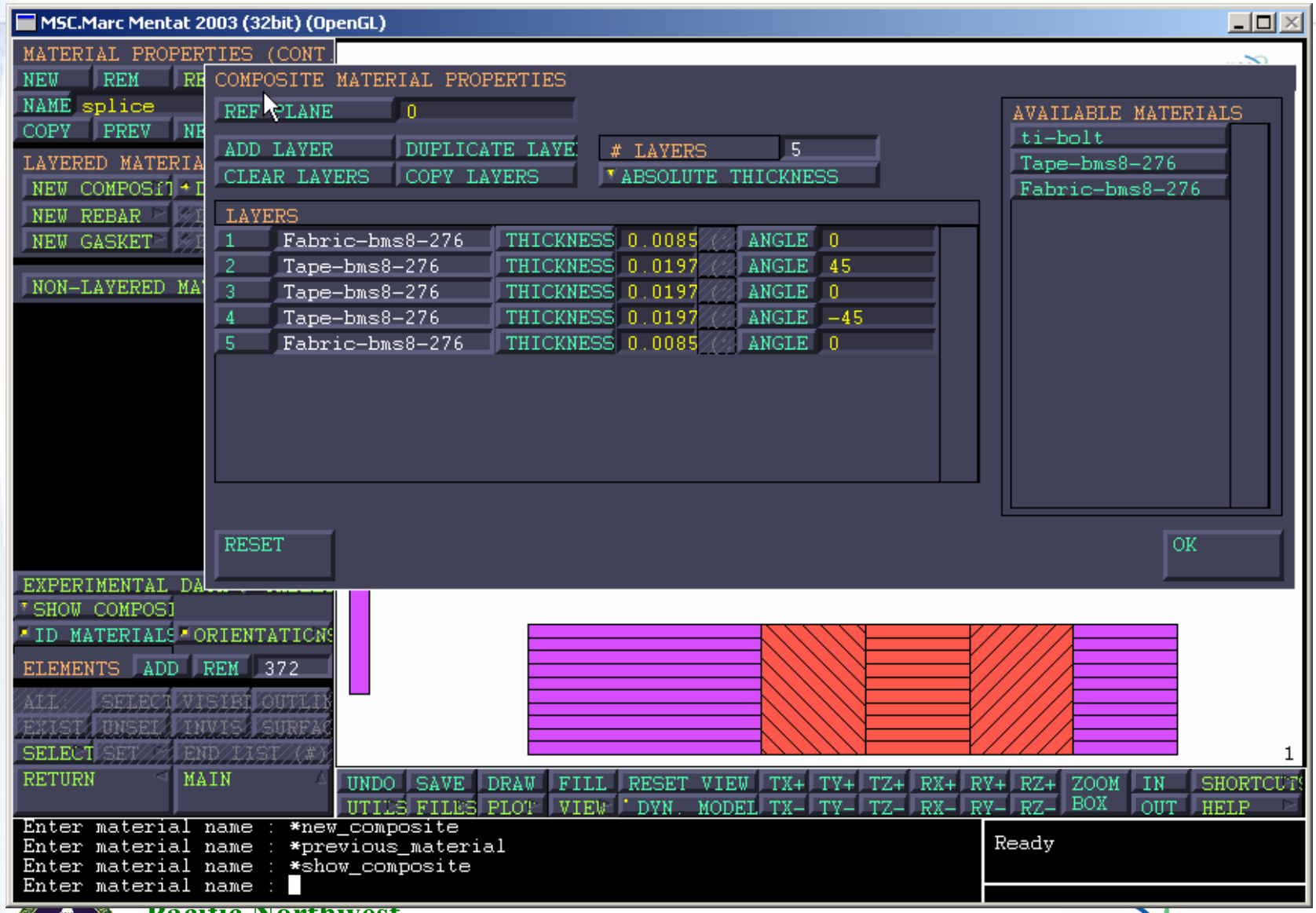
Analysis of Composite Materials

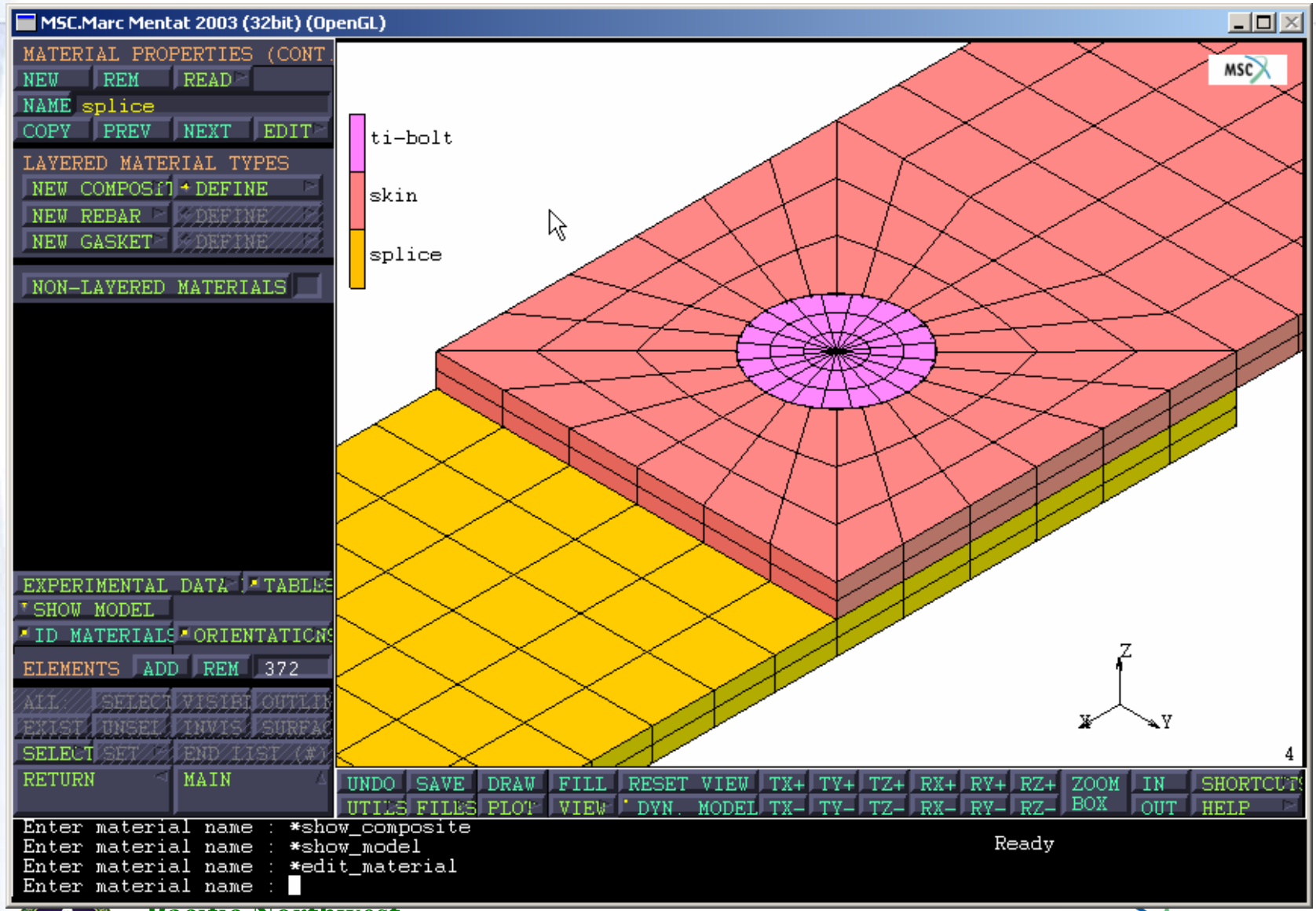


Shells and Solids

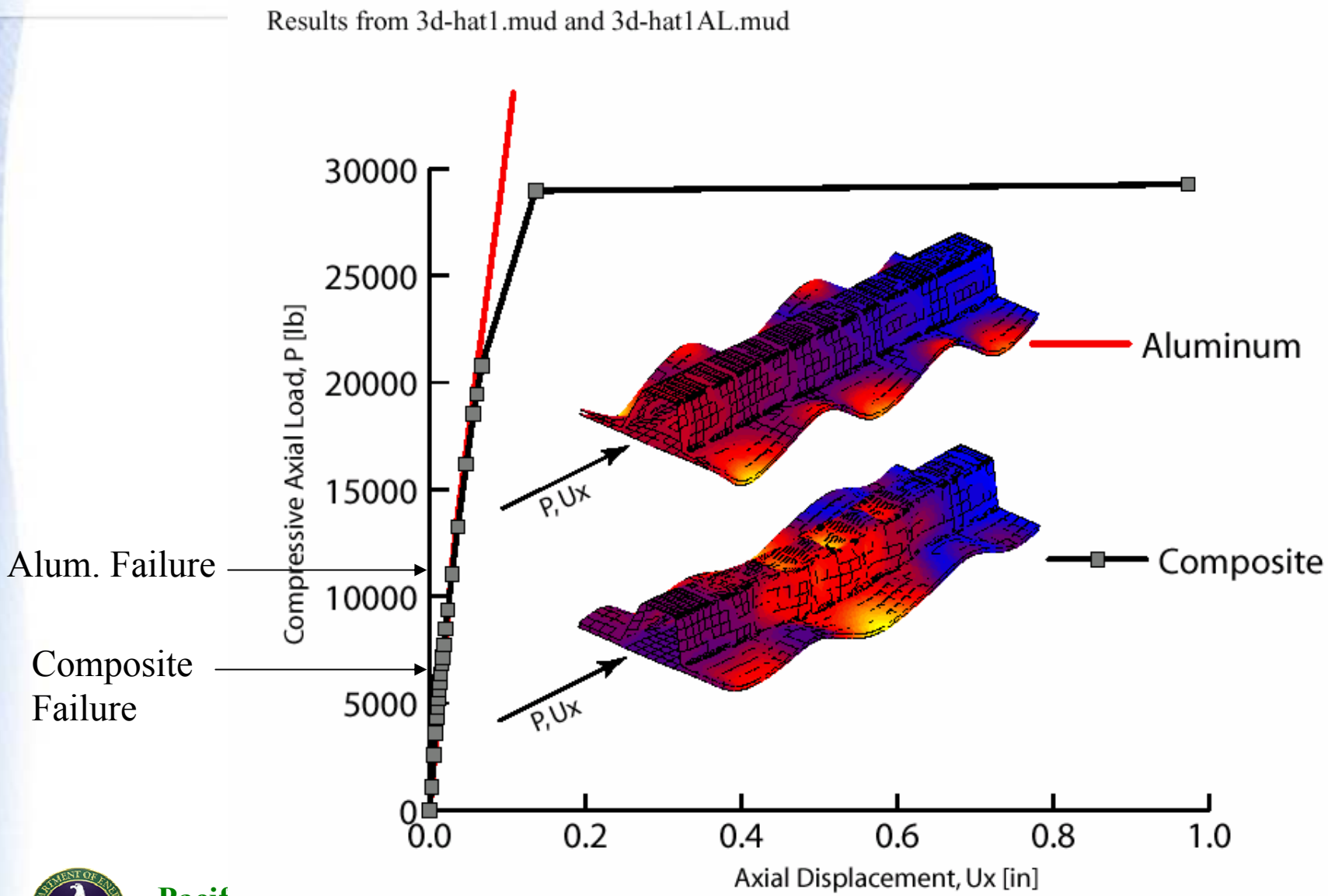
Composite Shell and Bricks



Composite Bricks



7E7 Mid Skin Buckling



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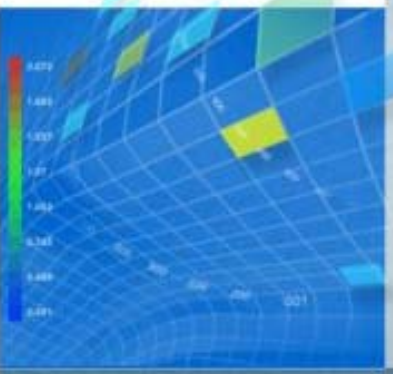
Fracture Mechanics



J-Integral Estimations

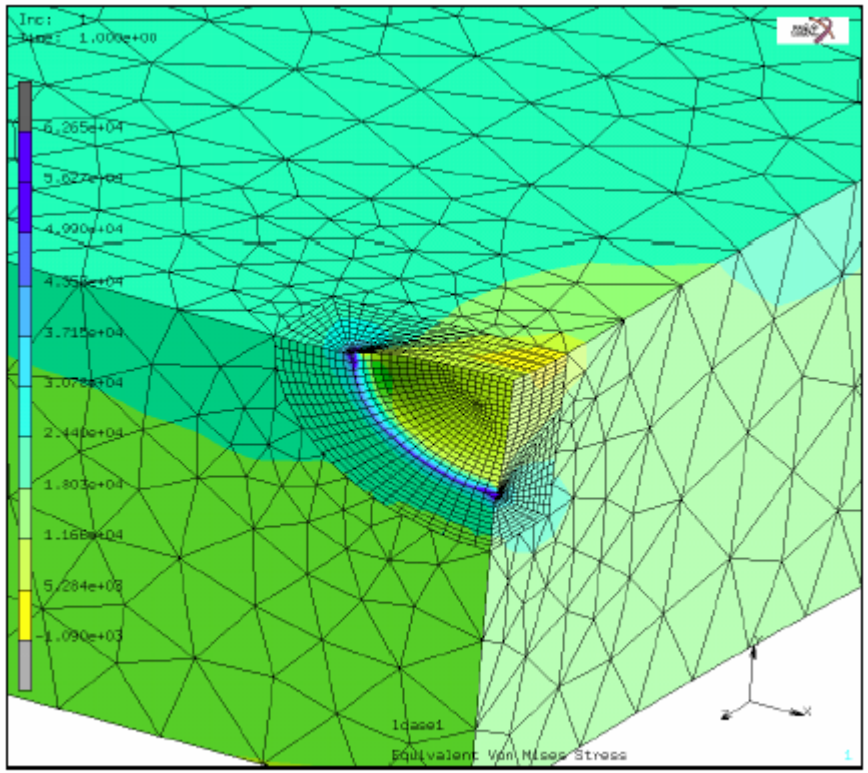


Figure 19-6 Equivalent von Mises Stress Contours

Table 19-1 J-integral Estimations

Crack Tip Node	Path Radius	J-integral Value
1235	1.1180E-01	3.1508E+03
1235	2.2361E-01	3.2027E+03
1235	3.3541E-01	3.1918E+03
1235	4.4721E-01	3.1984E+03
1235	5.5902E-01	3.1961E+03
1235	6.7082E-01	3.1947E+03
1235	7.8262E-01	3.1934E+03
3656	1.1187E-01	3.1553E+03
3656	2.2375E-01	3.2247E+03
3656	3.3562E-01	3.2335E+03
3656	4.4750E-01	3.2378E+03
3656	5.5937E-01	3.2338E+03
3656	6.7125E-01	3.2276E+03
3656	7.8312E-01	3.2216E+03

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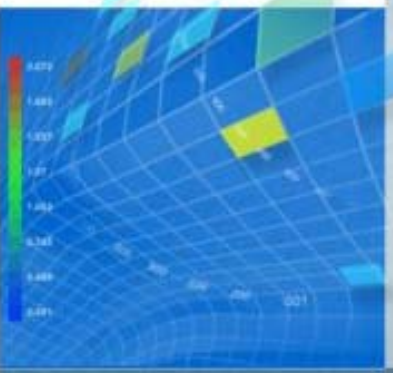
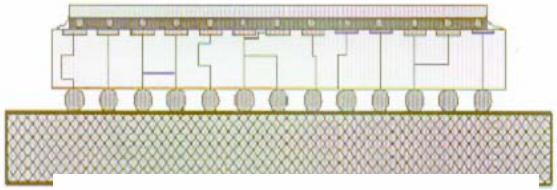
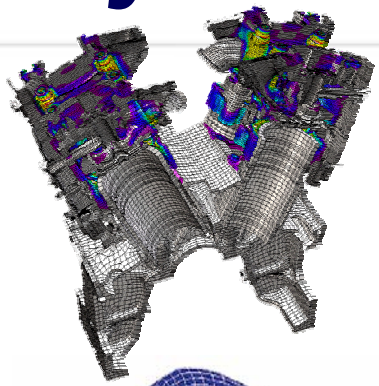
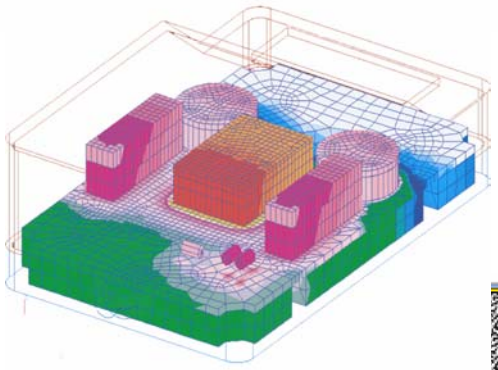
Heat Transfer and Coupled Thermal Stress

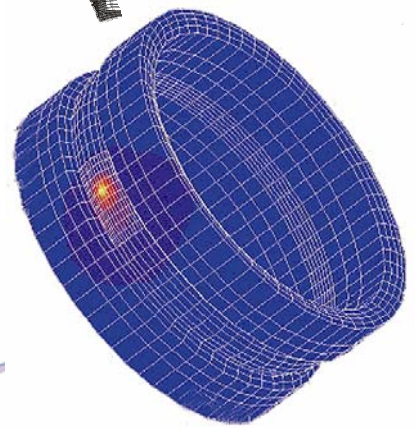


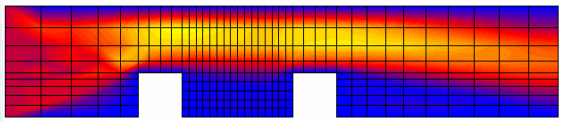
The World of Thermal Analysis

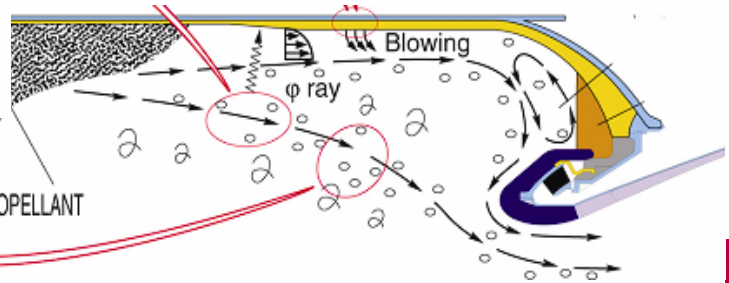


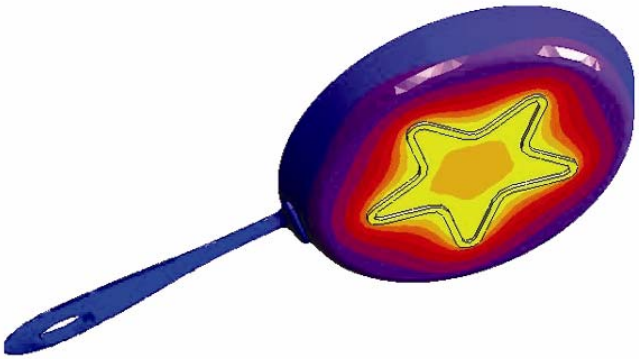


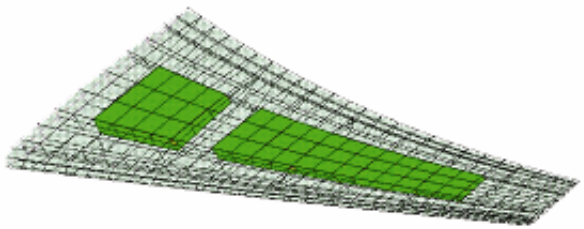


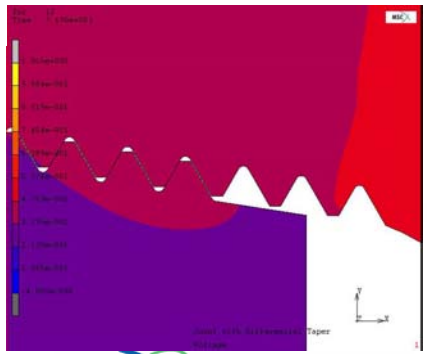












MSC SOFTWARE
SIMULATING REALITY

Capabilities

- Steady State Simulation
- Transient Simulation
- Temperatures can be easily used in uncoupled thermal stress analysis
- Coupled Thermal-Structural Analysis
- Coupled Thermal-Electric (Joule Heating)
- Coupled Thermal-Electric-Structural
- Choice of Time Step Procedures
  - Fixed Time Steps
  - Adaptive Time Steps

Capabilities

- 1-d
- 2-d (planar and axisymmetric solid and axisymmetric shells)
- 3-d (solid, and shells)
- Heat transfer shells may have any number of layers, temperature varies either linearly or quadratically through layer
- Nonlinear Transient Cyclic Symmetry
- All heat transfer elements have comparable structural elements for thermal stress analysis or coupled analysis

Capabilities

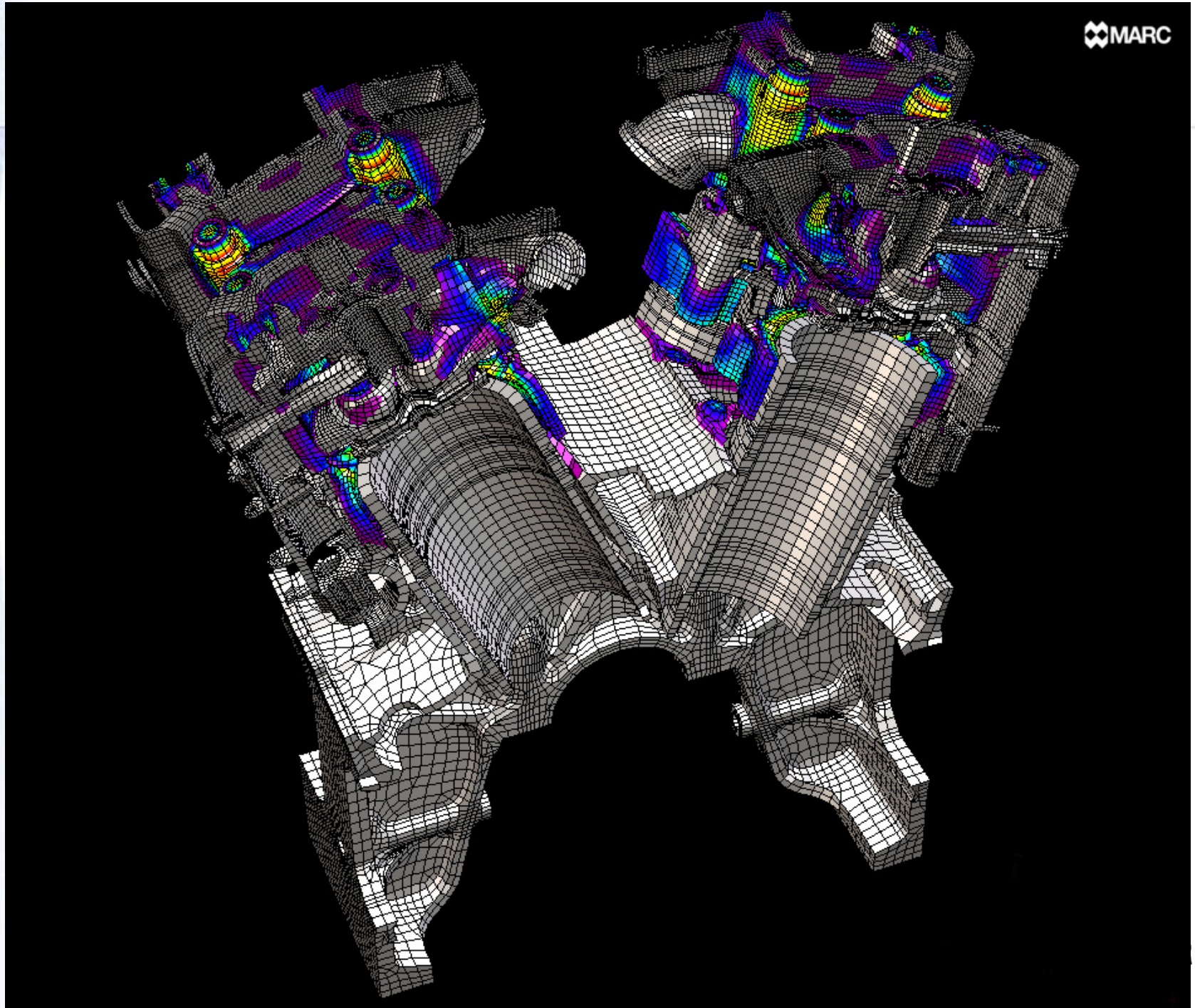
- Isotropic , Orthotropic or Anisotropic thermal properties.
- All properties may be function of temperature.
- Latent heat effects included to model phase changes

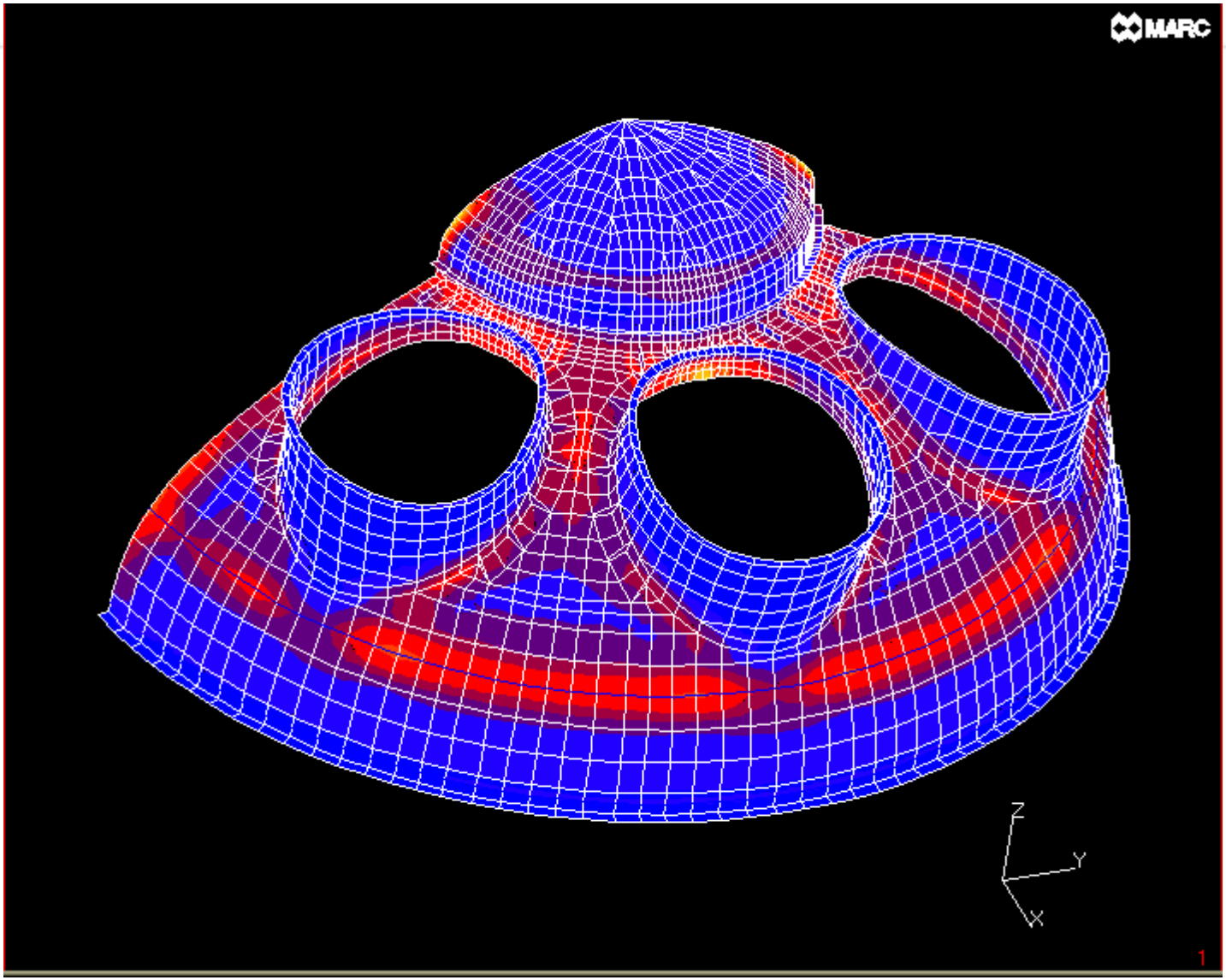
Capabilities

- Point or Distributed Fluxes
- Convective Boundary Conditions
- Radiative Heating
- View Factor Calculations efficiently done using Monte Carlo method
- Internal Heating due to plasticity or friction in coupled structural analysis.
- Thermal Contact in coupled structural analysis.

Applications

- Energy Industry
- Engines (Gas Turbine, Diesel, Automotive)
- Rockets
- Electronics
- Fire Safety
- Manufacturing
- Welding





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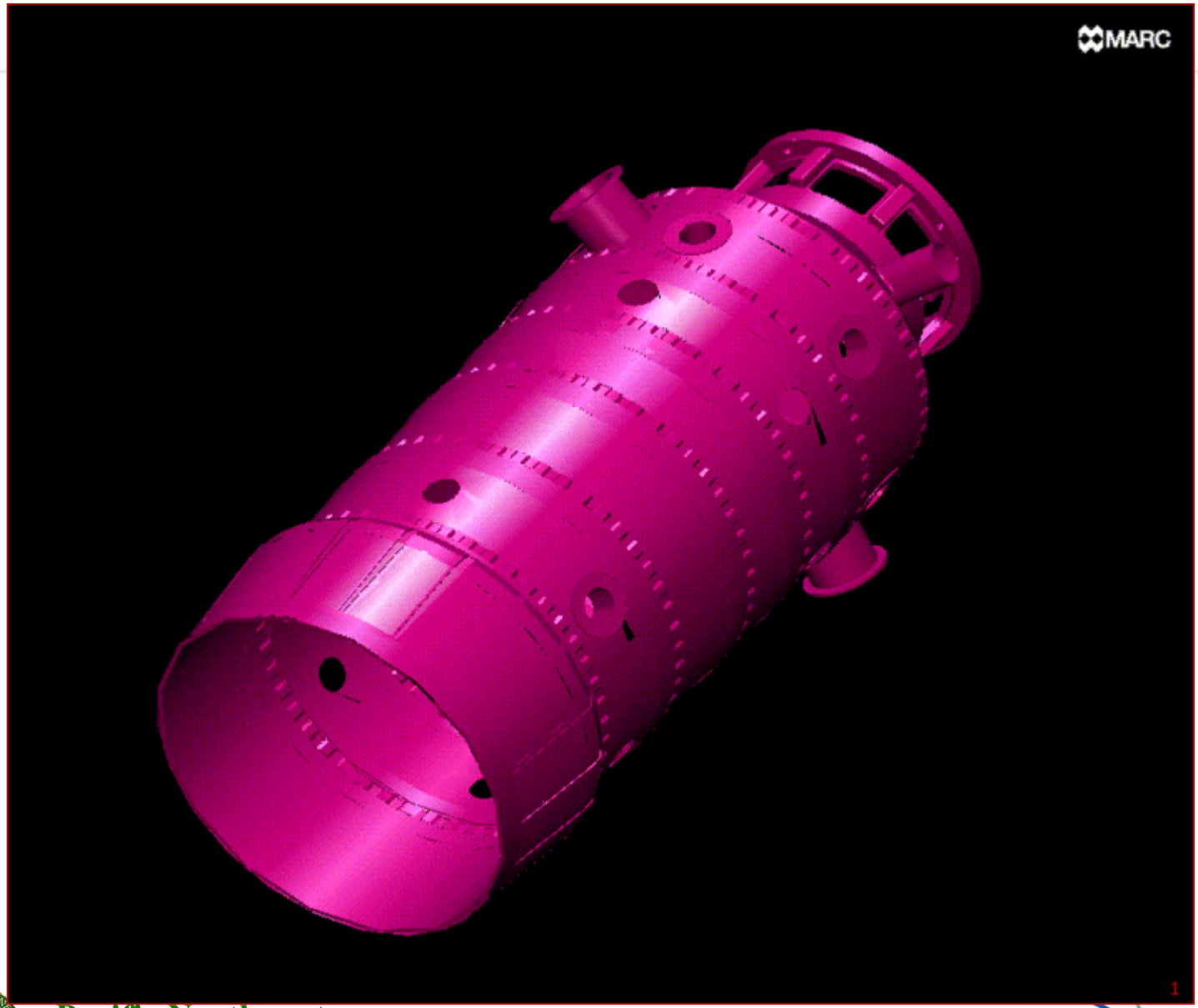

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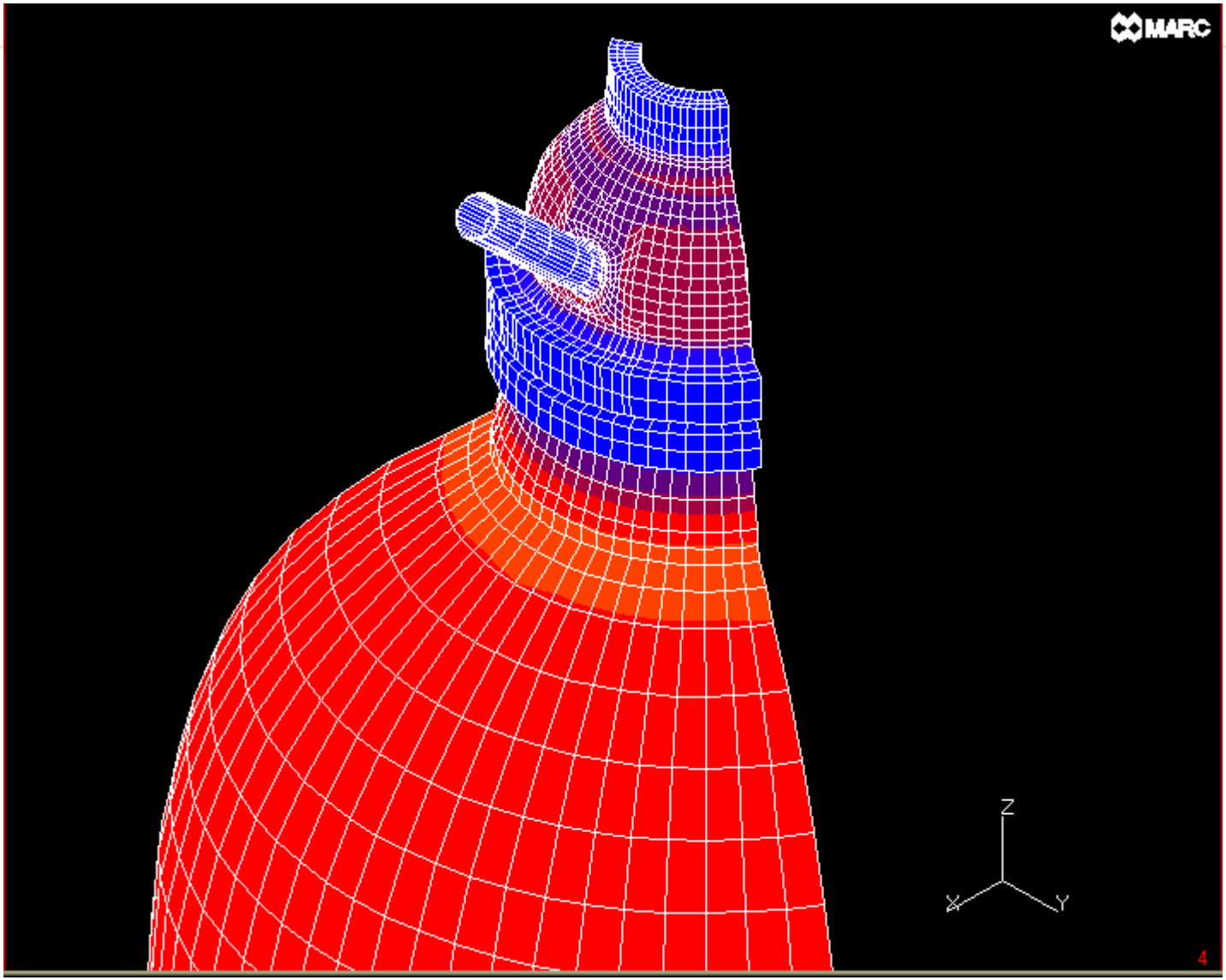

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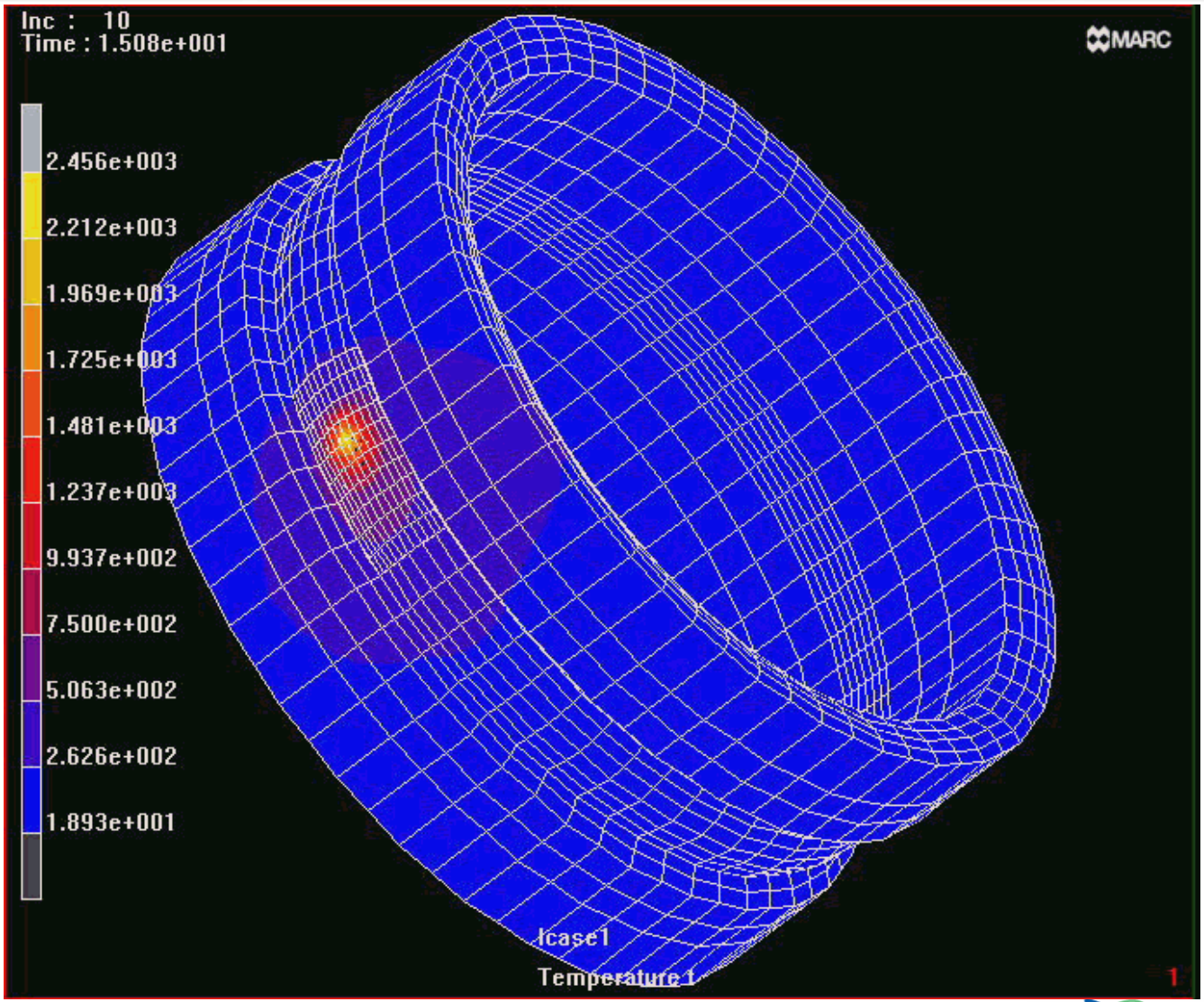
Welding Simulation



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Channel

- Special Modeling techniques to represent fluid flow in channels

- Special modeling techniques to model convection and radiation across small gaps.

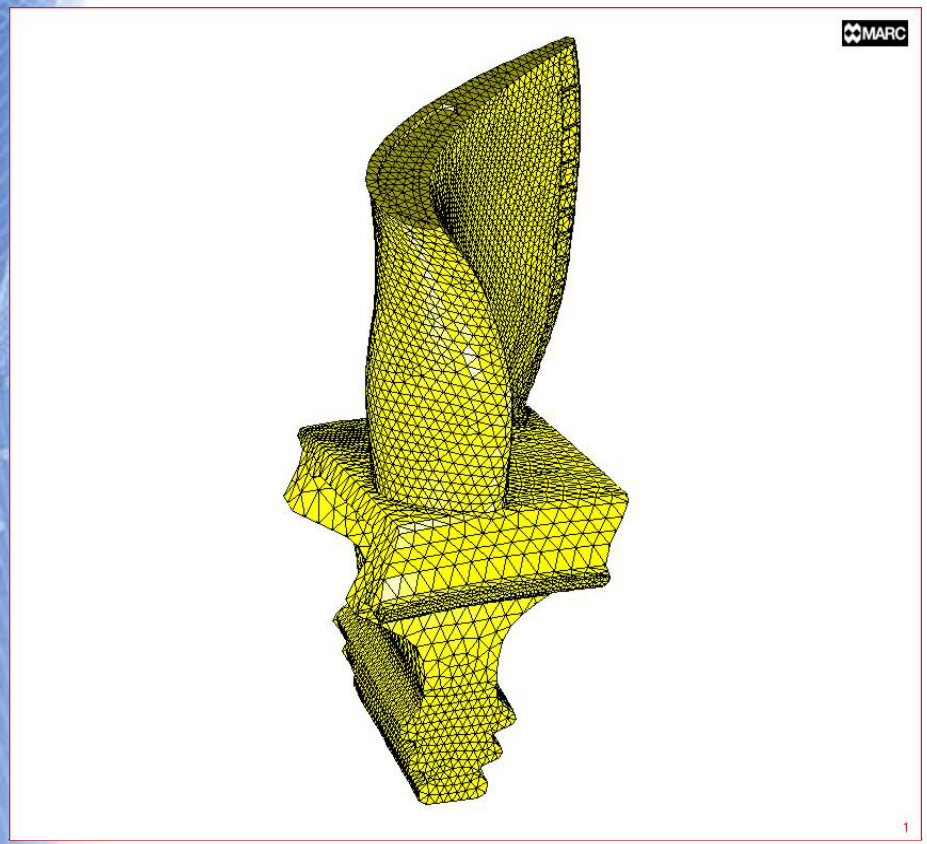
Computationally Efficient Solution Methods

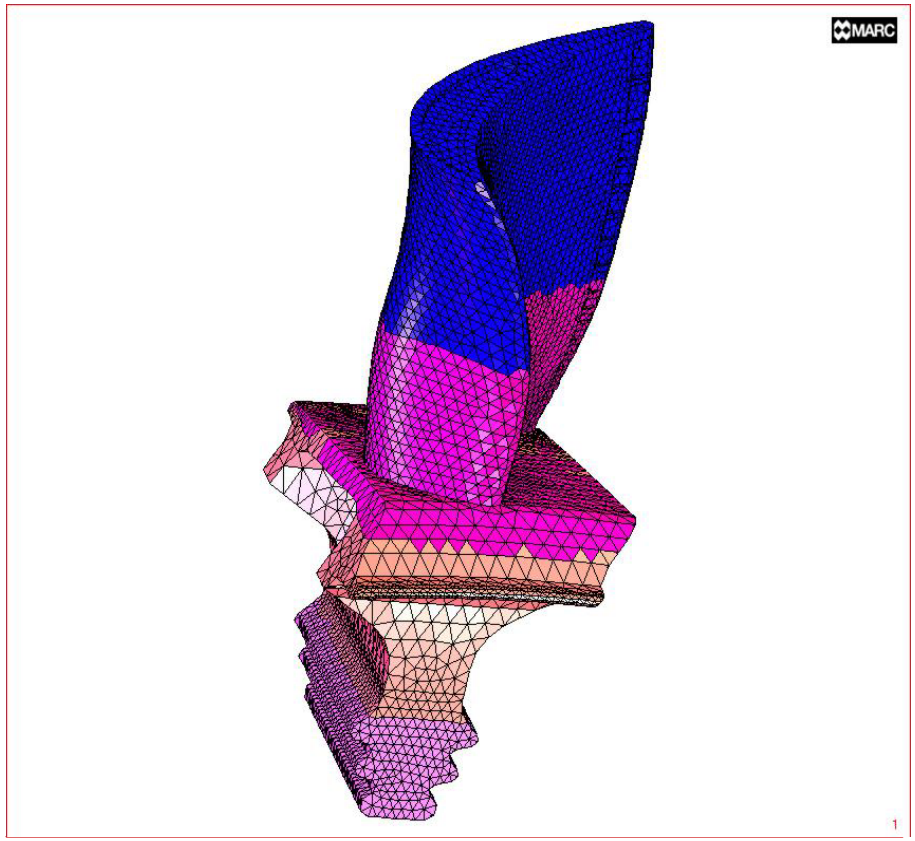
- Direct Sparse Solvers
- Iterative Solvers
- Parallel Processing using Domain Decomposition

Turbine Blade Structural Analysis

- Number of Domains: 4
- Number of Elements: 72K
- Degrees of Freedom: 55K
- Scaling: 4.2X

Turbine Blade Structural Analysis





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Thermal Contact

- If dist < d1 then thermal conduction
- If d1< dist < d2 then simplified thermal radiation
- If d2 < dist then no contact

Near Contact

- Convection
- Natural convection
- Radiation
- Distance dependent convection

- Q = hcv*(T2-T1)+hnt*(T2-T1)ent +
- sigma*eps*(T24-T14) +
- (hct – (hct-hbl)*gap/dqnear)*(T2-T1)

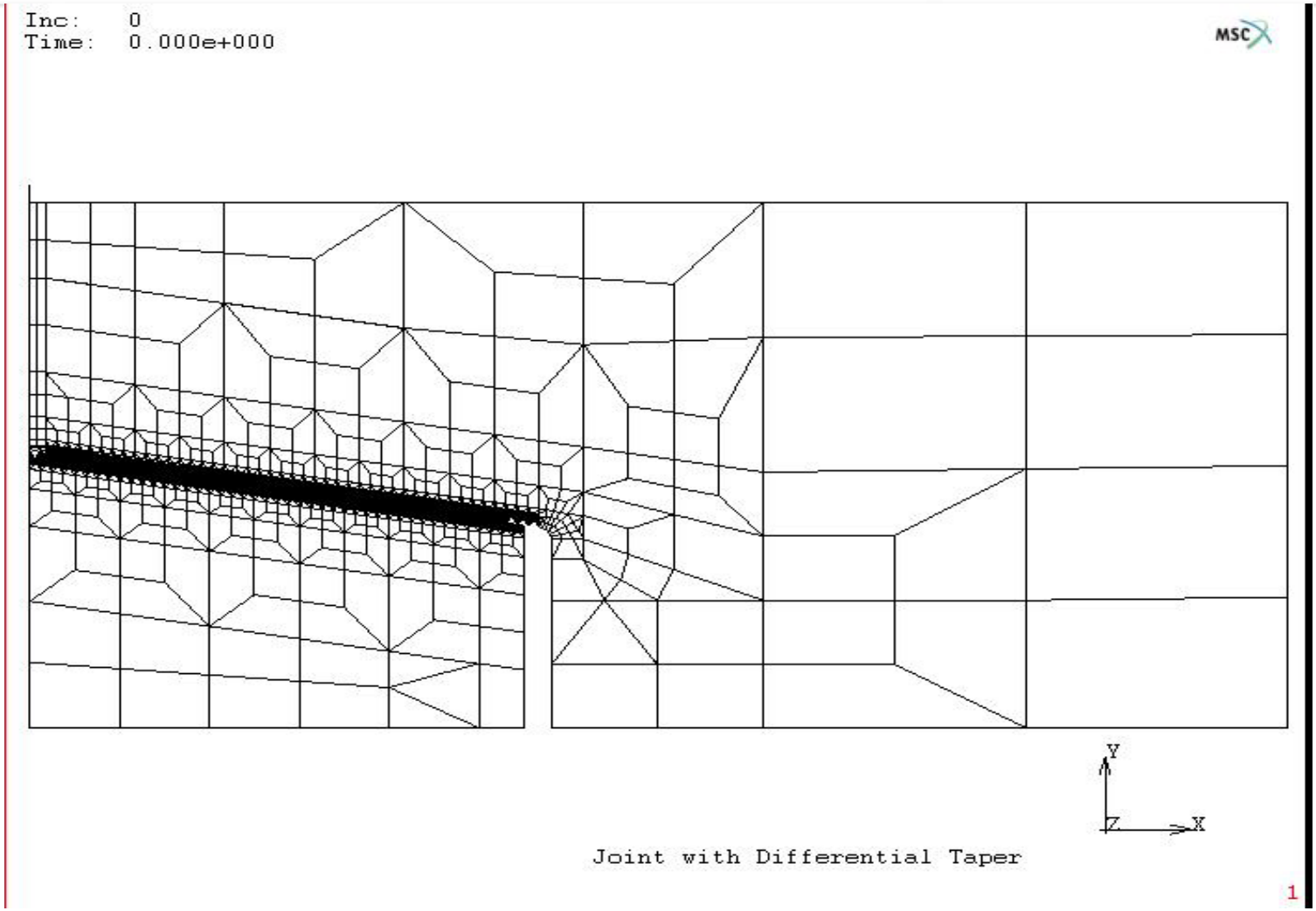
Thermal Contact Input

- Hct – contact thermal coefficient
- Hcve – environment thermal coefficient
- Tsink – sink temperature
- Hcv – near convective coefficient
- Hnc – near natural convection coefficient
- Bnc – exponent for natural convection
- Em – emissivity
- Hbl – lower limit of distance dependent convection coeff
- Dqnear – distance below which near thermal behavior is applied

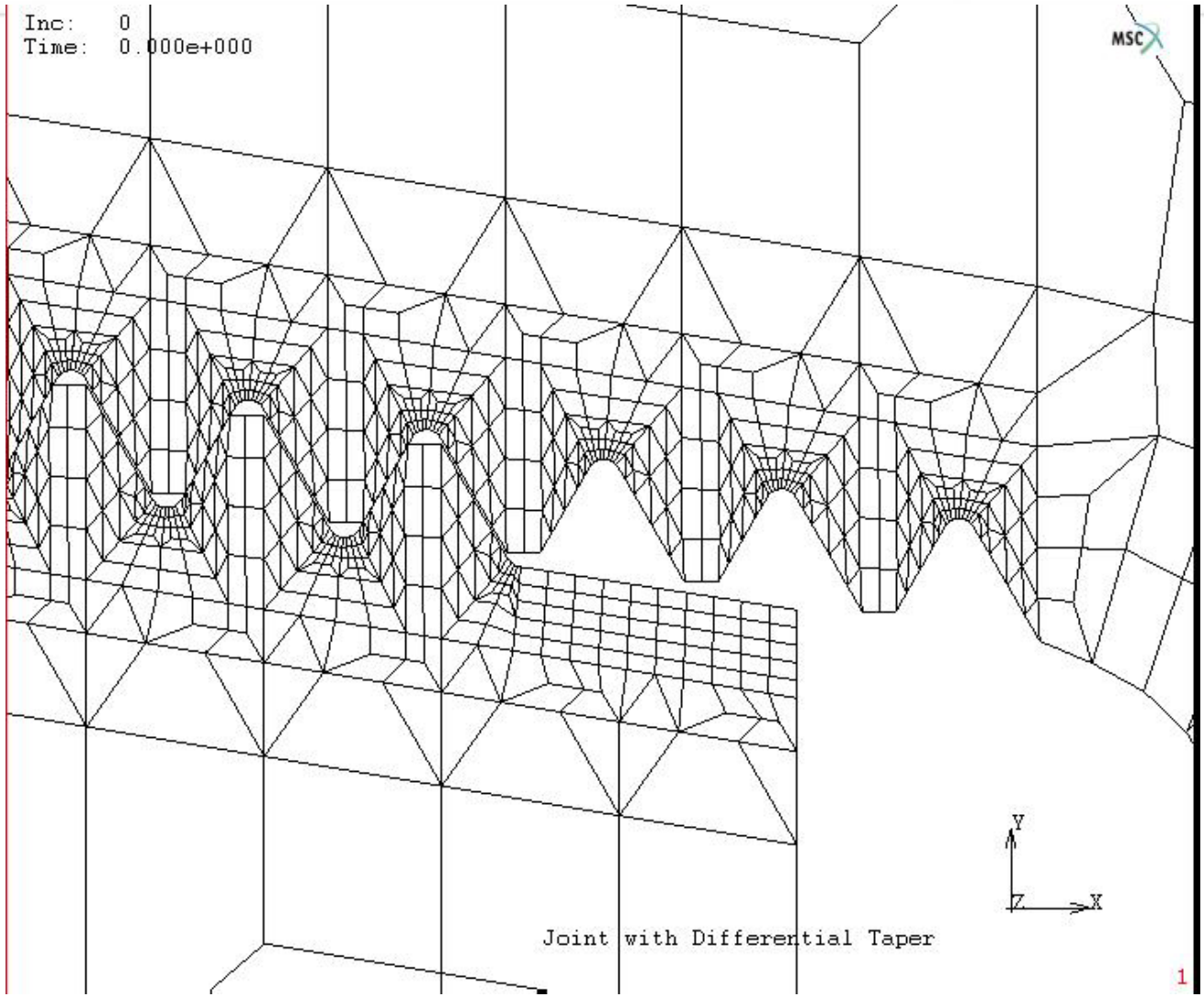
Coupled Joule Heating

- Weak coupling between mechanical, thermal, and electrical fields
- Typical application: high voltage electrical switch
- Electronic circuits

High Voltage Device



Close up of Threads



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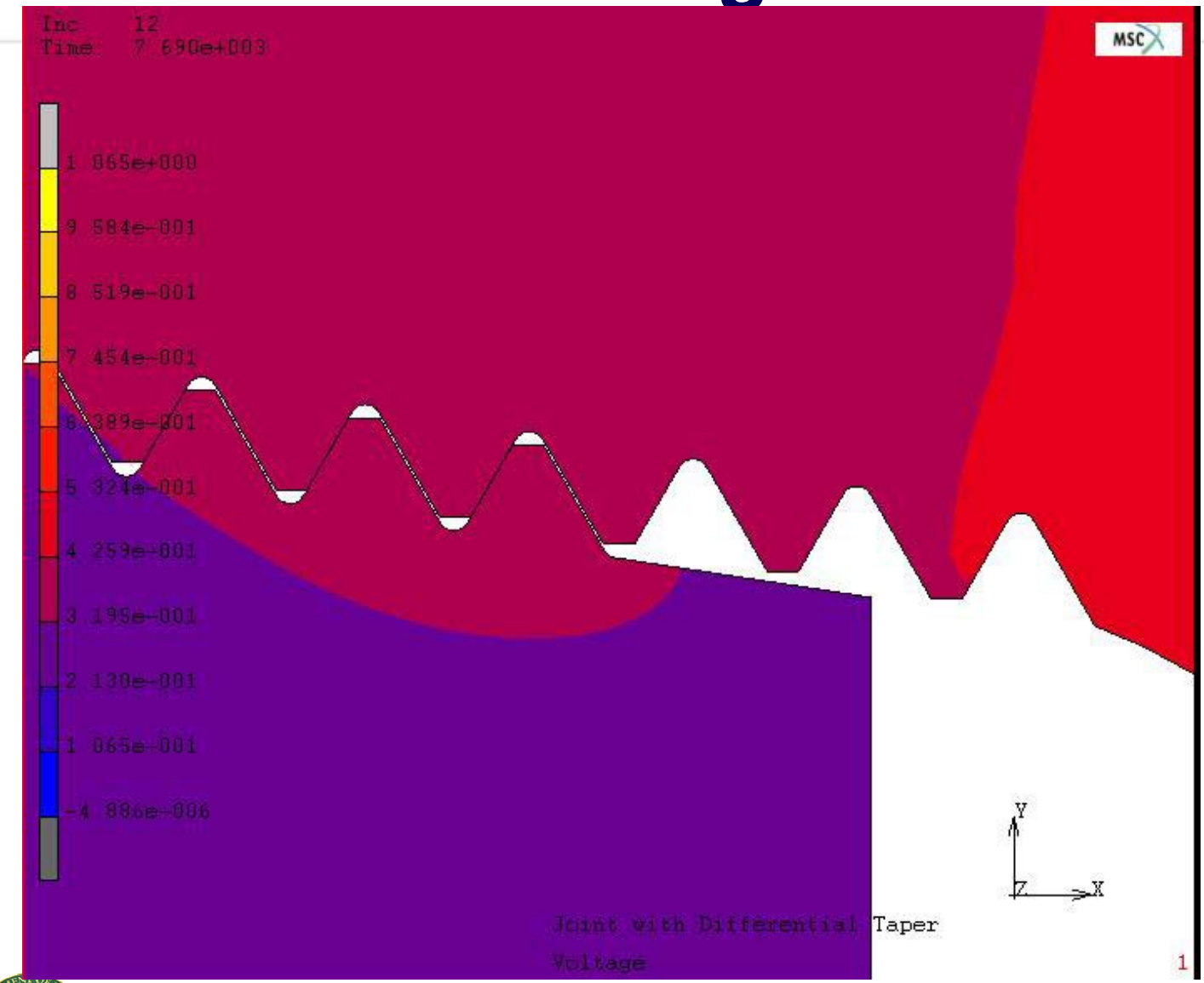
Voltage



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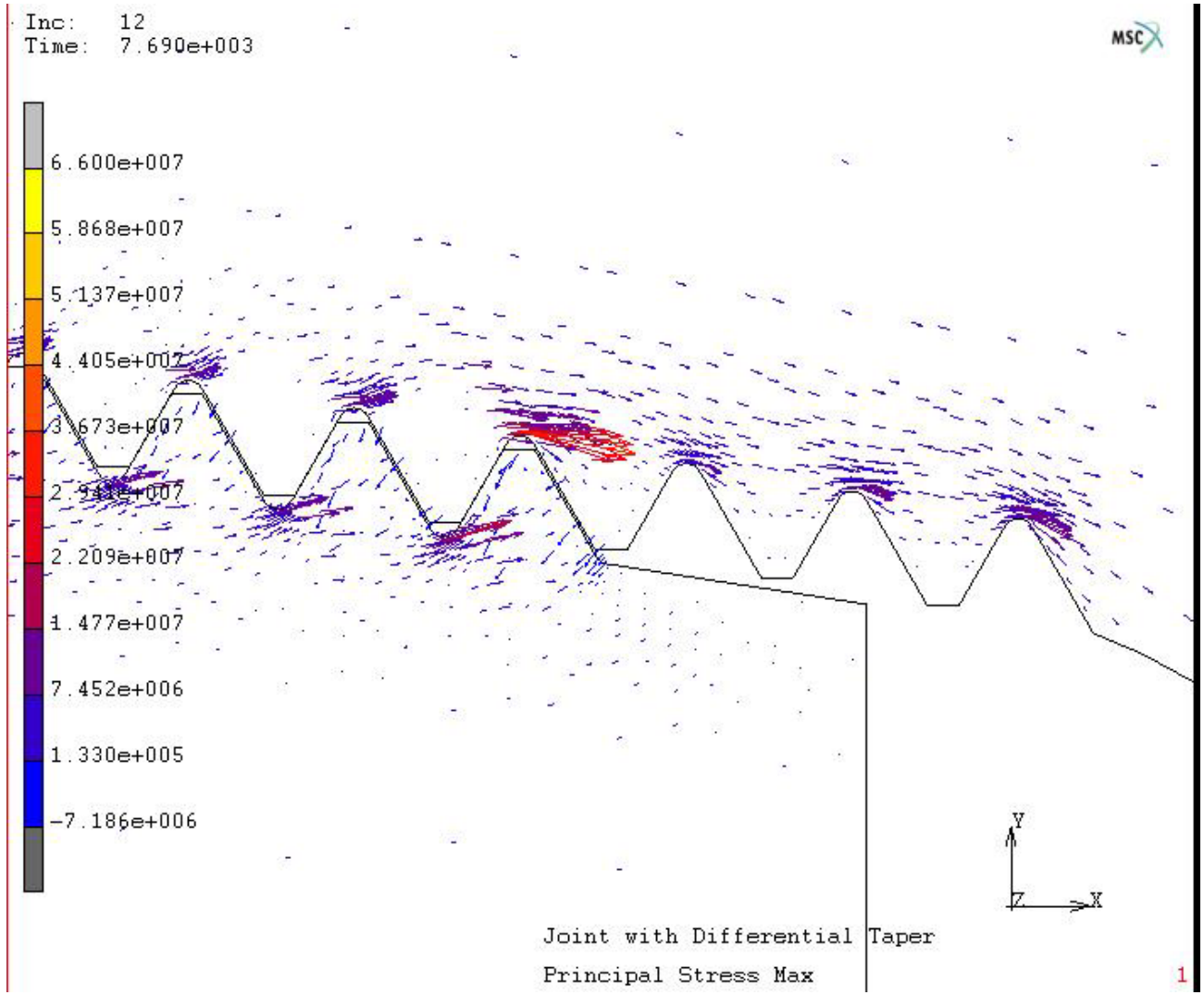
Induced Stress Due to Contact and Thermal Strains



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MSC SOFTWARE SIMULATING REALITY

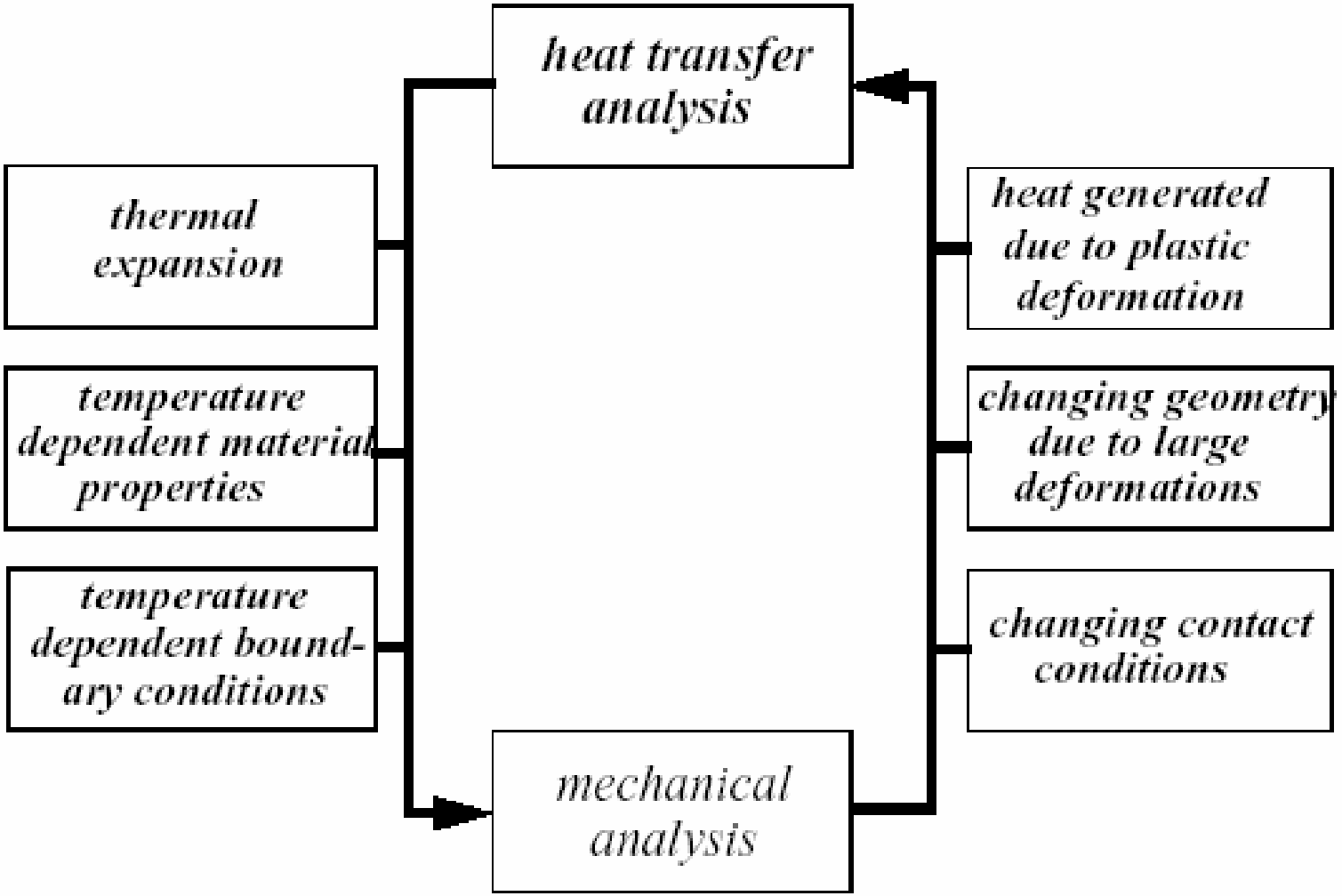
Fluid –Thermal Analysis

- Navier Stokes Finite Element Procedure Used
- Tightly Coupled Analysis
- Incompressible Fluid
- Laminar Flow
- Newtonian or Non-Newtonian Fluid
- 2D or 3D fluid flow with any type of element
- Forced or Free Convection

Fluid-Thermal Applications

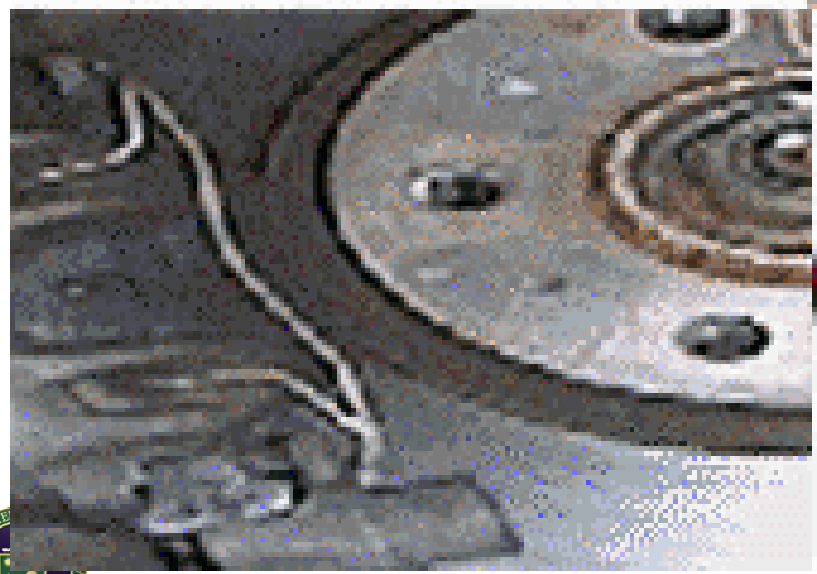
- Electronic Packaging
- Quenching
- Fuel Cells

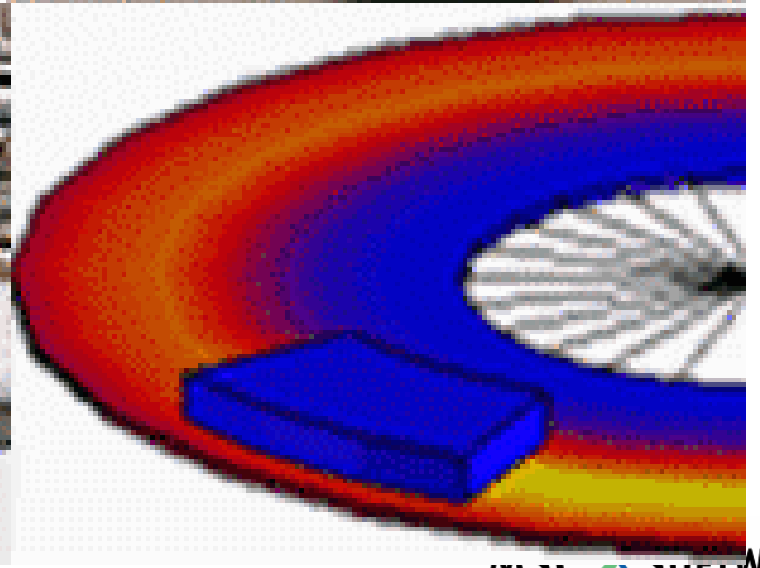
Coupled Thermal Stress



Disc Brake

Disc Brake
Dynamics
Coupled
Contact





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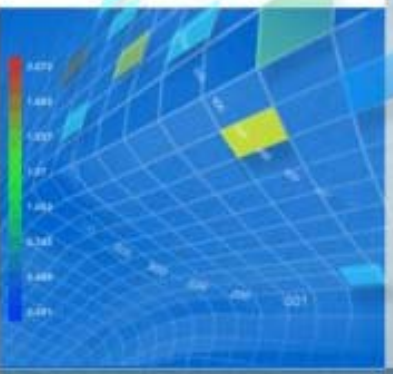
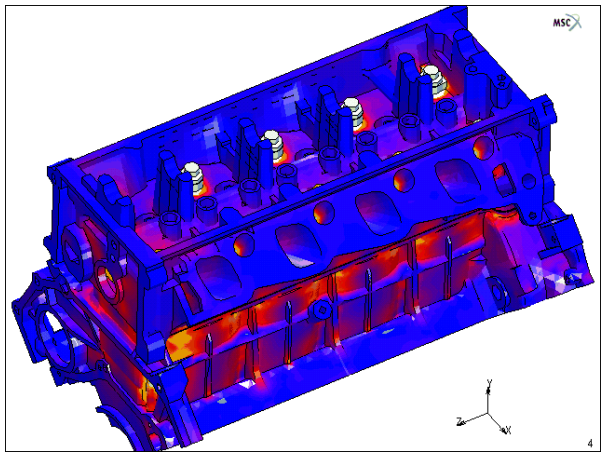
Parallelization

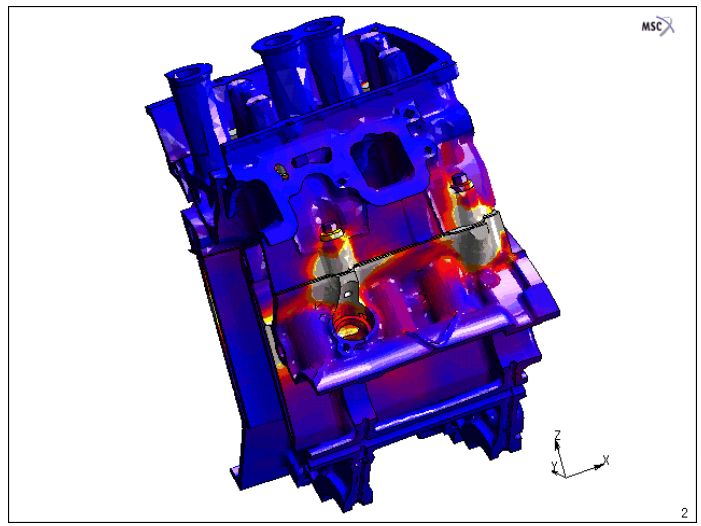


Super Scalable Parallel

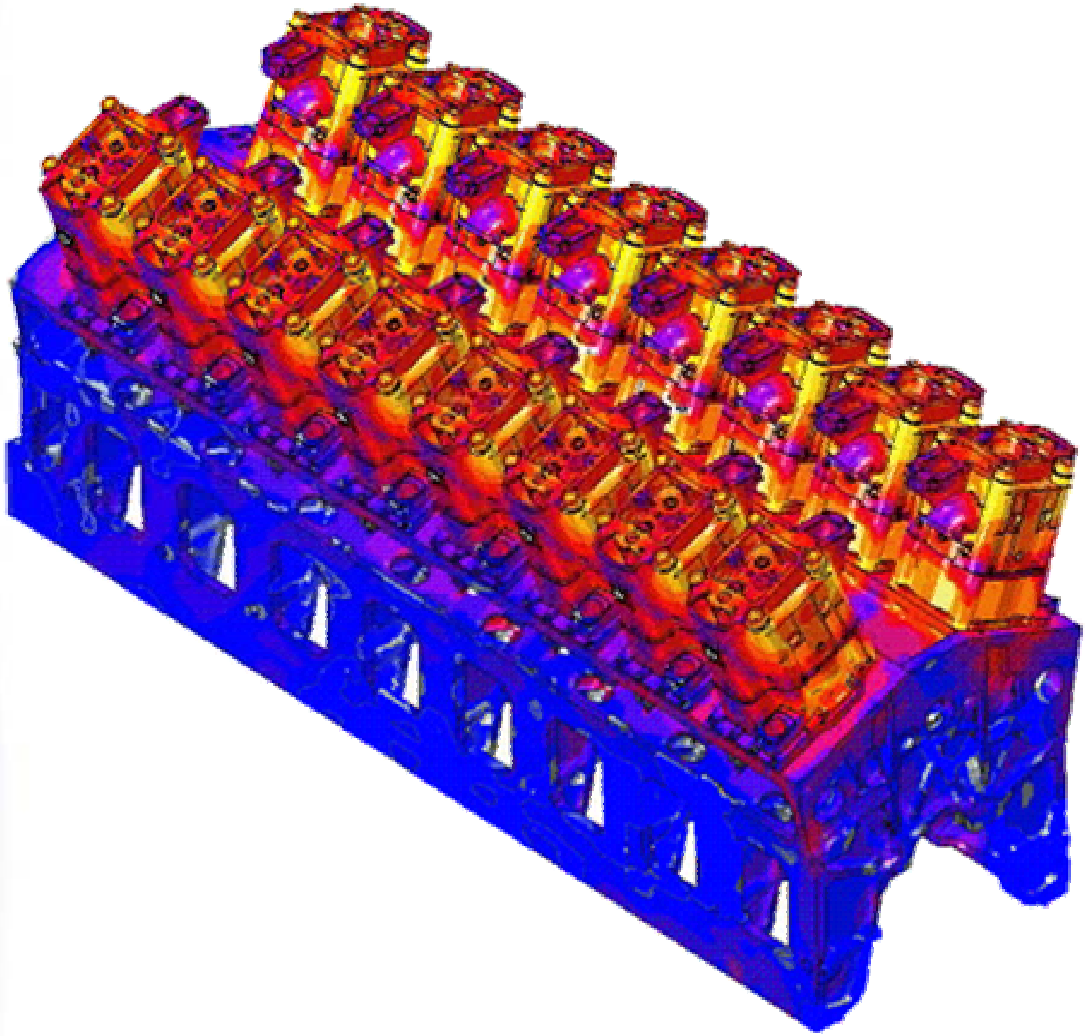
Number Of CPU's	1	2	4
CPU Time (sec)	6429	2491	1128
Speedup	1.0	2.6	5.7

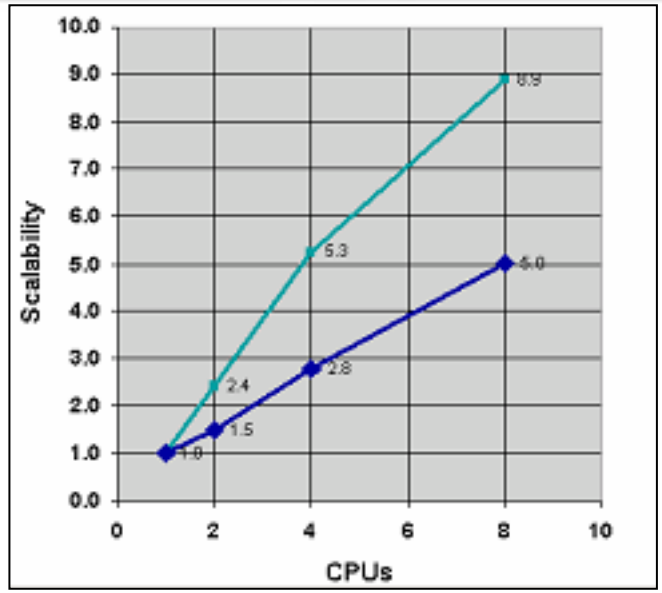
Linux cluster of 4 HP workstation xL-class with two of Intel's® Pentium® III 1GHz processors and 4GB of RAM/CPU





Parallel for Engine Assembles





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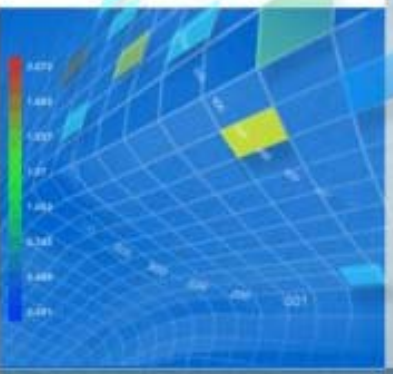
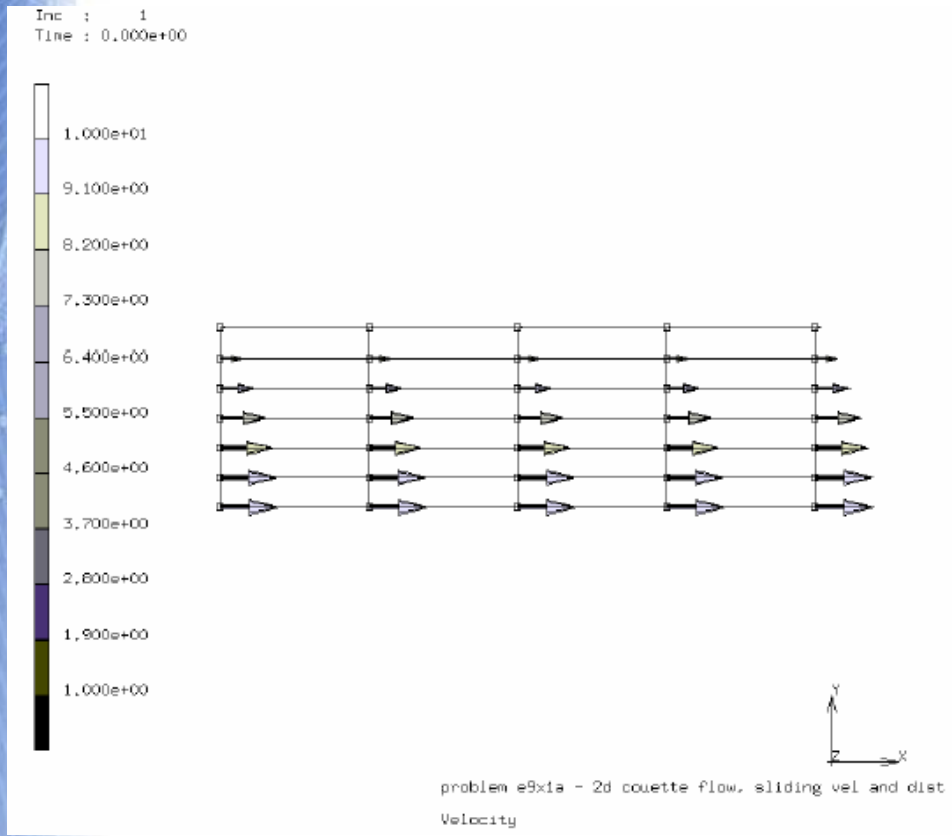
Fluids



MSC.Marc Volume E: Fluid Demonstration Problems

9.1	Planar Couette Flow, 9.1-1
9.2	Poiseuille Flow, 9.2-1
9.3	Fluid Squeezed Between Two Long Plates, 9.3-1
9.4	Driven Cavity Flow, 9.4-1
9.5	Flow Past a Circular Cylinder, 9.5-1
9.6	Flow Over Electronic Chip, 9.6-1
9.7	Natural Convection, 9.7-1
9.8	Flow Around Tubes, 9.8-1

Plot of the Couette Flow Velocity Field



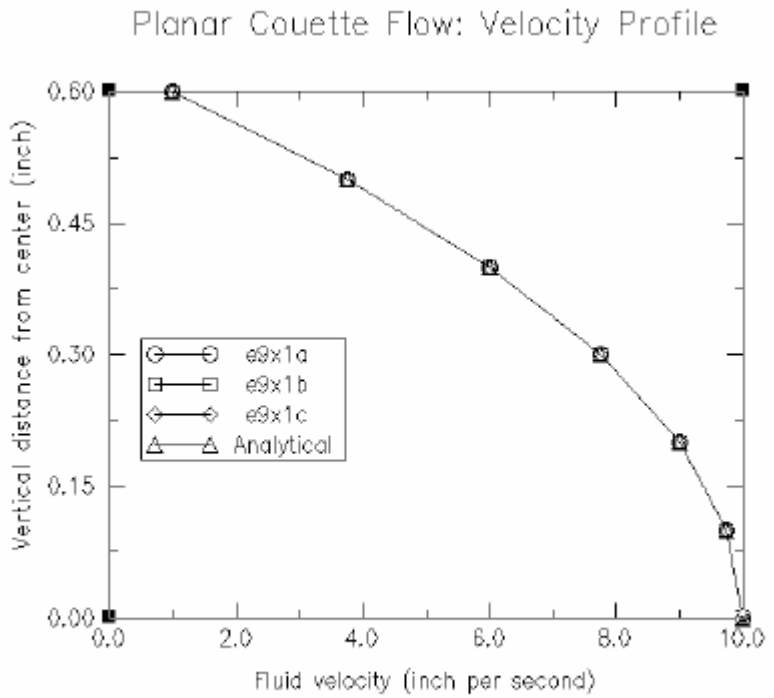


Figure 9.1-4 Comparison of Computation and Analytical Results

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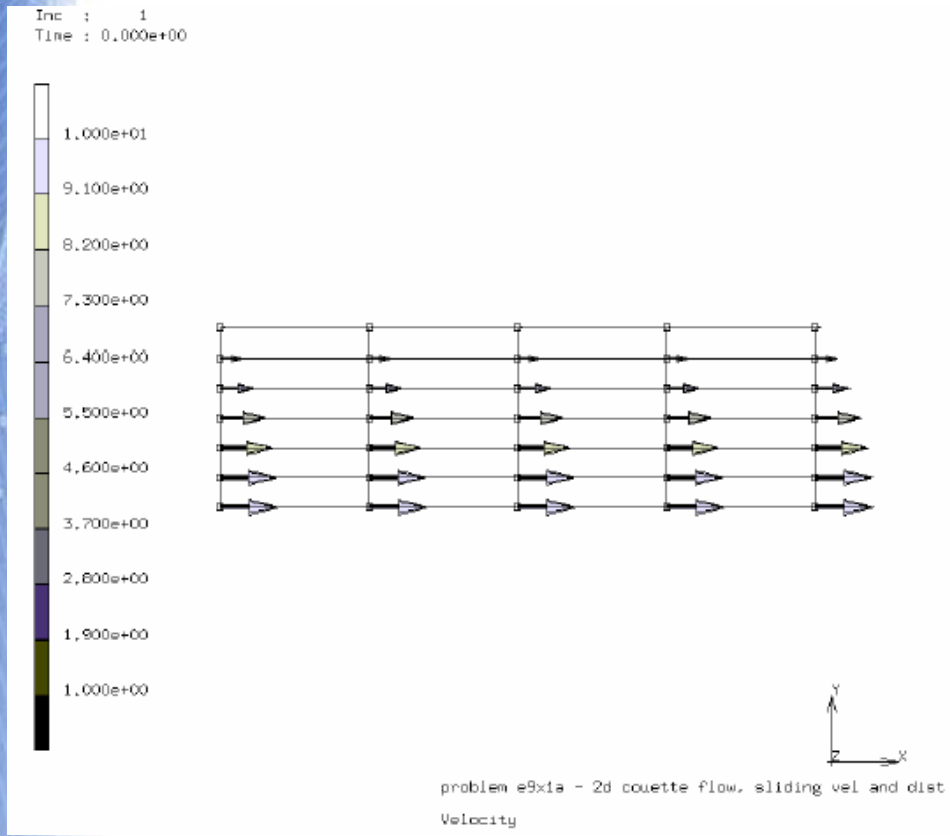
Plot of the Poiseuille Flow Velocity Field



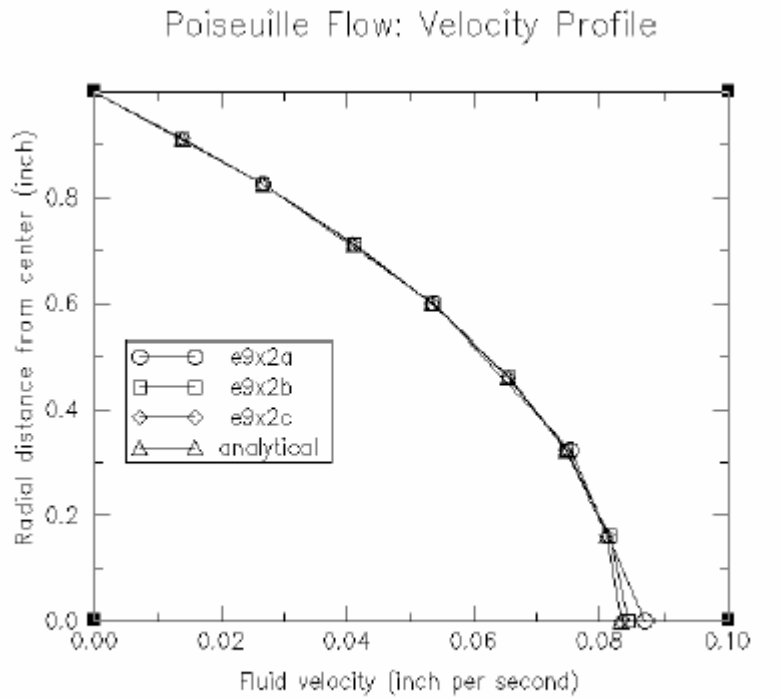


Figure 9.2-4 Comparison of Computation and Analytical Results

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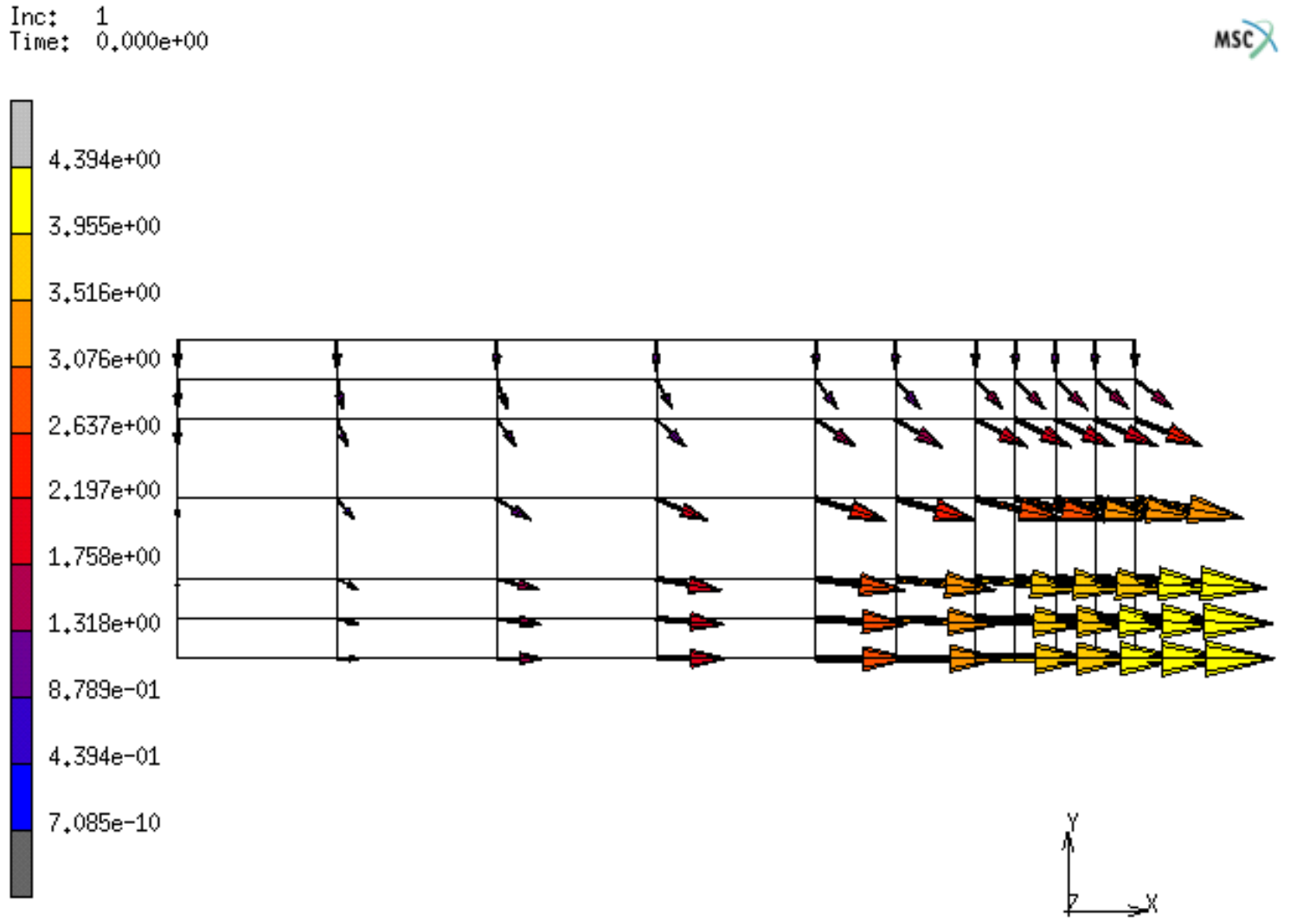
Fluid Squeezed Between Two Long Plates



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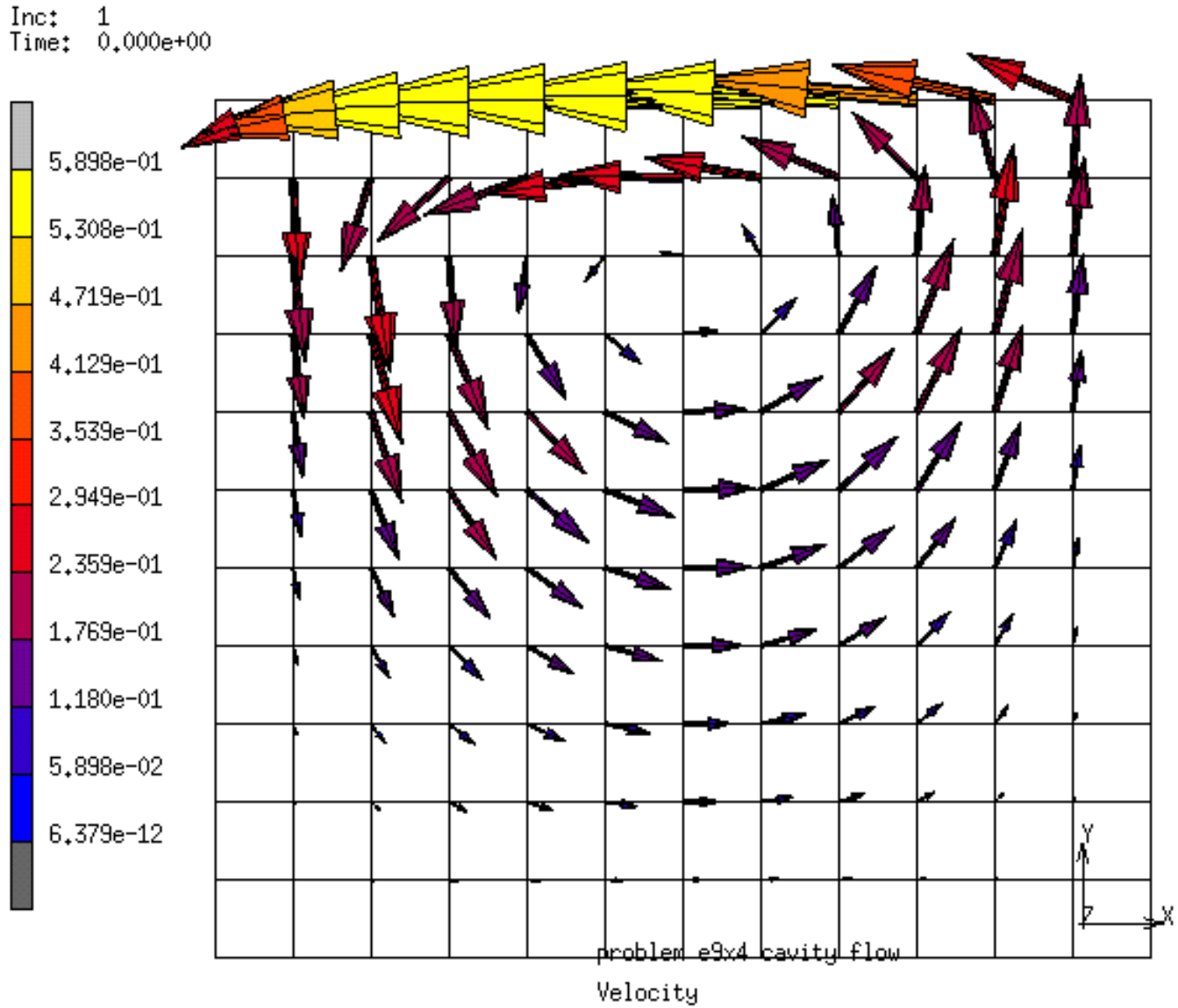
Vector Plot: Driven Cavity Flow Velocity Field



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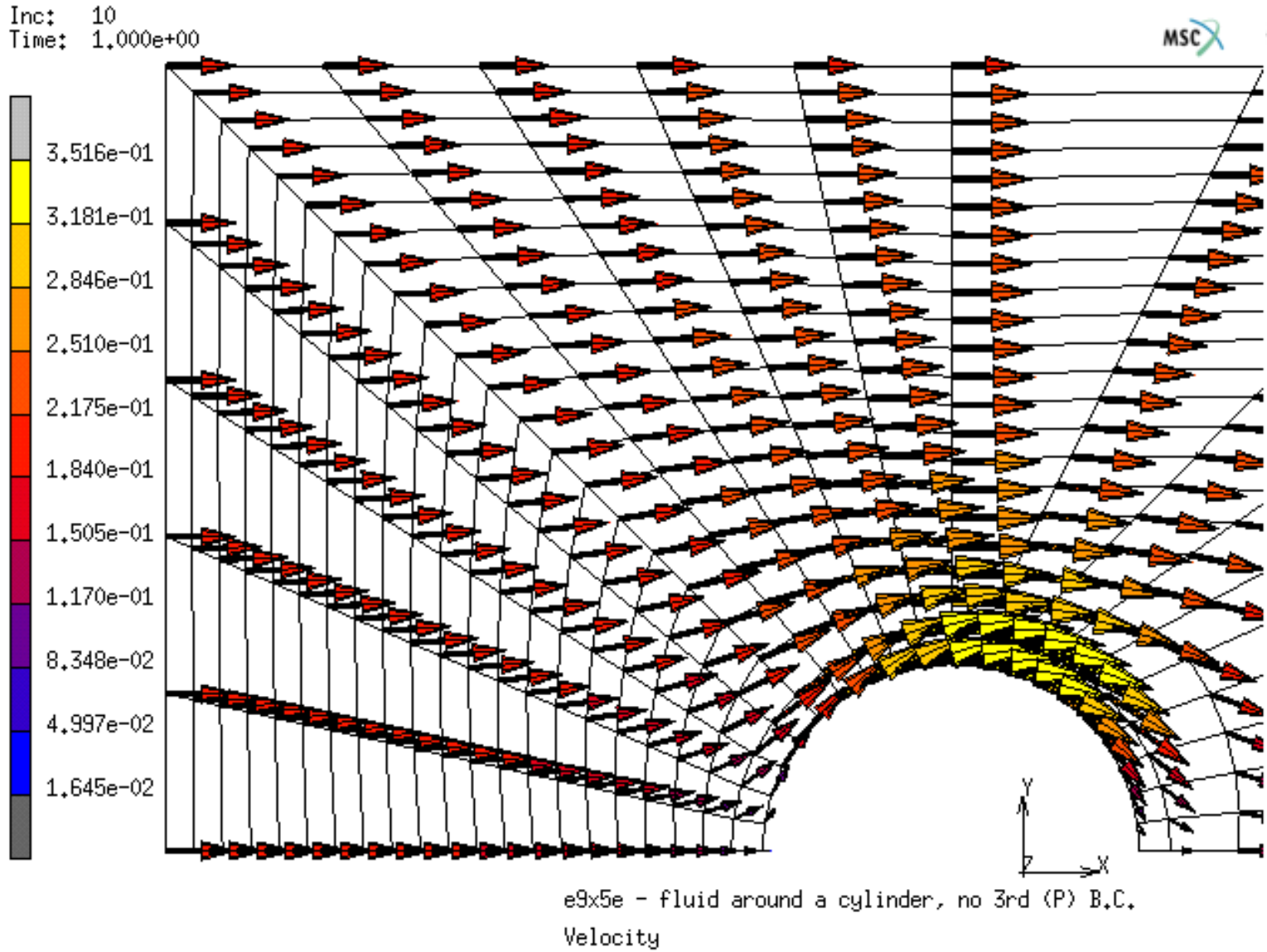
Flow Over Cylinder Transient Velocity Field



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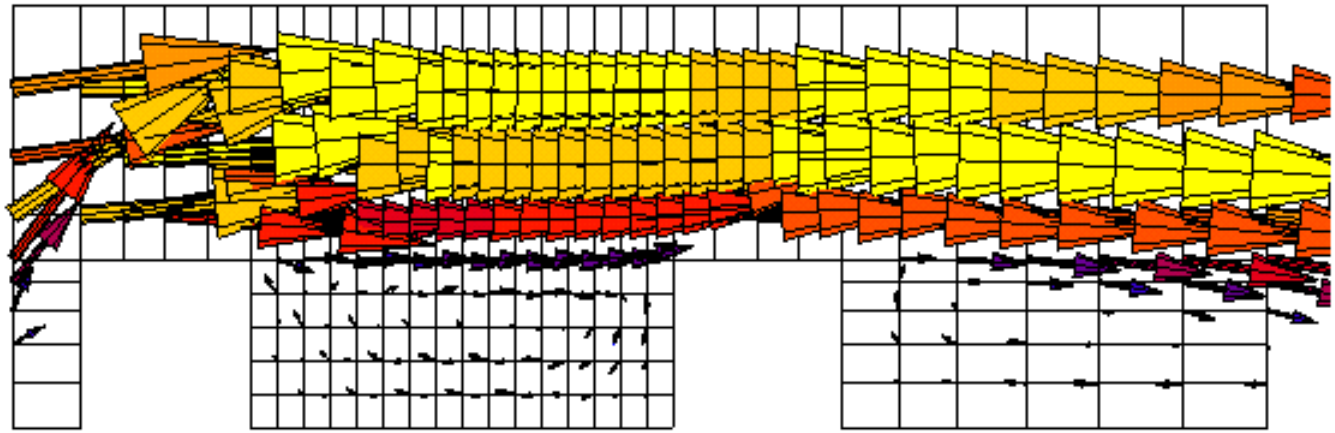
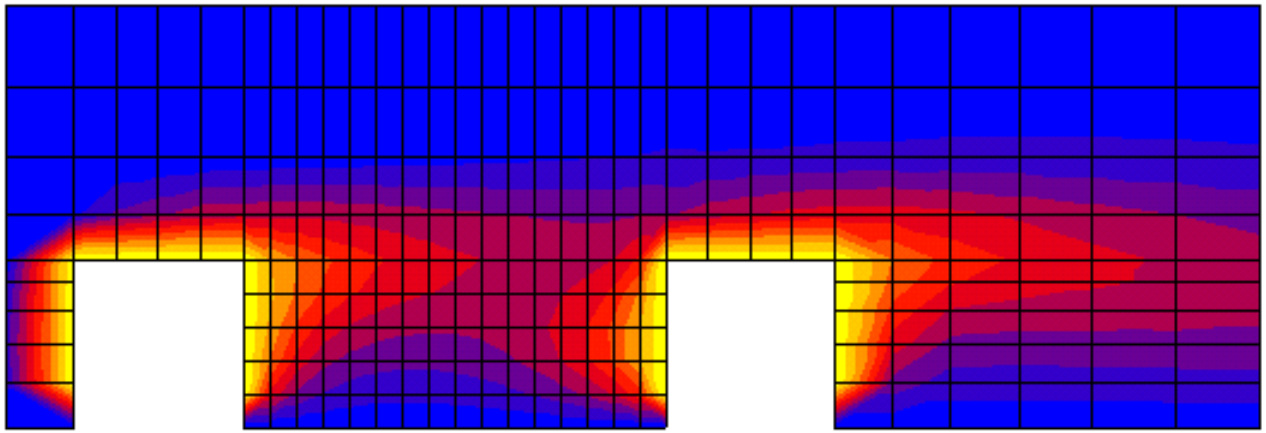
Flow Over Electronic Chip

Velocity Vector

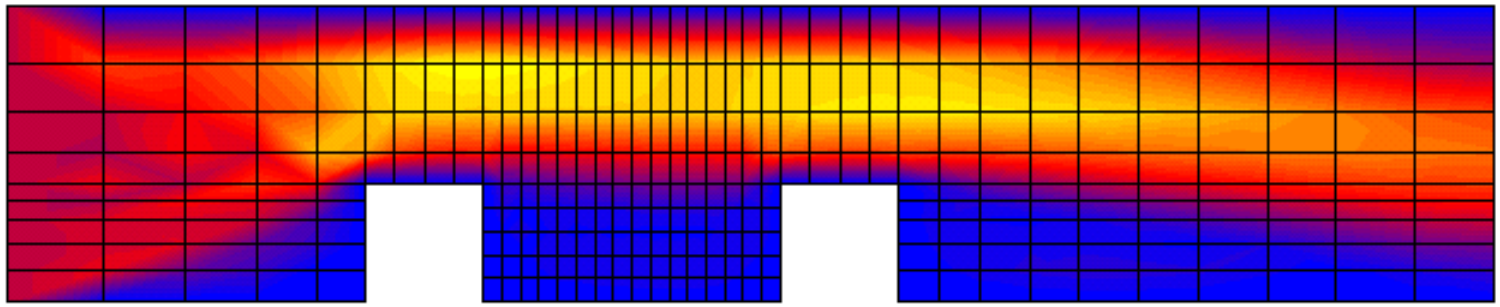


Temperatue



Flow Over Electronic Chip

Velocity Magnitude



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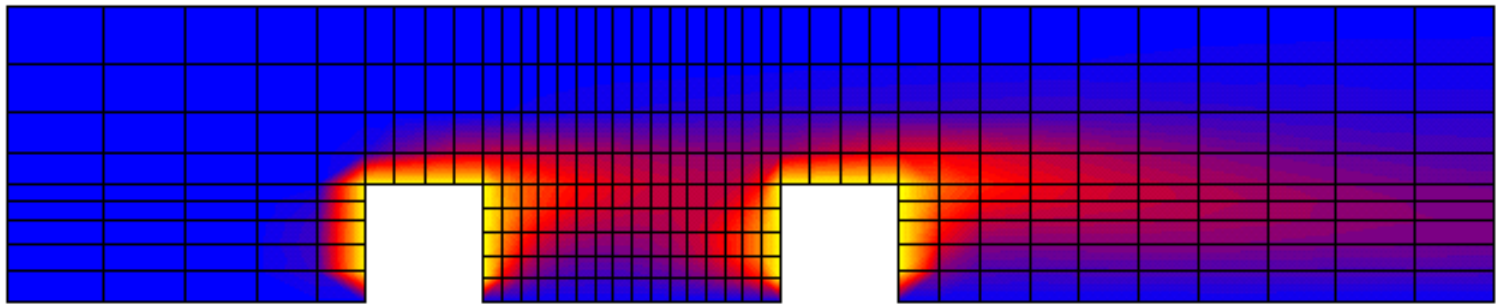

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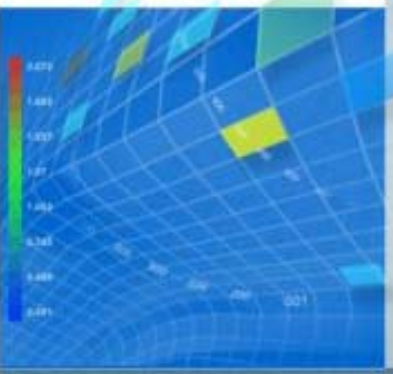
User Subroutines



Over 100 User Subroutines

Output Quantities Subroutines

User Subroutine	Required Parameters or Model Definition Options	Purpose
ELEVAR	UDUMP	Allows postprocessing of element results.
ELEVEC	UDUMP	Allows postprocessing of element results in harmonic analysis.
INTCRD		Makes available integration point coordinates.
IMPD	UDUMP	Allows postprocessing of nodal vector results.
PLOTV	POST	Defines element quantity to be written to post file.
UBGINC		Dummy routine available at the beginning of each increment.
UBGITR		Dummy routine available at the beginning of
UEDINC		
UELOOP		
UPOSTV	POST	

Loads and Boundary Conditions Subroutines

User Subroutine	Required Parameters or Model Definition Options	Purpose
CREDE	THERMAL LOADS	Definition of state variable including temperature.
CUPLFX	COUPLE DIST FLUXES (flux type 101)	Heat generated due to inelastic behavior in coupled analysis.
DIGEOM	CONTACT (2D) CONTACT (3D)	Definition of rigid surface.
FILM	HEAT or COUPLE FILMS (Model Definition) FILMS (History Definition)	Definition of convective heat transfer coefficient and sink temperature.
FLOW	HEAT CHANNEL	Definition of mass flow rate.
FLUX	HEAT or COUPLE DIST FLUXES (Model Definition) DIST FLUXES (History Definition)	Definition of distributed flux.
FORCDF	FORCDT FIXED DISP or DISP CHANGE	Definition of point load or kinematic boundary condition in a harmonic analysis.

Example

```
c*********************************************************************
      subroutine flux(f,ts,n,time)
c*********************************************************************
      implicit real*8 (a-h,o-z)                                        dp
c dimensions for FLUX subroutine
      dimension ts(6),n(7),thick(5)
c
c  dimension of arrays for passing data to the Electrochemistry Module
c
      integer ncell,ngridx,ngridy,ngridair,ngridz,ivchange
      integer i,j,k,l,m,ivflag,iu,iv
      integer ngridzi(4),ivflag,nd,nfueltype,nspecies,iflowtype
.................................
c
c   initialize parameters
       call ini_set(lxcell,lycell,ivflag,lair,lfuel,
     &   vtot,itot,ufuel,
     &   pin,iflowtype,nfueltype,ngridair,
     &   ncell,ngridx,ngridy,ngridz,nspecies,txyzn,qxyzn,pxyn,
     &   up,fuelvxn,tfuelxn,ap,thick,
     &   lzcell,airvn,tairn,tairxyn,tfuelxyn)

       nbhb = 999
.................................
c     FOLLOWING SECTION CALCULATES INTEGRATION POINT TEMPERATURES
c
c     Code is valid for any kind of problem where temperature at
c     integration points is available
c     Following code is set up for continuum elements (number of layers = 1)
c     icode = 9 = temperatures at integration points
c
            layer = 1
            icode=9
c  average temperatures for number of integration points per element
            ttl = 0.0
c  nn= integration point number
            do nn=1,numip
             call elmvar(icode,m,nn,layer,var)
             tmp = var
             ttl = ttl + tmp
            enddo
 ....................................
c  run EC code once per increment and update state variables
       call udf_qiv(ivflag,itot,vtot,ufuel,nD,ivpower,heattot,
     *  iflowtype,nfueltype,nspecies,
     &  lxcell,lycell,lzcell,
```

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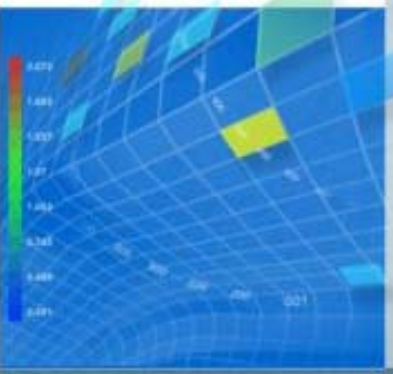

Future Work

On Fuel Cells

Proposed Development

- To develop a customized graphical user interface for fuel cell stacks.
- To integrate an EC module currently used by PNNL into MSC.Marc to be able to analyze the thermal stresses arising as a consequence of the heat production due to chemical reaction in the fuel cell and heat transfer due to convection effects.
- To conduct a feasibility study of the accuracy and efficiency of MSC.Marc for simulating flow fields in a typical fuel cell stack and to use the results of this feasibility study to determine areas of possible improvement in MSC.Marc's fluid capabilities.

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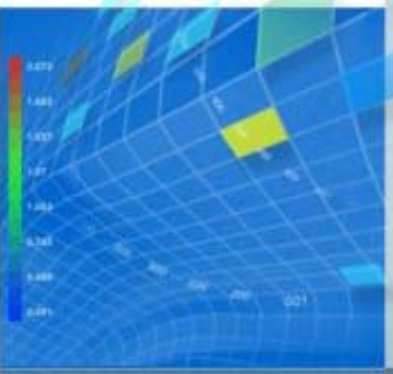
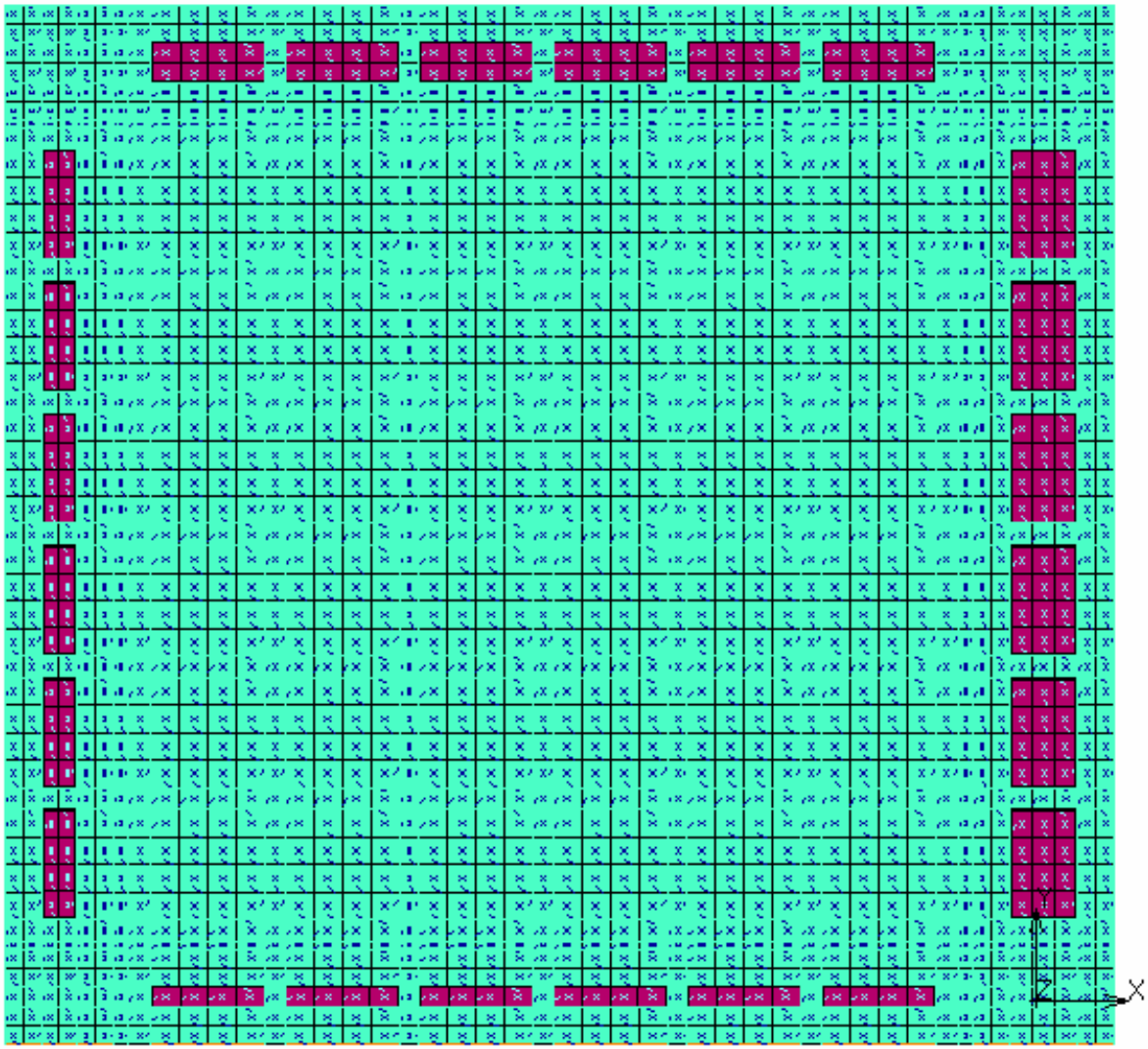
PEN Fuel Cell Modeling



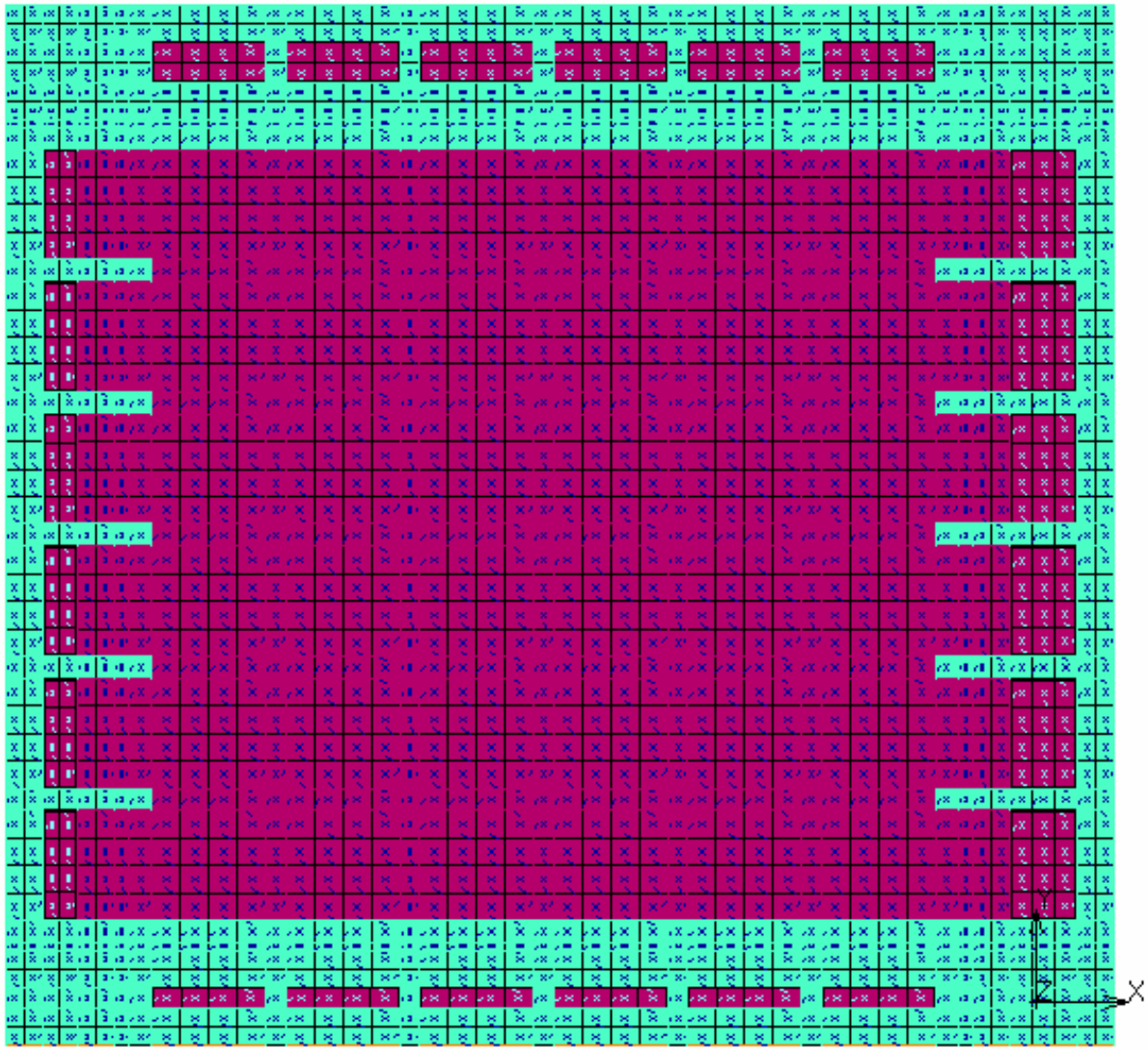
Fuel Cell Layer Configuration

- The following slides show the layers of a typical planar fuel cell design.
- In the example design, the layers stack up to make up air and fuel flow channels on each side of the PEN.
- The PEN has 3 layers, Cathode (air-side), Electrolyte, and Anode (fuel-side). The center area (inside where the PEN seals to the picture-frame) is where the electrochemistry occurs.
- The following slides show "footprints" of the various layers (the selected areas show in the blue-green color).
- The layers are listed in the order from the interconnect (conductive layer between stacked cells), to the cathode-side layers,the PEN, anode-side layers, to the interconnect on the anode-side.
- The last 2 slides show the layers from bottom (cathode) and top (anode) views with the interconnect layers removed.
- The flow/ heat transfer/EC/stress model must have the necessary connectivity through all these layers, including through the flow channels where no mesh is shown in the last 2 slides.

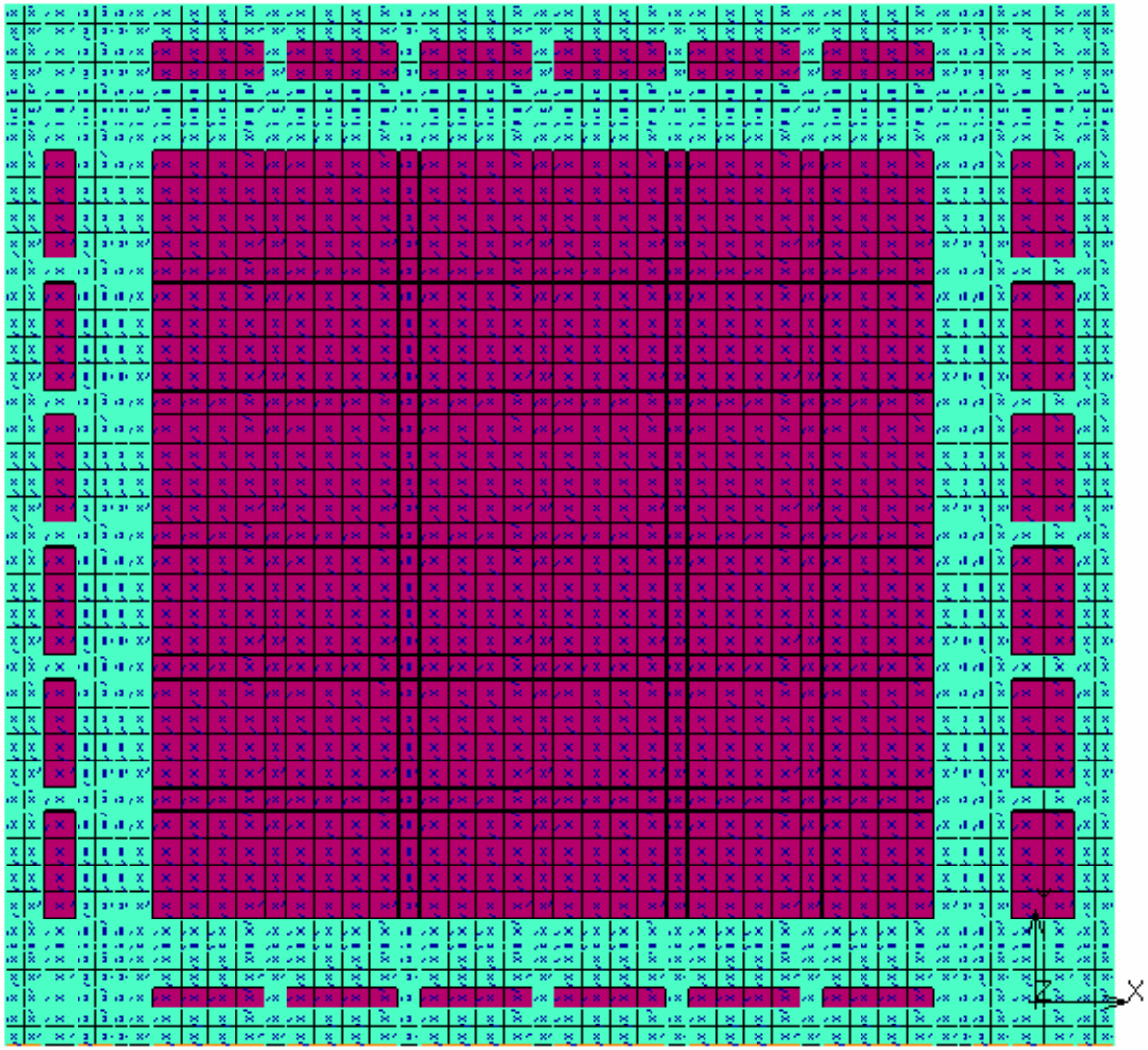
Interconnect



Cathode Spacer



Picture Frame

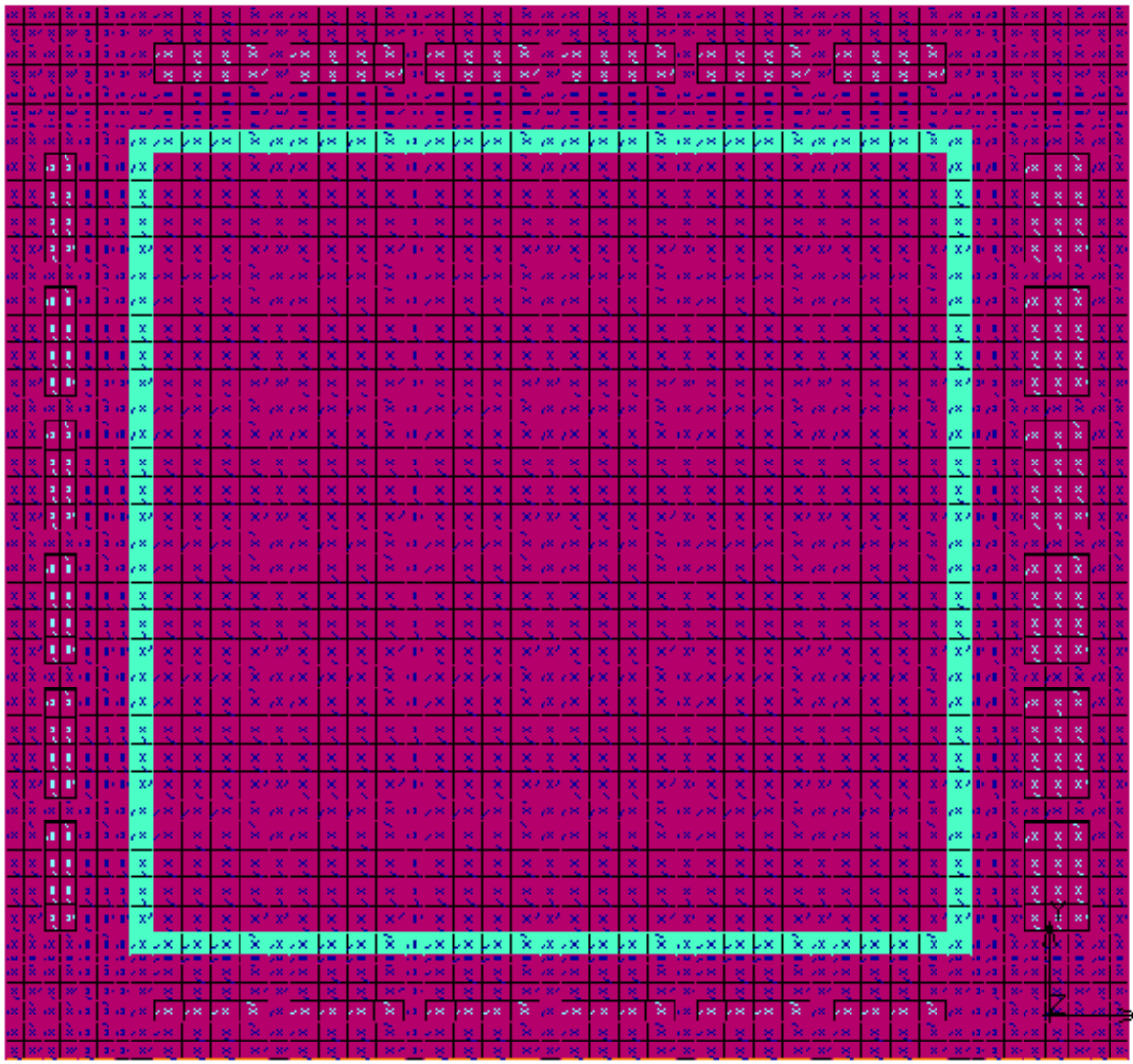


PEN Inactive Area

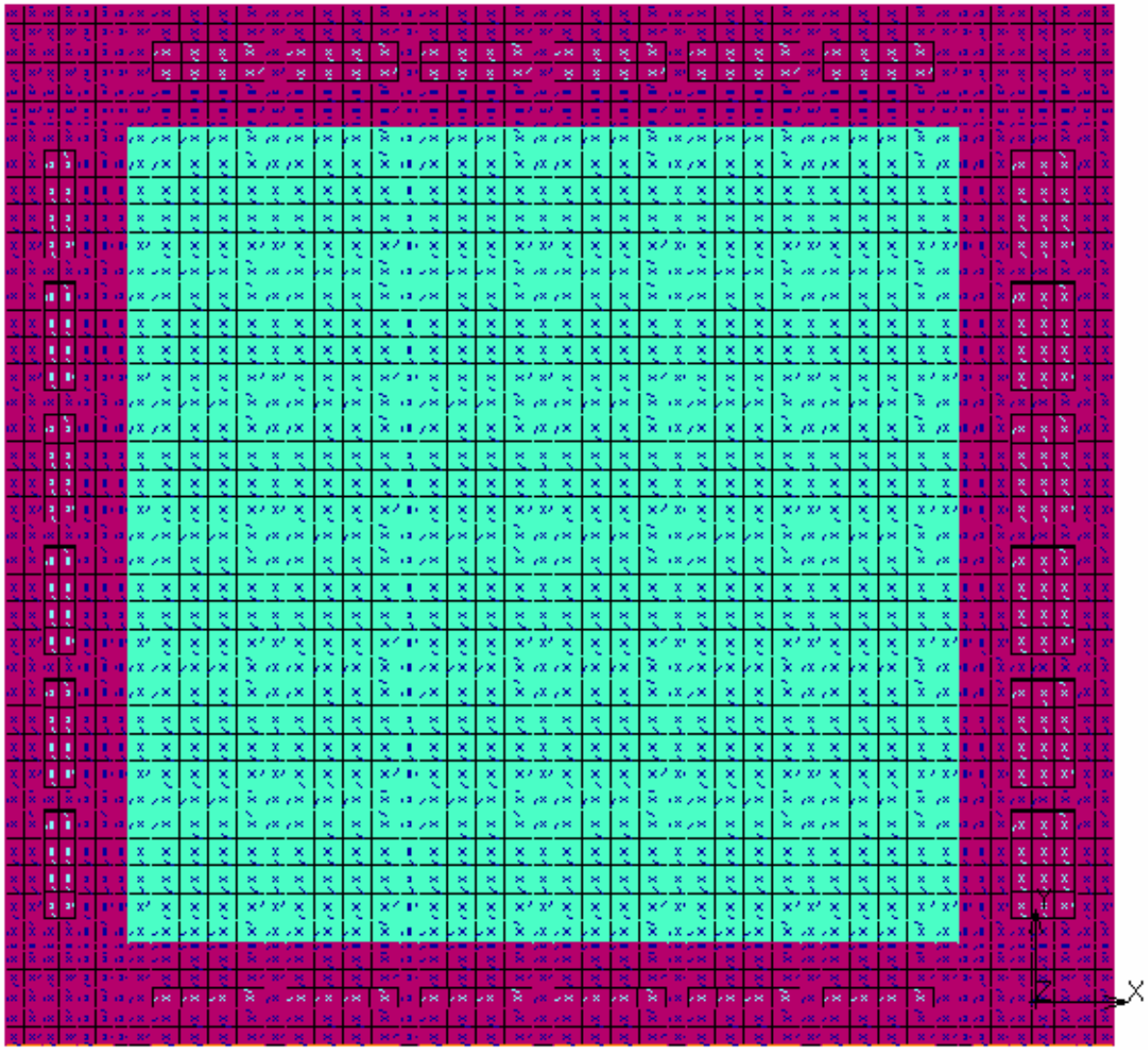
Pen Inactive Area,

Pen-to-Picture frame Seal

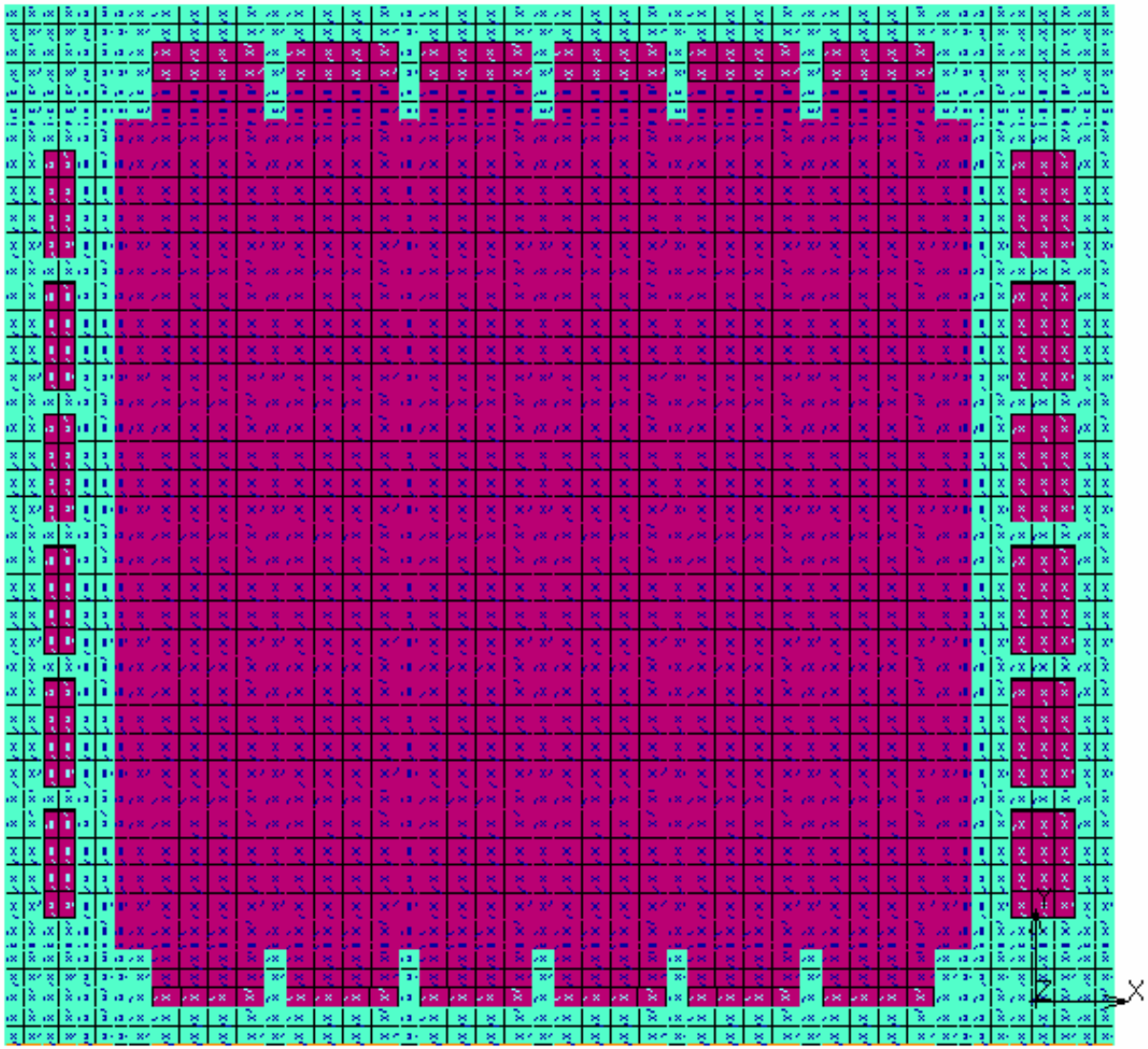
(both same Footprint)



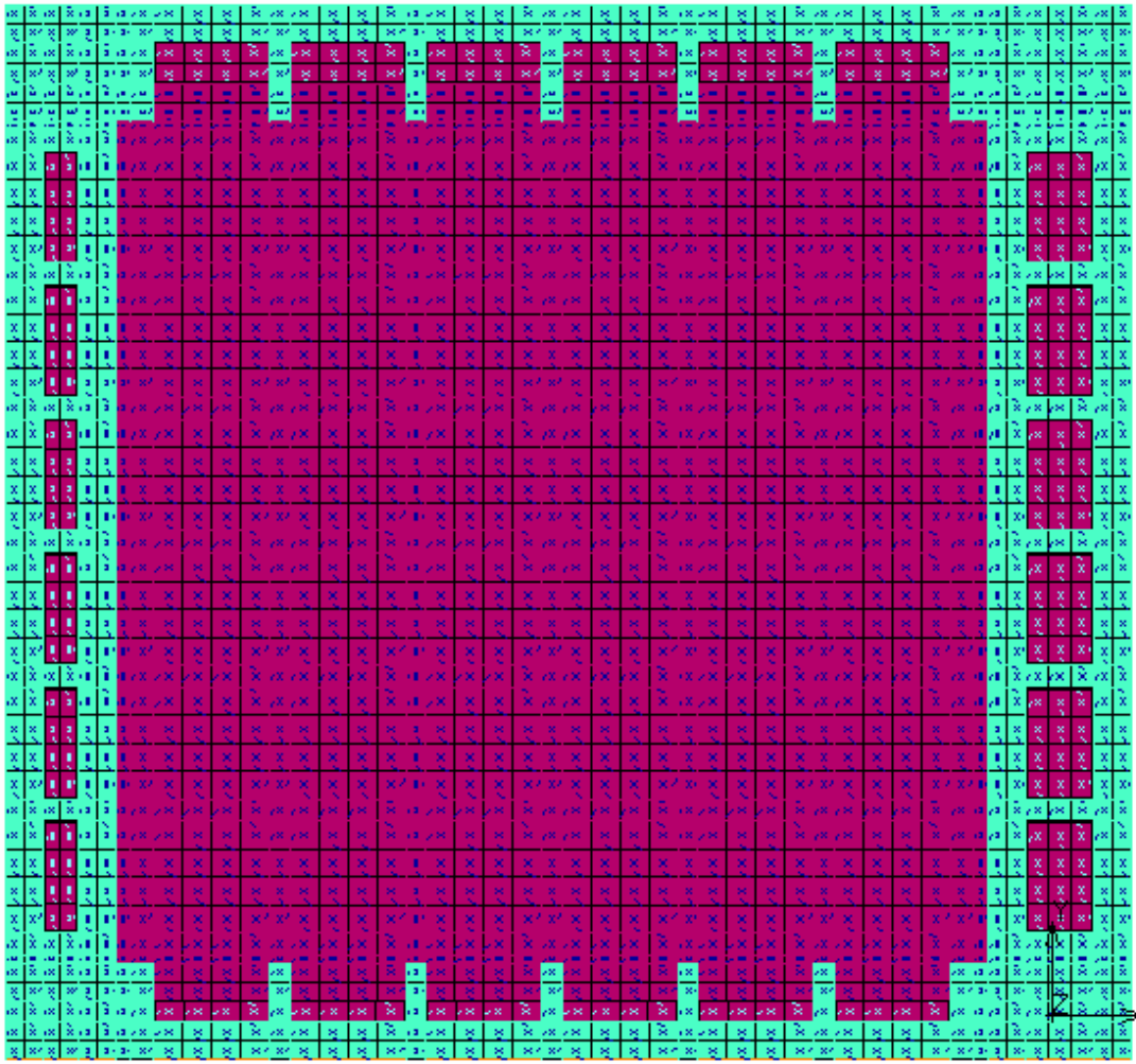
PEN



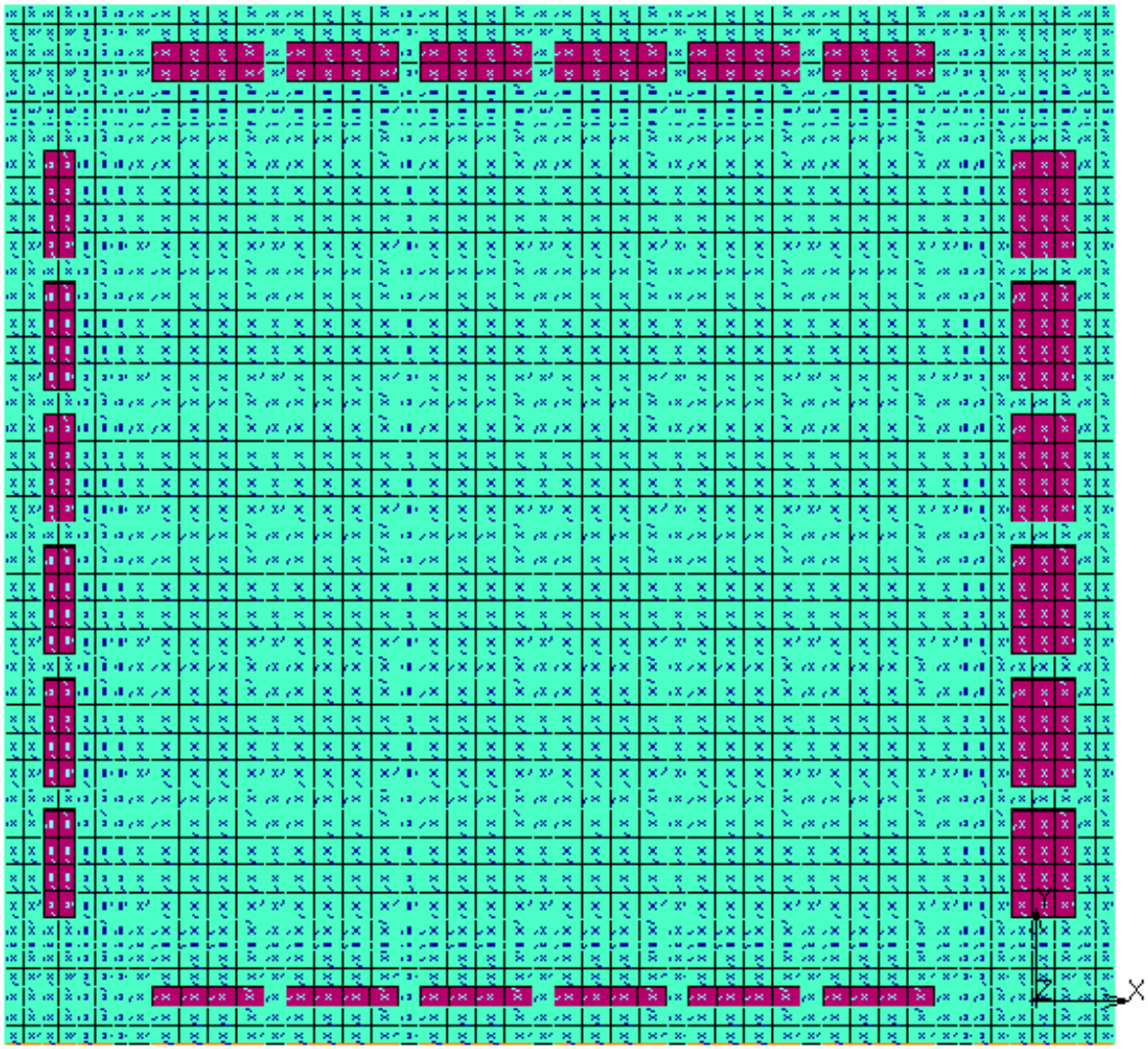
Anode Spacer



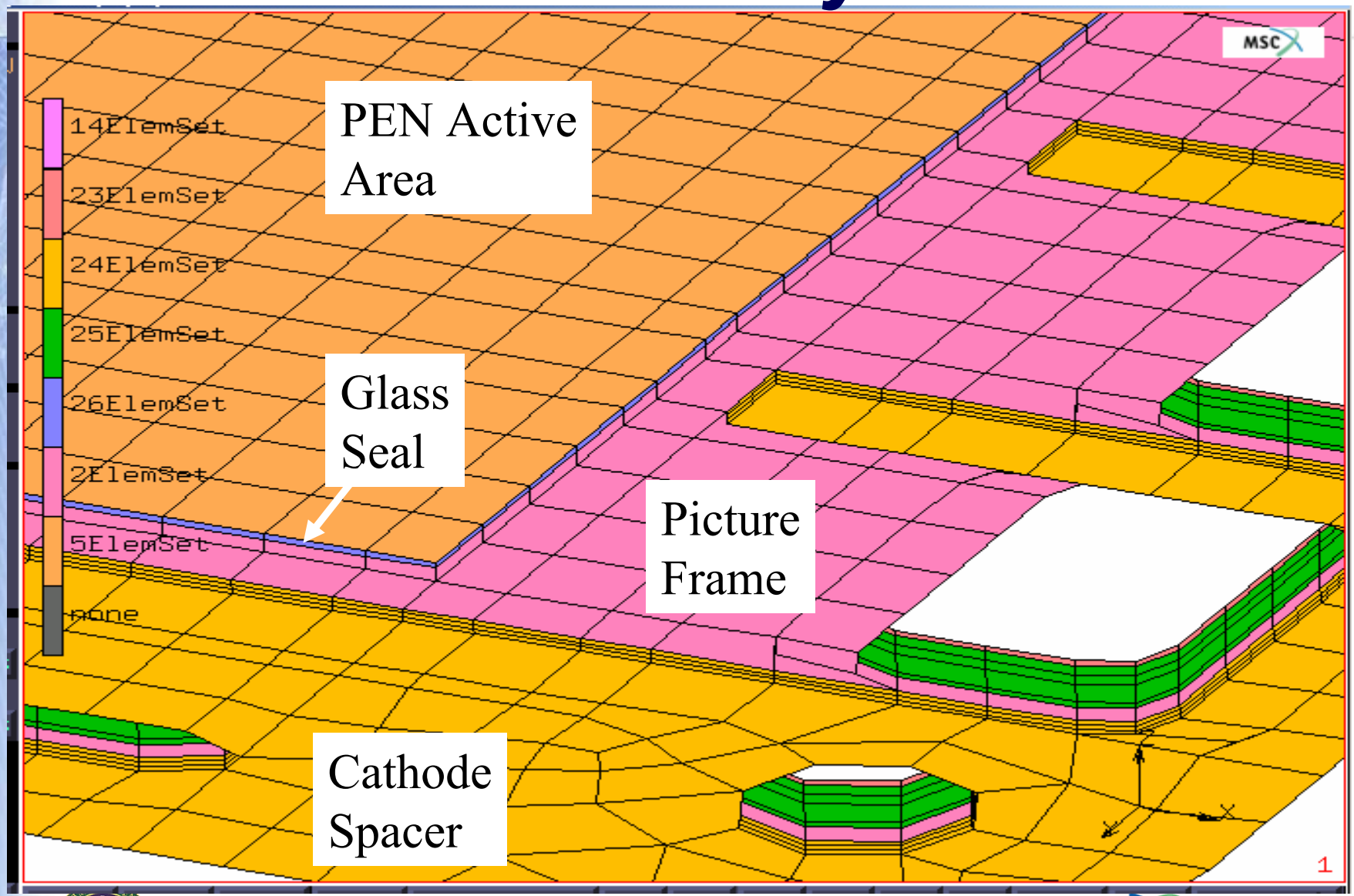
Seal to Interconnect



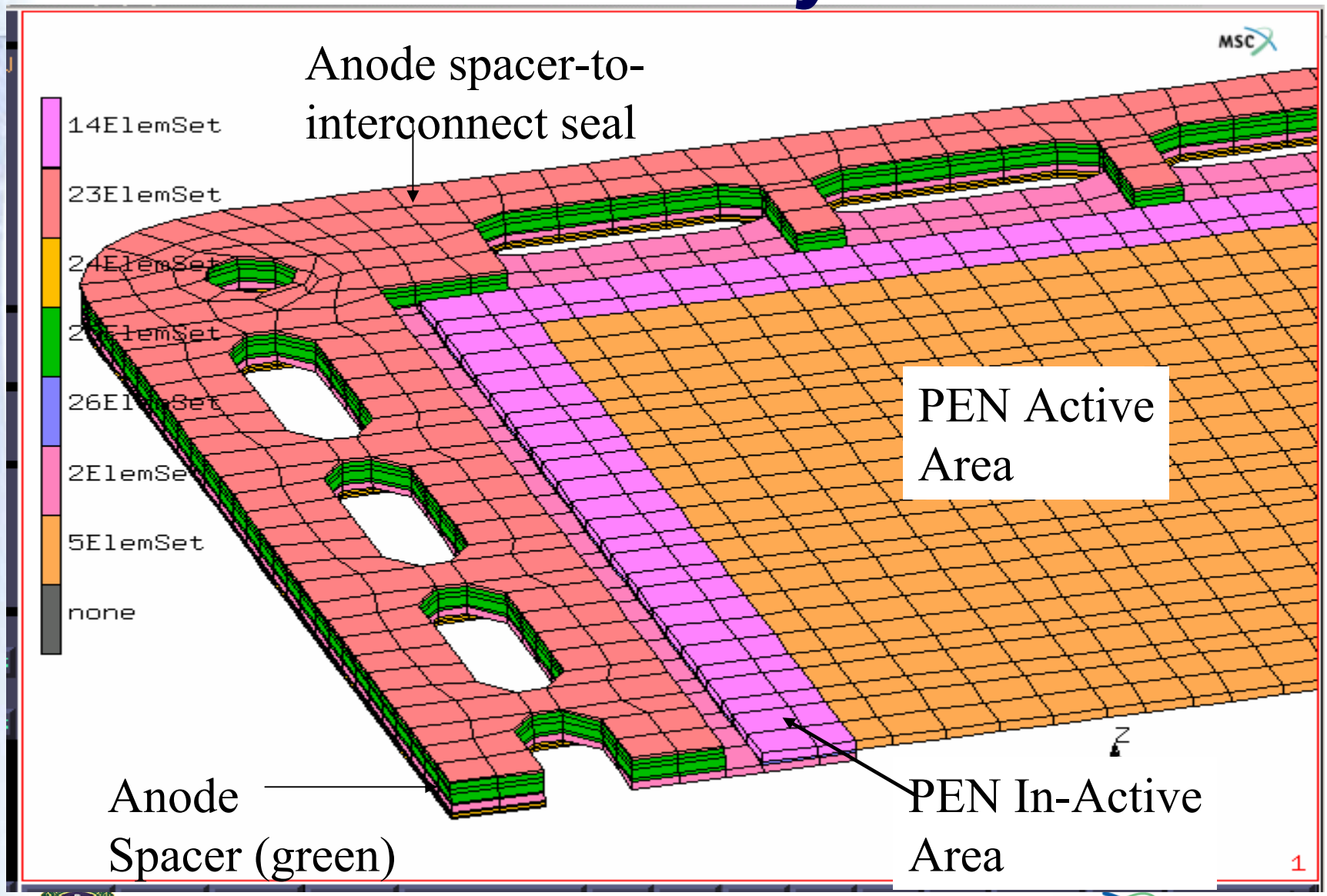
Interconnect



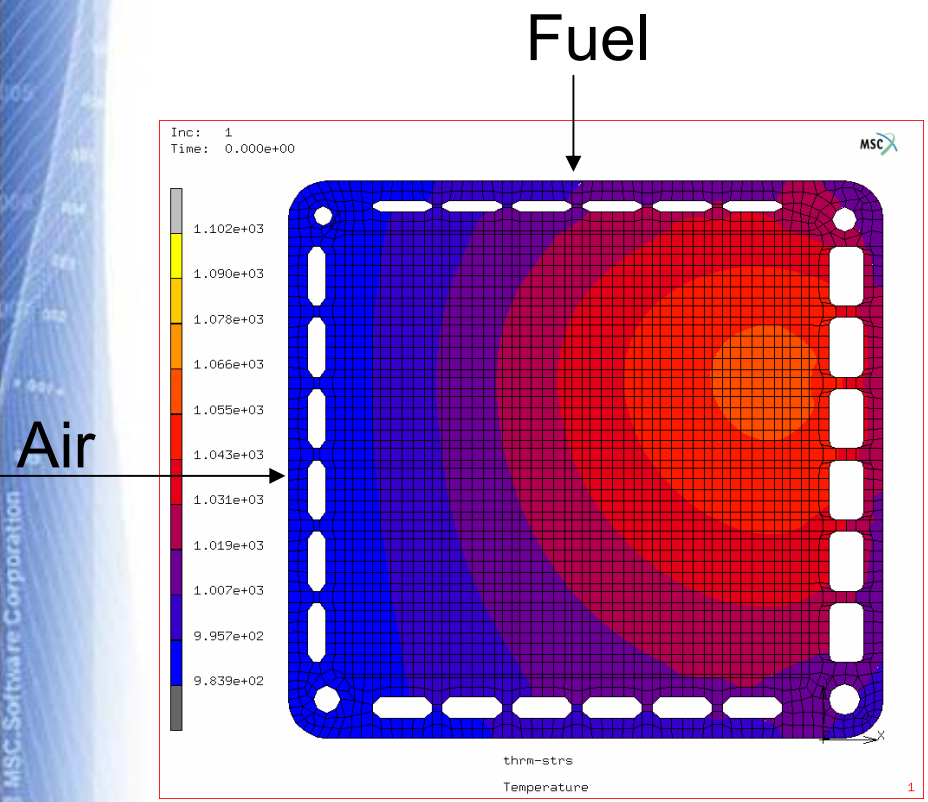
Assembly

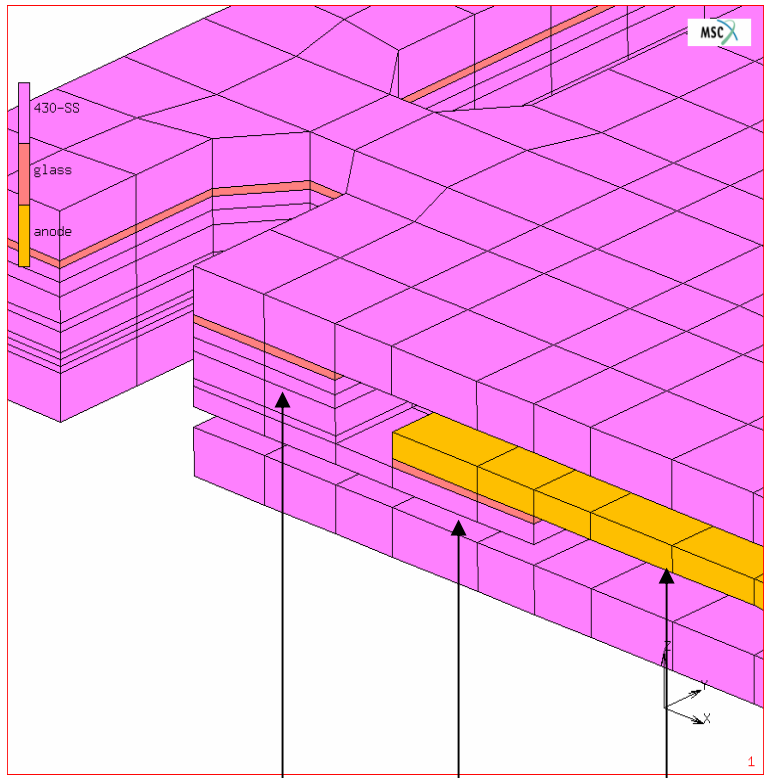


Assembly



Fuel Cell Geometry





Seal Seal Cell

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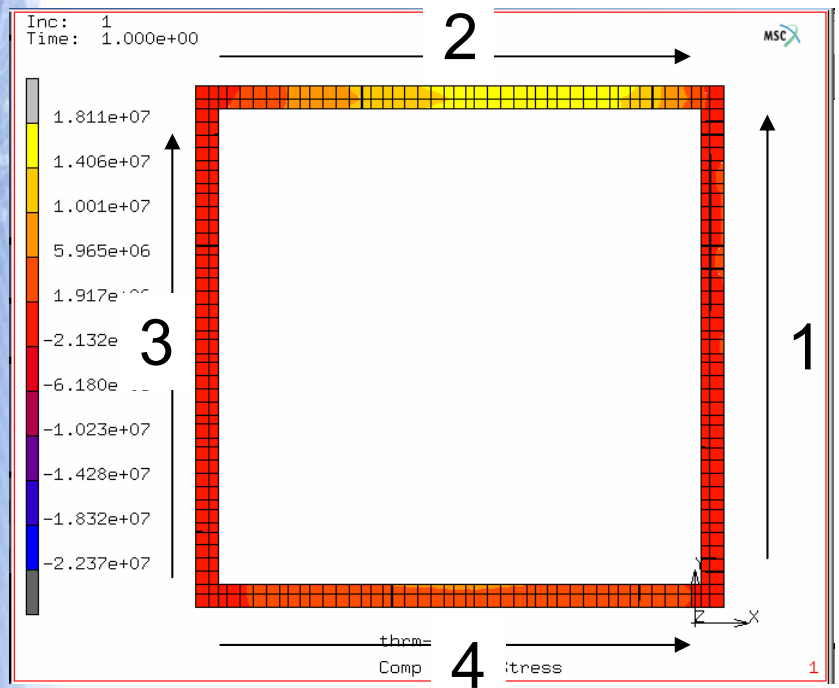
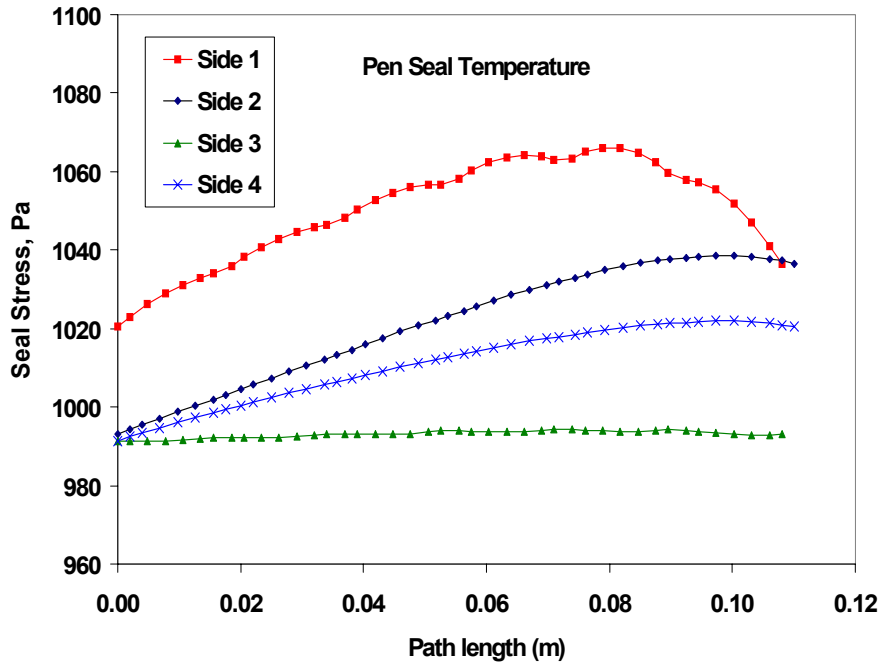
Seal Temperature Profiles





Glass Seal Temperature

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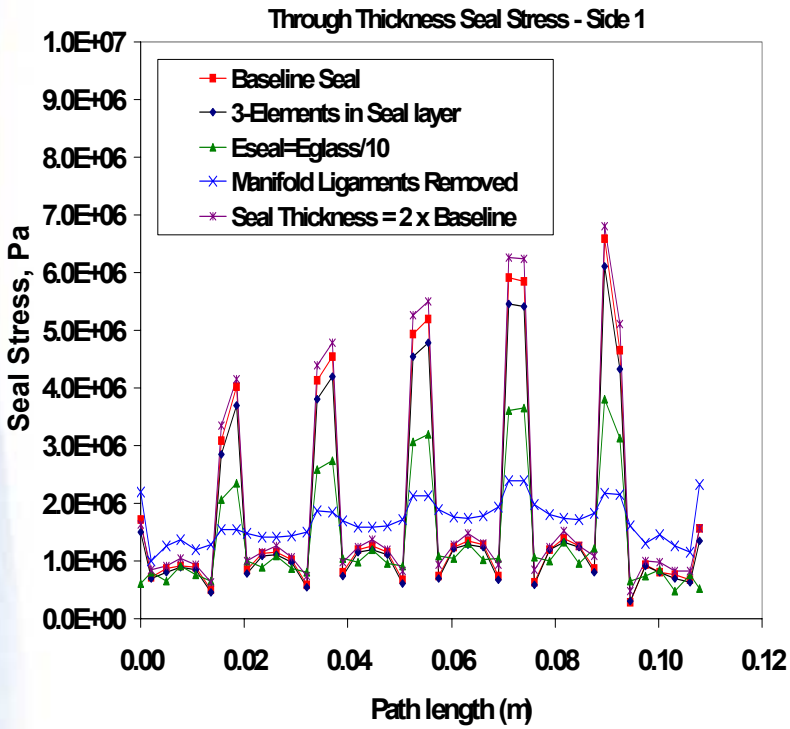
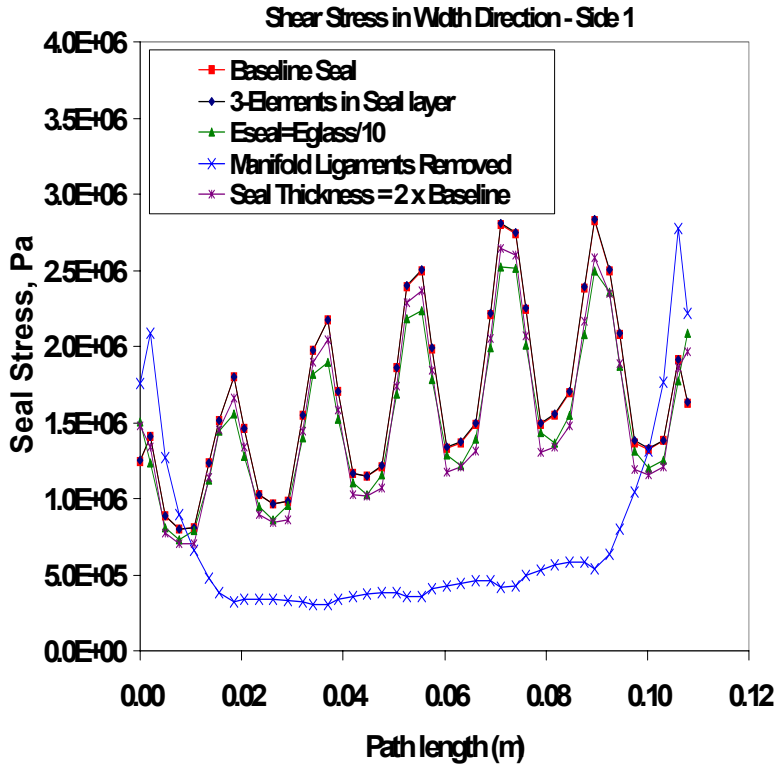
Through Thickness Stress





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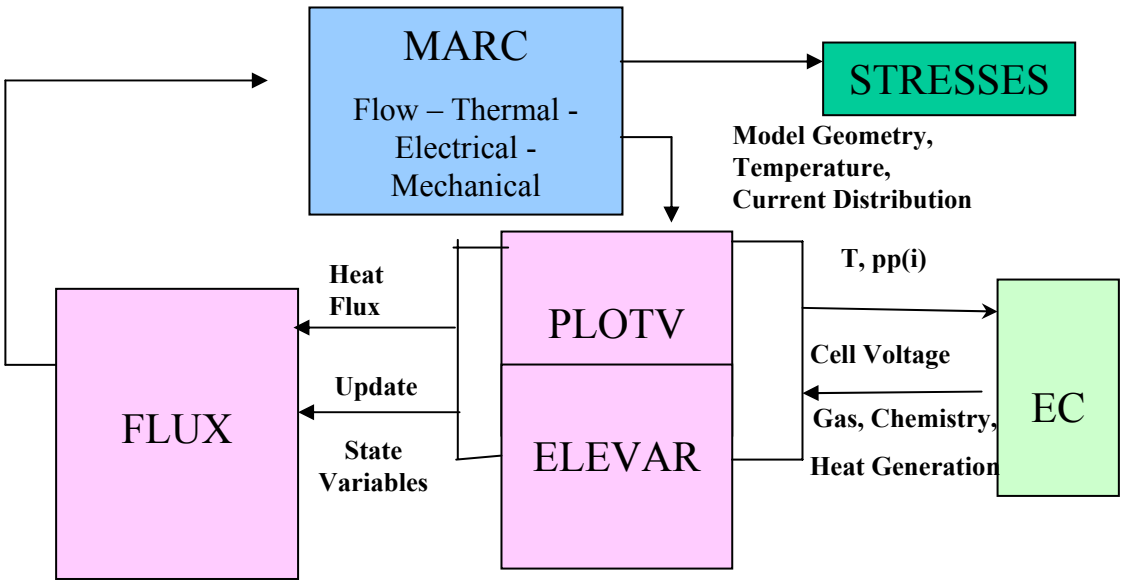
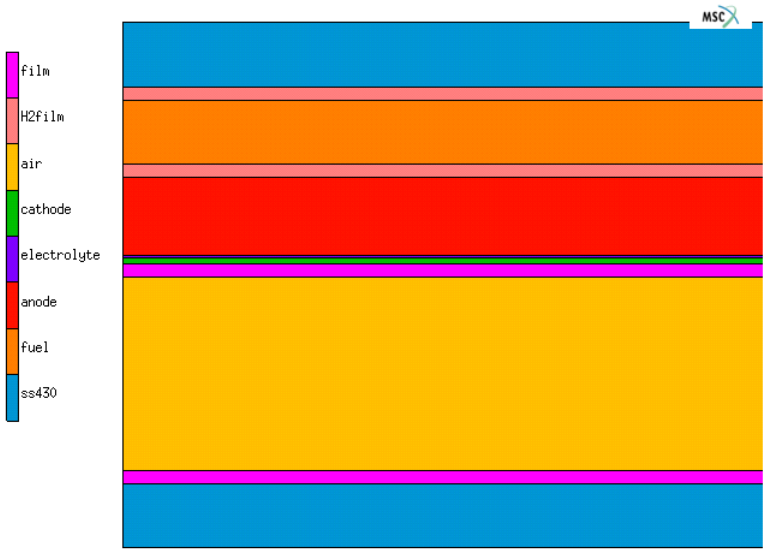
EC in FEA Framework

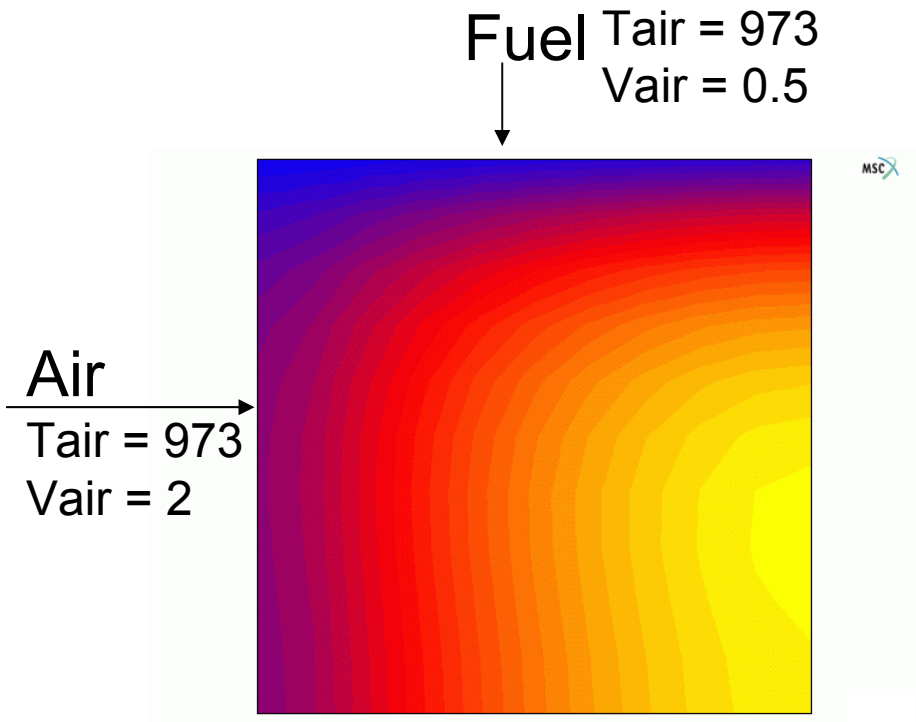
- Fuel cell operations involve multi-physics processes; the constitutive thermal, chemical, electrochemical and transport processes are strongly coupled => requiring versatile multi-physics tool for realistic description
- Technology development involves design optimization of various geometric, material and operation parameters; the cost of such parametric studies increases exponentially with the number of the working parameters and there are many such parameters involved

=> Computational efficiency is critically important



EC in FEA Framework





Material Layers Thickness 4mm

.11m square