ACE3P Simulation Workflow on NERSC

ACE3P Webinar

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November 19, 2025

SLAC NATIONAL ACCELERATOR LABORATORY

Stanford University | U.S. DEPARTMENT OF ENERGY

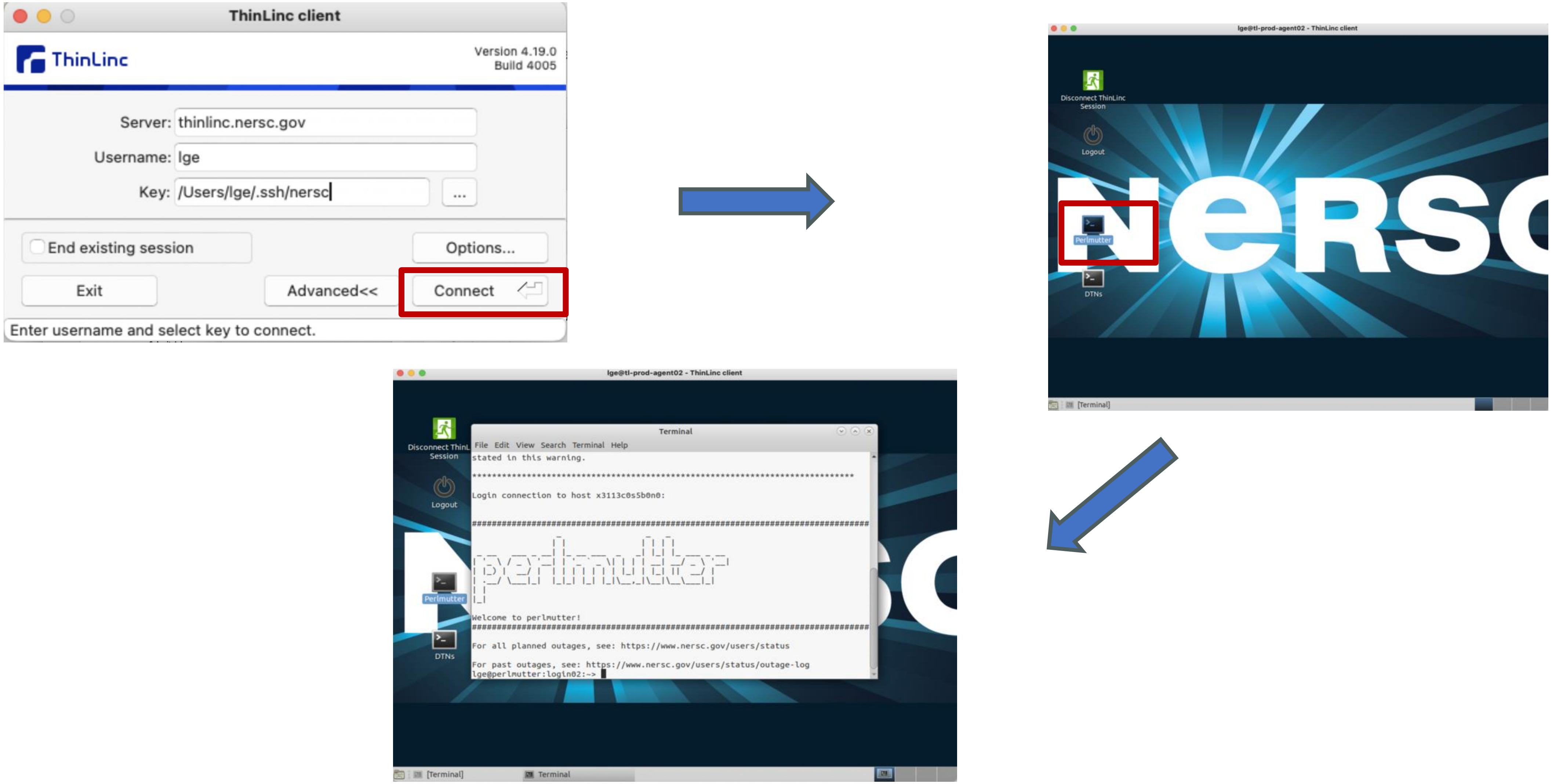
Simulation Workflow on NERSC via ThinLinc

- Log in to NERSC via ThinLinc
- ACE3P Setup on Perlmutter
- Run ACE3P: Example on Omega3P
    - Generate mesh
        - Generate mesh using Cubit
        - Convert mesh by acdtool
    - Execute Omega3P
        - Prepare input file
        - Prepare Omega3P run script
        - Submit job
    - Postprocess results
        - Visualization with ParaView
        - Analysis with acdtool

Log in to NERSC via ThinLinc

- Remote desktop at NERSC: https://docs.nersc.gov/connect/thinlinc/
- Simulation workflow entirely on Perlmutter without the need for data transfer
- ThinLinc at NERSC is hosted via the SSH protocol, so you must configure your connection to NERSC to authenticate via SSH.

Log in to NERSC via ThinLinc (Cont'd)



ACE3P Setup on Perlmutter

- ACE3P executables path: /global/cfs/cdirs/ace3p/perlmutter/CPU/
- Instructions to run ACE3P on Perlmutter:

```
source $CFS/ace3p/perlmutter/CPU/perlmutter-ace3p-spack.sh
```

Recommended practice: Perlmutter login nodes use bash by default, so put your environment setup in ~/.bashrc

- Copy examples folder to scratch:

```
cp -r $CFS/ace3p/cw23/examples/omega3p/demo .
```

Recommended practice: copy the examples folder to your scratch directory

Run ACE3P: Example on Omega3P

* Generate mesh
  - Generate mesh using Cubit
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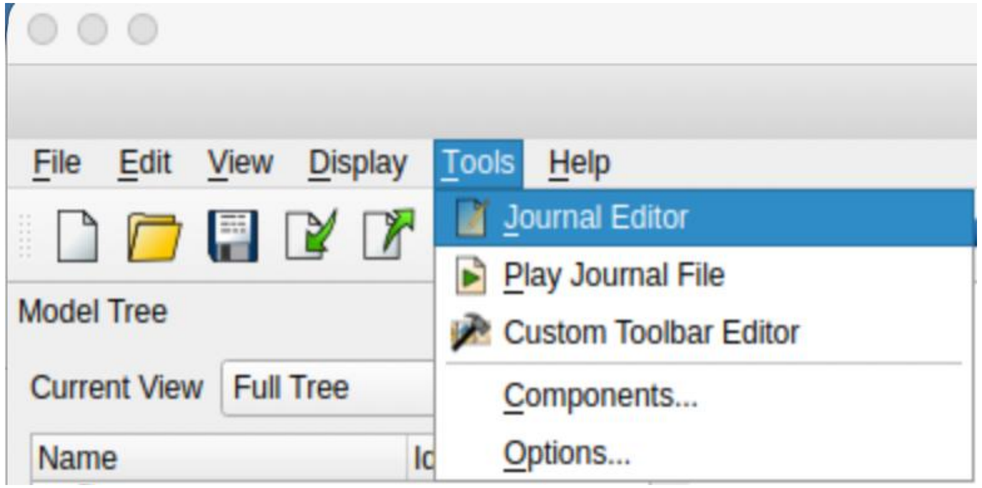
Example: Rounded top pillbox cavity

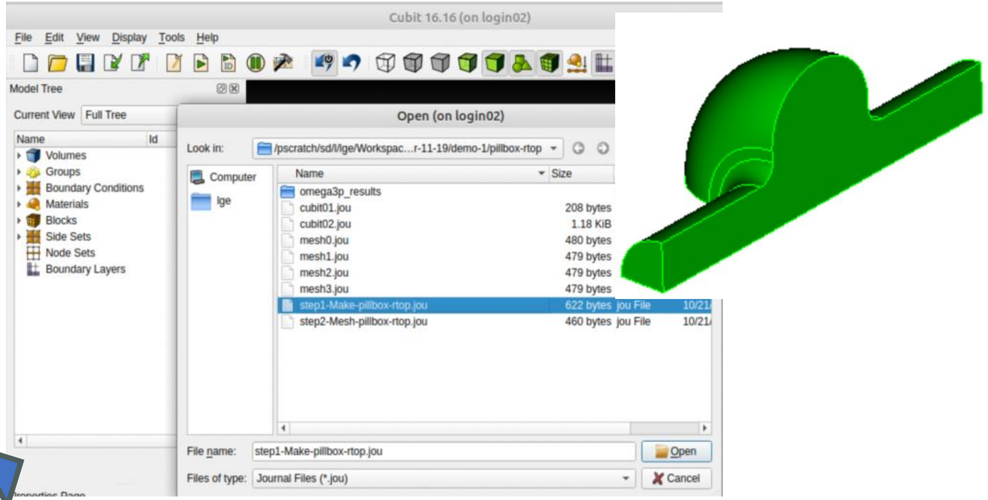
- Example: https://s3df.slac.stanford.edu/people/cho/cw23/examples/omega3p/pillbox-rtop/
- Tutorial: https://s3df.slac.stanford.edu/people/cho/cw23/presentations/omega3p-Tutorial.pdf

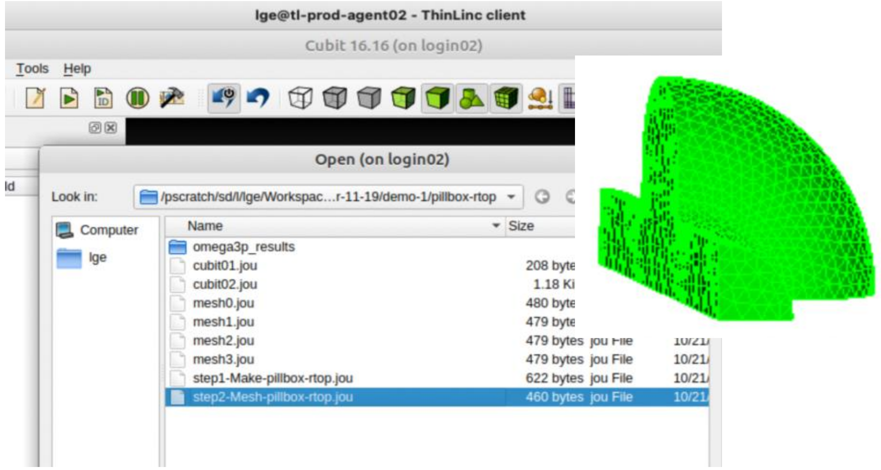
Generate Mesh

Launch cubit: `cubit`

- Model: step1-Make-pillbox-rtop.jou
  - Output: pillbox-rtop4.sat
- Mesh: step2-Mesh-pillbox-rtop.jou
  - Output: pillbox-rtop4.gen







Cubit website: https://cubit.sandia.gov/

Convert Mesh – acdtool

Convert mesh from '.gen' format (pillbox-rtop4.gen) to '.ncdf' format (pillbox-rtop4.ncdf) using acdtool

```
acdtool meshconvert pillbox-rtop4.gen
```

Convert Mesh - Standard Output

TOTALS:
  elements: 100822
  coordinates: 19327

EULER CHARACTER:
  Surf Euler Char = 2
  Vol Euler Char = 1
  Euler Char is OK.

ASPECT RATIO:
  min = 1.00476
  max = 2.36626 <- GREAT
  average = 1.43417
  std dev = 0.175048

SHAPE MEASURE:
  min = 0.494908 <- GREAT
  max = 0.999981
  average = 0.874053
  std dev = 0.0763151

ELEMENT VOLUME:
  min = 2.75555e-09
  max = 1.85833e-08
  average = 7.82677e-09
  std dev = 1.6013e-09

BOUNDING BOX:
  min = (0, 0, -0.15)
  max = (0.0999999, 0.0998816, 0.15)

EDGE LENGTH:
  min = 0.00289644
  max = 0.0207435
  average = 0.00800165
  std dev = 0.00243162

Existing boundary IDs:
1 2 6

Output mesh file: pillbox-rtop4.ncdf

Omega3P Input File - pillbox-rtop.omega3p

```
ModelInfo : {
  File: ./pillbox-rtop4.ncdf
  BoundaryCondition : {
    Magnetic: 1, 2
    Exterior: 6
  }
  SurfaceMaterial : {
    ReferenceNumber: 6
    Sigma: 5.8e7
  }
}

FiniteElement: {
  Order:         2
  CurvedSurfaces: on
}

EigenSolver : {
  NumEigenvalues: 2
  FrequencyShift:  1.0e9
}
```

- ModelInfo : Model used for omega3p simulation
- File: File name of the mesh (in netcdf format)
- BoundaryCondition: Boundary conditions, specifies the boundary conditions on all the surfaces of the mesh.
- SurfaceMaterial: External wall material properties, which are used to calculate the power loss on the surface.
- FiniteElement: Parameters for the finite element method.
- EigenSolver: How many eigenmodes with frequency above a shifted frequency will be searched.

Omega3P input file syntax:
https://s3df.slac.stanford.edu/people/cho/cw23/commands/omega3p-commands.pdf

Omega3P Run Script

```
#!/bin/bash -l
#SBATCH -C cpu
#SBATCH -q debug
#SBATCH -A m349
#SBATCH -N 1
#SBATCH -t 00:10:00
#SBATCH -J dump
#SBATCH -e myjob.%j.err
#SBATCH -o myjob.%j.out
export DIR=$PWD
cd $DIR
srun -n 64 -c 4 --cpu-bind=cores $CFS/ace3p/Perlmutter/CPU/omega3p pillbox-rtop.omega3p
```

Guidance for resource allocation on Perlmutter

acdtool resource <input>

Input - the input parameter file

NERSC Documentation: https://docs.nersc.gov/jobs/

Submit Job & Check Job Status

- Submit batch job

```
sbatch <run_script>
```

- Check job queue status

```
sqs
```

- Cancel a job

```
scancel  <Job ID>
```

NERSC Documentation: https://docs.nersc.gov/jobs/

Files in “omega3p_results” Directory

pillbox-rtop.omega3p ← Input file
omega3p.warn
omega3p.out ← Standard output
omega3p.log ← Run information
omega3p.l0.m0001.2.3291311e+09.mod
omega3p.l0.m0000.1.3138154e+09.mod
VECTOR

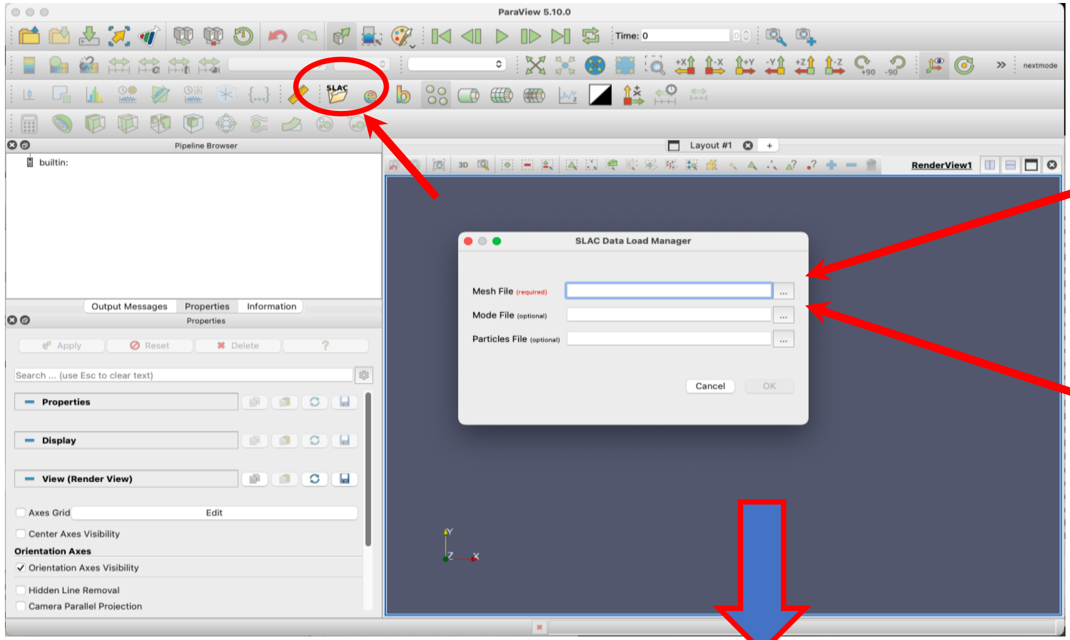
Eigenvector (VECTOR)

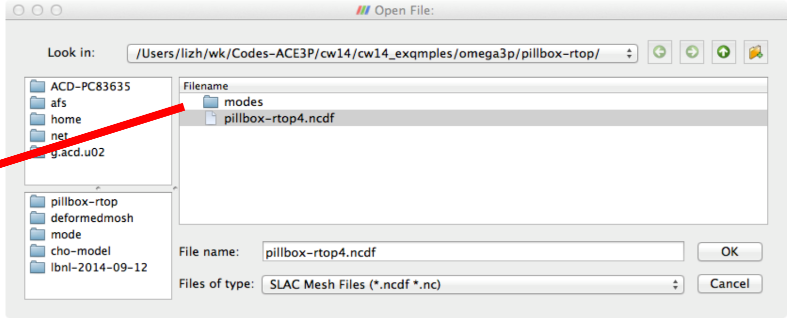
eigensystem.omega3p
postprocess.in

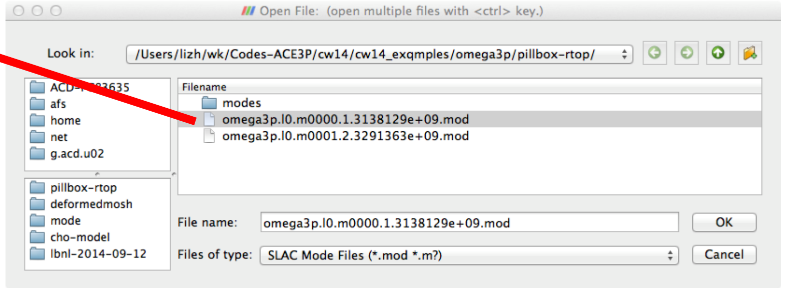
.mod files for Paraview visualization of fields

Visualization Using Paraview: Load Mesh and Field

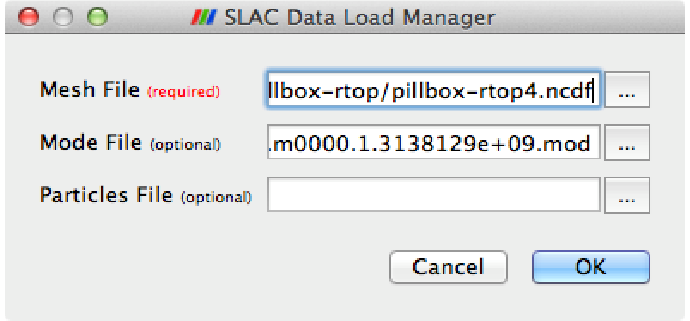
Launch Paraview: paraview





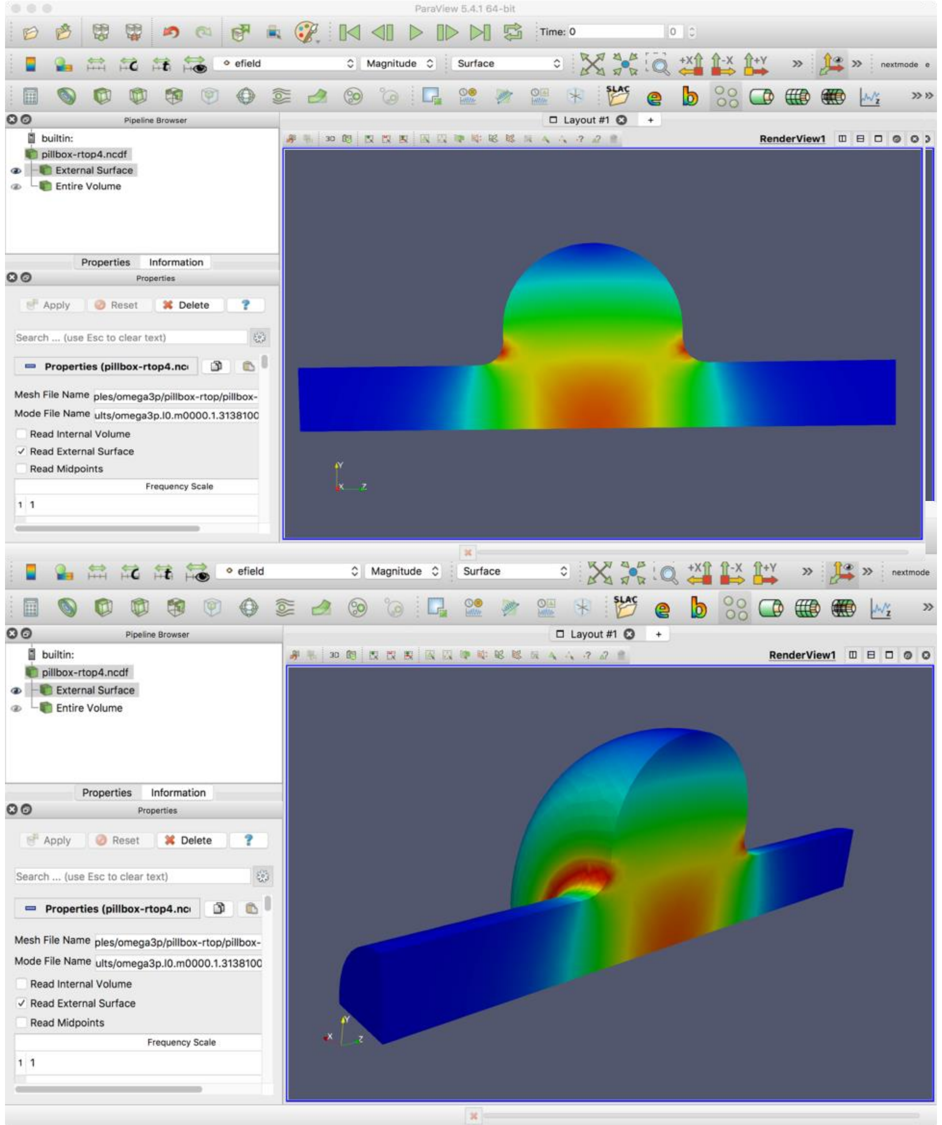


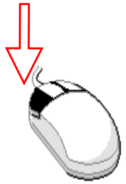
Load mesh and field files using SLAC toolbar



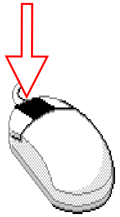
Paraview website: https://www.paraview.org/

Visualization Using Paraview: Electric Field Contour

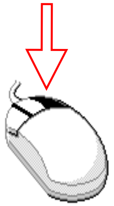




Left-button to
Rotate

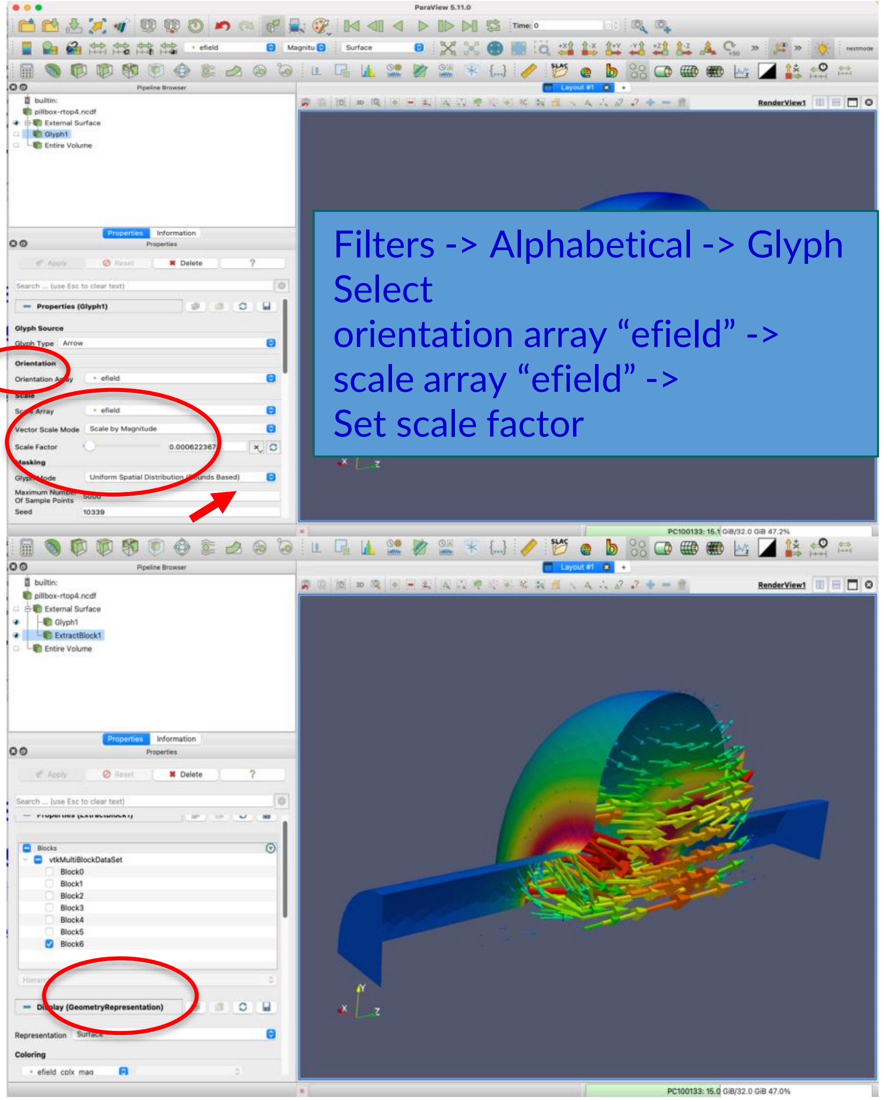


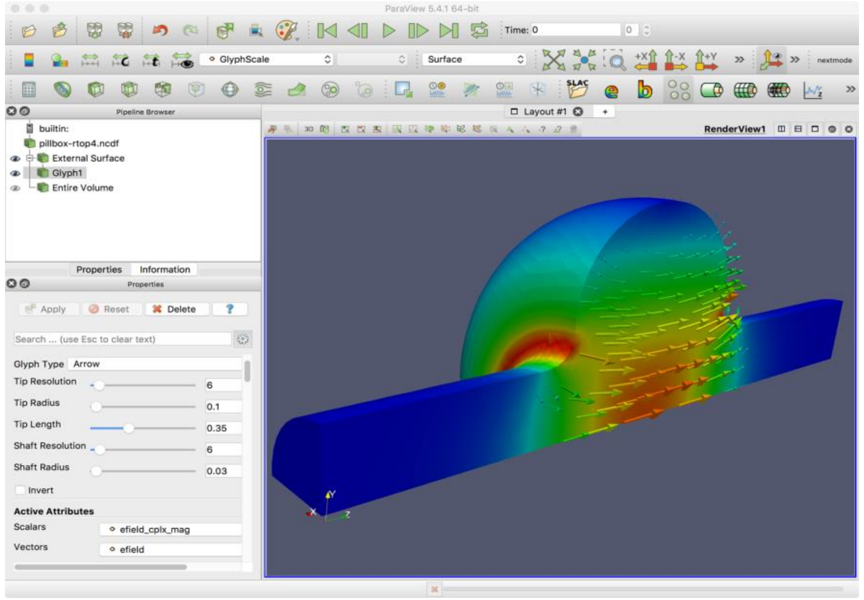
Mid-button to
Pan



Right-button to
Zoom

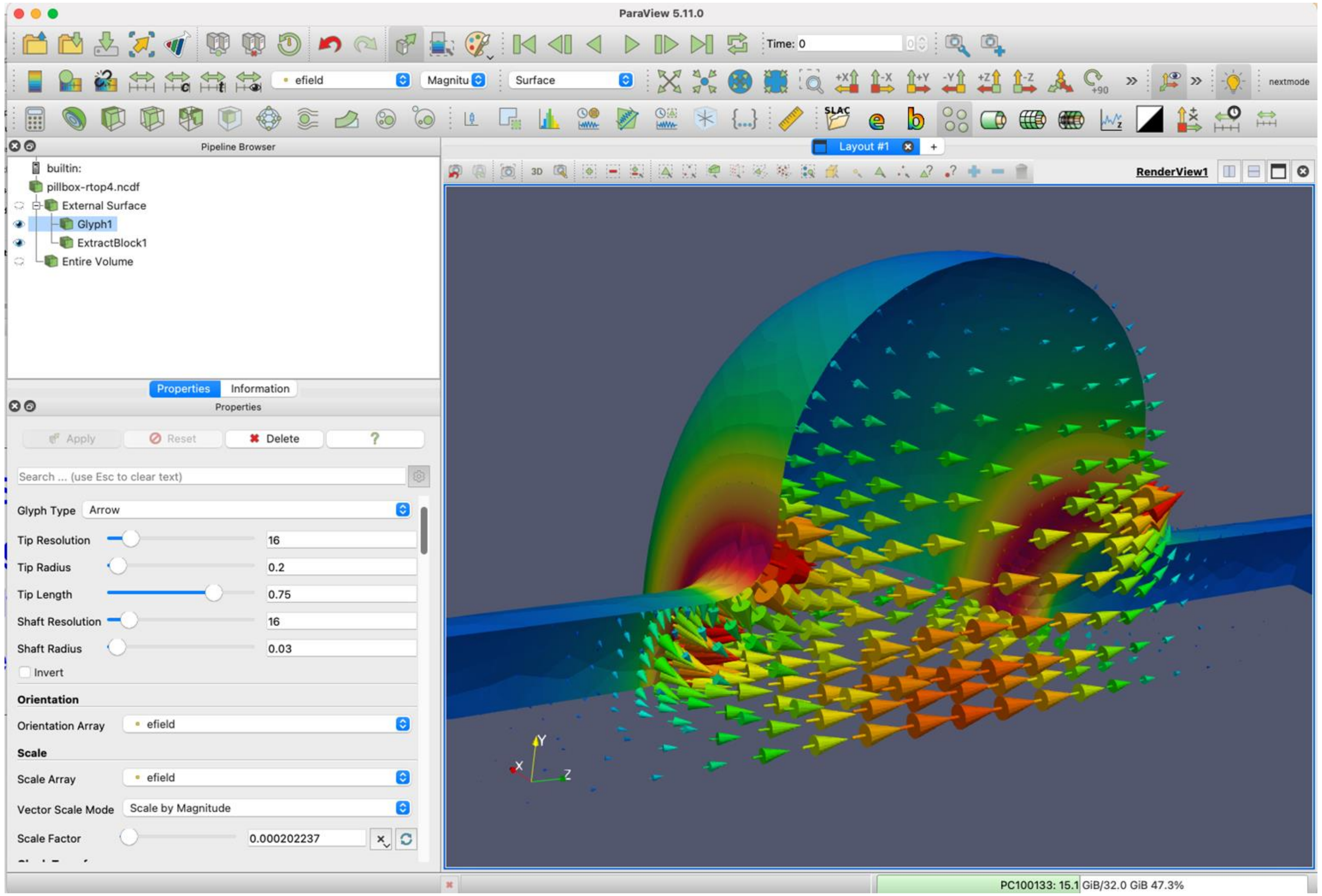
Visualization Using Paraview: Vector Field Plot



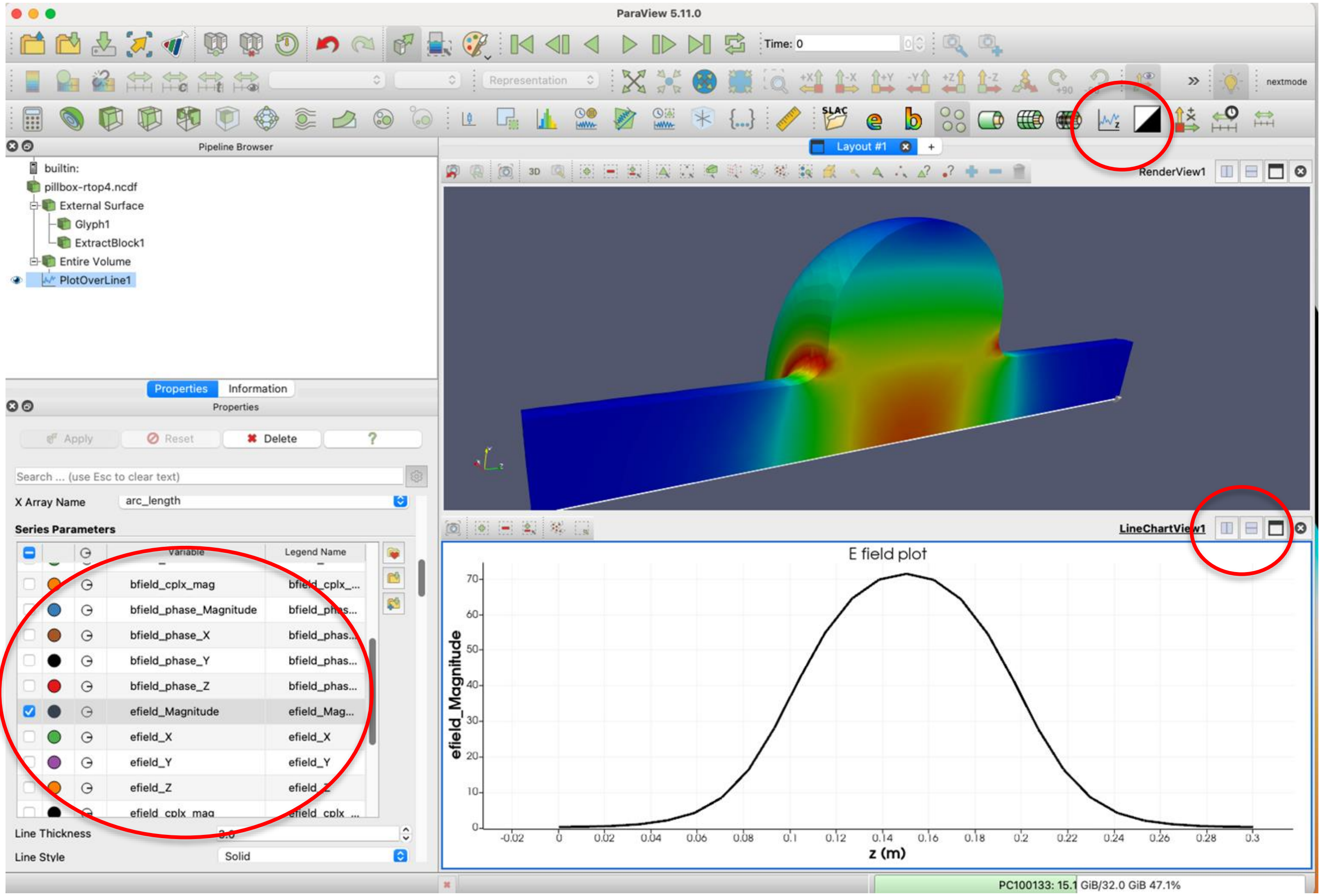


To see through the symmetry plane
High light “External Surface”
Filter -> Alphabetical -> Extract Block
select “[DataSet 6]”

Visualization Using Paraview: Vector Field Plot (Cont'd)



Visualization Using Paraview: Line Plot



Line plot

Layout of plots

Select item to plot

acdtool

acdtool - a set of utility tools for preprocessing and postprocessing

* acdtool meshconvert: mesh convertor
* acdtool mesh:
  - stats
  - check
  - deform
  - fix
  - warpsurface
* acdtool resource

"acdtool" command syntax:
https://s3df.slac.stanford.edu/people/cho/cw23/commands/acdtool-commands.pdf

* acdtool postprocess
  - **rf**
  - eigentomode
  - volmontomode
  - wake_new
  - wake_direct
  - Transwake
  - Coaxsignal
  - Pic3pstats
  - Pic3pconvert
  - Track3p
  - project
  - ...

Post-processing: RF Analysis with adctool

RoverQ

RoverQT

KickFactor

FieldMap

FieldAtPoint

FieldOnLine

FieldOn2DBoundary

FieldOnSurface

MaxFieldsOnSurface

….

“acdtool” Usage

* acdtool postprocess rf
  - Produce a “sample.rfpost” file containing inputs for all functions
  - Modify and rename it to pillbox-rtop.rfpost

* acdtool postprocess rf pillbox-rtop.rfpost
  - perform calculations specified in “pillbox-rtop.rfpost”

sample.rfpost - RFField

```
RFField: {
  ResultDir     = omega3p_results
  FreqScanID  =     0
  ModeID      =     0
  xsymmetry   =     magnetic
  ysymmetry   =     magnetic
  gradient    =  -1
  cavityBeta  =     1.00000
  reversePowerFlow=     0
  x0          =     0.00000
  y0          =     0.00000
  gz1         =    -0.057
  gz2         =     0.057
  npoint      =    300
  fmnx        =     10
  fmny        =     10
  fmnz        =     50
}
```

RFField: Field information

- ResultDir: The name of the directory where the field solver results are stored
- FreqScanID: Frequency scan
- ModeID: The mode index
- x/ysymmetry: symmetry type
- gradient: E field gradient
- reversePowerFlow: For omega3p calculation with open ports
- x0/y0/gz1/gz2: Integration path for gradient calculation

sample.rfpost – R/Q

```
RoverQ :
{
   ionoff      =    1
   modelD1     =   -1
   modelD2     =   -1
   x1          =     0.0
   x2          =     0.0
   y1          =     0.00
   y2          =     0.0
   z1          = 1000.0
   z2          = 1000.0
}
```

- Calculate R/Q
- The unit of R/Q: ohm/cavity
- ionoff: Switch to perform or skip calculation
- modelD1/modelD2: The range of modes for the R/Q calculation
- x1/y1/z1/x2/y2/z2: Start and end points of the integration path for R/Q calculation.

sample.rfpost - FieldMap

```
FieldMap
{
   ionoff     =    1
   nx         =   20
   ny         =   20
   nz         =   50
   x1         =    0.00000
   x2         =    0.00000
   y1         =    0.00100
   y2         =    0.00100
   z1         = 100000.0
   z2         = 100000.0
}
```

- Outputs a field map on a regular grid
- The field map data:
  - Efieldmap.dat
  - Bfield-map.dat
- ionoff: Switch to perform or skip FieldMap calculation
- nx/ny/nz: The numbers of grid lines in x, y, z
- x1/x2/y1/y2/z1/z2: The range of grid lines in x /y/z

sample.rfpost - FieldonLine

```
FieldOnLine
{
   ionoff      =     1
   npoint      =   300
   filename    = filename1
   rfphase     =     0.00000
   x1          =     0.00000
   x2          =     0.00000
   y1          =     0.0000
   y2          =     0.0000
   z1          = 100000000.0
   z2          = 100000000.0
}
```

- Calculate E and B fields along a line
- npoint: The number of points along the line to be calculated
- rfphase: The rf phase at which the fields will be evaluated
- filename: The output file for the fields along the line.
- x1/y1/z1/x2/y2/z2: Start and end points of the line for the field evaluation

sample.rfpost - maxFieldsOnSurface

```
maxFieldsOnSurface
{
  ionoff     =    1
  surfaceID  =    6
}
```

- Calculate the maximum fields on a surface
- surfaceID: The ID of the surface where the maximum surface fields are evaluated. It is set in Cubit.
- The mode with ModeID specified in RFField.

Postprocess Output – General Information

```
**************************** Omega3P/S3P Mode Summary ***********************************
** Omega3P/S3P Mode Summary:
**
**   Total number of modes :      2
**      ModeID        Frequency(r,i)                  Qext
**        0         1.31381e+09, 0.00000e+00         0.00000e+00
**        1         2.32914e+09, 0.00000e+00         0.00000e+00
**
**   Model bounding box: ( 0.00000e+00,  0.00000e+00 -1.50000e-01)
**                       ( 1.00005e-01,  1.00123e-01  1.50000e-01)
**
** ------------
**   Mode used:
**      ModeID    =      0
**      Frequency =  1.31381e+09,    0.00000e+00
*****************************************************************************************
[scaling]
{
   ModeID:   0
   Integral:  x0    = 0.0000e+00,   y0  = 0.0000e+00
              gz1   =-5.7000e-02,   gz2 = 5.7000e-02
              V     =(-6.0358e-03, -4.5814e+00) (normalized field)
              ga    = 4.01881e+01   (normalized field)
   E,B m_factor = 4.97660e+05
}
```

Postprocess Output – R/Q

```
RoverQ: {
   ionoff      =     1
   modeID1     =    -1
   modeID2     =    -1
   x1          =     0.00000
   x2          =     0.00000
   y1          =     0.0000
   y2          =     0.0000
   z1          =    -0.15000
   z2          =     0.15000
}
[RoverQ]
{  // RoverQ=V^2/(omega*U)
   Integral:  x1  = 0.0000e+00,  y1  = 0.0000e+00,  z1  =-1.5000e-01
              x2  = 0.0000e+00,  y2  = 0.0000e+00,  z2  = 1.5000e-01
 ModeID  Frequency        |V|             RoQ(ohm/cavity)
    0   1.31381e+09     4.18073e+00     1.19567e+02
    1   2.32914e+09     6.26119e-04     1.51273e-06
}
```

Postprocess Output – Surface Field

```
maxFieldsOnSurface
{
  ionoff      =     1
  surfaceID   =     6
}

[maxFieldsOnSurface]
{
  surfaceID :   6
     ModelD :   0
     Emax :  3.92574e+07 (V/m)     at ( 0.0000e+00,  4.2739e-02,  4.5782e-02)
    Hmax :  5.80786e+04 (A/m)       at ( 5.8915e-03,  8.8207e-02,  3.0153e-02)
}
```

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Demo