

Calypso Tutorial

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July 16, 2014
CIDER2014

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Goal of this tutorial



- Learn to run a geodynamo model using Calypso
- Understand parameter files for Calypso
- Run a non-magnetic convection model
- Check scaling with changing Rayleigh number



What is Calypso?

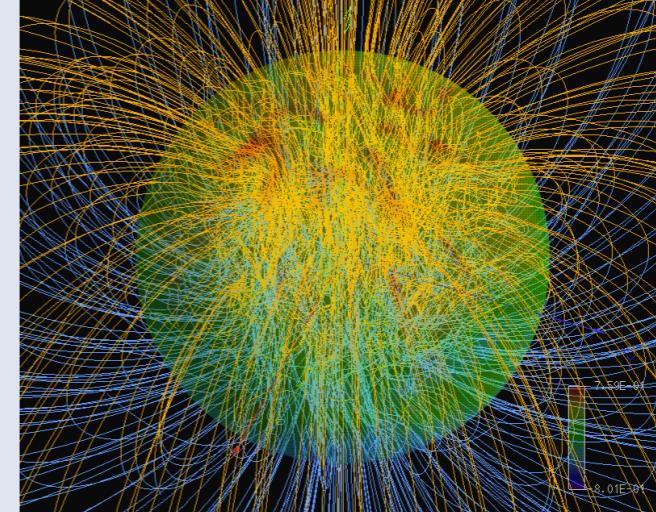


- Geodynamo model using spherical harmonics transform and Finite Difference method
 - MPI / OpenMP parallelization
 - Large flexibility
 - Various output
- More than 80 pages of documentation

COMPUTATIONAL INFRASTRUCTURE FOR GEODYNAMICS (CIG)



User Manual
Version 1.1



Hiroaki Matsui
www.geodynamics.org



What can Calypso do?



- Magnetohydrodynamics (MHD) simulation in a rotating spherical shell
 - Boussinesq fluid
 - Double diffusive (temperature and composition)
 - Thermal and compositional buoyancy
 - Conductive or insulated inner core
 - Thermal and compositional heterogeneity at boundaries
- Data output
 - Time history (Energies, Nusselt number)
 - Field data in Cartesian coordinates for visualization



Governing equations for non-magnetic rotating convection



- Momentum equation

$$\left[\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} \right] + \boxed{\text{Coriolis force}} + 2(\boldsymbol{\Omega} \times \mathbf{u}) = -\nabla P + \nu \nabla^2 \mathbf{u} - \alpha T \mathbf{g}$$

- Energy equation

$$\frac{\partial T}{\partial t} + (\mathbf{u} \cdot \nabla) T = \kappa \nabla^2 T,$$

- Conservation of Mass

$$\nabla \cdot \mathbf{u} = 0.$$

$\boldsymbol{\Omega}$: Rotation of system

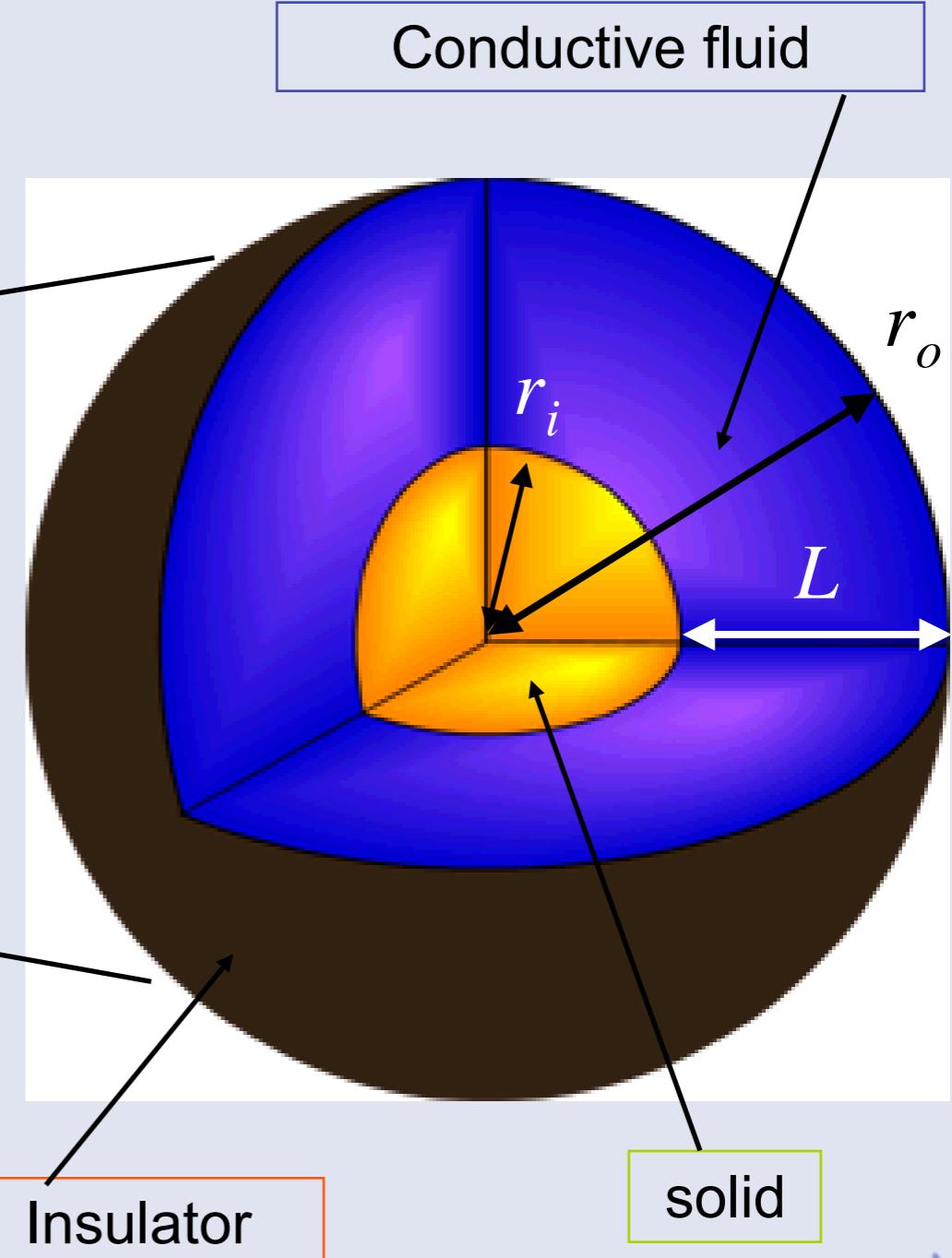
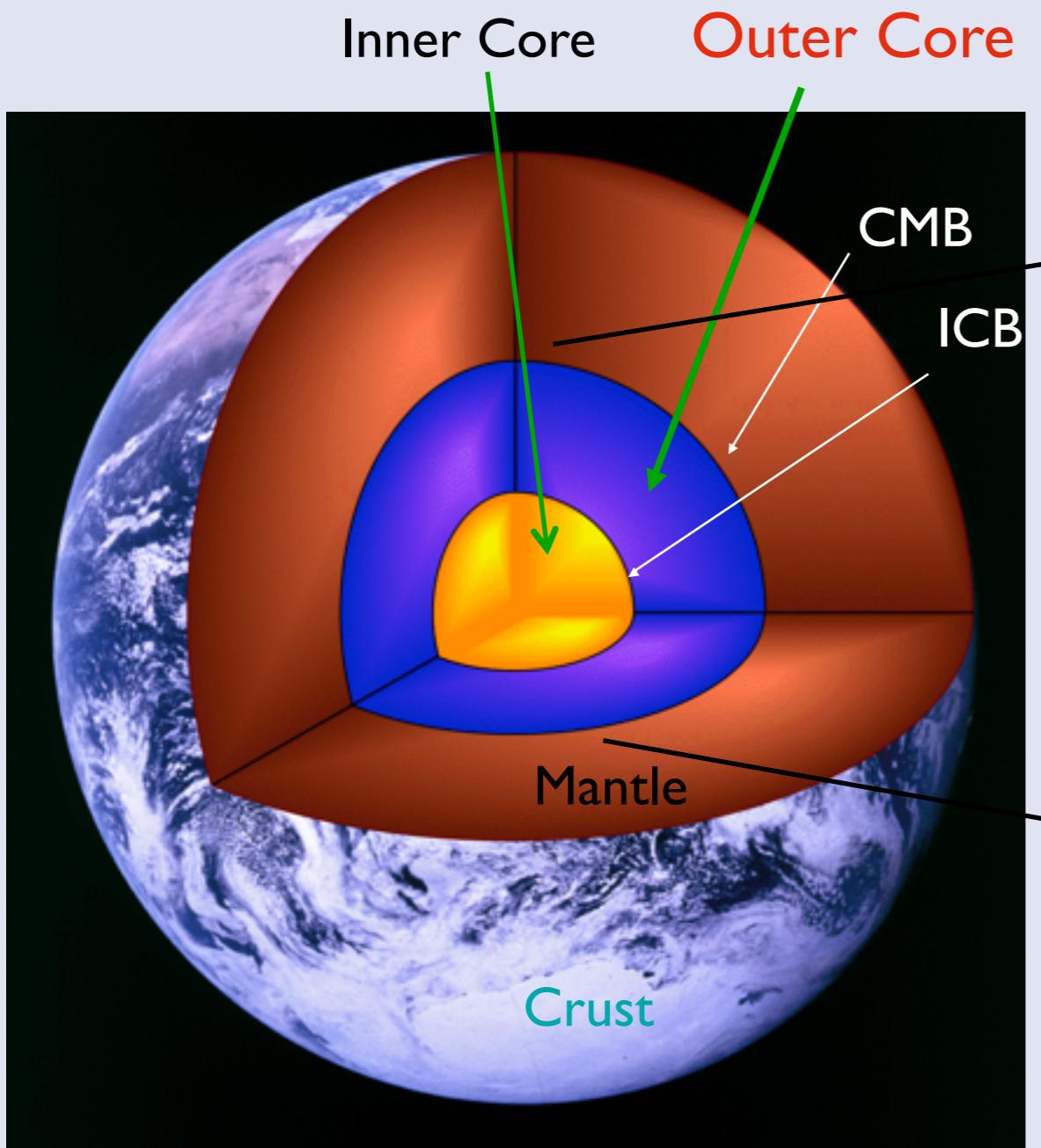
α : Thermal expansion

ν : Kinetic viscosity

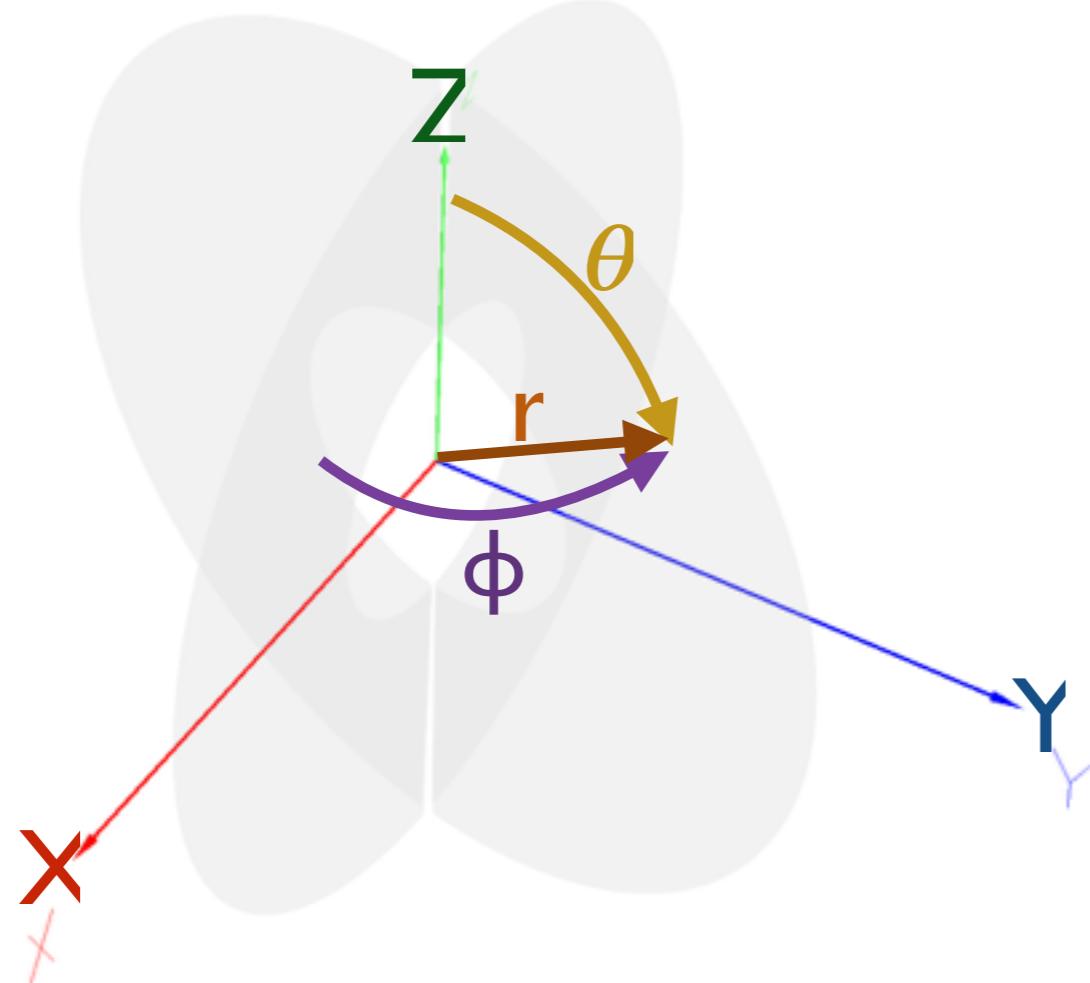
κ : Thermal diffusivity



Rotating spherical shell for geodynamo simulations



Spherical coordinate system



- r : Radial direction
- θ : Meridional direction
- ϕ : Zonal direction (Longitudinal)
- Domain is discretized to evaluate nonlinear terms

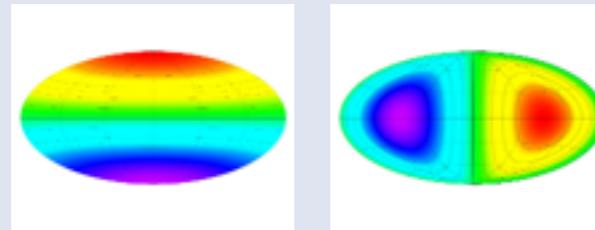
Spherical harmonics Y_l^m



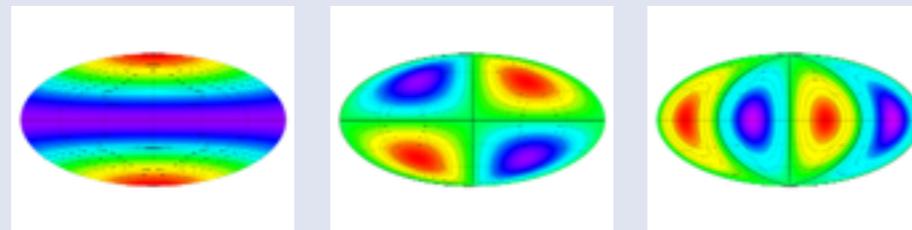
See <http://mathworld.wolfram.com/SphericalHarmonic.html>

$m = 0 \quad m = 1 \quad m = 2 \quad m = 3 \quad m = 4 \quad m = 5$

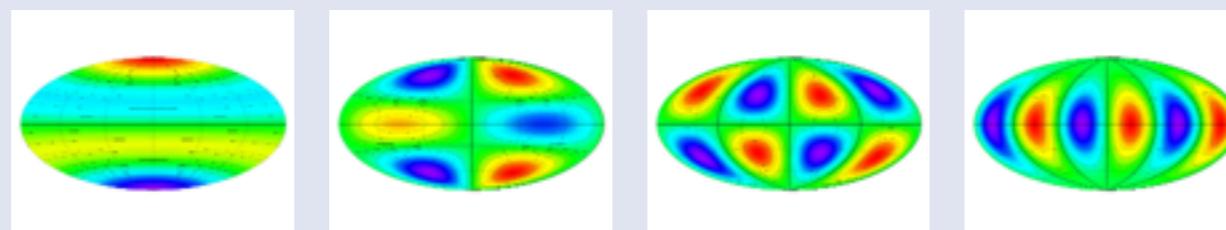
$l = 1$



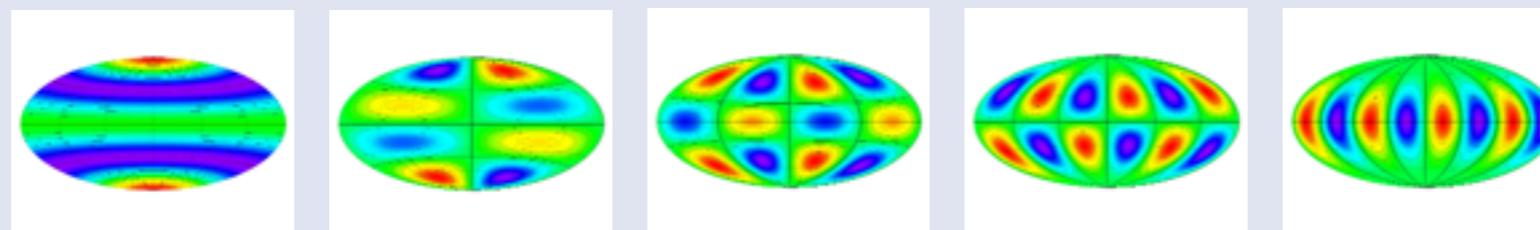
$l = 2$



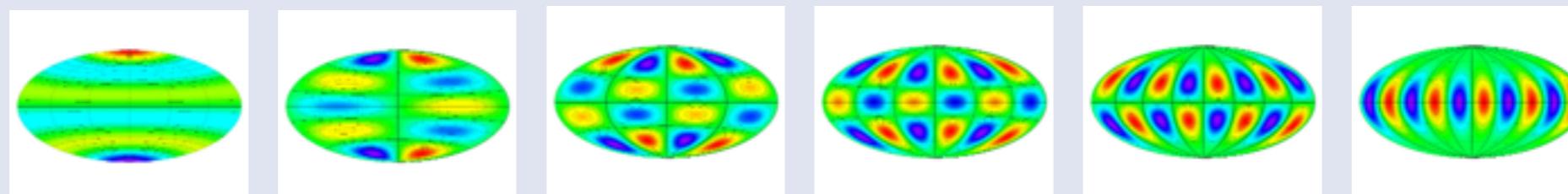
$l = 3$



$l = 4$



$l = 5$



⋮

Truncation degree l_{max}



Contacts for Calypso



- Homepage
 - <http://geodynamics.org/cig/software/calypso/>
- Mailing list
 - cig-geodyn@geodynamics.org
- Wiki
 - <http://wiki.geodynamics.org/software:calypso:start>



Procedure of simulation



1. Preprocessing: Prepare spherical harmonics index table
2. Run simulation
3. Postprocessing



Data for the tutorial

I. Open Terminal

2. \$ cd tutorial/calypso

```
Terminal
cig@cig-VirtualBox: ~tutorial/calypso/Convection_RaXXX
cig@cig-VirtualBox:~$ ls
aspect-bin calypso Desktop Downloads local  resetTutorial.sh  tutorial
cig@cig-VirtualBox:~$ cd tutorial/calypso/
cig@cig-VirtualBox:~/tutorial/calypso$ ls
Convection_RaXXX MHD_Example
cig@cig-VirtualBox:~/tutorial/calypso$ cd Convection_RaXXX/
cig@cig-VirtualBox:~/tutorial/calypso/Convection_RaXXX$ ls
average_KE.gnu  control_MHD      field          README    sph_lm23t36r48c_1
average_Nu.gnu  control_sph_shell gen_sph_grids restart  sph_mhd
cig@cig-VirtualBox:~/tutorial/calypso/Convection_RaXXX$
```

3. \$ cd Convection_RaXXX

Check file list

- Type \$ ls
- Programs and input files are ready

Parameter files

Empty folder for data output

```
cig@cig-VirtualBox:~/tutorial/calypso/Convection_RaXXX$ ls
average_KE.gnu    control_MHD      field          README        sph_Lm23t36r48c_1
average_Nu.gnu    control_sph_shell gen_sph_grids restart      sph_mhd
cig@cig-VirtualBox:~/tutorial/calypso/Convection_RaXXX$
```

Script for Gnuplot

programs



Procedure of simulation

1. Preprocessing: Prepare spherical harmonics index table
 - Command: `$./gen_sph_grid`
 - Parameter file: `control_sph_shell`
2. Run simulation
3. Postprocessing



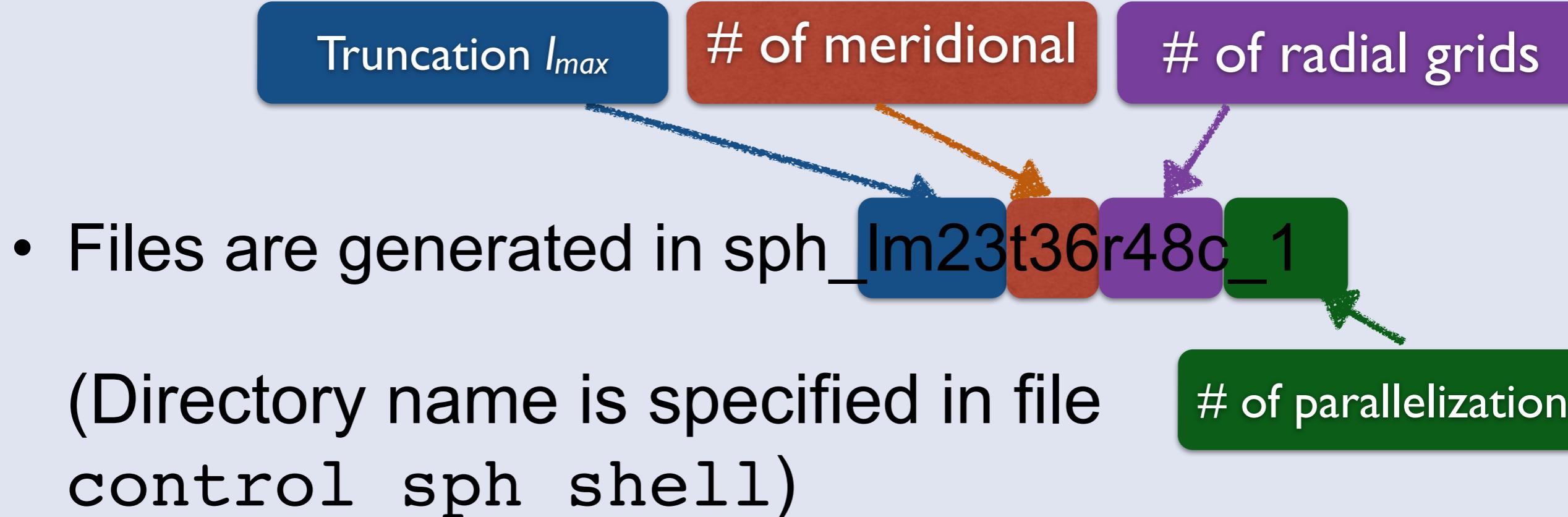
Start preprocessing program

1. Preprocessing: Prepare spherical harmonics index table

- Command: `$./gen_sph_grids`
- Parameter file: `control_sph_shell`

```
average_Nu.gnu control_sph_shell gen_sph_grids restart sph_mhd
cig@cig-VirtualBox:~/tutorial/calypso/Convection_RaXXX$ ./gen_sph_grids
truncation degree: 23
number of grid for f(r,t,p): 49 36 72
subdomain for f(r,t,p): 1 1 1
subdomain for f(r,t,m): 1 1 1
subdomain for f(r,l,m): 1 1 1
subdomain for spectr f(r,j): 1 1
radial grid is written in radial_point.dat
Write ascii spectr modes file: sph_lm23t36r48c_1/in.0.rlm
Write ascii grid file: sph_lm23t36r48c_1/in.0.rtm
```

Start preparation program



```
Write ascii spectr modes file: sph_lm23t36r48c_1/in.0.rj
Spherical modes and grids for domain      0 is done.
Write ascii mesh file: sph_lm23t36r48c_1/in.0.gfm
FEM mesh for domain      0 is done.
program is normally terminated
cig@cig-VirtualBox:~/tutorial/calypso/Convection_RaXXX$ ls
average_KE.gnu    control_sph_shell    radial_point.dat    sph_lm23t36r48c_1
average_Nu.gnu    field                  README             sph_mhd
control_MHD      gen_sph_grids       restart
cig@cig-VirtualBox:~/tutorial/calypso/Convection_RaXXX$ ls sph_lm23t36r48c_1/
in.0.gfm  in.0.rj  in.0.rlm  in.0.rtm  in.0.rtp  README
cig@cig-VirtualBox:~/tutorial/calypso/Convection_RaXXX$
```

Procedure of simulation



1. Preprocessing: Prepare spherical harmonics index table
2. Run simulation
 - Command: `$ mpirun -np 1 ./sph_mhd`
 - Parameter file: `control_MHD`
3. Postprocessing



Dimensionless numbers

Prandtl number: $Pr = \frac{\nu}{\kappa} = \frac{\text{Viscous diffusivity}}{\text{Thermal diffusivity}}$

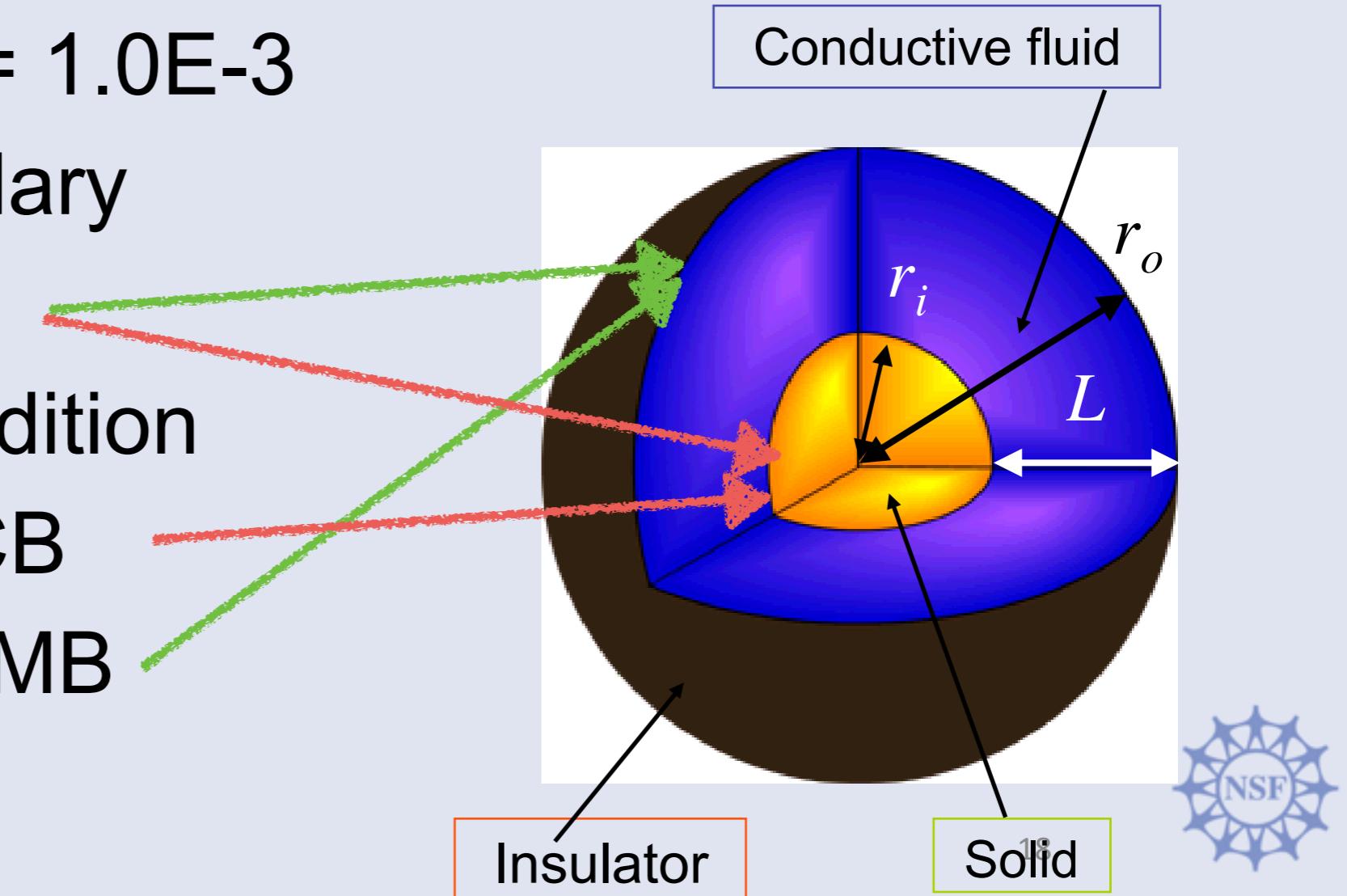
Ekman number: $E = \frac{\nu}{\Omega L^2} = \frac{\text{Viscous diffusivity}}{\text{Coriolis force}}$

Rayleigh number: $Ra = \frac{\alpha g \Delta T L^3}{\nu \kappa} = \frac{\text{Buoyancy}}{\text{Diffusivity}}$



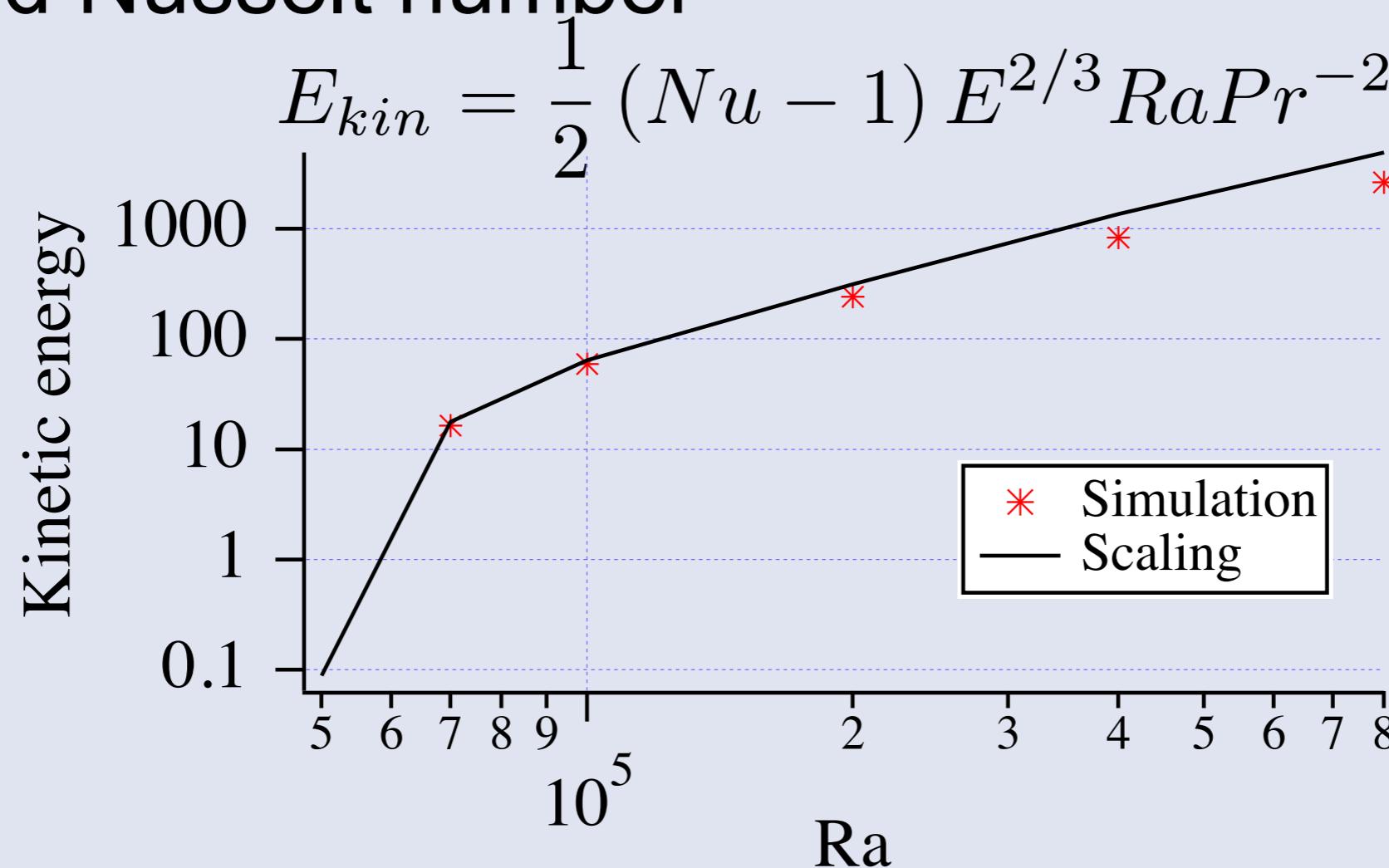
Model for tutorial

- You will perform simulation by changing Rayleigh number
 - $Ra = 7.0\text{e}4, 1.0\text{e}5, 2.0\text{e}5, 4.0\text{e}5, 8.0\text{e}5$
- The other dimensionless number is fixed
 - $Pr = 1.0, E = 1.0\text{E}-3$
- Non-slip boundary
 - $u = 0$
- Isothermal condition
 - $T = 1.0$ at ICB
 - $T = 0.0$ at CMB



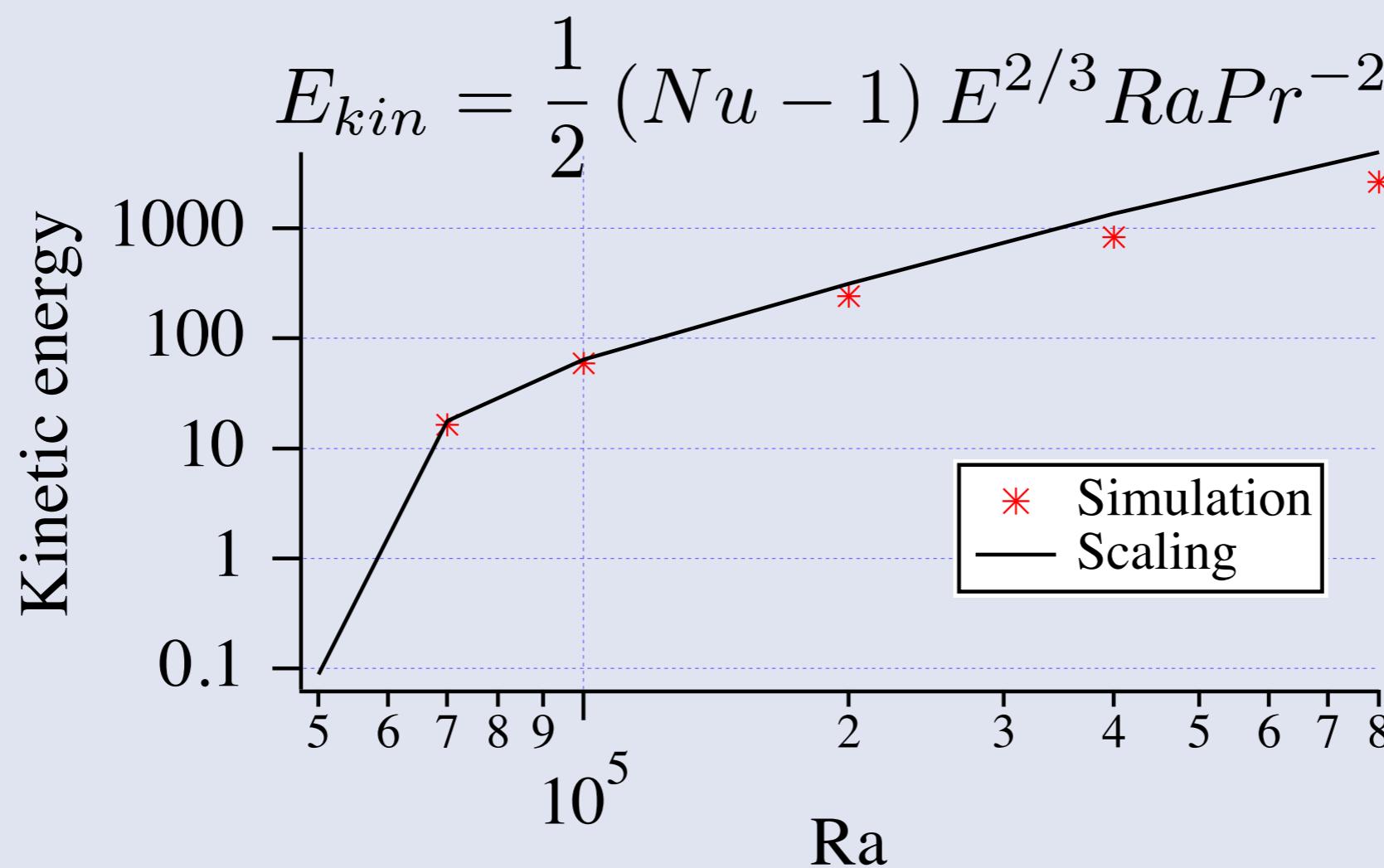
Expected scaling plot

- You will perform simulation by changing Rayleigh number
 - $Ra = 7.0\text{e}4, 1.0\text{e}5, 2.0\text{e}5, 4.0\text{e}5, 8.0\text{e}5$
- Obtain scaling law between kinetic energy and Nusselt number

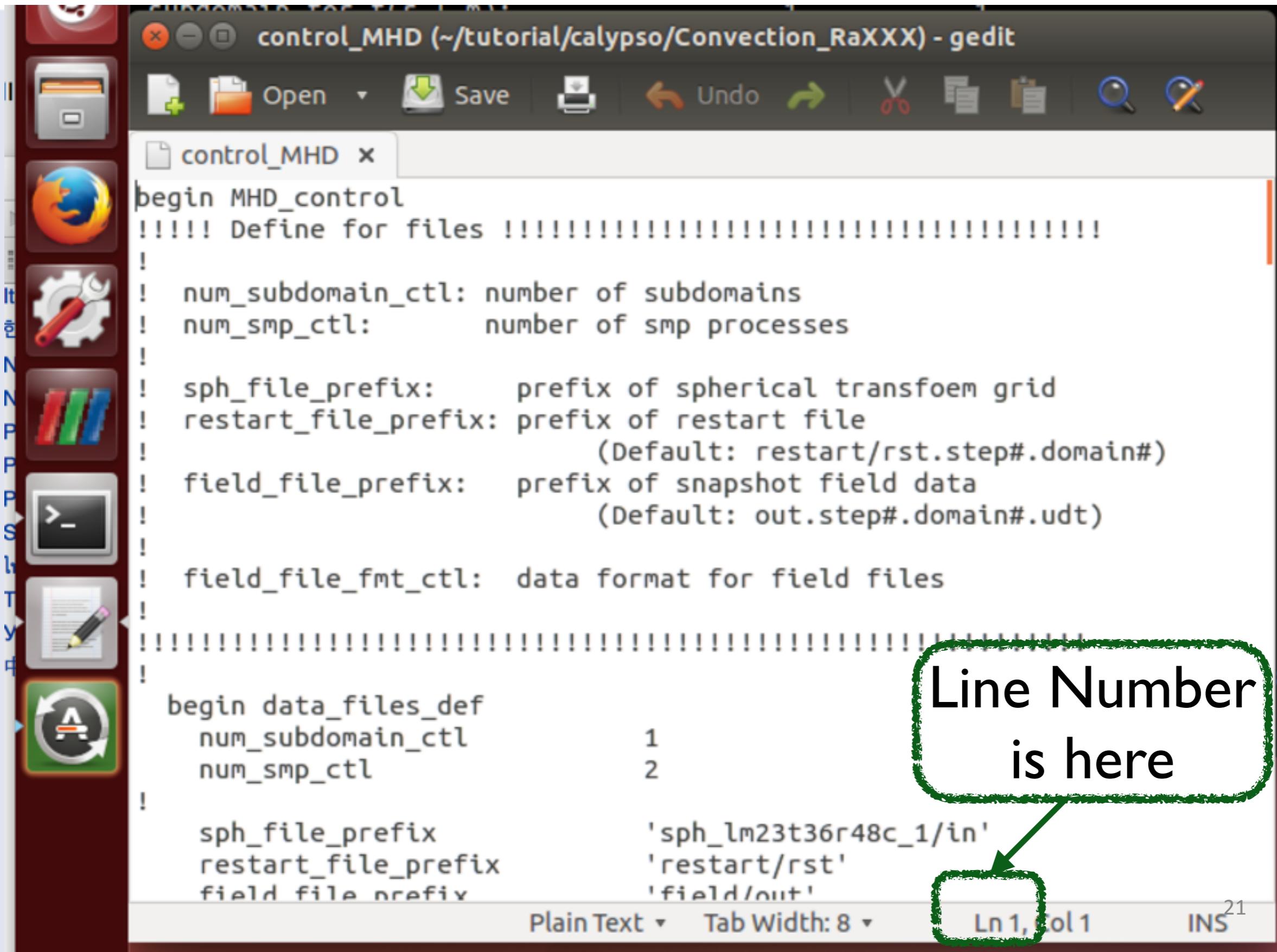


Expected scaling plot

- Details of the scaling law will be explained in Bruce's Lecture on this Friday



Open Control_MHD



control_MHD (~/tutorial/calypso/Convection_RaXXX) - gedit

control_MHD

```
begin MHD_control
!!!! Define for files !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
! num_subdomain_ctl: number of subdomains
! num_smp_ctl:       number of smp processes
!
! sph_file_prefix:   prefix of spherical transfoem grid
! restart_file_prefix: prefix of restart file
!                               (Default: restart/rst.step#.domain#)
! field_file_prefix:  prefix of snapshot field data
!                               (Default: out.step#.domain#.udt)
!
! field_file_fmt_ctl: data format for field files
!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
begin data_files_def
    num_subdomain_ctl          1
    num_smp_ctl                 2
!
    sph_file_prefix             'sph_lm23t36r48c_1/in'
    restart_file_prefix          'restart/rst'
    field_file_prefix            'field/out'
```

Plain Text ▾ Tab Width: 8 ▾ Ln 1, col 1 INS²¹

Line Number
is here

Parameter file format

```
143: begin dimensionless_ctl
144:   array dimless_ctl 4
145:     dimless_ctl  Pr           1.0e+0
146:     dimless_ctl  Ra          1.0E+5
147:     dimless_ctl  E            1.0e-3
148:     dimless_ctl  r_o         1.53846154e+0
149:   end array dimless_ctl
150: end dimensionless_ctl
```



Parameter name

- (defined by program)



If many parameters are defined with the same name, number of items is defined by ‘array [name] # of item’ block.



Parameter block is defined by ‘begin’ and ‘end’



Modification for control_MHD

- Perform simulation by changing Rayleigh number
- $\text{Ra} = 7.0\text{e}4, 1.0\text{e}5, 2.0\text{e}5, 4.0\text{e}5, 8.0\text{e}5$
- If $\text{Ra} = 8.0\text{e}5$ is chosen, one more modification is required for the shorter time stepping

```
143: begin dimensionless_ctl
144:   array dimless_ctl 4
145:     dimless_ctl Pr           1.0e+0
146:     dimless_ctl Ra          1.0E+5
147:     dimless_ctl E           1.0e-3
148:     dimless_ctl r_o         1.53846154e+0
149:   end array dimless_ctl
150: end dimensionless_ctl
```



Change here!

Change time step length for Ra = 8.0E5 Case

```
155: begin time_step_ctl
156:   i_step_init_ctl      0
157:   i_step_finish_ctl    4000
158:!
159:   i_step_check_ctl     20
160:   i_step_RST_ctl       2000
161:   i_step_field_ctl     500
162:!
163:   dt_ctl               2.0e-4
164:   time_init_ctl        0.0e-8
165: end time_step_ctl
```

- Change the total number of time steps to 8000

- Change length of time step to 1.0e-4



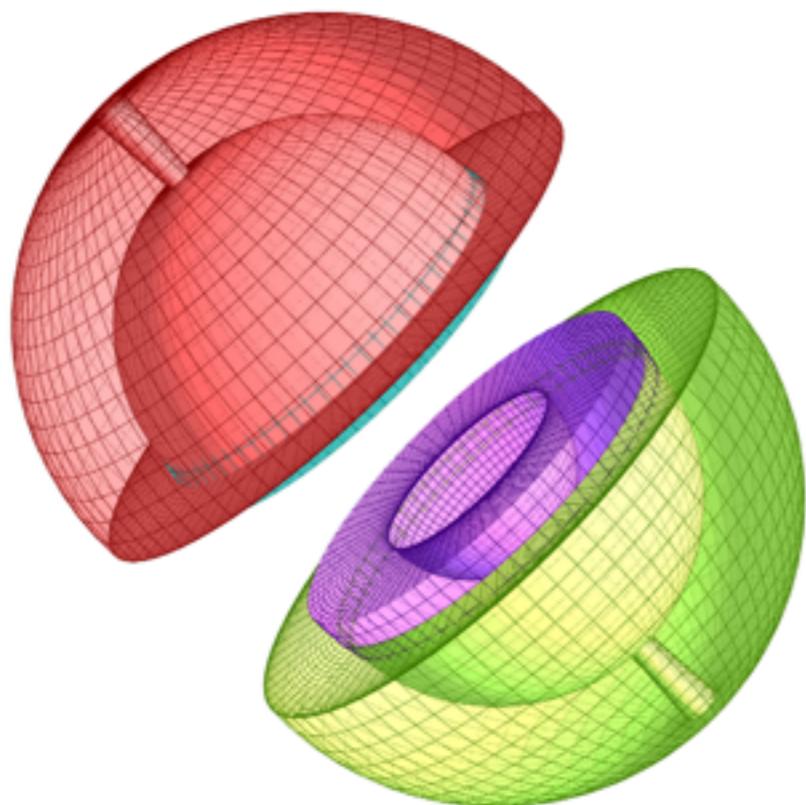
How to run MPI programs?

```
$ mpirun -np 4 ./sph_mhd
```

Command to invoke MPI program

Number of Processes

Executable file name



Process 0

Process 1

Process 2

Process 3

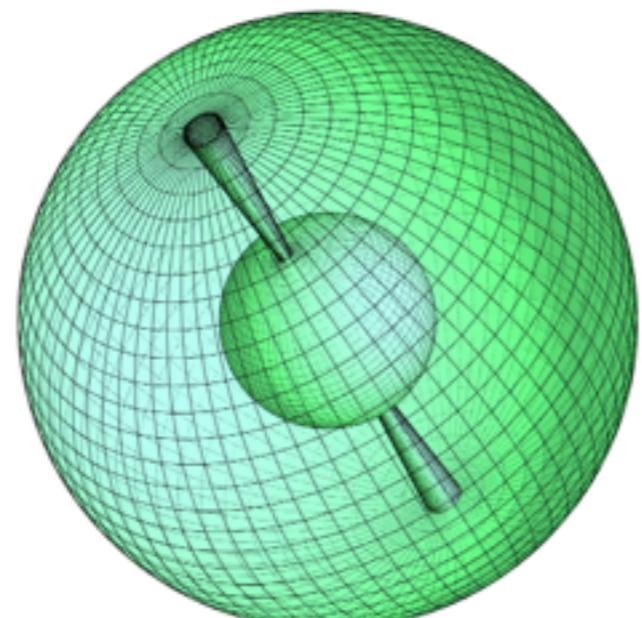
Now, we use only one process

```
$ mpirun -np 1 ./sph_mhd
```

Command to
invoke MPI program

Number of
Processes

Executable
file name



Process 0



Start simulation

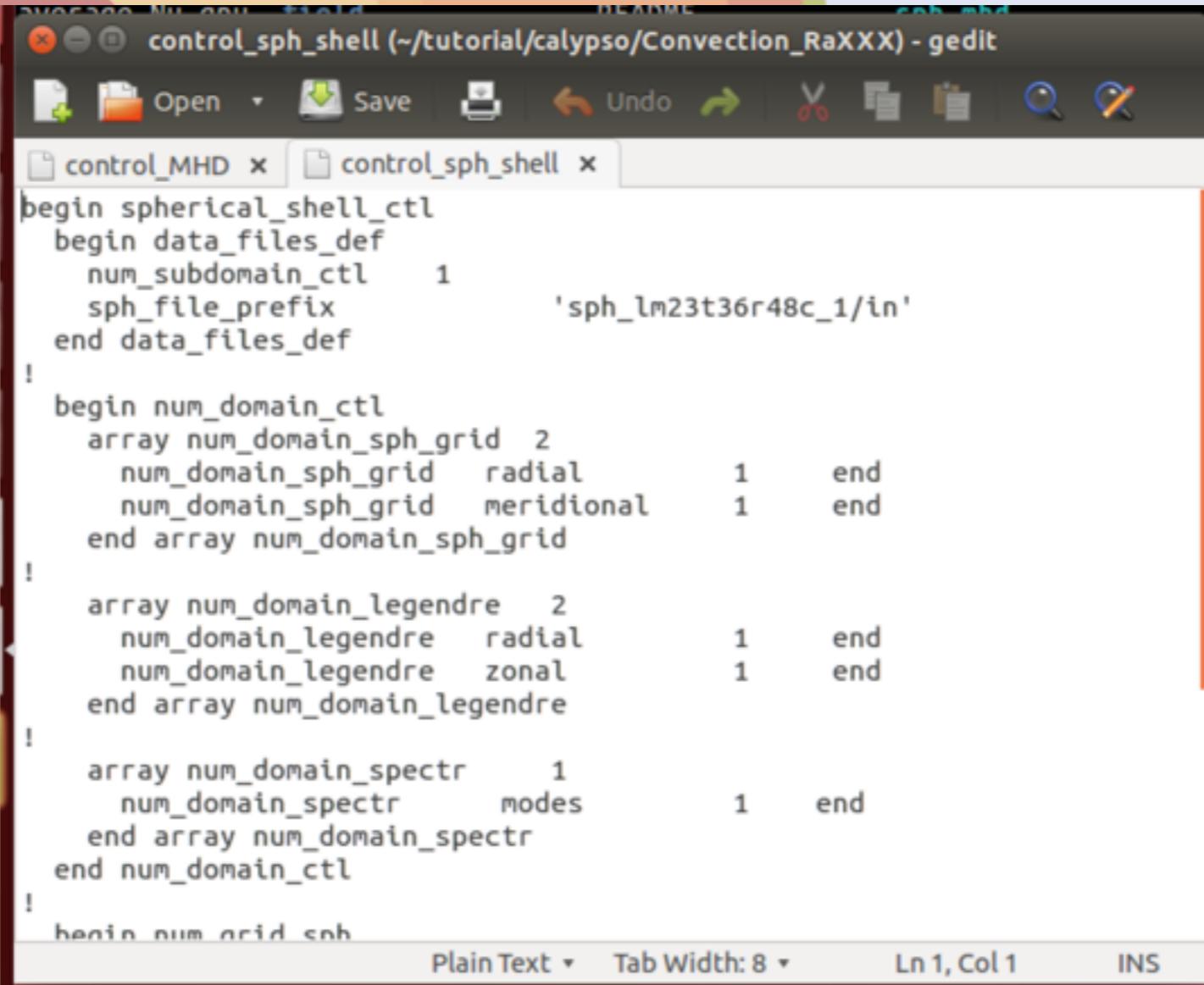
2. Run simulation

- Command: `$ mpirun -np 1 ./sph_mhd`
- Parameter file: `control_MHD`

```
in.0.gfm  in.0.rj  in.0.rlm  in.0.rtm  in.0.rtp  README
cig@cig-VirtualBox:~/tutorial/calypso/Convection_RaXX$ mpirun -np 1 ./sph_mhd
Simulation start: PE.          0
Read ascii mesh file: sph_lm23t36r48c_1/in.0.gfm
Read ascii grid file: sph_lm23t36r48c_1/in.0.rtp
Read ascii spectr modes file: sph_lm23t36r48c_1/in.0.rj
Read ascii grid file: sph_lm23t36r48c_1/in.0.rtm
Read ascii spectr modes file: sph_lm23t36r48c_1/in.0.rlm
```

coefficient for velocity:	1.0000000000000000
coefficient for pressure:	1000.0000000000000
coefficient for viscous diffusion:	1.0000000000000000
coefficient for buoyancy:	64999.999935000007
coefficient for composit buovanc:	1.0000000000000000

Input file for preprocessing (control_sph_shell)



```
control_sph_shell (~tutorial/calypso/Convection_RaXXX) - gedit
control_MHD x control_sph_shell x
control_sph_shell (~tutorial/calypso/Convection_RaXXX) - gedit
control_sph_shell (~tutorial/calypso/Convection_RaXXX) - gedit

begin spherical_shell_ctl
  begin data_files_def
    num_subdomain_ctl      1
    sph_file_prefix         'sph_lm23t36r48c_1/in'
  end data_files_def
!
  begin num_domain_ctl
    array num_domain_sph_grid 2
      num_domain_sph_grid radial      1      end
      num_domain_sph_grid meridional 1      end
    end array num_domain_sph_grid
!
    array num_domain_legendre 2
      num_domain_legendre radial      1      end
      num_domain_legendre zonal      1      end
    end array num_domain_legendre
!
    array num_domain_spectr   1
      num_domain_spectr modes      1      end
    end array num_domain_spectr
  end num_domain_ctl
!
begin num_grid sph
```

Blocks for control_sph_shell



File prefix

Parallelization

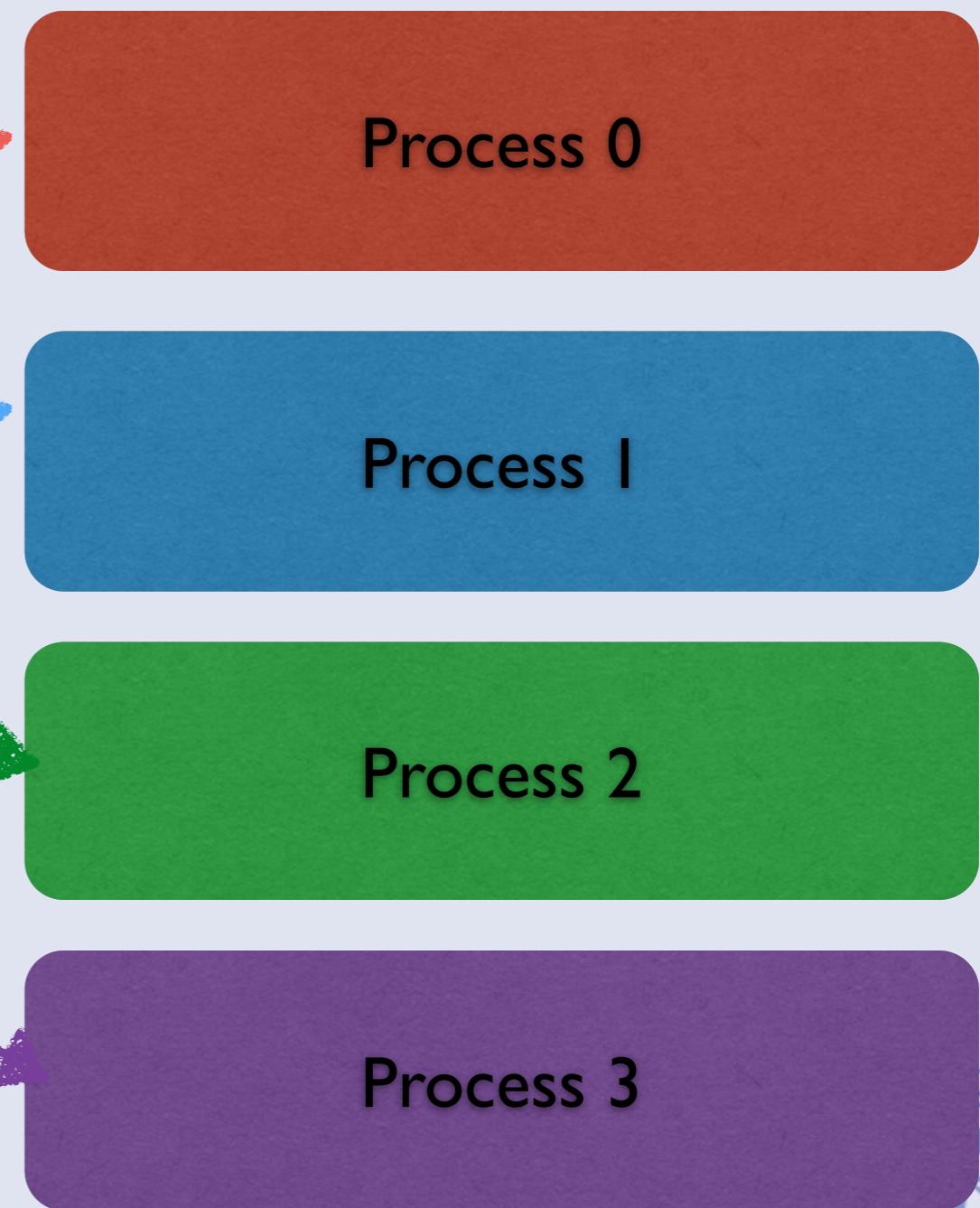
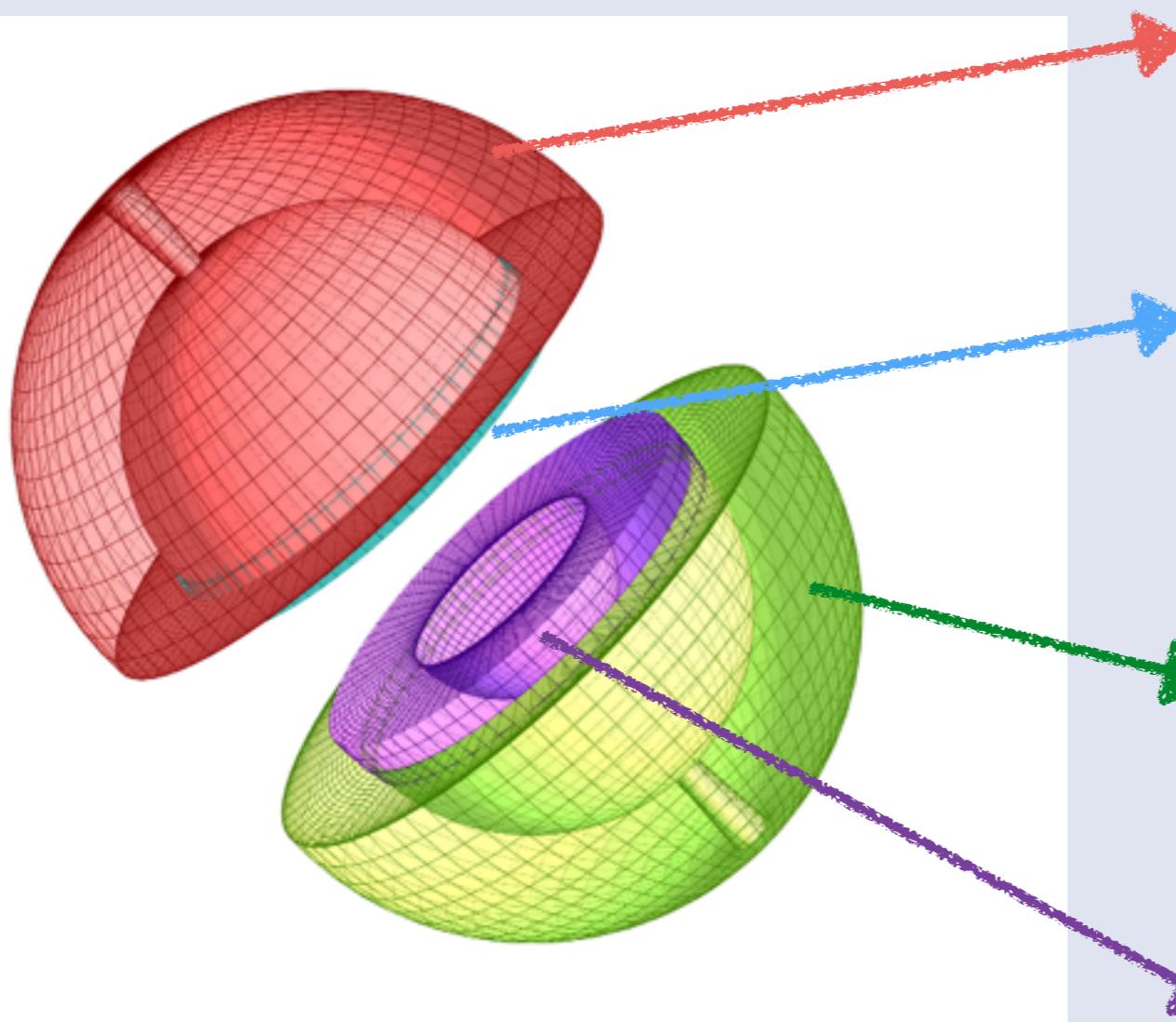
Spatial resolution

```
1: begin spherical_shell_ctl
2: begin data_files_def
3: ...
4: ...
5: end data_files_def
6: !
7: begin num_domain_ctl
8: ...
9: ...
10: end num_domain_ctl
11: !
12: begin num_grid_sph
13: ...
14: ...
15: end num_grid_sph
16: !
17: end spherical_shell_ctl
```



Parallel computation with MPI

- Number of subdomain is equal to MPI processes

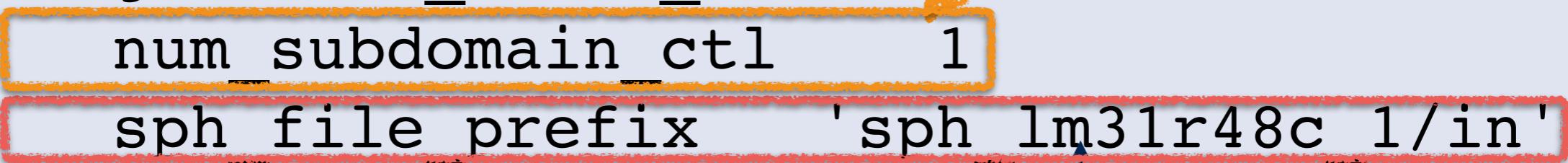


File names

```
2: begin data_files_def
3:   num_subdomain_ctl      1
4:   sph_file_prefix        'sph_lm31r48c_1/in'
5: end data_files_def
```

of MPI process

File prefix for harmonics
indexing data

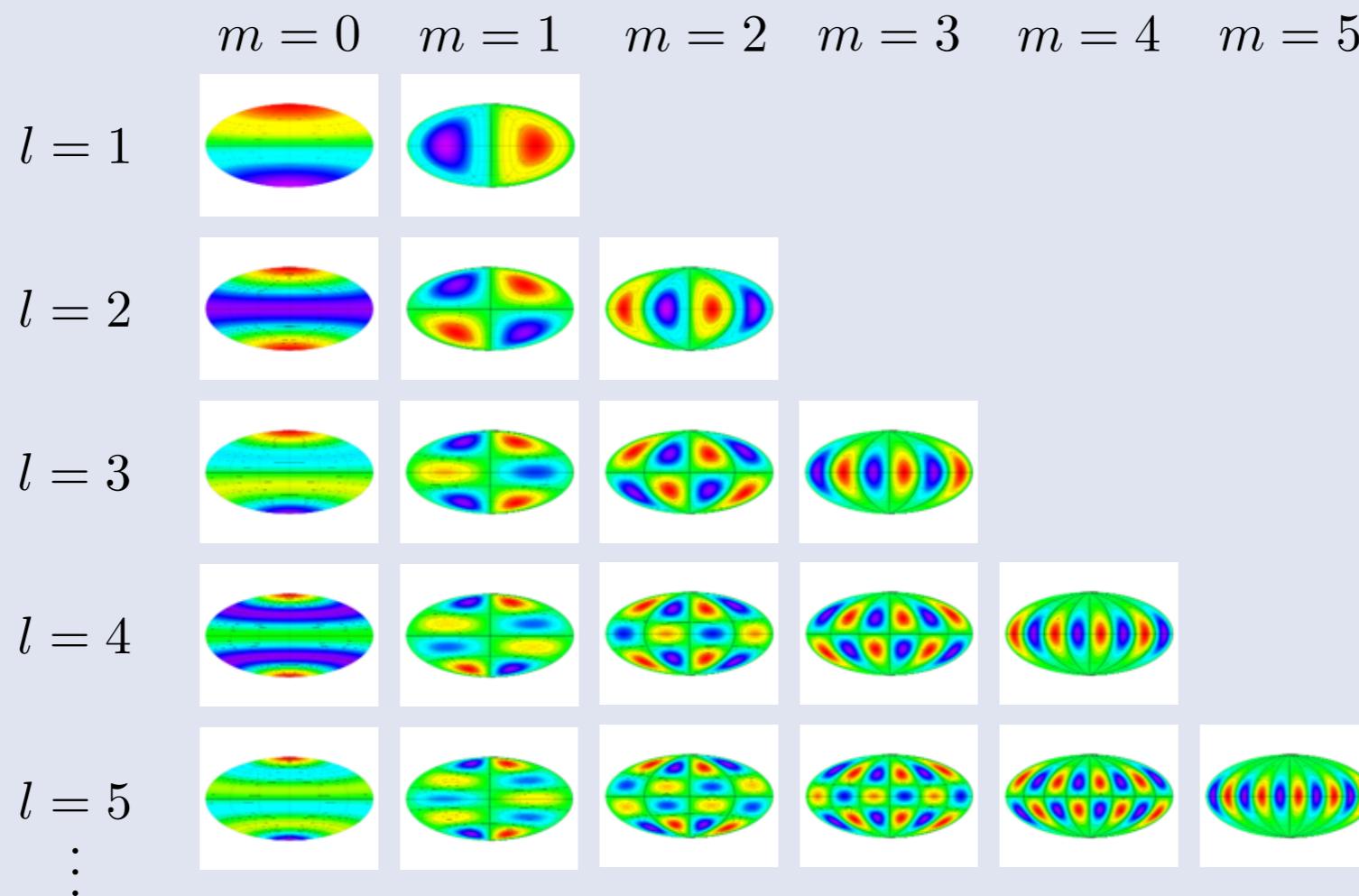


```
cig@cig-VirtualBox:~/tutorial/calypso/Convection_RaXXX$ ls
average_KE.gnu    control_MHD          field          README      sph_lm23t36r48c_1
average_Nu.gnu    control_sph_shell    gen_sph_grids  restart    sph_mhd
cig@cig-VirtualBox:~/tutorial/calypso/Convection_RaXXX$
```

Definition of spatial resolution

-Horizontal direction-

24:	truncation_level_ctl	23	Truncation degree	l_{max}
25: !				
26:	ngrid_meridonal_ctl	36		
27:	ngrid_zonal_ctl	72		



Definition of spatial resolution

-Horizontal direction-

```
24:      truncation_level_ctl    23  
25: !  
26:      ngrid_meridonal_ctl  
27:      ngrid_zonal_ctl
```

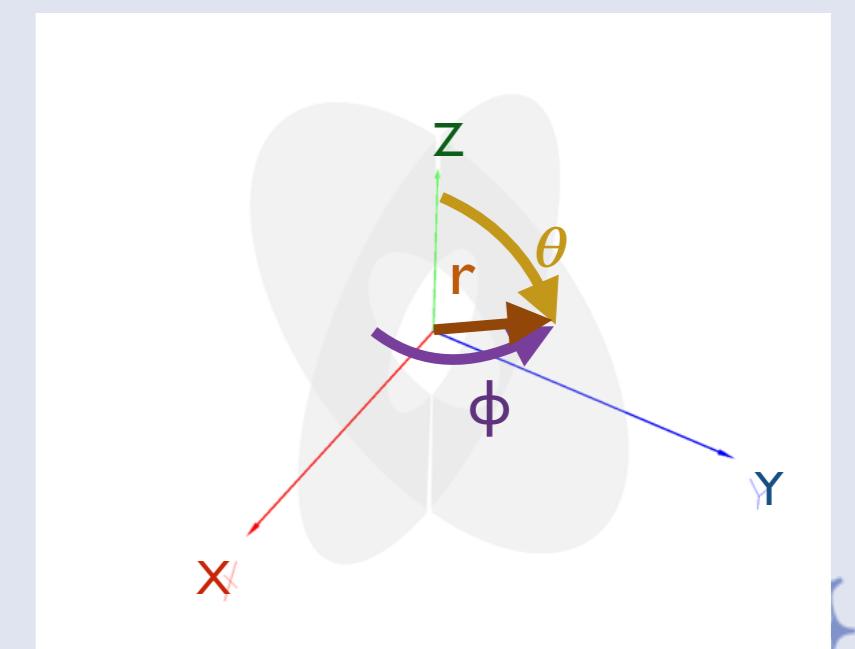
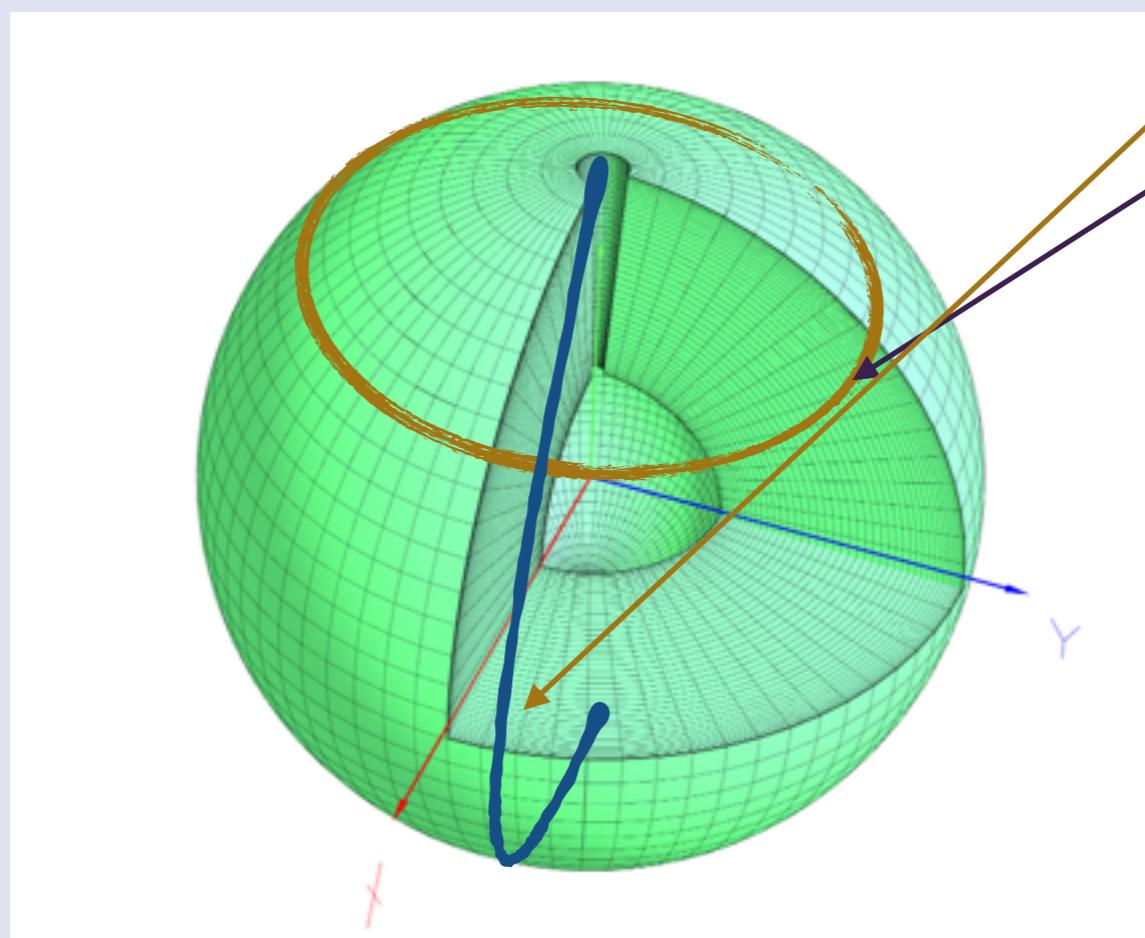
23

36

72

Number of
meridional grid N_θ

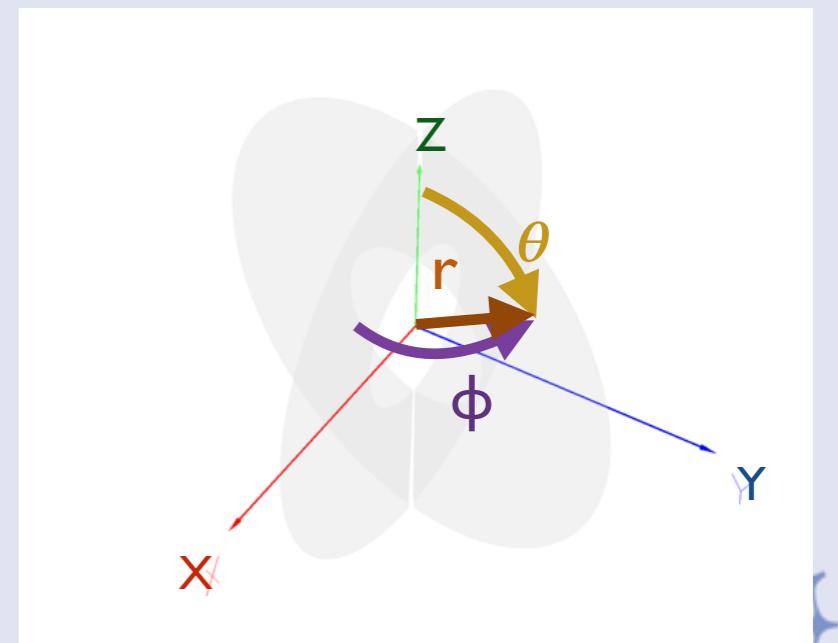
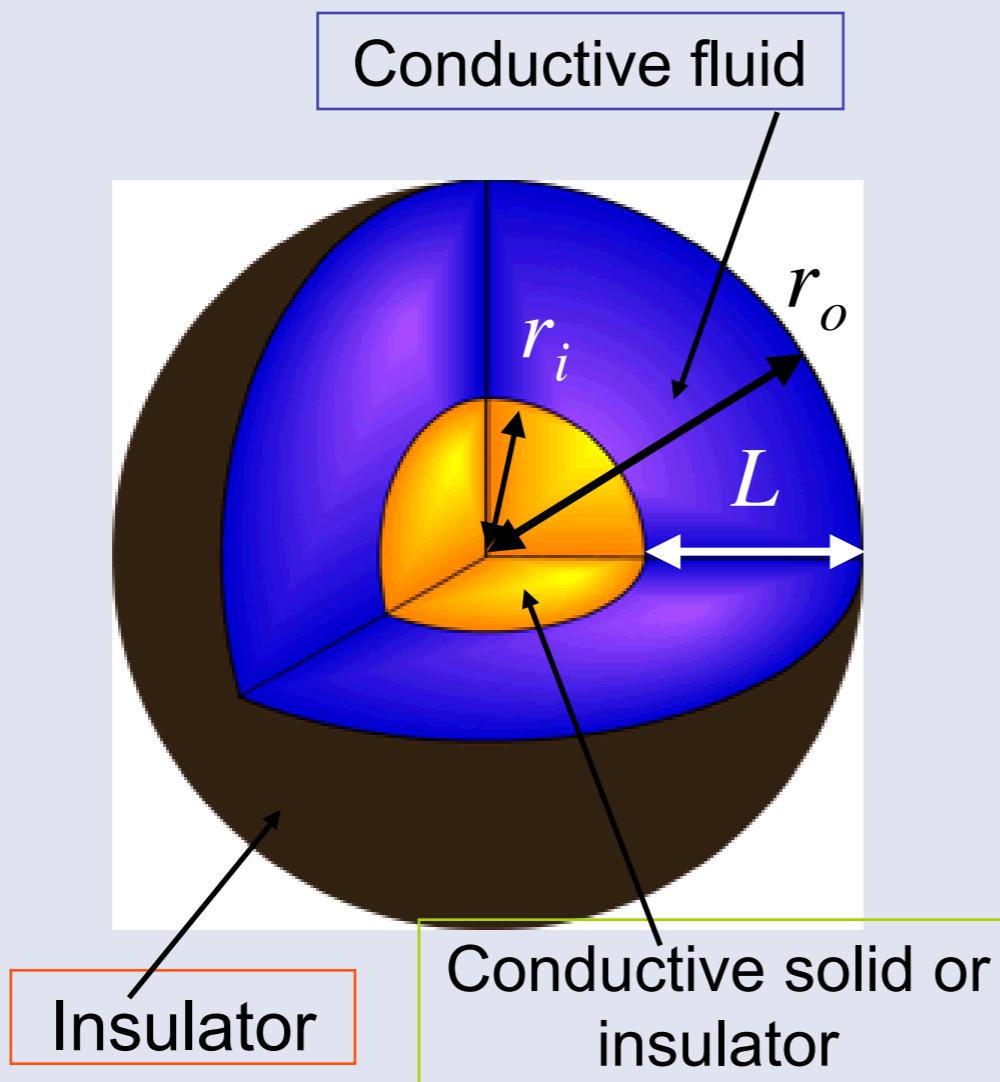
Number of
zonal grid N_ϕ



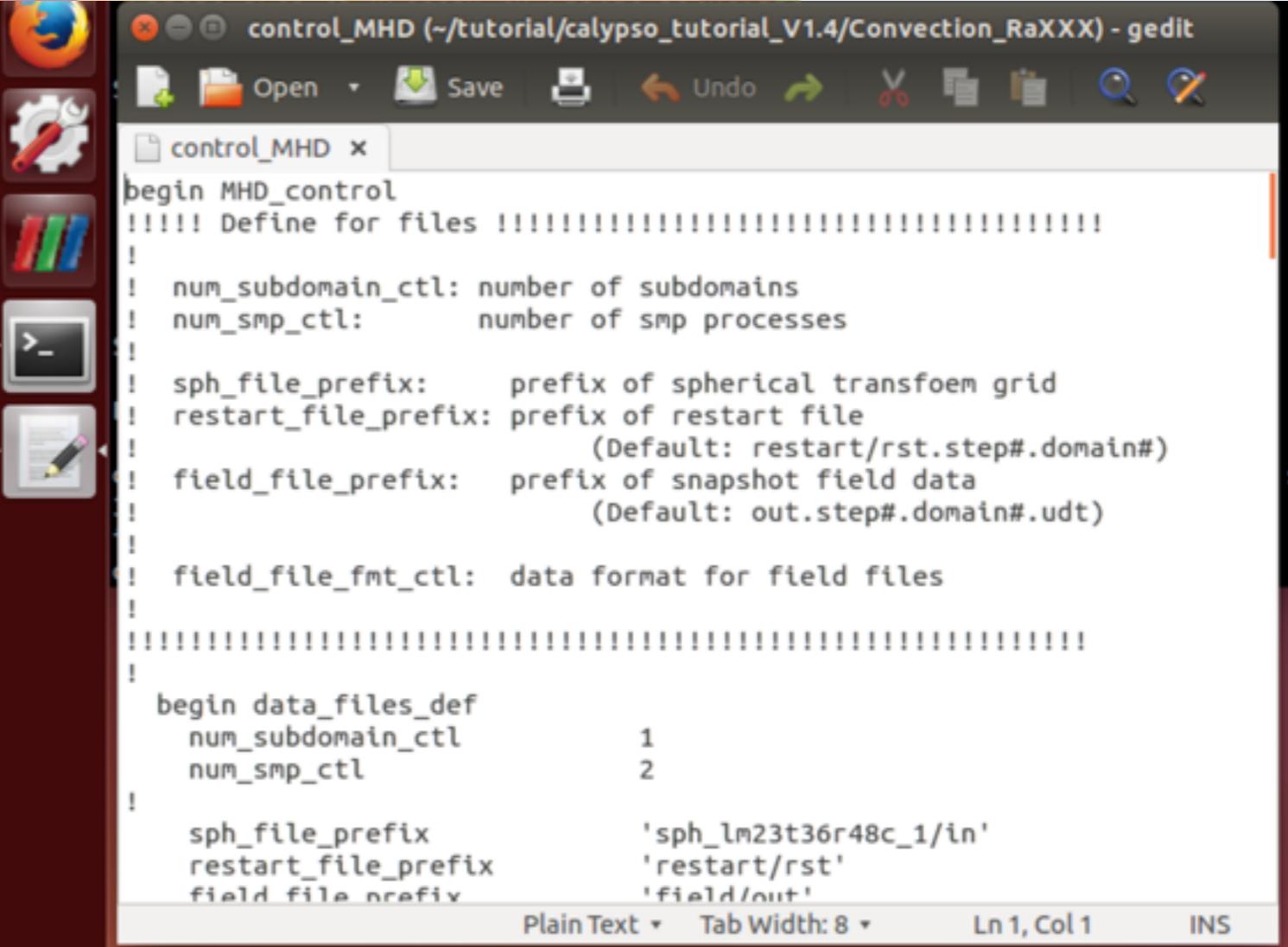
Definition of radial grid

```
30: num_fluid_grid_ctl  
31: fluid_core_size_ctl  
32: ICB_to_CMB_ratio_ctl
```

48 ← Number of Layers
1.0 ← Size of fluid shell L
0.35 ← Ratio of inner core $\frac{r_i}{r_o}$
to whole shell



Parameter file for simulation (control_MHD)



```
control_MHD (~/tutorial/calypso_tutorial_V1.4/Convection_RaXXX) - gedit
control_MHD x
begin MHD_control
!!!! Define for files !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
! num_subdomain_ctl: number of subdomains
! num_smp_ctl:      number of smp processes
!
! sph_file_prefix:   prefix of spherical transfoem grid
! restart_file_prefix: prefix of restart file
!                               (Default: restart/rst.step#.domain#)
! field_file_prefix:  prefix of snapshot field data
!                               (Default: out.step#.domain#.udt)
!
! field_file_fmt_ctl: data format for field files
!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
begin data_files_def
  num_subdomain_ctl           1
  num_smp_ctl                 2
!
  sph_file_prefix             'sph_lm23t36r48c_1/in'
  restart_file_prefix          'restart/rst'
  field_file_prefix            'field/out'
```



data_files_def

File setting

```
17: begin data_files_def
18:   num_subdomain_ctl      1
19:   num_smp_ctl            2
20: !
21:   sph_file_prefix         'sph_lm23t36r48c_1/in'
22:   restart_file_prefix     'restart/rst'
23:   field_file_prefix       'field/out'
24: !
25:   field_file_fmt_ctl     'VTK'
26: end data_files_def
```

```
cig@cig-VirtualBox:~/tutorial/calypso/Convection_RaXXX$ ls
average_KE.gnu    control_MHD      field          README      sph_lm23t36r48c_1
average_Nu.gnu    control_sph_shell gen_sph_grids  restart    sph_mhd
cig@cig-VirtualBox:~/tutorial/calypso/Convection_RaXXX$
```

Data definition phys_values_ctl

```
37: begin phys_values_ctl
38:   array nod_value_ctl 4
39:     nod_value_ctl velocity
40:     nod_value_ctl temperature
41:     nod_value_ctl pressure
42:     nod_value_ctl vorticity
43:   end array nod_value_ctl
44: end phys_values_ctl
```

The code defines a structure for physical values control. It begins with a 'begin phys_values_ctl' block, followed by an array declaration 'array nod_value_ctl 4'. Inside the array, four field names are listed: 'velocity', 'temperature', 'pressure', and 'vorticity'. The array is closed with an 'end array nod_value_ctl' statement, and the entire block is closed with an 'end phys_values_ctl' statement.

Field name

Field data
output flag

Time series
output flag

Choose of time integration

time_evo_ctl

```
50: begin time_evolution_ctl
51:   array time_evo_ctl 2
52:     time_evo_ctl temperature
53:     time_evo_ctl velocity
54:   end array time_evo_ctl
55: end time_evolution_ctl
```



Field for time integration

label	field name	Description
velocity	Velocity	\mathbf{u}
temperature	Temperature	T
composition	Composition variation	C
magnetic_field	Magnetic field	\mathbf{B}

Boundary conditions

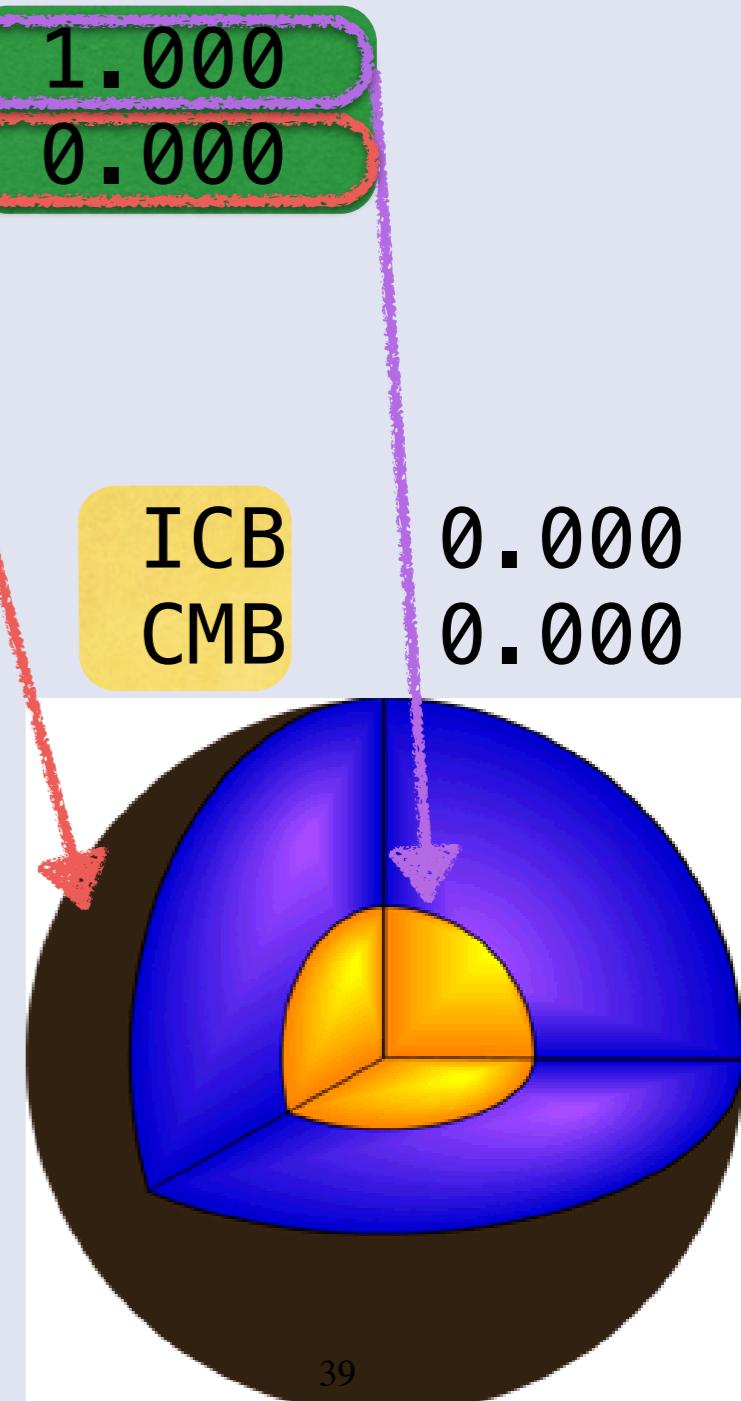
boundary_condition

```
59: begin boundary_condition
60:     array bc_temperature 2
61:         bc_temperature fixed ICB 1.000
62:         bc_temperature fixed CMB 0.000
63:     end array bc_temperature
64: !
65:     array bc_velocity 2
66:         bc_velocity non_slip_sph
67:         bc_velocity non_slip_sph
68:     end array bc_velocity
69: end boundary_condition
```

Boundary condition type

Place to be defined

B.C. Value



Forcing terms

forces_define

```
75: begin forces_define
76:   array force_ctl      2
77:     force_ctl    gravity
78:     force_ctl    Coriolis
79:   end array force_ctl
80: end forces_define
```

Available forces

Label	Field name	Equation
Coriolis	Coriolis force	$-2\Omega\hat{z} \times \mathbf{u}$
Lorentz	Lorentz force	$\mathbf{J} \times \mathbf{B}$
gravity	Thermal buoyancy	$-\alpha_T T g$
Composite_gravity	Compositional buoyancy	$-\alpha_C C g$



Governing equations for rotating convection

Coriolis force

$$\begin{aligned} 1 \left[\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} \right] + 2E^{-1} (\hat{z} \times \mathbf{u}) &= -E^{-1} \nabla P + 1 \nabla^2 u + r_o^{-1} Ra Pr Tr \\ 1 \left[\frac{\partial T}{\partial t} + (\mathbf{u} \cdot \nabla) T \right] &= Pr^{-1} \nabla^2 T, \\ \nabla \cdot \mathbf{u} &= 0. \end{aligned}$$

$$Pr = \frac{\nu}{\kappa}, \quad E = \frac{\nu}{\Omega L^2}, \quad Ra = \frac{\alpha g \Delta T L^3}{\kappa \nu}$$

Coefficients to be defined by the control file



Scaling for momentum equation momentum (Cont'd)

$$1 \left[\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} \right] + 2E^{-1} (\hat{z} \times \mathbf{u}) = -E^{-1} \nabla P + 1 \nabla^2 \mathbf{u} + r_o^{-1} Ra Pr Tr$$

```
125: array coef_4_v_diffuse_ctl           1
126:   coef_4_v_diffuse_ctl  One          1.0
127: end array coef_4_v_diffuse_ctl
128: !
129: array coef_4_buoyancy_ctl            3
130:   coef_4_buoyancy_ctl  r_o          -1.0
131:   coef_4_buoyancy_ctl  Ra           1.0
132:   coef_4_buoyancy_ctl  Pr           1.0
133: end array coef_4_buoyancy_ctl
```

Dimensionless numbers

dimensionless_ctl

```
143: begin dimensionless_ctl
144:   array dimless_ctl 4
145:     dimless_ctl E
146:     dimless_ctl Pr
147:     dimless_ctl Ra
148:     dimless_ctl r_o
149:   end array dimless_ctl
150: end dimensionless_ctl
```

Name of numbers

Values

- Name of parameters are arbitrary.
- Parameter names are **case sensitive**



Parameters for time integration

time_step_ctl

```
155: begin time_step_ctl
156:   i_step_init_ctl
157:   i_step_finish_ctl
158: !
159:   i_step_check_ctl      20
160:   i_step_RST_ctl       2000
161:   i_step_field_ctl     500
162: !
163:   dt_ctl
164:   time_init_ctl
165: end time_step_ctl
```

- 0 ← • Time step to start
- 3000 ← • Time step to finish
- 2.0e-4 ← • Length of time step
- 0.0e-8 ← • Initial time



Parameters for time integration

time_step_ctl

```
155: begin time_step_ctl
156:   i_step_init_ctl
157:   i_step_finish_ctl
158: !
159:   i_step_check_ctl
160:   i_step_RST_ctl
161:   i_step_field_ctl
162: !
163:   dt_ctl
164:   time_init_ctl
165: end time_step_ctl
```

- Increment for time sequence data
 - Increment for restarting data
 - Increment for field data output
-
- The diagram illustrates the mapping of parameters from the configuration file to their descriptions. Red arrows point from the values 0, 3000, 20, 2000, 500, 2.0e-4, and 0.0e-8 to their respective definitions in the list.
- | Parameter Value | Description |
|-----------------|------------------------------------|
| 0 | • Increment for time sequence data |
| 3000 | • Increment for time sequence data |
| 20 | • Increment for restarting data |
| 2000 | • Increment for restarting data |
| 500 | • Increment for restarting data |
| 2.0e-4 | • Increment for field data output |
| 0.0e-8 | • Increment for field data output |

Time series data setting

sph_monitor_ctl

```
181: begin sph_monitor_ctl
182:   volume_average_prefix      'sph_ave_volume'
183:   volume_pwr_spectr_prefix   'sph_pwr_volume'
184: !
185:   nusselt_number_prefix      'Nusselt'
186: end sph_monitor_ctl
```

name	Parallelization	I/O
control_MHD	Serial	Input
[sph_prefix]. [domain#]. rj	Distributed	Input
[sph_prefix]. [domain#]. rlm	Distributed	Input
[sph_prefix]. [domain#]. rtm	Distributed	Input
[sph_prefix]. [domain#]. rtp	Distributed	Input
[sph_prefix]. [domain#]. gfm	Distributed	Input
[boundary_data_name]	Single	Input
[rst_prefix]. [step#]. [domain#]. fst	Distributed	Input/Output
[vol_pwr_prefix]. dat	Single	Output
[vol_pwr_prefix]_l.dat	Single	Output
[vol_pwr_prefix]_m.dat	Single	Output
[vol_pwr_prefix]_lm.dat	Single	Output
[vol_ave_prefix]. dat	Single	Output
[layer_pwr_prefix]_l.dat	Single	Output
[layer_pwr_prefix]_m.dat	Single	Output
[layer_pwr_prefix]_lm.dat	Single	Output
[gauss_coef_prefix]. dat	Single	Output
[picked_sph_prefix]. dat	Single	Output
[nusselt_number_prefix]. dat	Single	Output
[fld_prefix]. [step#]. [domain#]. [extension]	-	Output



Postprocessing



Procedure of simulation

1. Preprocessing: Prepare spherical harmonics index table
2. Run simulation
3. Postprocessing
 - Check Scaling law by Gnuplot
 - Visualization by Paraview



files after simulation

Field data
for visualization

Time sequence
data

```
time step= 3940      time= 7.88000000E-01 E_kin = 5.84177111E+01
time step= 3960      time= 7.92000000E-01 E_kin = 5.84177134E+01
time step= 3980      time= 7.96000000E-01 E_kin = 5.84177157E+01
Write ascii data file: restart/rst.4.0.fst
time step= 4000      time= 8.00000000E-01 E_kin = 5.84177178E+01
Write parallel VTK file: field/out.8.pvtk
Write ascii VTK file: field/out.8.0.vtk
cig@cig-VirtualBox:~/tutorial/calypso/Convection_RaXXX$ ls
average_KE.gnu      Nusselt.dat          sph_mhd
average_Nu.gnu       radial_point.dat    sph_pwr_volume.dat
control_MHD          README               sph_pwr_volume_l.dat
control_sph_shell    restart              sph_pwr_volume_lm.dat
field                sph_ave_volume.dat  sph_pwr_volume_m.dat
gen_sph_grids        sph_lm23t36r48c_1  time_total.dat
cig@cig-VirtualBox:~/tutorial/calypso/Convection_RaXXX$ ls field/
out.1.0.vtk  out.2.pvtk  out.4.0.vtk  out.5.pvtk  out.7.0.vtk  out.8.pvtk
out.1.pvtk   out.3.0.vtk  out.4.pvtk   out.6.0.vtk  out.7.pvtk   README
out.2.0.vtk   out.3.pvtk  out.5.0.vtk  out.6.pvtk   out.8.0.vtk
cig@cig-VirtualBox:~/tutorial/calypso/Convection_RaXXX$
```

Data analysis by Gnuplot



- Mean square data consists of time series data
- Make a line plot and take a time average by Gnuplot



Which column should be used? CIG COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

- Time is in the 2nd column
- Nu at ICB is in the 3rd column
- Nu at CMB is in the 4th column

```
out.1.vtk  out.2.vtk  out.3.vtk  out.4.vtk  out.5.vtk  out.6.vtk  out.7.vtk  out.8.vtk  README
out.2.0.vtk  out.3.pvtk  out.5.0.vtk  out.6.pvtk  out.8.0.vtk
cig@cig-VirtualBox:~/tutorial/calypso/Convection_RaXXX$ more Nusselt.dat
# Inner_radius, Outer_radius
 5.384615384615384E-001    1.538461538461538E+000
t_step      time    Nu ICB    Nu CMB
 20  4.00000000000000E-003  1.00201594246366E+000  1.00213480315182E+000
 40  7.99999999999999E-003  1.00619668098559E+000  1.00743933682635E+000
 60  1.20000000000000E-002  1.01430018065005E+000  1.01432829581630E+000
 80  1.60000000000000E-002  1.02607049869886E+000  1.02032185400044E+000
100  2.00000000000000E-002  1.04100666627049E+000  1.02587679487352E+000
120  2.40000000000000E-002  1.05968146246822E+000  1.03149275995523E+000
```

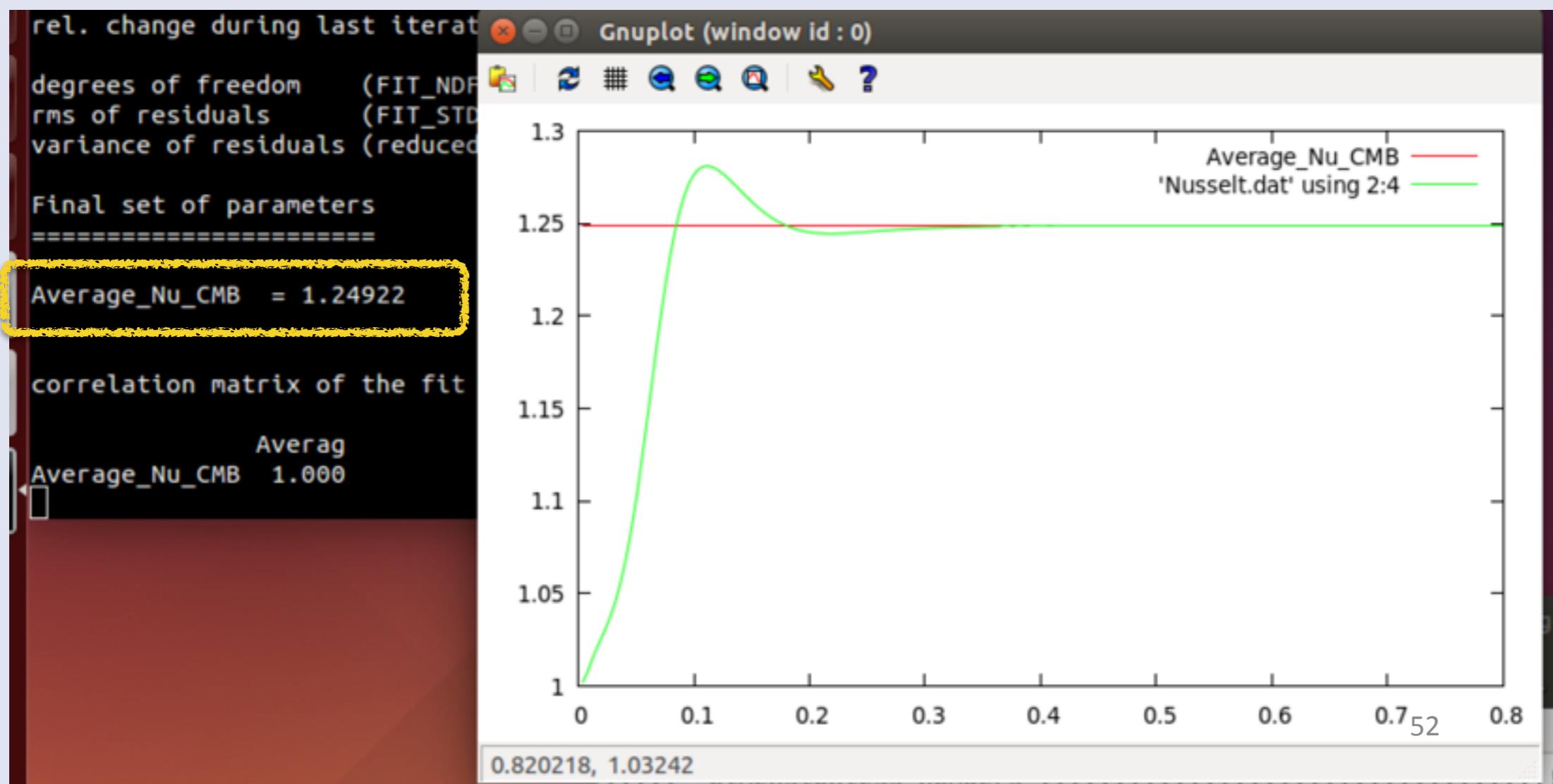


Obtain time averaged Nusselt number

- Run Gnuplot with “average_Nu.gnu”

```
cig@cig-VirtualBox:~/tutorial/calypso_tutorial_V1.4/Convection_RaXXX$ gnuplot average_Nu.gnu
```

- Averaged Nusselt number is displayed on Terminal



Which column should be used? CIG COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

- Time is in the 2nd column
- Kinetic energy is in the 5th column

```
cig@cig-VirtualBox:~/tutorial/calypso/Convection_RaXXX$  
cig@cig-VirtualBox:~/tutorial/calypso/Convection_RaXXX$ more sph_pwr_volume.dat  
radial_layers, truncation  
    49          23  
ICB_id, CMB_id  
    1          49  
number of components  
    3          7  
    3  1  3  
t_step  time   K_ene_pol   K_ene_tor   K_ene   temperature   vorticity_po  
l  vorticity tor  vorticity  
    20  4.0000000000000E-003  1.79583422259195E+000  3.36798559698955E+000  
5.16381981958150E+000  8.35965158490096E-002  4.79449697263297E+002  3.22878754  
242708E+002  8.02328451506006E+002  
    40  7.9999999999999E-003  3.03586924148587E+000  5.87318860233336E+000  
8.90905784381922E+000  8.34712341521374E-002  9.18593101631710E+002  5.31664748  
513151E+002  1.45025785014486E+003  
sum_domain_spectr modes      1      end      53
```

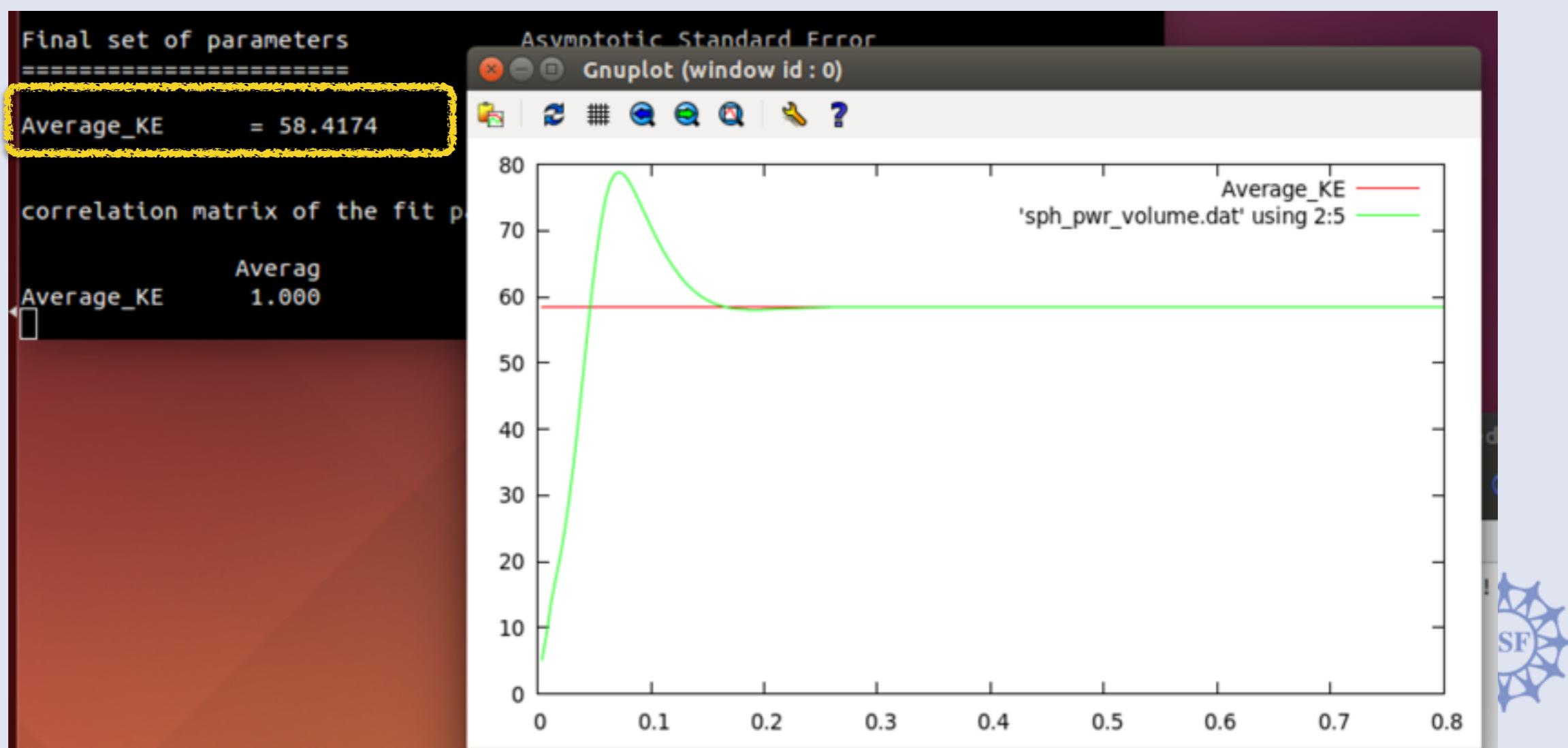
Obtain time averaged kinetic energy



- Run Gnuplot with “average_KE.gnu”

```
out.2.0.vtk  out.3.pvtk  out.5.0.vtk  out.6.pvtk  out.8.0.vtk  
cig@cig-VirtualBox:~/tutorial/calypso_tutorial_V1.4/Convection_RaXXX$ gnuplot av  
erage_KE.gnu
```

- Averaged kinetic energy is displayed on Terminal



Results

$$E_{kin} = \frac{1}{2} (Nu - 1) E^{2/3} Pr^{-2} Ra \frac{1}{r_o} \frac{dT_{diff}}{dr}$$

Effect of geometry

Ra	E	Nu	E
7.0×10	15.9	1.10	15.6
1.0×10	58.4	1.25	58.0
2.0×10	234.2	1.57	266.2
4.0×10	820.5	2.24	1151.4
8.0×10	2651.4	3.42	4483.4

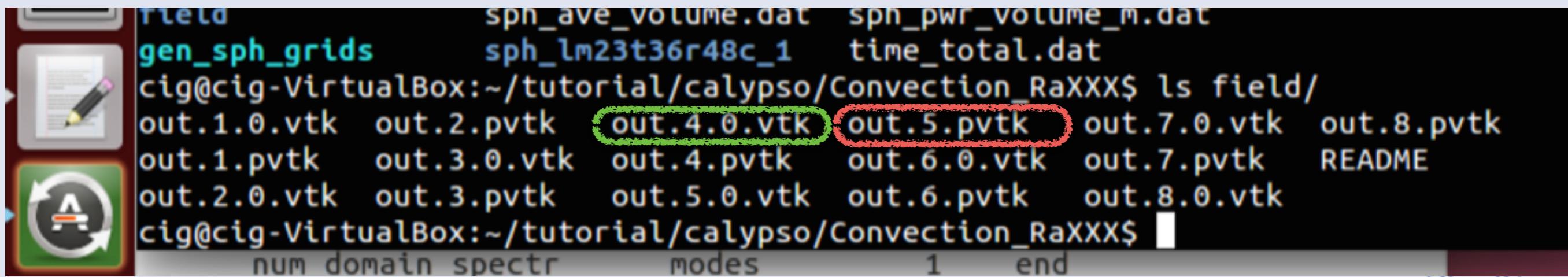
- Kinetic energy departs from the scaling with the larger Ra .
- Need more resolution



Visualization by ParaView

Look a flow pattern aligned with rotation axis

- Open Parallel VTK data by paraview
`out.[step#].vtk`
- Field data for each subdomain are in
`out.[step#].[domain#].vtk`



A screenshot of a terminal window showing the output of the command `ls field/`. The directory contains several files and folders:

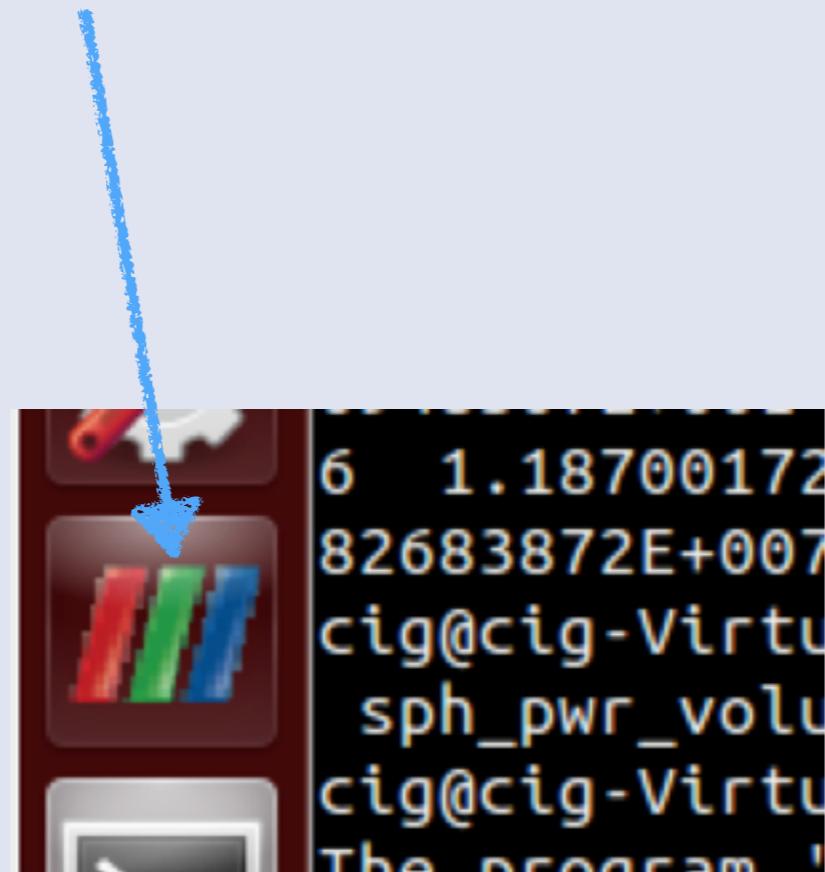
- Field
- gen_sph_grids
- cig@cig-VirtualBox:~/tutorial/calypso/Convection_RaXXX\$ ls field/
- out.1.0.vtk
- out.2.pvtk
- out.4.0.vtk
- out.5.pvtk
- out.7.0.vtk
- out.8.pvtk
- out.1.pvtk
- out.3.0.vtk
- out.4.pvtk
- out.6.0.vtk
- out.7.pvtk
- README
- out.2.0.vtk
- out.3.pvtk
- out.5.0.vtk
- out.6.pvtk
- out.8.0.vtk

The files `out.4.0.vtk` and `out.5.pvtk` are highlighted with green and red circles respectively.



Start ParaView

- Click ParaView Icon!!



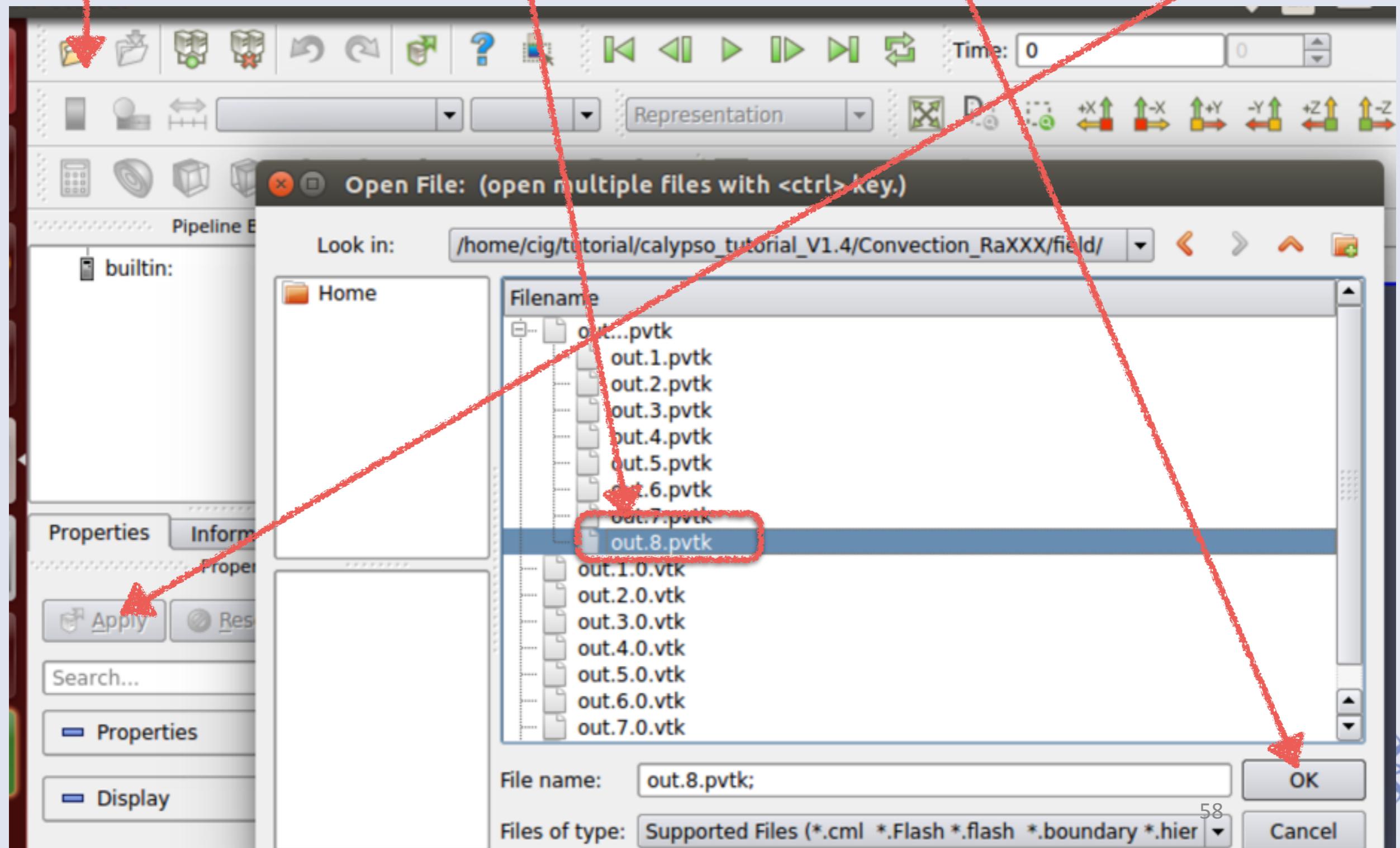
Open field data by Paraview

1. Push “open file”

2. Select a file

3. Push “OK”

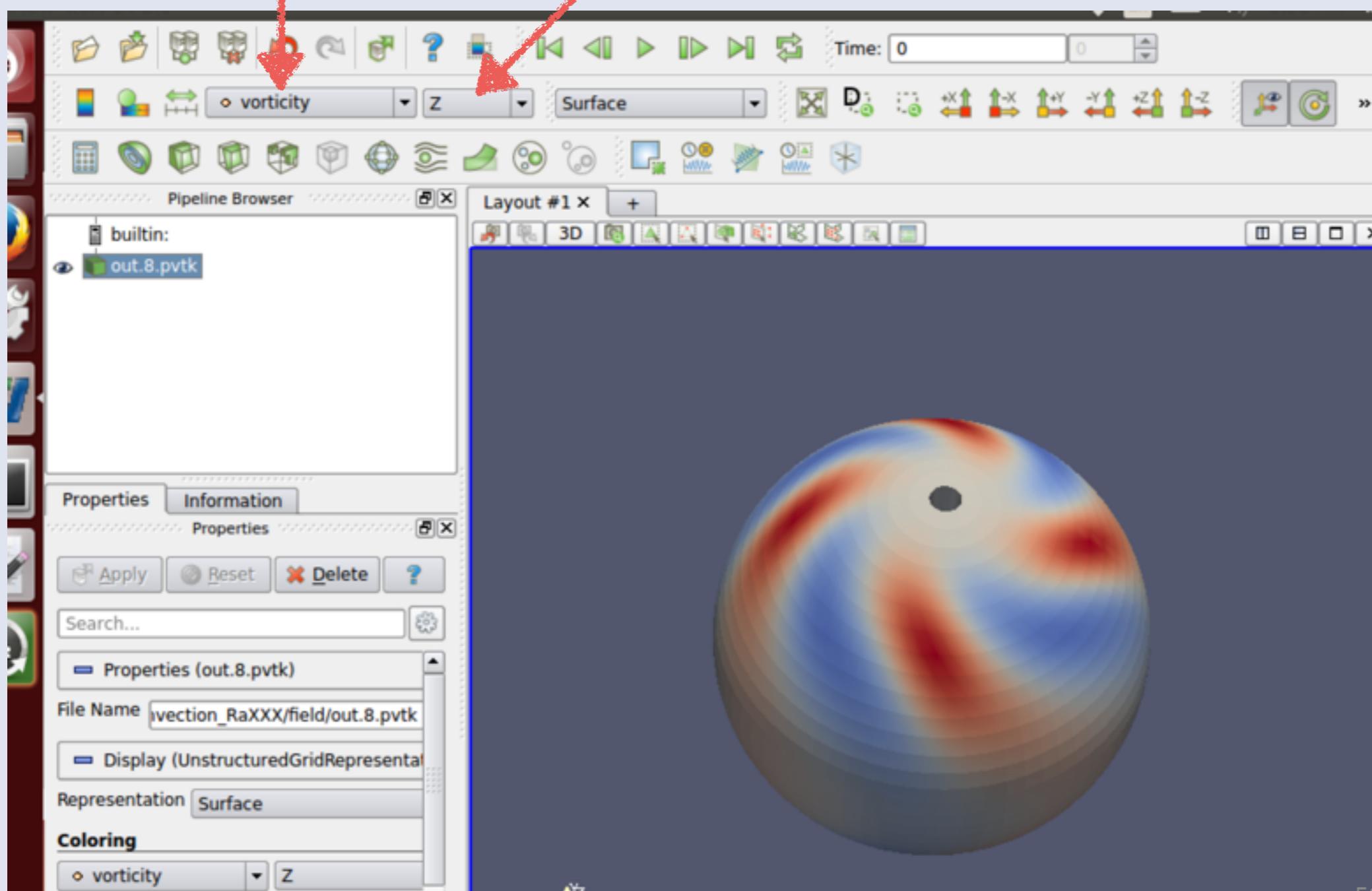
4. Push “Apply”



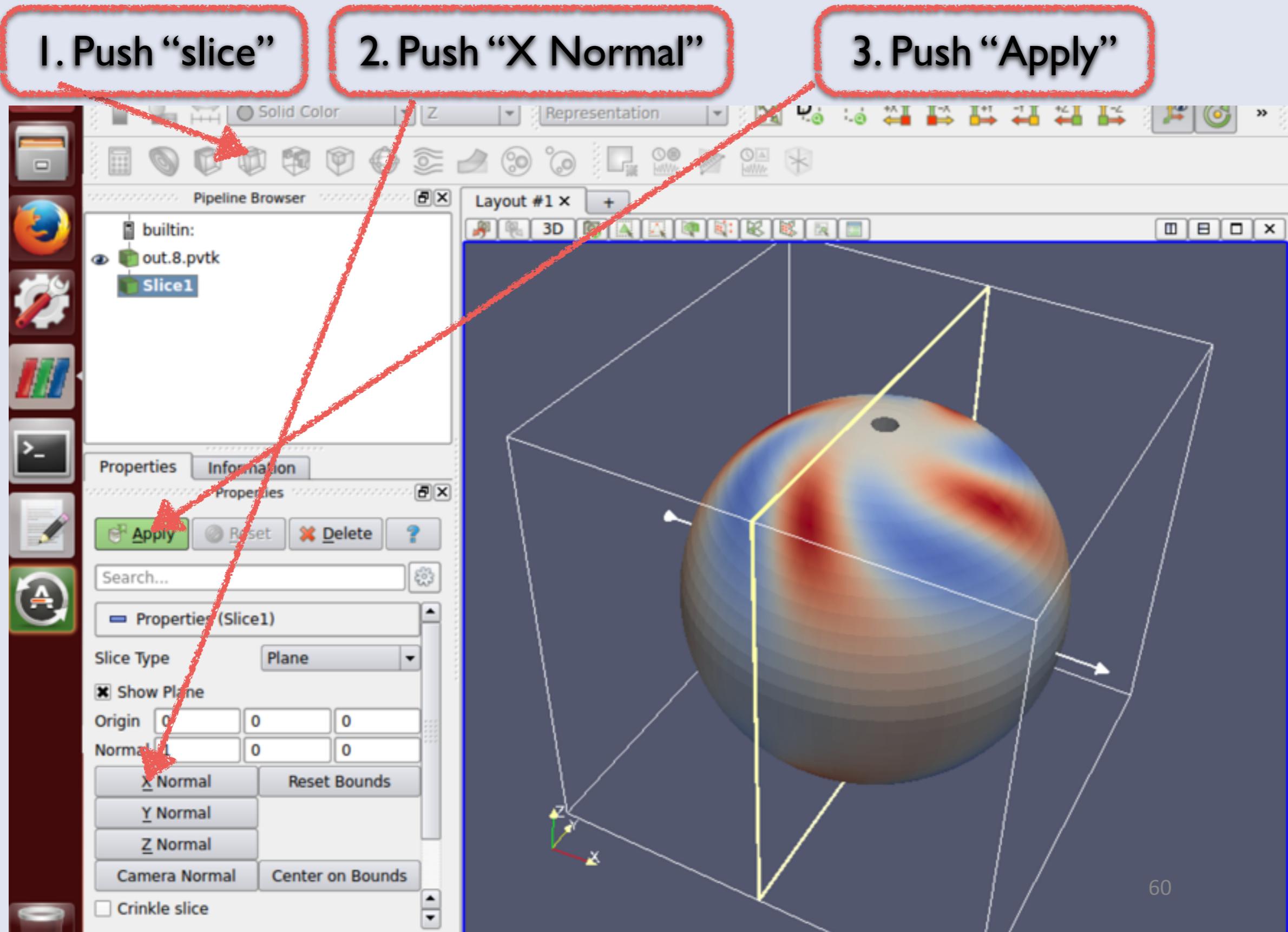
Choose z-component of vorticity

I. Select “vorticity”

2. Select “Z”



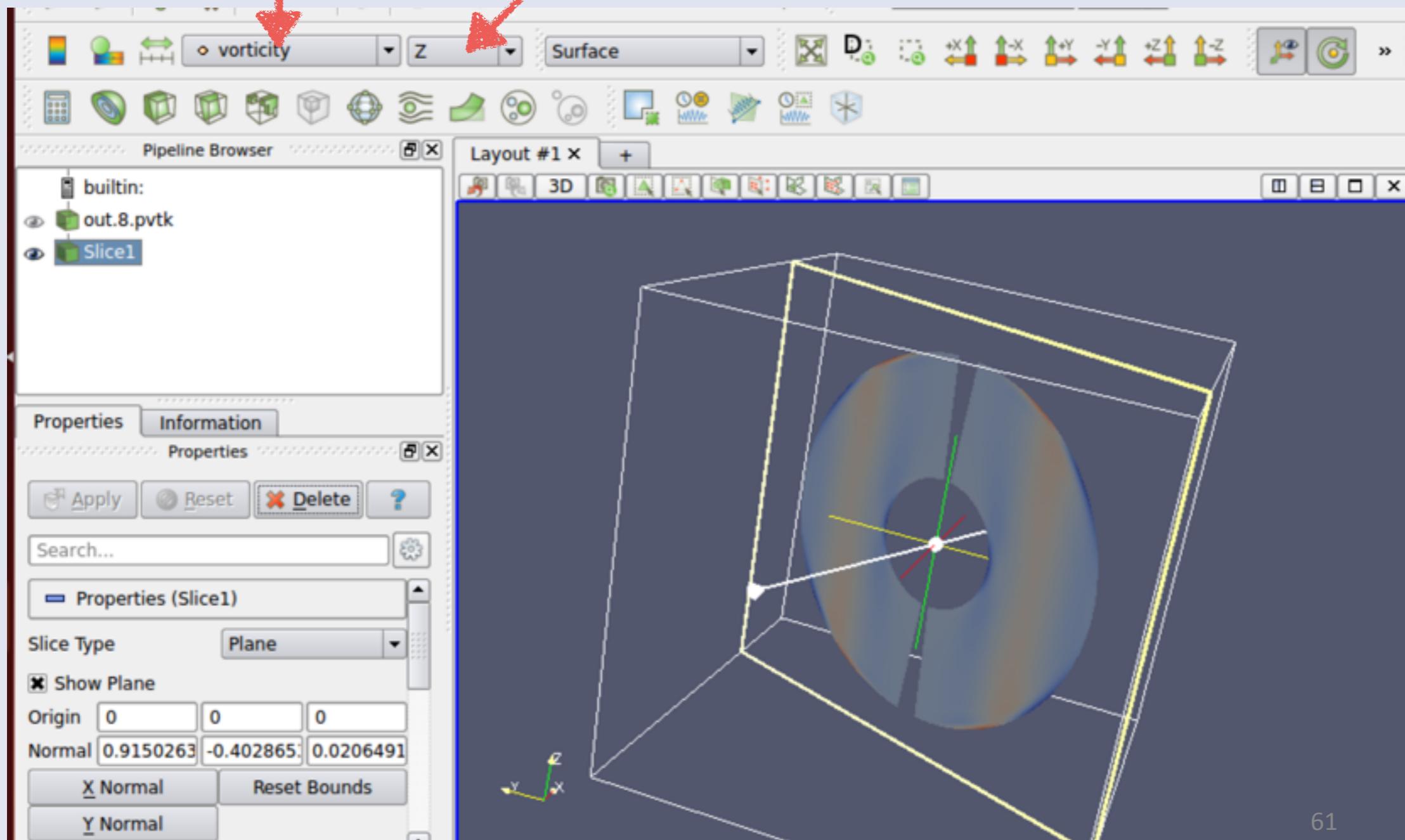
Look vorticity at a meridional section



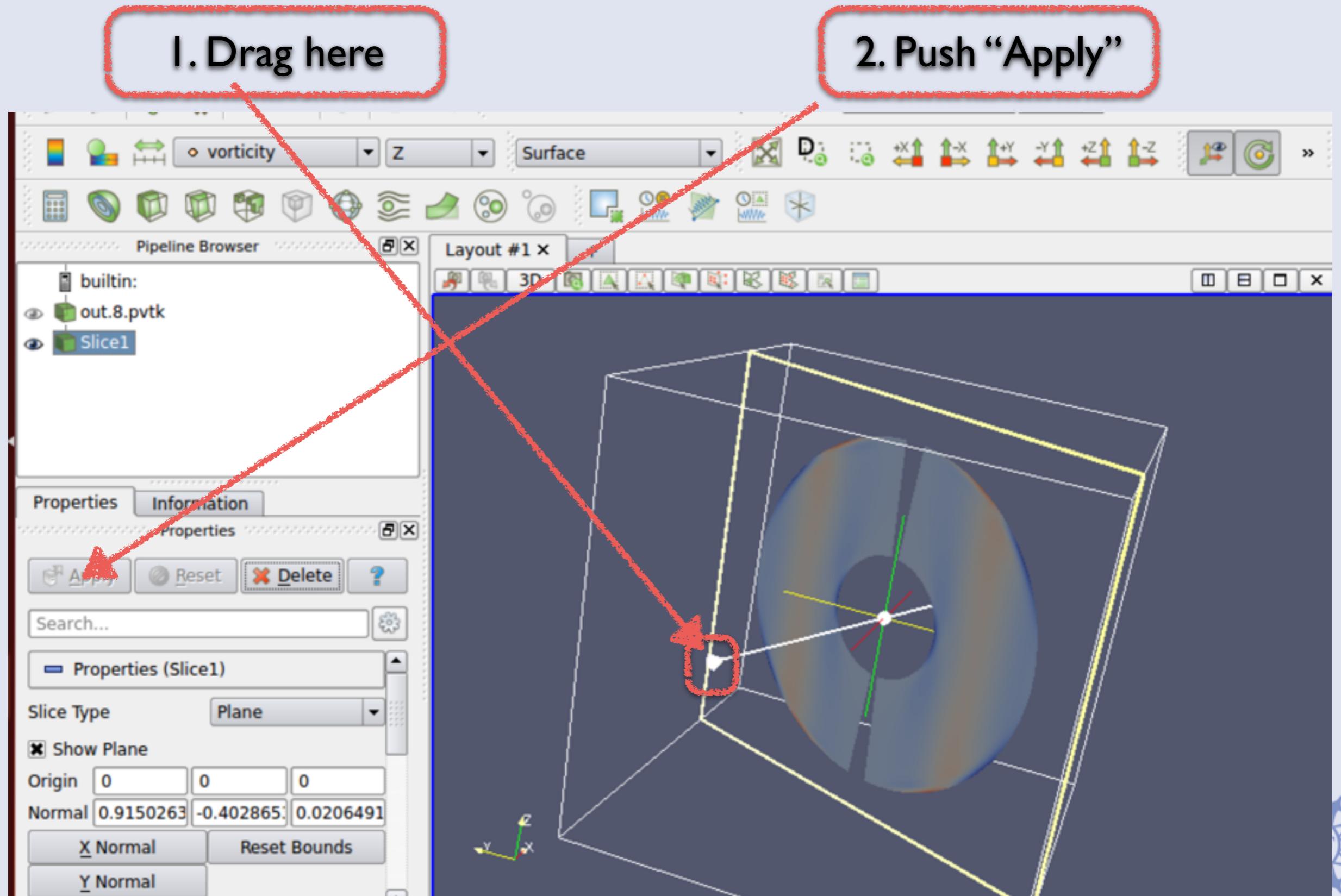
Choose vorticity-z (Again!!)

I. Select “vorticity”

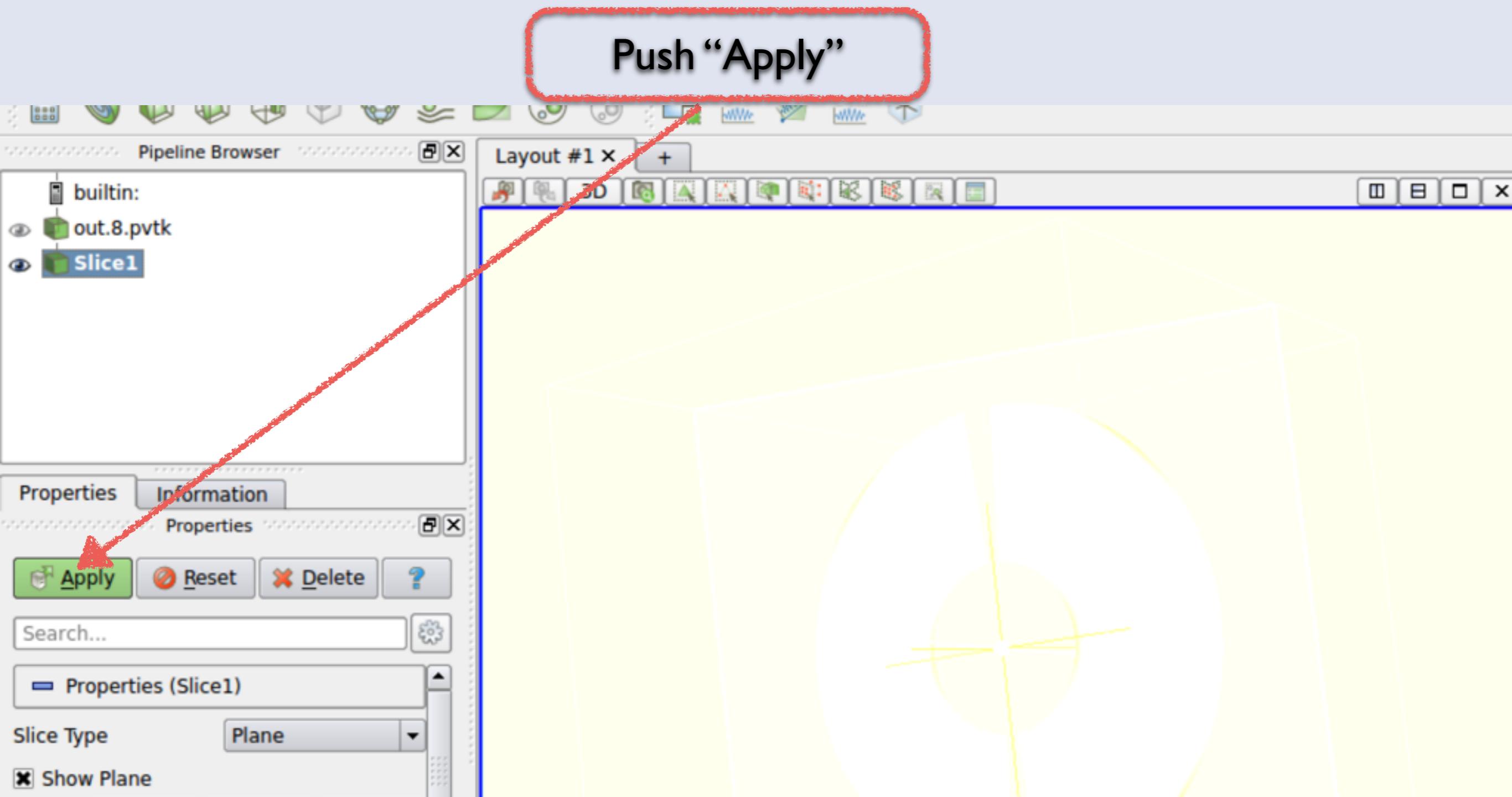
2. Select “Z”



To look a different section...

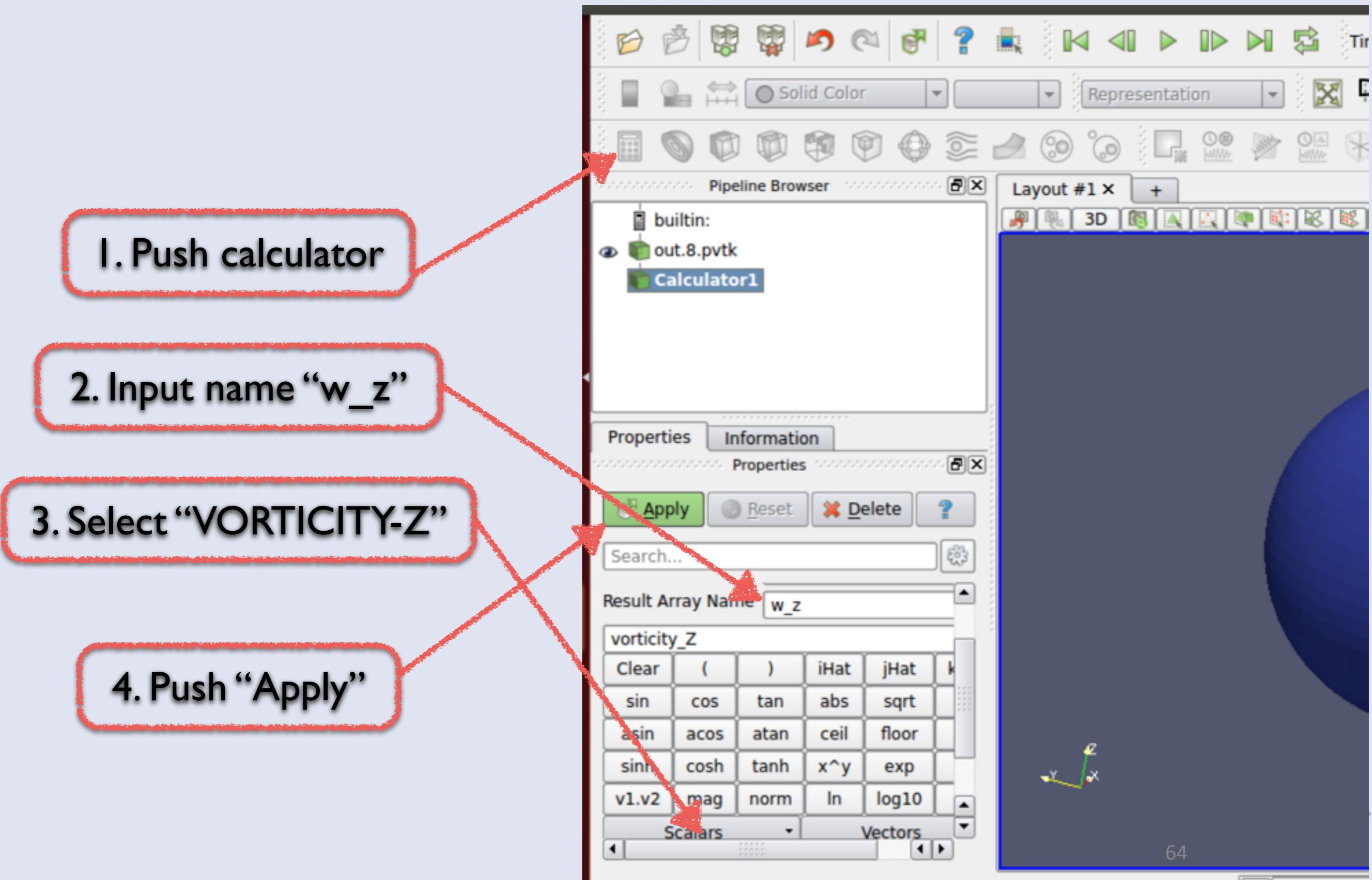


If screen becomes white...

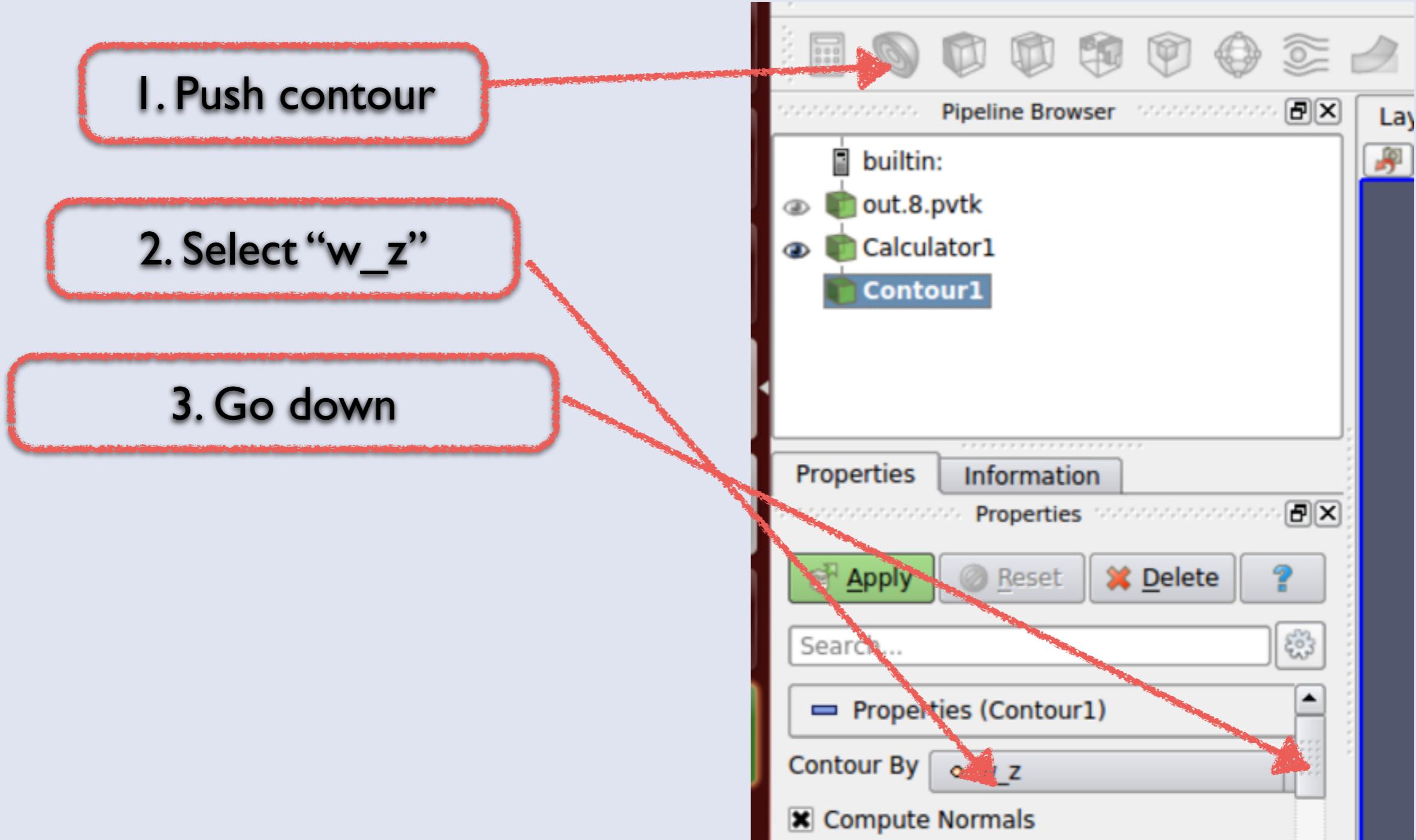


Virtualbox's graphic emulation makes this problem.

Pick z-component of vorticity



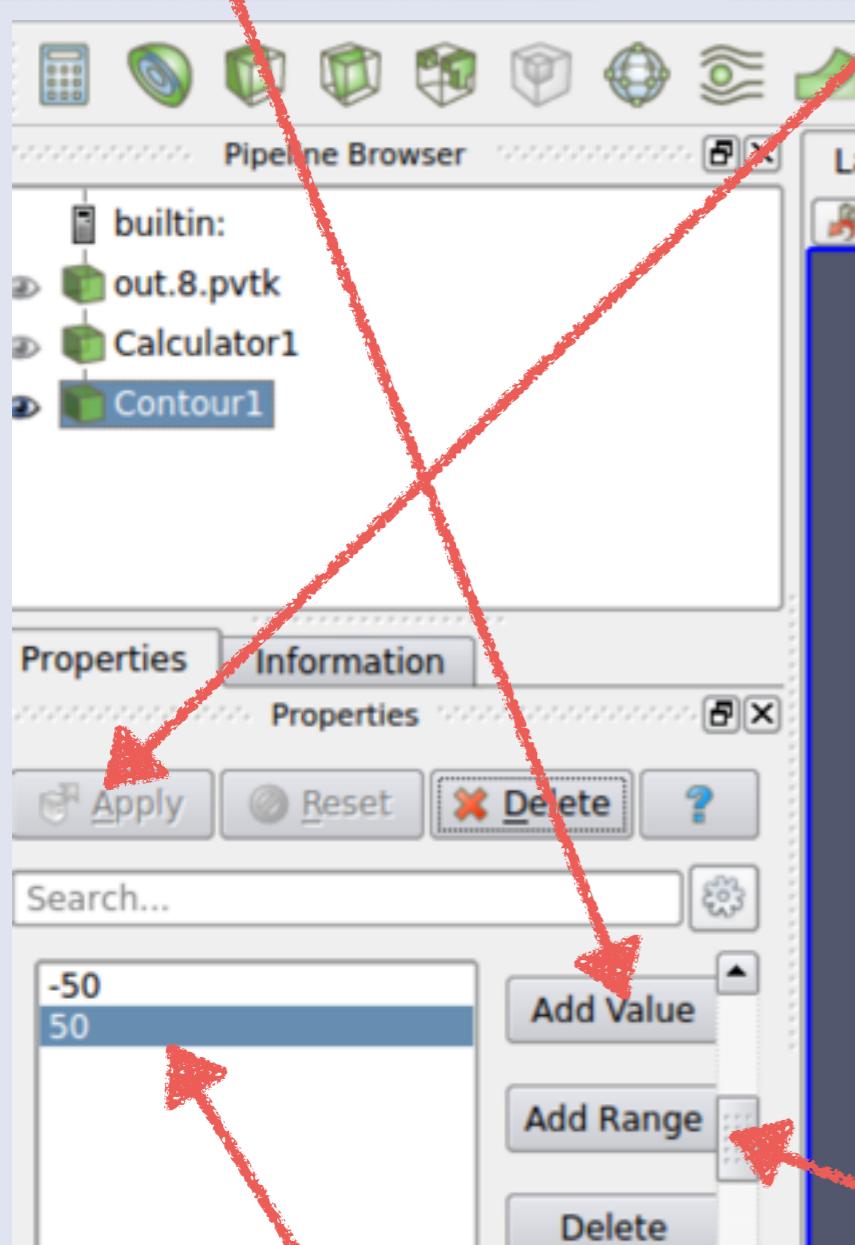
Generate Isosurfaces



Set Isosurface parameters

1. Push “Add value”

3. Push Apply



2. Input values for isosurface

4. Go down

- Suggested values:
 - $Ra=100\dots -50, 50$

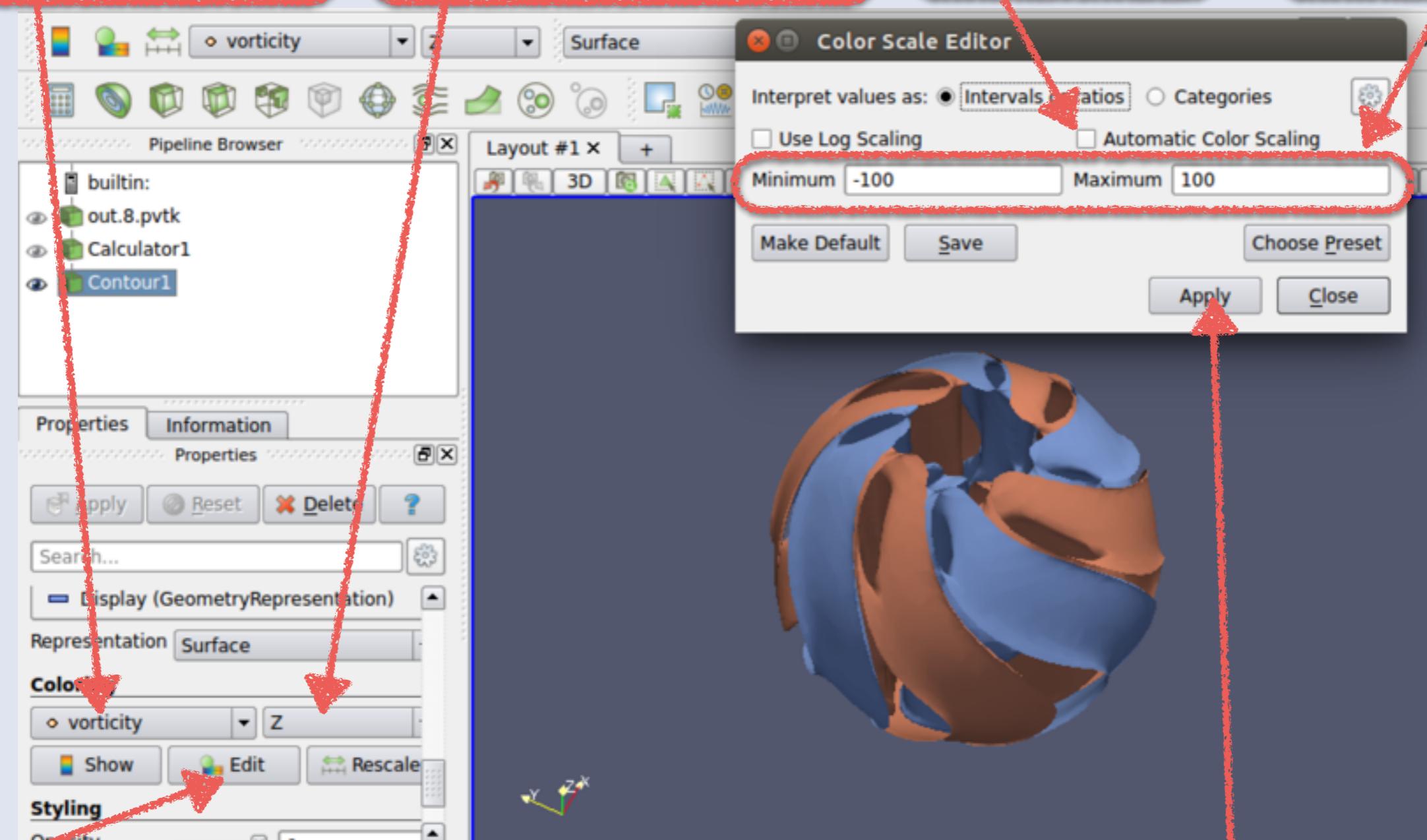
Set color for Isosurface

1. Select “vorticity”

2. Select “Z”

4. Turn Off

5. Set range



3. Push “Edit”

6. Push Apply

Delete boundary layer

1. Select “Contour1”

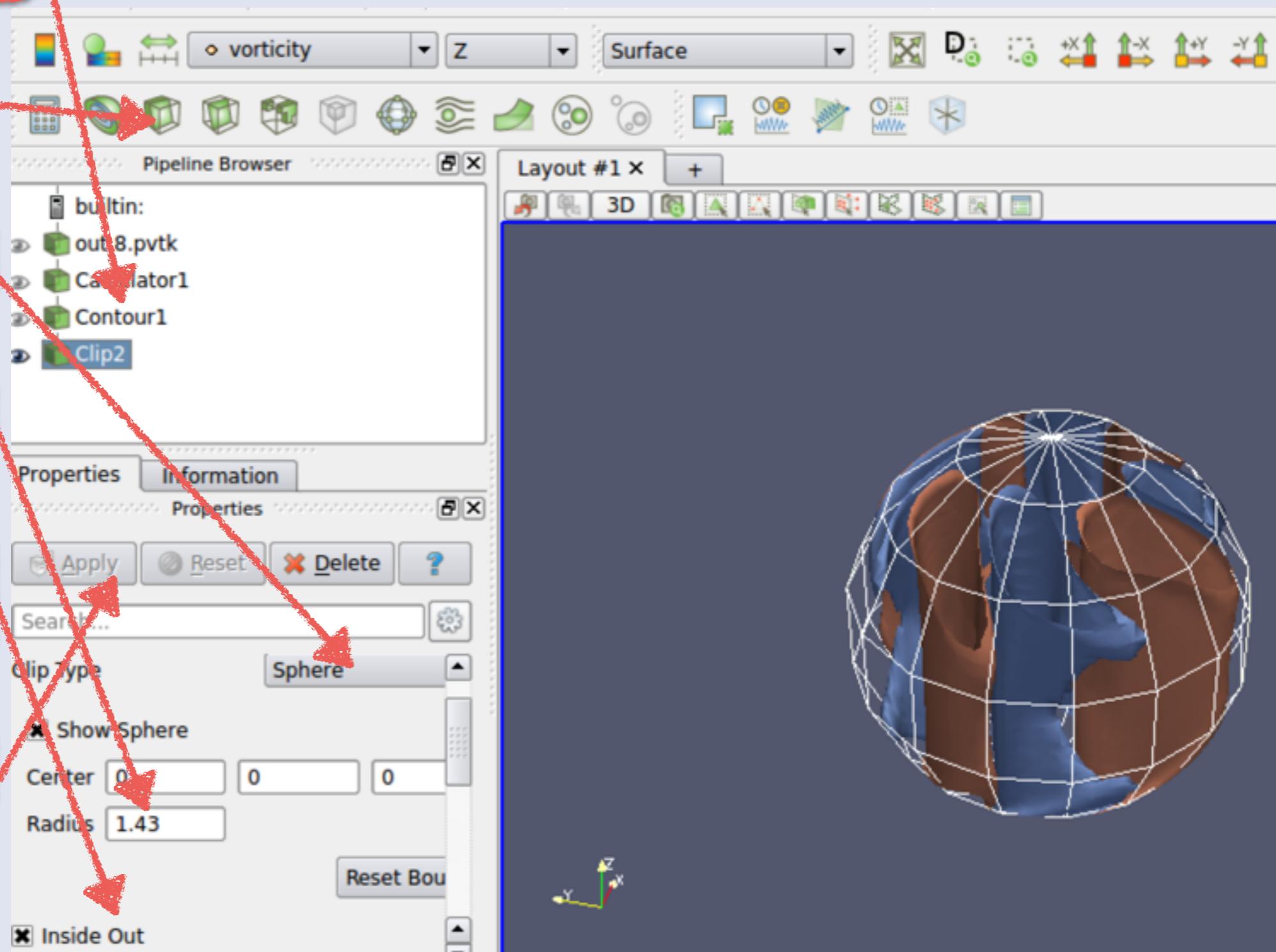
2. Push “Clip”

3. Select “Sphere”

4. Set $r=1.43$

5. Check “Inside Out”

6. Push Apply



How to run MHD dynamos?



Example for MHD dynamo

Go to MHD_example folder

```
cig@cig-VirtualBox:~/tutorial/calypso$ ls
Convection_RaXXX  MHD_example
cig@cig-VirtualBox:~/tutorial/calypso$ cd MHD_example/
cig@cig-VirtualBox:~/tutorial/calypso/MHD_example$ ls
control_MHD  control_sph_shell  field  README  restart  sph_lm31r48r48c_2
cig@cig-VirtualBox:~/tutorial/calypso/MHD_example$ █
```

Example of control file



Governing Equations

$$\begin{aligned}
 \frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} &= -\frac{1}{E} \nabla P + \nabla^2 \mathbf{u} - 2 \frac{1}{E} (\hat{\mathbf{z}} \times \mathbf{u}) \\
 &\quad + \frac{Ra}{E} E^{-1} T \frac{\mathbf{r}}{r_o} + \frac{1}{EPm} (\nabla \times \mathbf{B}) \times \mathbf{B}, \\
 \frac{\partial T}{\partial t} + (\mathbf{u} \cdot \nabla) T &= \frac{1}{Pr} \nabla^2 T, \\
 \frac{\partial \mathbf{B}}{\partial t} &= \frac{1}{Pm} \nabla^2 \mathbf{B} + \nabla \times (\mathbf{u} \times \mathbf{B}), \\
 \nabla \cdot \mathbf{u} &= \nabla \cdot \mathbf{B} = 0.
 \end{aligned}$$

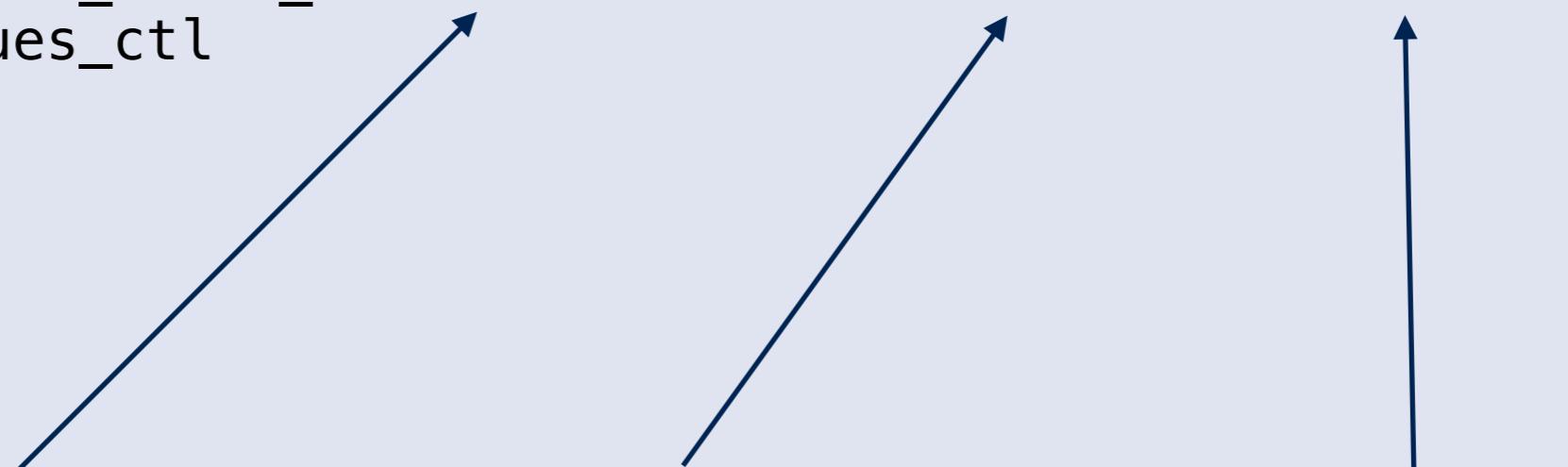
Data definition phys_values_ctl

```
49: begin phys_values_ctl
50:   array nod_value_ctl  6
51:     nod_value_ctl velocity      Viz_On    Monitor_On
52:     nod_value_ctl temperature   Viz_On    Monitor_On
53:     nod_value_ctl pressure    Viz_On    Monitor_On
54:     nod_value_ctl vorticity   Viz_On    Monitor_On
55:     nod_value_ctl magnetic_field Viz_On    Monitor_On
56:     nod_value_ctl current_density Viz_On    Monitor_On
57:   end array nod_value_ctl
58: end phys_values_ctl
```

Field name

field data
output flag

Monitoring data
output flag

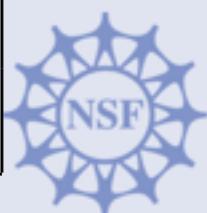


Choose of time integration time_evo_ctl

```
64: begin time_evolution_ctl
65:   array time_evo_ctl 3
66:     time_evo_ctl temperature
67:     time_evo_ctl velocity
68:     time_evo_ctl magnetic_field
69:   end array time_evo_ctl
70: end time_evolution_ctl
```

Field for time integration

label	field name	Description
velocity	Velocity	u
temperature	Temperature	T
composition	Composition variation	C
magnetic_field	Magnetic field	B



Boundary conditions

boundary_condition

```
74: begin boundary_condition
75:   array bc_temperature 2
76:     bc_temperature fixed ICB 1.000
77:     bc_temperature fixed CMB 0.000
78:   end array bc_temperature
79: !
80:   array bc_velocity 2
81:     bc_velocity non_slip_sph ICB 0.000
82:     bc_velocity non_slip_sph CMB 0.000
83:   end array bc_velocity
84: !
85:   array bc_magnetic_field 2
86:     bc_magnetic_field insulator ICB 0.000
87:     bc_magnetic_field insulator CMB 0.000
88:   end array bc_magnetic_field
89: end boundary_condition
```

Place to be defined

Boundary condition type

B.C. Value



Forcing terms forces_define

```
97: begin forces_define
98:   array force_ctl      3
99:     force_ctl  gravity
100:    force_ctl Coriolis
101:    force_ctl Lorentz
102:  end array force_ctl
103: end forces_define
```

3



List for forces

Label	Field name	Equation
Coriolis	Coriolis force	$-2\Omega\hat{z} \times \mathbf{u}$
Lorentz	Lorentz force	$\mathbf{J} \times \mathbf{B}$
gravity	Thermal buoyancy	$-\alpha_T T g$
Composite_gravity	Compositional buoyancy	$-\alpha_C C g$



Governing Equations

$$\begin{aligned}
 \frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} &= -\frac{1}{E} \nabla P + \nabla^2 \mathbf{u} - 2 \frac{1}{E} (\hat{\mathbf{z}} \times \mathbf{u}) \\
 &\quad + \frac{Ra}{E} E^{-1} T \frac{\mathbf{r}}{r_o} + \frac{1}{EPm} (\nabla \times \mathbf{B}) \times \mathbf{B}, \\
 \frac{\partial T}{\partial t} + (\mathbf{u} \cdot \nabla) T &= \frac{1}{Pr} \nabla^2 T, \\
 \frac{\partial \mathbf{B}}{\partial t} &= \frac{1}{Pm} \nabla^2 \mathbf{B} + \nabla \times (\mathbf{u} \times \mathbf{B}), \\
 \nabla \cdot \mathbf{u} &= \nabla \cdot \mathbf{B} = 0.
 \end{aligned}$$

Scaling for momentum equation momentum (Cont'd)

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} = -E^{-1} \nabla P + \nabla^2 \mathbf{u} - 2E^{-1} (\hat{\mathbf{z}} \times \mathbf{u}) \\ + \frac{Ra}{Er_0} Tr + \frac{1}{PmE} (\nabla \times \mathbf{B}) \times \mathbf{B},$$

```
170: array coef_4_Coriolis_ctl          2
171:   coef_4_Coriolis_ctl Two        1.0
172:   coef_4_Coriolis_ctl E         -1.0
173: end array coef_4_Coriolis_ctl
174:!
175: array coef_4_Lorentz_ctl          2
176:   coef_4_Lorentz_ctl Pm       -1.0
177:   coef_4_Lorentz_ctl E         -1.0
178: end array coef_4_Lorentz_ctl
179: end momentum
```

Scaling for magnetic induction

$$\frac{\partial \mathbf{B}}{\partial t} = \frac{1}{Pm} \nabla^2 \mathbf{B} + \nabla \times (\mathbf{u} \times \mathbf{B})$$

```
182: begin induction
183:   array coef_4_magnetic_ctl  1
184:     coef_4_magnetic_ctl      One                      1.0
185:   end array coef_4_magnetic_ctl
186: !
187:   array coef_4_m_diffuse_ctl  1
188:     coef_4_m_diffuse_ctl      Pm                     -1.0
189:   end array coef_4_m_diffuse_ctl
190: !
191:   array coef_4_induction_ctl  1
192:     coef_4_induction_ctl      One                     -1.0
193:   end array coef_4_induction_ctl
194: end induction
```

Dimensionless numbers

dimensionless_ctl

```
106: begin dimensionless_ctl
107:   array dimless_ctl[5]
108:     dimless_ctl  Pr           1.0e-0
109:     dimless_ctl  mod_Ra      1.0E+2
110:     dimless_ctl  E            1.0e-3
111:     dimless_ctl  Pm          5.0e+0
112:     dimless_ctl  r_o         1.53846154e+0
113:   end array dimless_ctl
114: end dimensionless_ctl
```

Name of parameters

Values

- Name of parameters are arbitrary.
- Same parameter names are used in coefficients_ctl



Enjoy!!

Delete header and insert space in the beginning of label

- % tail -n +8 sph_pwr_volume.dat | sed -e 's/t_step/ t_step/g' > sph_pwr_volume.csv

```
radial_layers, truncation
        49          31
ICB_id, CMB_id
        1          49
number of components
        8          16
        3          1          1          3          3          3          1          1
t_step    time    K_ene_pol   K_ene_tor   K_ene     temperature   pressure
vorticity_pol  vorticity_tor  vorticity   M_ene_pol   M_ene_tor   M_ene
current_density_pol  current_density_tor  current_density  Lorentz_work
buoyancy_flux
      5  2.5000000000000E-004  1.26868799936036E-001  3.89151176117312E-001
5.16019976053348E-001  8.37240378379609E-002  2.87882823435135E+000  9.86686975519297E+001
2.78615124115976E+001  1.26530209963527E+002  2.88644913094851E+000  3.17830080113554E+000
6.06474993208405E+000  1.02956456982691E+002  3.74881891640869E+001  1.40444646146778E+002
4.61481885954648E+007  9.01911785957379E+005
      10  5.0000000000000E-004  6.08060955924017E-001  1.34833005116663E+000
1.95639100709064E+000  8.37155261627966E-002  3.08165583167533E+000  2.64575310917710E+002
1.00469814016078E+002  3.65045124933788E+002  2.88536695611089E+000  3.16660213693698E+000
6.05196909304787E+000  1.03024858411853E+002  3.75526416948364E+001  1.40577500106689E+002
1.58027270251743E+008  3.74865939636243E+006
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