Scientific visualization with ParaView
Part 2

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✔ slides, data, codes at `https://bit.ly/paraviewzipp`
  ▶ the link will download a file `paraview.zip` (∼36MB)
  ▶ unpack it to find `codes/`, `data/` and `slides{1,2}.pdf`
  ▶ command line: `wget https://bit.ly/paraviewzipp -O paraview.zip`

✔ install ParaView 5.11.x on your laptop from
  `http://www.paraview.org/download`

EXPORTING SCENES (PRE-COMPUTED POLYGONS)

ParaView Glance

https://kitware.github.io/paraview-glance

PV Glance is an open-source standalone web app for in-browser 3D sci-vis

- very easy to use, ideal for sharing pre-built 3D scenes via the web
- no server ⇒ up to medium-size data (server support planned in future versions)
- interactive manipulation of pre-computed polygons
  - ▶ volumetric images, molecular structures, geometric objects, point clouds
- written in JavaScript and vtk.js + can be further customized with vtk.js and ParaViewWeb for custom web and desktop apps
- source and installation instructions
  https://github.com/kitware/paraview-glance

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1. Create a visualization with several layers, make **all layers visible in the pipeline**

2. Many options in $\boxed{\text{File}} \to \boxed{\text{Export Scene...}}$ ⇒ save as VTKJS to your laptop

3. Open https://kitware.github.io/paraview-glance/app

4. Drag the newly saved file to the dropzone on the website

5. Interact with individual layers in 3D: rotate and zoom, change visibility, representation, variable, colourmap, opacity

Automatically load a visualisation into Glance

https://discourse.paraview.org/t/customise-pv-glance/2831

- Use the query syntax
  <u>GLANCEAPPURL?name=FILENAME&url=FILEURL</u>
  to pass `name` and `url` to the web server

- E.g. using ParaView Glance website
  `https://kitware.github.io/paraview-glance/app?name=`
  `sineEnvelope.vtkjs&url=https://raw.githubusercontent.`
  `com/razoumov/publish/master/data/sineEnvelope.vtkjs`
  - shortened to `https://bit.ly/2KtPWNf`

- You can parse long strings with JavaScript (next slide)

Embed your vis into a website with an iframe (`embed.html`)

```html
<!DOCTYPE html>
<html>
  <head>
    <title>Sine envelope function</title>
  </head>
  <body>
    <h1>3D sine envelope function</h1>

    <script>
      var app = "https://kitware.github.io/paraview-glance/app";
      var dir = "https://raw.githubusercontent.com/razoumov/publish/master/data/";
      var file = "sineEnvelope.vtkjs";
      document.write("<iframe src='" + app + "?name=" + file + "&url=" +
                     dir + file +
                     "' id='iframe' width='1100' height='900'></iframe>");
    </script>

    <p>More stuff in here</p>
  </body>
</html>
```

- JavaScript here only to parse long strings

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ANIMATION IN PARAVIEW

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Animation methods

1. Use ParaView's built-in animation of any property of any pipeline object
   - ▶ easily create snazzy animations, somewhat limited in what you can do
   - ▶ in Animation View: select object, select property, create a new track with "+", double-click the track to edit it, press "▶"

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   - ▶ easily create snazzy animations, somewhat limited in what you can do
   - ▶ in Animation View: select object, select property, create a new track with "+", double-click the track to edit it, press "▶"

2. Use ParaView's ability to recognize a sequence of similar files
   - ▶ time animation only, very convenient
   - ▶ try loading `data/2d*.vtk` sequence and animating it (visualize one frame and then press "▶")

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3. Script your animation in Python (covered in next section)
   - ▶ steep learning curve, very powerful, can do anything you can do in the GUI
   - ▶ typical usage scenario: generate one frame per input file
   - ▶ a simpler exercise without input files: see next slide
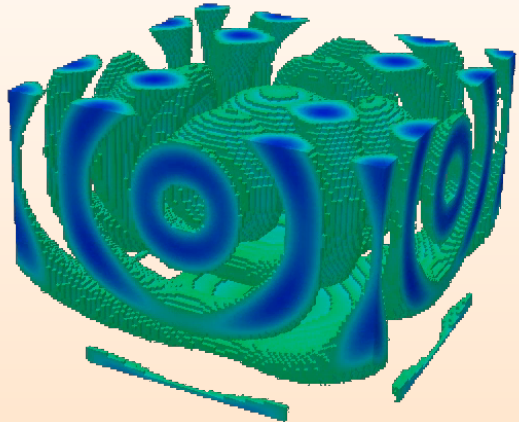
Exercise: animating function growth

➠ 3D sine envelope wave function defined inside a unit cube ($x_i \in [0, 1]$)

$$f(x_1, x_2, x_3) = \sum_{i=1}^{2} \left[\frac{\sin^2\left(\sqrt{\xi_{i+1}^2 + \xi_i^2}\right) - 0.5}{\left[0.001(\xi_{i+1}^2 + \xi_i^2) + 1\right]^2} + 0.5 \right], \text{ where } \xi_i \equiv 15(x_i - 0.5)$$

➠ Reproduce the movie on the screen

https://vimeo.com/248501176

or   hidden/growth.mp4 on

presenter's laptop

Exercise: animating function growth (cont.)

To visualize a single frame of the movie:

1. load data/sineEnvelope.nc (discretized on a 100^3 grid)
2. apply Threshold keeping only data from 1.2 to 2
3. apply Clip: origin $O = (49.5, 15, 49.5)$, normal $N = (0, -1, 0)$
4. colour by the right quantity

Two possible solutions:

1. bring up **Animation View** to animate Clip's O_2 from 0 to 99, for best results save animation as a sequence of PNG files
2. covered in the next section: Start/Stop Trace to record the workflow, save the corresponding **Python script**, enclose parts of it into a loop changing O_2 from 0 to 99 and writing a series of PNG screenshots, run it inside ParaView to produce 100 frames

   in either case, merge PNGs using a 3rd-party tool, e.g.

   ```
   ffmpeg -r 30 -i frame%04d.png -c:v libx264 -pix_fmt yuv420p \
          -vf "scale=trunc(iw/2)*2:trunc(ih/2)*2" movie.mp4
   ```

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Camera animation in the GUI

Good introductory resource `https://www.paraview.org/Wiki/Advanced_Animations`

1. Start with any static visualization

2. Click on 'Adjust Camera' icon (one of the left-side icons on top of the visualization window)
   - adjust / write down Camera Focal Point

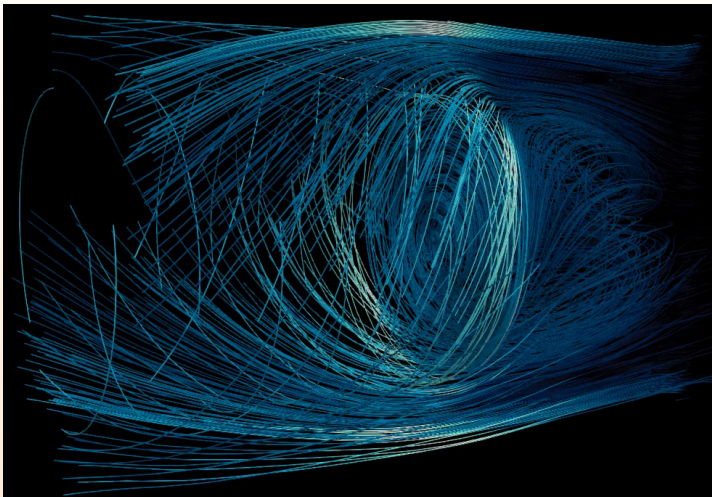3. Bring up Animation View (or erase all previous timelines)

(3a) In Animation View:

- select Camera - Orbit
- click "+" to create a new timeline
- set Center = Camera Focal Point, for the rest accept default settings
- adjust the number of frames

(3b) In Animation View:

- select Camera - Follow Path
- click "+" to create a new timeline
- double-click on the white (or black) timeline
- double-click on Path... in the right column
- click on Camera Position
  - a yellow path with spheres will appear
  - drag the spheres around
- also can change Camera Focus and Up Direction

4. Click "▶"

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Animating stationary flow: streamlines through a slice

- https://vimeo.com/248501893   or   hidden/radialSlice.mp4 on presenter's laptop
- https://vimeo.com/248502086   or   hidden/xySlice.mp4 on presenter's laptop

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Animating stationary flow: streamlines through a slice (cont.)

1. Load disk_out_ref.ex2 making sure to load velocity

2. Draw a radius-z plane slice through the center, origin $O = (0, 0, 0)$ and normal $N = (1, 0, 0)$

3. Stream Tracer With Custom Source: *input*=disk_out_ref.ex2, *seedSource*=Slice1

4. Tube filter with $r = 0.015$

5. Animation View: animate Slice's O_0 from -1 to 1 (full range [-5.75,5.75])

6. Use 100 frames, black background, blue2cyan colourmap, colour with vorticity

7. Unselect "Show Plane"

8. Save animation as PNGs, encode at 10 fps

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Animating a stationary flow: time contours
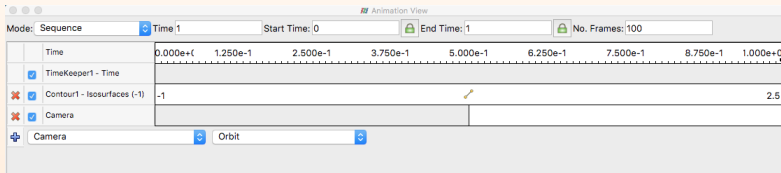

https://vimeo.com/248509153 **or** hidden/timeContours.mp4 **on presenter's laptop**
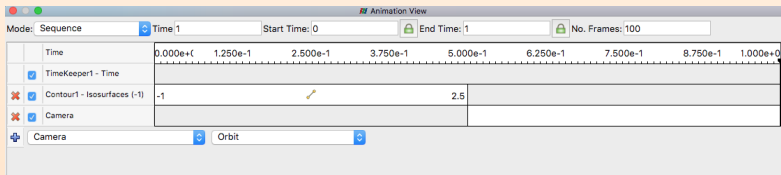
Animating a stationary flow: time contours (cont.)

1. Start with the streamtracer lines, however drawn

2. Apply a Countour filter to the output of Streamtracer
   - contour by Integration Time
   - probe the range of values that works best

3. Apply Glyph filter to the output of Countour

4. Animation View: animate Contour | Isosurfaces

5. This video was recorded with 2000 frames at 60 fps
   - such high resolution only for the final production video
   - debugging animation with 100 frames is perfectly Ok

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Exercise: several timelines in one animation

1. Start with the previous integration-time-contour animation

2. Add the second timeline to the animation: Camera - Orbit from $t = 0.5$ to $t = 1$ (while the first animation is still playing for its second half)
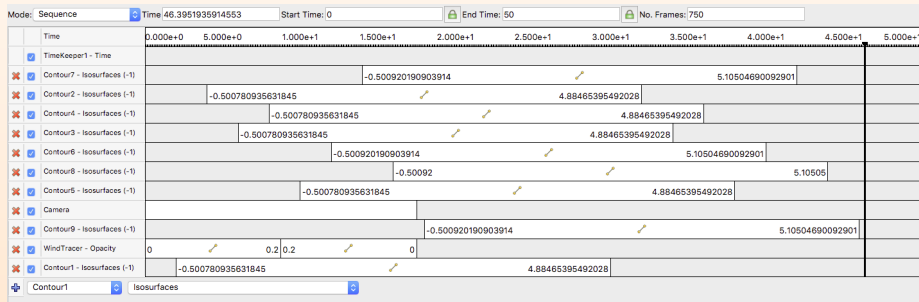

3. Now complete integration-time-contour animation before rotation

Combining many timelines in one animation (cont.)

- In principle, can add as many timelines (with their individual time intervals and variables!) to the animation as you want

- Here is an example from WestGrid's 2017 *Visualize This* competition submission by Nadya Moisseeva (UBC)

hidden/complexAnimation.mp4 on presenter's laptop

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PYTHON SCRIPTING IN PARAVIEW

Batch scripting for automating visualization

Official documentation at https://www.paraview.org/Wiki/ParaView/Python_Scripting

- Why use scripting?
  - ▶ automate mundane or repetitive tasks, e.g., making frames for a movie
  - ▶ document and store your workflow
  - ▶ use ParaView on clusters from the command line and/or via batch jobs
- In the GUI: View | Python Shell opens a Python interpreter
  - ▶ write or paste your script there
  - ▶ use the button to run an external script from a file
- *[/usr/bin/   /usr/local/bin/   /Applications/Paraview*.app/Contents/bin/]*
  pvpython will give you a Python shell connected to a ParaView server (local or remote) without the GUI
- *[/usr/bin/   /usr/local/bin/   /Applications/Paraview*.app/Contents/bin/]*
  pvbatch *--force-offscreen-rendering script.py* is a serial (on some machines parallel) application using a local ParaView server ✐ make sure to save your visualization
- *[/usr/bin/   /usr/local/bin/   /Applications/Paraview*.app/Contents/MacOS/]*
  paraview --script=codes/displayWireframe.py to start ParaView GUI and auto-run the script

First script

- Bring up View | Python Shell
- "Run Script" `codes/displaySphere.py`

displaySphere.py

```python
from paraview.simple import *

sphere = Sphere() # create a sphere pipeline object

print(sphere.ThetaResolution) # print one of the attributes of the sphere
sphere.ThetaResolution = 16

Show() # turn on visibility of the object in the view
Render()
```

- Can always get help from the command line

```python
help(paraview.simple)      # will display a help page on paraview.simple module
help(Sphere)
help(Show)
help(sphere)    # to see this object's attributes
dir(paraview.simple)
```

Using filters

- "Run Script" `codes/displayWireframe.py`

displayWireframe.py

```
from paraview.simple import *

sphere = Sphere(ThetaResolution=36, PhiResolution=18)

wireframe = ExtractEdges(Input=sphere) # apply Extract Edges to sphere

Show() # turn on visibility of the last object in the view
Render()
```
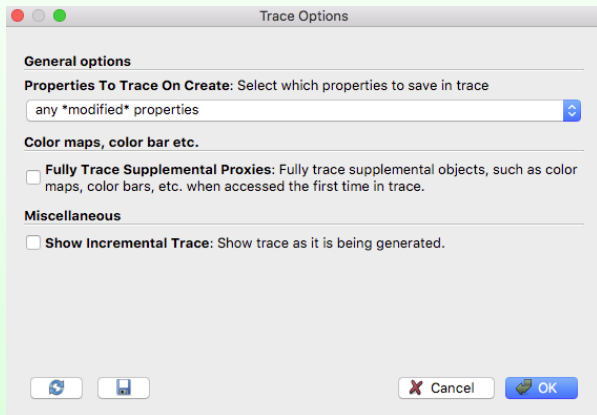
- Try replacing Show() with Show(sphere)

- Also try replacing `Render()` with
  `SaveScreenshot('/path/to/wireframe.png')` and running via
  `pvbatch`

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Trace tool

Generate Python code from GUI operations

- <u>Newer ParaView</u>:
  Tools | Start / Stop
  Trace

- <u>Older ParaView</u>: Tools
  | Python Shell | Trace
  | Start / Stop / Show
  Trace

Passing information down the pipeline

... and other useful high-level workflow functions

- GetSources() gets a list of pipeline objects
- GetActiveSource() gets the active object
- SetActiveSource() sets the active object
- GetRepresentation() returns the *view representation* for the active pipeline object and the active view
- GetActiveCamera() returns the active camera for the active view
- GetActiveView() returns the active view
- CreateRenderView() creates standard 3D render view
- ResetCamera() resets the camera to include the entire scene but preserve orientation (or does nothing ☺)

There is quite a bit of overlap between these two:

```
help(GetActiveCamera())
help(GetActiveView())
```

Camera animation with scripting

1. Let's load `data/sineEnvelope.nc` and draw an isosurface at $\rho = 0.15$

2. Compare the focal point to the center of rotation (must be the same for object to stay in view)

   ```
   v1 = GetActiveView()
   print(v1.CameraFocalPoint)
   print(v1.CenterOfRotation)
   ```

   if not $\Rightarrow$ `ResetCamera()`

3. Look up azimuthal rotation

   ```
   dir(GetActiveCamera())
   help(GetActiveCamera().Azimuth)
   ```

4. Rotate by $10°$ around the view-up vector

   ```
   camera = GetActiveCamera()
   camera.Azimuth(10)
   Render()
   ```

Camera animation: full rotation

✎ Can paste longer commands from `clipboard.txt`

5. Do full rotation and save to disk

```
nframes = 360
for i in range(nframes):
    print(v1.CameraPosition)
    camera.Azimuth(360./nframes)   # rotate by 1 degree
    SaveScreenshot('/path/to/frame%04d'%(i)+'.png')
```

6. Merge all frames into a movie at 30 fps

```
ffmpeg -r 30 -i frame%04d.png -c:v libx264 -pix_fmt yuv420p \
      -vf "scale=trunc(iw/2)*2:trunc(ih/2)*2" spin.mp4
```

Camera animation: flying towards the focal point

1. Optionally reset the view manually or with `ResetCamera()`

2. Now let's fly 2/3 of the way towards the focal point

```
initialCameraPosition = v1.CameraPosition[:]    # force a real copy
nframes = 100
for i in range(nframes):
    coef = float(i+0.5)/float(1.5*nframes)  # runs from 0 to 2/3
    print(coef, v1.CameraPosition)
    v1.CameraPosition = [((1.-coef)*a + coef*b) \
      for a, b in zip(initialCameraPosition,v1.CameraFocalPoint)]
    SaveScreenshot('/path/to/out%04d'%(i)+'.png')
```

3. Create a movie

```
ffmpeg -r 30 -i out%04d.png -c:v libx264 -pix_fmt yuv420p \
       -vf "scale=trunc(iw/2)*2:trunc(ih/2)*2" approach.mp4
```

Exercise: write and run a complete off-screen script

1. Mac/Linux/Windows: create a script with standalone ParaView GUI
   - ▶ use Start/Stop Trace
   - ▶ load `data/sineEnvelope.nc` and draw an isosurface at $\rho = 0.15$
   - ▶ save the image as PNG

2. Test-run your script with `pvbatch` on your laptop

   ```
   $ pvbatch --force-offscreen-rendering script.py
   ```

   - ▶ Linux: `pvbatch` should be in one of your system's `bin` directories
   - ▶ Mac: `pvbatch` should be in `/Applications/ParaView*.app/Contents/bin`
   - ▶ Windows: `pvbatch` does not exist (or so I am told), but you can use `pvpython`
     ➥ you will need to locate it yourself
   - ▶ those of you with a Compute Canada account can run this script on one of our HPC clusters with

   ```
   $ module load gcc/9.3.0 paraview-offscreen/5.10.0
   $ pvbatch --force-offscreen-rendering script.py
   ```

3. Modify the script to create some animation

Extracting data from VTK objects

Do this from *View | Python Shell* or from *pvpython* (either shell will work)

```python
# codes/extractValues.py
from paraview.simple import *

dir = '/Users/razoumov/training/paraviewWorkshop/data/'
data = NetCDFReader(FileName=[dir+'stvol.nc'])
local = servermanager.Fetch(data) # get the data from the server
print(local.GetNumberOfPoints())

for i in range(10):
    print(local.GetPoint(i))    # coordinates of first 10 points

pd = local.GetPointData()
print(pd.GetArrayName(0))    # the name of the first array

result = pd.GetArray('f(x,y,z)')
print(result.GetDataSize())
print(result.GetRange())

for i in range(10):
    print(result.GetValue(i))    # values at first 10 points
```
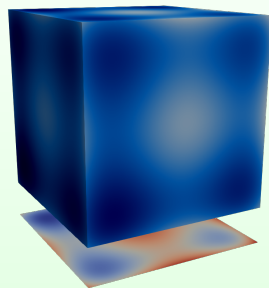
This is useful for post-processing, e.g., feeding these into **numpy arrays** and
doing further calculations in a Python script

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Creating/modifying VTK objects

Let's say we want to plot a projection
of a cubic dataset along one of its
principal axes, or do some other
transformation for which there is no
filter

- Calculator / Python Calculator filter cannot modify the geometry ...

Programmable filter

Watch our webinar `https://bit.ly/programmablefilter`

1. Apply Programmable Filter with OutputDataSetType = vtkUnstructuredGrid
2. Paste the following code `codes/projectionUnstructured.py` into the filter (this code was tested in ParaView 5.10.1)

```python
numPoints = inputs[0].GetNumberOfPoints()
side = int(round(numPoints**(1./3.)))    # round() in this Python returns float type
layer = side*side
rho = inputs[0].PointData['density']      # 1D flat array
points = vtk.vtkPoints()       # create vtkPoints instance, to contain 100^2 points in the projection
proj = vtk.vtkDoubleArray(); proj.SetName('projection')   # create the projection array
for i in range(layer):         # loop through 100x100 points
    x, y = inputs[0].GetPoint(i)[0:2]
    z, column = -20., 0.
    for j in range(side):
        column += rho.GetValue(i+layer*j)
    points.InsertNextPoint(x,y,z)          # also points.InsertPoint(i,x,y,z)
    proj.InsertNextValue(column)           # add value to this point

output.SetPoints(points)                   # add points to vtkUnstructuredGrid
output.GetPointData().SetScalars(proj)     # add projection array to these points

quad = vtk.vtkQuad()               # create a cell
output.Allocate(side, side)        # allocate space for side^2 'cells'
for i in range(side-1):
    for j in range(side-1):
        quad.GetPointIds().SetId(0,i+j*side)
        quad.GetPointIds().SetId(1,(i+1)+j*side)
        quad.GetPointIds().SetId(2,(i+1)+(j+1)*side)
        quad.GetPointIds().SetId(3,i+(j+1)*side)
        output.InsertNextCell(vtk.VTK_QUAD, quad.GetPointIds())
```

Using 3rd-party libraries from ParaView's Python

- `pvpython` includes few common 3rd-party libraries such as `numpy,scipy,pandas`
- What if you want to use other libraries that were not bundled with ParaView?

Using 3rd-party libraries from ParaView's Python

- pvpython includes few common 3rd-party libraries such as numpy, scipy, pandas
- What if you want to use other libraries that were not bundled with ParaView?

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1. Let's assume you work on a CC cluster; check your ParaView's Python version

```
module load gcc/9.3.0 paraview/5.10.0
pvpython    # let's assume it says Python 3.9.6
```

2. Load the closest Python module, create a virtual env. and install your library there

```
module avail python   # python/3.9.6 is one of them
module load python/3.9.6
virtualenv --no-download astro   # this will install a new virtual environment into ~/astro
source ~/astro/bin/activate
pip install --no-index --upgrade pip
pip install --no-index xarray   # install an external package into this new environment
```

3. Next time you log in to the cluster, start pvpython:

```
module load gcc/9.3.0 paraview/5.10.0
pvpython
```

4. Load your new virtual environment directly from Python:

```
filename = '/home/username/astro/bin/activate_this.py'
exec(open(filename).read(), {'__file__': filename})
from paraview.simple import *
import xarray    # this xarray comes from your new virtual environment
```

REMOTE AND DISTRIBUTED VISUALIZATION

Visualizing remote data

If your dataset is on a remote cluster, there are several options:

✗ **download data** to your desktop and visualize it locally
  - limited by the dataset size and your desktop's CPU/GPU + memory

✗ run ParaView remotely on a larger machine via **X11 forwarding**
  - your desktop $\xrightarrow{\text{ssh } -Y}$ larger machine running ParaView
  - remote OpenGL apps with either (1) software rasterizer on the cluster (usually the default) or (2) on your laptop's GPU (need to re-enable INdirect GLX inside X11 server and set `LIBGL_ALWAYS_INDIRECT=1`)

✓ run ParaView remotely on a larger machine **via remote desktop**
  - your desktop $\xrightarrow{\text{VNC}}$ larger machine running ParaView
  - you can always start a VNC server on an interactive cluster compute node by hand as described in our documentation `https://bit.ly/startVNC`
  - remote OpenGL apps will run either (1) using software rasterizer on the cluster (usually the default) or (2) on cluster's GPU(s) via VirtualGL wrapper (see our VNC docs)
  - the VNC slide is coming up

✓ run ParaView in **client-server mode**
  ParaView client on your desktop ⇌ ParaView server on larger machine

✓ run ParaView via a GUI-less **batch script** (interactively or scheduled)
  - render server can run with GPU rendering or purely in software
  - data/render servers can run on single-core, or across several cores/nodes with MPI
  - for interactive GUI work on clusters you should schedule interactive jobs, as opposed to running on the login nodes
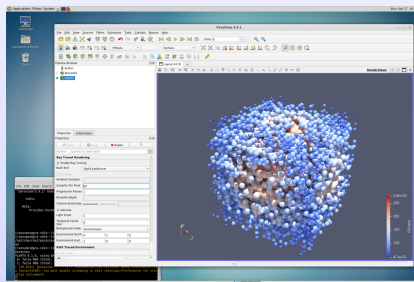
Special remote vis cases

1. In-situ visualization = instrumenting a simulation code on the cluster to
   1.1 output graphics and/or
   1.2 act as on-the-fly server for a visualization frontend (ParaView/VisIt client on your laptop)
   ▶ need to use a special library (ParaView's Catalyst or VisIt's libsim)
   ▶ very advanced topic for another time

2. Web-based visualization with data served from another location

ParaView via remote desktop

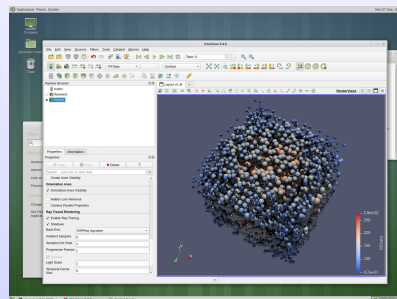https://docs.alliancecan.ca/wiki/VNC or https://docs.alliancecan.ca/wiki/JupyterHub

You have several options:

(1) run a VNC server on compute nodes with SSH tunnelling, connect via a VNC client
https://docs.alliancecan.ca/wiki/VNC#Compute_Nodes

(2) VNC on gra-vdi.computecanada.ca,
connect via a VNC client

(3) Remote Desktop via JupyterHub on
Béluga, point your web browser at
https://jupyterhub.beluga.
computecanada.ca

Cedar, Graham, Béluga, Narval clusters

- General-purpose CC clusters for a variety of workloads
  - ▶ entered production in phases since June 2017
  - ▶ located at SFU, UofWaterloo, École de technologie supérieure (Montreal)
  - ▶ 101,568 / 44,444 / 39,120 / 80,720 CPUs
  - ▶ many hundred NVIDIA GPUs (with 12GB/16GB/32GB on-board memory)
  - ▶ multiple types of nodes, with 128GB/256GB/0.5TB/1.5TB/3TB memory
  - ▶ specs at `https://docs.alliancecan.ca/wiki/Cedar`
    (replace `Cedar` with `Graham` or `Beluga` or `Narval`)

- Batch-oriented environment for parallel and serial jobs $\Rightarrow$ use Slurm scheduler and workload manager

- Identical software setup
  `https://docs.alliancecan.ca/wiki/Available_software`

Interactive jobs on Cedar / Graham / Béluga

- **Client-server workflow** is by definition interactive

- On Cedar interactive jobs should automatically go to one of Slurm's interactive partitions (CPU or GPU)

```
$ sinfo -p cpubase_interac
    # will list nodes and their states (idle, mixed, allocated, ...)
```

- salloc without a script name will start an interactive shell inside a submitted job on a compute node

```
$ salloc --time=1:0:0 --ntasks=4 ... --account=def-someuser
$ echo $SLURM_...      # access Slurm variables
$ module load ...      # set your environment
$ ./serialCode
$ srun ./mpiCode       # run an MPI code
$ exit                 # terminate the job (go back to the login node)
```

- You might need to specify pvserver --server-port=11112 (etc.) if someone else is already using the default port 11111 on the same node

Question 1: should I use CPUs or GPUs for rendering?

- Can render on GPUs (*hardware acceleration*) or CPUs (*software rendering*) with both interactive and batch visualizations
  - ▶ GPUs have traditionally been faster for rendering graphics
  - ▶ in recent years better open-source software rendering libraries such as OSPRay (Intel's ray tracing) and OpenSWR (Intel's rasterizer) have largely closed the performance gap for many types of visualizations
  - ⇒ I recommend starting with CPU rendering
    since you already likely have many CPUs! (see next slide)

- One might have to resort to software rendering if no GPUs are available, e.g., all taken by GP-GPU jobs

- I suggest doing **all hands-on exercises with CPU rendering**; also included slides on **GPU rendering** on the cluster

Question 2: how many CPUs/GPUs do I need?

- How many processors do we need? From *ParaView documentation*:
  - ▶ structured data (Structured Points, Rectilinear Grid, Structured Grid): one CPU core per ∼20 million cells
  - ▶ unstructured data (Unstructured Points, Polygonal Data, Unstructured Grid): one CPU core per ∼1 million cells
- Your main bottlenecks will be physical memory and disk read speed, and to a lesser extent CPU/GPU rendering time ⇒ to simplify things, to decide on the number of CPU cores for initial dataset exploration, use the dataset size
  - ▶ consider 80 GB dataset
  - ▶ base nodes have 128 GB memory with 32 cores ⇒ 3.5 GB/core (accounting for the OS, system tools, etc.) ⇒ 23 cores for this dataset
  - ▶ need to account for filters (and other processing), MPI buffers ⇒ minimum 32 cores
  - ▶ for comfortable processing with complex filters use $48 - 64$ cores
- On large HPC systems ParaView is known to scale to $\sim 10^{12}$ cells (Structured Points) on ∼10,000 cores and beyond
- Always do a scaling study before attempting to visualize large datasets
- It is important to understand memory requirements of filters
  - ▶ a typical structured → unstructured filter increases memory footprint by $\sim$ 3X

Remote Render Threshold

In ParaView's preferences can set | Render View | →

| Remote/Parallel Rendering Options | → | Remote Render Threshold |

beyond which rendering will be remote

- default 20MB ⇒ small rendering will be done on your laptop's GPU, interactive rotation with a mouse will be fast, but anything modestly intensive (under 20MB) will be shipped to your laptop and <u>might</u> be slow
- 0MB ⇒ all rendering (including rotation) will be remote, so you will be really using the cluster's CPU(s)/GPU(s) for everything
    - good for large data processing
    - not so good for interactivity, especially on a slower connection
- experiment with the threshold to find a suitable value

Next few pages: remote rendering exercises

<u>Short version:</u>

1. create your visualization via interactive client-server using CPU rendering
2. save your visualization to PNG

<u>Long version:</u>

1. create your visualization via interactive client-server using CPU rendering
2. save your visualization to PNG
3. convert this workflow into a Python script
4. upload this Python script to the cluster
5. try running the script inside an interactive (`salloc`) job; debug if needed
6. once happy with the result, write a Slurm job submission script and submit this rendering as a batch (`sbatch`) job

Exporting
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Animation
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Scripting
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Remote
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Summary
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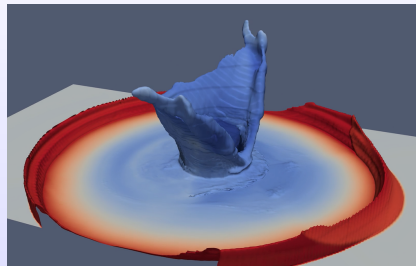# Exercise 1 (on Cedar): deep impact dataset

Dataset from IEEE 2018 SciVis Contest

- Dataset from *Deep Water Impact* simulation
  by John Patchett (LANL) and Galen Gisler
  (Univ. of Oslo)
  - ▶ dataset details at `https://bit.ly/2SXmjsq`
  - ▶ you can work with 269 low-resolution
    ($460 \times 280 \times 240$) snapshots in time
  - ▶ the original simulation is much higher
    resolution

- You can render this dataset in serial
  - ▶ try to adapt the client-server instructions from
    "Parallel software rendering" slide (forward a
    few pages) to render on one CPU

- Data in `cedar:/project/6003910/razoumov/ieeevis2018/460x280x240`
  (115GB in total)

- To simplify navigating to the dataset in ParaView, I highly recommend creating a
  symbolic link:

```
[cedar]$ mkdir -p ~/data
[cedar]$ ln -s /project/6003910/razoumov/ieeevis2018/460x280x240/ ~/data/deepImpact
```

Exporting
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Animation
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Scripting
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Summary
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Exercise 2 (on Cedar): Earth's mantle convection

Dataset from IEEE 2021 SciVis Contest `https://scivis2021.netlify.app`
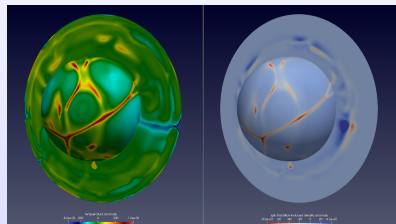
- Dataset from *Earth's Mantle Convection* simulation by Hosein Shahnas and Russell Pysklywec (U. of Toronto)
  - ▶ dataset details at `https://scivis2021.netlify.app/data`
  - ▶ 251 timesteps on a spherical $180 \times 201 \times 360$ grid

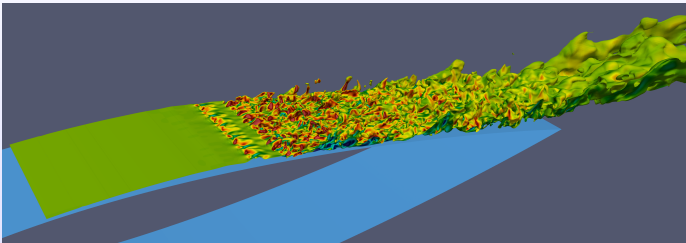- You can render this dataset in serial
  - ▶ try to adapt the client-server instructions from "Parallel software rendering" slide (forward a few pages) to render on one CPU

- Data in `cedar:/project/6003910/razoumov/ieeevis2021/spherical` (89GB in total)

- Create a symbolic link to simplify navigating to the dataset in ParaView

Exporting
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Animation
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Scripting
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Remote
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Summary
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Exercise 3 (on Cedar): airflow over a turbine blade

Dataset from WestGrid's 2019 `https://computecanada.github.io/visualizeThis`
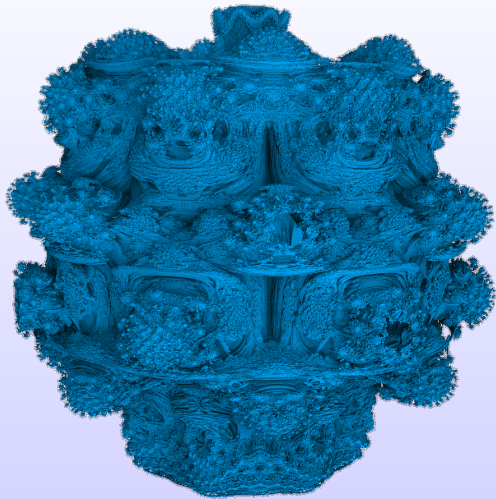

- OpenFOAM *decomposed* dataset: 512 cores, 86 timesteps, 5 hydro variables, ∼1TB in total
  - ▶ kindly provided for this competition by Joshua Brinkerhoff (UBC Okanagan)
  - ▶ unstructured mesh ⇒ loading a single timestep from the 3D internal mesh requires 200GB+ physical RAM
  - ▶ the 2D airfoil mesh takes only 13.7 GB virtual memory for 1 timestep + 1 variable
  - ▶ data in `cedar:/project/6003910/razoumov/visThis2019`
- Image at the top shows the isosurface of constant air speed coloured by the Y-component of the vorticity, full animation rendering (86 timesteps) took 17 minutes on 128 Cedar CPU cores
- Create a symbolic link to simplify navigating to the dataset in ParaView

Exporting
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Animation
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Scripting
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Remote
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Summary
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Exercise 4 (on the training cluster): Mandelbulb

- Visualize power-8 Mandelbulb
- Use the file `mandelbulb800.nc` – now sampled at 800^3
- Use 4–8 CPU cores on the training cluster via `salloc`
  1. consult the next three pages, use critical thinking – you will need to modify some of the commands!
  2. try to recreate the picture on the right: pay attention to the lights and shadows
  3. use View → Memory Inspector to keep an eye on memory usage
  4. optionally colour your dataset by `processID`


```
$ unzip /home/razoumov/shared/paraview.zip data/mandelbulb800.nc
$ ls -lh data/mandelbulb800.nc
```

Parallel software rendering

From interactive client-server debugging to remote batch rendering

1. On the cluster start remote parallel ParaView server:

```
$ cd scratch    # necessary on Cedar
$ module load StdEnv/2020 gcc/9.3.0 openmpi/4.0.3 paraview-offscreen/5.10.0
$ salloc --time=0:60:0 --ntasks=128 --mem-per-cpu=3600 --account=def-someuser
$ mpirun -np 128 pvserver
```

2. Wait for it to start waiting for incoming connection:

```
Waiting for client...
Connection URL: cs://cdr774.int.cedar.computecanada.ca:11111
Accepting connection(s): cdr774.int.cedar.computecanada.ca:11111
```
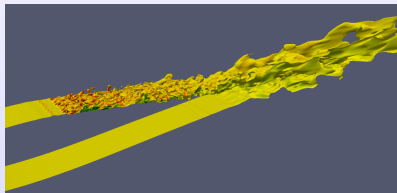
3. On your laptop start SSH port forwarding:

```
$ ssh cedar.computecanada.ca -L 11111:cdr774:11111   # use the actual compute node
```

4. On your laptop start ParaView 5.10.x, click Connect, then connect to
   `cs://localhost:11111`

Parallel software rendering (cont.)

5. $\boxed{\text{Tools}}$ → $\boxed{\text{Start Trace}}$

6. Load OpenFOAM data, set Case Type = Decomposed

7. Apply Calculator: speed = mag(U)

8. Apply Contour at `speed=0.8`

9. Colour by $(vorticity)_y$

10. Load *Rainbow Desaturated* colourmap

11. Save the image as a PNG file

12. $\boxed{\text{Tools}}$ → $\boxed{\text{Stop Trace}}$

13. Save the generated script as `airflow.py` locally
    ▶ edit it in a text editor, simplify (most generated lines will be setting defaults)
    ▶ provide the correct output PNG path on the remote system

Parallel software rendering (cont.)

14. Upload the script to the cluster:

```
$ scp airflow.py cedar.computecanada.ca:scratch/
```

15. On the cluster try running it as a parallel interactive job:

```
$ cd ~/scratch
$ salloc --time=0:60:0 --ntasks=128 --mem-per-cpu=3600 --account=def-someuser
$ module load gcc/9.3.0 paraview-offscreen/5.10.0
$ mpirun -np 128 pvbatch --force-offscreen-rendering airflow.py
```

16. Once you are happy with the result, write a Slurm job submission script and submit it with `sbatch`

OpenGL context for off-screen rendering on a GPU

To render on a GPU from an OpenGL application such as ParaView, **traditionally you would require**:

1. OpenGL support in the GPU driver, and
2. an X server that handles windows and surfaces onto which client APIs can draw
   - ▶ run X11 server (typically started by root) on the GPU compute node, set DISPLAY=:0.$gpuindex (get GPU index from Slurm)

Latest NVIDIA GPU drivers include EGL (*Embedded-System Graphics Library*) support enabling creation of an OpenGL context for off-screen rendering without an X server.

- Your OpenGL application needs to be **recompiled with EGL support** ⇒ use a special version of ParaView for GPU rendering without an X server; currently compiled into a module `paraview-offscreen-gpu/5.10.0` that provides both **pvserver** for client-server and **pvbatch** for batch rendering
- Unlike X11, EGL does not require any special setting to scale to very high resolutions, e.g., 4K (3840×2160) – simply ask it to render a 4K image

Interactive client-server rendering on a cluster's GPU

Details in `http://bit.ly/2wrSvKV`

1. On Cedar/Graham/Béluga **submit an interactive job** to the GPU partition, e.g., a serial job:

   ```
   $ salloc --time=0:30:0 --ntasks=1 --gpus-per-node=[type:]count \
            --mem-per-cpu=3600 --account=def-someuser
   ```

   When the job starts, it'll return a prompt on the assigned compute node.

2. On the compute node inside the job **start the ParaView server** using a special version of ParaView with EGL support

   ```
   $ module load gcc/9.3.0 paraview-offscreen-gpu/5.10.0
   $ unset DISPLAY   # so that PV does not attempt to use X11 rendering context
   $ pvserver        # --egl-device-index=0 not needed: first available GPU
                     #    is #0 inside the job
   ```

   For multiple GPUs can use

   ```
   $ nvidia-smi -L   # will return 0, 1, ...
   ```

   The `pvserver` command will return something like

   ```
   Waiting for client...
   Connection URL: cs://cdr347.int.cedar.computecanada.ca:11111
   Accepting connection(s): cdr347.int.cedar.computecanada.ca:11111
   ```

Interactive client-server rendering on a cluster's GPU (cont.)

3. On your desktop **set up ssh forwarding** to the ParaView server port:
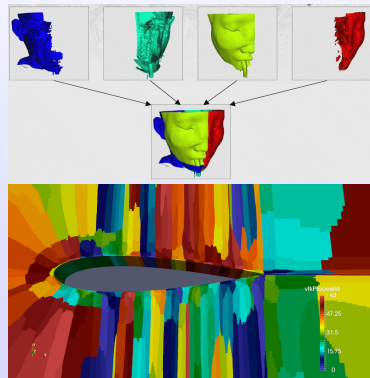
   ```
   $ ssh username@cedar.computecanada.ca -L 11111:cdr347:11111
   ```

4. On your desktop **start ParaView 5.10.x** and **edit its connection properties** under *File - Connect - Add Server* (name = Cedar, server type = Client/Server, host = localhost, port = 11111), click *Configure* → *Manual* → *Save*, then select the server from the list and click on *Connect*

   _____

   - ParaView's client and server must have matching major versions (5.10.x)

Data partitioning in parallel ParaView

- If loading unpartitioned data ⇒ dynamic load balancing is handled automatically for <u>structured data</u>:
  - ▶ structured points
  - ▶ rectilinear grid
  - ▶ structured grid

- Unpartitioned <u>unstructured data</u> will usually be read in serial, then must be passed through D3 (Distributed Data Decomposition) filter for dynamic load balancing:
  - ▶ particles/unstructured points
  - ▶ polygonal data
  - ▶ unstructured grid

- Some unstructured file formats can be read in parallel, e.g. the OpenFOAM reader will automatically read its unstructured data in parallel, distributing it among all available CPU cores

- After passing your unstructured data through D3, you can save it as parallel PVTU file ⇒ you'll get a statically distributed dataset that you can load next time with the same number of CPU cores

- Reading time ⇒ you can usually tell if your dataset is being read in serial or in parallel

- Look for `vtkProcessID` variable

Data partitioning in parallel ParaView (cont.)

If you have a large (many GBs) .vtu file:

1. Read your serial .vtu file into parallel ParaView on 16 cores - slow
   - ▶ and hope that it does not run out of memory on the reading core!
   - ▶ at this point the dataset is sitting in memory on one core
   - ▶ example: serial .vtu file at 9.1GB $\Rightarrow$ 1'49" reading time

2. Apply D3 filter to distribute the dataset - slowish (memory + MPI)

3. $\boxed{\text{File}} \rightarrow \boxed{\text{Save data}}$ as .pvtu with lz4 level-6 (fast) compression - fast
   - $\Rightarrow$ 16 files + 1 header file
   - ▶ now you have a statically decomposed dataset

4. Restart parallel ParaView on 16 cores, read .pvtu from scratch into - fast!
   - ▶ at this point the dataset is distributed across all 16 cores
   - ▶ example: same (but now decomposed) .pvtu dataset at 5.1GB (fast compression) $\Rightarrow$ 11" reading time

   - ● The same I/O speeds logic applies to .vti $\rightarrow$ .pvti (but there is no need for D3)

Exercise: parallel rendering of partitioned data

This is an extremely concise step-by-step guide for the turbine dataset:

1. Submit an interactive job
   `salloc --time=0:60:0 --ntasks=16 --mem-per-cpu=3600`

2. Start client-server ParaView session on 16 cores

3. Load all .vtm files (all 10 timesteps)

4. Apply Merge Blocks, output type = Unstructured Grid

5. Apply Cell Data to Point Data (so that you could use Contour)

6. Apply D3

7. Save data as `decomposed.pvtu`, write all timesteps as series, fast compression

8. Restart client-server ParaView session on 16 cores

9. Load all `decomposed.pvtu` files

10. Create visualization interactively

11. Save animation as 1000×800 PNG files ✍ this step should take $\sim$ 1min of processing time

12. Merge them into a movie with `ffmpeg`

Remote rendering summary: some orthogonal decisions

(1) interactive vs. batch

- interactive client-server for a quick look, exploration or debugging
  - ▶ another option is to download a scaled-down version of your dataset, debug a script locally on your laptop, and then run it as a batch job on the original full-resolution dataset on the cluster
- batch really preferred for production jobs and producing animations

(2) CPU vs. GPU

- in general, no single answer which one is better
  - ▶ you can throw many CPUs at your rendering job
  - ▶ modern software rendering libraries such as OSPRay (Intel's ray tracing) and OpenSWR (Intel's rasterizer) can be very fast, depending on your visualization
- might have to resort to software rendering if no GPUs are available (e.g., all are taken by GP-GPU jobs)
- for initial exploration, I would use the dataset size (GBs) to figure out the best number of CPU cores, and adjust from there

Exporting
oooo

Animation
ooooooooooo

Scripting
ooooooooooooo

Remote
ooooooooooooooooooooooo

Summary
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SUMMARY

Further resources

- ParaView Discourse
  https://discourse.paraview.org

- Self-directed ParaView tutorial
  https://docs.paraview.org/en/latest/Tutorials/SelfDirectedTutorial/index.html

- ParaView User's Guide
  https://docs.paraview.org/en/latest/UsersGuide/index.html

- ParaView F.A.Q.
  http://www.itk.org/Wiki/ParaView:FAQ

- VTK wiki with webinars, tutorials, etc.
  http://www.vtk.org/Wiki/VTK

- VTK for C++/Python/Java/C#/JavaScript code examples
  https://kitware.github.io/vtk-examples

- VTK file formats (3rd-party intro)
  http://www.earthmodels.org/software/vtk-and-paraview/vtk-file-formats

Our visualization webinars

- ∼3-4 visualization webinars per academic year
  - ✏ keep an eye on our emails, Twitter,
    https://westgrid.github.io/trainingMaterials/blog
  - ▶ ∼50 mins + questions, usually on fairly specific or advanced topics

- Many past webinars are available with slides and screencasts at
  https://bit.ly/vispages
  - "In-situ visualization with ParaView Catalyst2"
  - "Highlights from the 2021 IEEE SciVis Contest"
  - "Remote visualization on Compute Canada clusters"
  - "Scientific visualization on NVIDIA GPUs"
  - "Workflows with Programmable Filter / Source in ParaView"
  - "The Topology ToolKit (TTK)"
  - "Web-based 3D scientific visualization" (ParaViewWeb, vtk.js, ParaView Glance)
  - "Photorealistic rendering with ParaView and OSPRay"
  - "Batch visualization on Compute Canada clusters"
  - "Molecular visualization with VMD" • "Intermediate VMD topics: trajectories, movies, scripting"
  - "Using YT for analysis and visualization of volumetric data" (part 1) • "Working with data objects in YT" (part 2)
  - "Scientific visualization with Plotly"
  - "Novel visualization techniques from 2017 VISUALIZE THIS competition"
  - "Camera animation in ParaView and VisIt"
  - "3D visualization on new Compute Canada systems"
  - "Using ParaViewWeb for 3D visualization and data analysis in a web browser"
  - "Visualization support in WestGrid / Compute Canada"
  - "Scripting and other advanced topics in VisIt visualization"
  - "CPU-based rendering with OSPRay"
  - "3D graphs with NetworkX, VTK, and ParaView" • "Graph visualization with Gephi"

- We are always looking for topic suggestions!

Documentation and getting help

- Visualization in the Alliance `https://ccvis.netlify.app` (online gallery)

- Official documentation
  `https://docs.alliancecan.ca/wiki/Visualization`

- Western Canada research computing visualization resources
  `https://bit.ly/vispages`

- Email **support@tech.alliancecan.ca** and mention *"visualization"* in the subject line (goes to our ticketing system)

- Email me **alex.razoumov@westdri.ca**

- ParaView documentation
  - official documentation `https://docs.paraview.org/en/latest`
  - wiki `http://www.paraview.org/Wiki/ParaView`
  - Python batch scripting `http://bit.ly/2wF5v0B`
  - VTK tutorials `http://www.itk.org/Wiki/VTK/Tutorials`