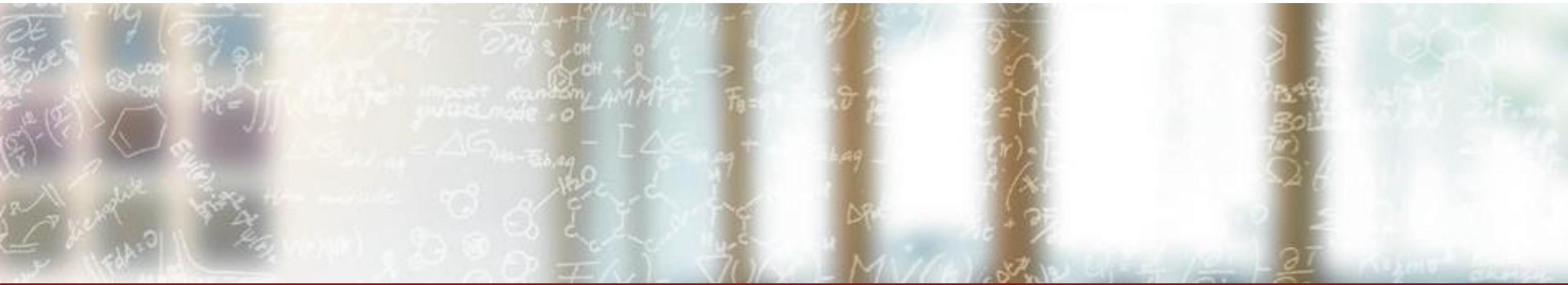




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# Scientific visualization

**PDC Summer School 2023**

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# Preamble 1

- We will use two different methods of using/demonstrating visualization in an HPC context
  - On your desktop with small data
  - In Dardel, with small and big data
- Paraview can be driven both by a Python script, and by interactive GUI-based actions (understand the diffs between *paraview*, *pvpypython*, *pvserver*, *pvbatch*)
- Thus, you should clone the repo on both sides to see the exercise/demo file, e.g.  
git clone <https://github.com/jfavre/PDC-SummerSchool> Visualization
- In my lecture notes, all examples for exercises should be written in green, i.e. [pvSphere.py](#). You should find them in the git repo.

## Preamble 2

- No training dedicated to HPC I/O in this summer school
- Difficult to know what is our common understanding of file I/O and file formats
- Most demonstration/exercises will use auto-generated data

# Outline of the day

- Scientific data analysis and visualization (1hr)
  - ParaView hands-on lab session
- Parallel data visualization (1hr)
  - ParaView hands-on lab session for parallel data visualisation
- Because of the limited time, I decided to focus on a single application (ParaView), to avoid context switching
- ParaView is open-source, available everywhere on earth, and a *de-facto* leader in HPC visualization apps.
- The comprehensive ParaView guide is here:

<https://docs.paraview.org/en/latest/UsersGuide/index.html>

## Definition, Data dimensions

*Information Visualization* is the study of visual representations of abstract data to reinforce human cognition. The abstract data include both numerical and non-numerical data, such as text and geographic information. However, information visualization differs from *Scientific Visualization*.

"It is *Information Visualization*, when the spatial representation is chosen, and it is *Scientific Visualization*, when the spatial representation is given"

The X,Y,Z,Time space will be our natural basis, and we will deal with grid-less or gridded data.

# Grid types

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# Grid Types. The VTK Data Model

<https://docs.paraview.org/en/latest/UsersGuide/understandingData.html#>

Take ParaView's ProgrammableSource and list its possible output types:

**pvpython**

```
>>> from paraview.simple import *
```

```
>>> a = ProgrammableSource()
```

```
>>> a.OutputDataSetType.Available
```

```
['vtkPolyData', 'vtkStructuredGrid', 'vtkRectilinearGrid', 'vtkUnstructuredGrid',  
'vtkImageData', 'vtkMultiblockDataSet', 'vtkHierarchicalBoxDataSet', 'vtkTable',  
'vtkMolecule', 'vtkPartitionedDataSet', 'vtkPartitionedDataSetCollection']
```

# Grid Types. The VTK Data Model

It is far more important to know the mesh type a reader will produce....

['vtkPolyData', 'vtkStructuredGrid', 'vtkRectilinearGrid', 'vtkUnstructuredGrid', 'vtkImageData', 'vtkMultiblockDataSet', 'vtkHierarchicalBoxDataSet', 'vtkTable', 'vtkMolecule']

...rather than its specific name

Said in a different manner “*you can encode the same data in multiple data formats*”

Implementation details will be important for time-series and parallel support



# ParaView's look at data

Properties Information

Apply Reset Delete ?

Search ... (use Esc to clear text)

Properties (snapshot\_400.h)

☒ Point Array Status

- ☒ PartType0/PhotonEnergy
- ☒ PartType0/Potential
- ☒ PartType0/SmoothingLength
- ☒ PartType0/StarFormationRate
- ☒ PartType0/Velocities
- ☒ PartType1/Masses
- ☒ PartType1/ParticleChildIDsNumber
- ☒ PartType1/ParticleIDGenerationNumber
- ☒ PartType1/ParticleIDs
- ☒ PartType1/Potential
- ☒ PartType1/Velocities

Cell Type: Poly-Vertex

Properties Information

Information

Data Hierarchy

- Multi-block Dataset
  - PartType0
  - PartType1
  - PartType2
  - PartType4
  - PartType5

Properties

Filename: snapshot\_400.hdf5  
Path: /mnt/data/Feldmann

Statistics

Type: Multi-block Dataset  
Number of Cells: 5  
Number of Points: 48673607  
Memory: 1.3e+03 MB

Data Arrays

Current data time: 0.0984848

| Name                  | Data Type | Data Ranges        |
|-----------------------|-----------|--------------------|
| Density (partial)     | float     | [1.56138e-15, ...] |
| Masses (partial)      | float     | [1.68492e-06, ...] |
| ParticleIDs (partial) | idtype    | [0, 1.51613e+...   |

Bounds

X Range: 0.0246315 to 400000 (delta: 400000)  
Y Range: 0.0159307 to 400000 (delta: 400000)  
Z Range: 0.00109296 to 400000 (delta: 400000)

Properties Information

Information

Data Hierarchy

- Multi-block Dataset
  - PartType0
  - PartType1
  - PartType2
  - PartType4
  - PartType5

Statistics

Type: Unstructured Grid  
Number of Cells: 1  
Number of Points: 15065389  
Memory: 4.8e+02 MB

Data Arrays

| Name        | Data Type | Data Ranges              |
|-------------|-----------|--------------------------|
| Density     | float     | [1.56138e-15, 0.0587404] |
| ParticleIDs | idtype    | [0, 1.51613e+07]         |

# Grid Types...and filtering

Each mesh type will have a corresponding subset of filters that can be applied to it.

Example:

| Mesh Type           | Can Use ExtractSubset ? |
|---------------------|-------------------------|
| vtkPolyData         | No                      |
| vtkStructuredGrid   | Yes                     |
| vtkUnstructuredGrid | No                      |
| vtkImageData        | Yes                     |

# Multiple view representations

- <https://docs.paraview.org/en/latest/UsersGuide/displayingData.html#id3>



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# Scalar field visualization

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# A quick look at the classic visualization methods

- Slicing
- Clipping
- Iso-contouring
- glyphing
- Volume rendering

# Exercise

- I suggest to use two different (internal) data sources in the ParaView GUI
  - Fast Uniform Grid
  - Wavelet
- Try out all techniques introduced above
- Add a “tetrahedralize” filter, and try again



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# Query-ing/filtering data

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# ParaView's Find Data menu

- Demonstrations
- Limitations in version  $\leq 5.11$
- The Python commands to reproduce a data selection are not saved in ParaView's session files. Following in the next 3 slides are examples of what you would have to do...



# Query-based filtering examples

<https://gitlab.kitware.com/paraview/paraview/blob/master/Wrapping/Python/paraview/selection.py>

```
qs1="rho > 1e-05"
```

```
sel1 = QuerySelect(QueryString=qs1, Source=mergeBlocks1)
```

```
extractSelection1 = ExtractSelection(Input=mergeBlocks1)
```

```
rep1 = Show(extractSelection1)
```

```
rep1.Representation = 'Points'
```

```
ColorBy(rep1, ('POINTS','rho'))
```

# Query-based filtering examples

# points is the array of coordinates. We select the 0-th coordinate  $< -12.15$  AND  $\rho > 1e-5$

```
Qs2 = "np.logical_and(rho > 1e-05, points[:,0] < -12.15)"
```

```
sel2 = QuerySelect(QueryString=Qs2, Source=mergeBlocks1)
```

```
extractSelection2 = ExtractSelection(registrationName='ExtractSelection2', Input=mergeBlocks1)
```

```
rep2 = Show(extractSelection2)
```

```
rep2.Representation = 'Points'
```

```
ColorBy(rep2, ('POINTS','rho'))
```

# Query-based filtering examples

# points is the array of coordinates. We select particles within a given Radius and Center

```
#Center = [-11.1431, 3.97869, -0.173805]; Radius = 10
```

```
Qs3 = "mag(points - [-11.1431, 3.97869, -0.173805]) < 10"
```

```
sel3 = QuerySelect(QueryString=Qs3, Source=mergeBlocks1)
```

```
extractSelection3 = ExtractSelection(registrationName='ExtractSelection3', Input=mergeBlocks1)
```

```
rep3 = Show(extractSelection3)
```

```
rep3.Representation = 'Points'
```

```
ColorBy(rep3, ('POINTS','rho'))
```

# Query-based filtering

<https://gitlab.kitware.com/paraview/paraview/blob/master/Wrapping/Python/paraview/selection.py>

## Other selections:

```
SelectThresholds(Thresholds=[-338000, 0], ArrayName= 'Potential', Source=GetActiveSource())
```

```
SelectIDs(IDs=[i for i in range(100000, 1100000)], , Source=GetActiveSource())
```

# Vector field visualization

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# Vector field visualization

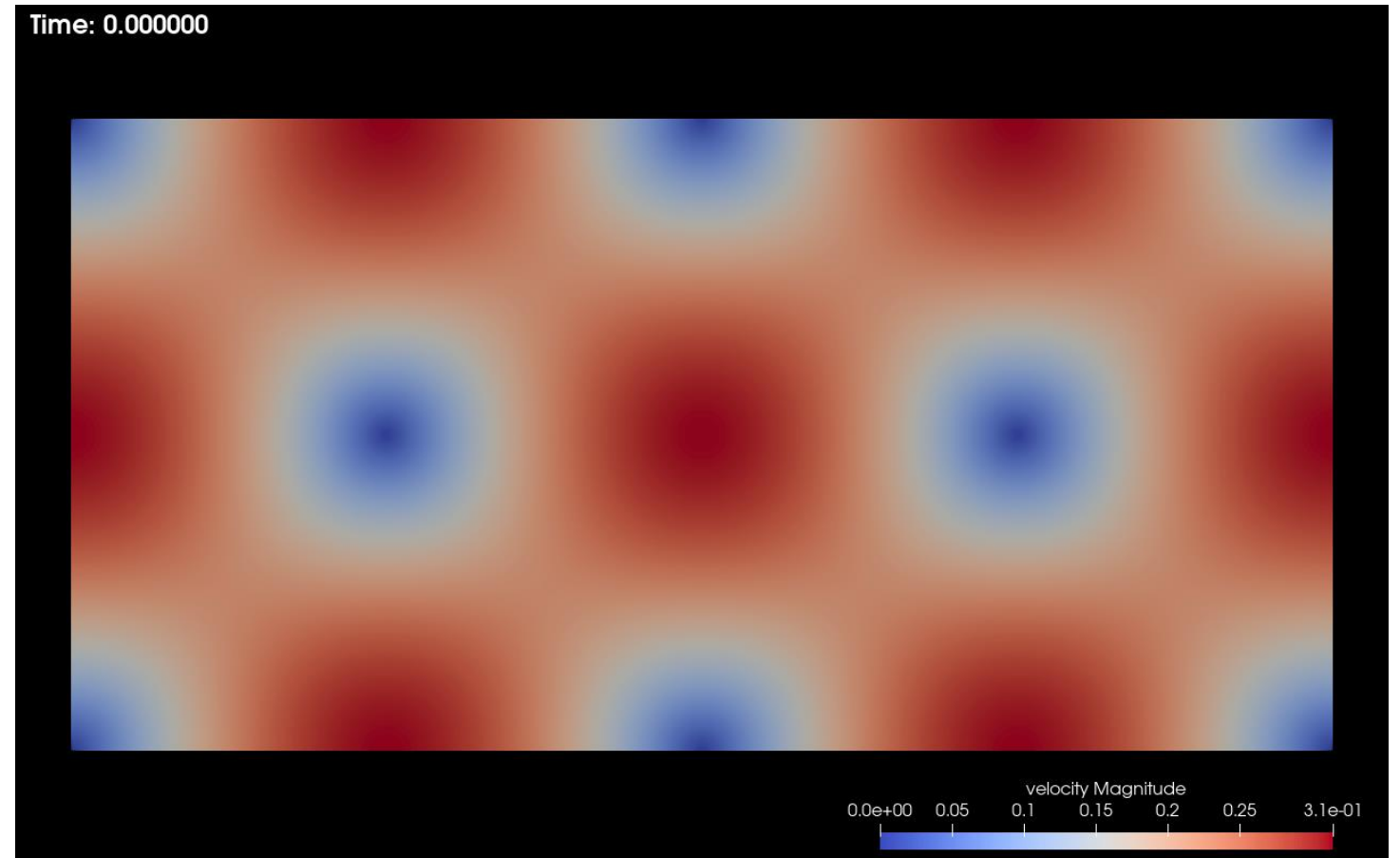
- Use a scalar field visualization technique
- Use glyphs representations (oriented arrows in the direction of the field)
- Use lines tangent to the vector field

Time-dependent data:

- Use particle traces
- Use pathlines

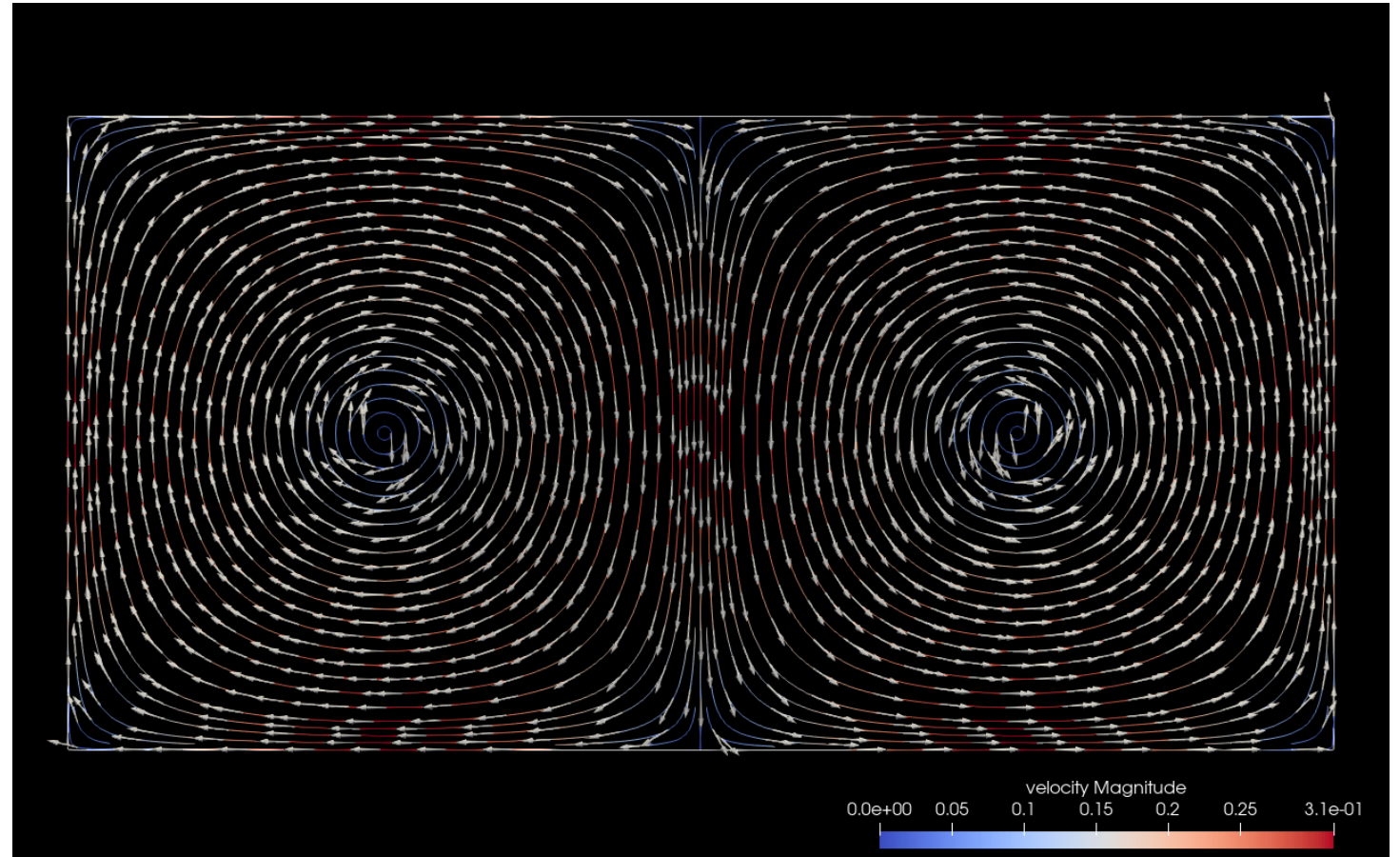
# Vector field visualization (1)

- Shade the vector field by its magnitude
- Missing cues?
  - direction



## Vector field visualization (2)

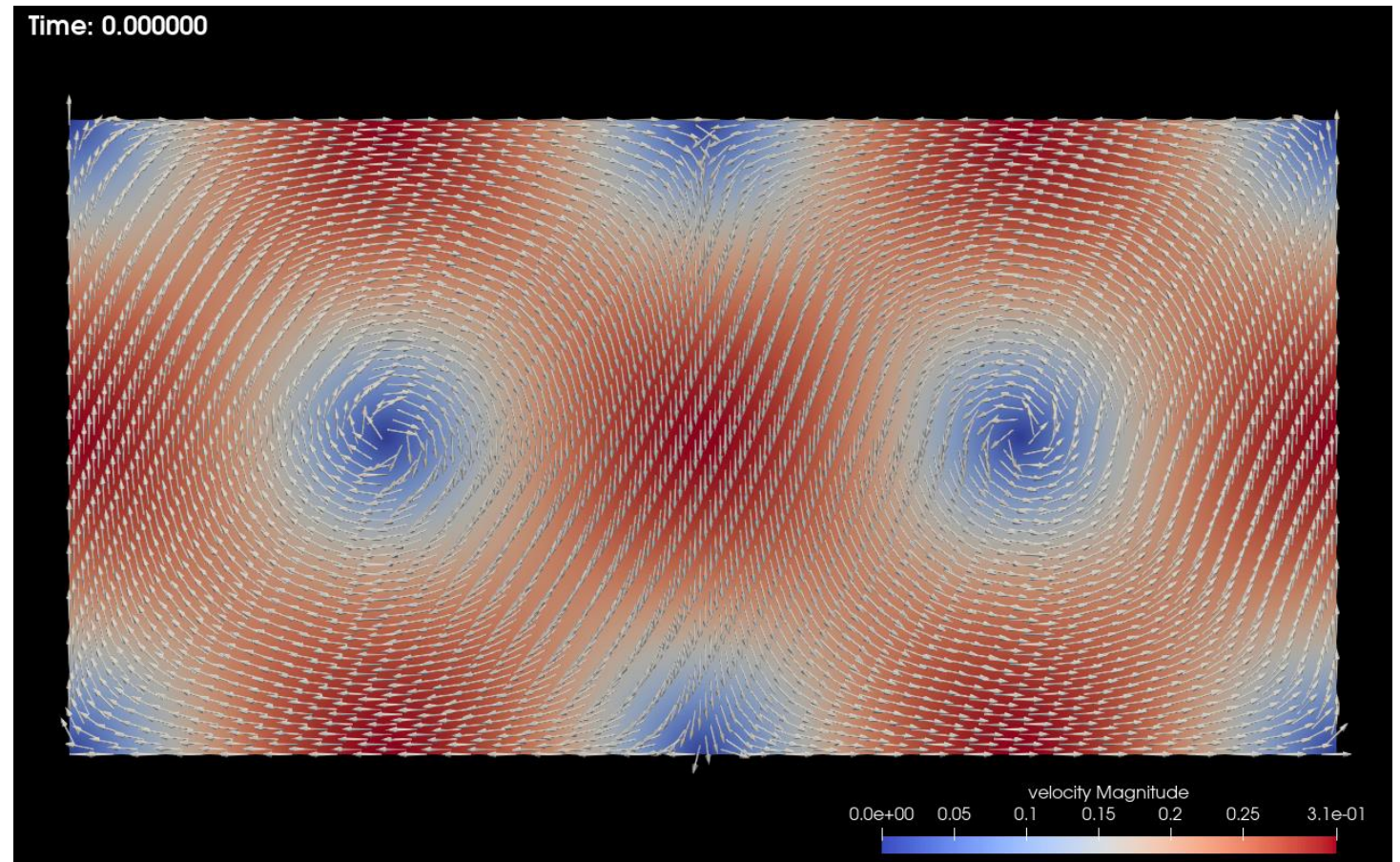
- Draw arrows oriented in the direction of the field
- Issues?
  - Make the density of arrows dependent on the zoom ration
- Difficulties?
  - Can be too complicated in 3D





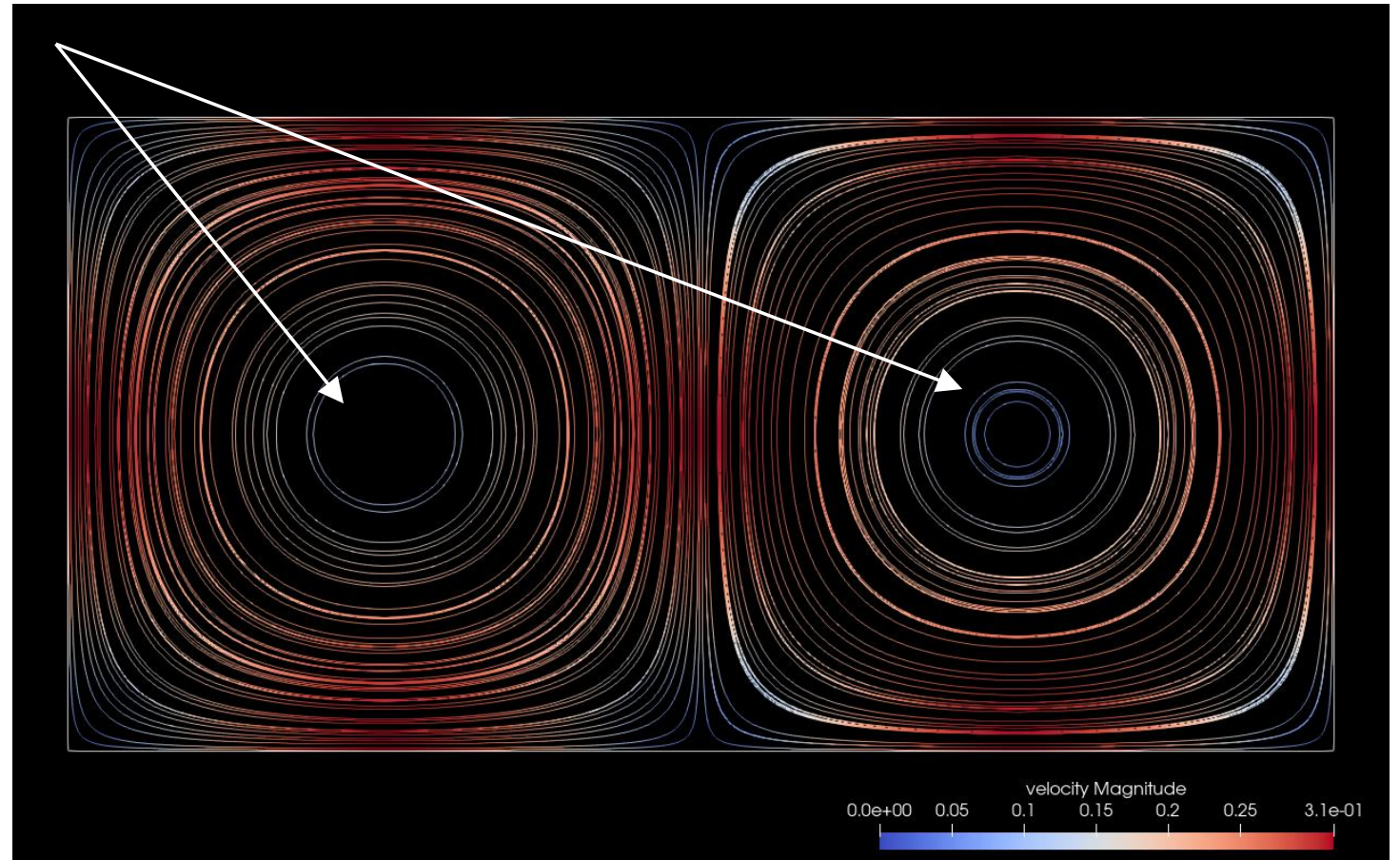
## Vector field visualization (2)

- Apply both techniques seen earlier



## Vector field visualization (2)

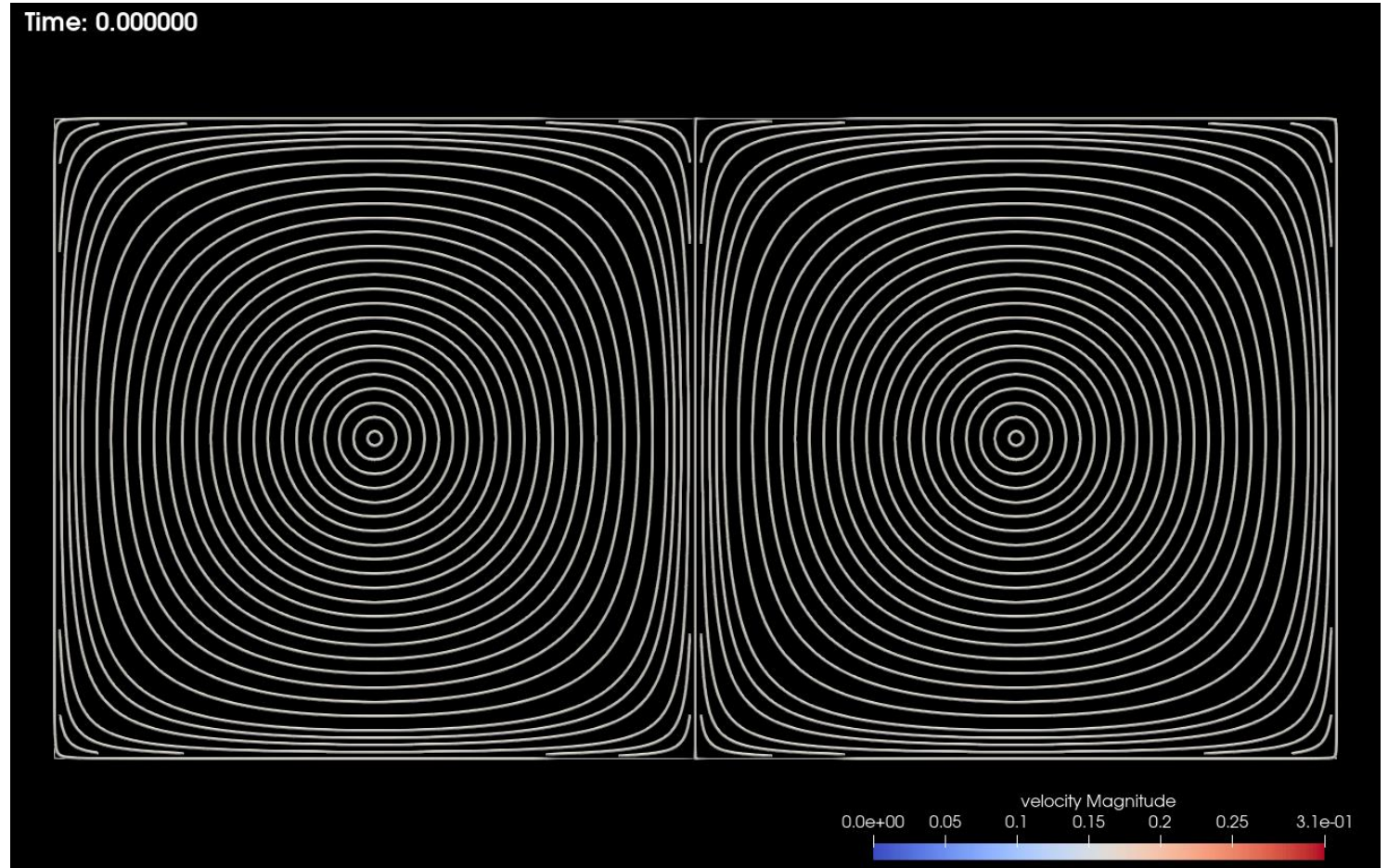
- Draw streamlines tangent to the vector field
- Difficulties?
  - too dense, or too sparse





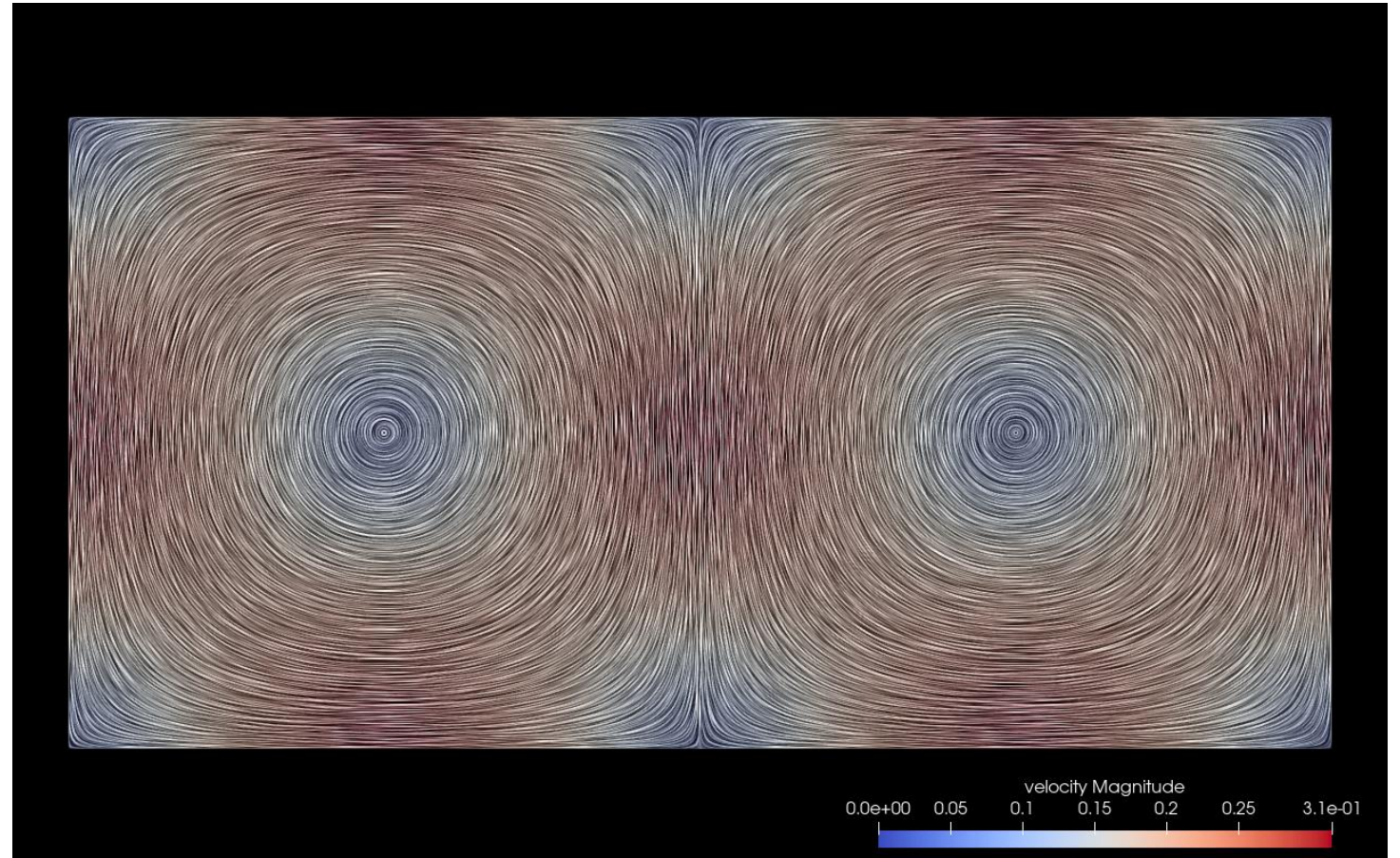
## Vector field visualization (2)

- Draw **evenly-spaced** streamlines tangent to the vector field
- Difficulties?
  - Missing in 3D



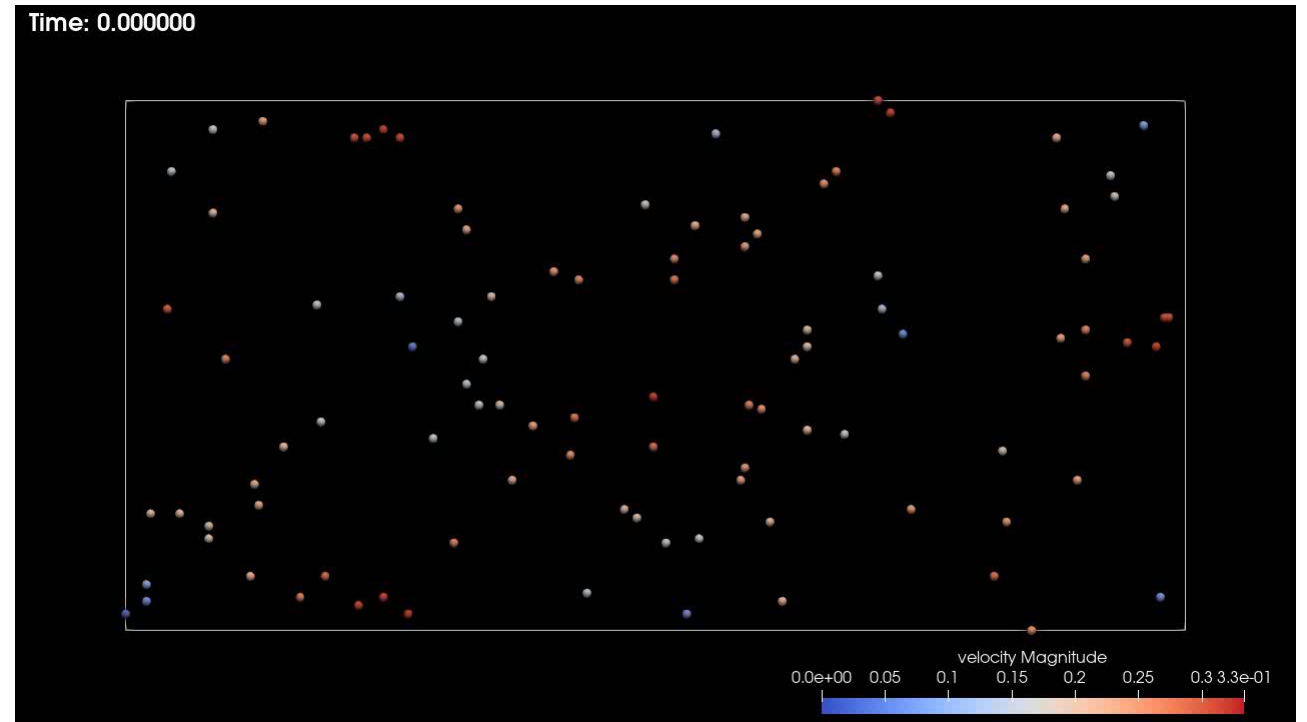
## Vector field visualization (2)

- Use a screen-space representation to do a Linear Integral Convolution
- Difficulties?
  - Missing in 3D
  - Not correct for transient data



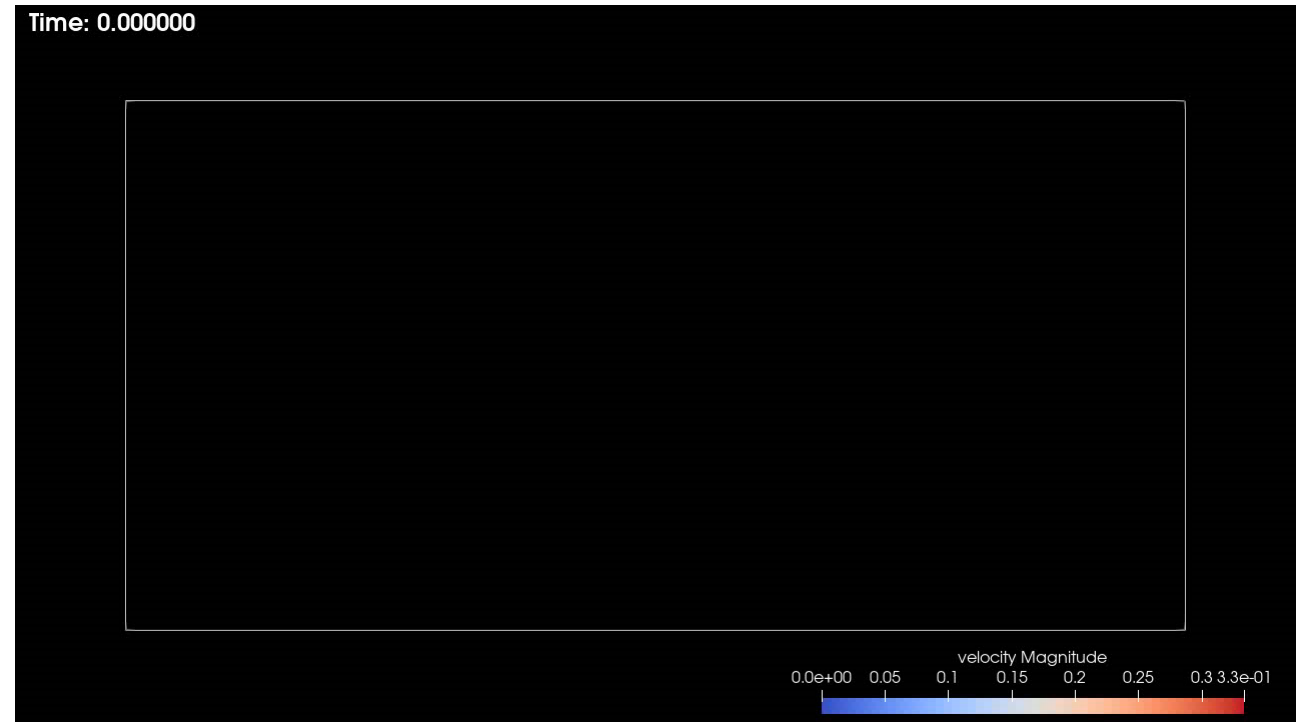
## Vector field visualization (2)

- Transient particles advected by the vector field
- Issues?
  - Particles disappearing
  - Can we re-inject particles at regular intervals?



## Vector field visualization (2)

- Transient particles advected by the vector field



# Exercise

- Login in to Dardel
- Execute `pvTransientDoubleGyre.0*.py`
- Make an animation (an mpeg file saved to disk) of temporal pathlines

# Time series

- <https://docs.paraview.org/en/latest/UsersGuide/dataIngestion.html#handling-temporal-file-series>
- <https://docs.paraview.org/en/latest/UsersGuide/dataIngestion.html#id1>