

CFD on HPC – OpenFOAM

01 – Introduction



Aleksander GRM – June, 2025



Short review

- Small introduction into PDEs

- Solution methods

- Mesh description

ParaVIEW

- Introduction

- GUI

- Basic usage

- Advanced usage

Introduction to OpenFOAM

- Structure

- Basic details

- Example

Short review



- ▶ Small introduction into PDEs
- ▶ Solution methods
- ▶ Mesh description



The mathematical modelling of real systems is in most cases narrowed down to the mathematical model described by **Partial Differential Equations (PDE)**.

Example: PDE describing waves motion on a free surface

$$\boxed{\frac{\partial^2 u}{\partial t^2} = c^2 \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right)} = c^2 \Delta u,$$

where the wave height is

$$u = u(t, \mathbf{x}), \quad \mathbf{x} \in \Omega, \quad \Omega \subseteq \mathbb{R}^2,$$

in the direction z , where $z \perp \Omega$.



In general we solve two types of problems

► **Initial Value problem (IVP):**

time t is independent variable of the problem, we solve **time-dependant** problem, so we need

initial condition: $u_0 = u(t = t_0, \mathbf{x})$, where $\mathbf{x} \in \Omega \subseteq \mathbb{R}^n$

► **Boundary Value Problem (BVP):**

time t is not part of the problem, we solve **time-independent** problem, so we need

boundary condition: $u_0 = u(\mathbf{x})$, where $\mathbf{x} \in \Gamma \subseteq \mathbb{R}^{n-1}$ ($\Gamma = \partial\Omega$),

where Γ is **boundary** of the computational domain. Many times you may see $\partial\Omega$.

IVP condition is obtained with the solution of BVP (start BVP with intuitive initialization)!

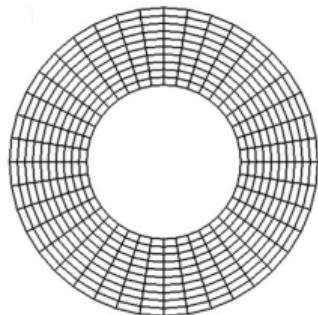


PDE can be solved in different ways

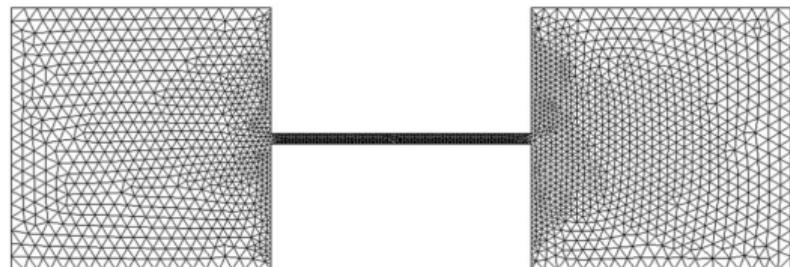
- ▶ **analytical methods:** mostly solving linear problems, or problems involving small parameter ϵ . Methods used are: separation of variables, series expansion, Perturbation methods, Laplace transform, Complex analysis methods, ...
- ▶ **numerical methods:** solve problems that is not possible to solve with analytical methods. In general we distinguish:
 - ▶ finite difference method (FDM) - solving **strong** form
 - ▶ finite volume method (FVM) - solving **weak** form
 - ▶ finite element method (FEM) - solving **weak** form
- ▶ **special numerical approaches:** use of FDM, FVM and FEM in different combinations
 - ▶ Immersed Boundary Method - IBM
 - ▶ Smoothed Particle Hydrodynamics - SPH (mesh less method)

All numerical methods, except SPH, need the mesh. Mesh divides computational domain onto cells/elements

Structured grid



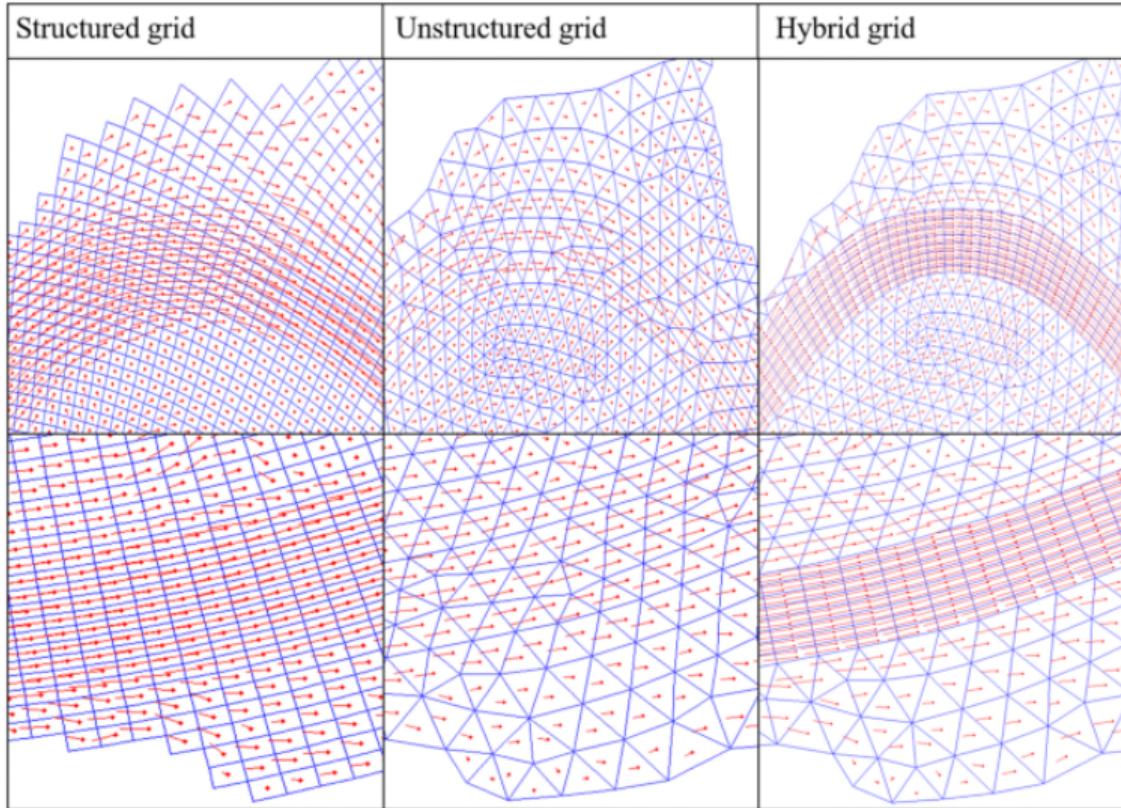
Unstructured grid



better convergence

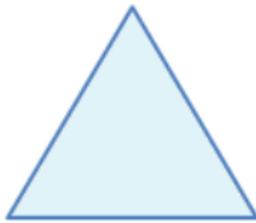
worse convergence

Very often we have a combination of both types! (next pages)





2D mesh

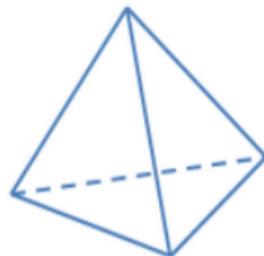


Triangle

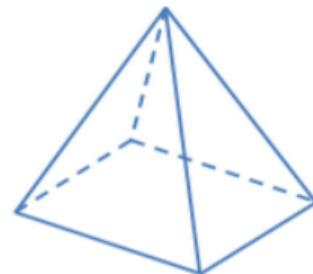


Quadrilateral

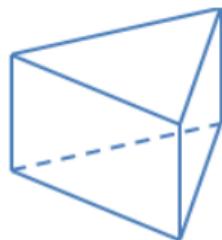
3D mesh



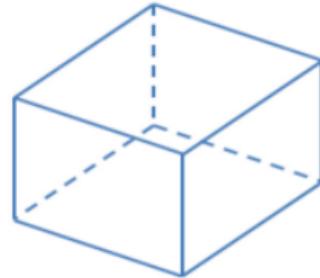
Tetrahedron



Pyramid

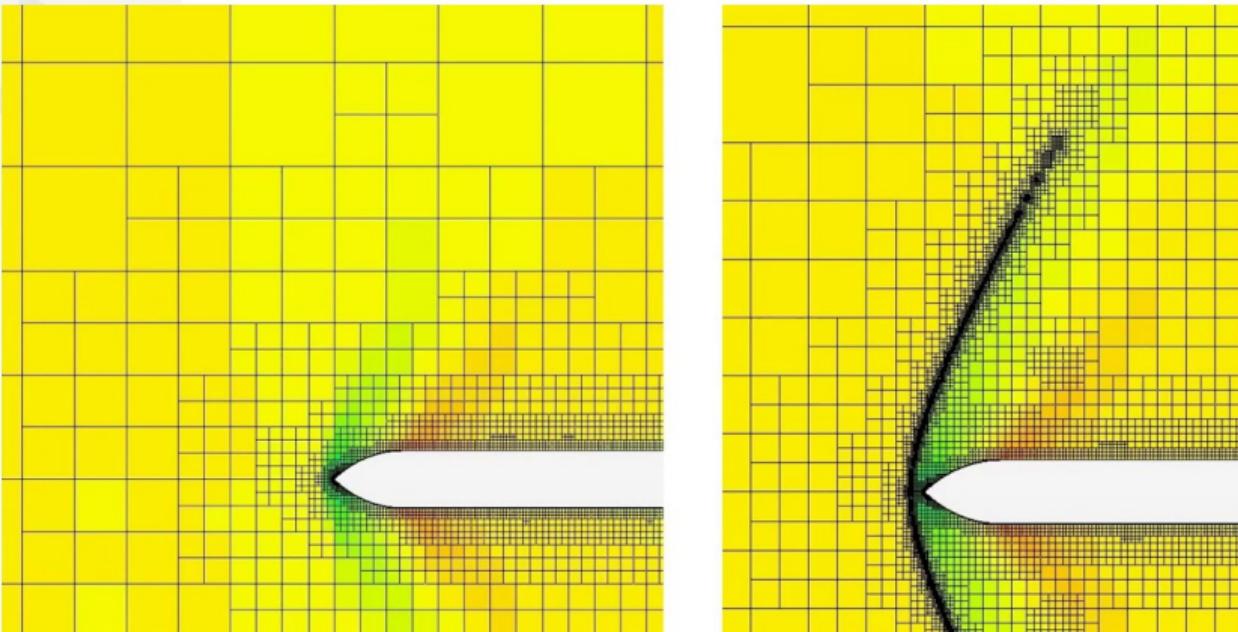


Triangular Prism

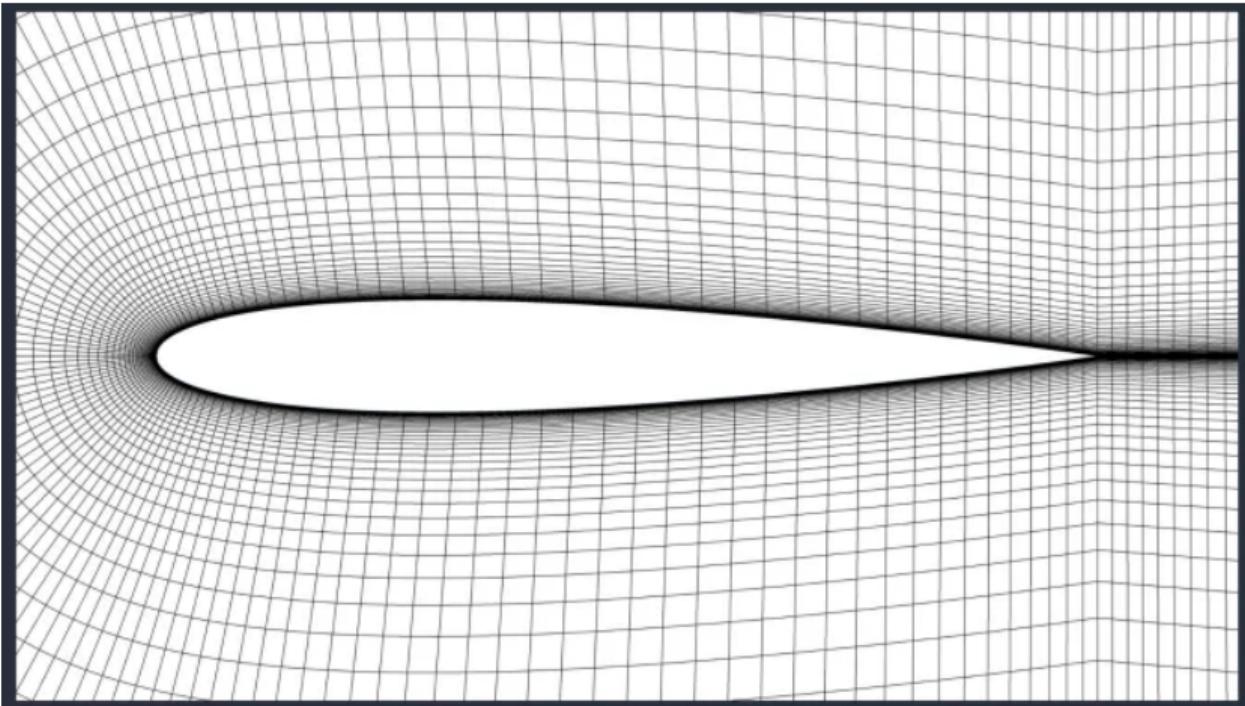


Hexahedron

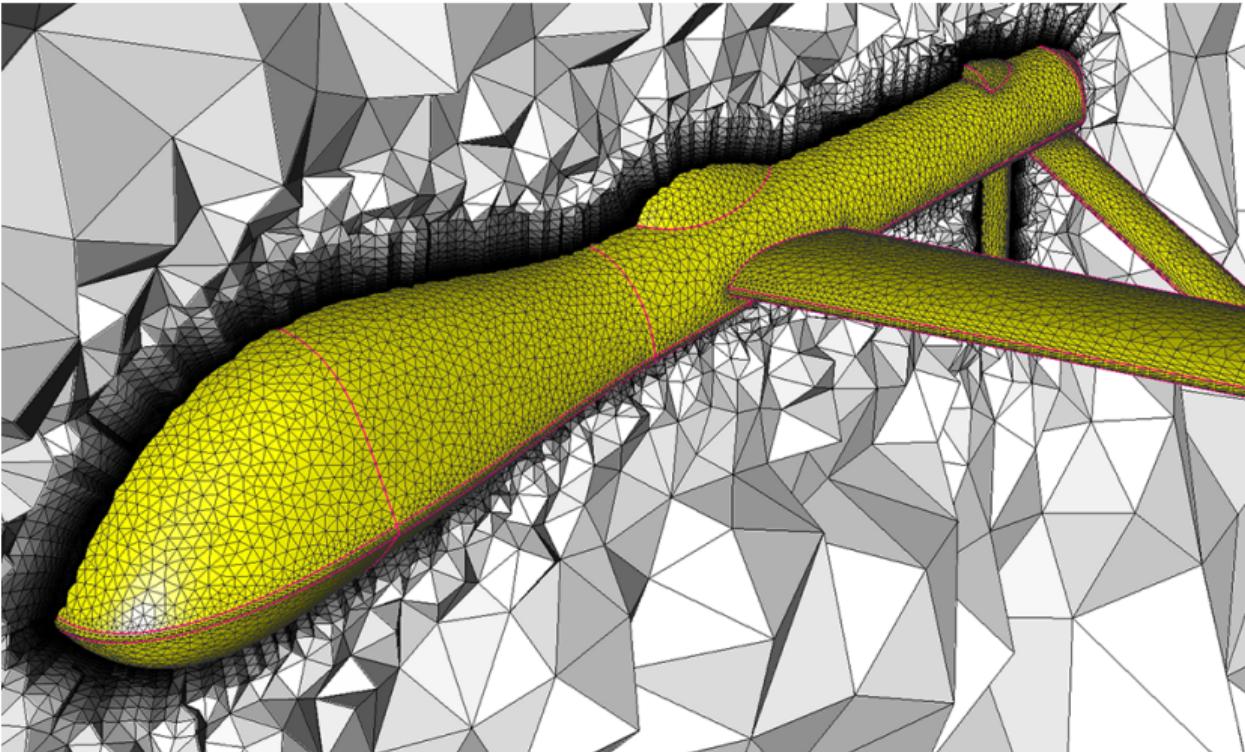
Some numerical solutions are only possible with **mesh refinement**!



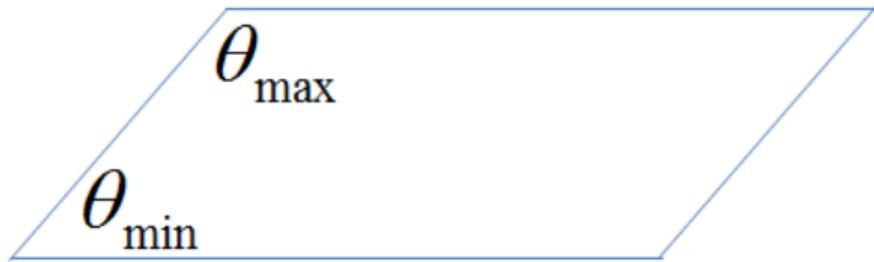
formation of shock waves - space entry simulation



external flow – foil geometry



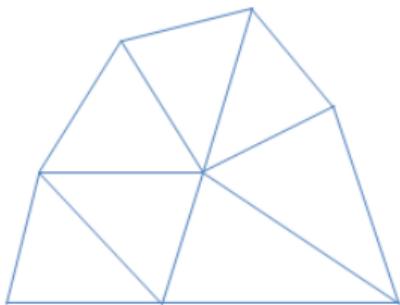
external flow – raptor geometry



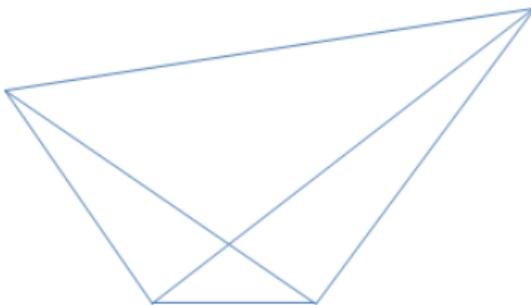
Skewness can be determined in many different ways, but always determines ratio of inner cell sides/angles!

$$\text{skewness} = \frac{\text{optimal cell size} - \text{cell size}}{\text{optimal cell size}}$$

It measures the deviation from optimal geometry (equidistant triangle)!



Smooth Change in cell size



Large jump in cell size

Smoothness measures the speed of cell size transition.



Aspect ratio = 1



High aspect ratio triangle



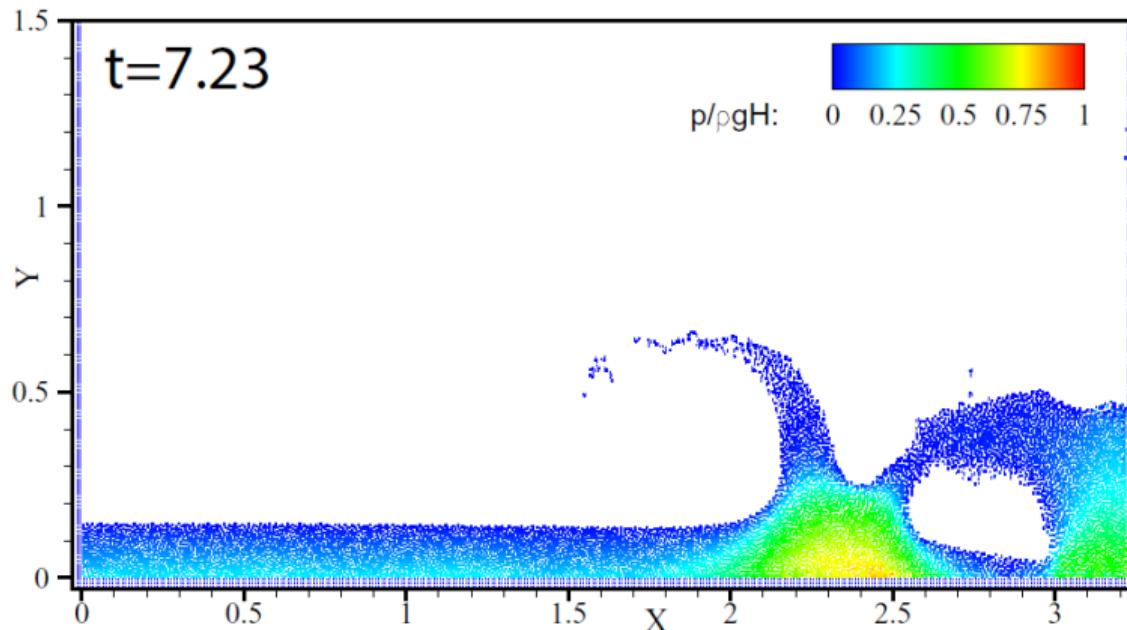
Aspect ratio = 1



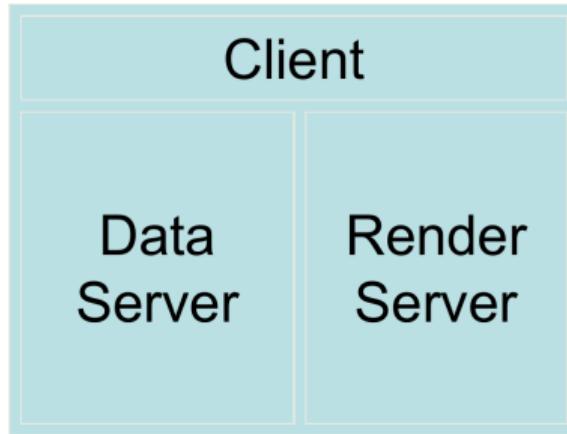
High aspect ratio quad

Aspect ratio measures the ratio of longest to the shortest side in a cell. Ideally it should be equal to 1 to ensure best results.

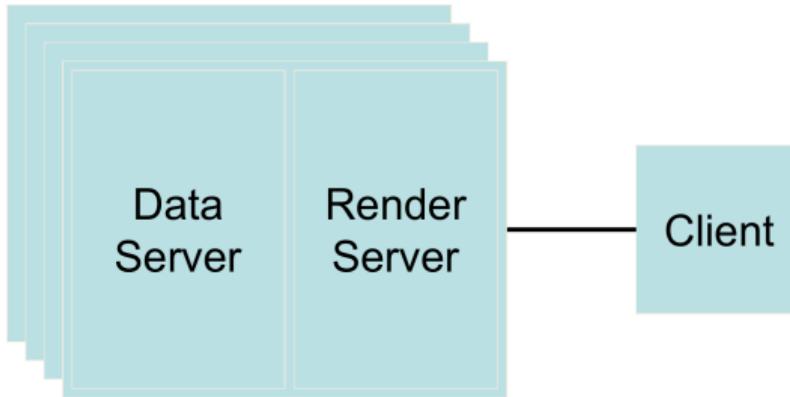
In mesh-less methods, we use particles that fill the space. They're mainly used where the shape of the surface changes over time, e.g. waves, continuous casting, solidification, etc.



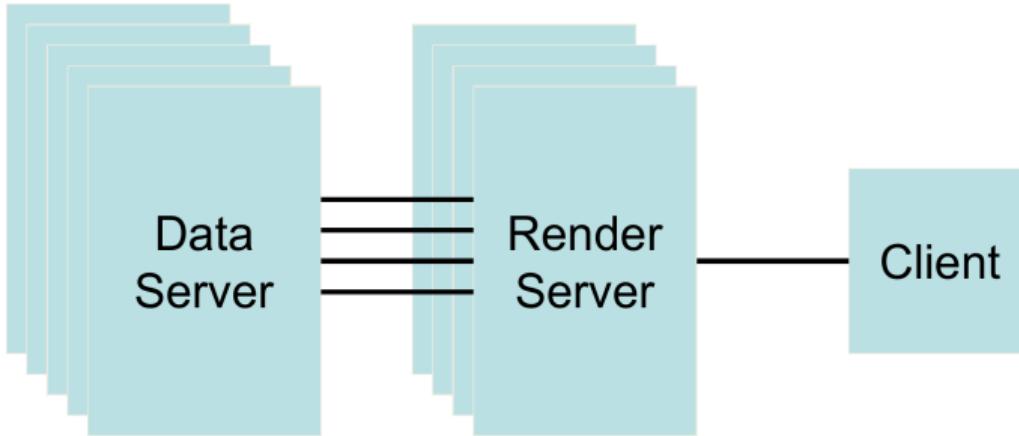
ParaVIEW



- ▶ In standalone mode, the client, data server, and render server are all combined into a single serial application.
- ▶ When you run the ParaView application, you are automatically connected to a built-in server so that you are ready to use the full features of ParaView.
- ▶ **This is how we are going to work.**



- ▶ In client-server mode, you execute the **pvserver** program on a parallel machine and connect to it with the ParaView client application.
- ▶ The **pvserver** program has both the data server and render server embedded in it, so both data processing and rendering take place there.
- ▶ The client and server are connected via a socket.



- ▶ In this mode, all three applications are running in separate programs.
- ▶ The client is connected to the render server via a single socket connection.
- ▶ The render server and data server are connected by many socket connections, one for each process in the render server.



<http://www.ParaView.org/in-situ/>

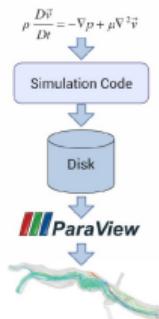
- ▶ **What is that?**

Catalyst is a library for in situ (also known as co-processing or co-visualization) integration into simulations and other applications. In other words, the post-processing is done as the simulation runs. No need to read the simulation data to do post-processing.

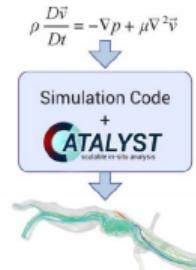
- ▶ **Where can I get it?**

You already have it. It is distributed with ParaView binaries.

- ▶ The post-processing is done as the simulation is running, we do not need to wait for the simulation to end.
- ▶ No more expensive IO.
- ▶ We have the full computational power of the supercomputer available to do this processing.
- ▶ Writing the results from the analysis and visualization will be much smaller and faster than the original full simulation data.



Traditional post-processing approach



In situ analysis and visualization,
co-processing or co-visualization



<http://www.ParaView.org/in-situ/>

- ▶ **What is that?**

Catalyst is a library for in situ (also known as co-processing or co-visualization) integration into simulations and other applications. In other words, the post-processing is done as the simulation runs. No need to read the simulation data to do post-processing.

- ▶ **Where can I get it?**

You already have it. It is distributed with ParaView binaries.



- ▶ paraFoam is the main post-processor distributed with OpenFOAM®.
- ▶ paraFoam is a wrapper of a third-party open source product named ParaView (www.ParaView.org).
- ▶ **In theory paraFoam and ParaView are the same.**
- ▶ The main post-processing tool provided with OpenFOAM® is a reader module to run with ParaView. The module is compiled into two libraries, `PV4FoamReader` and `vtkPV4Foam`.
- ▶ To visualize data obtained from OpenFOAM, you do not need to use paraFoam, you can use an stand-alone version of ParaView.
- ▶ In the user guide, it is written that it is highly recommended to use paraFoam.
- ▶ However, we have found that paraFoam can be slower than ParaView.
- ▶ **Therefore, we prefer to use ParaView.**



- ▶ Basically, when we use paraFoam we load the libraries `PV4FoamReader` and `vtkPV4Foam`.
- ▶ We also create the empty file `case.OpenFOAM` used by paraFoam to load the case.
- ▶ If you do not want to use paraFoam, just create the empty file `case.OpenFOAM` and open it with ParaView.

In the terminal type

- ▶ `$> touch case.OpenFOAM`
- ▶ `$> paraview case.OpenFOAM`

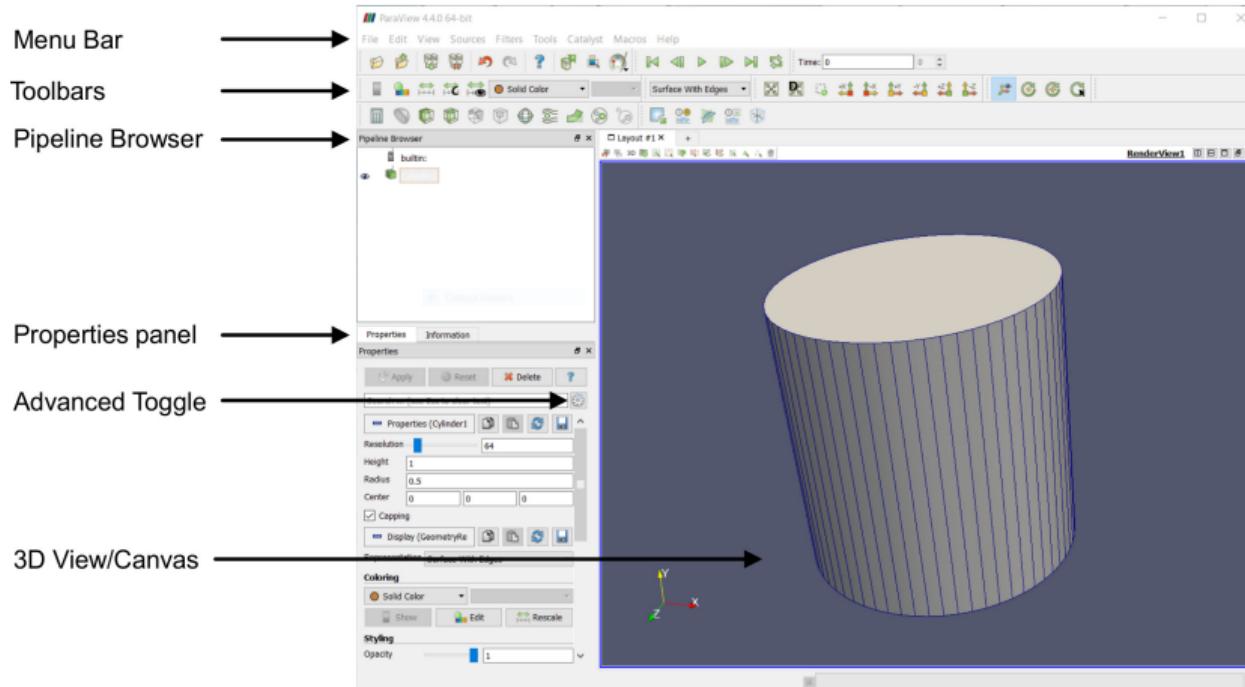
Or in one single step

- ▶ `$> touch case.OpenFOAM | paraview case.OpenFOAM`



Default User Interface

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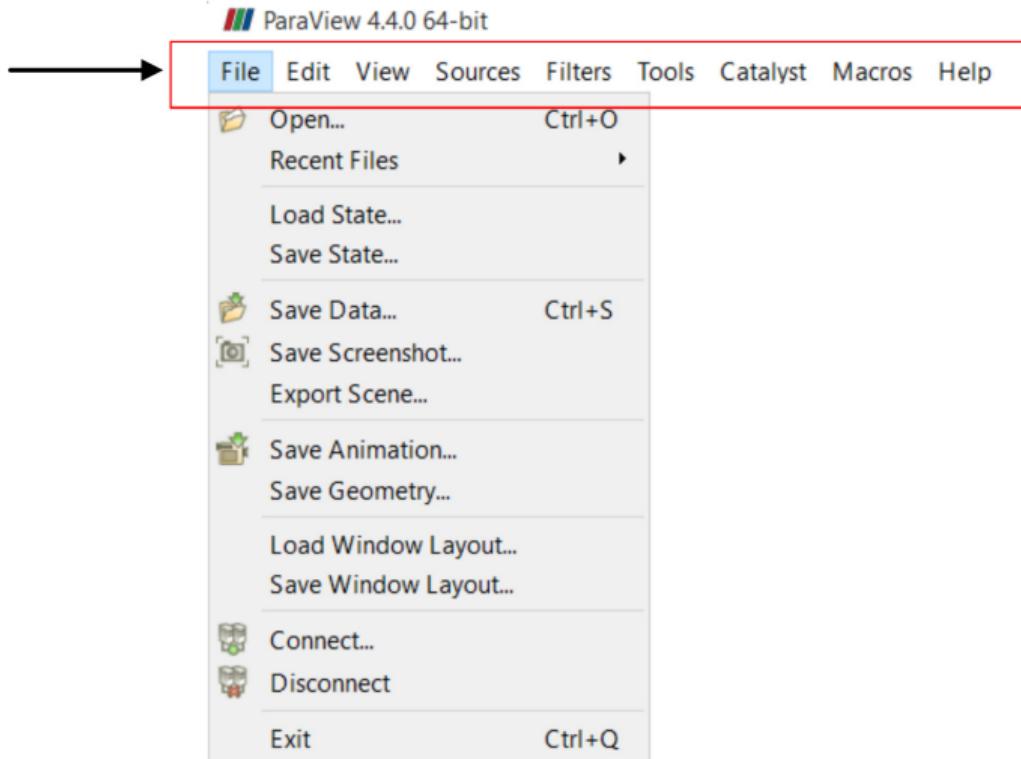


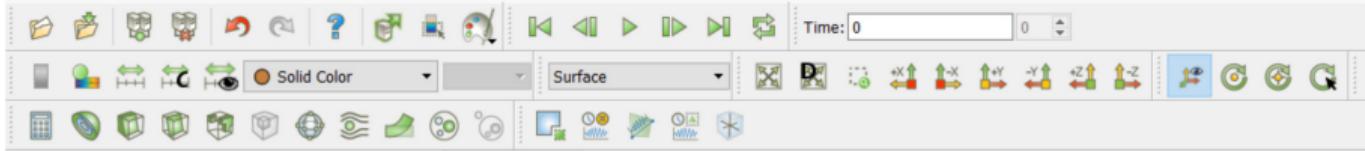
GUI layout is highly configurable, it is easy to change the look of the window.



Menu bar

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- ▶ The toolbars provide quick access to the most commonly used features within ParaView.
- ▶ By right clicking on the bar or selecting

[View → Toolbars](#)

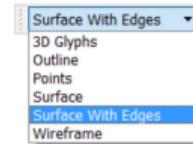
you can show/hide what features to see on the toolbar.



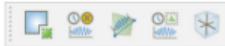
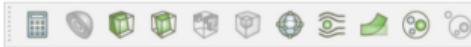
Toolbars



- Main Controls
- VCR Controls
- Current Time Controls
- Active Variable Controls
- Representation Toolbar

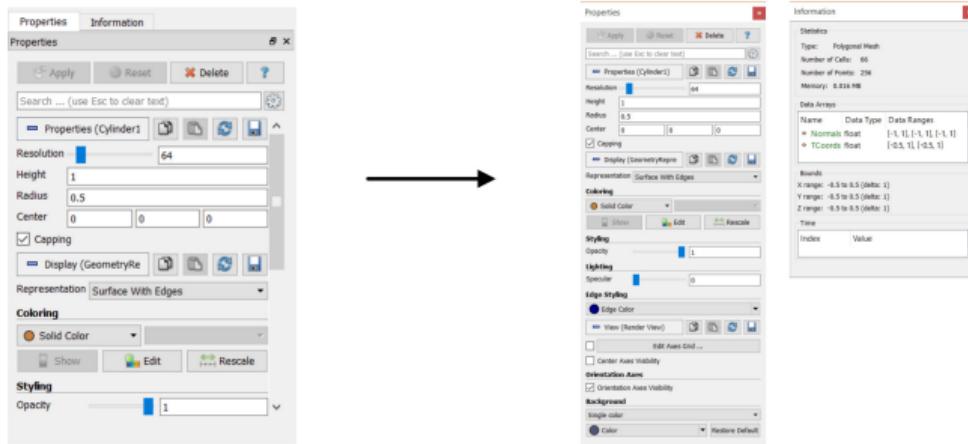


- Camera Controls
- Center Axes Controls
- Common Filters
- Data Analysis Toolbar





- ▶ ParaView manages the reading and filtering of data with a pipeline.
- ▶ The pipeline browser allows you to view the pipeline structure and select pipeline objects.
- ▶ It provides a convenient list of pipeline objects with an indentation style that shows the pipeline structure.
- ▶ By clicking on the eyeball icon you can show/hide objects.



- ▶ The properties panel allows you to view and change the parameters of the current pipeline object.
- ▶ On the properties panel there is an advanced properties toggle that shows and hides advanced controls.
- ▶ The properties are by default coupled with an information tab that shows basic summary of the data produced by the pipeline object.



ParaView 4.4.0 64-bit

File Edit View Sources Filters Tools Catalyst Macros Help

Toolbars

- Animation View
- Collaboration Panel
- Color Map Editor
- Comparative View Inspector
- Information
- Memory Inspector
- Multi-block Inspector
- Pipeline Browser
- Properties
- Selection Display Inspector
- Statistics Inspector
- Time Inspector

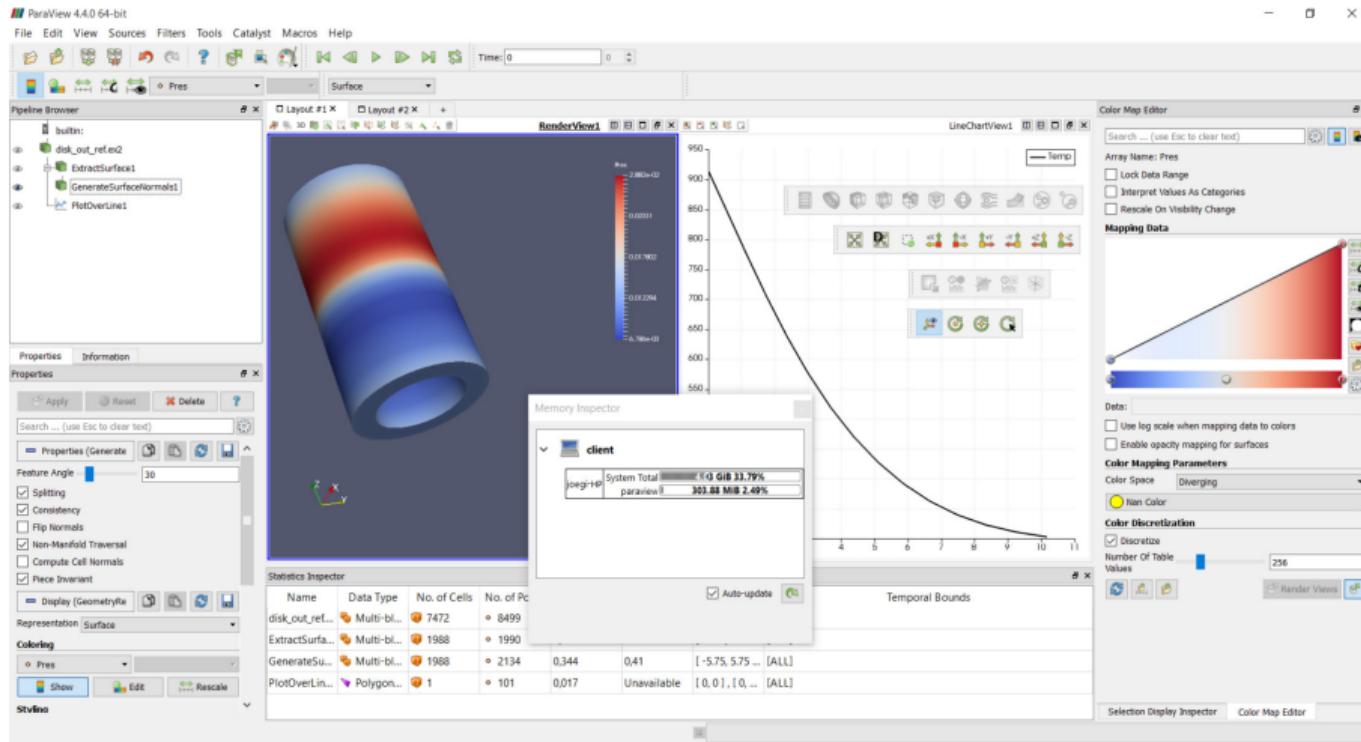
Toggle Borders Ctrl+D

Full Screen F11



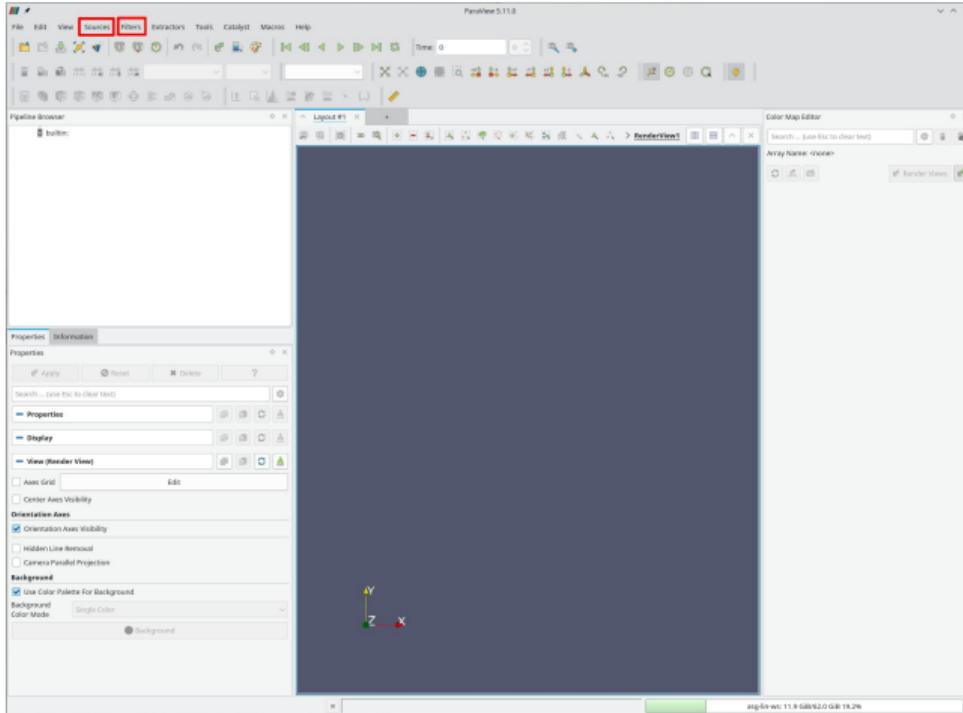
User Interface Customization

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Show the use of basic **Sources** and basic **Filters**





It will be shown in between the simple case of cylinder in cavity!

Introduction to OpenFOAM



- ▶ OpenFOAM folder structure
- ▶ Literature and Basic details
- ▶ Introductory example



Directory structure of OpenFOAM system as downloaded from a **GIT** repository

```
OF system folder
├── applications -- source code for solvers
├── bin -- bash scripts
├── doc -- documentation
├── etc -- compile & runtime controls
├── platforms -- platform specific compiled binaries
├── src -- source codes of the system
├── tutorials -- pre-configured cases
└── wmake -- compile script system
```



Files containing initial condition for all dependant variables

- 0
 - U -- velocity
 - p -- pressure
 - k -- turbulent
 - epsilon -- turbulent
 - T -- scalar transport



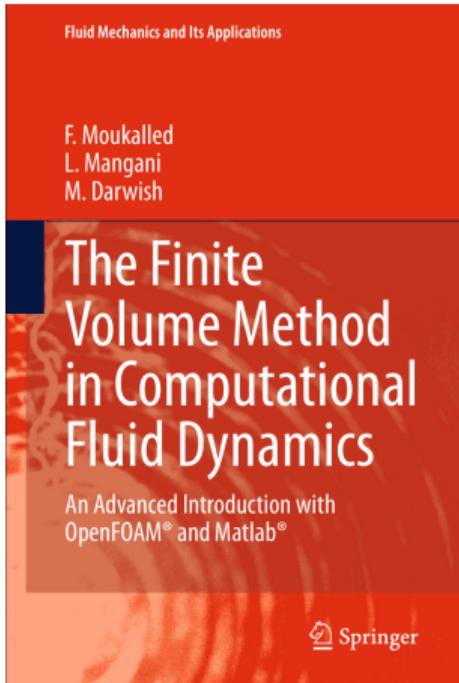
Folder containing files with constant data and mesh

```
constant
└── turbulenceProperties -- turbulent model properties
└── physicalProperties -- viscosity model & flow type
└── polyMesh -- computational mesh
    ├── boundary
    ├── points
    ├── faces
    ├── owner
    └── neighbour
```

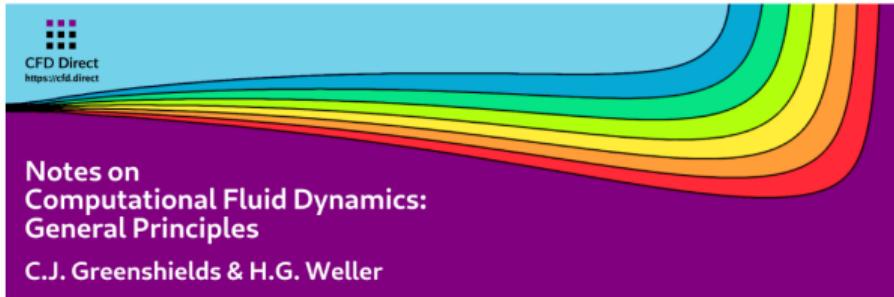


Folder containing system files

```
system
└── controlDict -- simulation controls
└── fvSchemes -- discretization schemes
└── fvSolution -- solution procedures
└── decomposeParDict -- domain decomposition & parallelization
└── residuals -- simulation residuals for post-process
└── ...
```



[link to the book](#)



About the Book

Notes on Computational Fluid Dynamics (CFD) was written for people who use CFD in their work, research or study, providing essential *knowledge* to perform CFD analysis with confidence. It offers a modern perspective on CFD with the finite volume method, as implemented in OpenFOAM and other popular general-purpose CFD software. Fluid dynamics, turbulence modelling and boundary conditions are presented alongside the numerical methods and algorithms in a series of short, digestible topics, or *notes*, that contain complete, concise and relevant information. The book benefits from the experience of the authors: Henry Weller, core developer of OpenFOAM since writing its first lines in 1989; and, Chris Greenshields, who has delivered over 650 days of CFD training with OpenFOAM.

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[8 Sample Problems](#)

[Index](#)

ISBN 978-1-3999-2078-0, 291 pages.

[link to the book](#)



Dimensions in OF are set in a list

No.	Property	SI unit	USCS unit
1	Mass	kilogram (kg)	pound-mass (lbm)
2	Length	metre (m)	foot (ft)
3	Time	second (s)	second (s)
4	Temperature	Kelvin (K)	degree Rankine ($^{\circ}$ R)
5	Quantity	mole (mol)	mole (mol)
6	Current	ampere (A)	ampere (A)
7	Luminous intensity	candela (cd)	candela (cd)

Example: kinematic viscosity ν [m^2/s]

- value is set in a file `constants/transportProperties`

```
nu [0 2 -1 0 0 0 0] 0.01;
```



OF diversity

- ▶ many turbulent flows ($k-\varepsilon$, $k-\omega$, $k-\omega$ -SST,...)
- ▶ many boundary conditions
- ▶ multi phase flows models
- ▶ internal combustion models
- ▶ DNS
- ▶ stress analysis + FSI
- ▶ and many more ...
- ▶ look into www.openfoam.org - User Guide



Example of a simple case in OF – Cavity flow

1. create mesh: `blockMesh`

2. check mesh quality: `checkMesh`

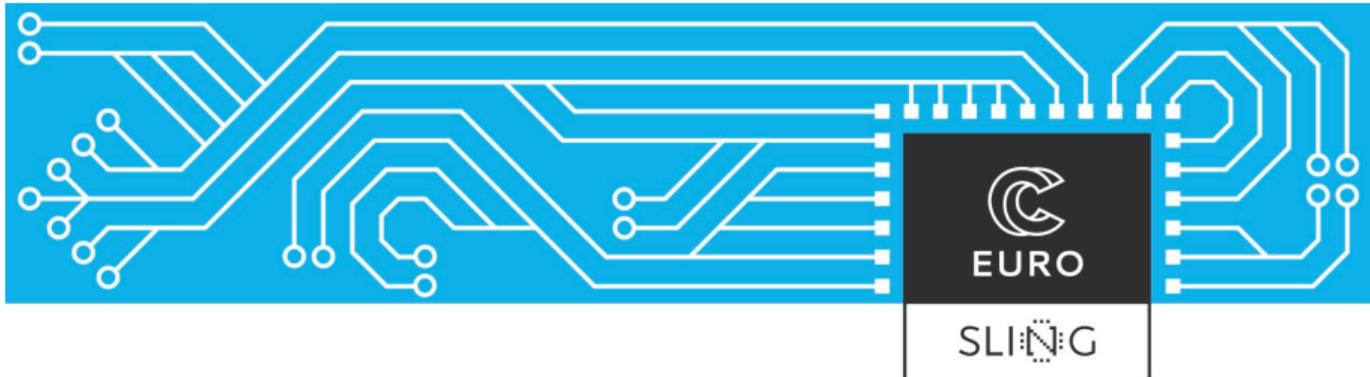
3. run solver: `foamRun`

4. check residuals:

```
foamMonitor -l postPorocessing/residuals/0/residuals.dat
```

5. preview results: `paraFoam -builtin`

Show and try in **HPC@FS** system!



Thank you for attention!



EuroHPC
Joint
Undertaking



REPUBLIC OF SLOVENIA
MINISTRY OF HIGHER EDUCATION,
SCIENCE AND INNOVATION

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