PPS 2024
30 Sept.-03 Oct. | Ferrol · Spain

Introduction to OpenFOAM® Computational Library and Viscoelastic Fluid Flow Simulation

P1 - Introduction do OpenFOAM

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iPC INSTITUTE FOR POLYMERS AND COMPOSITES
IPPD Institute of Polymer Processing and Digital Transformation
JOHANNES KEPLER UNIVERSITY LINZ

Outline

9:00 – 10:30	**Introduction to OpenFOAM (P1)**
10:30 – 12:00	**Mesh generation and post-processing (P2)**
12:00 – 13:00	Lunch break
13:00 – 14:30	**Case studies: Single- and two-phase flow solvers (P3)**
14:30 – 16:00	**Case studies: Viscoelastic fluid flow solvers (P4)**

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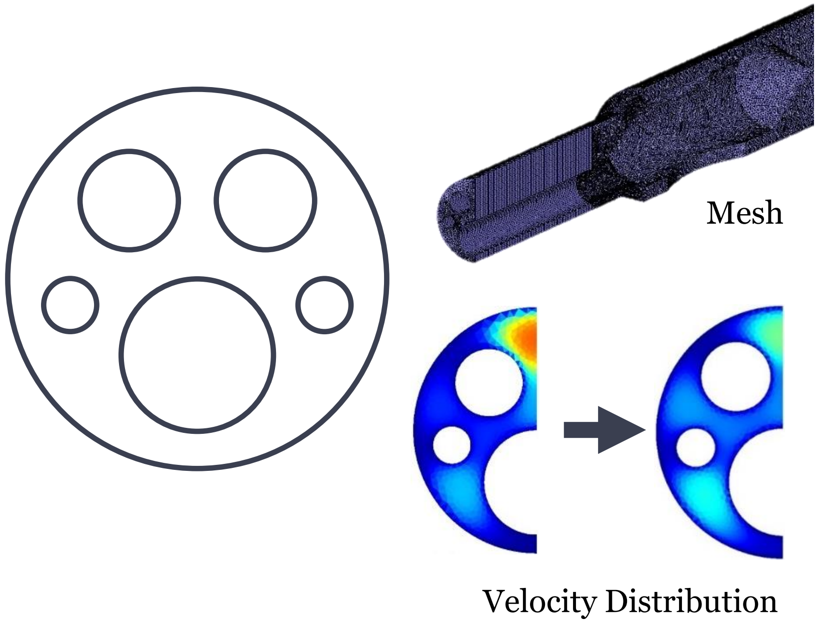
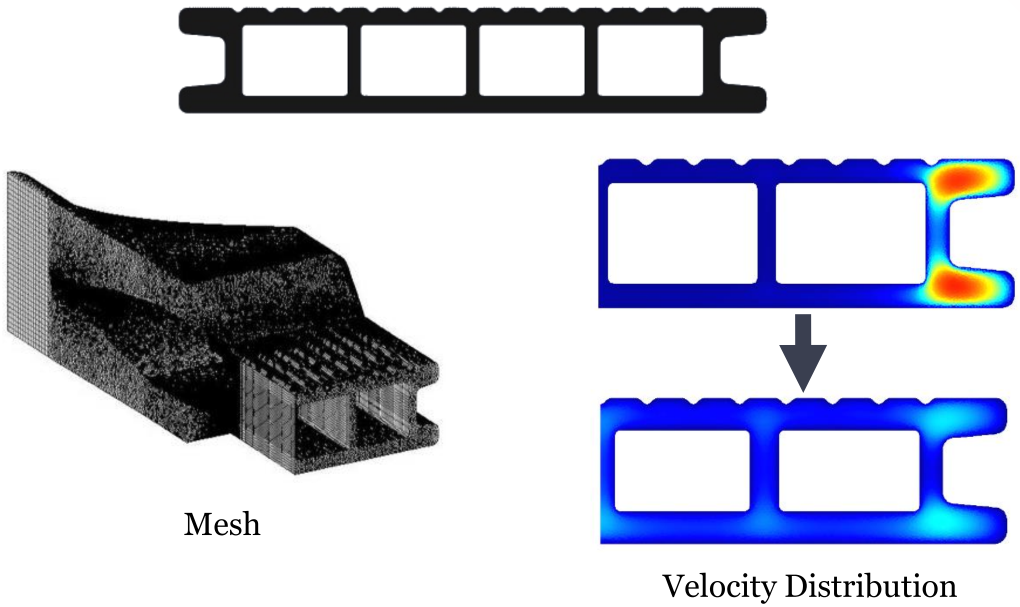
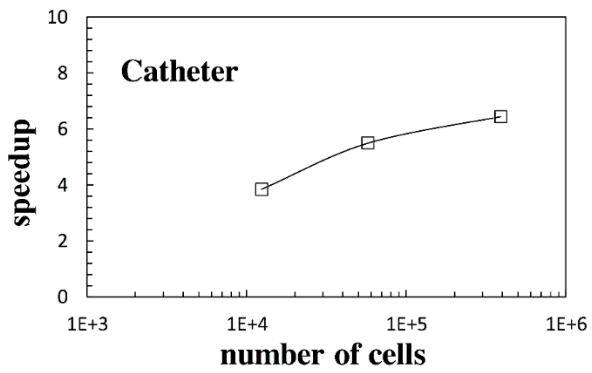
Motivation

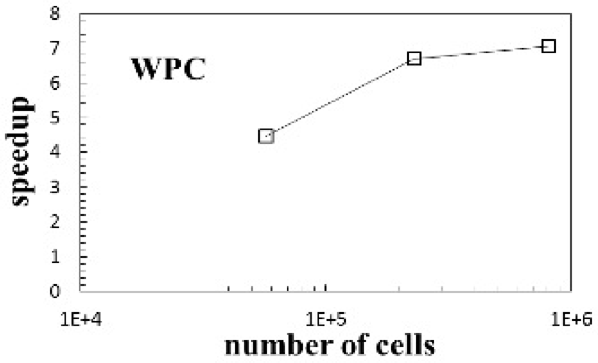
Unstructured Numerical Modeling Code





GPU Parallelization





ND Gonçalves, OS Carneiro, JM Nóbrega - Journal of Non-Newtonian Fluid Mechanics, 2013
ND Gonçalves, SP Pereira, LL Ferrás, OS Carneiro , JM Nóbrega - International Polymer Processing 2015

Motivation

New feature → New researcher

Hussaini Hanging Bridge, Pakistan

The OpenFOAM® Computational Library

OpenFOAM

- **<u>O</u>pen** source <u>F</u>ield <u>O</u>peration <u>A</u>nd <u>M</u>anipulation
- C++ Computational Library, Finite Volume Method, Unstructured meshes (and mesh generators)
- Multiphysics and Multiphase systems (FSI, Eulerian-Eulerian, Eulerian-Lagrangian)
- Parallelized
- Several **pre-compiled** solvers available

‘Basic’ CFD codes
Incompressible flow
Compressible flow
Multiphase flow
Large eddy simulation (LES)
Combustion
Particle-tracking flows
Heat transfer
Buoyancy-driven flows
Molecular dynamics methods
Direct simulation Monte Carlo methods
Electromagnetics
Solid Mechanics
Viscoelastic
Finance
…

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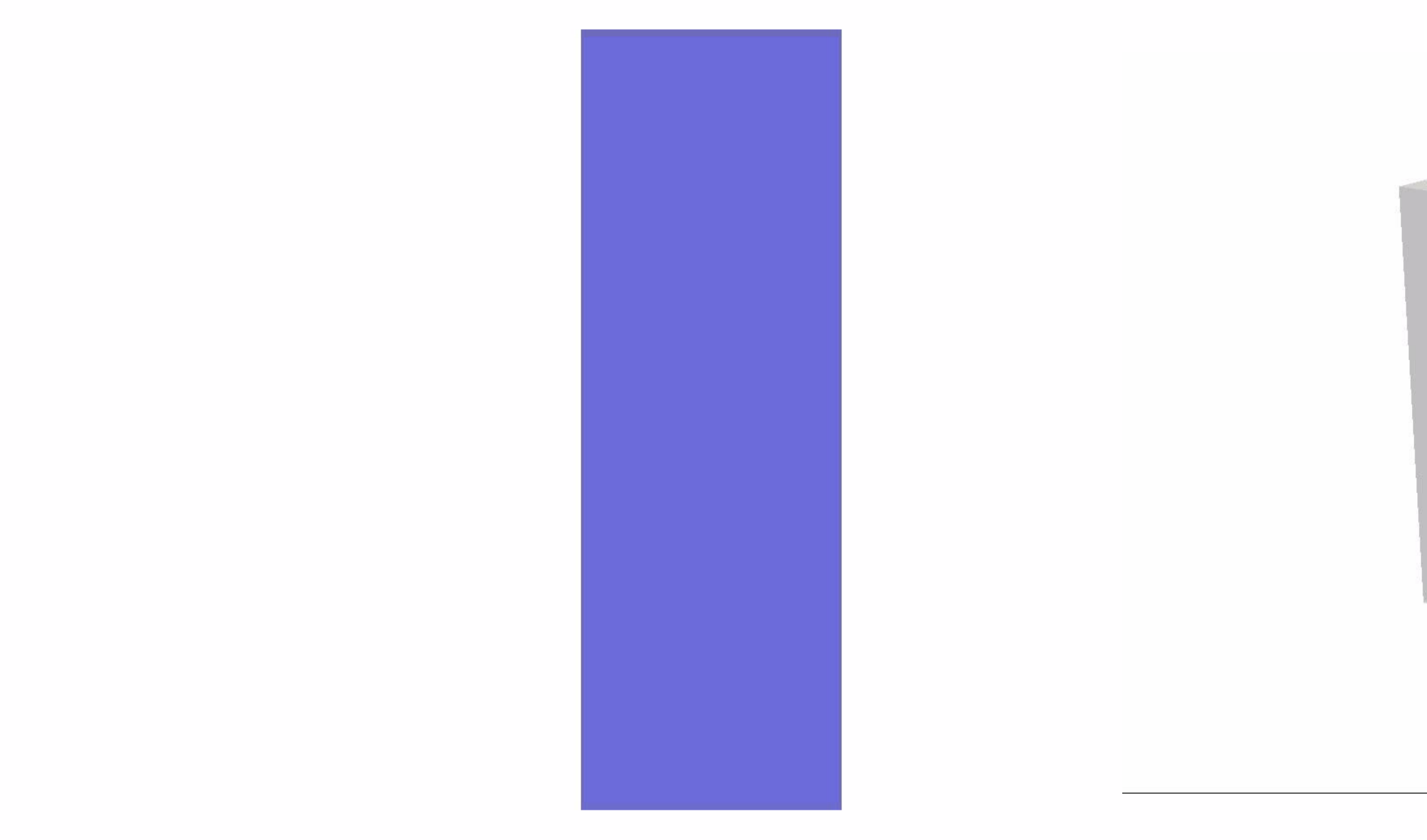
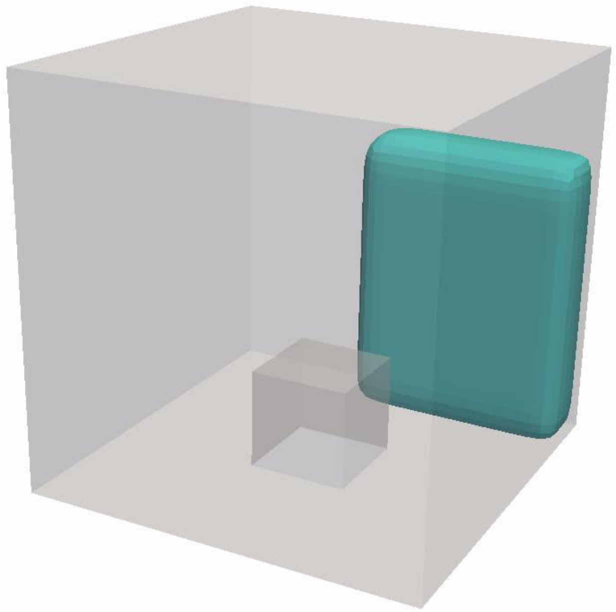
The OpenFOAM® Computational Library

OpenFOAM

Fluid Dynamics



Fluidized Bed
(Eulerian+Lagrangian)



Dam Break 3D - VOF
(Eulerian+Eulerian)

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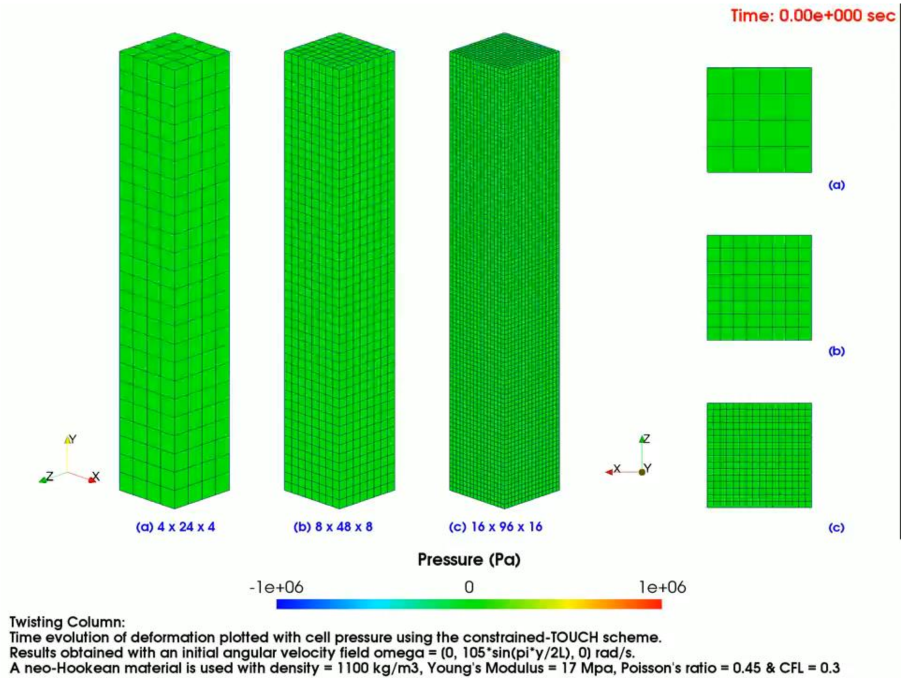
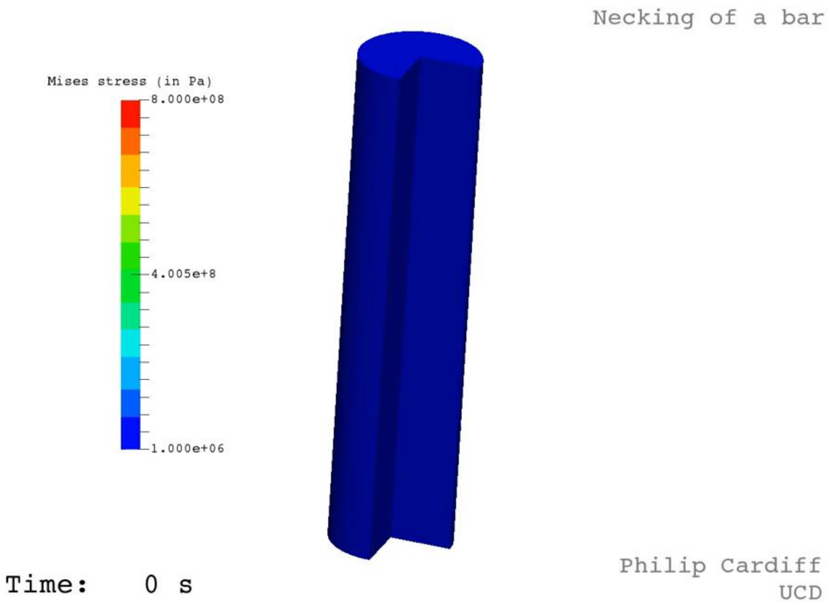
OpenFOAM

Solid Mechanics



Twisting Column(1)



Necking of a bar (2)

(1) From Jibran Haider's Youtube channel - https://tinyurl.com/ybosqbtq
(2) From Philip Cardiff's Youtube channel - https://tinyurl.com/pcardiff

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The OpenFOAM® Computational Library

A (very) brief history…

1996 – Hrvoje Jasak PhD Thesis, Imperial College

1998 – Weller, Tabor, Jasak, Fureby, Computers in Physics

A tensorial approach to computational continuum mechanics using object-oriented techniques

H. G. Weller and G. Tabor[a]
Department of Mechanical Engineering, Imperial College, London SW7 2BX, United Kingdom

H. Jasak
Computational Dynamics Limited, London W10 6RA, United Kingdom

C. Fureby
Department of Weapons and Protection, National Defense Research Establishment (FOA), S-17290 Stockholm, Sweden

2006 – **1st OpenFOAM Workshop** (Zagreb)

2010 – **Foam-Extend v1.6**

2013 – **1st OpenFOAM Conference** (Frankfurt)

2016 – **11th OpenFOAM Workshop** (Guimarães)
4th OpenFOAM Conference (Cologne)

2016 – **Discussions about "One OpenFOAM"**
Creation of OpenFOAM Wiki

2021 – **The OpenFOAM Journal**

OpenFOAM® Journal

1990

2000

2010

2020

1989 – **FOAM** v1 – Imperial College
Henry Weller and **Hrvoje Jasak**

?

2000 – **Nabla Ltd.** Foundation
FOAM released as commercial CFD Toolbox

2004 – **Nabla Ltd.** Closure
OpenFOAM v1.0 released as open-source by **OpenCFD**

2006 – **Trademarks OpenFOAM** and **OpenCFD** registration (to avoid misusage)

2011 – Acquisition of **OpenCFD** by **SGI** and creation of **OpenFOAM Foundation** (to assure the open-source nature)

2012 – Acquisition of **OpenCFD** by **ESI**

2018 – **OpenFOAM Governance**

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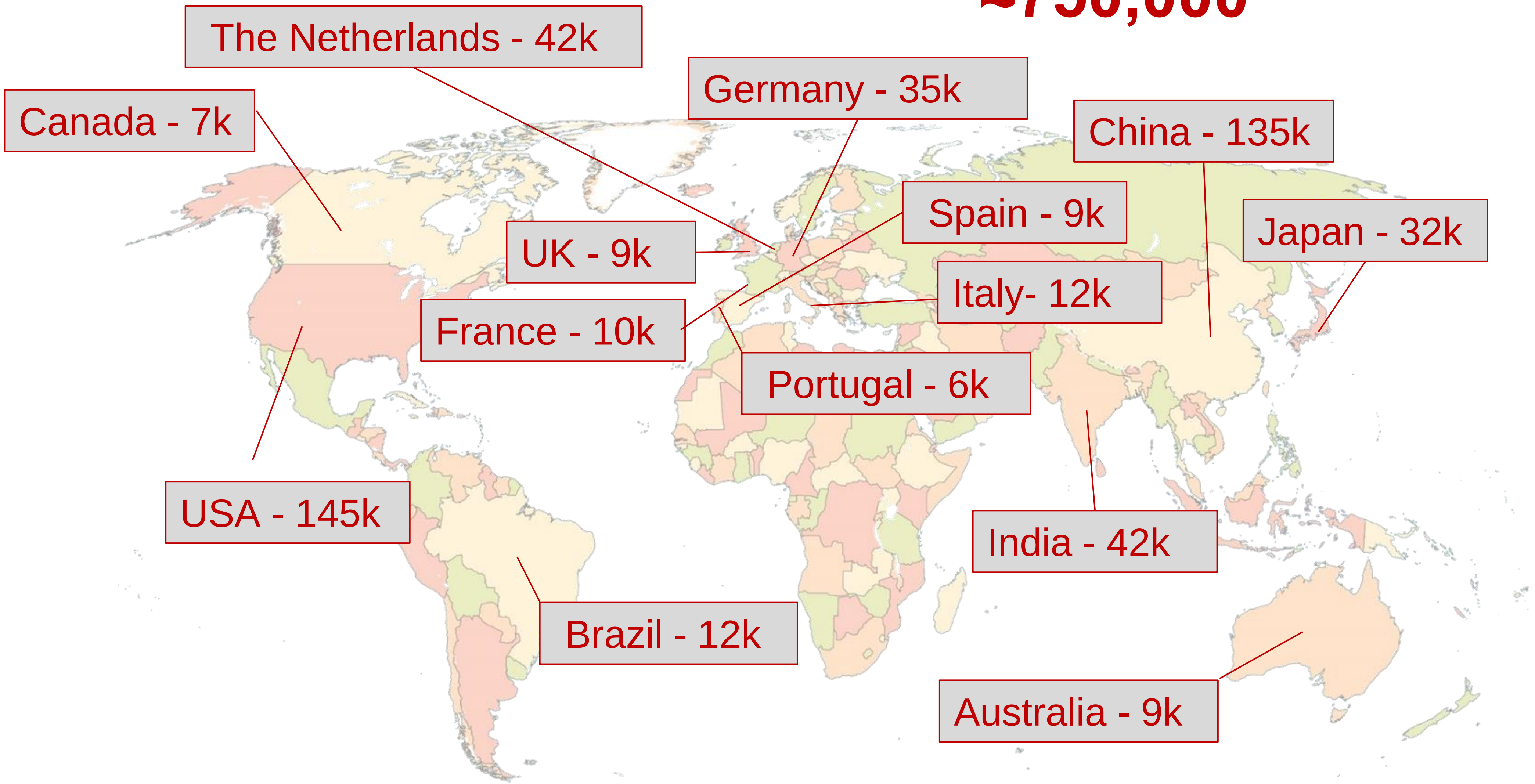
The OpenFOAM® Computational Library

Downloads during 2023 of the three major forks

≈750,000



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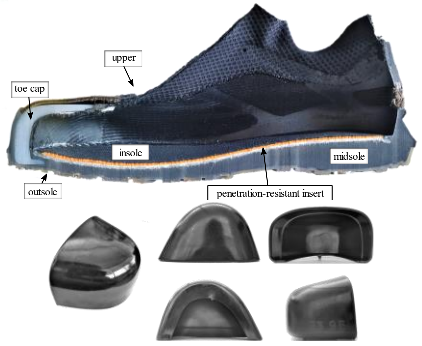
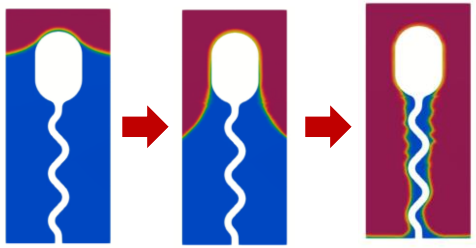
Introduction

FAMEST



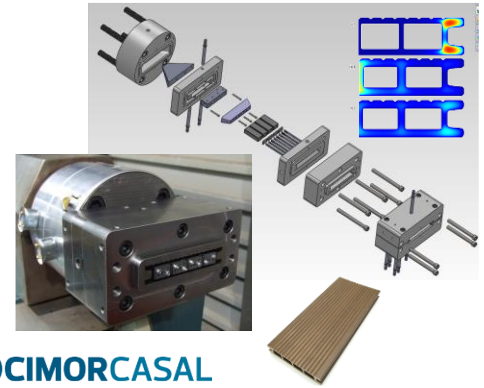
MICHELIN



Atlanta

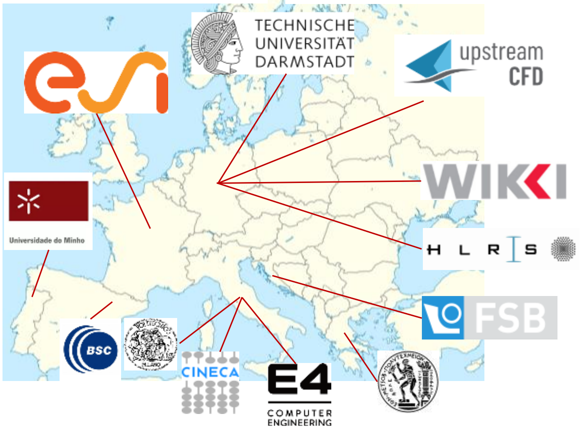
FAMEST

SOCIMORCASAL

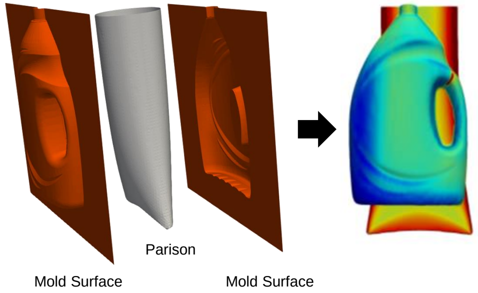


exaFOAM

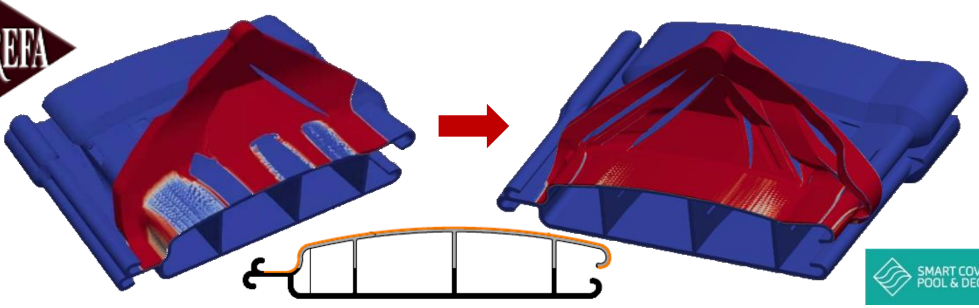
EuroHPC Joint Undertaking



LOGOPLASTE



SOPREFA



SMART COVER POOL & DECK

FORTISSIMO

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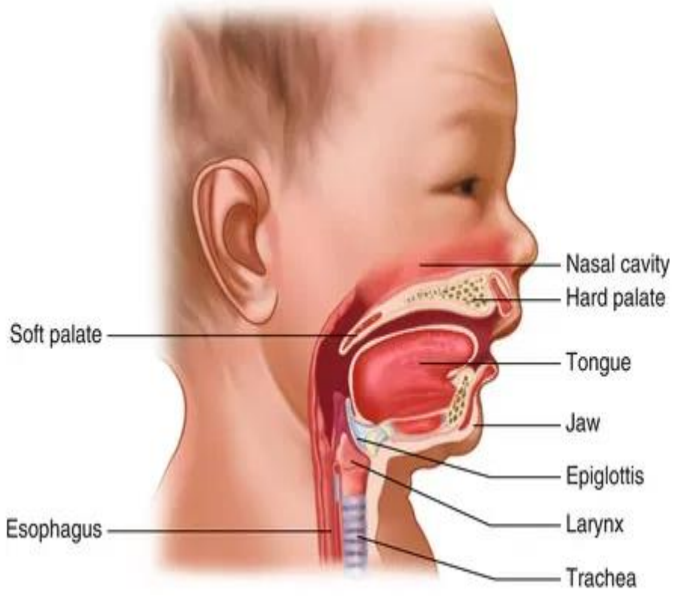
Pacifiers Assessment

Development of a computational methodology capable of predicting the newborn oral cavity behavior during pacifier sucking



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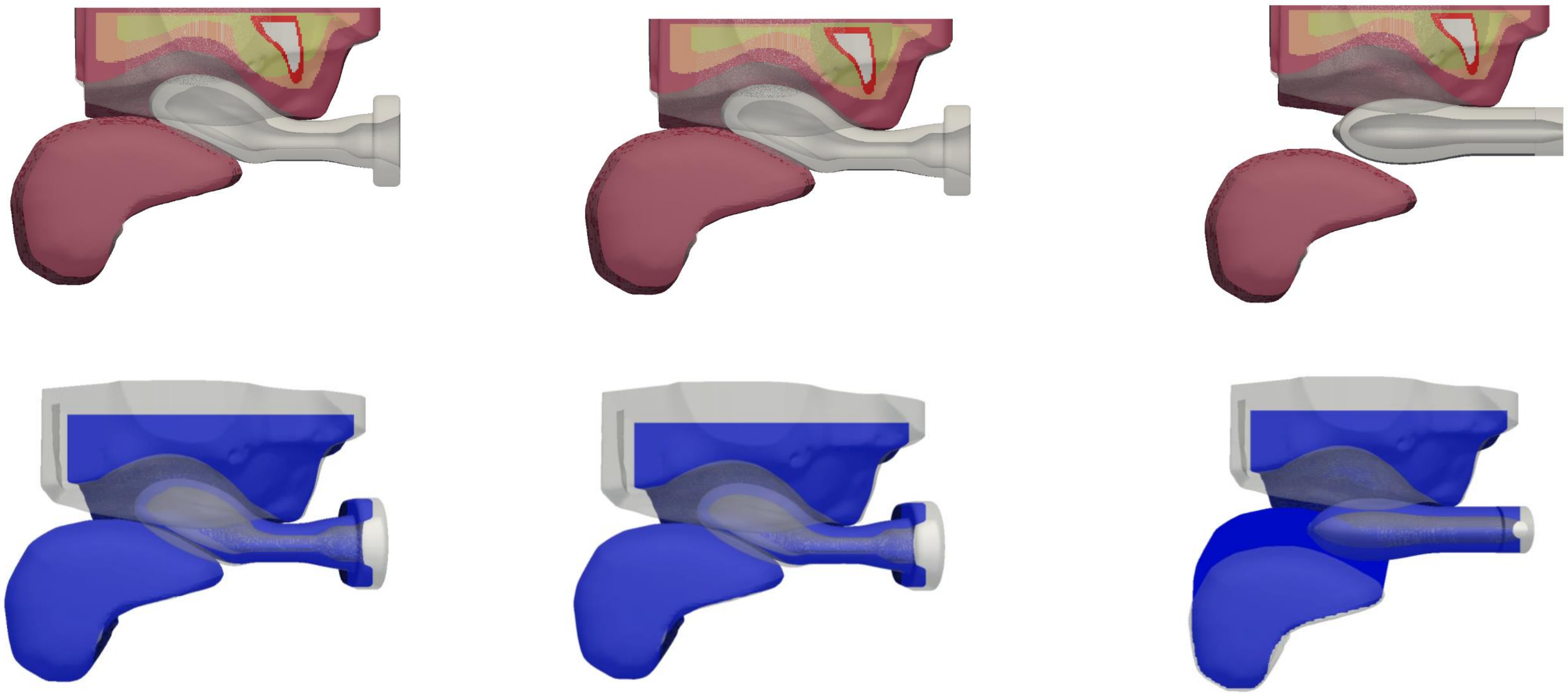
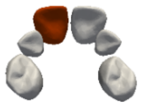
Pacifiers Assessment

NUK Genius Pacifier | NUK Standard Pacifier | Conventional Pacifier

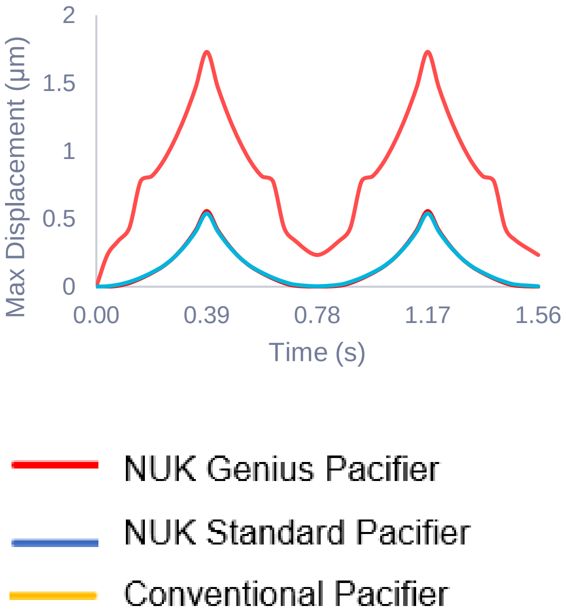


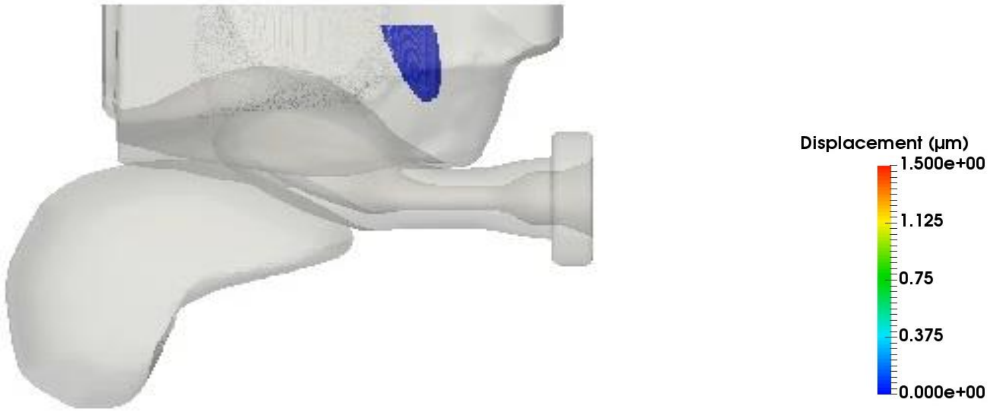
Introduction

Pacifiers Assessment

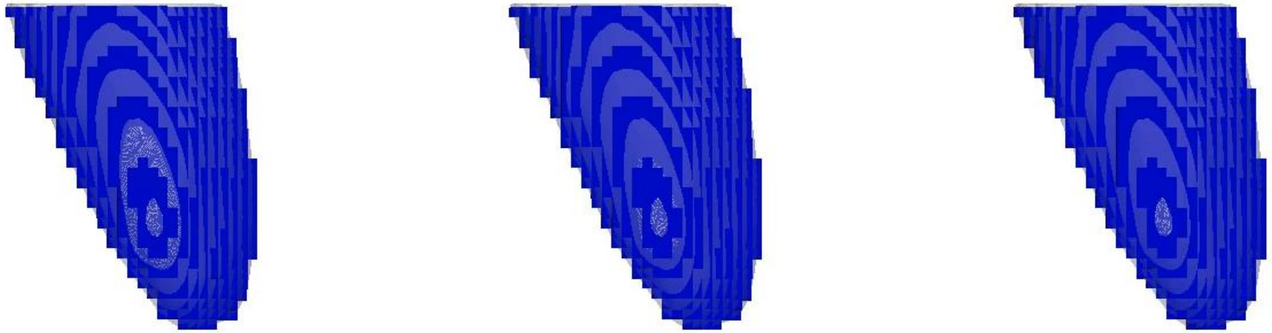


Central Incisor





Conventional Pacifier



Displacement 1000x

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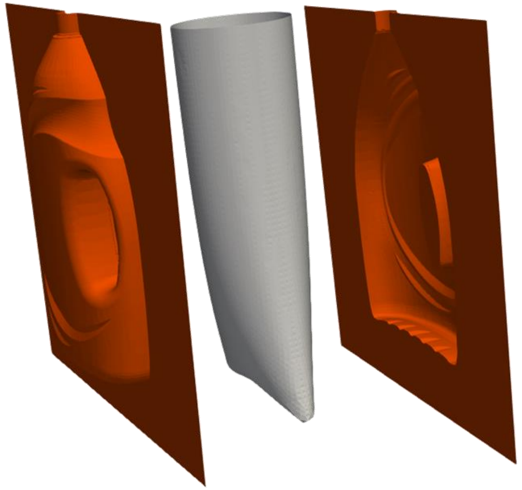
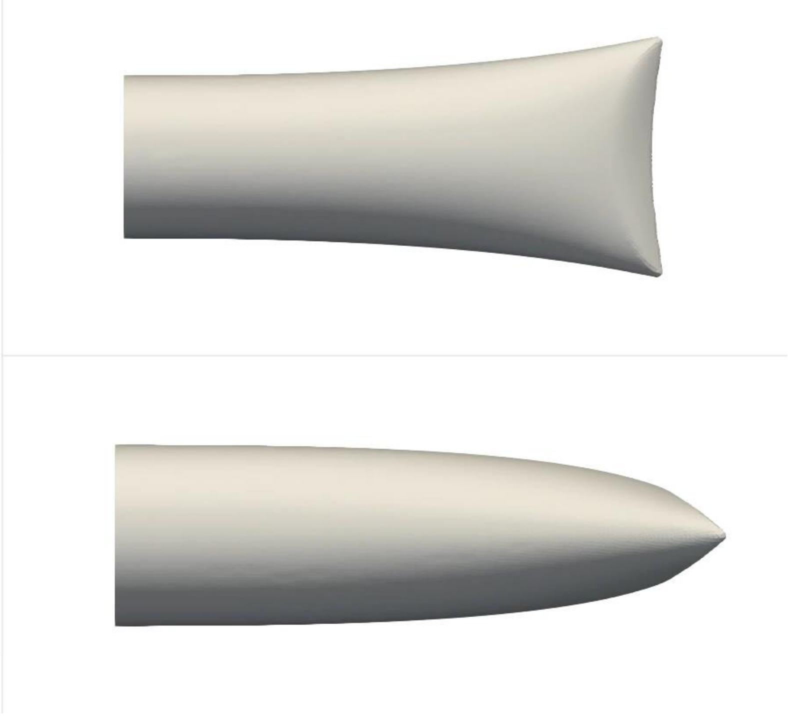
Extrusion Blow Molding Simulator

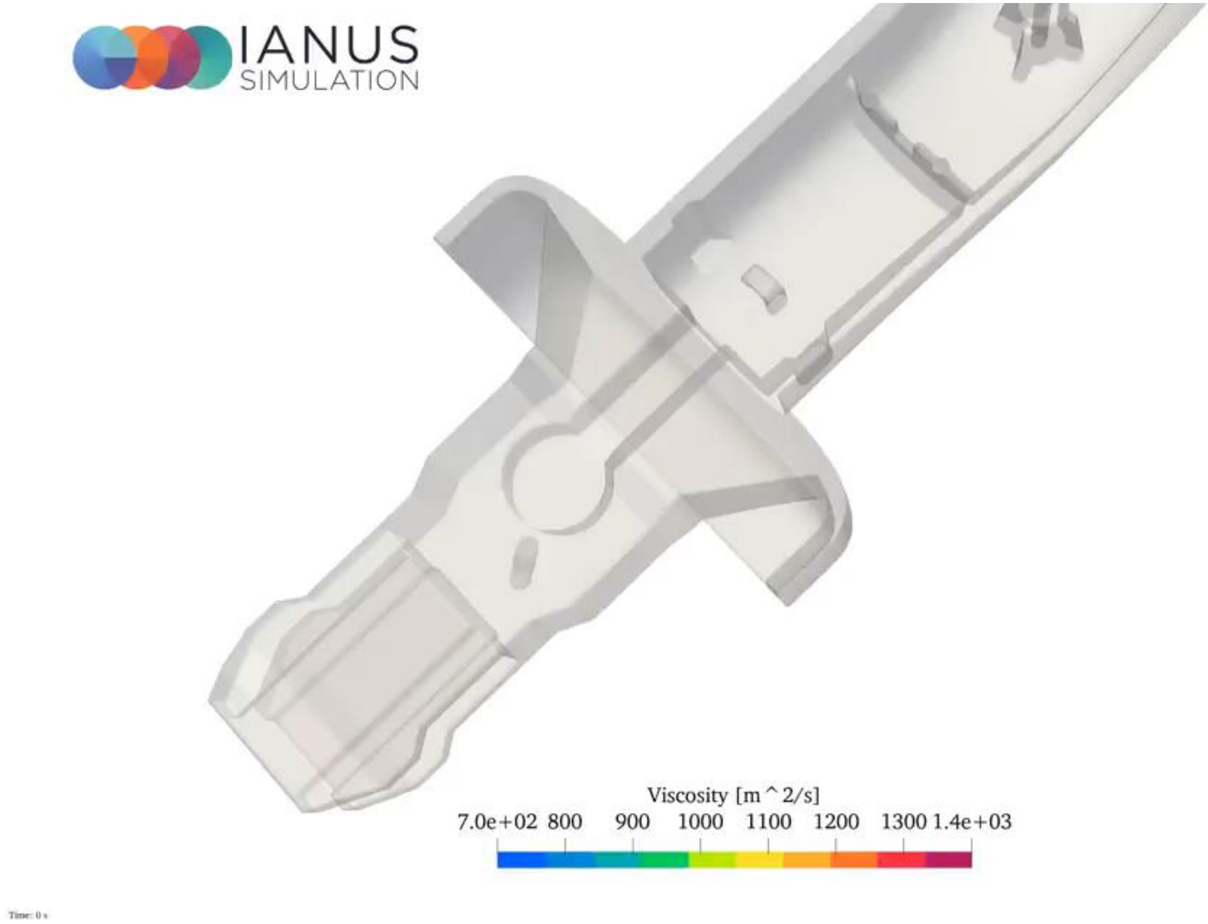
LOGOPLASTE





Introduction

Injection Molding



https://www.linkedin.com/feed/update/urn:li:activity:7187341849596940288/

Computational Modelling

Notation

- Scalars – plain characters - e.g. p, ρ, η_P, λ
- Tensors [ ] , vectors { } or bold characters – e.g. $\mathbf{U}, \boldsymbol{\tau}$
- Nabla (∇) the following differential operator

$$\nabla = \begin{Bmatrix} \dfrac{\partial}{\partial x} \\ \dfrac{\partial}{\partial y} \\ \dfrac{\partial}{\partial z} \end{Bmatrix}$$

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Computational Modelling

Governing Equations

- Continuity

$$\frac{\partial \rho}{\partial t} + \nabla \bullet \left(\rho \mathbf{U} \right) = 0$$

- Momentum

$$\frac{\partial \left(\rho \mathbf{U} \right)}{\partial t} + \nabla \bullet \left(\rho \mathbf{U} \mathbf{U} \right) + \nabla \bullet \left(p \mathbf{I} \right) + \nabla \bullet \boldsymbol{\tau} = 0$$

- Constituive Model (Oldroyd-B)

$$\boldsymbol{\tau} = \boldsymbol{\tau}_S + \boldsymbol{\tau}_P$$

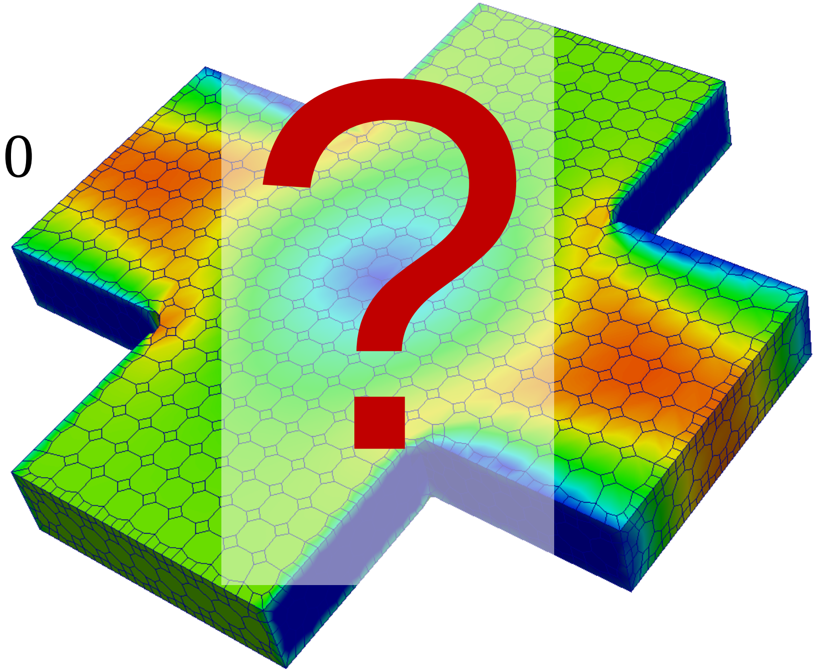
Solvent

$$\boldsymbol{\tau}_S = \eta_S \left(\nabla \mathbf{U} + \left(\nabla \mathbf{U} \right)^{\mathrm{T}} \right)$$

Polymeric

$$\boldsymbol{\tau}_P + \lambda \left(\frac{\partial \boldsymbol{\tau}_P}{\partial t} + \nabla \bullet \left(\mathbf{U} \boldsymbol{\tau}_P \right) \right) = \eta_P \left(\nabla \mathbf{U} + \nabla \mathbf{U}^{\mathrm{T}} \right) + \lambda \left(\boldsymbol{\tau}_P \bullet \nabla \mathbf{U} + \boldsymbol{\tau}_P \bullet \left(\nabla \mathbf{U} \right)^{\mathrm{T}} \right)$$

Velocity magnitude distribution



Computational Modelling

Governing Equations

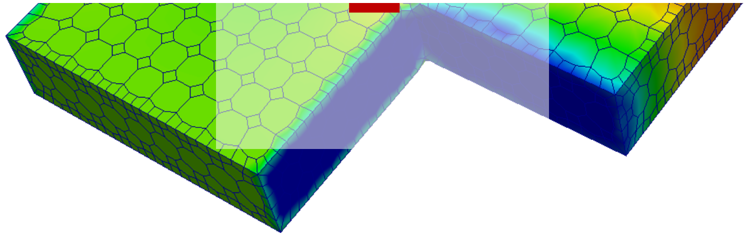
- Continuity

$$\frac{\partial \rho}{\partial t} + \nabla \bullet \left(\rho \mathbf{U} \right) = 0$$

- Momentum

$$\frac{\partial \left(\rho \phi \right)}{\partial t} + \nabla \bullet \left(\rho \mathbf{U} \phi \right) - \nabla \bullet \left(\rho \Gamma_{\phi} \nabla \phi \right) = S_{\phi} \left(\phi \right)$$

Velocity magnitude distribution



Solvent

$$\boldsymbol{\tau}_S = \eta_S \left(\nabla \mathbf{U} + \left(\nabla \mathbf{U} \right)^{\mathrm{T}} \right)$$

Polymeric

$$\boldsymbol{\tau}_P + \lambda \left(\frac{\partial \boldsymbol{\tau}_P}{\partial t} + \nabla \bullet \left(\mathbf{U} \boldsymbol{\tau}_P \right) \right) = \eta_P \left(\nabla \mathbf{U} + \nabla \mathbf{U}^{\mathrm{T}} \right) + \lambda \left(\boldsymbol{\tau}_P \bullet \nabla \mathbf{U} + \boldsymbol{\tau}_P \bullet \left(\nabla \mathbf{U} \right)^{\mathrm{T}} \right)$$

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Computational Modelling

The Standard Governing Equation

$$\underbrace{\frac{\partial(\rho\phi)}{\partial t}}_{\text{Time evolution}} + \underbrace{\nabla\bullet(\rho\mathbf{U}\phi)}_{\text{Advection}} - \underbrace{\nabla\bullet\left(\rho\Gamma_{\phi}\nabla\phi\right)}_{\text{Diffusion}} = \underbrace{S_{\phi}(\phi)}_{\text{Source}}$$

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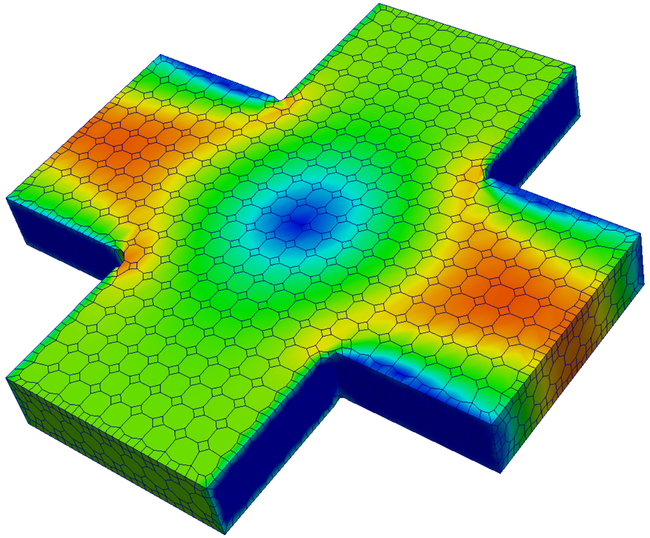
Computational Modelling

The Standard Governing Equation

$$\underbrace{\frac{\partial(\rho\phi)}{\partial t}}_{\text{Time evolution}} + \underbrace{\nabla\bullet(\rho\mathbf{U}\phi)}_{\text{Advection}} - \underbrace{\nabla\bullet(\rho\Gamma_\phi\nabla\phi)}_{\text{Diffusion}} = \underbrace{S_\phi(\phi)}_{\text{Source}}$$

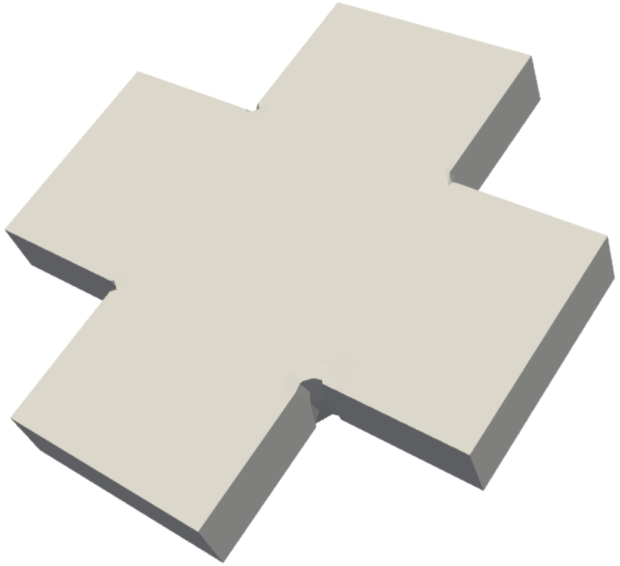
?



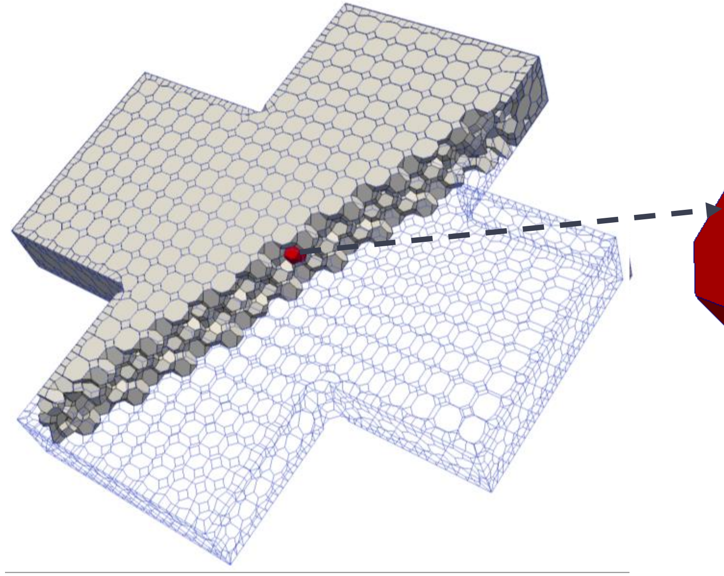
Computational Modelling

The Finite Volume Method

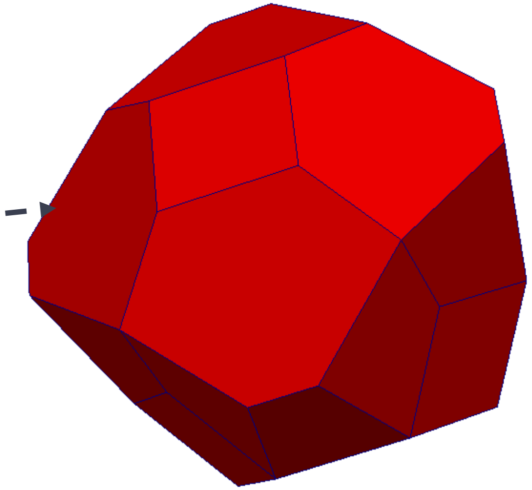
$$\frac{\partial(\rho\phi)}{\partial t} + \nabla\bullet(\rho\mathbf{U}\phi) - \nabla\bullet\left(\rho\Gamma_{\phi}\nabla\phi\right) = S_{\phi}(\phi)$$



Geometry



Mesh



Cell

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Computational Modelling

The Finite Volume Method

$$\frac{\partial(\rho\phi)}{\partial t}+\nabla\bullet(\rho\mathbf{U}\phi)-\nabla\bullet\left(\rho\Gamma_{\phi}\nabla\phi\right)=S_{\phi}(\phi)$$

$$\begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1N} \\ a_{21} & a_{21} & \cdots & a_{21} \\ \cdots & \cdots & \cdots & \cdots \\ a_{N1} & a_{N2} & \cdots & a_{NN} \end{bmatrix}\begin{Bmatrix} \phi_1 \\ \phi_2 \\ \cdots \\ \phi_N \end{Bmatrix}=\begin{Bmatrix} b_1 \\ b_2 \\ \cdots \\ b_N \end{Bmatrix}$$

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Computational Modelling

The Finite Volume Method

$$\frac{\partial(\rho\phi)}{\partial t} + \nabla\bullet(\rho\mathbf{U}\phi) - \nabla\bullet(\rho\Gamma_\phi\nabla\phi) = S_\phi(\phi)$$

$$\begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1N} \\ a_{21} & & & \\ \cdots & & & \\ a_{N1} & a_{N2} & \cdots & a_{NN} \end{bmatrix} \begin{Bmatrix} \phi_1 \\ \\ \\ \phi_N \end{Bmatrix} = \begin{Bmatrix} b_1 \\ \\ \\ b_N \end{Bmatrix}$$

$$[A]\{\phi\} = \{b\}$$

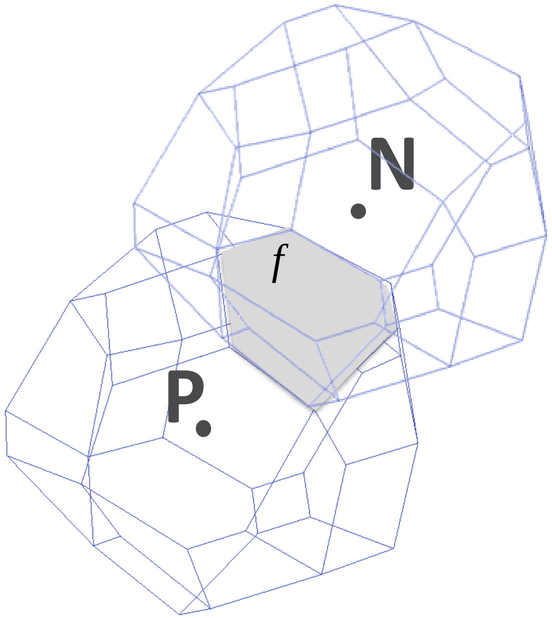
The Finite Volume Method

$$\frac{\partial(\rho\phi)}{\partial t} + \nabla\bullet(\rho\mathbf{U}\phi) - \boxed{\nabla\bullet(\rho\Gamma_\phi\nabla\phi)} = S_\phi(\phi)$$

Discretization (fvSchemes)

$$\frac{\phi_N - \phi_P}{|\boldsymbol{d}|} = \boxed{\frac{-1}{|\boldsymbol{d}|}}\phi_P + \boxed{\frac{1}{|\boldsymbol{d}|}}\phi_N$$

Add to P cell equation



Cell P and N share face *f*

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Computational Modelling

System of Equations

Solve the system(s) of equations (fvSolution)

$$[A]\{\phi\} = \{b\}$$

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System of Equations

Solve the system(s) of equations (fvSolution)

$$[A]\{\phi\} = \{b\}$$

- Direct Solvers
- Iterative Solvers

Computational Modelling

System of Equations – Iterative Solvers

$$[A]\{\phi\}-\{b\}=\{R\}$$

- $|\boldsymbol{R}|$ quantifies the error of the current solution

  - Relative tolerance
  - Absolute Tolerance

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Linux/OpenFOAM - Memory Aid

General

- ❑ WSL App ## Open Ubuntu Terminal
- ❑ ParaView App ## open Paraview for post processing
- ❑ right mouse button ## paste clipboard contents in command line
- ❑ tab key ## complete commands
- ❑ Ctrl+R ## Repeat previous Commands
- ❑ Arrow up or down ## Browse by previous commands
- ❑ >> code . ## open VSCode in the current folder
- ❑ >> shopt -s direxpand #allow tab in WSL
- ❑ >> explorer . ## Open the current folder in windows explorer

Linux

- ❑ >> cd <name> ## Change to directory <name>
- ❑ >> cd .. ## Change to previous folder
- ❑ >> cd ## Change to home folder
- ❑ >> pwd ## print current (working) directory
- ❑ >> rm <file> ## remove file named <file>
- ❑ >> rm –rf <folder> ## remove folder named <folder>
- ❑ >> chmod +x <file> ## make the <file> executable
- ❑ >> touch x.foam ## create empty file named x.foam

OpenFOAM

- ❑ >> openfoam2206 ## load OpenFOAM variables
- ❑ $FOAM_TUTORIALS ## Folder for tutorial cases
- ❑ $FOAM_RUN ## folder to run cases
- ❑ >> tut ## change to tutorial folder
- ❑ >> run ## change to run folder
- ❑ >> <solverName> ## run solver named <solverName>
- ❑ >> <solverName> > log & ## run solver named <solverName> in background and send output to log file

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OpenFOAM 1st case study

1. Open WSL
2. Load OpenFOAM variables
3. >> run
4. >> wget https://github.com/Computational-Rheology/PPS2024_OFCourse/raw/main/2-CaseFiles/CaseFiles.zip
5. >> unzip CaseFiles.zip
6. >> cd case 11
7. >> code .
8. Check the case structure with the instructor, in folders *0*, *constant* and *system*

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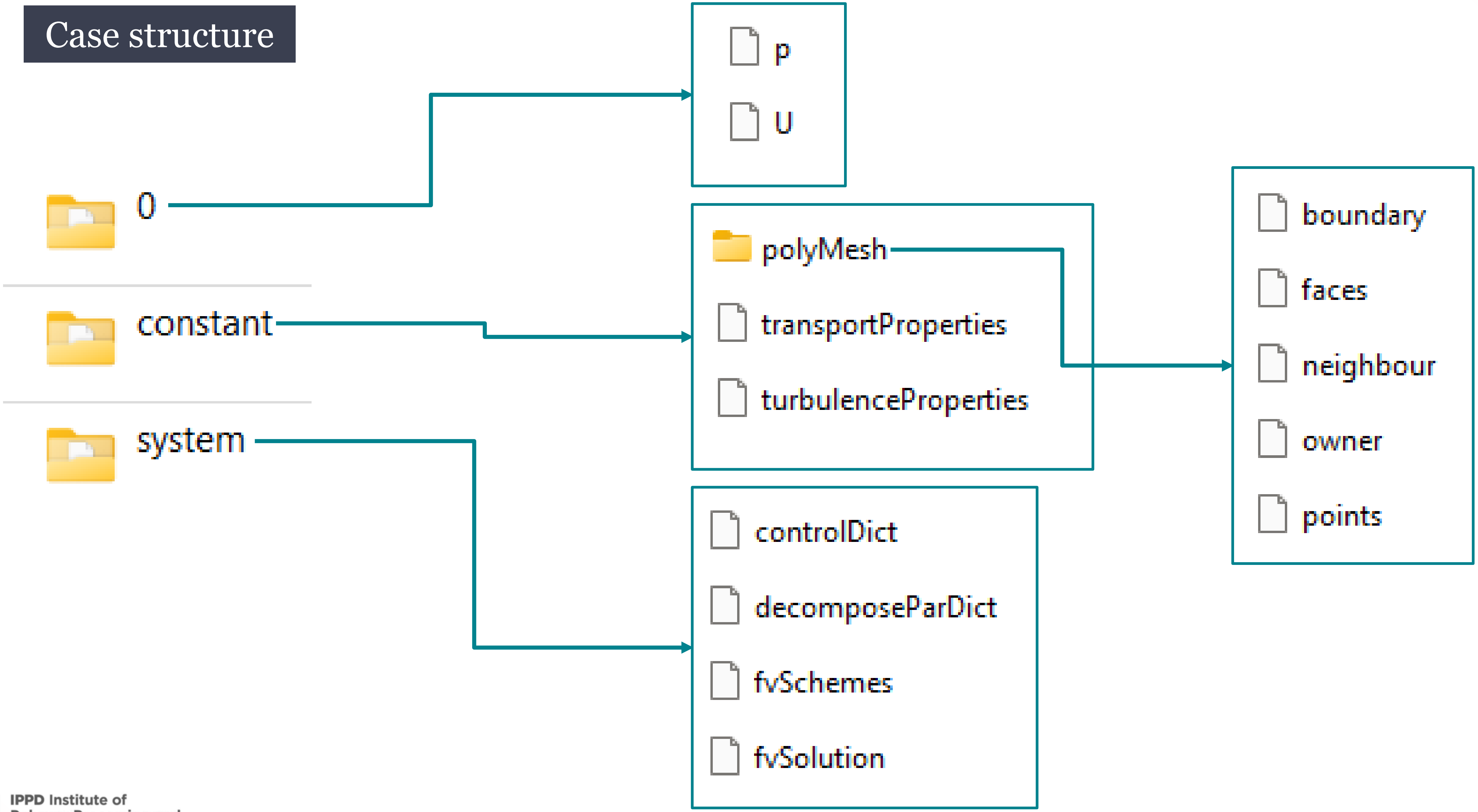
OpenFOAM 1st case study

Case structure



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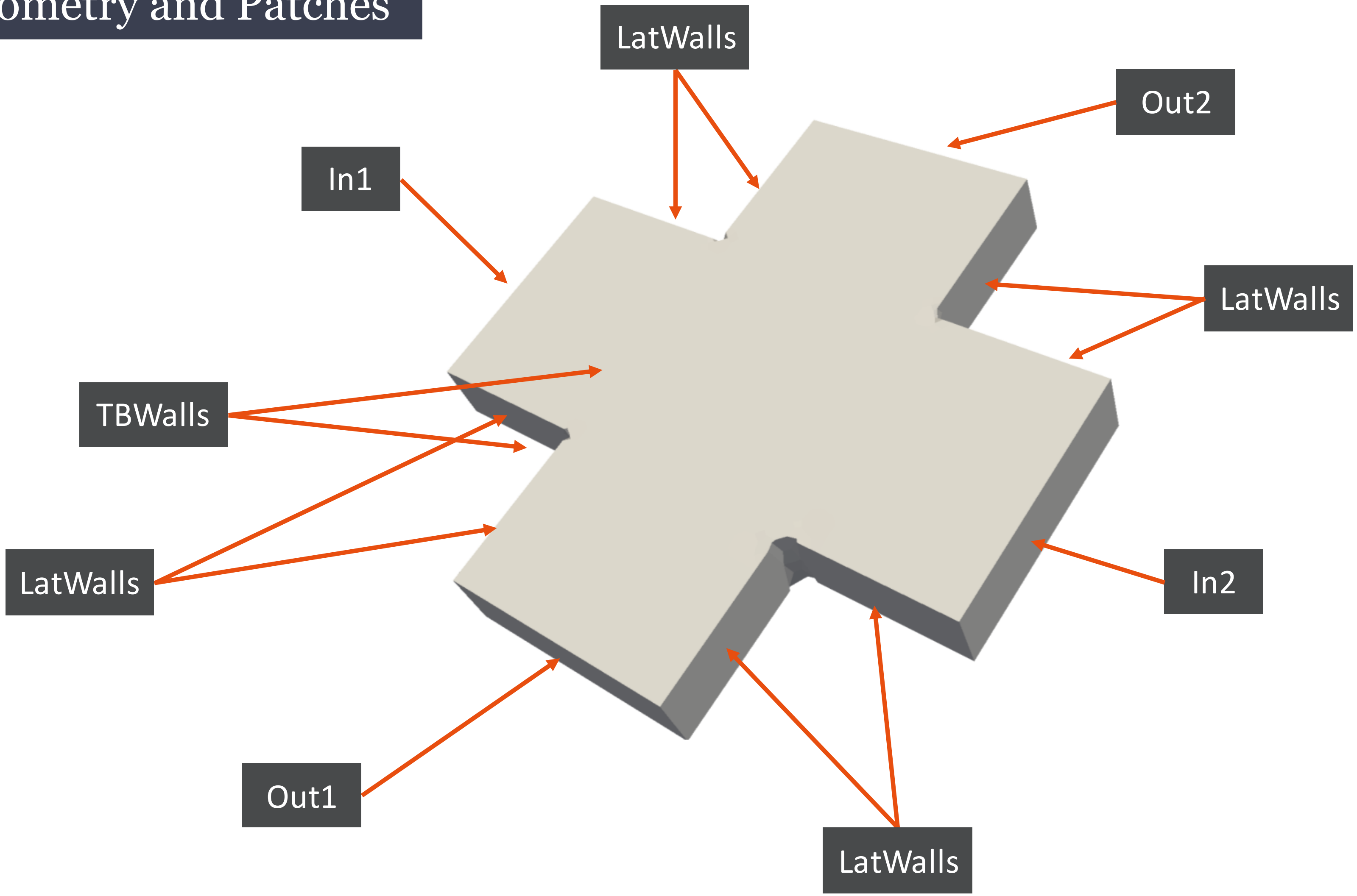
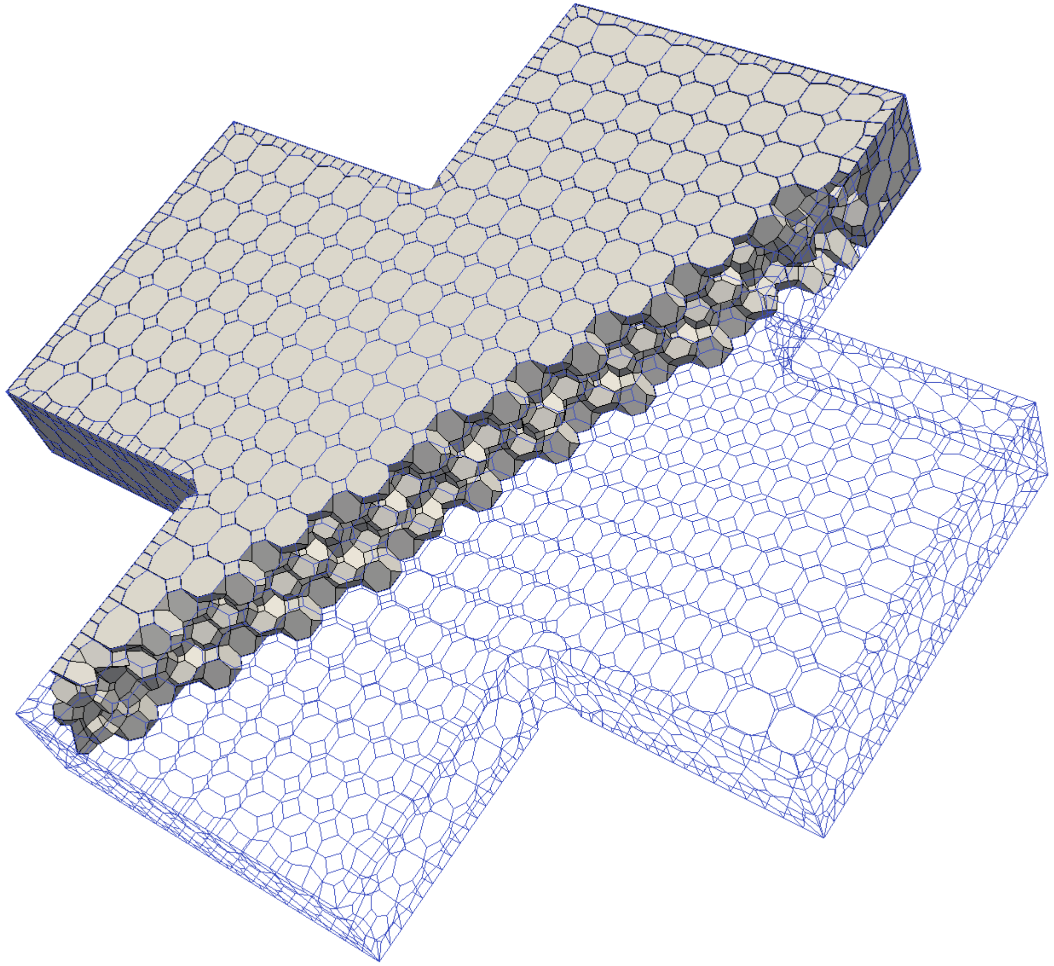
OpenFOAM 1st case study

Geometry and Patches



OpenFOAM 1st case study

Mesh



Session P2

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30 Sept.-03 Oct. | Ferrol - Spain
CRheo@IPC
iPC
JKU IPPD Institute of Polymer Processing and Digital Transformation

OpenFOAM 1st case study

File 0/U

```
………….
dimensions      [0 1 -1 0 0 0 0];

internalField   uniform (0 0 0);

boundaryField
{

    In1
    {
        type            fixedValue;
        value           uniform (0.01 0 0);
    }

    In2
    {
        type            fixedValue;
        value           uniform (-0.01 0 0);
    }

    Out1
    {
        type            zeroGradient;
    }

    ……..
```

No.	Property
1	Mass
2	Length
3	Time
4	Temperature
5	Quantity
6	Current
7	Luminous intensity

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OpenFOAM 1st case study

File 0/p

```
.....

boundaryField
{
    In1
    {
        type            zeroGradient;
    }

    In2
    {
        type            zeroGradient;
    }

    Out1
    {
        type            fixedValue;
        value            uniform 0;
    }

    .......
```

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File constant/transportProperties

```
.....

transportModel  Newtonian;

nu              nu [0 2 -1 0 0 0 0] 1e-05;
.......
```

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File system/controlDict

```
......
application simpleFoam;

startFrom       startTime;

startTime       0;

stopAt          endTime;

endTime         1000;

deltaT          1;

writeControl    timeStep;

writeInterval   500;

purgeWrite      0;

.......
```

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File system/fvSchemes

```
ddtSchemes
{
    default         steadyState;
}

gradSchemes
{
    default         Gauss linear;
}

divSchemes
{
    default         none;
    div(phi,U)      bounded Gauss linearUpwind grad(U);
    …
    div((nuEff*dev2(T(grad(U))))) Gauss linear;
    div(nonlinearStress) Gauss linear;
}

laplacianSchemes
{
    default         Gauss linear corrected;
}
….
```

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File system/fvSolution

```
….
solvers
{
    p
    {
        solver         GAMG;
        tolerance      1e-07;
        relTol         0.1;
        smoother       GaussSeidel;
    }
….
SIMPLE
{
    nNonOrthogonalCorrectors 2;
    consistent      yes;

    residualControl
    {
        p              1e-6;
        U              1e-6;
        "(k|epsilon|omega|f|v2)" 1e-6;
    }
}
…..
```

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1. >> simpleFoam #run the solver and output screen
2. >> rm –rf 112 #remove the lastTime results folder
3. >> simpleFoam >log.simpleFoam #run the solver and output to log.simpleFoam file
4. >> rm –rf 112 #remove the lastTime results folder
5. >> simpleFoam >log.simpleFoam & #run the solver in background and output to log.simpleFoam file
6. Check the contents of the logfile with the instructor

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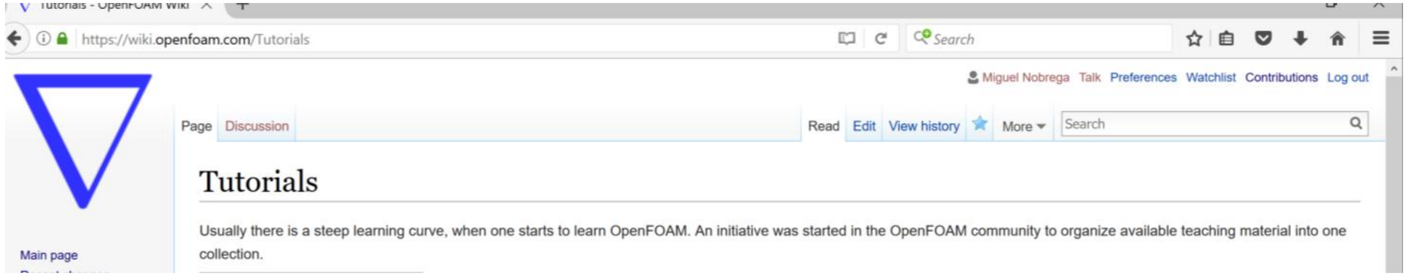
1. >> touch x.foam
2. >> explorer.exe .
3. Open *x.foam* file with paraview
4. Visualize the results
   a) Show/hide mesh
   b) FV results or interpolated
   c) Rescale color map
   d) Show/hide interior cells and patches
   e) Stream tracer (source line and point cloud)
   f) Contour, clip, slice, threshold and glyph
5. Adapt the velocity boundary conditions
6. Visualize the results in paraview

OpenFOAM 1st case study

1. Check the contents of the file system/decomposeParDict with the instructor
2. The banana trick
3. >> decomposePar
4. Use the scotch method to decompose
5. >> mpirun -np 4 simpleFoam -parallel > log.simpleFoamP
6. >> simpleFoam > log.simpleFoam
7. Compare the execution time of both runs

Where to get more information?

OpenFOAM Wiki - wiki.openfoam.com



OpenFOAM Journal

journal.openfoam.com / youTube @openfoamjournal6606

FOAM@Iberia 2023 – November 2-3, 2023 – Guimarães, Portugal

https://2023.foam-iberia.eu/

FOAM@Iberia 2024 – October 3-4, 2024 – Ferrol, Spain

www.foam-Iberia.eu

OpenFOAM Workshop 2025 – ????? – ??????, Europe

www.openfoamworkshop.org