

Computational
Rheology
@IPC

Computational Rheology with OpenFOAM®: From Code Development to Industrial Application

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University of Minho
School of Engineering

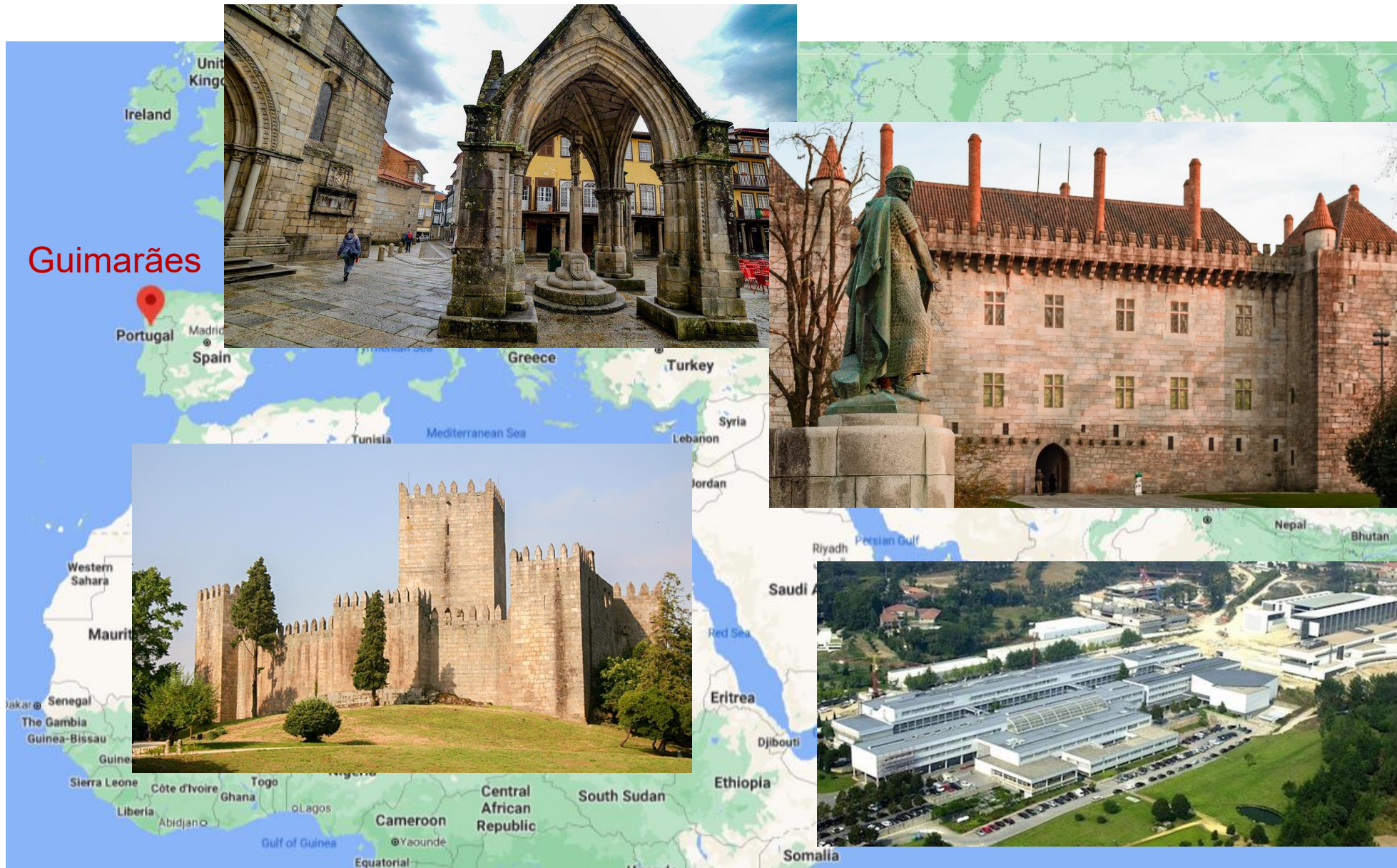


IPC – Institute for Polymers and Composites



PIEP - Pole for Innovation in Polymer Engineering

Guimarães / Portugal



- The OpenFOAM® Computational Library
- Industrial Applications
 - Design of profile extrusion dies
 - Extrusion Blow Molding
 - Injection Molding
 - Footwear Components/Soles
 - Pacifiers
- Solvers/Numerical Developments
 - Integral Viscoelastic Solver
 - Improved Both Sides Diffusion (iBSD)
 - Fiber Orientation
- Recent Works
- Conclusion

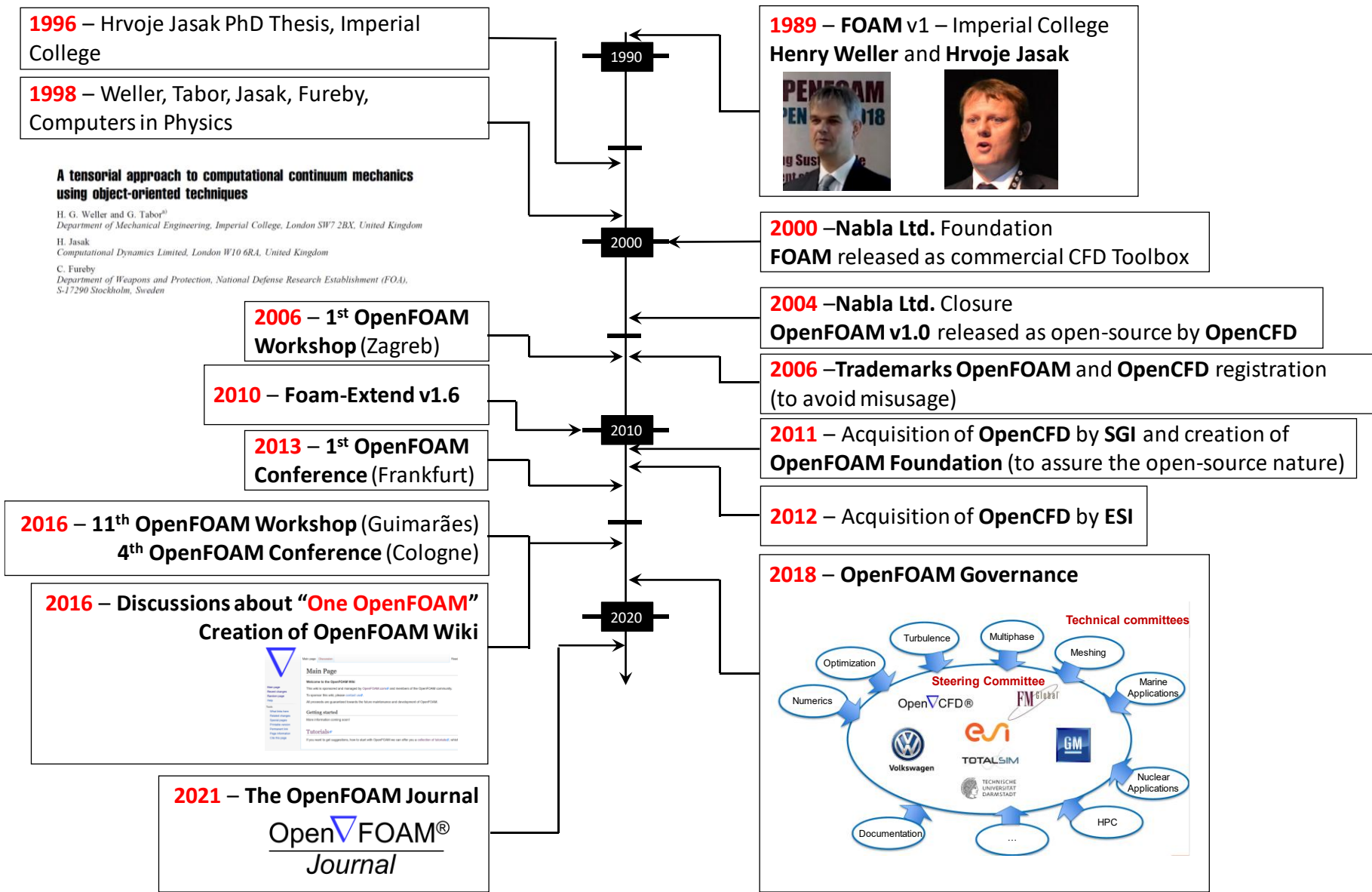


OpenFOAM

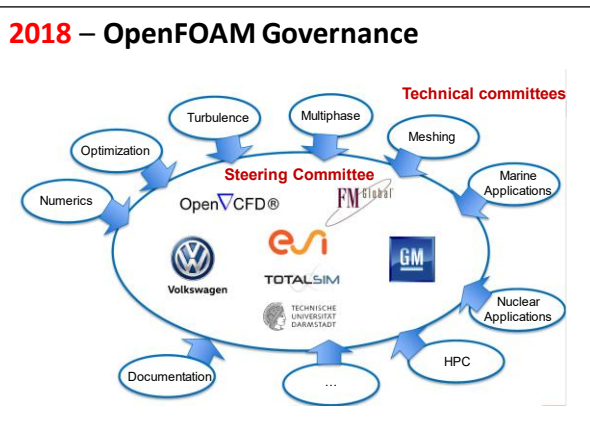
- **Open** source **Field Operation **And Manipulation****
 - C++ Computational Library, Finite Volume Method, Unstructured meshes (and mesh generators)
 - Multiphysics and Multiphase systems (FSI, Eulerian-Eulerian, Eulerian-Lagrangian)
 - Parallelized
 - Several **pre-compiled** solvers available
- '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
 - ...

The OpenFOAM® Computational Library

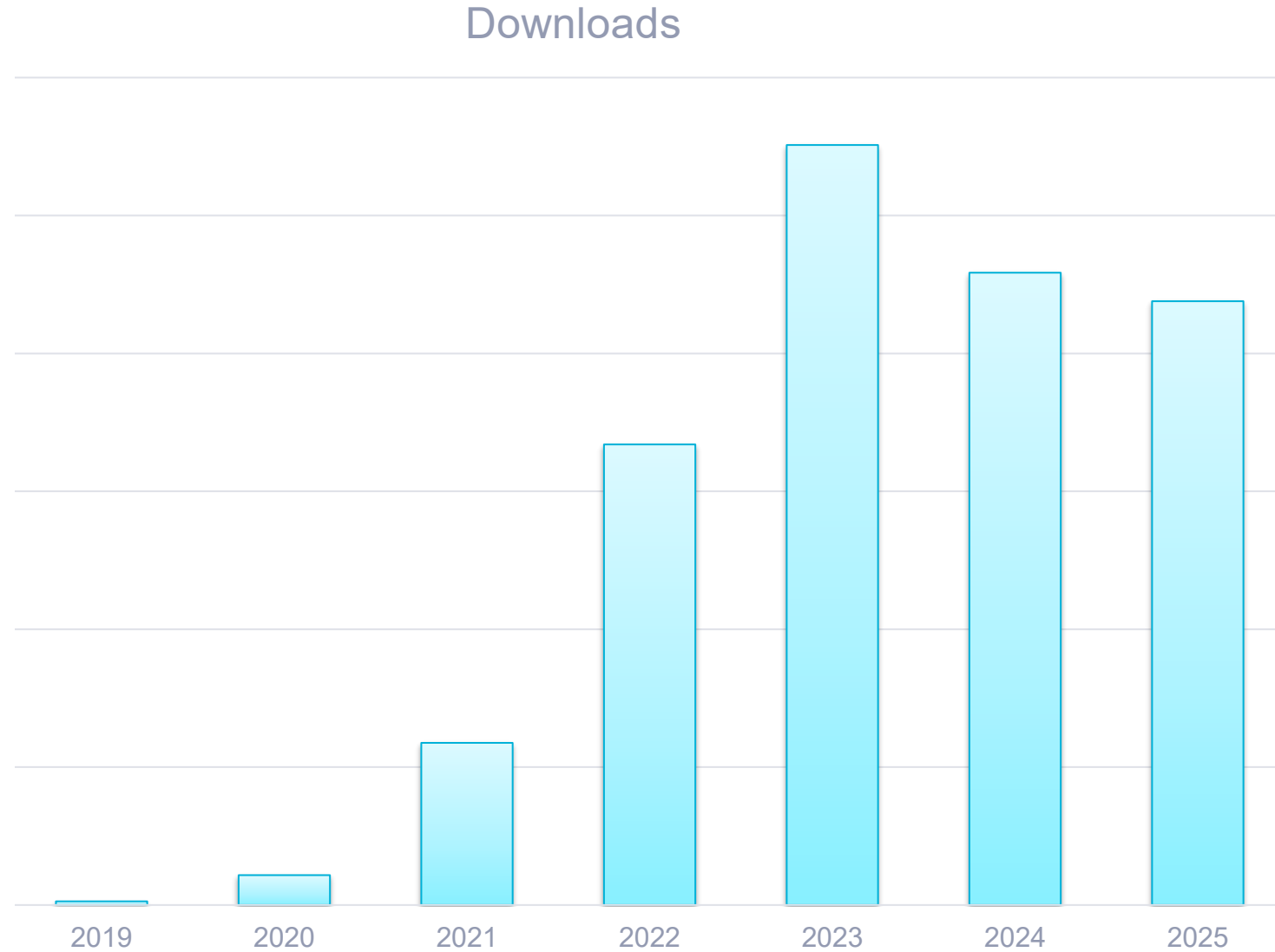
A (very) brief history...



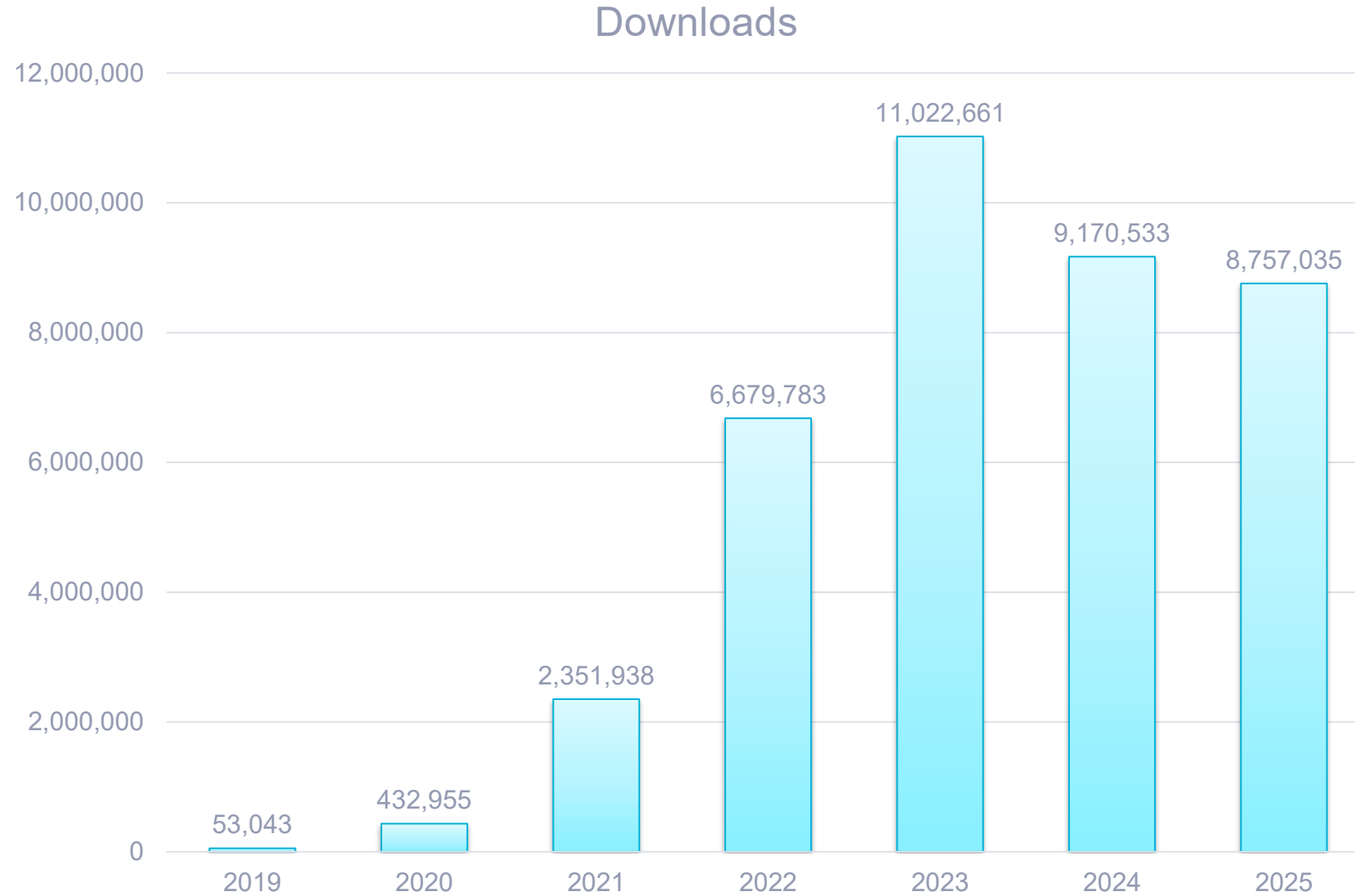
A tensorial approach to computational continuum mechanics using object-oriented techniques
 H. G. Weller and G. Tabor¹
 Department of Mechanical Engineering, Imperial College, London SW7 2BX, United Kingdom
 H. Jasak
 Computational Dynamics Limited, London W10 6RA, United Kingdom
 C. Fureby
 Department of Weapons and Protection, National Defense Research Establishment (FOA), S-17290 Stockholm, Sweden



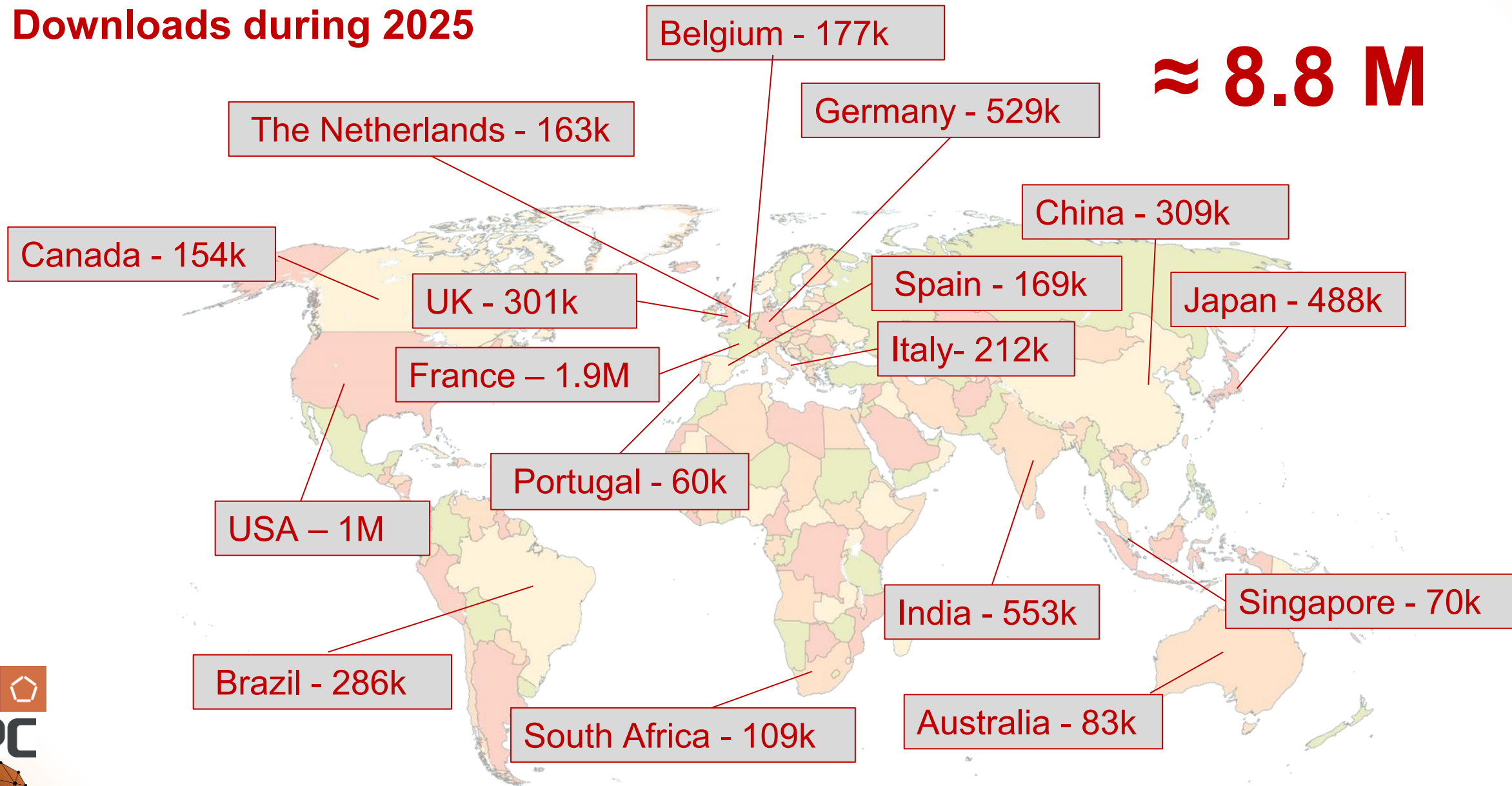
Downloads 2019-2025



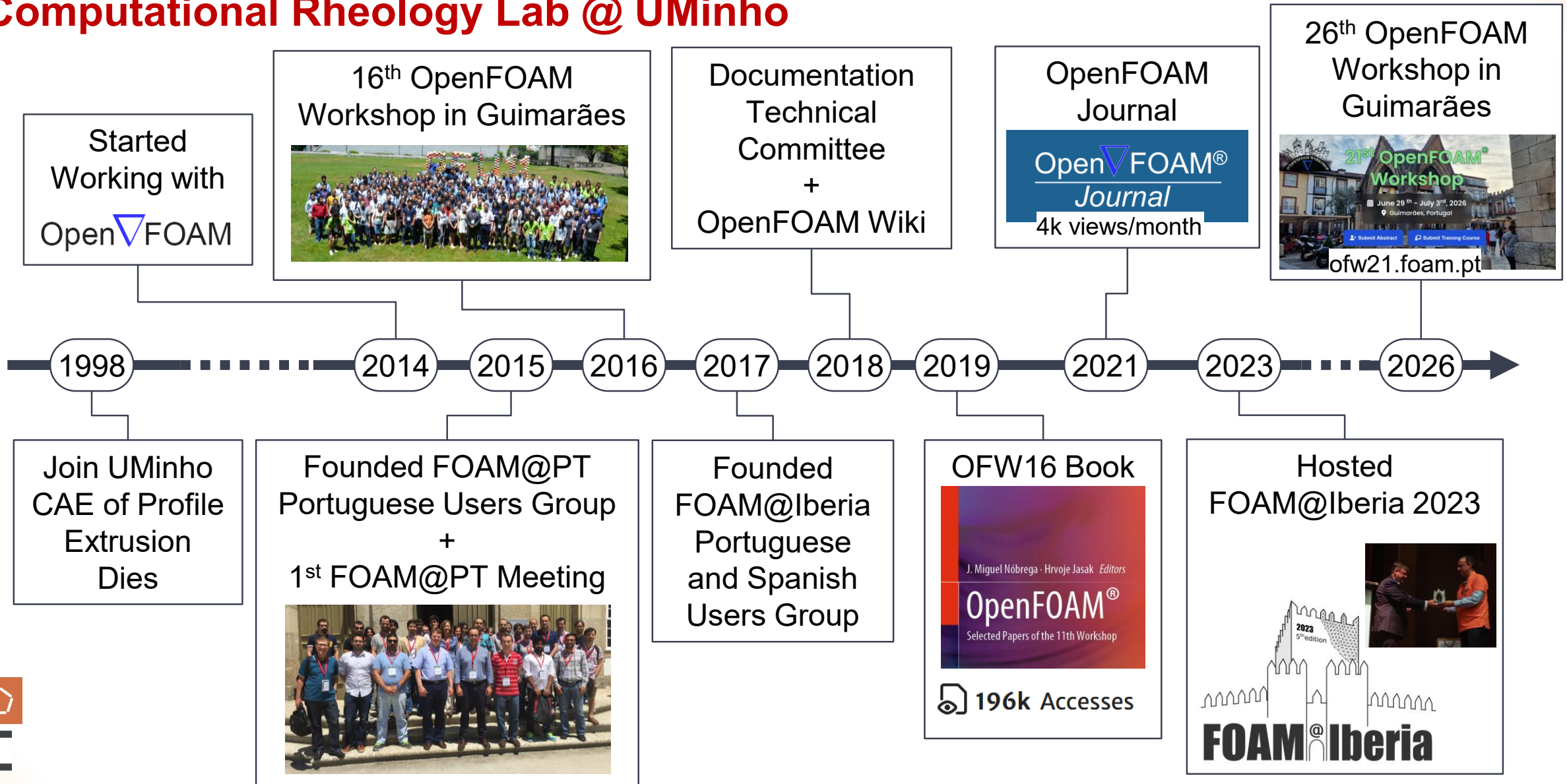
Downloads 2019-2025



Downloads during 2025



Computational Rheology Lab @ UMinho

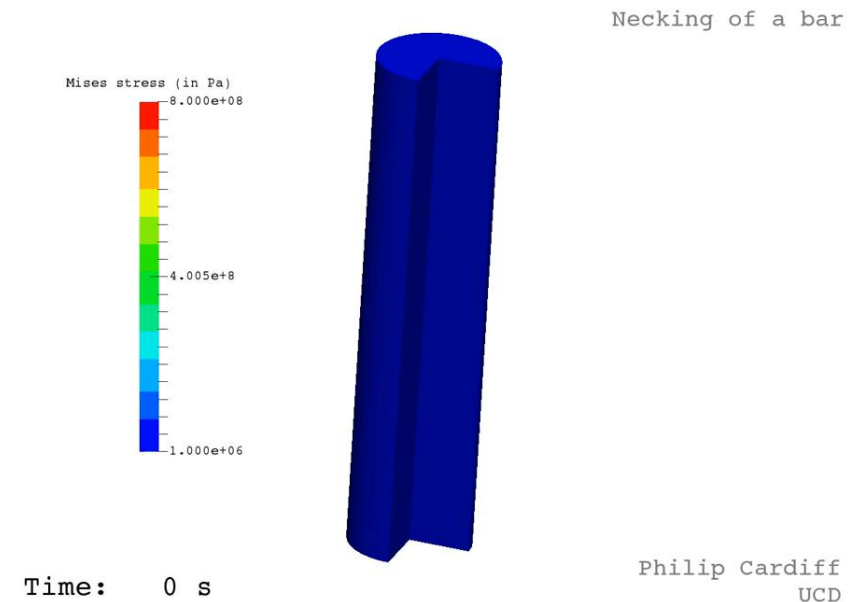




Fluid Dynamics



Solid Mechanics



Necking of a bar

Fluidized Bed (Eulerian+Lagrangian)

From Philip Cardiff's Youtube channel - <https://tinyurl.com/pcardiff>



Equation mimicking

$$\rho \frac{\partial \mathbf{U}}{\partial t} + \nabla \cdot (\rho \mathbf{U} \mathbf{U}) - \mu \nabla^2 \mathbf{U} = -\nabla p$$

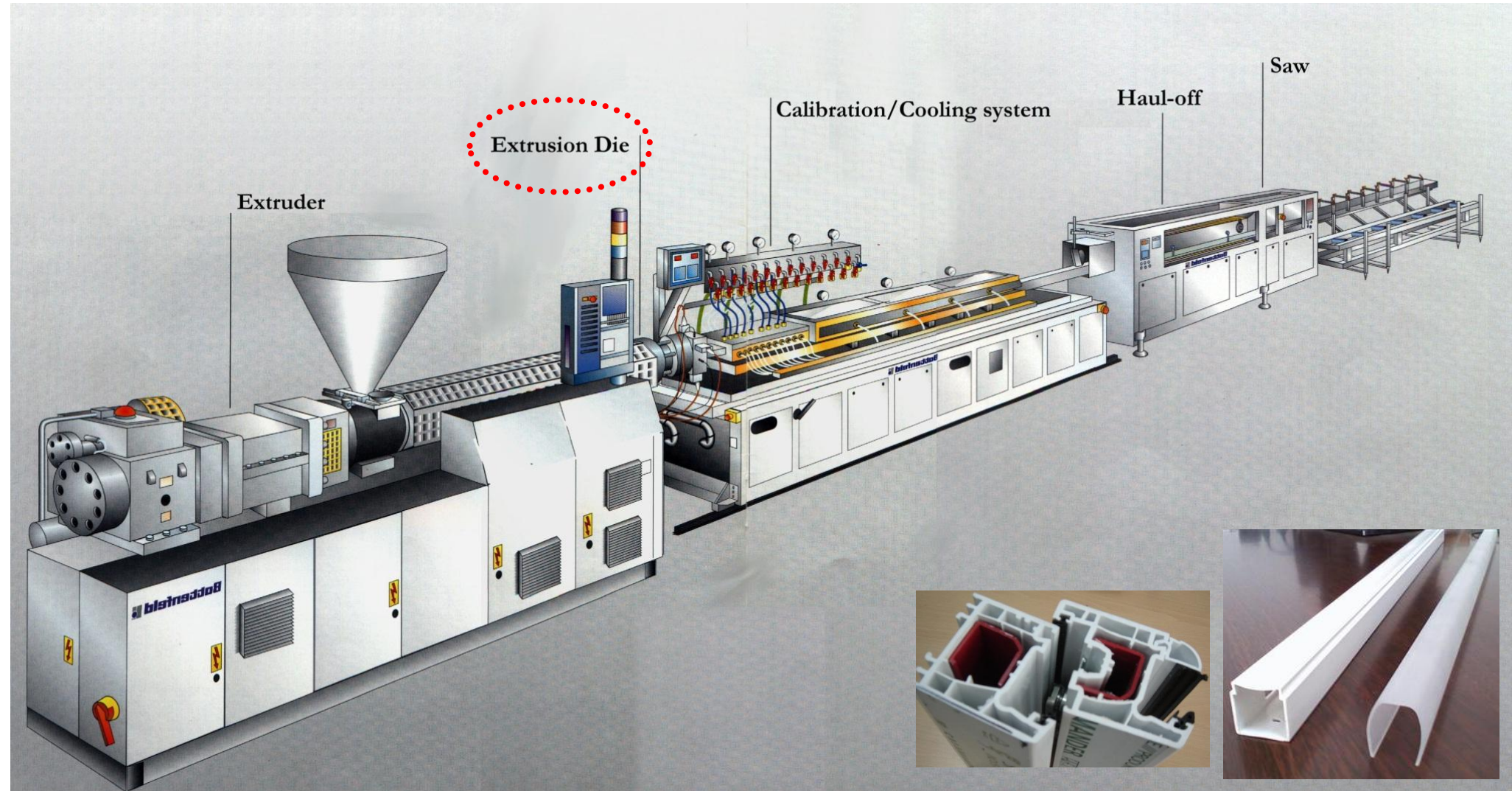
solve

```
(  
    fvm::ddt(rho,U) + fvm::div(phi,U) - fvm::laplacian(mu,U) == -fvc::grad(p)  
);
```

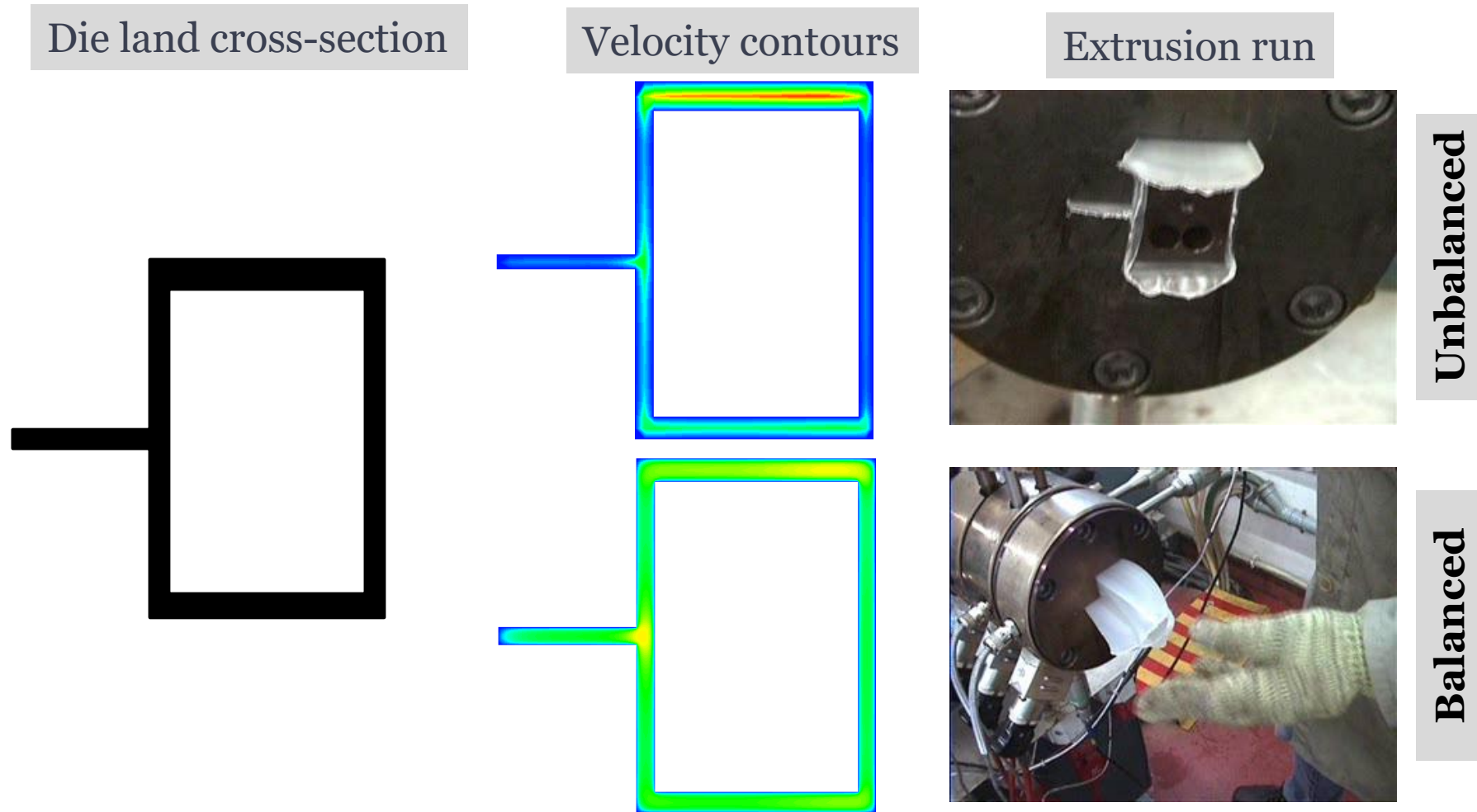


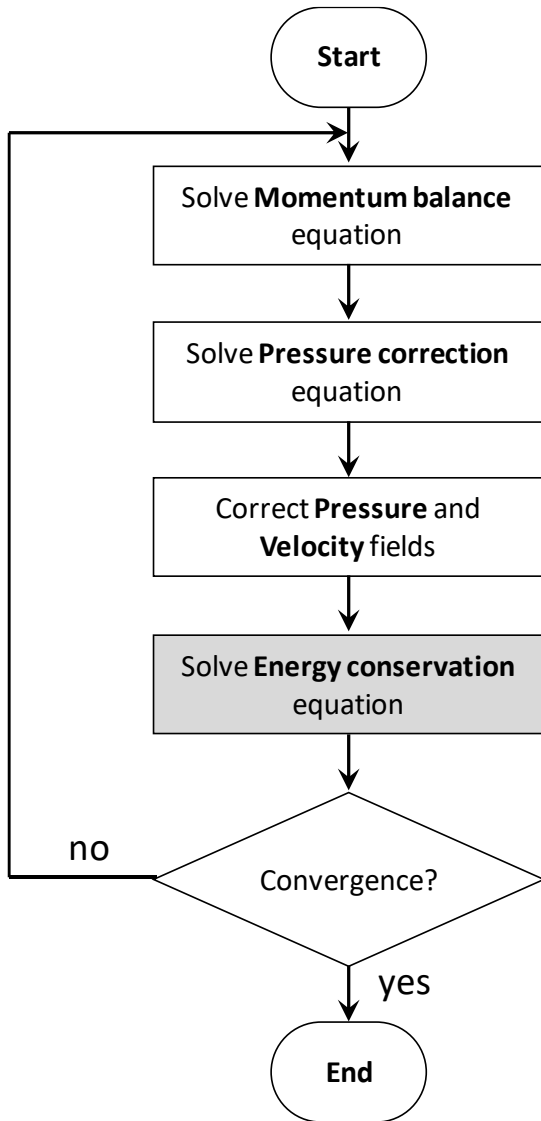
Industrial Applications (IA)





Flow Balance





Methodology Employed

Energy conservation equation (Steady State)

$$\nabla \cdot (UT) - \nabla \cdot \left(\frac{k}{\rho c_p} \nabla T \right) = \frac{1}{\rho c_p} \tau : \nabla U$$

OpenFOAM Code

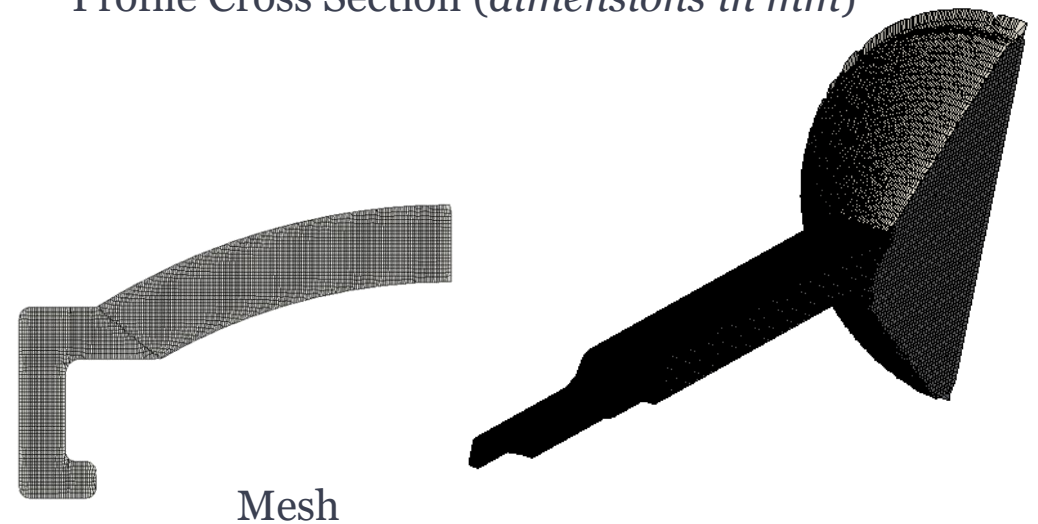
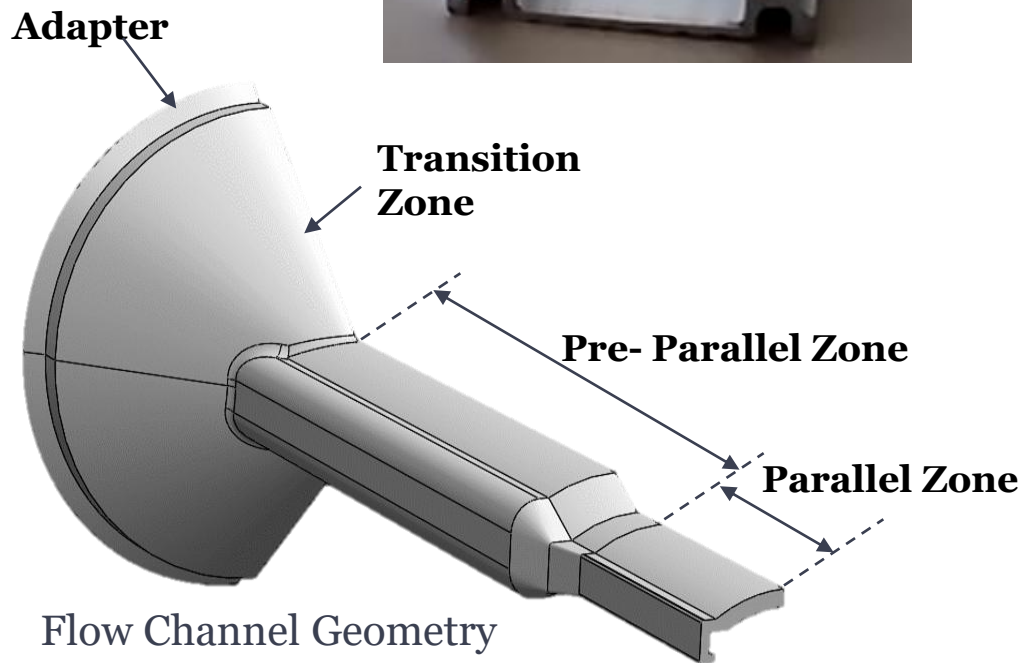
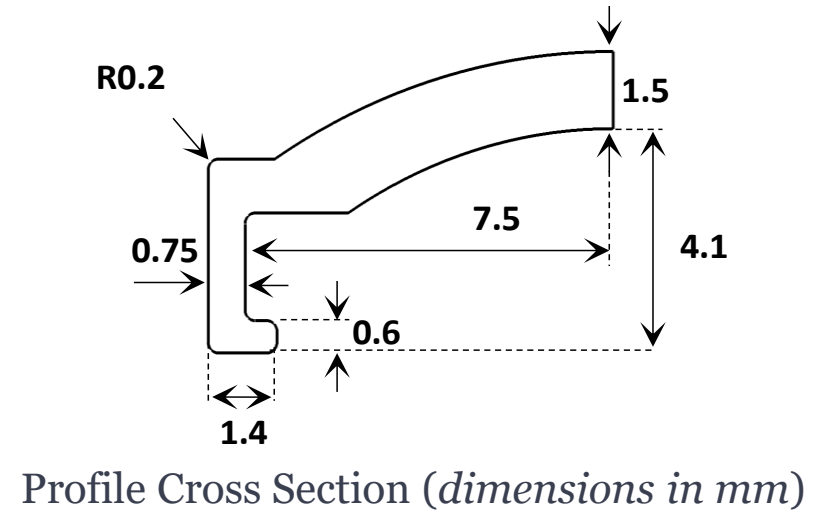
```

Solve
(
    fvm :: div (phi , T)
    - fvm :: laplacian (DT , T)
    == (1 / c_p) * (tau && grad U)
)
  
```





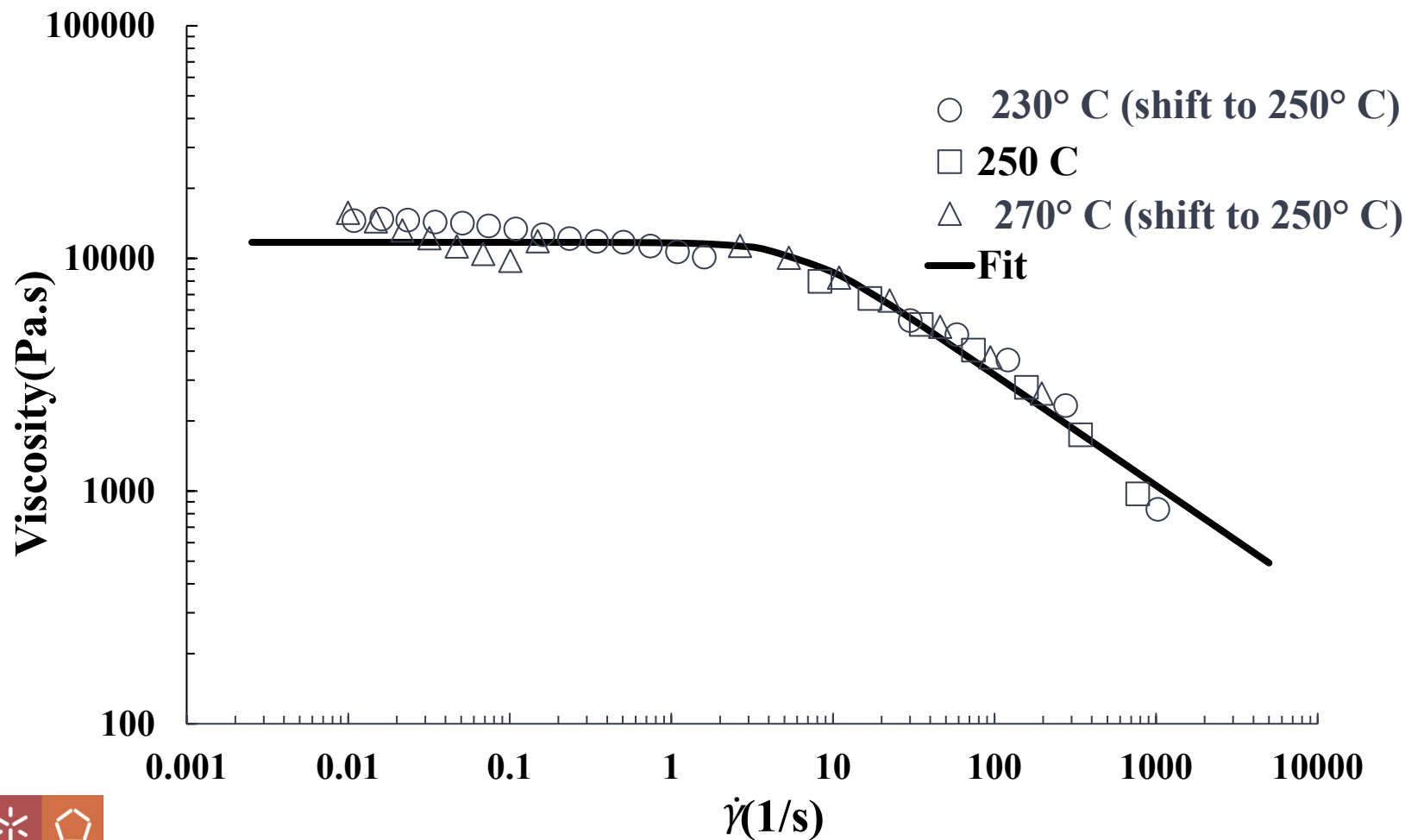
Case Study



A Rajkumar et al., An Open-source framework for the CAD of Complex Profile Extrusion Dies, International Polymer Processing, 33, 2018



Material characterization



**PC extrusion grade
(TRIREX 3027U(M1))**

Bird Carreau + Arrhenius Law

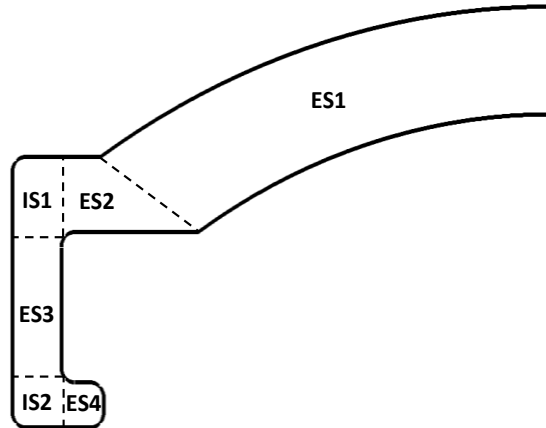
$$\eta(\dot{\gamma}, T) = a_T \eta_\infty + \frac{a_T (\eta_0 - \eta_\infty)}{\left(1 + (a_T \lambda \dot{\gamma})^2\right)^{\frac{1-n}{2}}}$$

Shift Factor

$$a_T = \exp\left(\frac{E}{R} \left(\frac{1}{T} - \frac{1}{T_0}\right)\right)$$

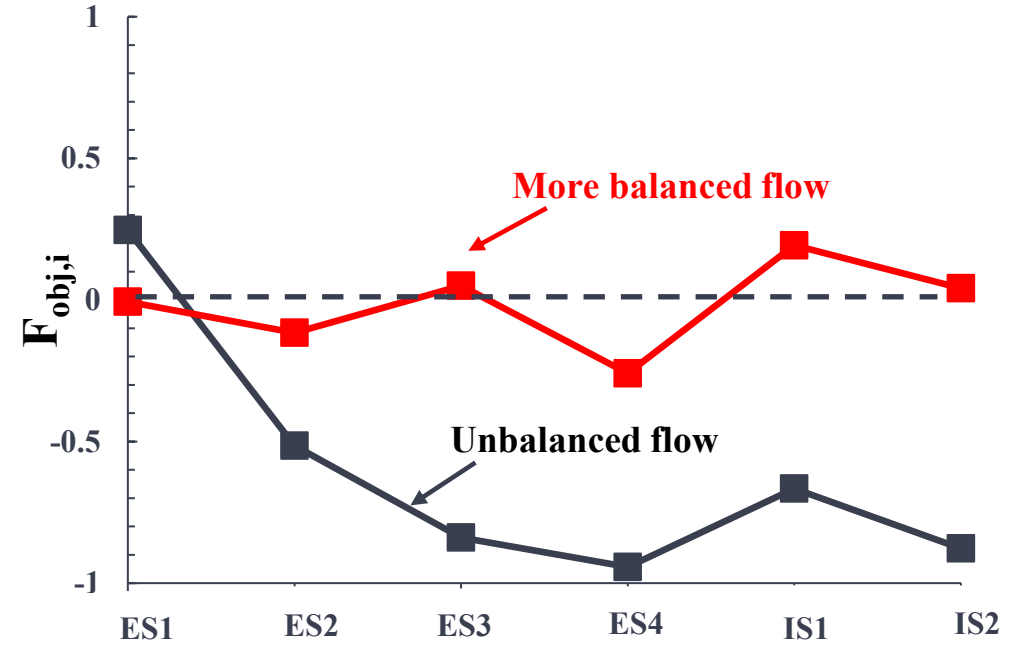


Methodology



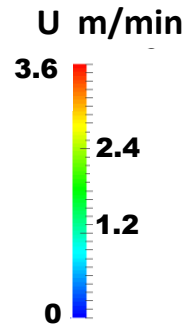
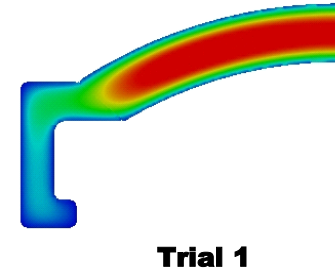
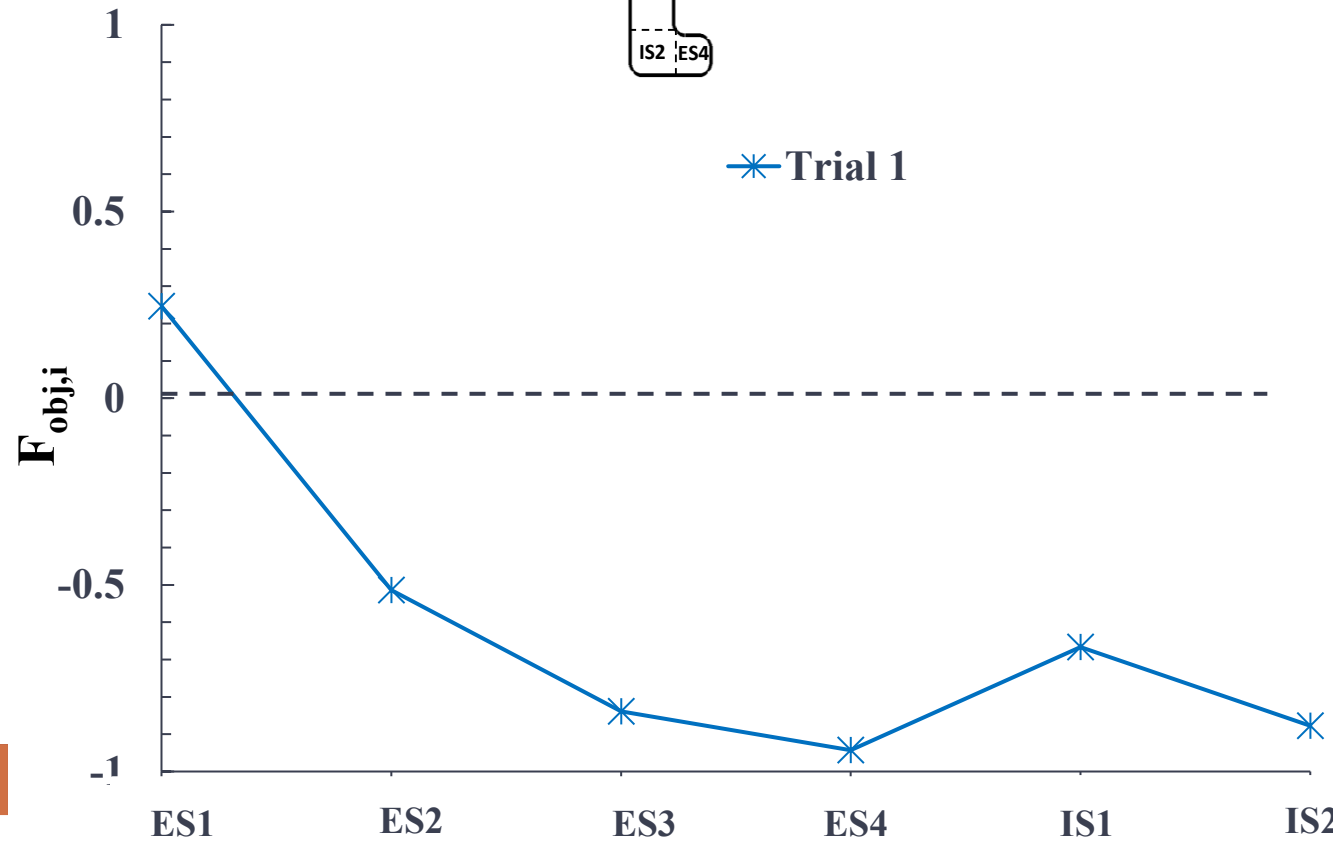
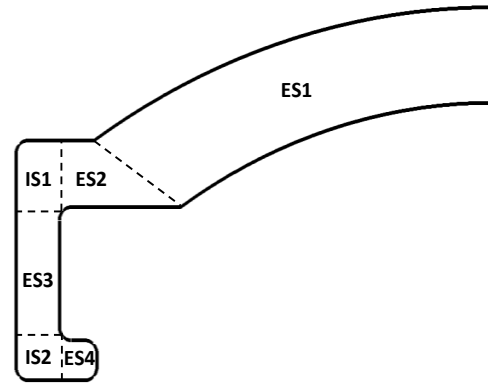
Objective Function

$$F_{obj,i} = \frac{\frac{U_i}{U_{av}} - 1}{\max\left(\frac{U_i}{U_{av}}, 1\right)}$$

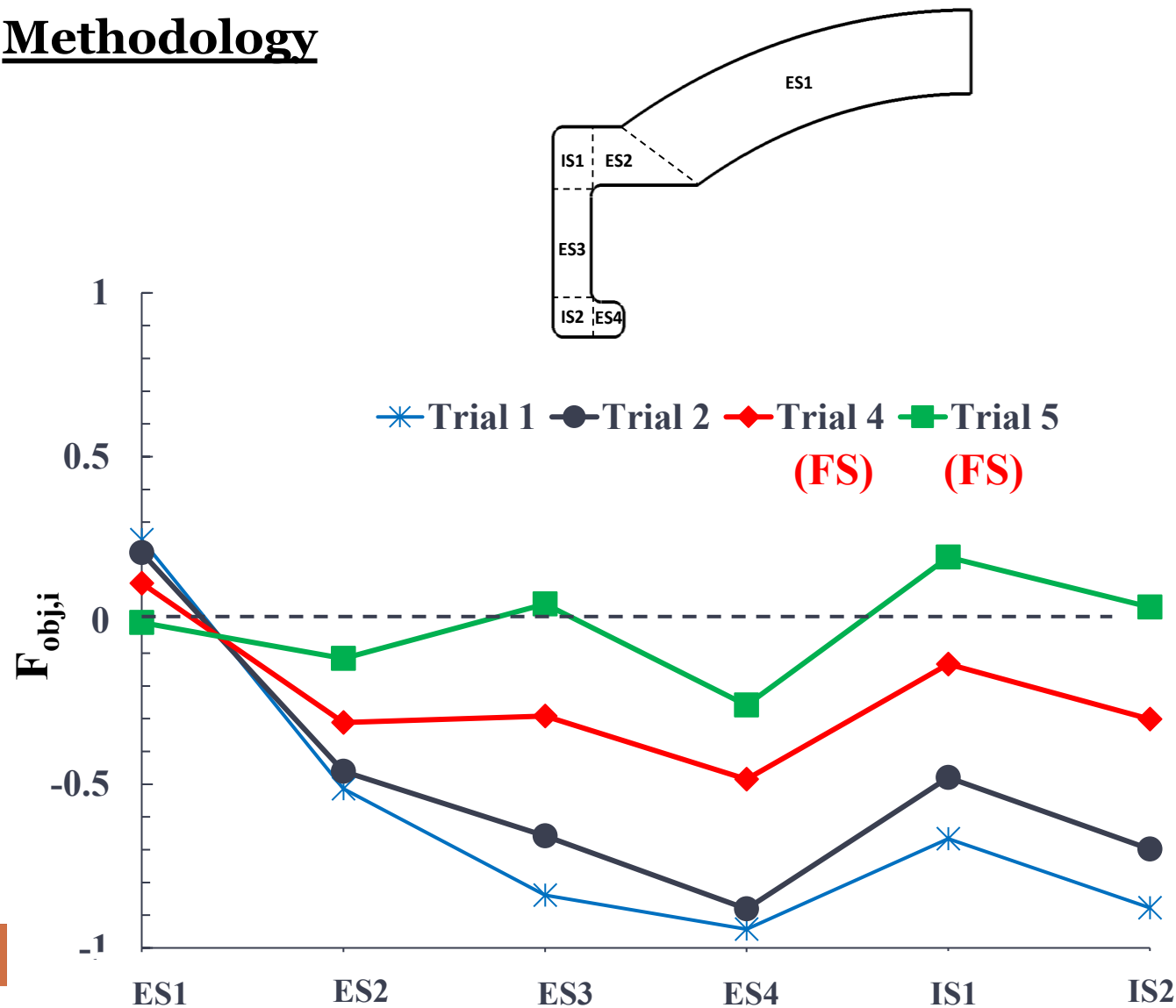




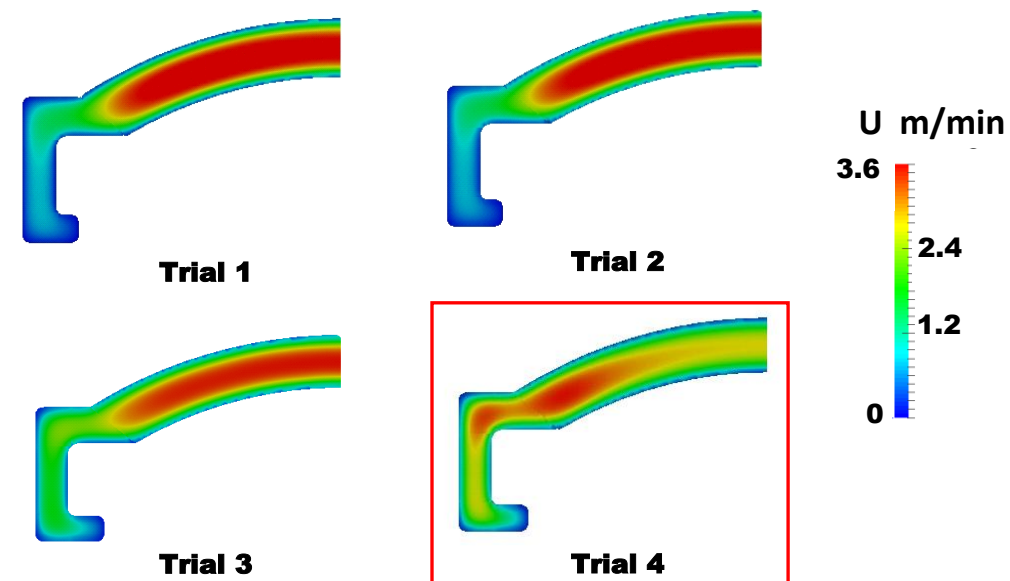
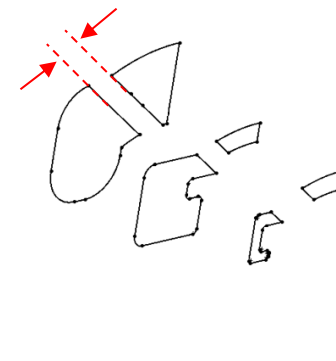
Methodology



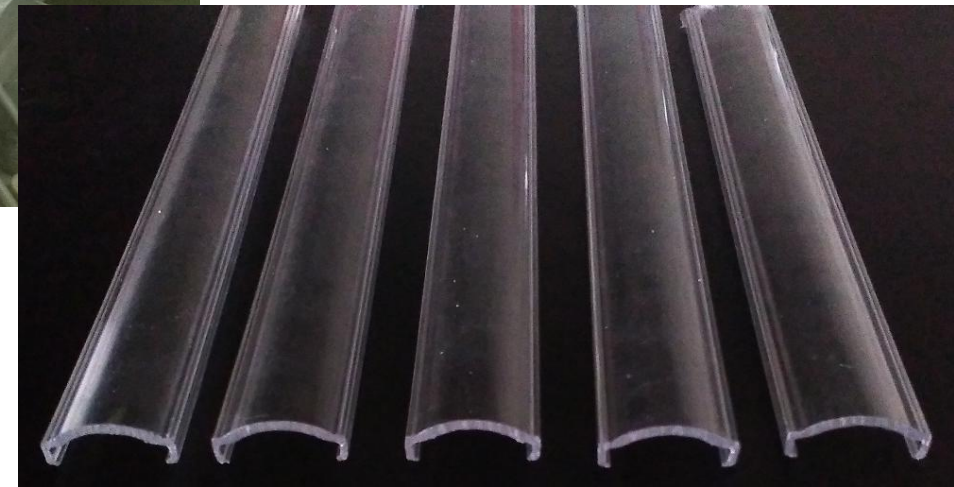
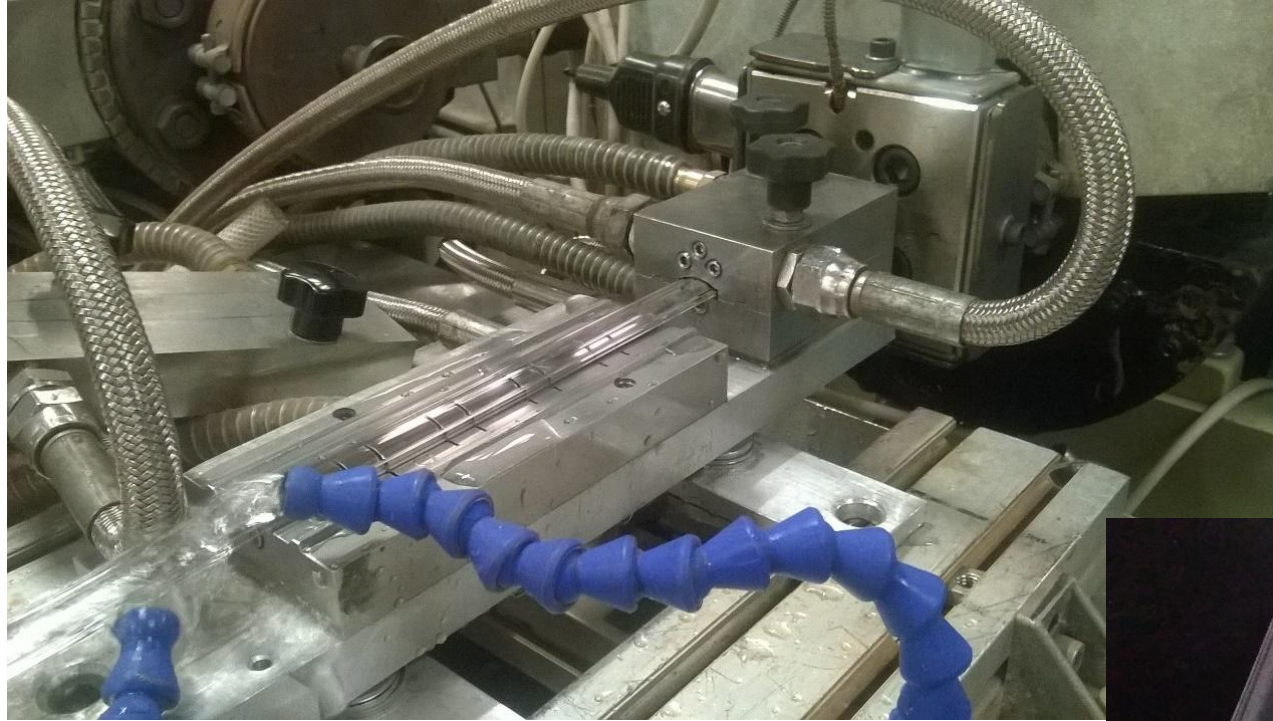
Methodology



Flow Separator (FS)



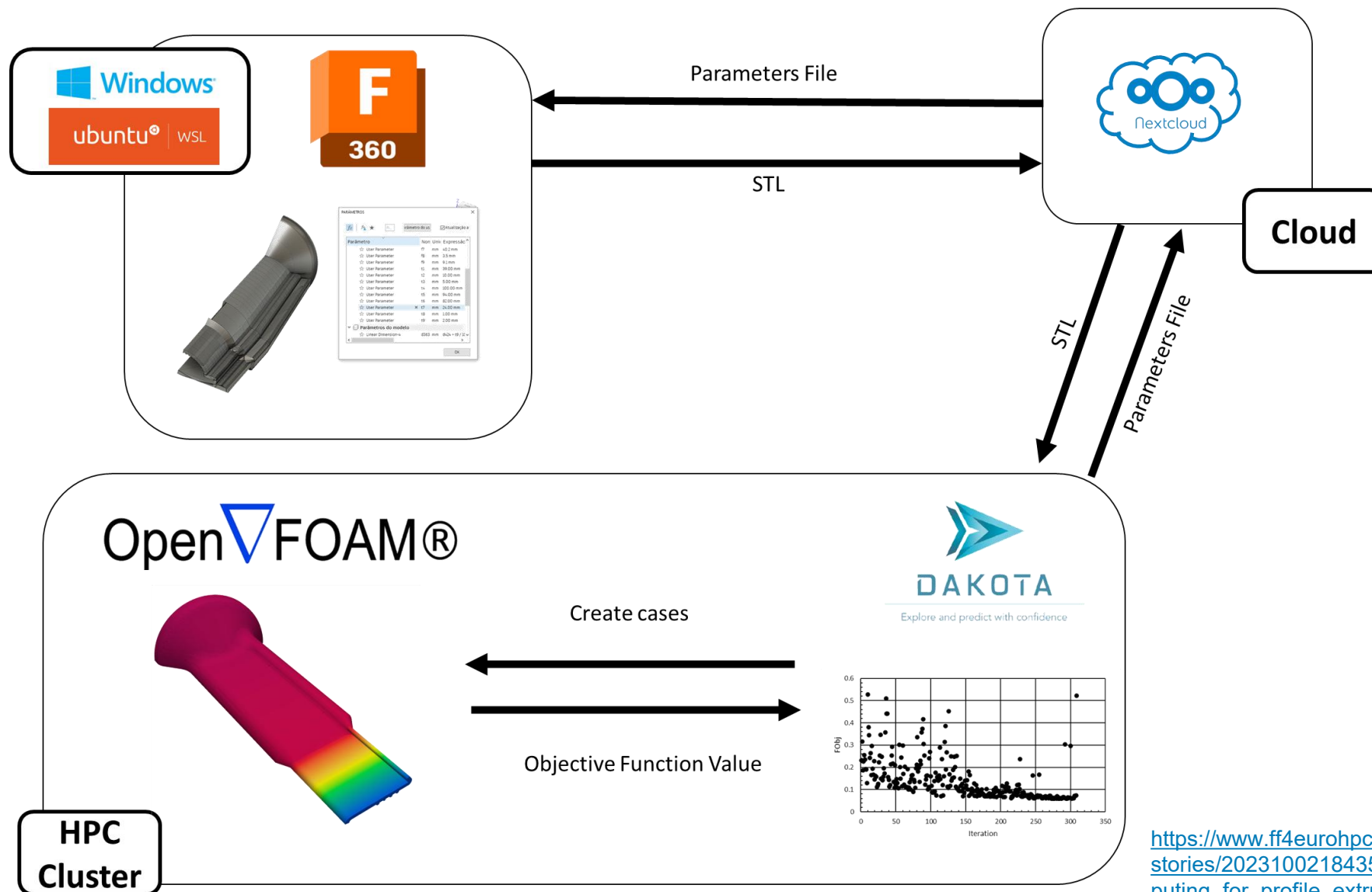
Experimental trial



A Rajkumar et al., An Open-source framework for the CAD of Complex Profile Extrusion Dies, International Polymer Processing, 33, 2018



Optimization in HPC systems



https://www.ff4eurohpc.eu/en/success-stories/2023100218435592/high_performance_computing_for_profile_extrusion

Vidal, J. P. O., et al. (2024). Enhancing extrusion die design efficiency through high-performance computing based optimization. *Meccanica*, 1-12.

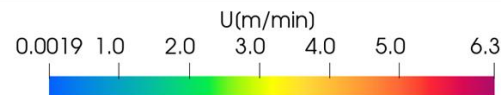




Optimization in HPC systems

ID	Material	F _{obj} Improvement	Velocity Distribution		Cores	Trials	Time (Hours)	Cost (€)
			Initial	Final				
								45
P3	HDPE	2.3			512	409	23	115

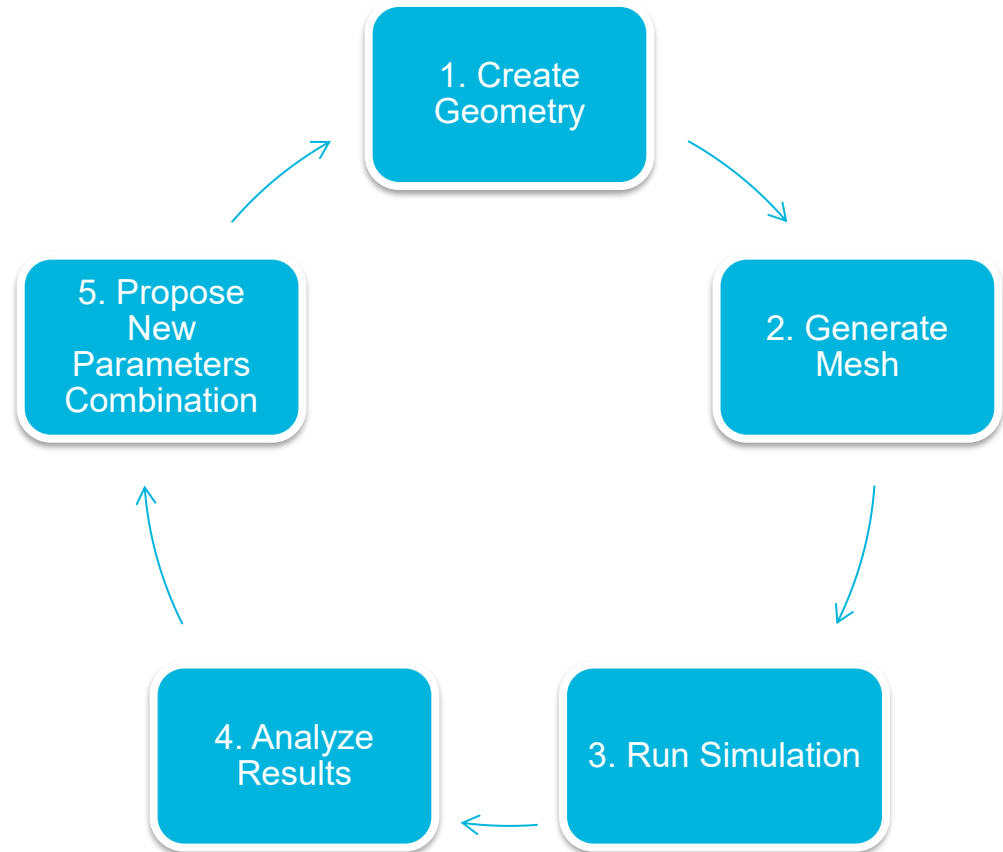
- Reduction of 30-40% on the product time to market
- Reduction at least in 40% of the raw materials spent in experimental trials
- Estimated savings of 23 % in tools development



https://www.ff4eurohpc.eu/en/success-stories/2023100218435592/high_performance_computing_for_profile_extrusion

Vidal, J. P. O., et al. (2024). Enhancing extrusion die design efficiency through high-performance computing based optimization. *Meccanica*, 1-12.



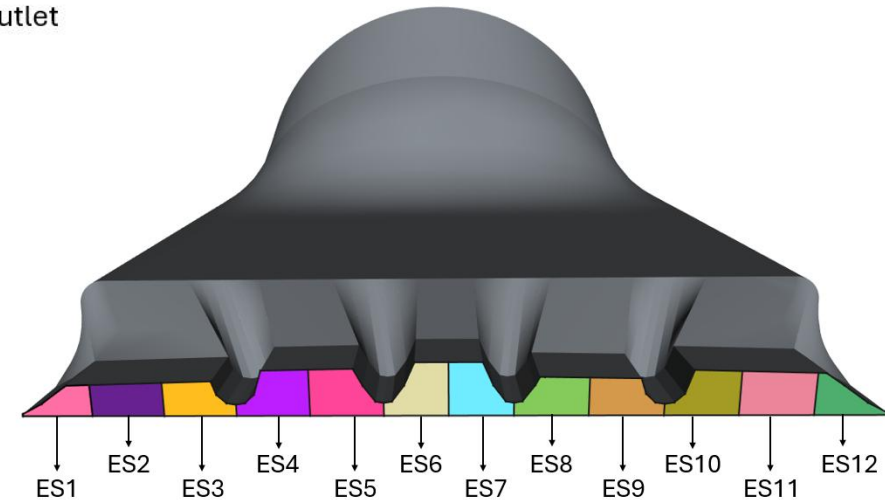
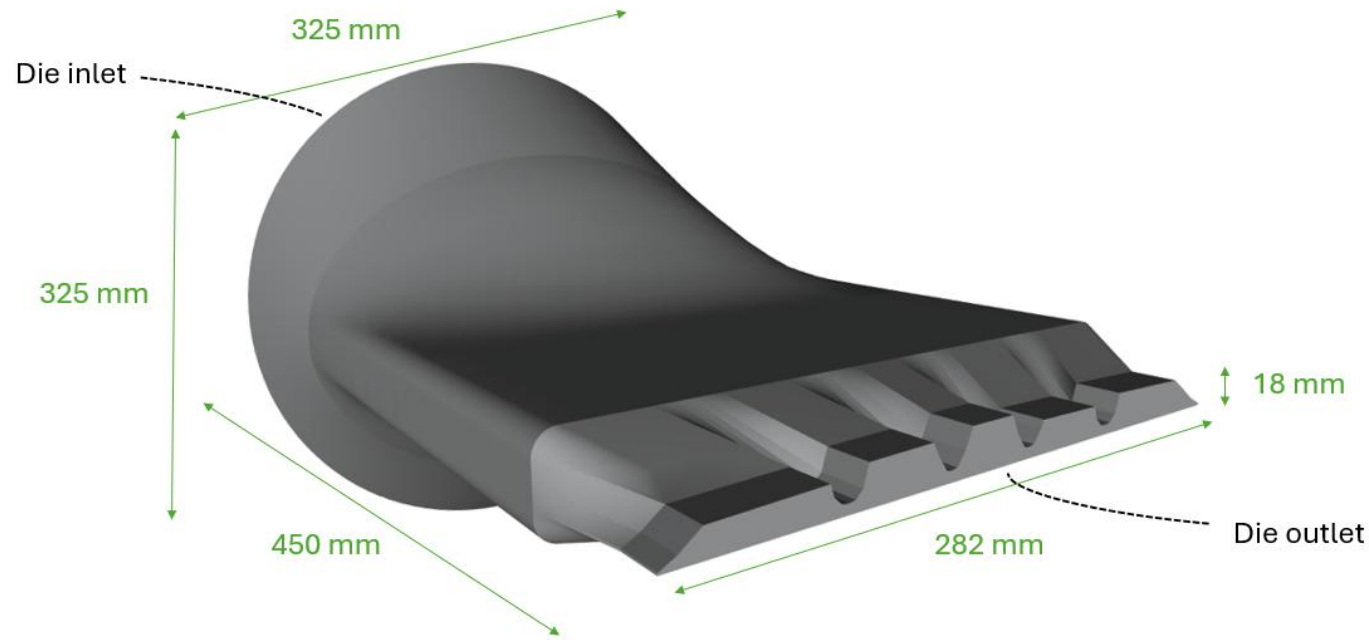


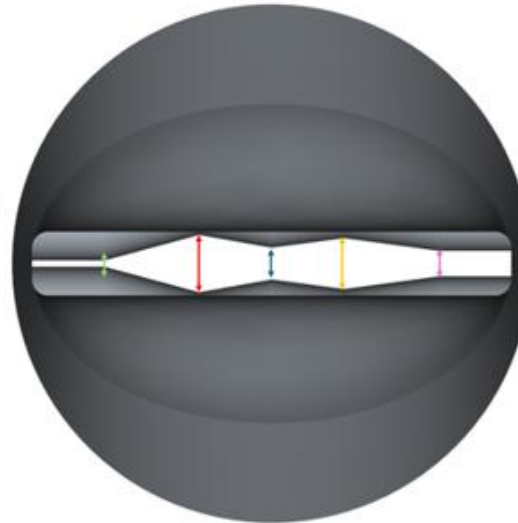
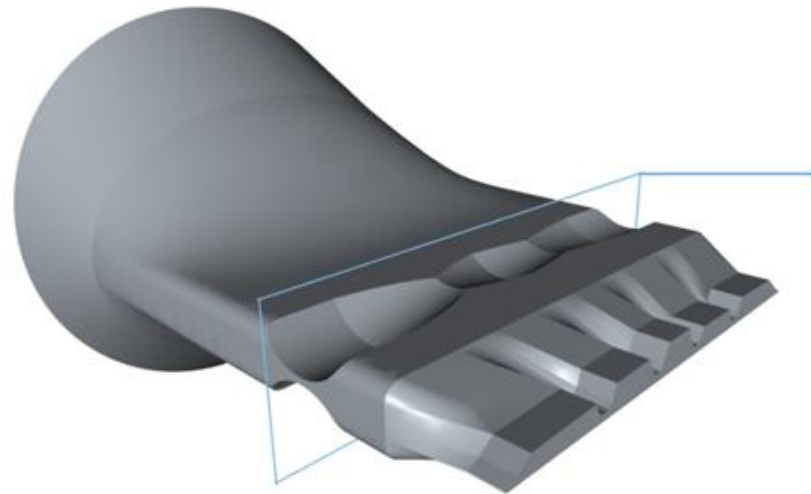
1. Initial geometry is created with proposed parameters combination based on the dataSet provided in ParetoOptimalParameters.txt
2. Uses cartesianMesh utility (cfMesh) to generate mesh
3. Run the simulation through Allrun script
4. Analyze the results of outlet velocity uniformity and total pressure drop
5. Proposes a new parameters combination and creates a new geometry (Bayesian Optimization)



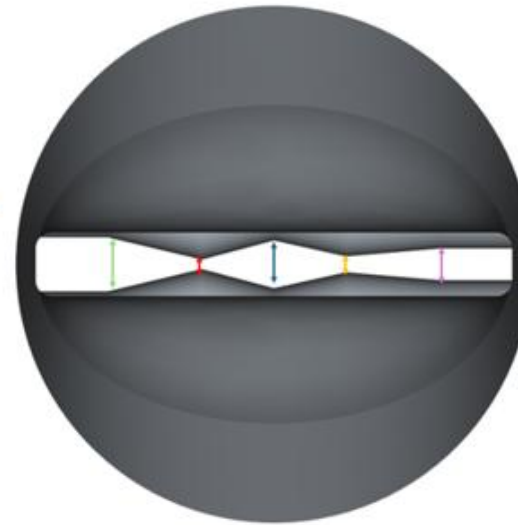
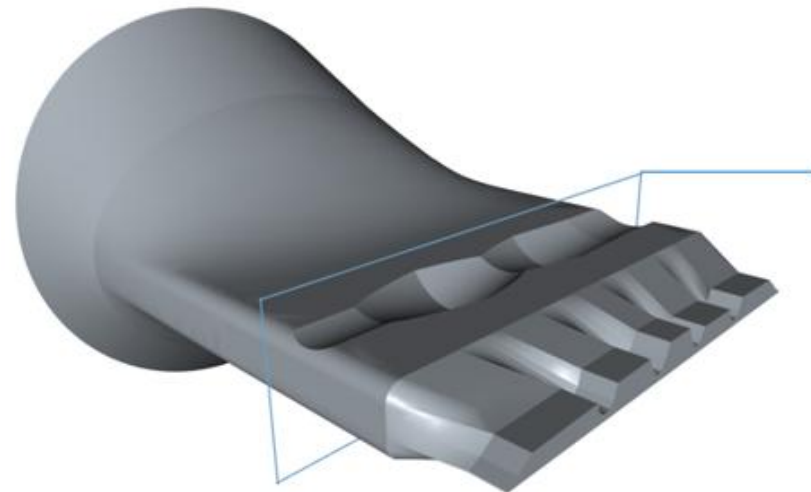
scikit-optimize

https://scikit-optimize.github.io/stable/auto_examples/bayesian-optimization.html

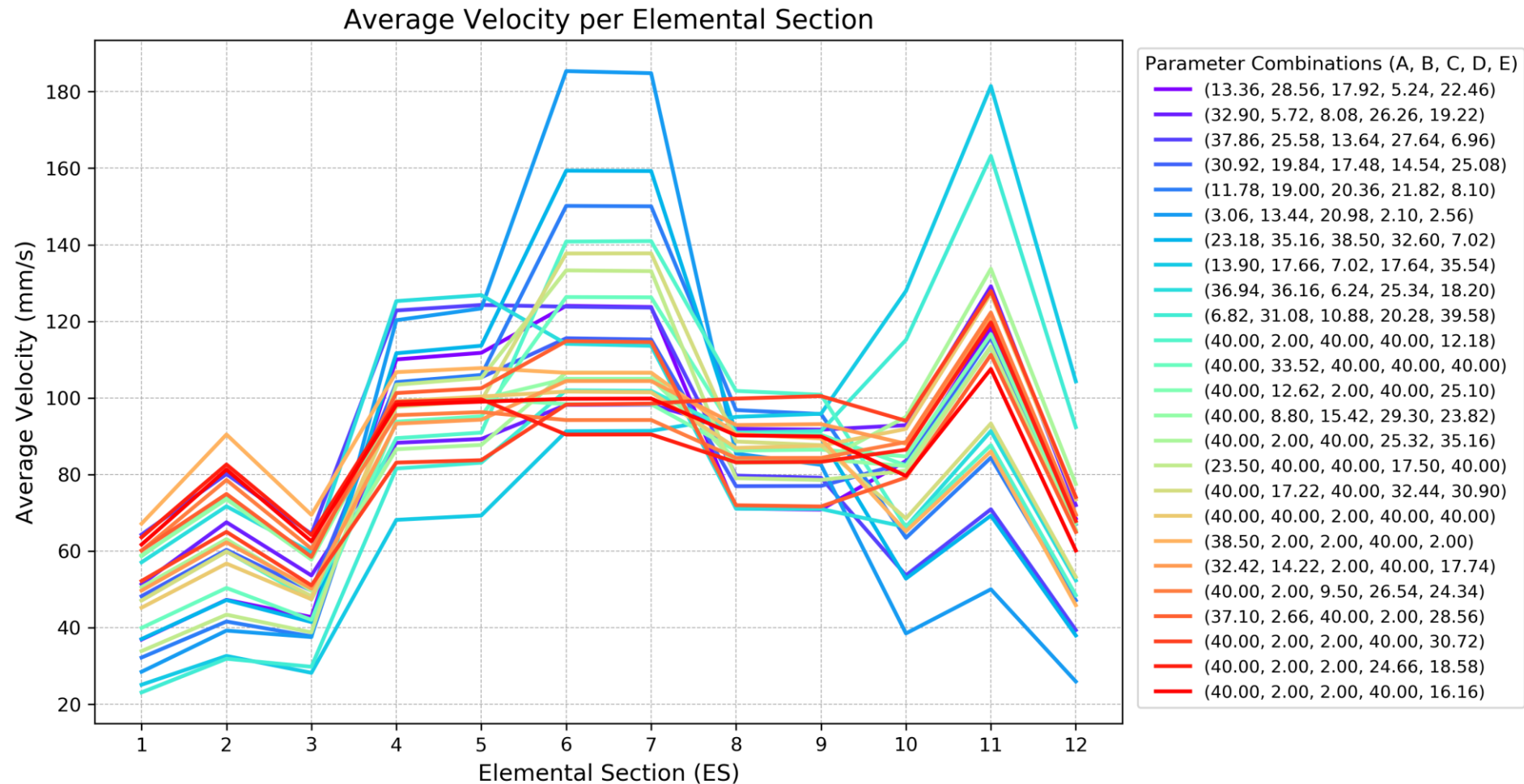


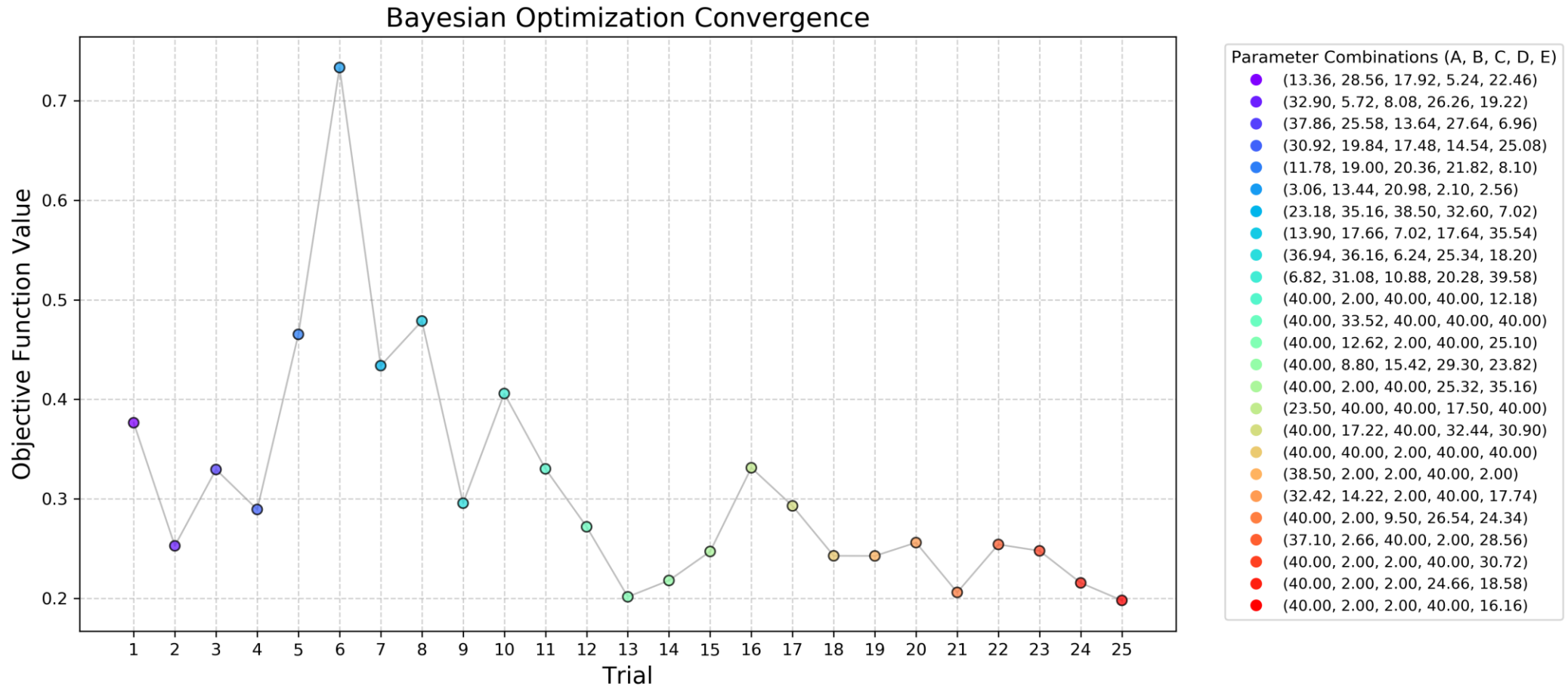


A = 4 mm
B = 36 mm
C = 20 mm
D = 32 mm
E = 16 mm

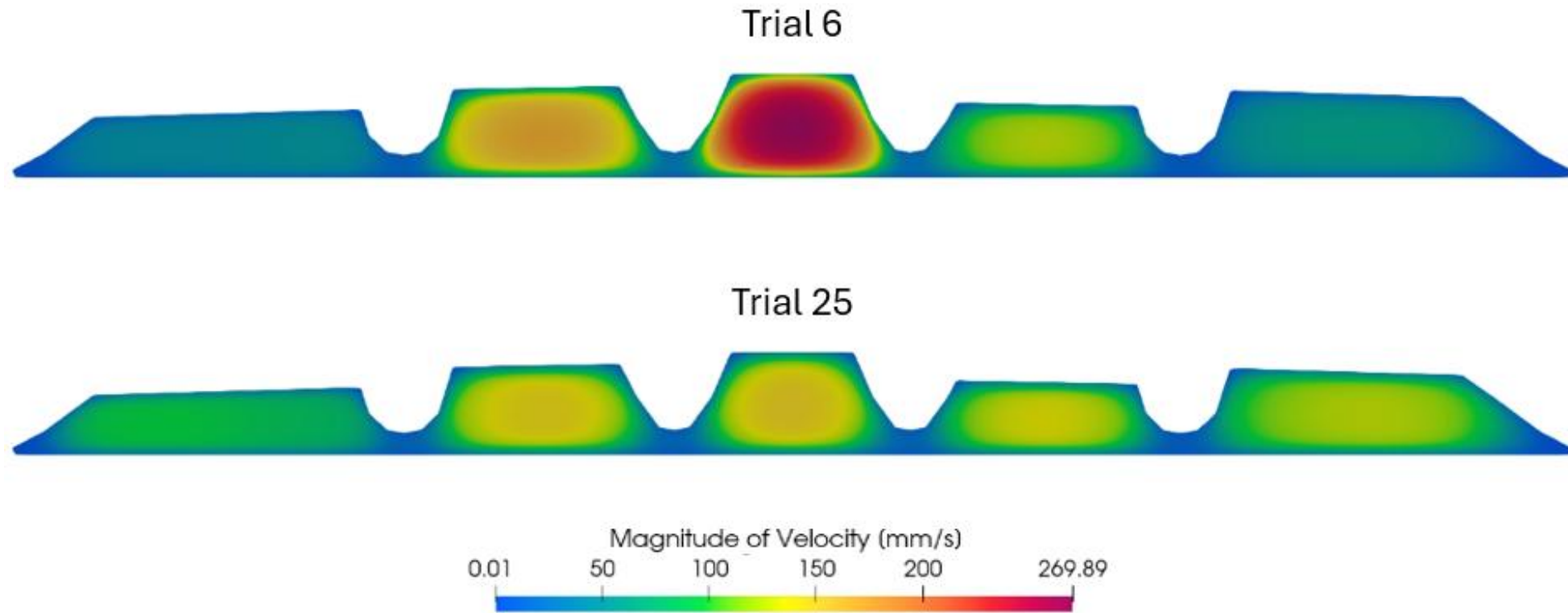


A = 34 mm
B = 6 mm
C = 30 mm
D = 10 mm
E = 20 mm

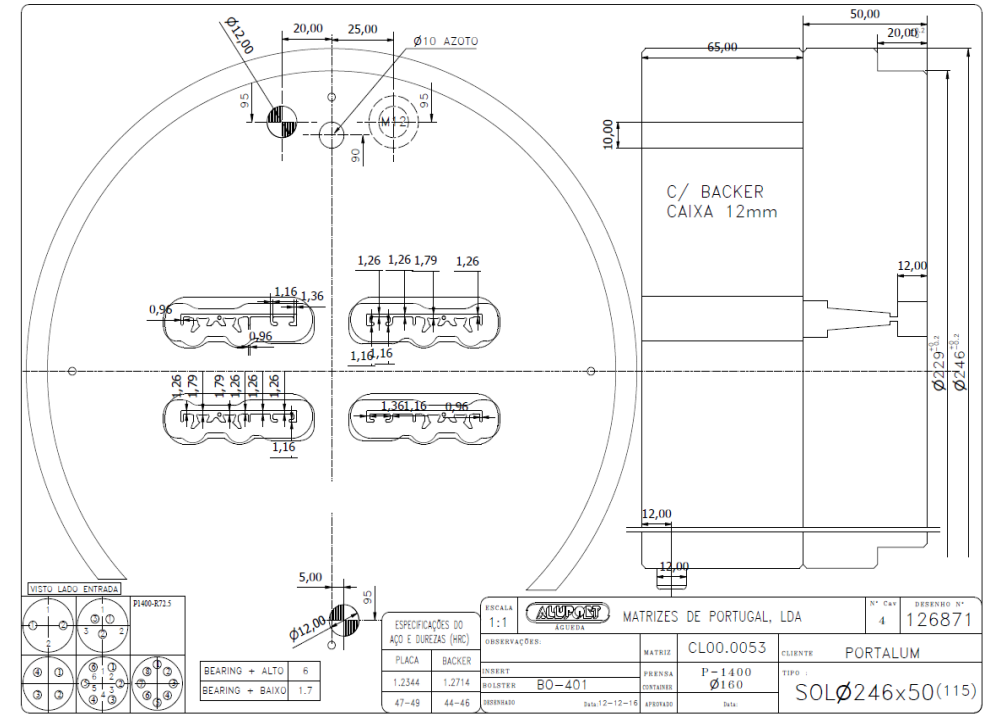
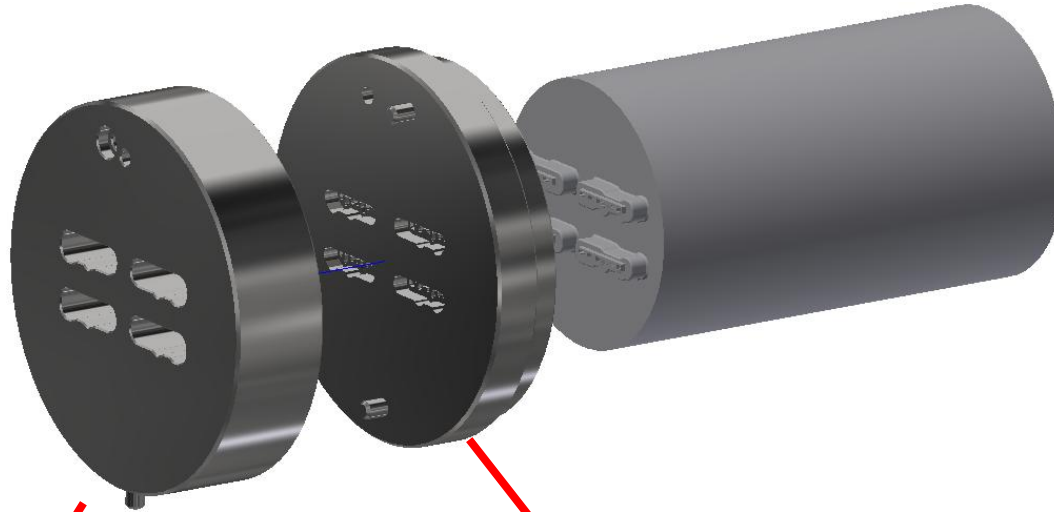




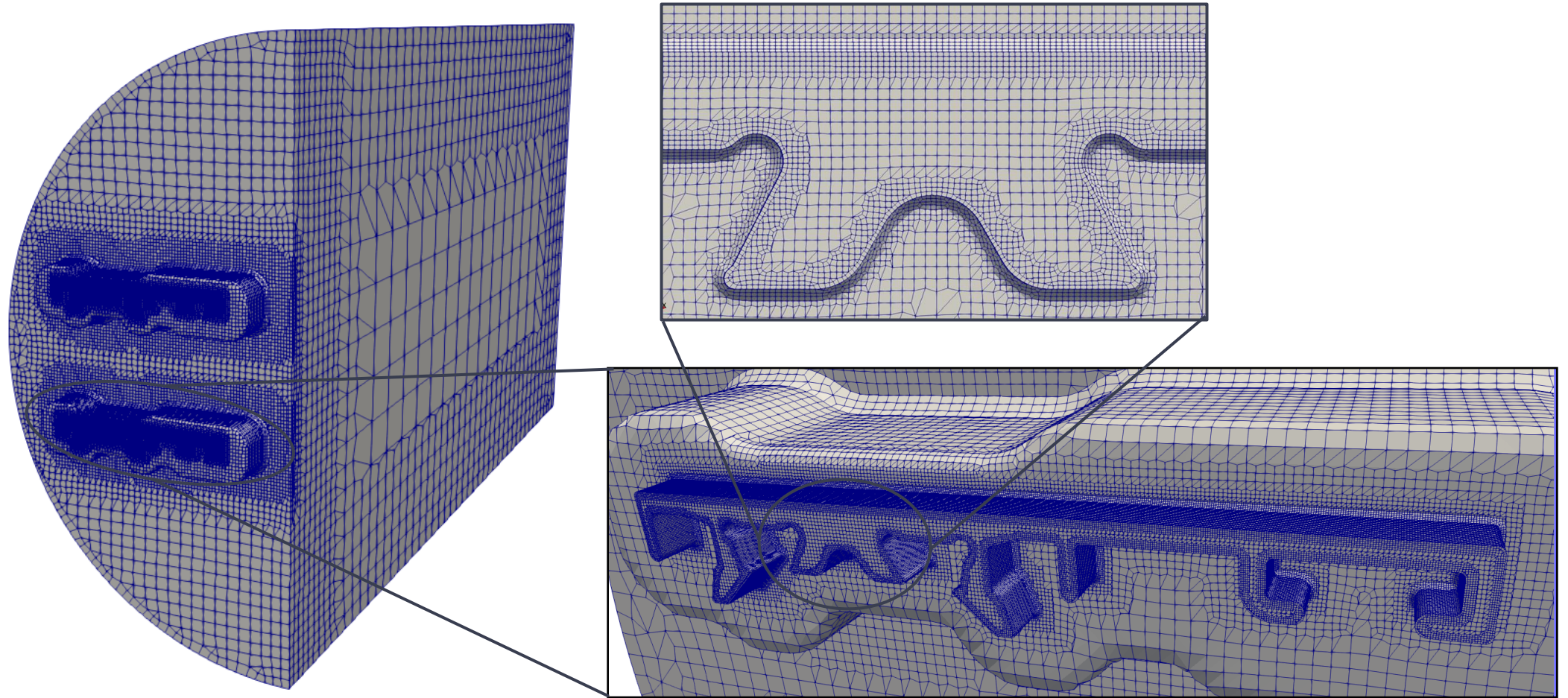
Outlet Velocity Distribution



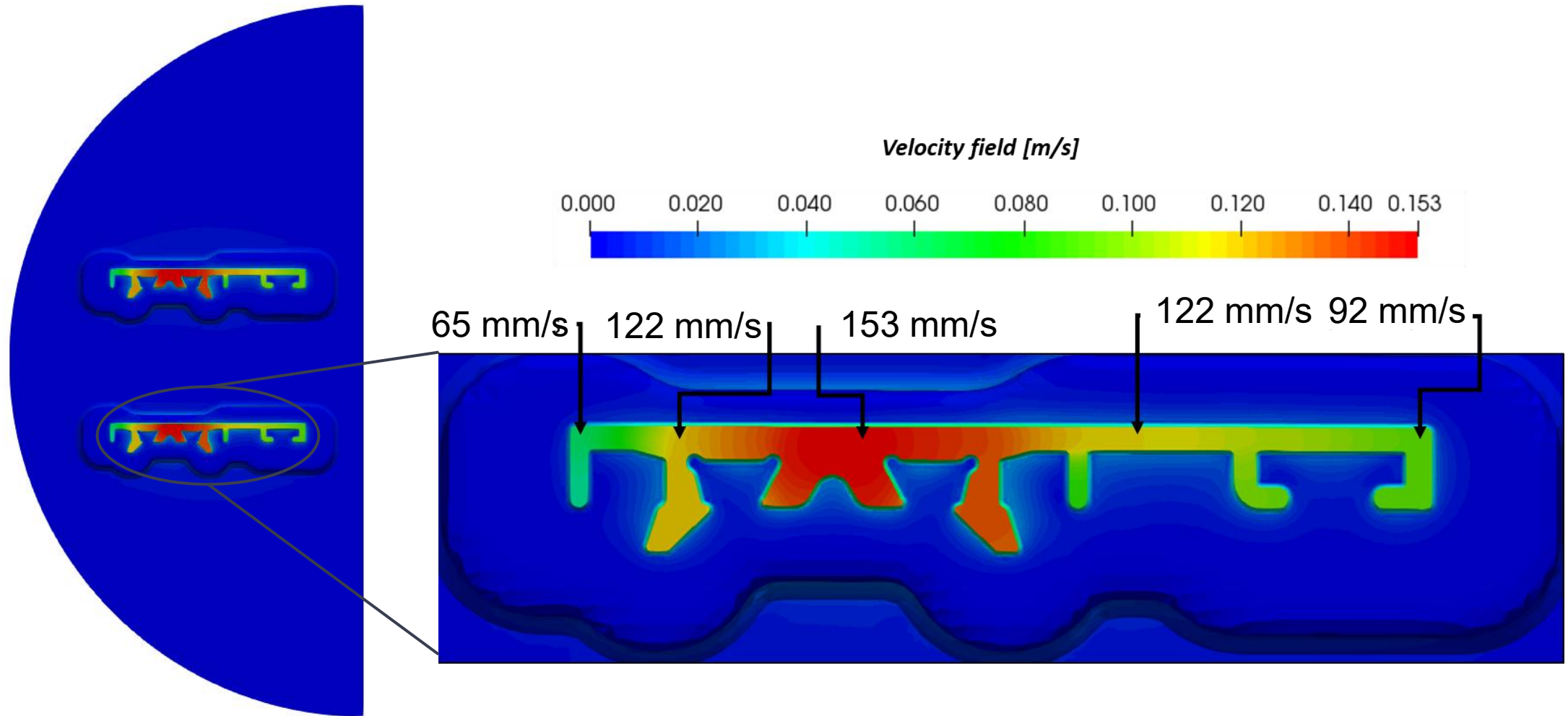
alExtFoam



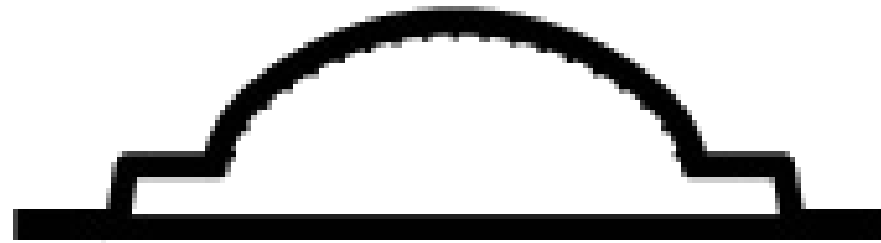
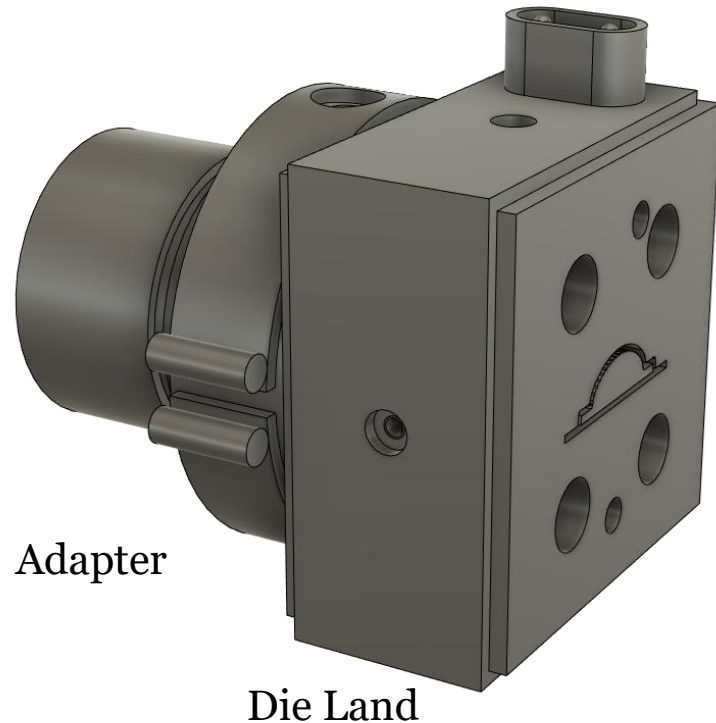
alExtFoam



alExtFoam



Profile extrusion



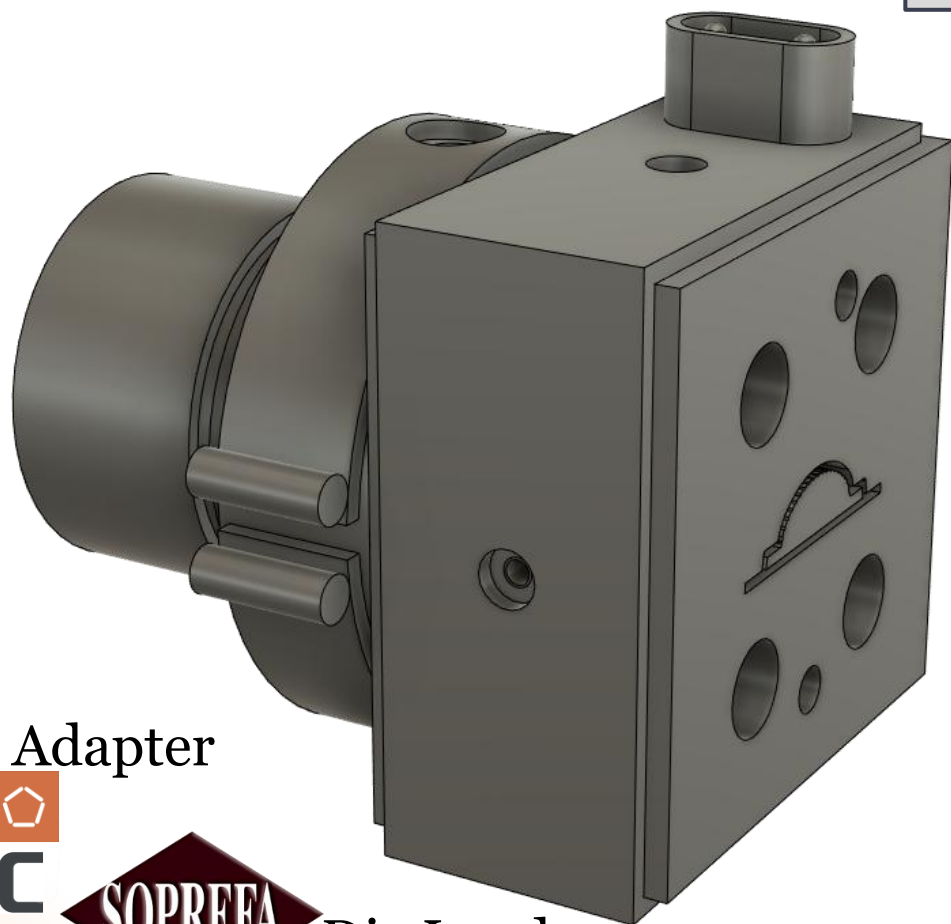
Process Data

- **Material:** Polycarbonate
- **Average linear outlet velocity:** 3 m/min
- **Temperature:**
 - **Inlet:** 245 °C
 - **Adapter:** 228 °C
 - **Die Land:** 220 °C



**How to model
this system?**

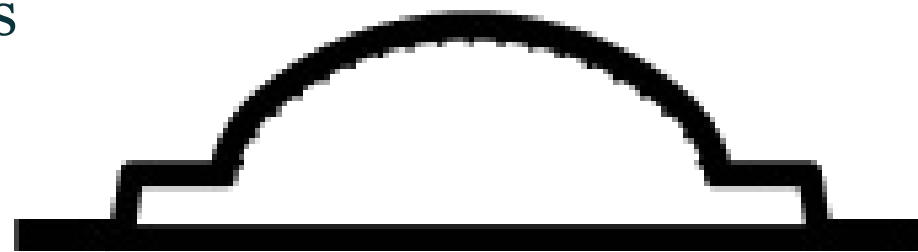
Profile extrusion



Adapter



Die Land



T=245 °C

T=228 °C

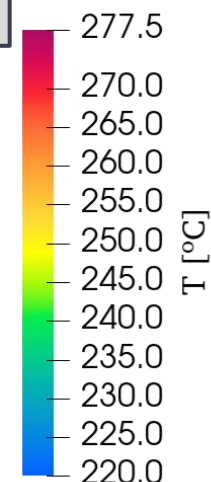


Flow Channel

T=220 °C

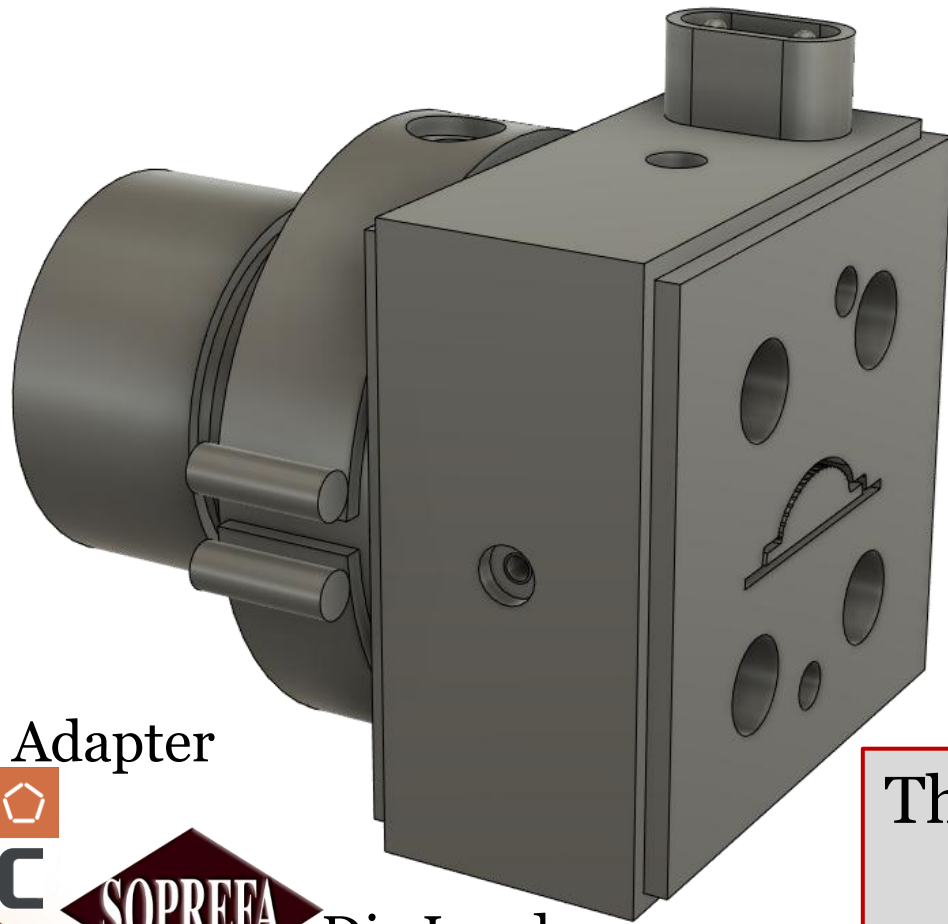
Insulated?

Boundary Conditions



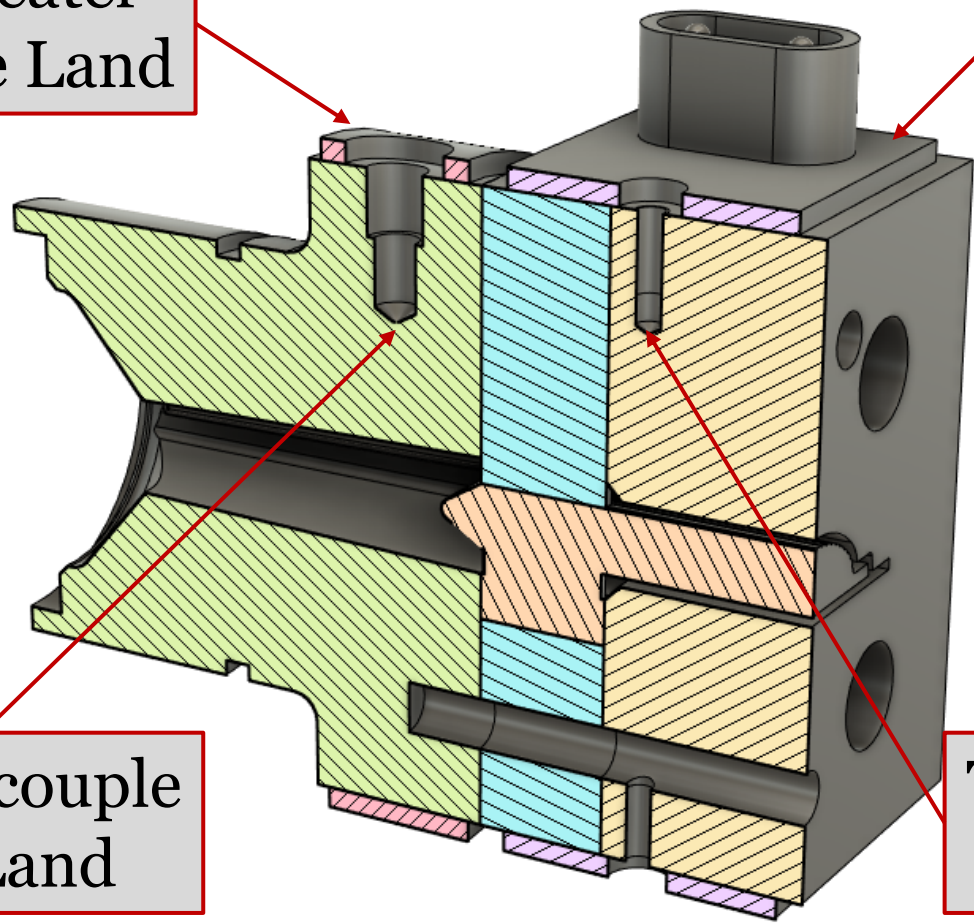
Profile extrusion

How is the temperature controlled?



Heater Die Land

Heater Die Land



Themocouple Die Land

Themocouple Die Land

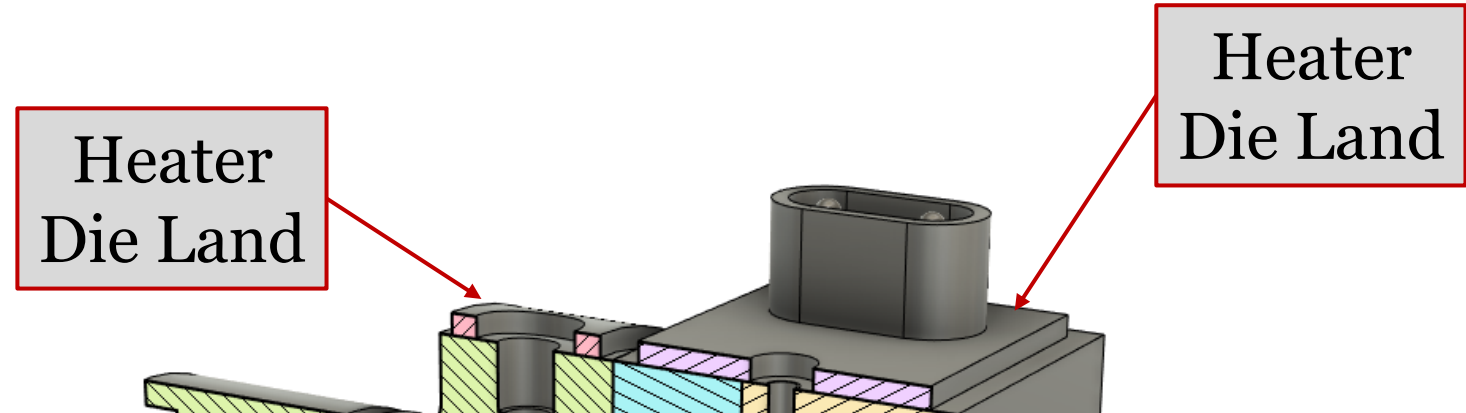
Adapter

Die Land

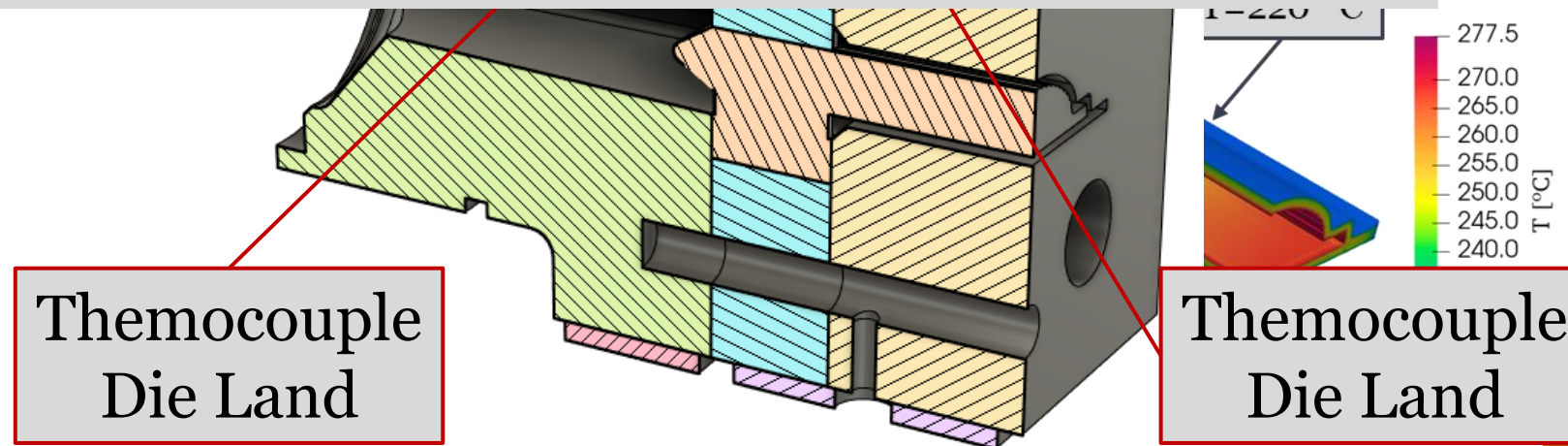


Vidal, J., Nóbrega, J. M. (2024). An Enhanced Temperature Control Approach to Simulate Profile Extrusion. *Polymers*, 16(7), 904.

Profile extrusion



Does it make any difference?



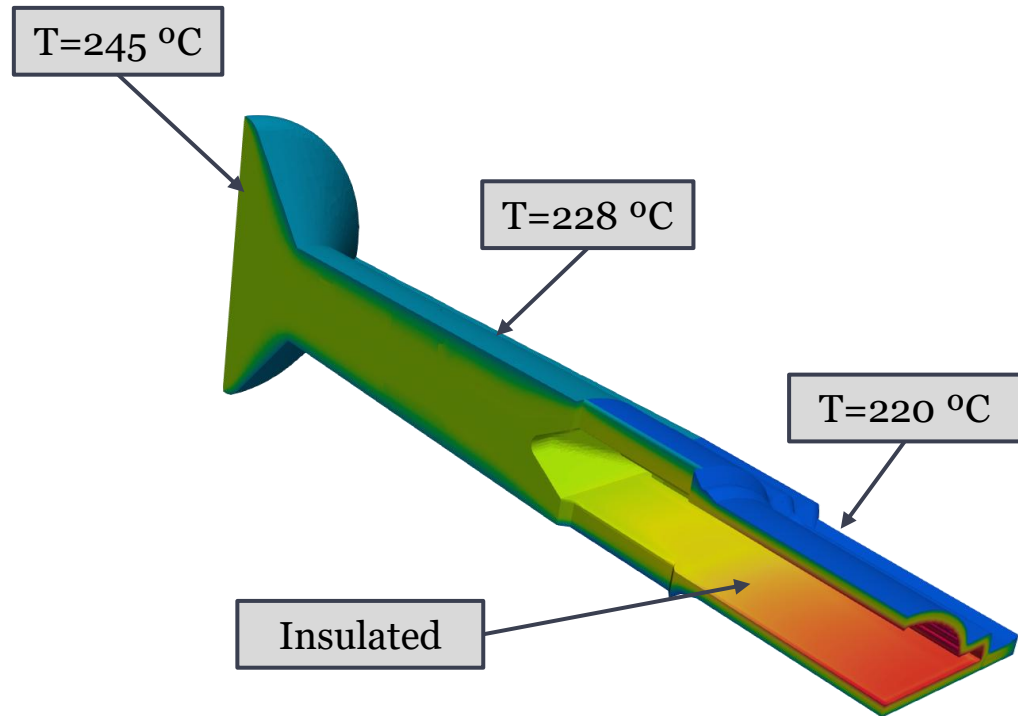
The new solver

OpenFOAM

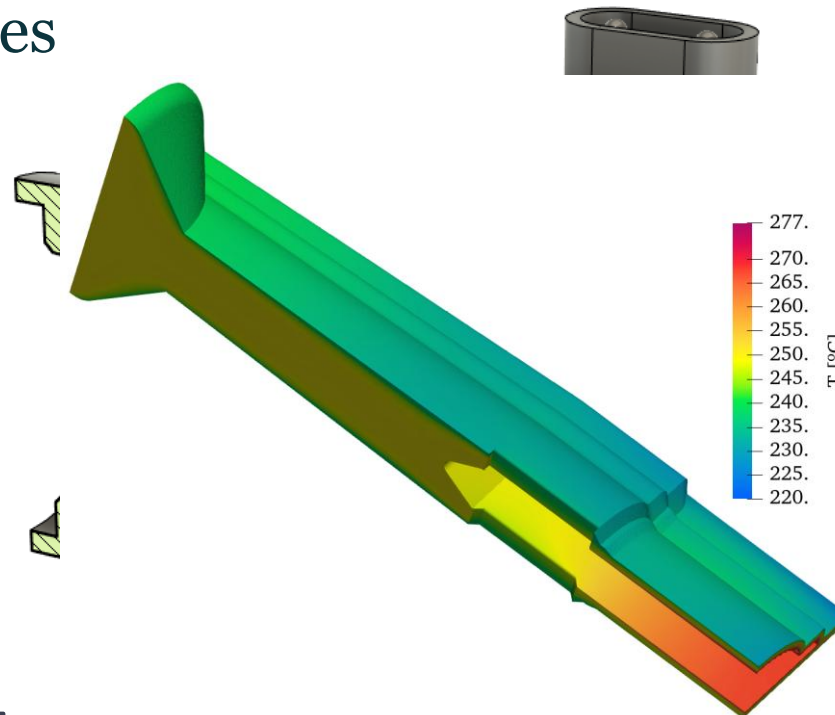
chtMultiRegionFoam Solver

- Transient
- Multiple ~~in~~compressible fluid and solid regions
- ~~Turbulence~~
- Heat transfer
- **New Boundary Condition**

Case Studies

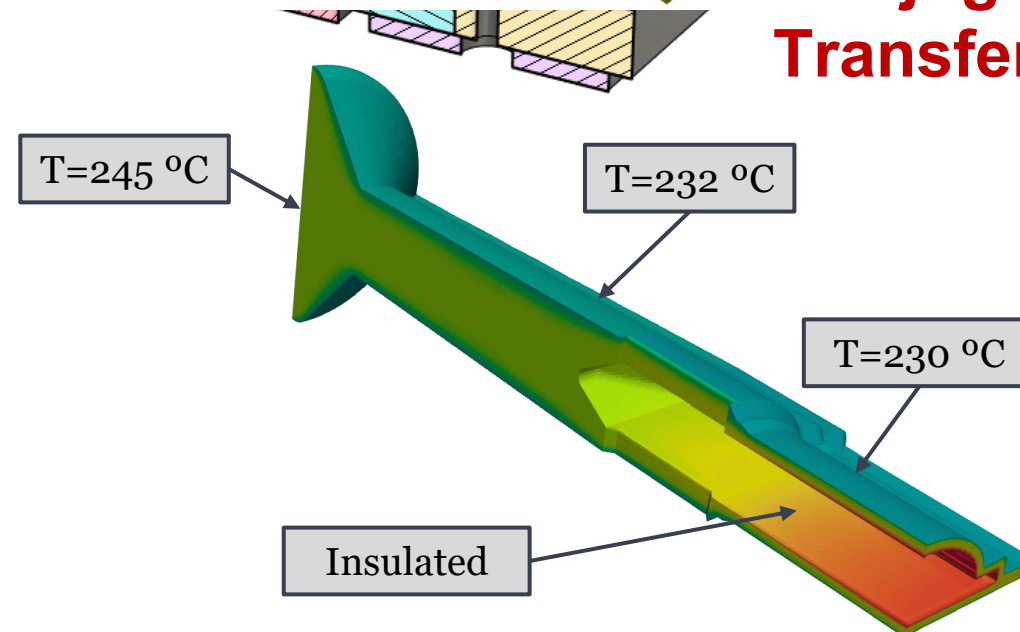


Conventional (CV)



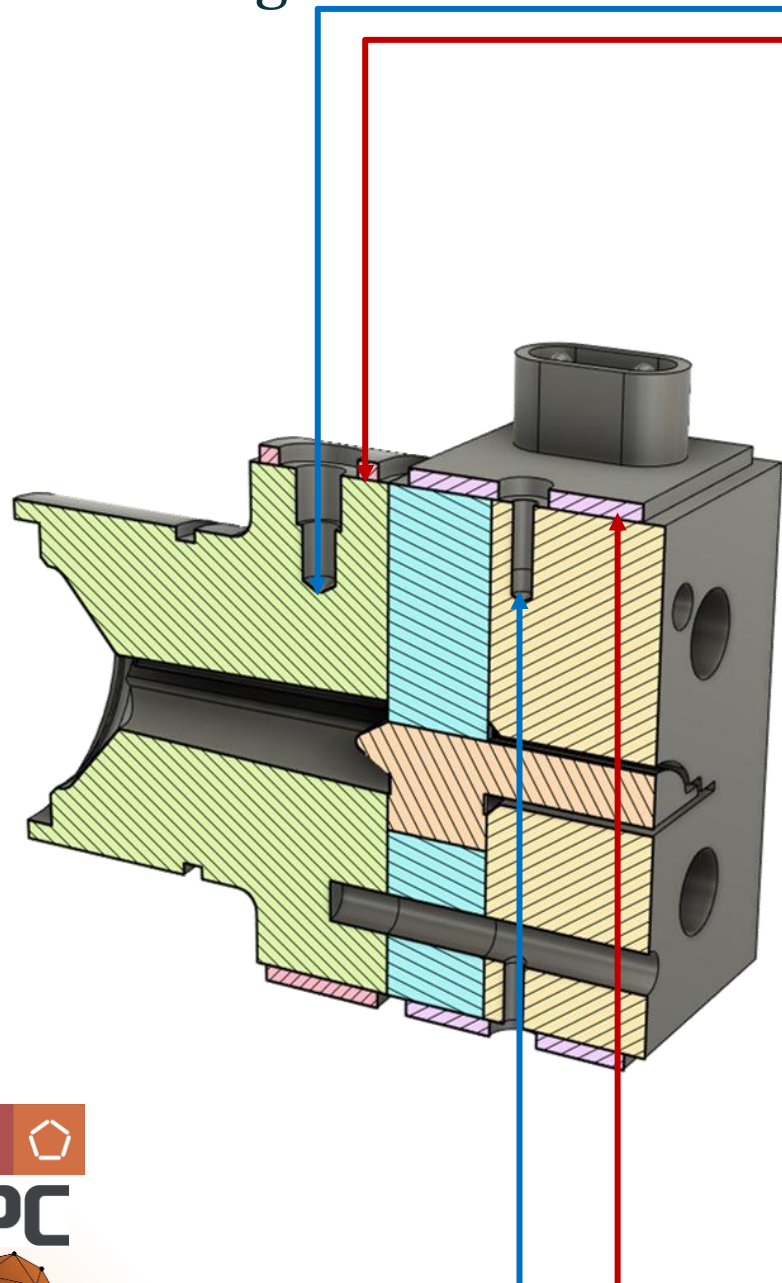
- Boundary Conditions
- Heater BC
 - Temperature continuity at the fluid /solid interface
 - External walls with natural convection

Conjugate Heat Transfer (CHT)

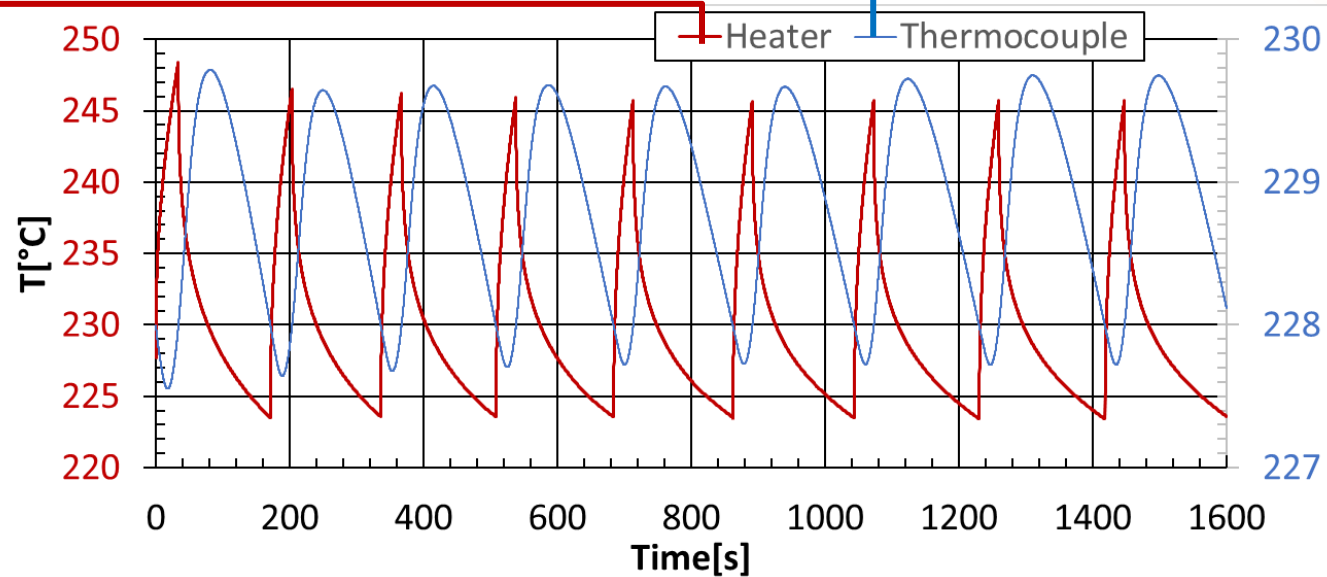


CV+CHT

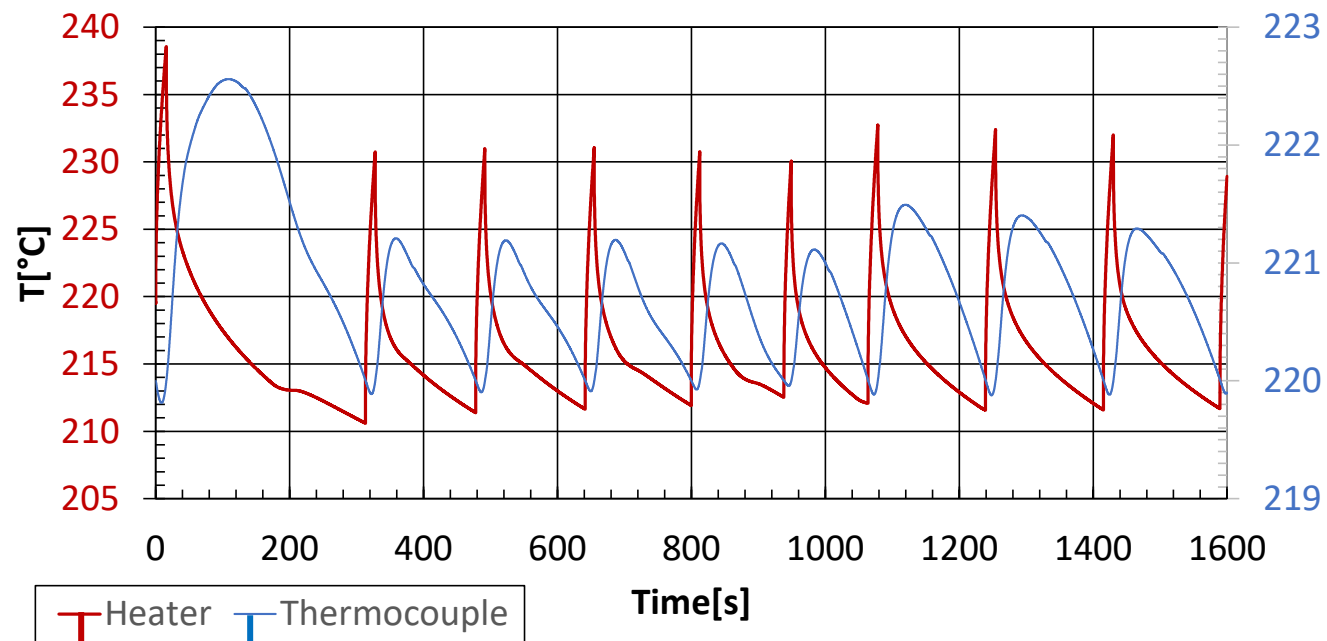
IA - Design of Profile Extrusion Dies



Adapter

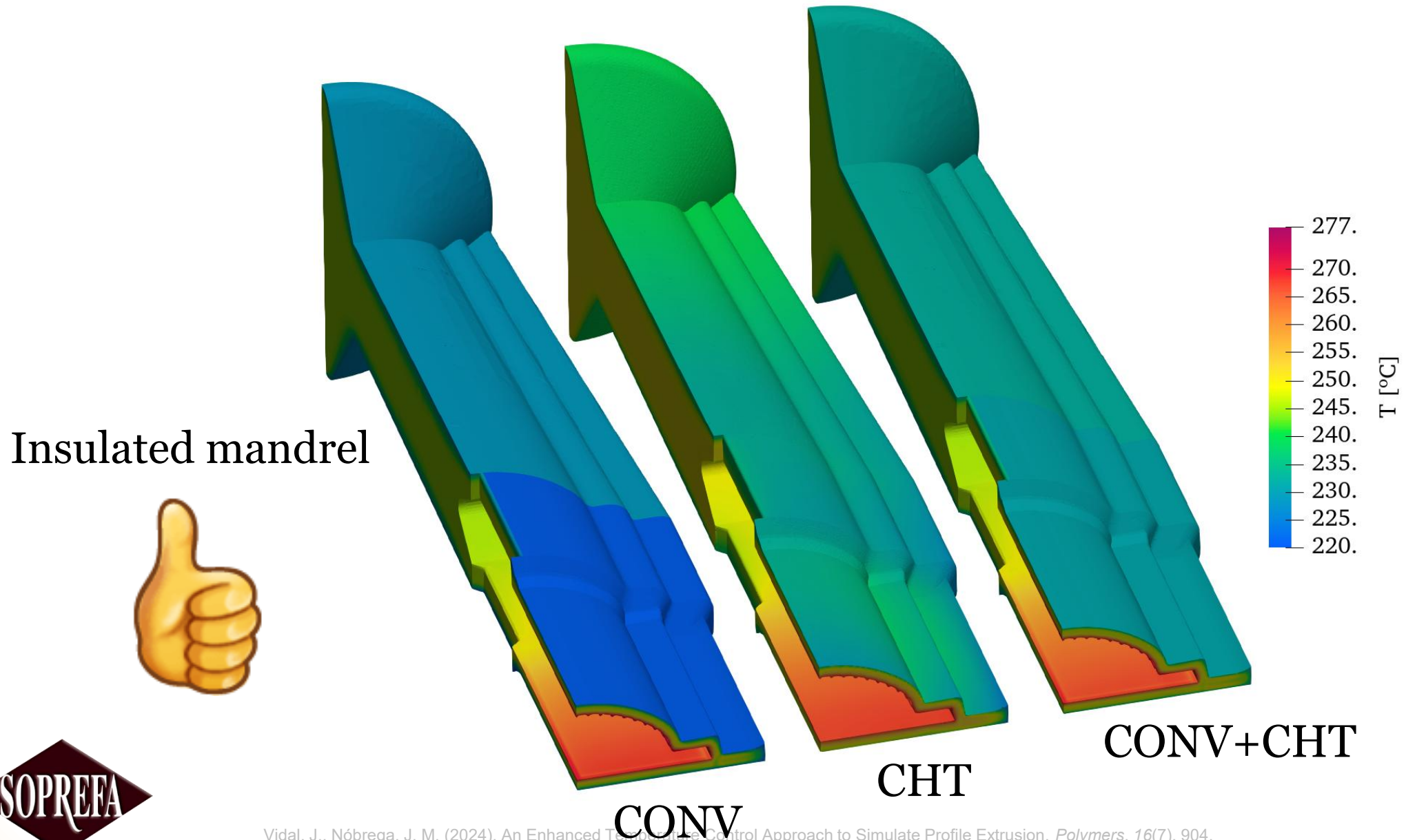


Die Land

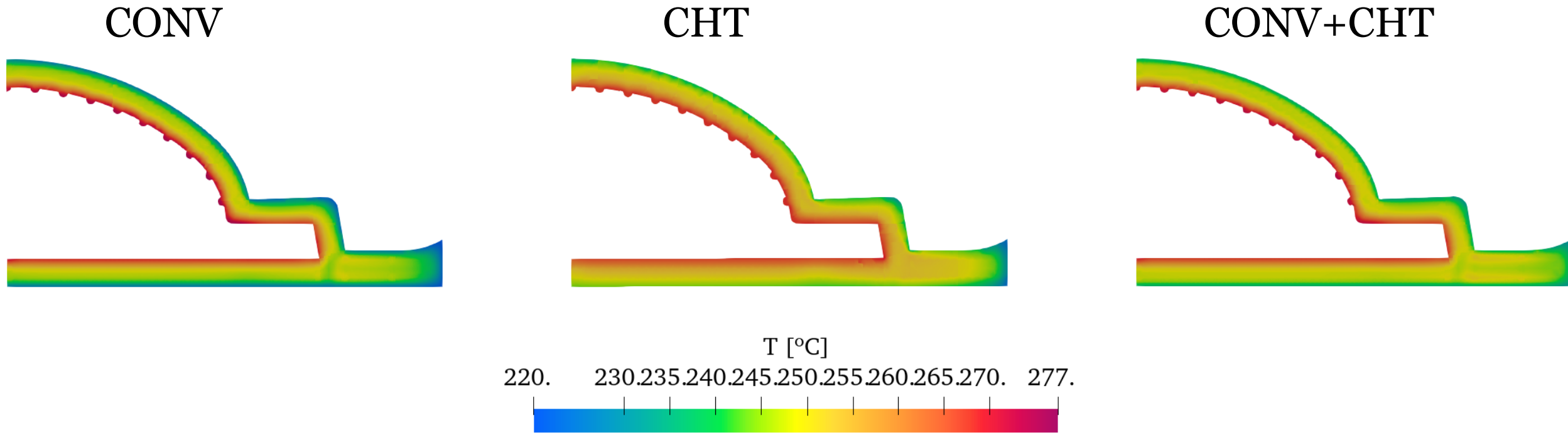


Vidal, J., Nóbrega, J. M. (2024). An Enhanced Temperature Control Approach to Simulate Profile Extrusion. *Polymers*, 16(7), 904.

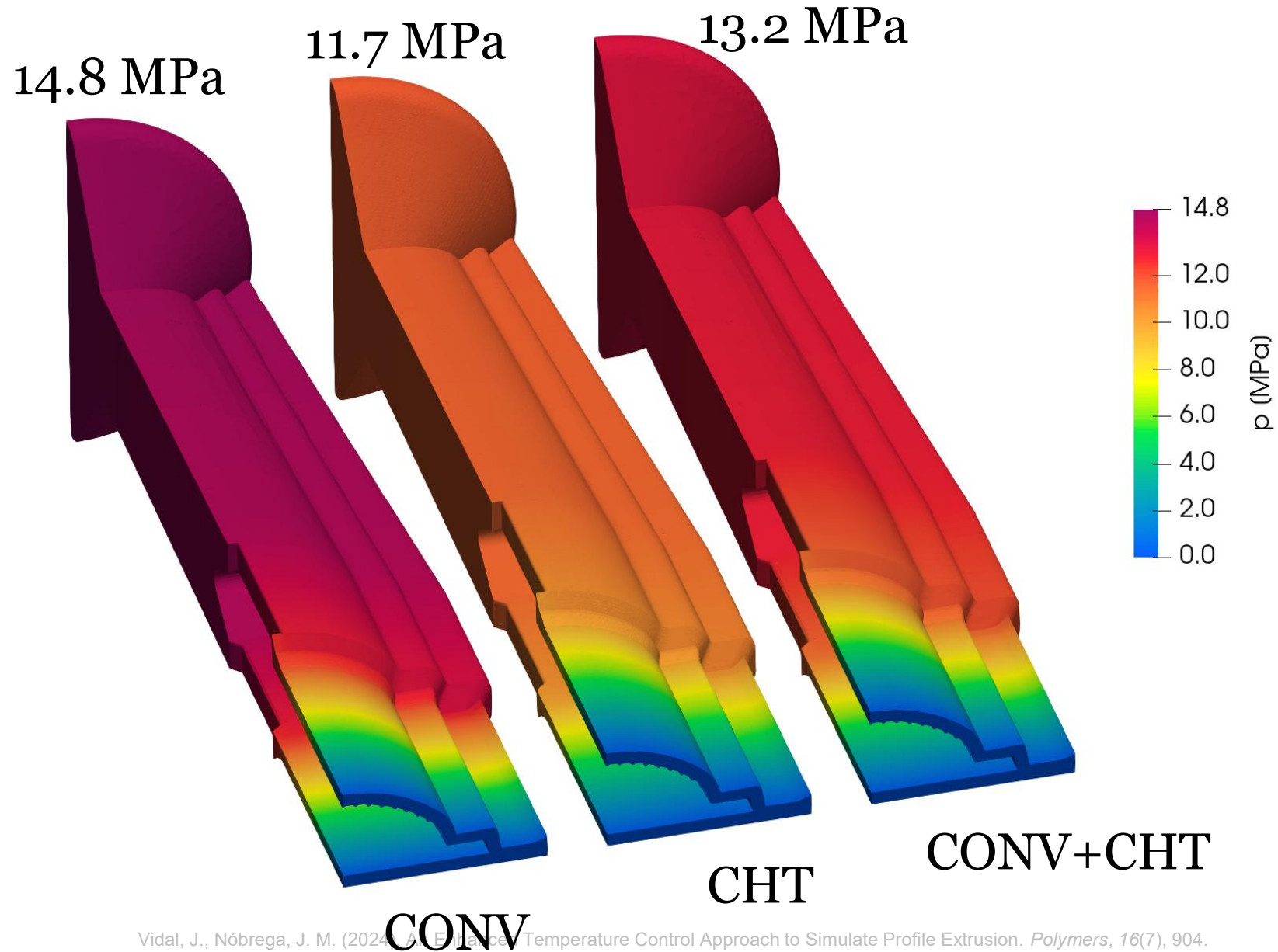
Results and Discussion



Results and Discussion

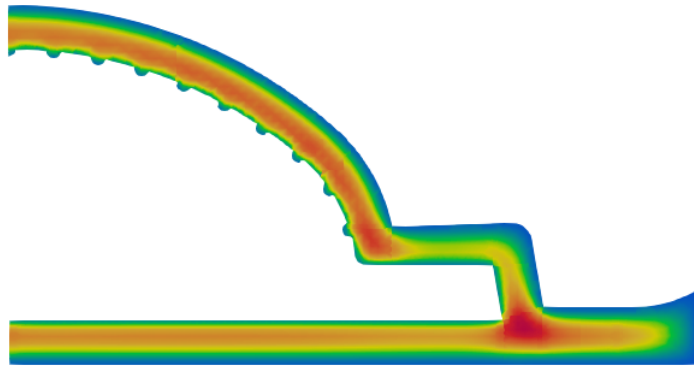


Results and Discussion

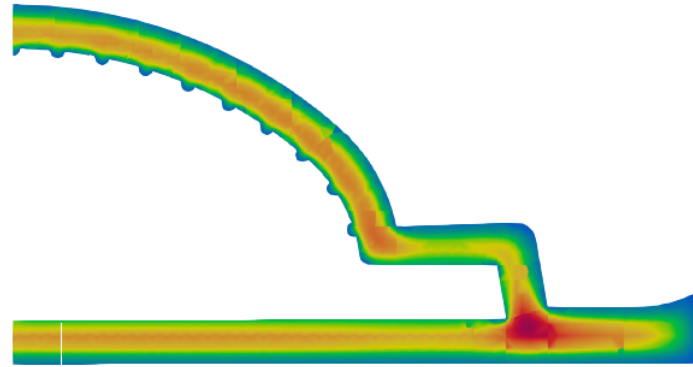


Results and Discussion

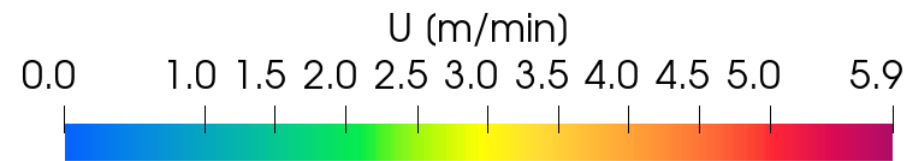
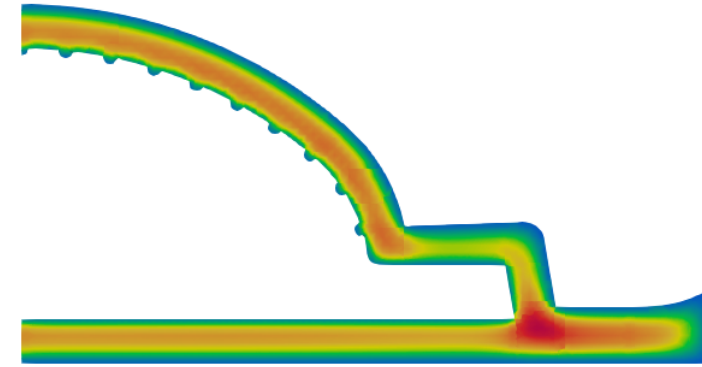
CONV



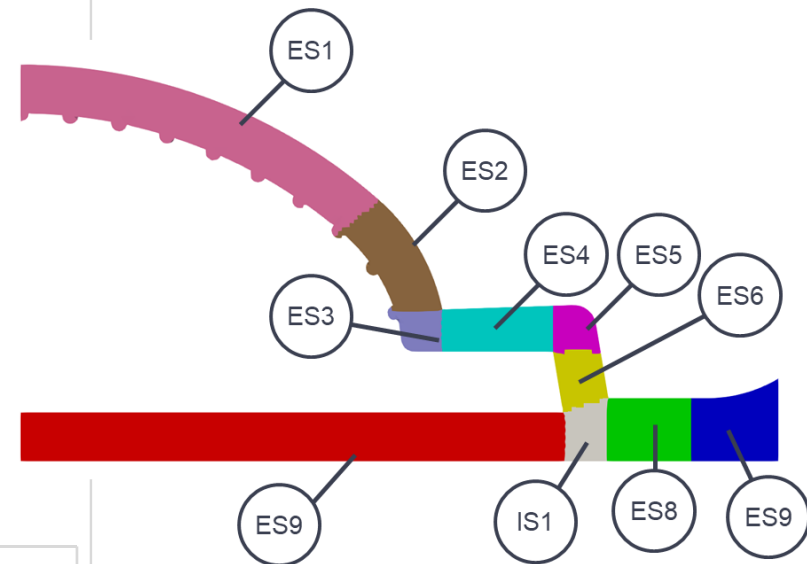
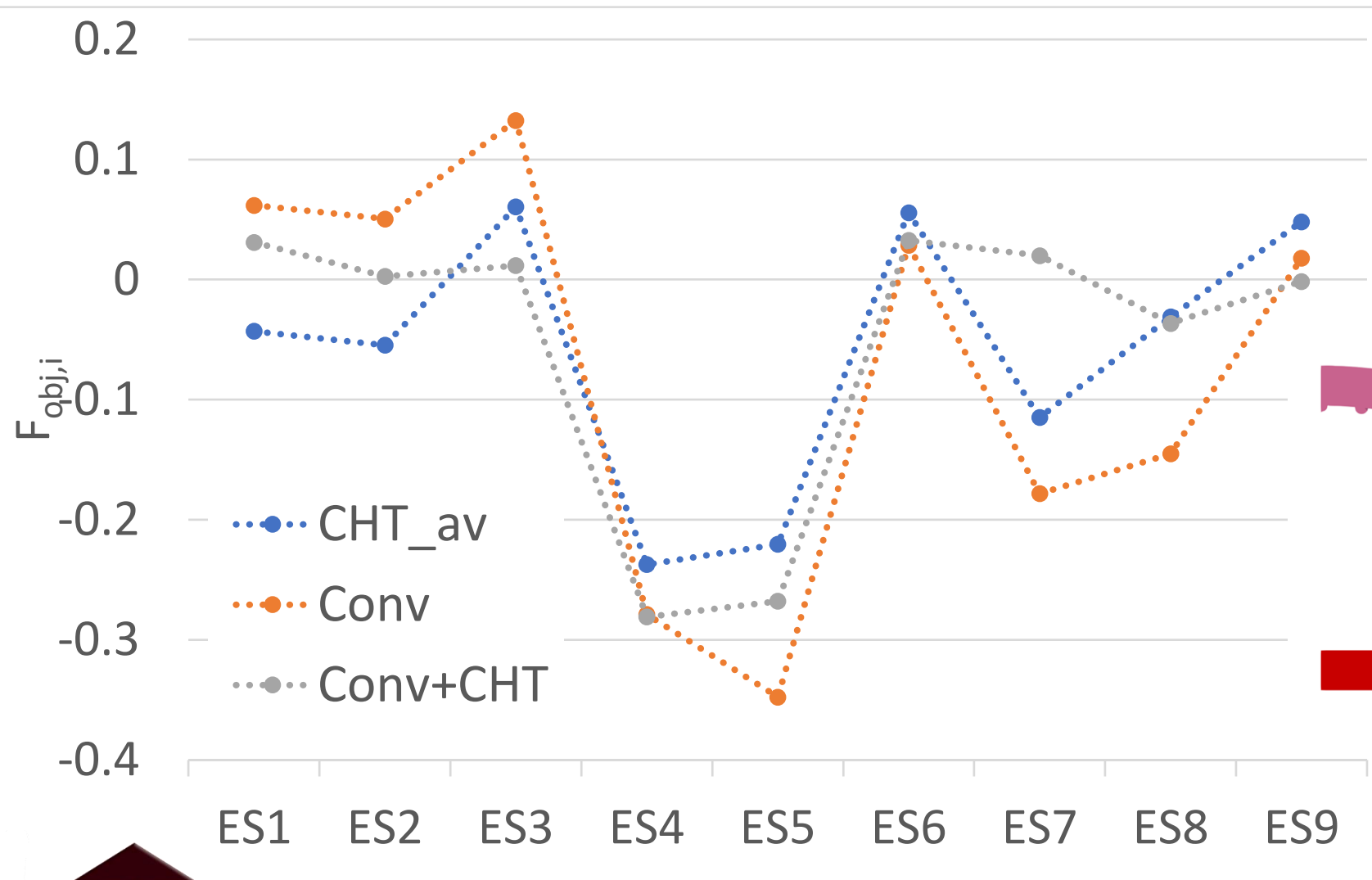
CHT



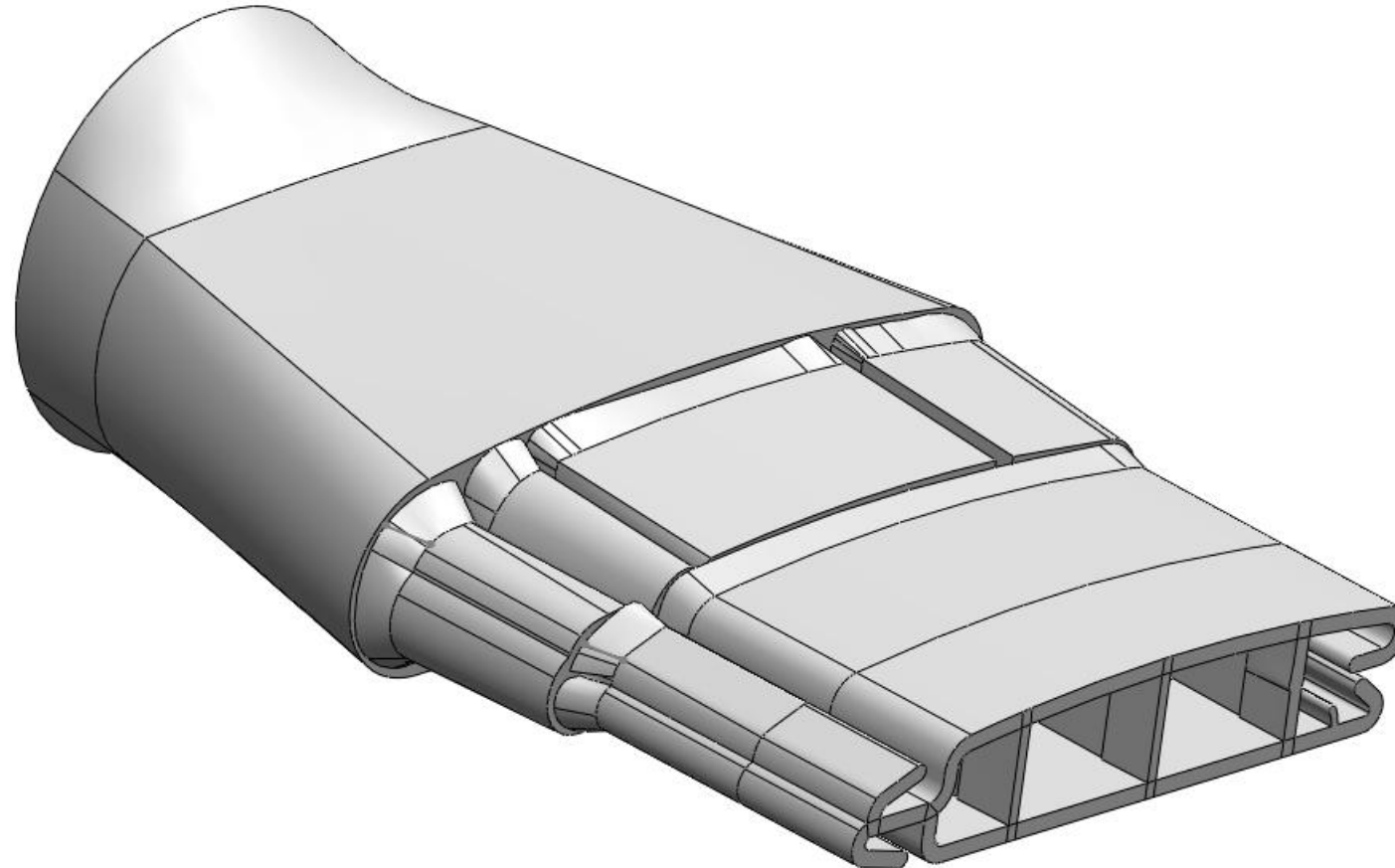
CONV+CHT



Results and Discussion



Case Study II

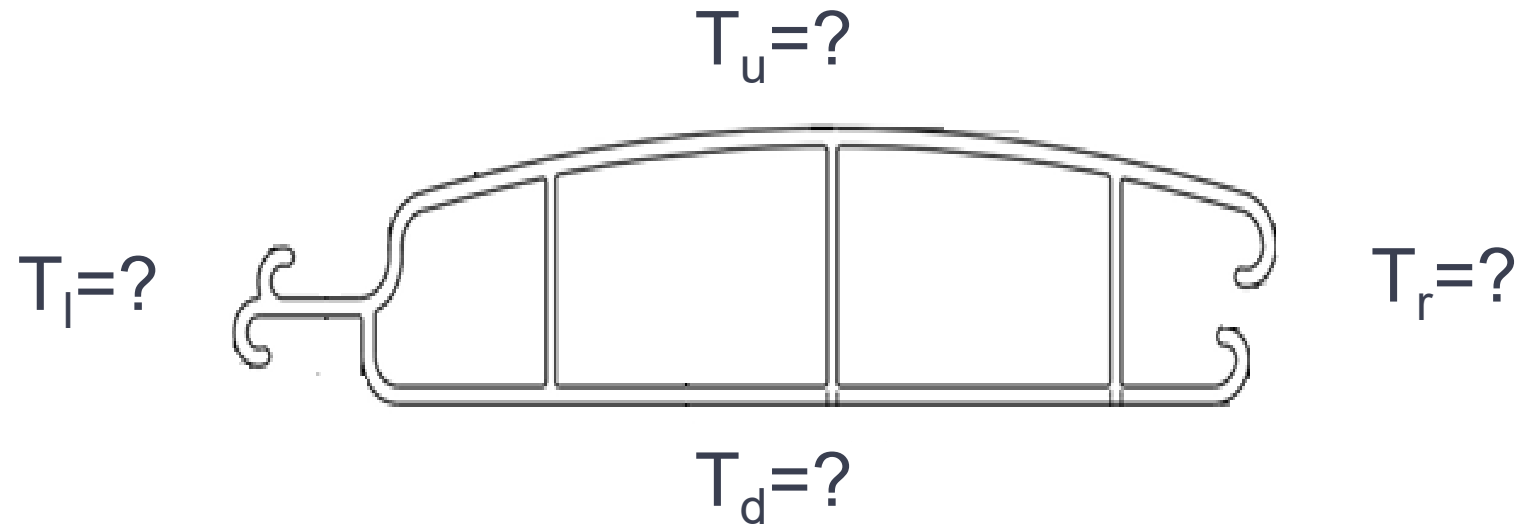


Previously designed Flow Channel

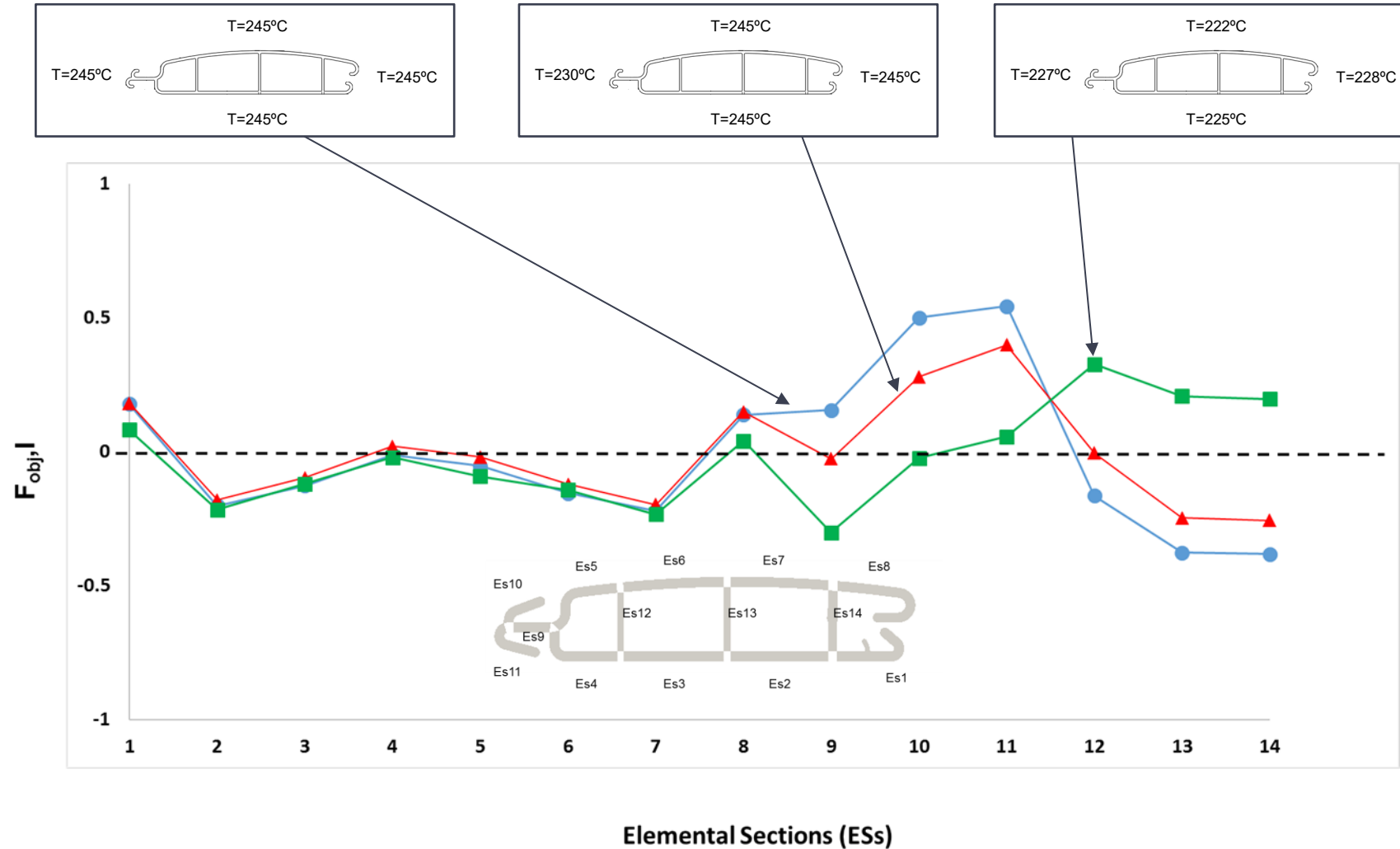
A Rajkumar et al., Differential Heating as a Strategy for Controlling the Flow Distribution in Profile Extrusion Dies, OFW11 Book, Springer, 2019

Case Study II

Test the effect of non-uniform temperature distribution

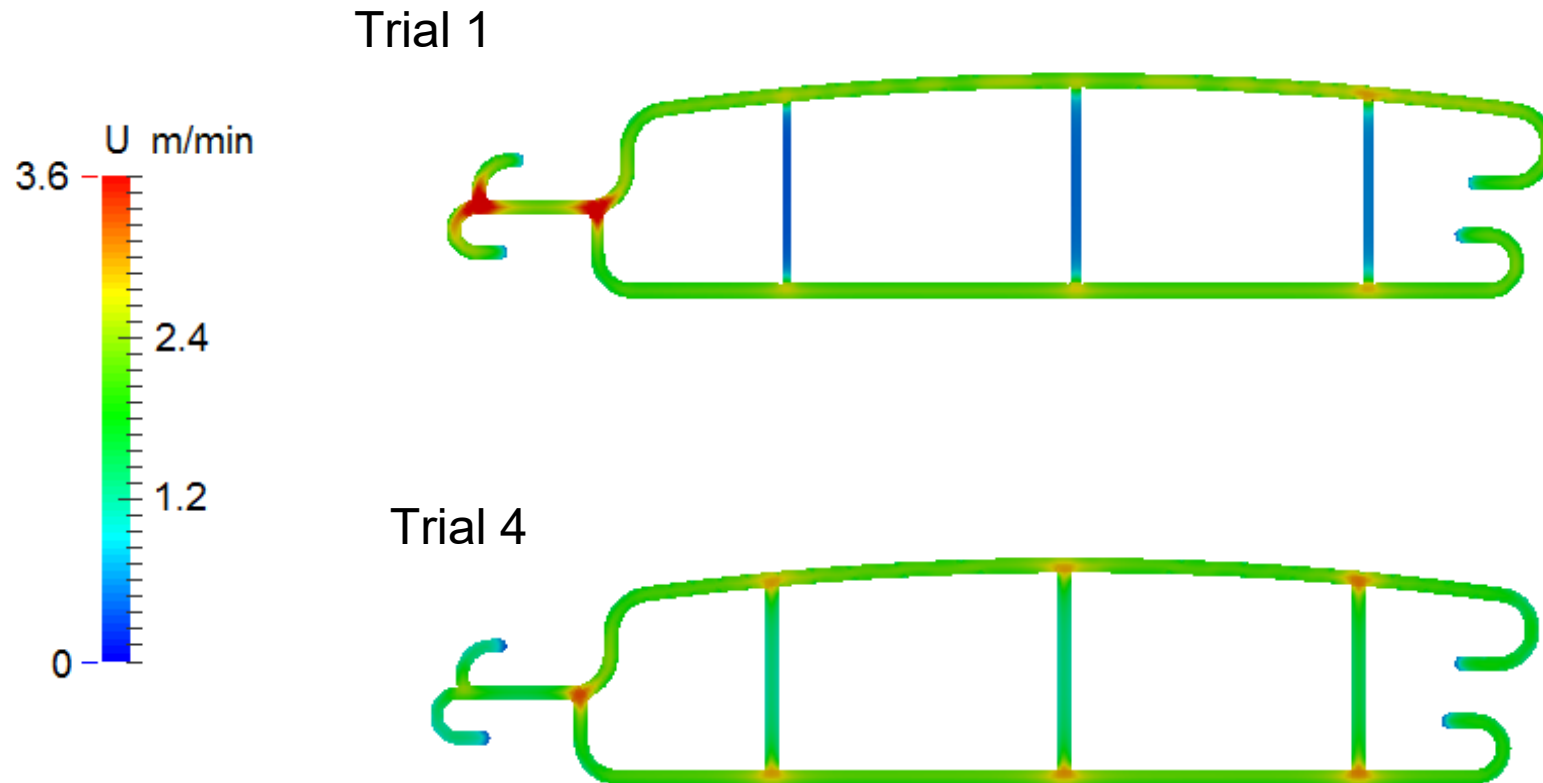


Case Study II – Design Iterations



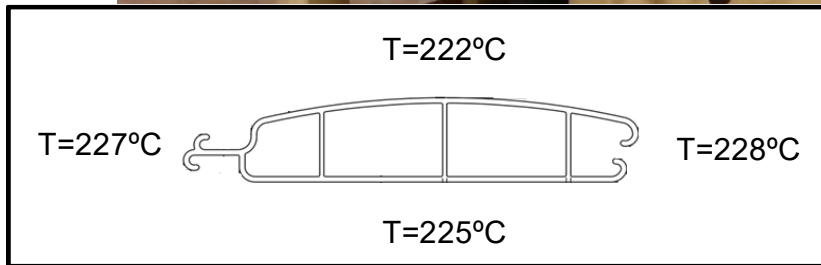
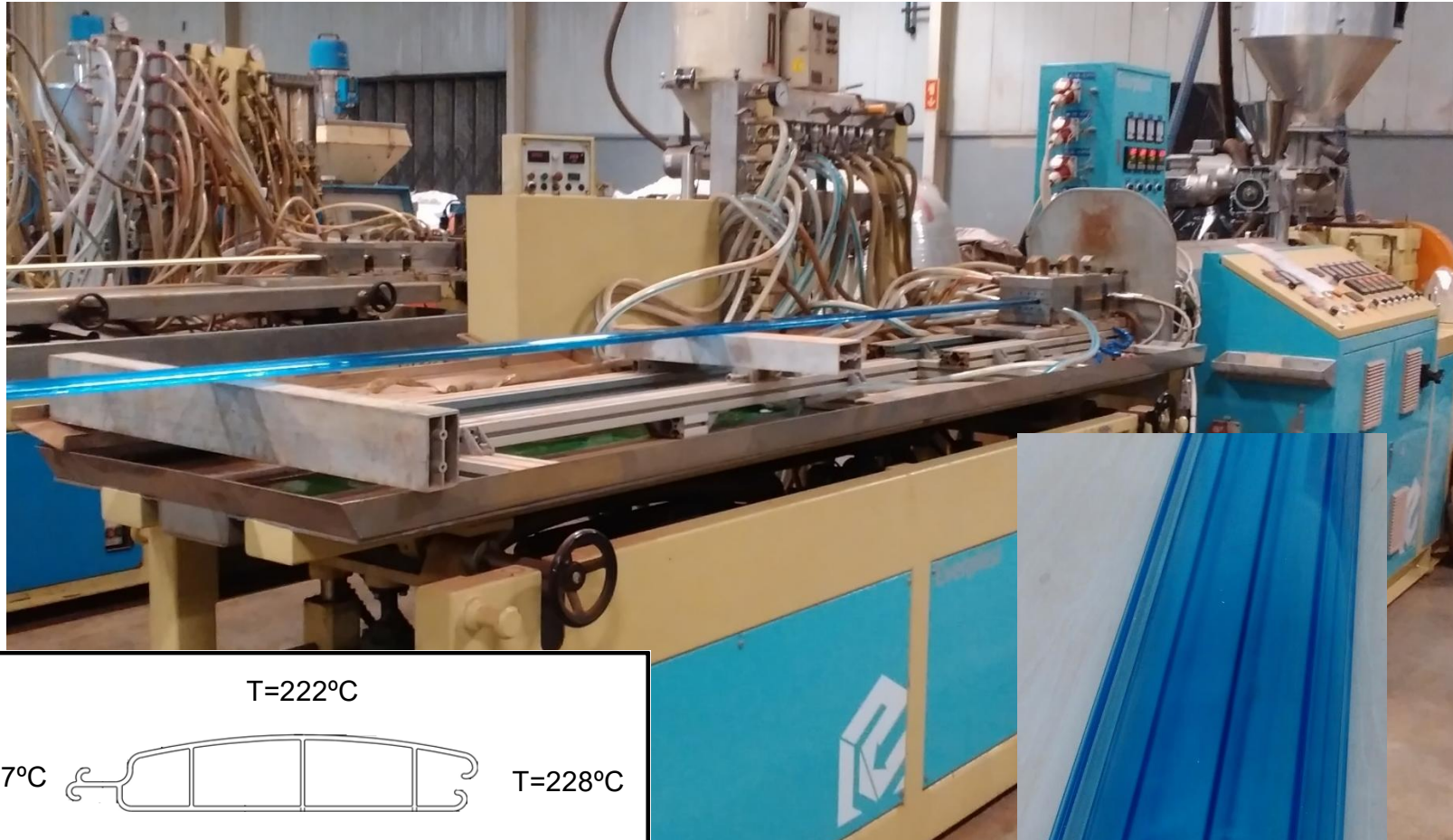
A Rajkumar et al., Differential Heating as a Strategy for Controlling the Flow Distribution in Profile Extrusion Dies, OFW11 Book, Springer, 2019

Case Study II – Design Iterations

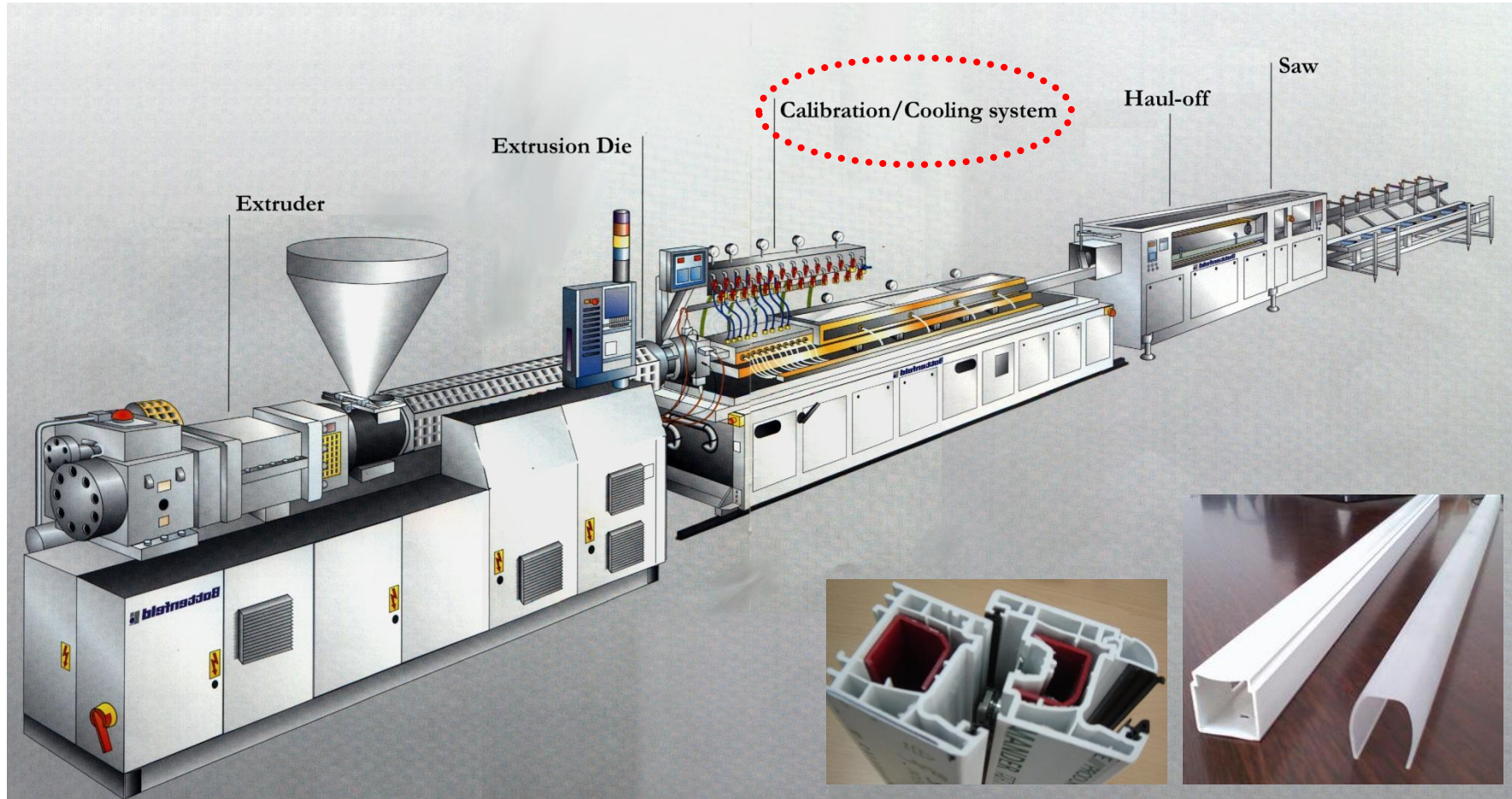


A Rajkumar et al., Differential Heating as a Strategy for Controlling the Flow Distribution in Profile Extrusion Dies, OFW11 Book, Springer, 2019

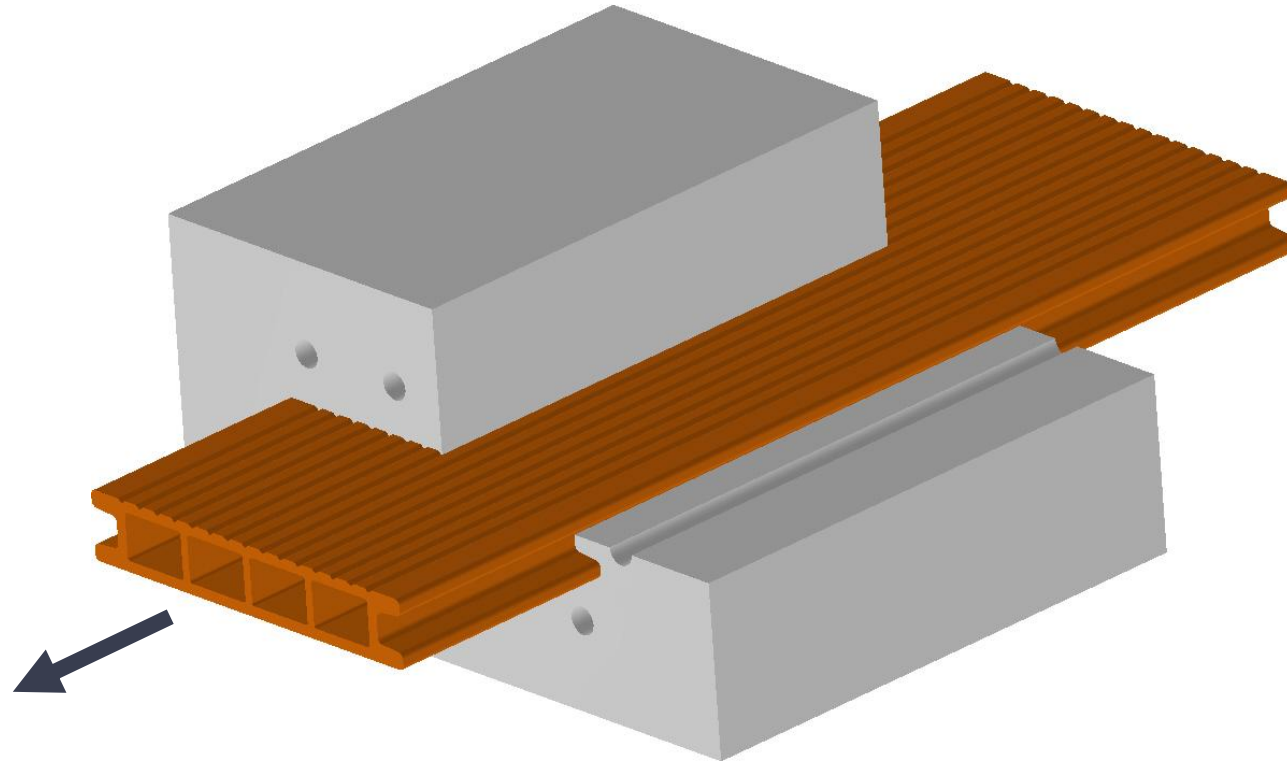
Case Study II – Experimental Trial



A Rajkumar et al., Differential Heating as a Strategy for Controlling the Flow Distribution in Profile Extrusion Dies, OFW11 Book, Springer, 2019



Problems to solve: obtain the distribution of T



Methodology Employed

- **Coupled approach**
- **Conditional Volume Averaging** technique was used to derive an equation for the mixture temperature T_m

Final governing equation:

$$\frac{\partial(\rho_m c_{P,m} T_m)}{\partial t} + \nabla \cdot (\mathbf{U}_m \rho_m c_{P,m} T_m) - \nabla \cdot k_m \nabla T_m =$$

$$-\nabla \cdot \left[\frac{k_m \nabla \alpha_p - \alpha_p \alpha_c (\bar{k}^p - \bar{k}^c) (\frac{1}{\bar{k}^p} - \frac{1}{\bar{k}^c}) h \mathbf{n}}{h (\frac{\alpha_p}{\bar{k}^p} + \frac{\alpha_c}{\bar{k}^c}) + \nabla \alpha_p \cdot \mathbf{n}} \nabla T_m \cdot \mathbf{n} \right]$$

OpenFOAM Code

```
// Temperature equation with jump
tmp<fvScalarMatrix> TEqn
(
    fvm::ddt(rhoCp, T)
    + fvm::div(phi * rhoCpf, T, "div(phi,T)")
    - fvm::laplacian(k, T, "laplacian(k,T)")
    ==
    - fvc::div(sjump)
);
```

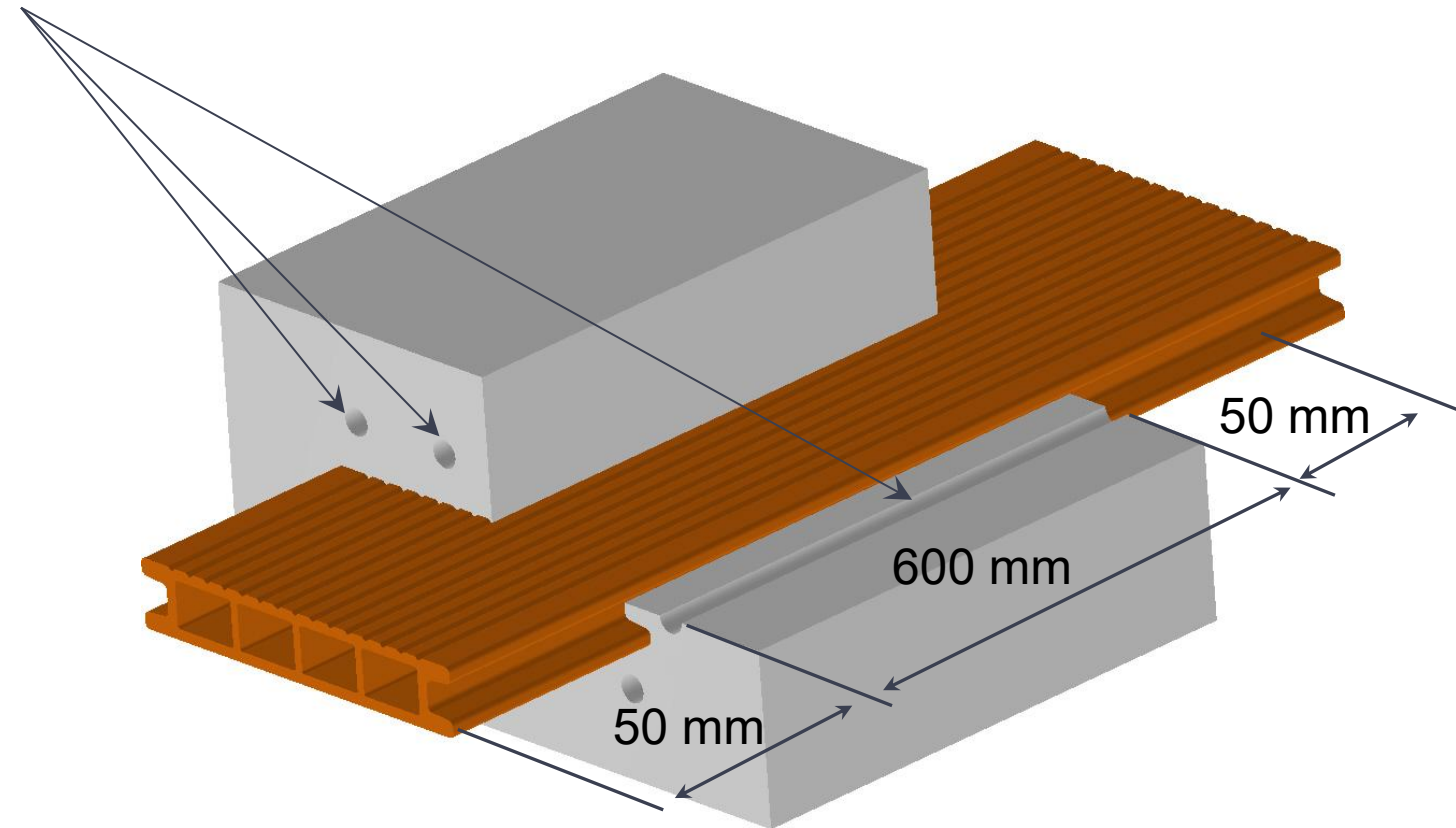
Subscripts

p -polymer
 c -calibrator



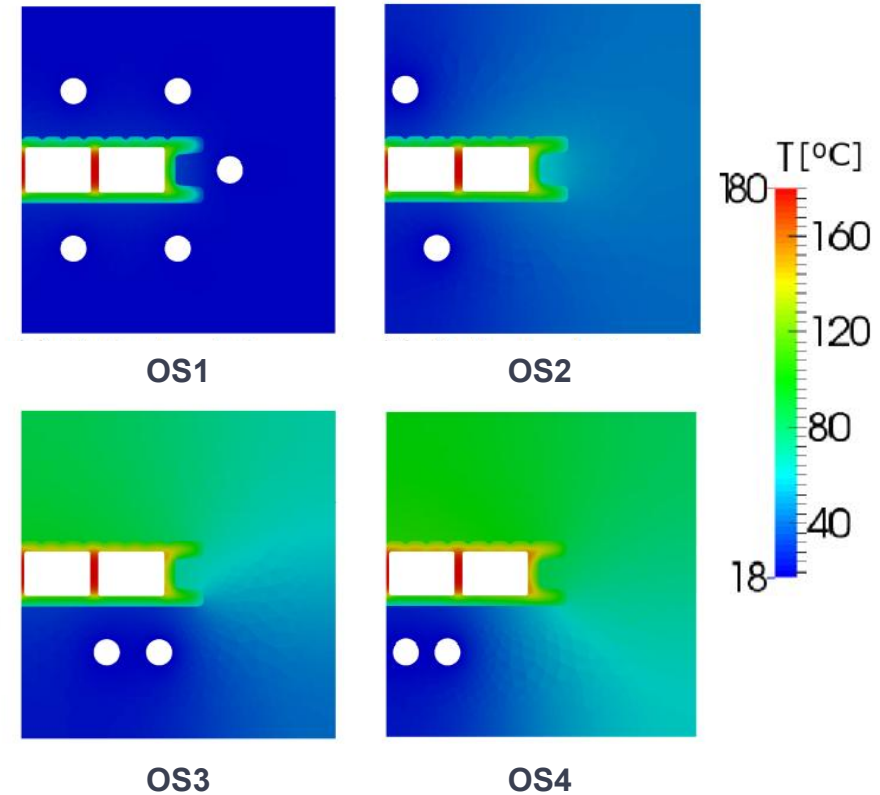
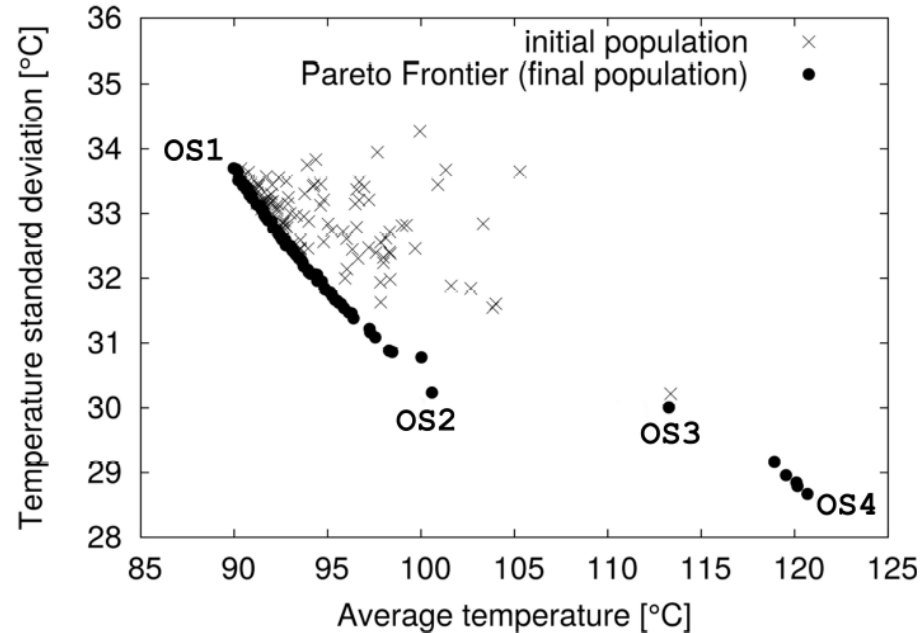
Case Study I

10 cooling channels (\varnothing 10 mm)



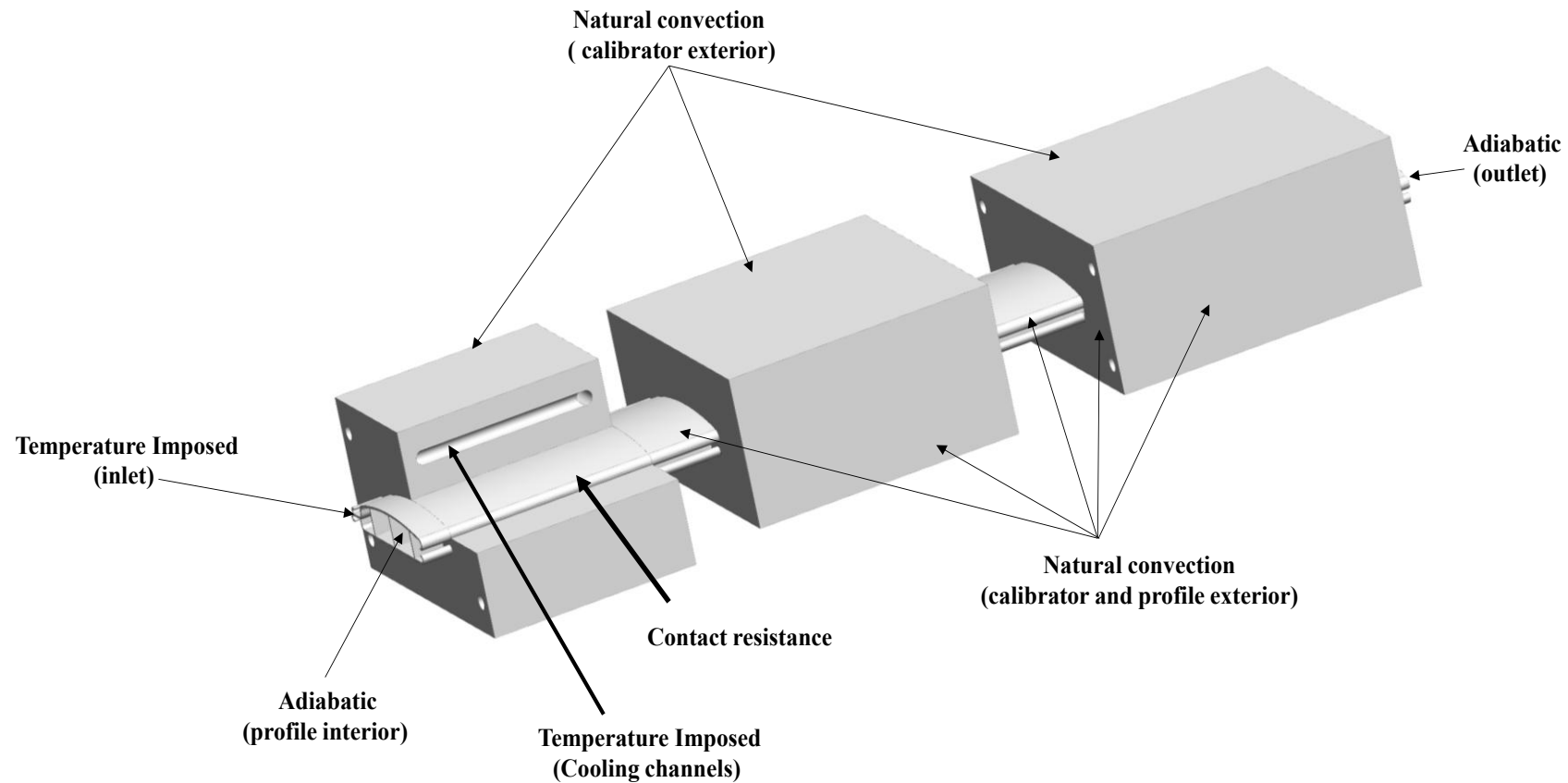
Case Study I

Coupling OpenFOAM with  (<https://dakota.sandia.gov/>)
Study on the effect of the cooling channel location



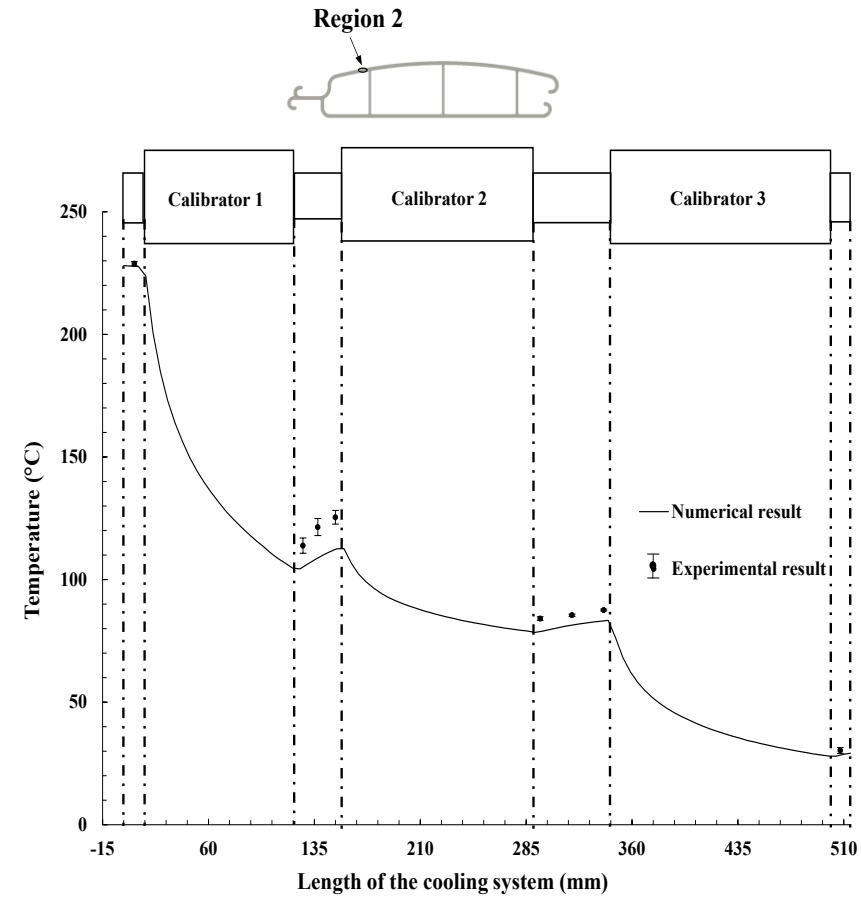
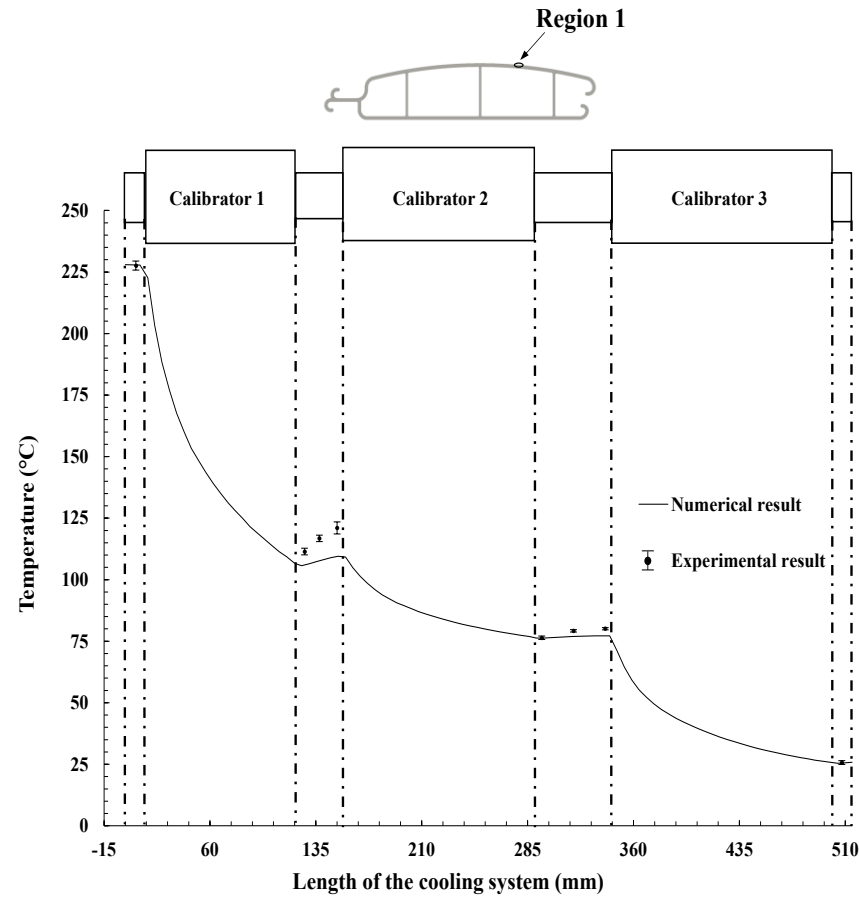
F Habla, et al., Development and validation of a model for the temperature distribution in the extrusion calibration stage, Applied Thermal Engineering, 100, 2016

Case Study - Experimental Assessment



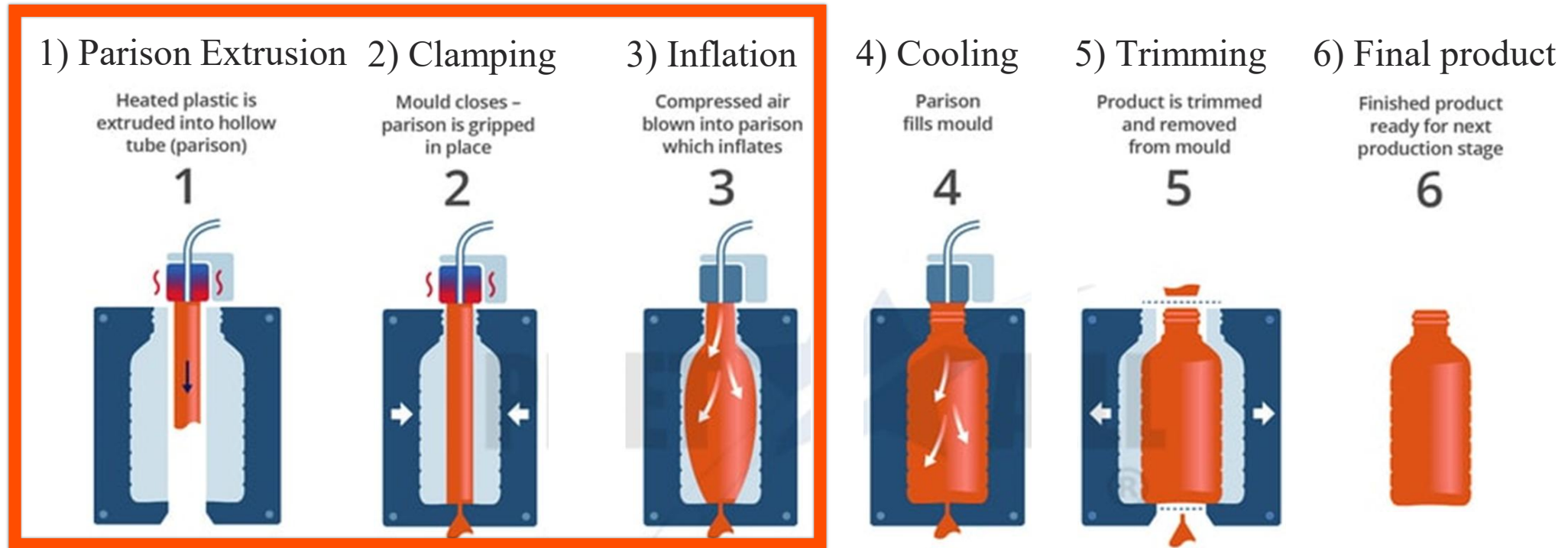
A Rajkumar et al., Profile extrusion: experimental assessment of a numerical model for heat transfer in the cooling/calibration stage, PES, 2019

Case Study - Experimental Assessment



A Rajkumar et al., Profile extrusion: experimental assessment of a numerical model for heat transfer in the cooling/calibration stage, PES, 2019

Extrusion Blow Molding Simulator

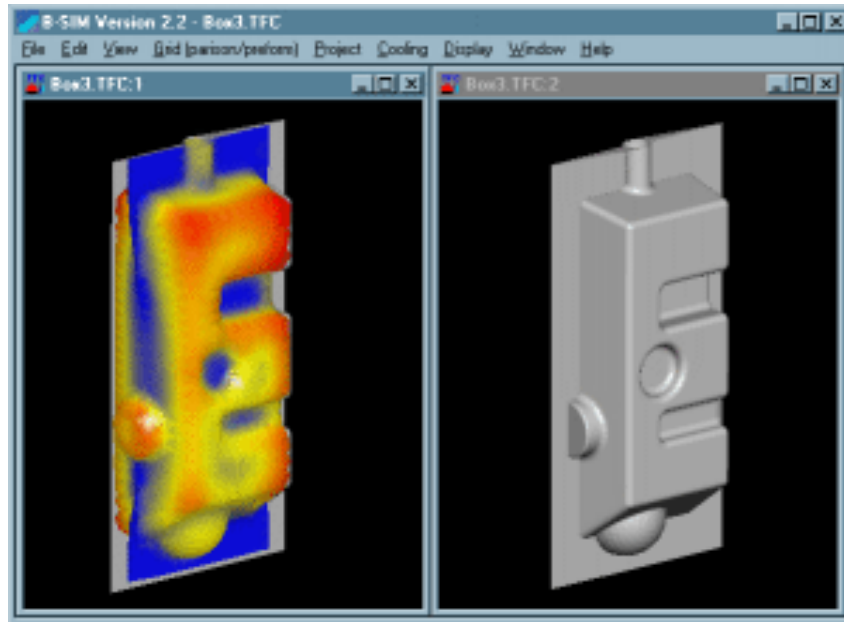


MOTIVATION

Available software

B-Sim

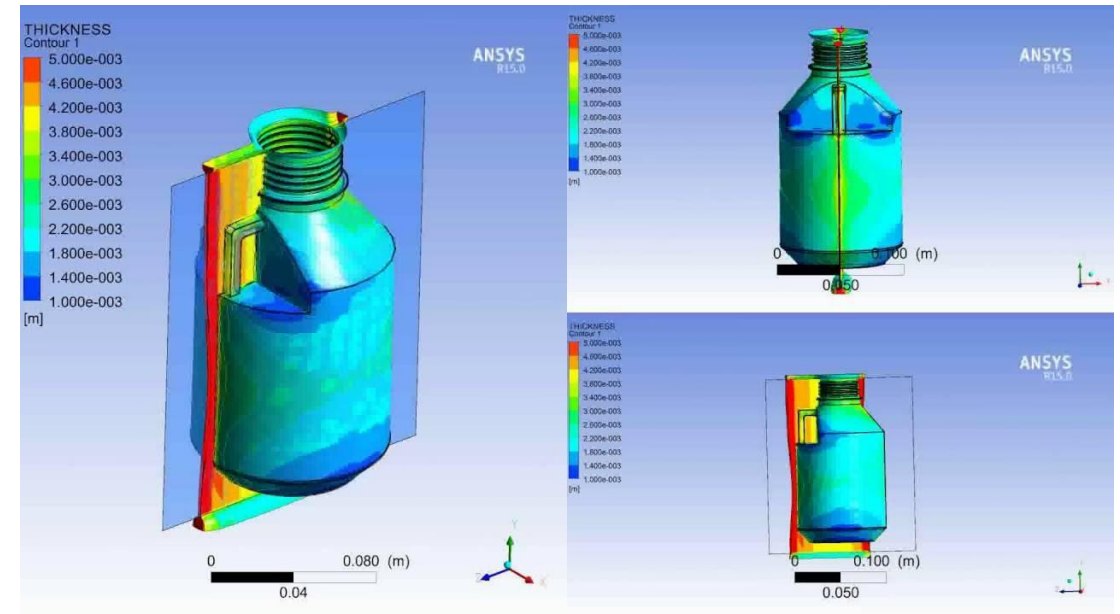
Can only simulate clamping and inflation



Adapted from “Tutorial - Extrusion blow molding”, by Accuform, retrieved from <https://www.t-sim.com/Refbsim/Example3.htm>

Ansys Polyflow

Simulates extrusion, clamping and inflation



Adapted from “Fluid Flow Blow Molding of a cane using Ansys Polyflow”, by Sameera Weeratunga, retrieved from <https://youtu.be/ABRukstpIX8>

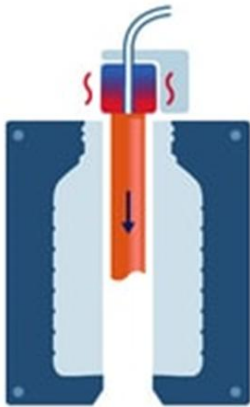
Separate extrusion and mold clamping and inflation steps (~~Automatic optimization~~)

Extrusion Blow Molding Simulator

1) Parison Extrusion

Heated plastic is extruded into hollow tube (parison)

1



2) Clamping

Mould closes - parison is gripped in place

2



3) Inflation

Compressed air blown into parison which inflates

3



4) Cooling

Parison fills mould

4



5) Trimming

Product is trimmed and removed from mould

5



6) Final product

Finished product ready for next production stage

6



Constitutive Models

Linear Elastic and Hyperelastic

- Linear Elastic Generalized Hooke's law for plane stresses
- Mooney–Rivlin
- Total Lagrangian Approach

Viscoelastic K-BKZ Model

- Updated Lagrangian approach

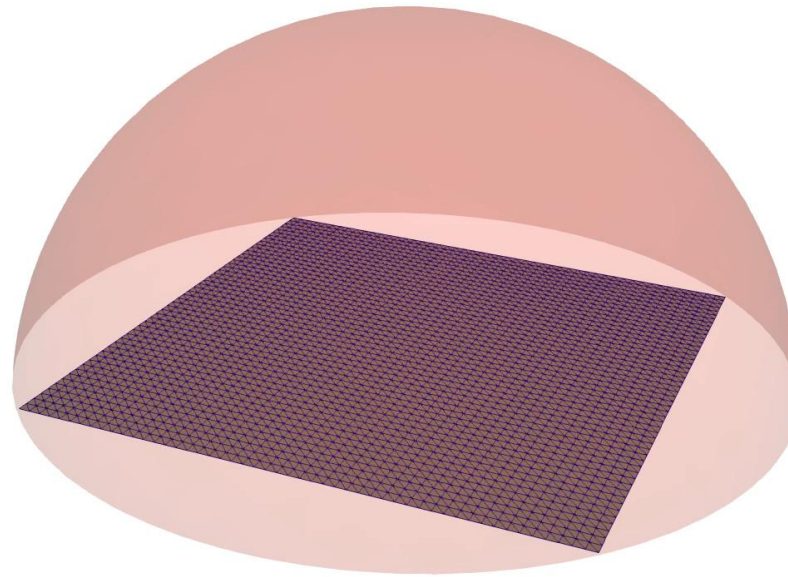
$$\boldsymbol{\sigma} = \int_{-\infty}^t m(t-t') h(\mathbf{I}_1, \mathbf{I}_2) \mathbf{C}_t^{-1}(t') dt'$$

- $m(t-t')$ - linear-viscoelastic memory function
- $h(\mathbf{I}_1, \mathbf{I}_2)$ - damping function
- \mathbf{C}_t^{-1} - Finger tensor

J. Vlachopoulos, B.L. Koziey, M.O. Ghafur, SIMULATION OF THERMOFORMING AND BLOWMOLDING - THEORY AND EXPERIMENTS, (1995) 321–383.

Time evolution (Newton's 2nd Law):

$$\text{mass} \times \text{acceleration} = \sum (\text{Force}_{\text{body}} + \text{Force}_{\text{pressure}} + \text{Force}_{\text{internal}})$$

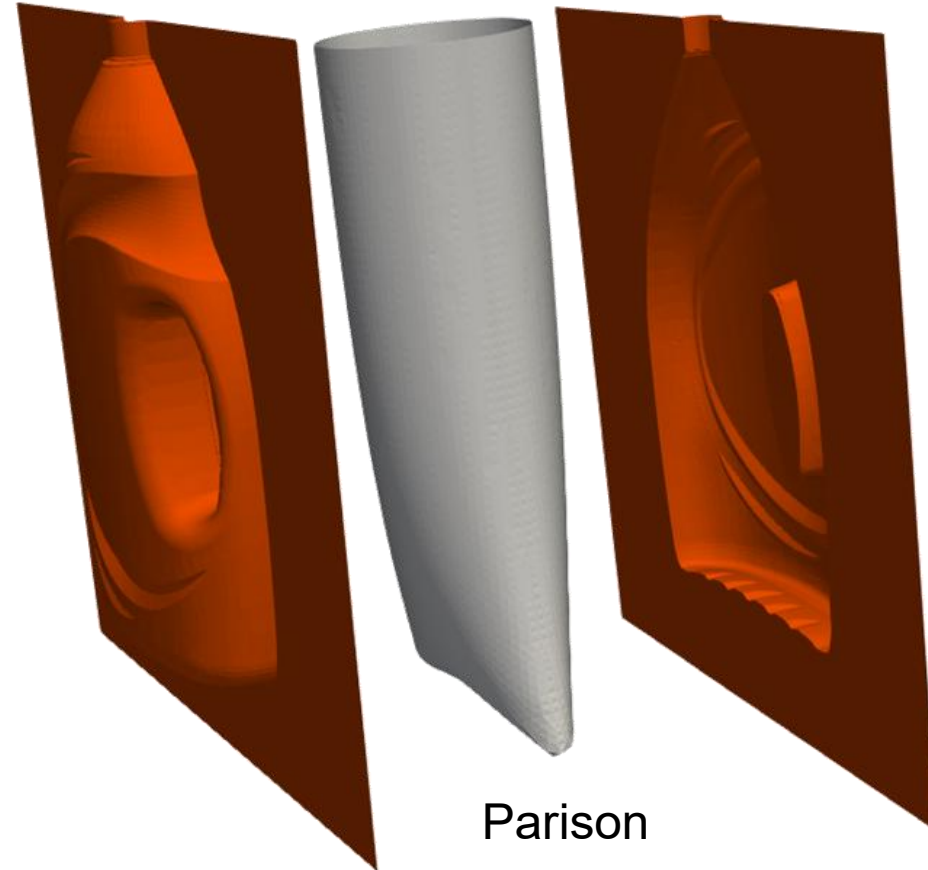


Case Study

Container



Data for simulation

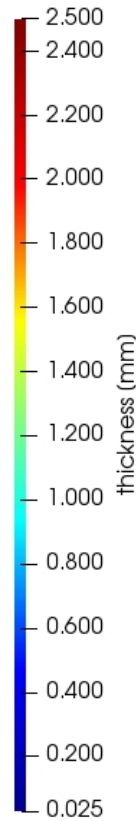
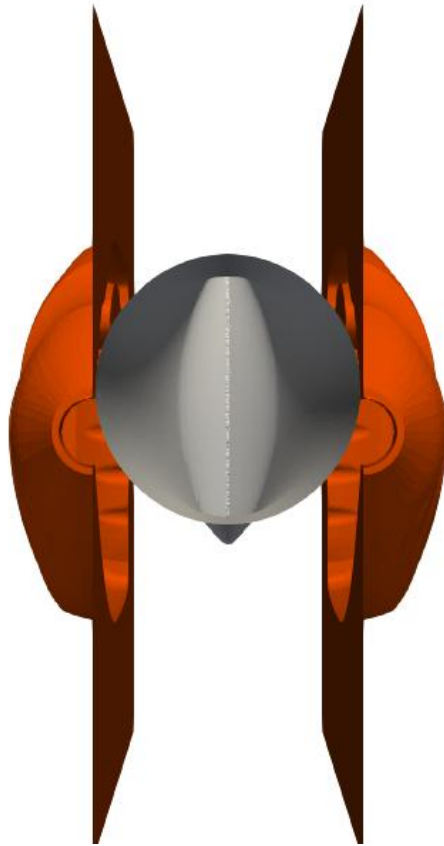


Parison

Mold Surface

Mold Surface

Case Study

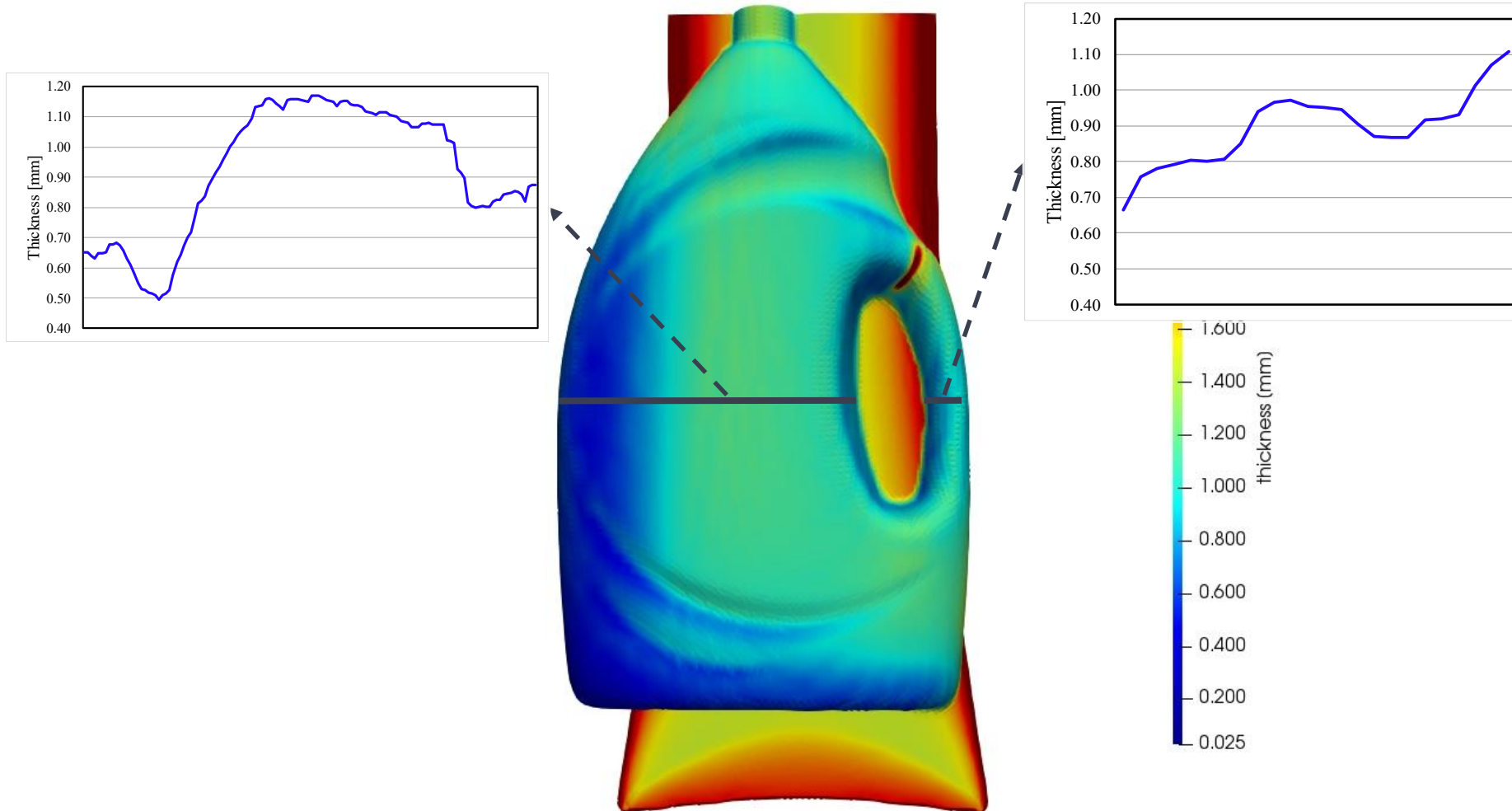


Thickness Distribution



Case Study

Thickness Distribution

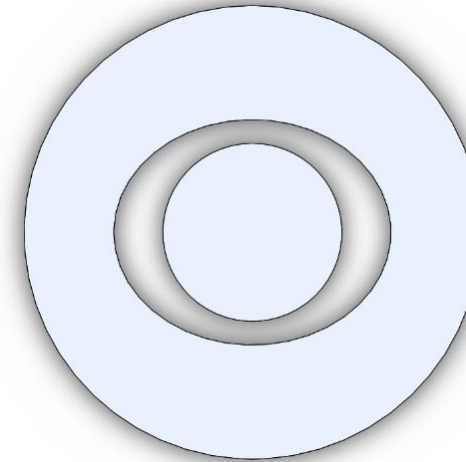


Parison thickness optimization – *Methodology*

Variables to consider



Moving mandrel

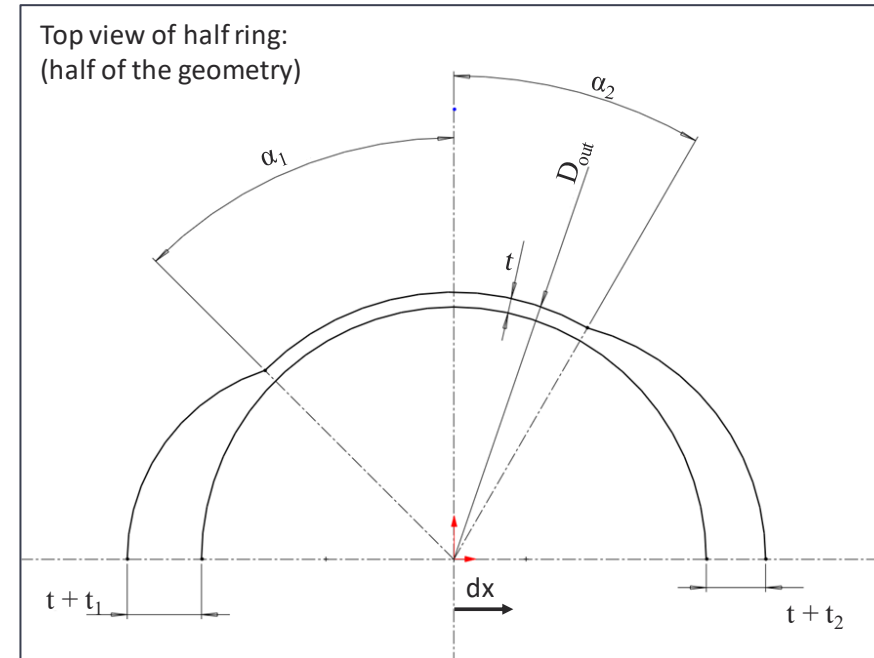


Extrusion Die Ovalization

Parison thickness optimization – Methodology



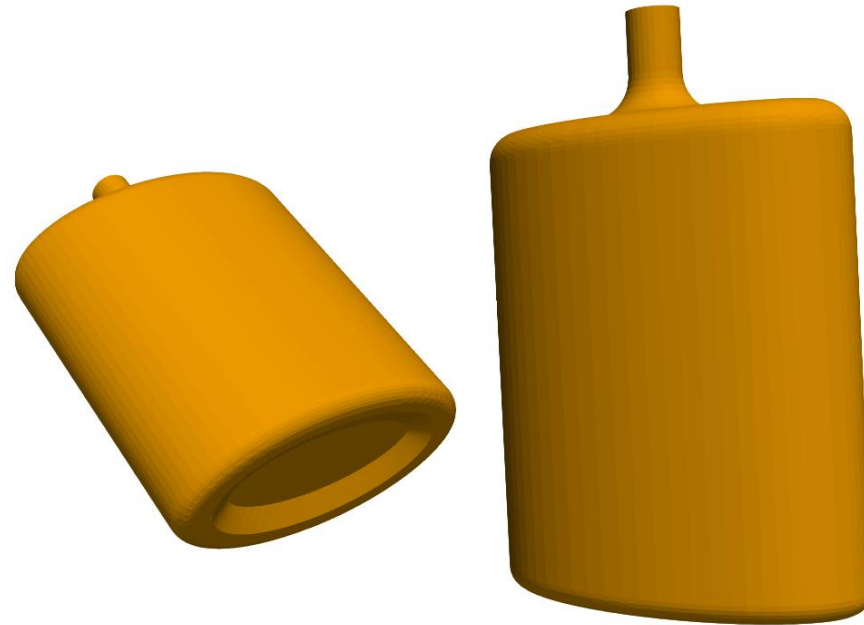
Thickness of n layers (t_{h_i})
(spline fitting)



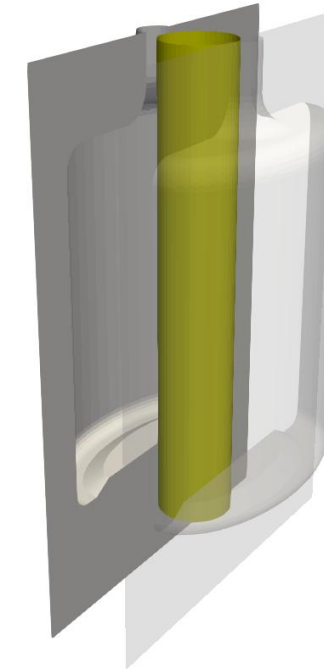
Ovalization ($t_1, t_2, \alpha_1, \alpha_2$)

Mold Clamping and Inflation

Parison thickness optimization – *Case Study*



Container

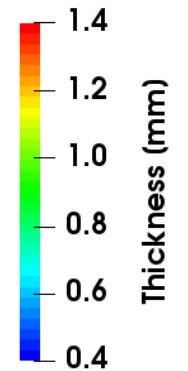


Mould and Parison

Target thickness 0.9 mm / double symmetry / $\alpha_1 = \alpha_2 = 45^\circ$

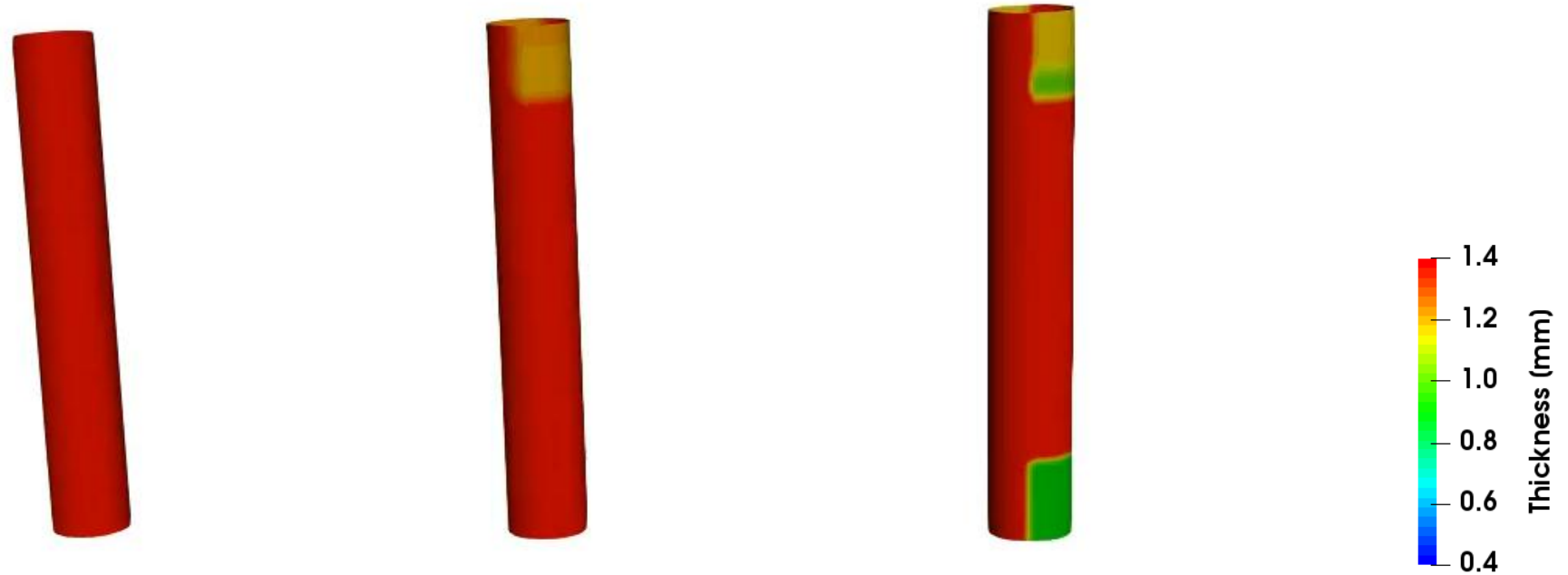
Parison thickness optimization – Case Study

Initial trial

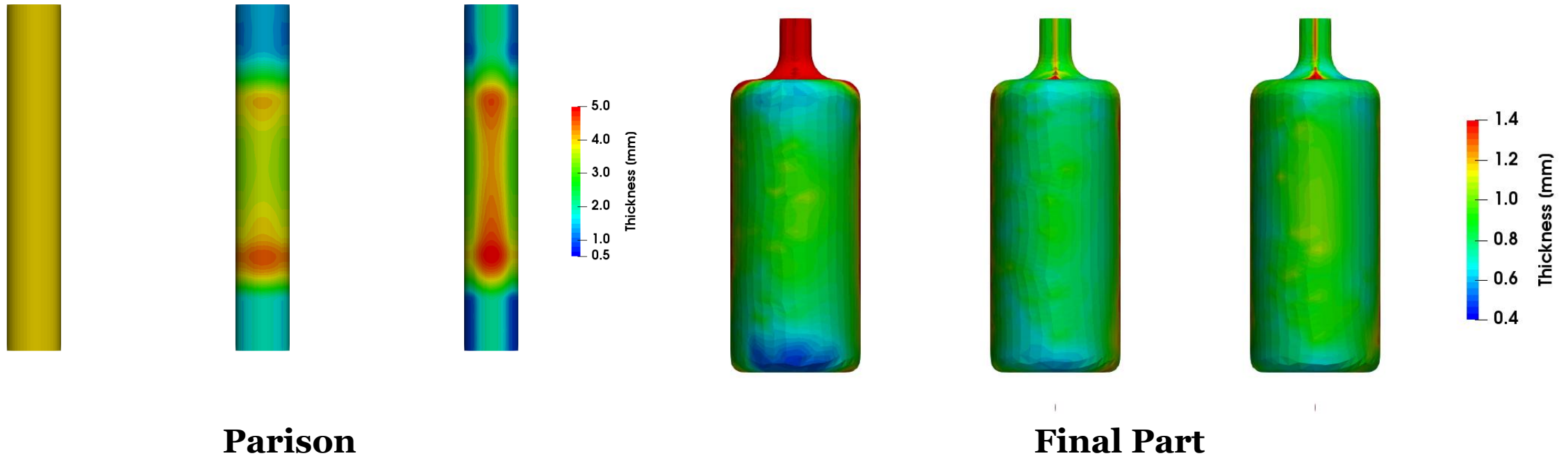


$$th_i = 3.95 \text{ mm} / t_1 = t_2 = 0$$

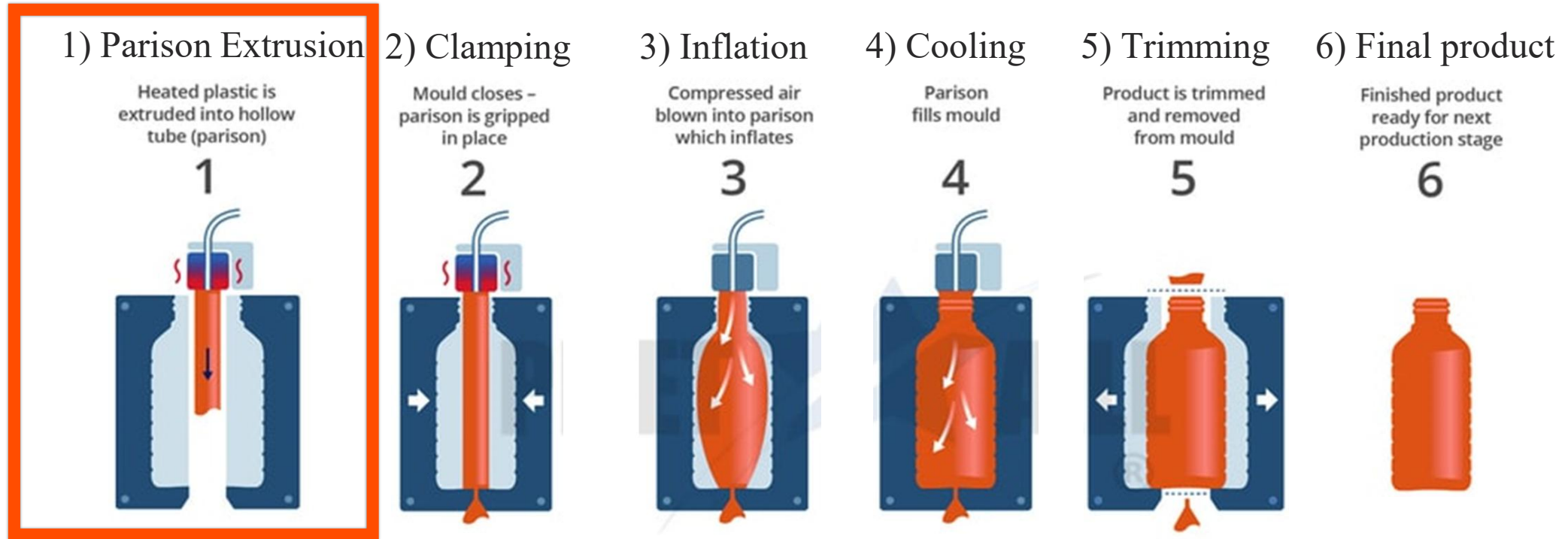
Parison thickness optimization – Case Study



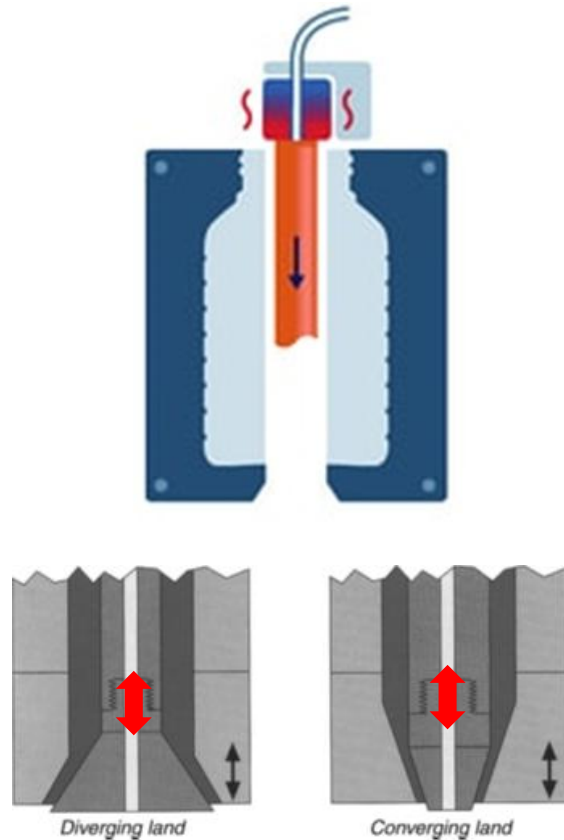
Parison thickness optimization – Case Study



Extrusion Blow Molding Simulator



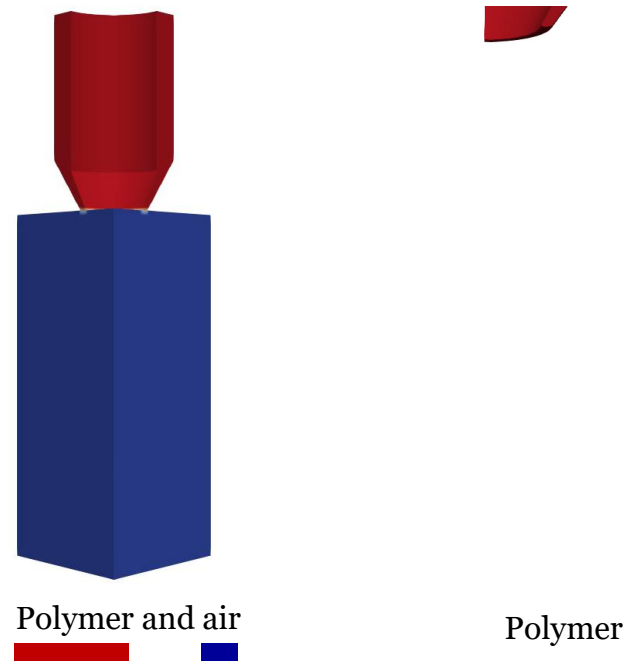
Parison Extrusion – Methodology



Moving mandrel

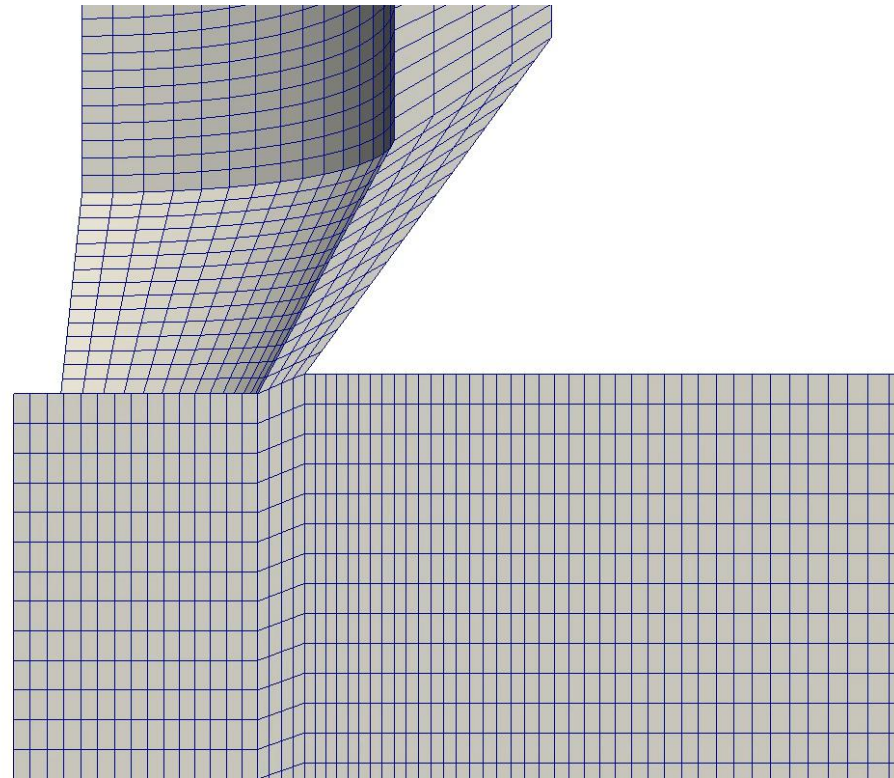
Numerical approach

- New multiphase solver in OpenFOAM
- Volume-of-Fluid Formulation
- Differential viscoelastic models



Parison Extrusion – Methodology

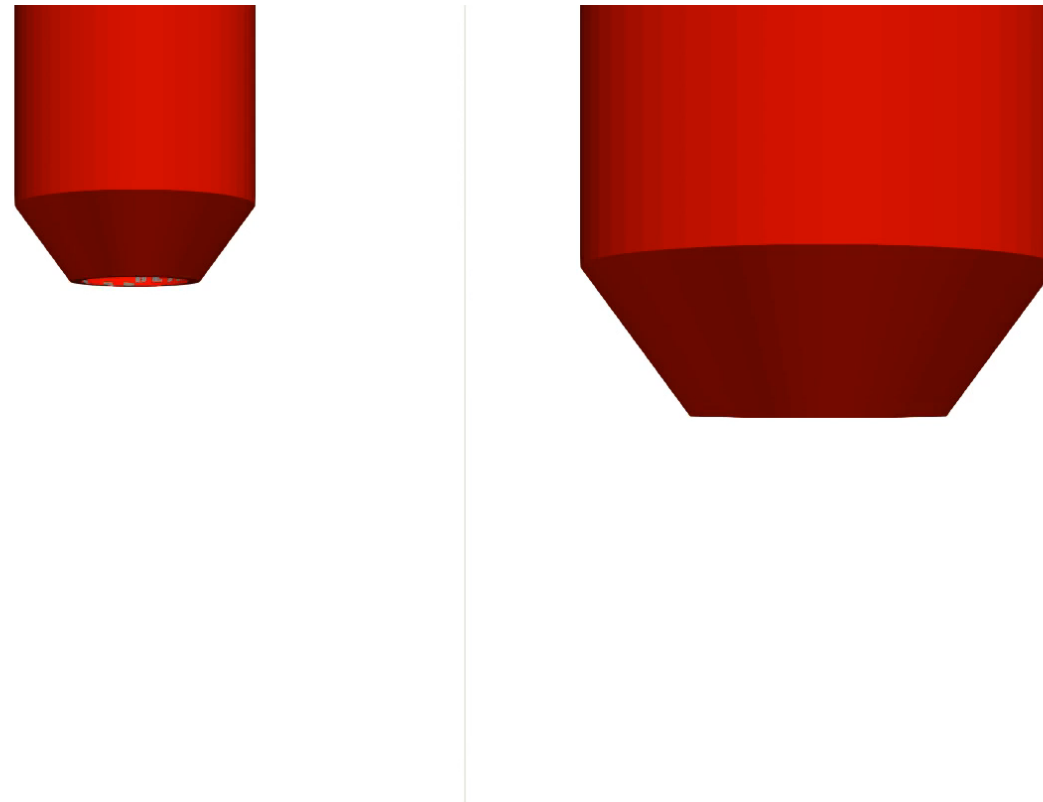
Moving Mandrel



Computational mesh

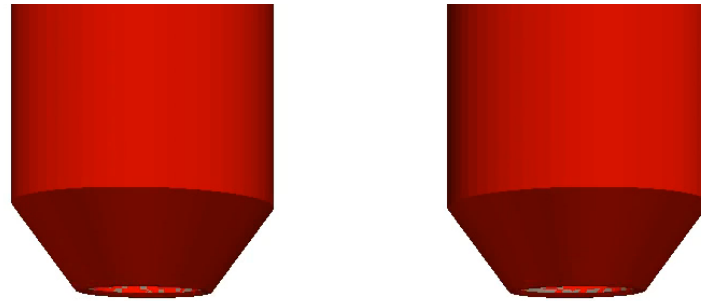
Parison Extrusion

Typical run



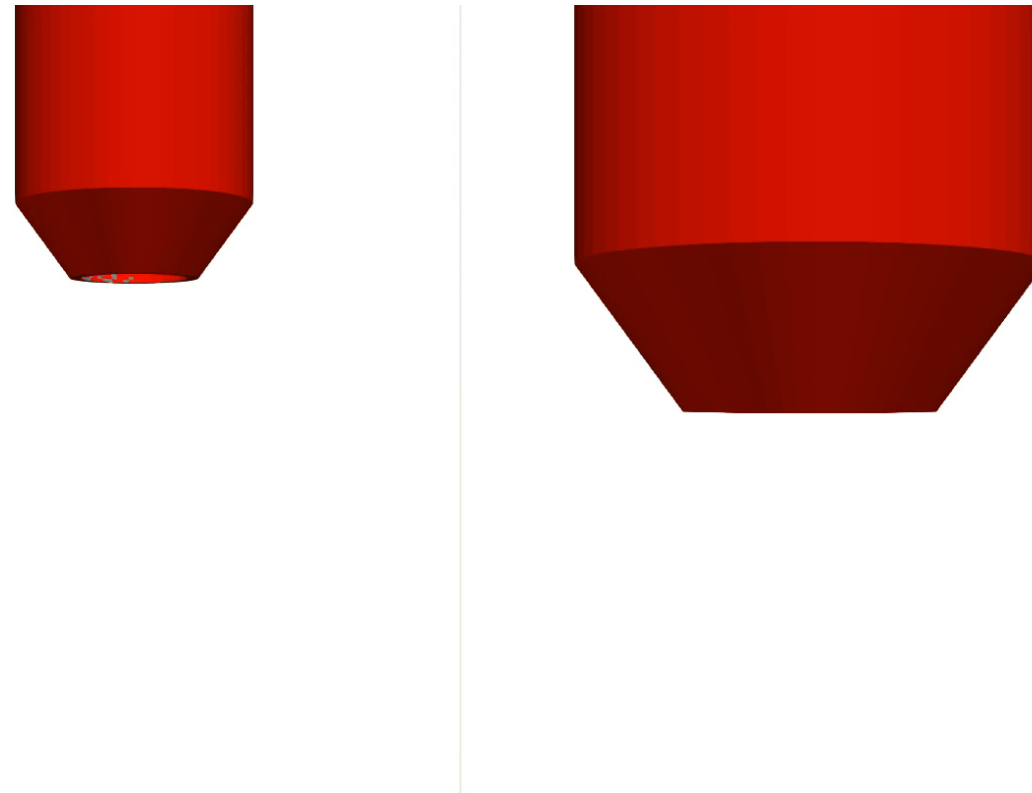
Parison Extrusion

Effect of density



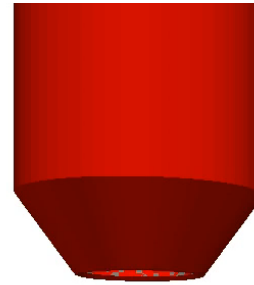
Parison Extrusion

Moving Mandrel

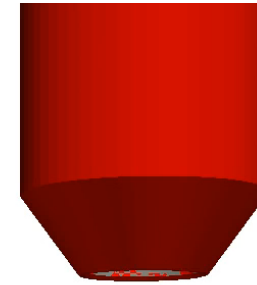


Parison Extrusion

Effect of elasticity

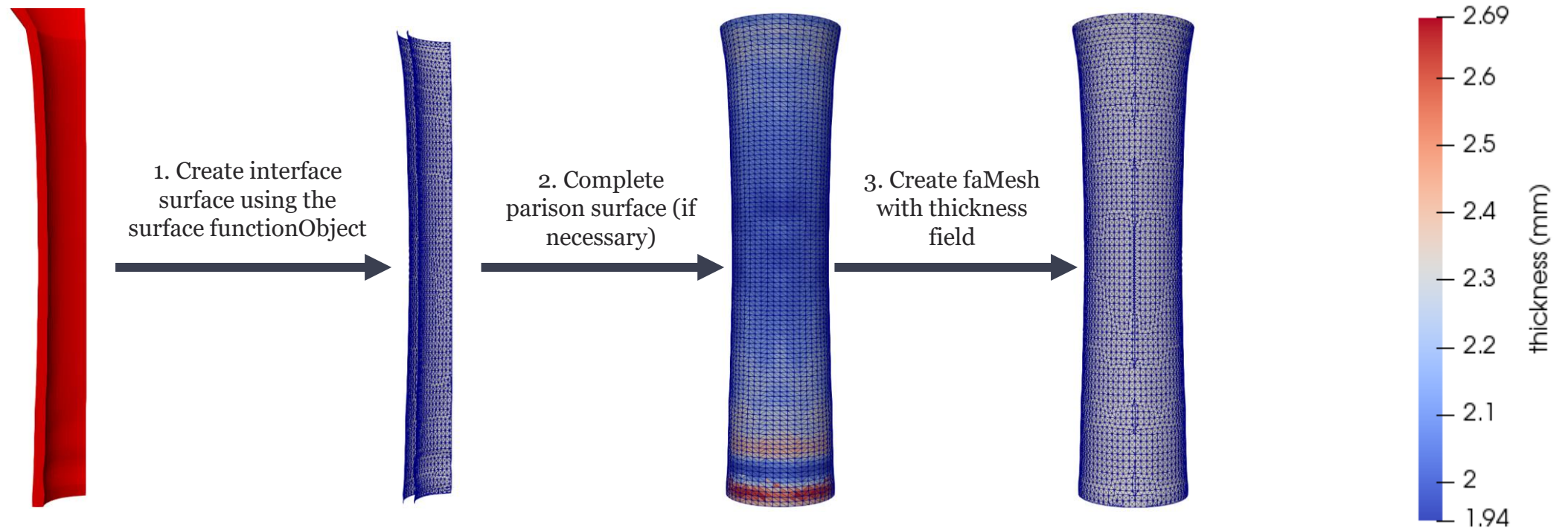


Low

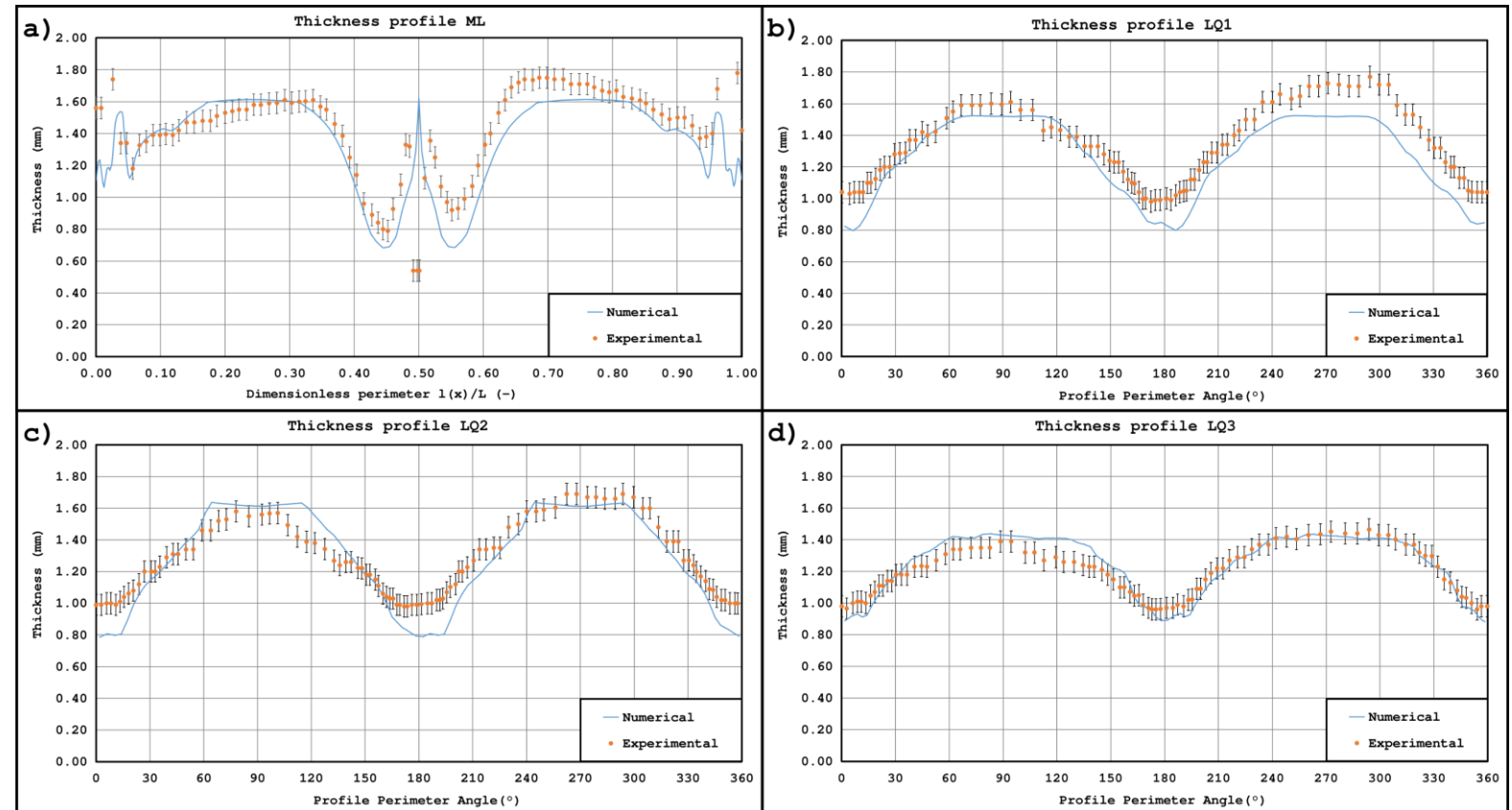
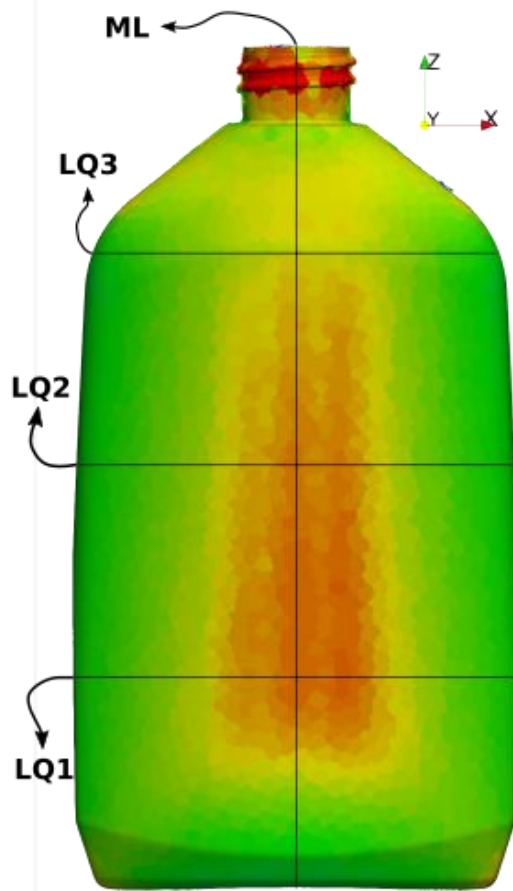


Moderate

Link Extrusion and Inflation



Experimental Validation



openInjMoldsim Solver

- Compressible, non-isothermal, laminar cavity flow.
- Tait equation of state.
- Cross-WLF viscosity model.
- Specific heat and thermal conductivity may depend on temperature and pressure (tabular form).
- Elastic stress in the solid phase.
- Fiber orientation (*openInjMoldSimF*).

Current activities

- Starting a new implementation from the scratch in the framework of a PhD



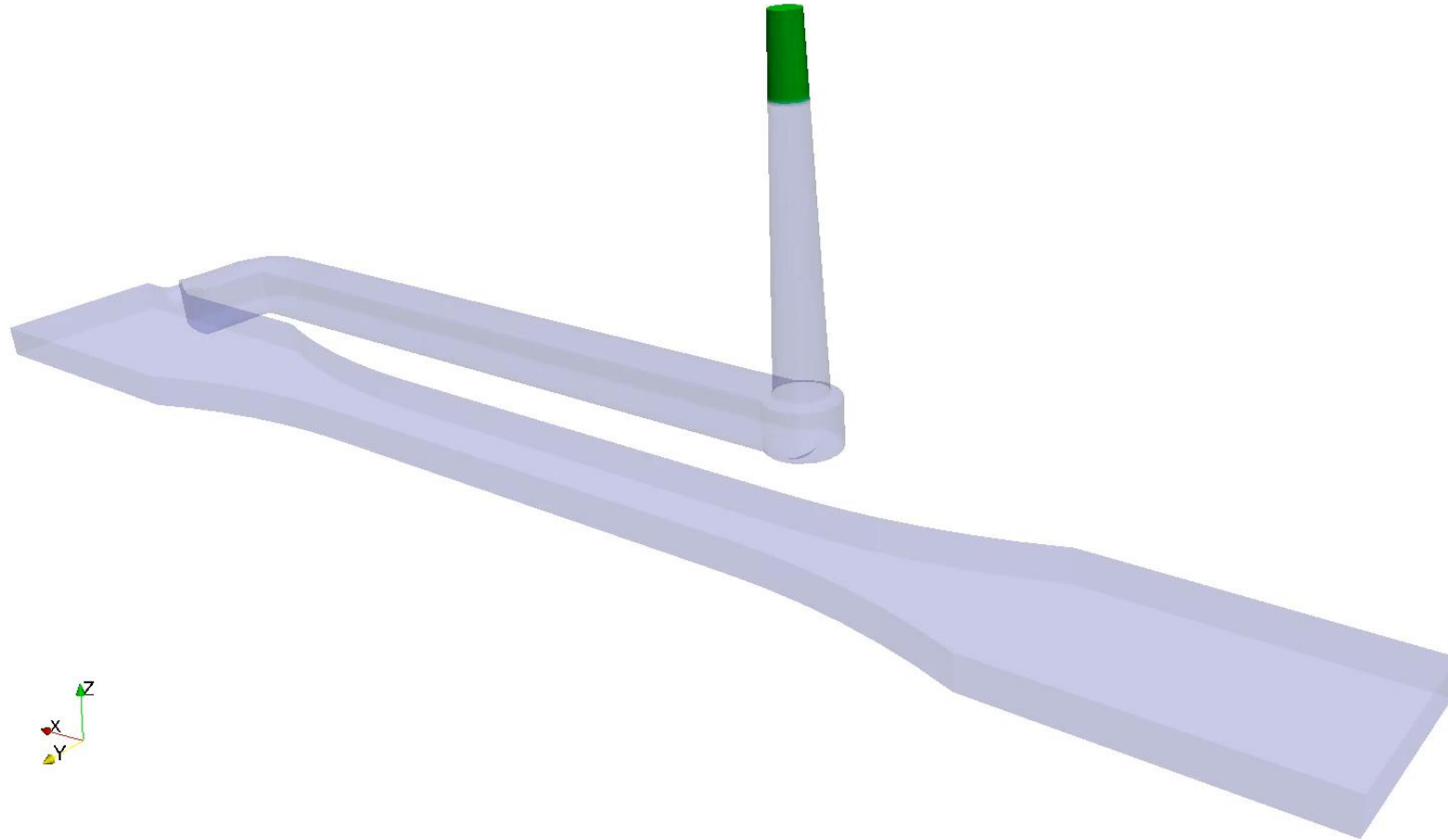
IPC



<https://github.com/krebeljk/openInjMoldSim>

N. Mole, K. Krebelj, and B. Stok.. International Journal of Advanced Manufacturing Technology, 93:4111{4124, 2017. DOI: <https://doi.org/10.1007/s00170-017-0847-3>.

Case Study

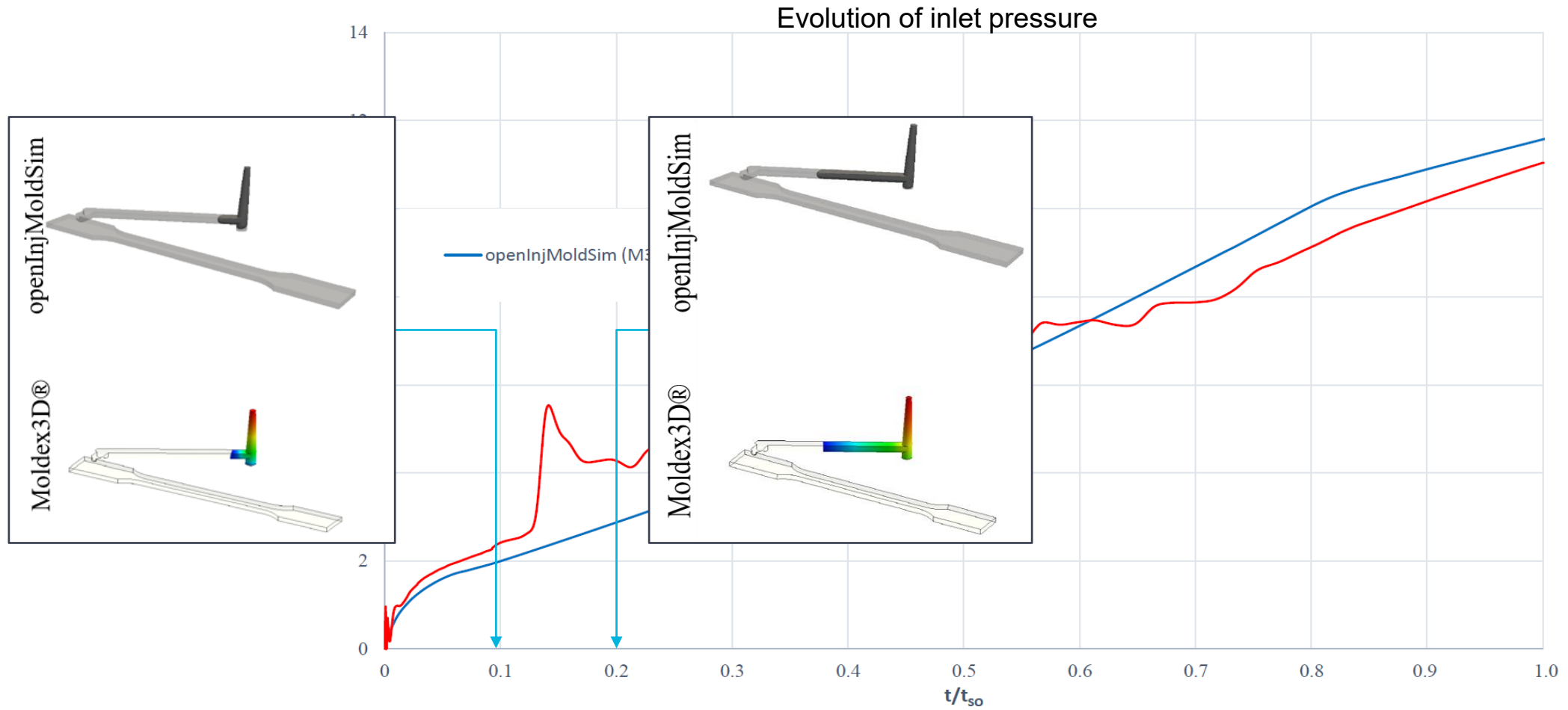


IPC

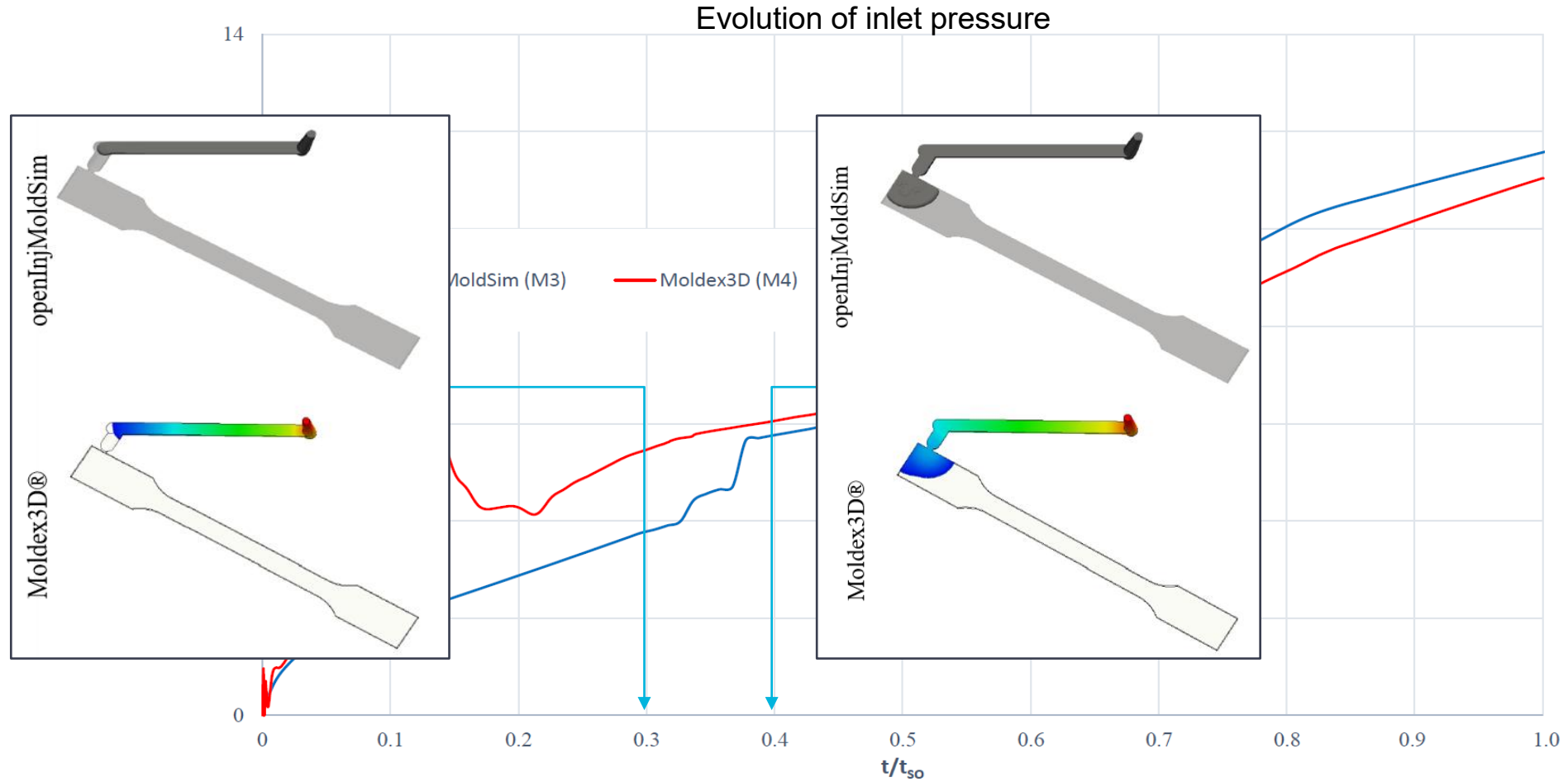


J Pedro et al., Verification and validation of openInjMoldSim, an open-Source solver to model the filling stage of thermoplastic injection molding, *Fluids* 5 (2), 84, 2020

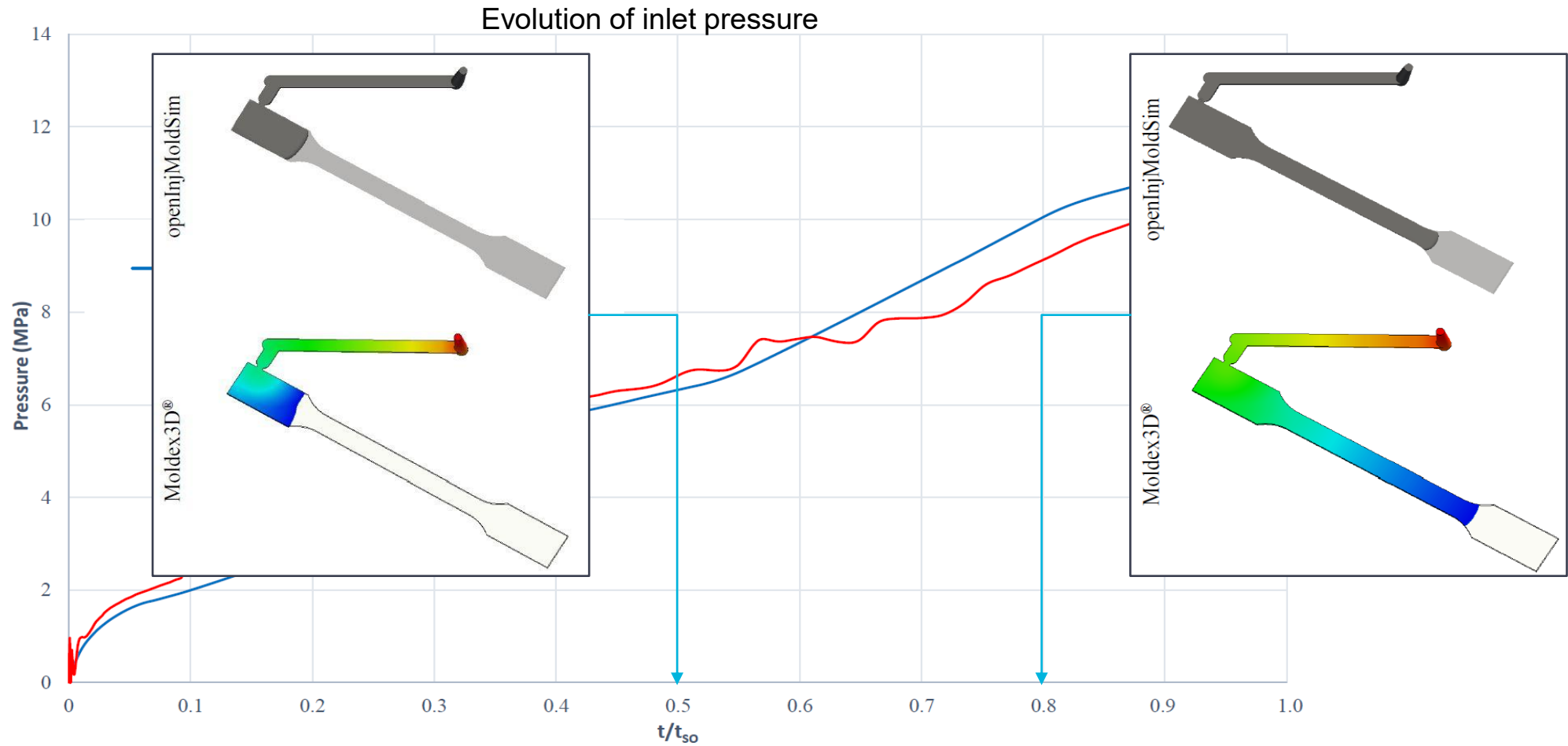
Case Study



Case Study



Case Study

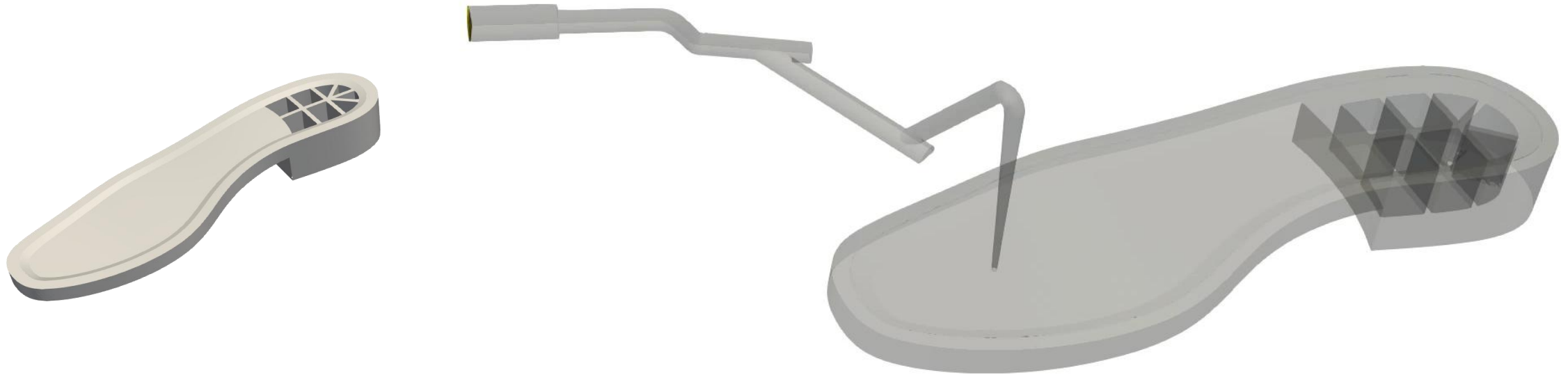


Case Study

Performance and accuracy

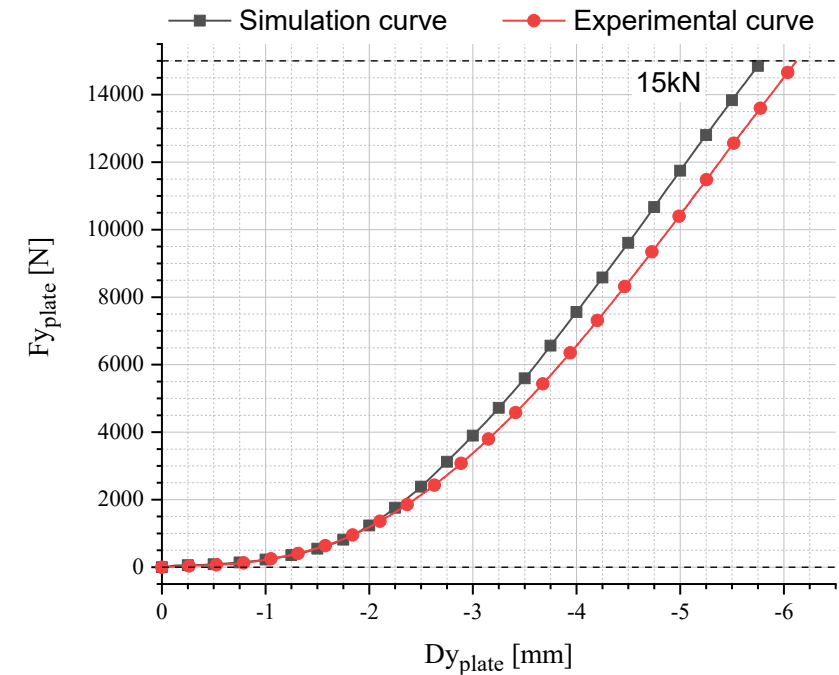
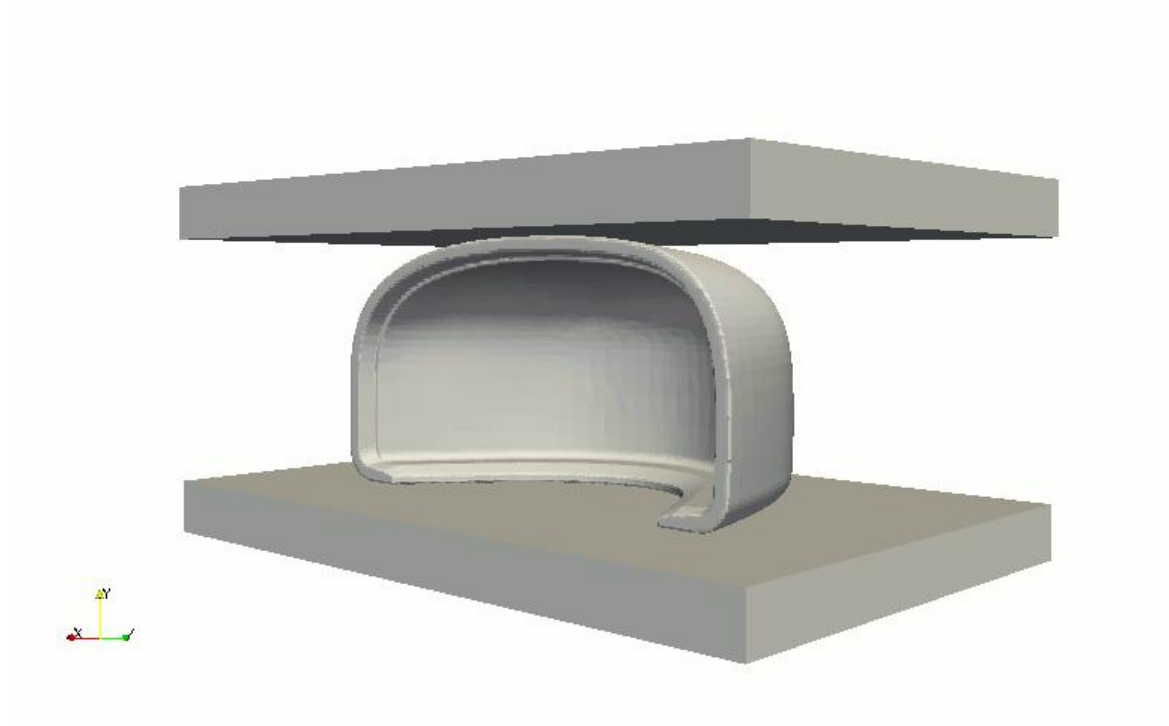
Software	Mesh	Difference	Number of cores	Run Time	
		p_{\max} (%)			
Moldex3D®	M1	43.4	1	88 seconds	
	M2	34.4	1	23 minutes	
	M3	23.8	8	3.8 hours	
	M4	8.41	8	24.5 hours	
openInjMoldSim	M1	29.6	1	12.8 hours	
	M2	27.8	8	41 hours	
	M3			48	98.5 hours
			9.1	96	59 hours
				192	34 hours





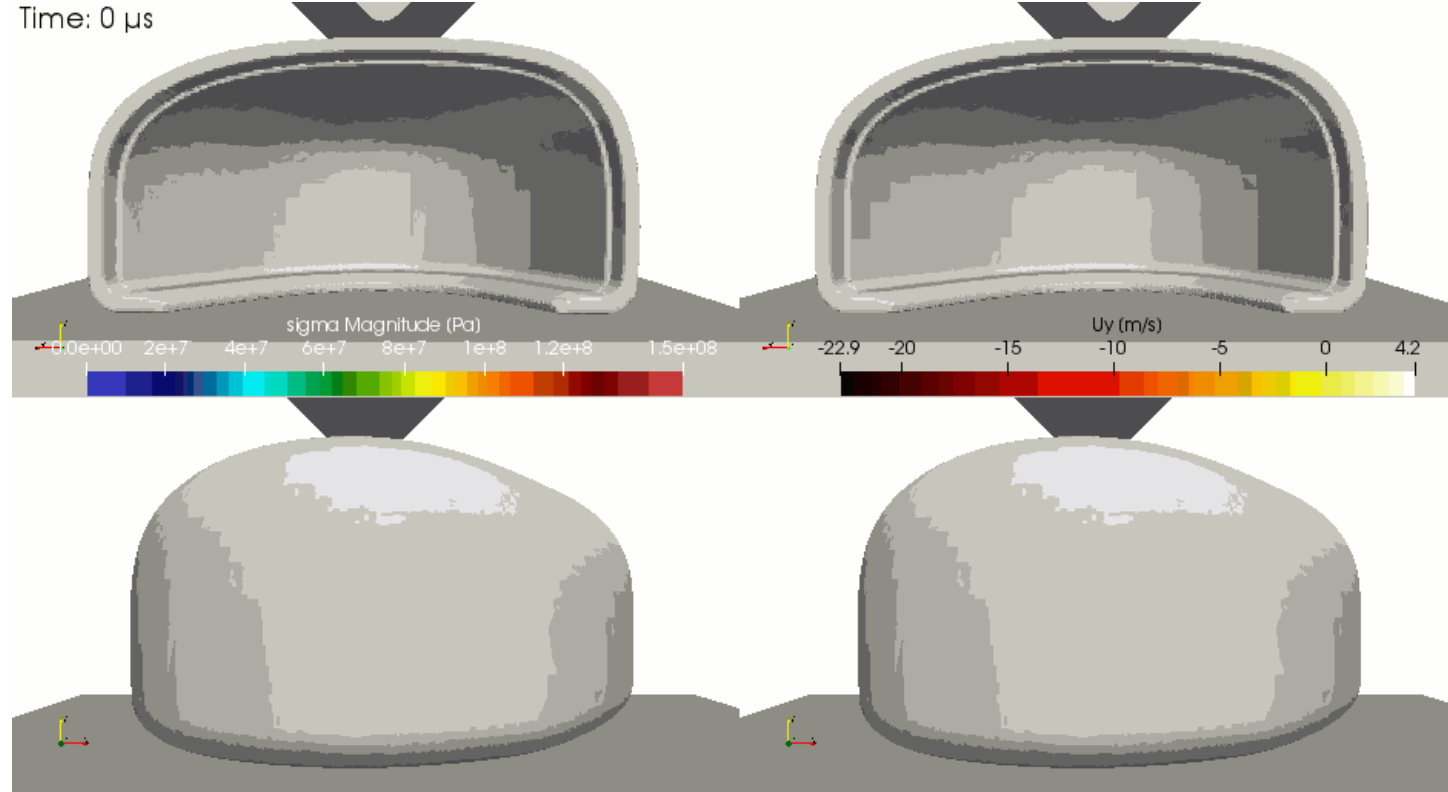


Compression test



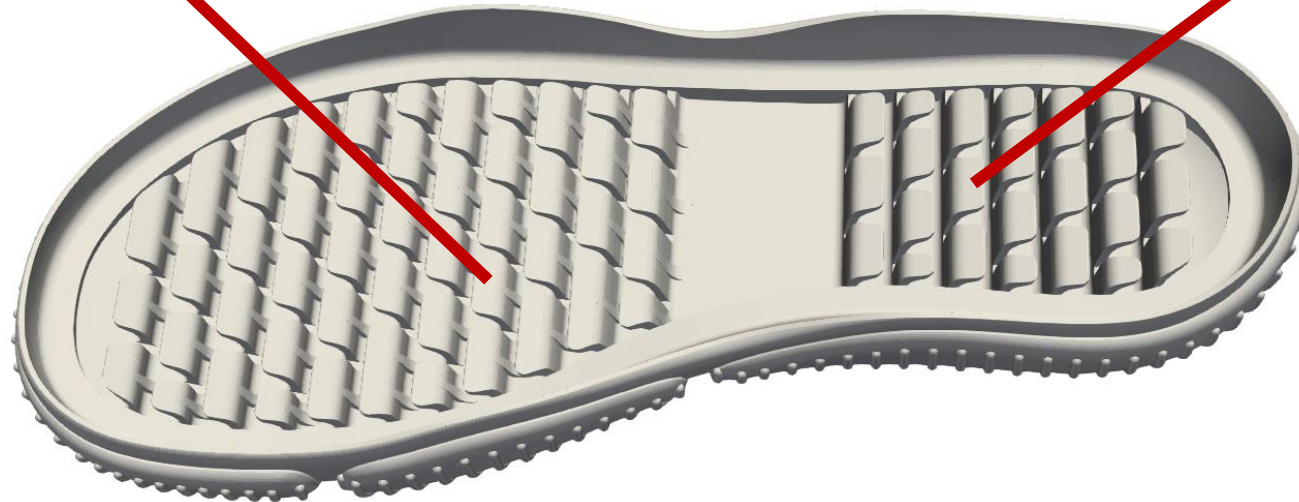
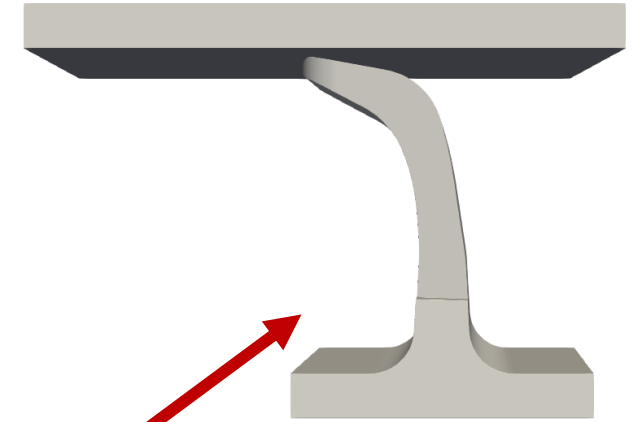
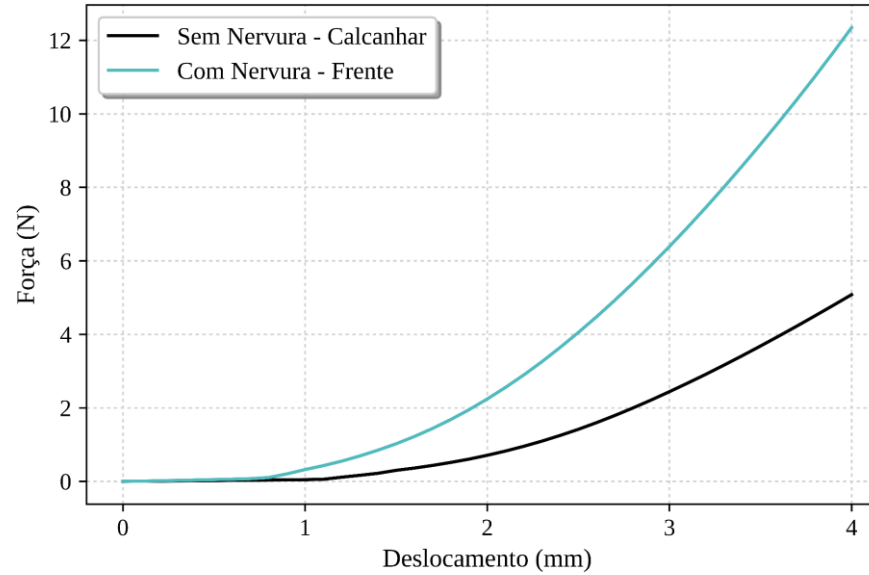
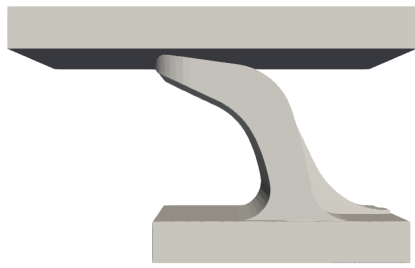


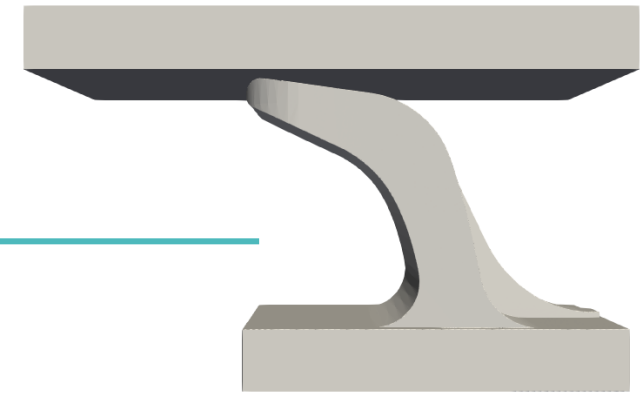
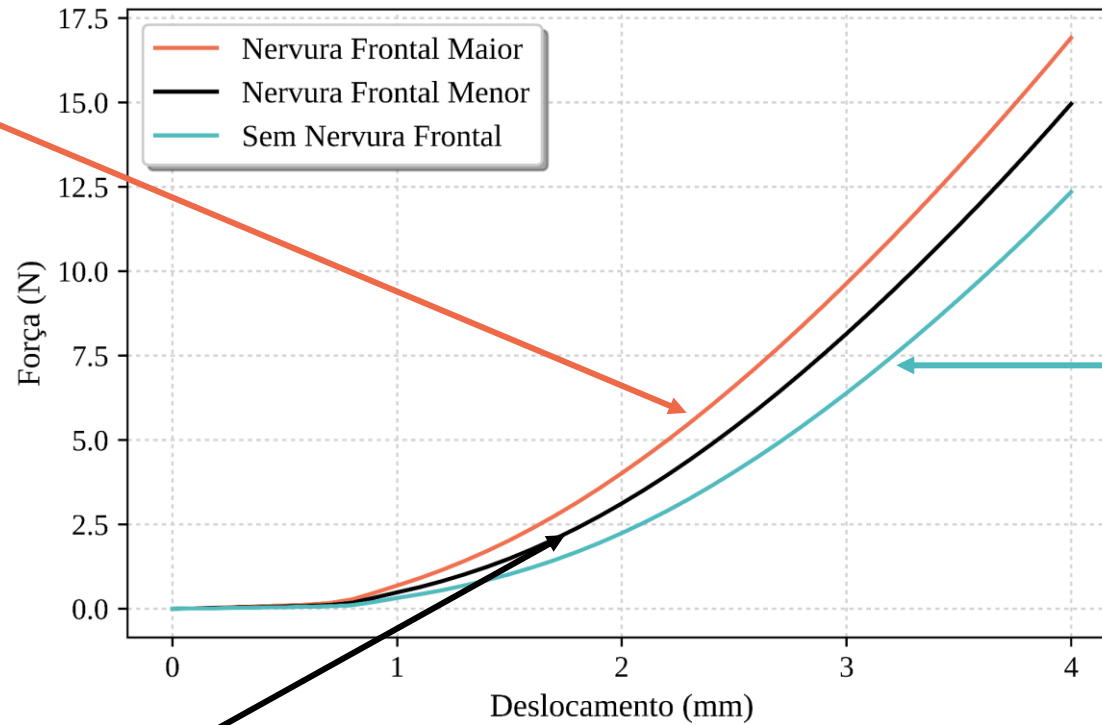
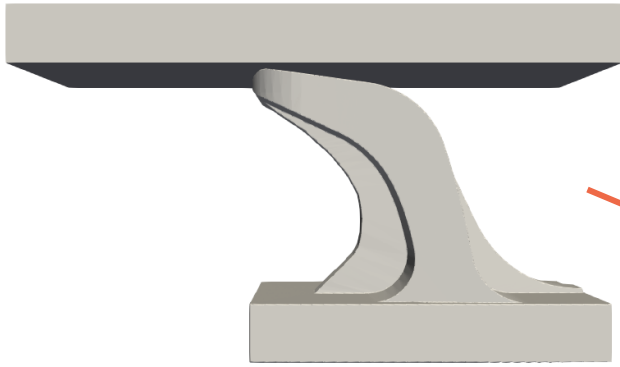
Impact test





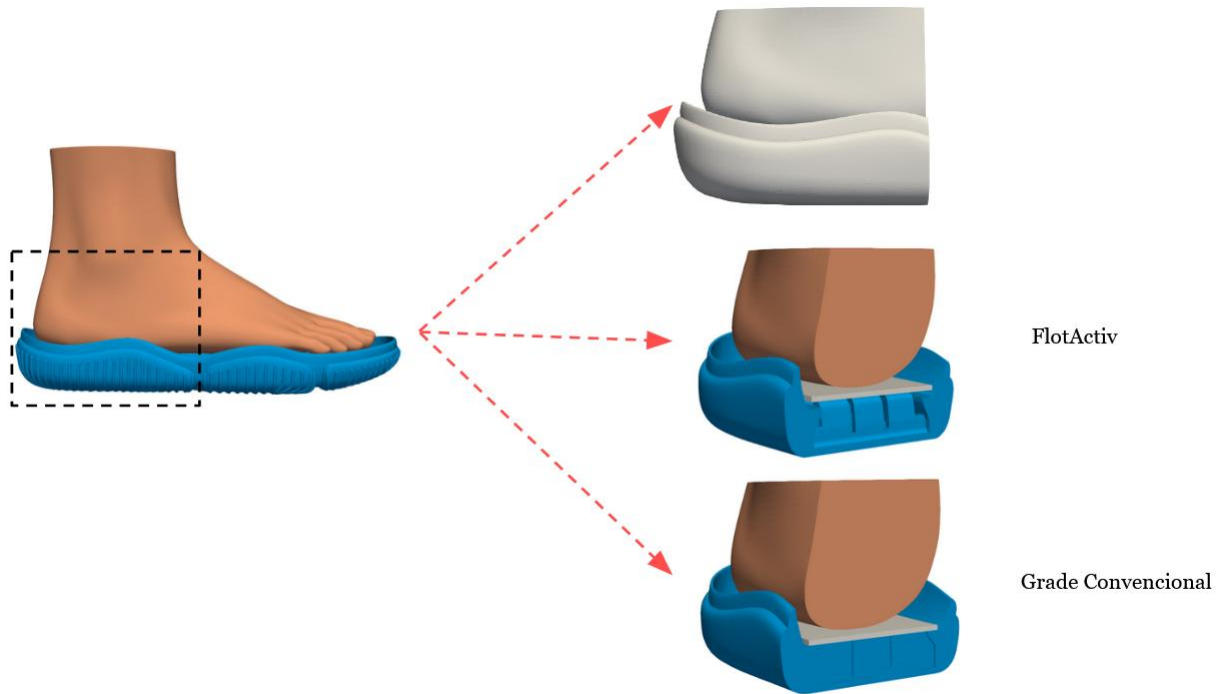
GREENSHOES 4.0





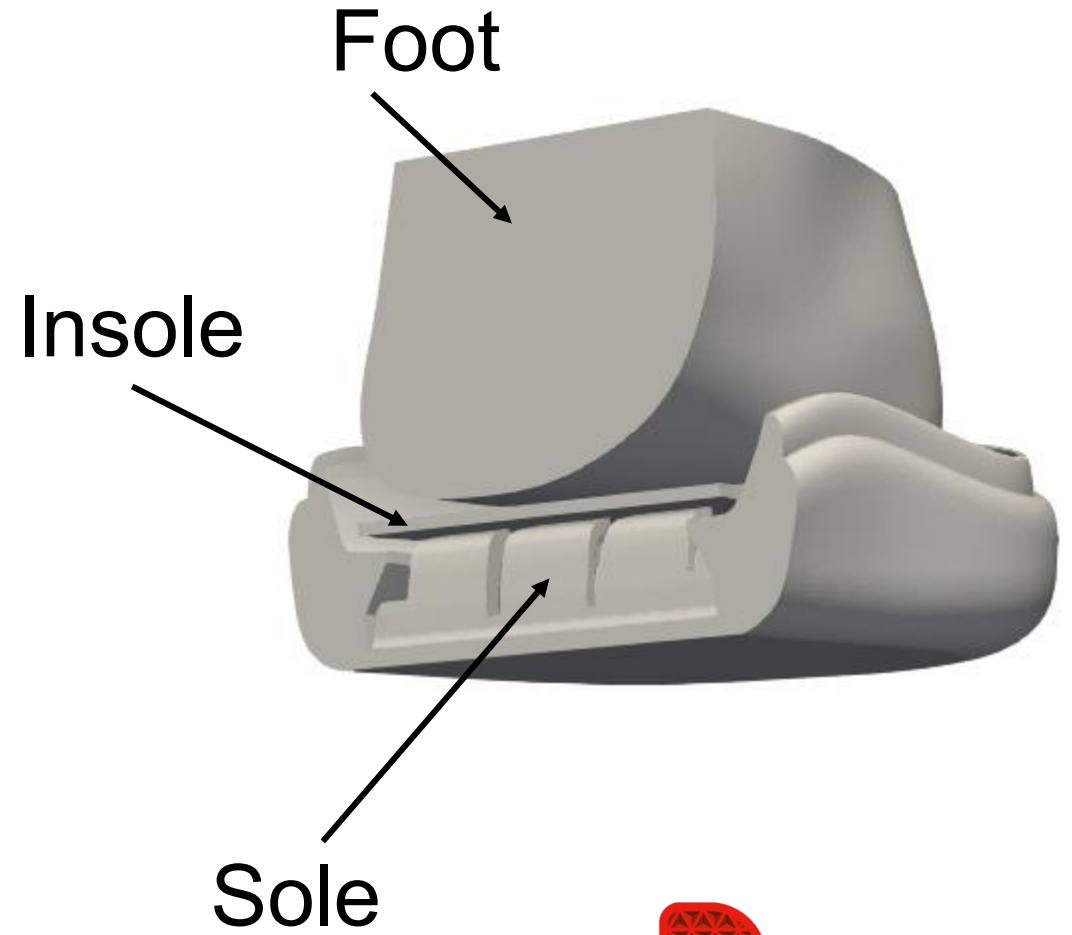


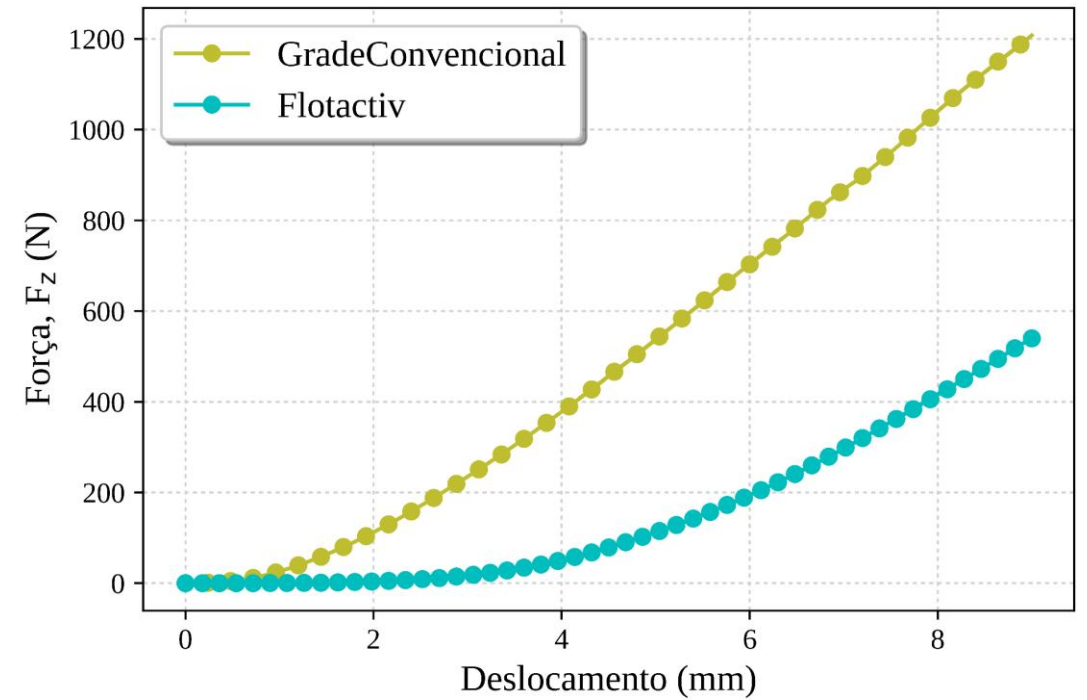
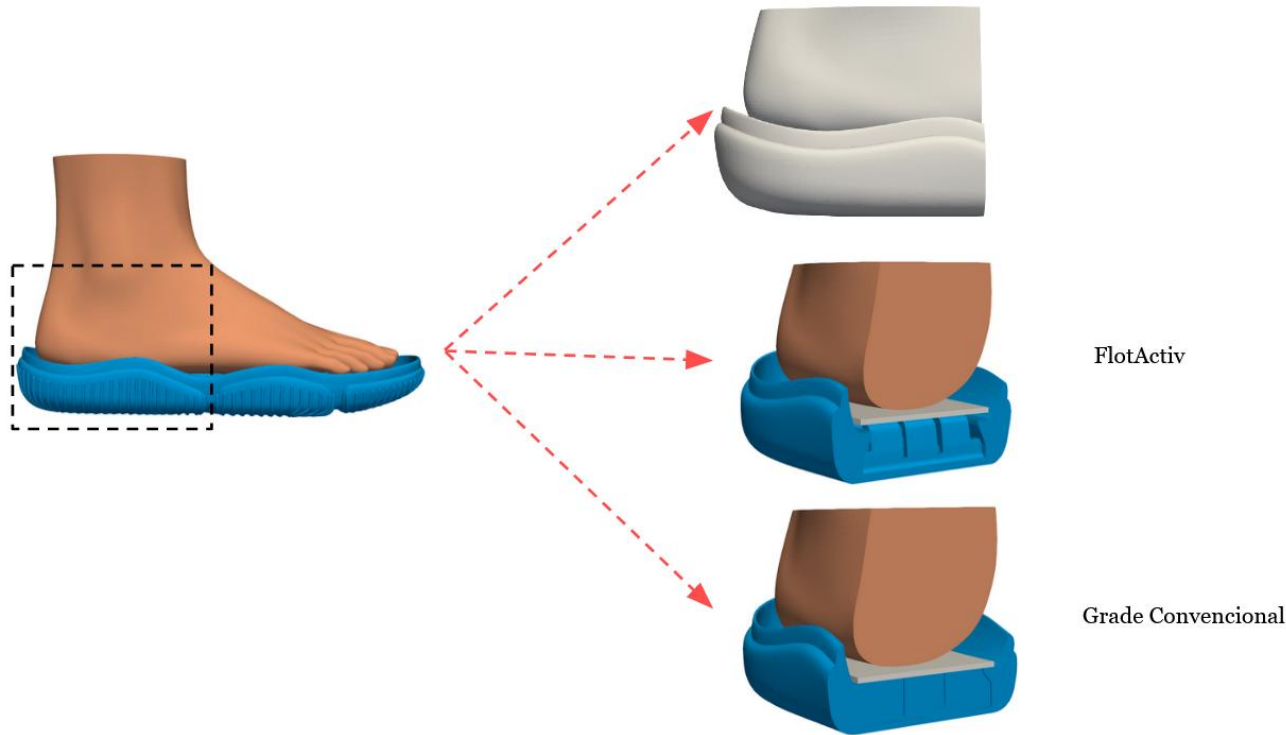
GREENSHOES 4.0



FlotActiv

Grade Convencional

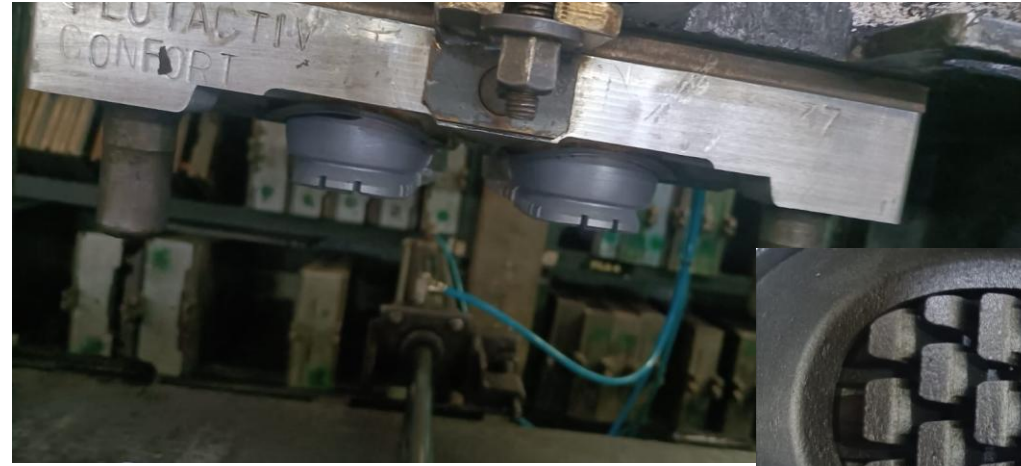




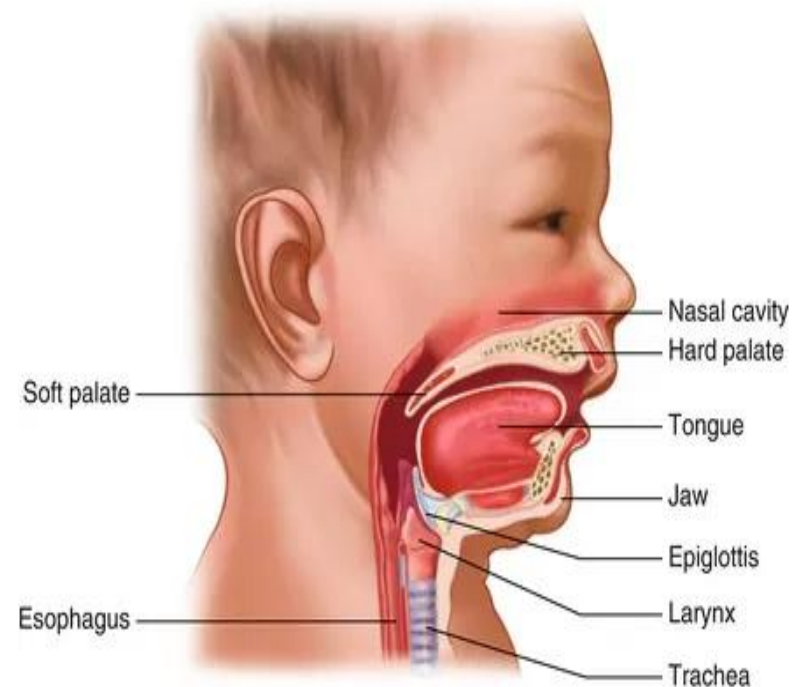
IA – Manufacturing of Footwear Soles (additive)

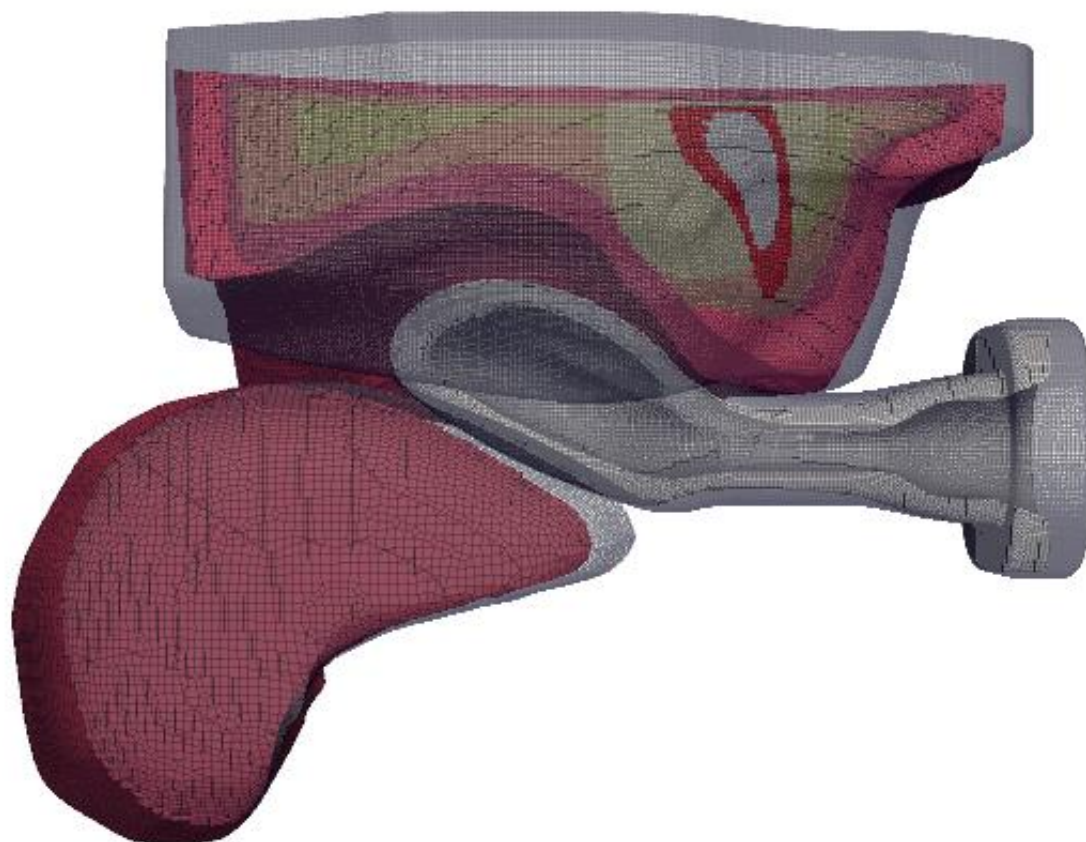


SLS

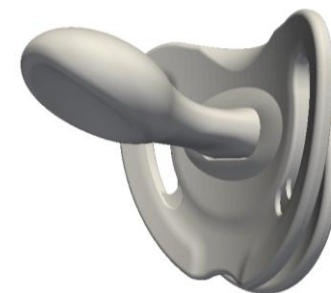


Development of a computational methodology capable of predicting the newborn oral cavity behavior during pacifier sucking

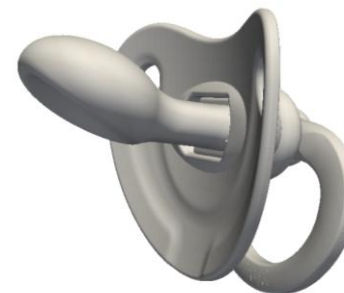




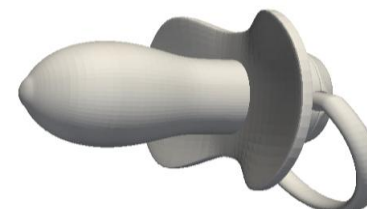
Orthodontic Pacifier

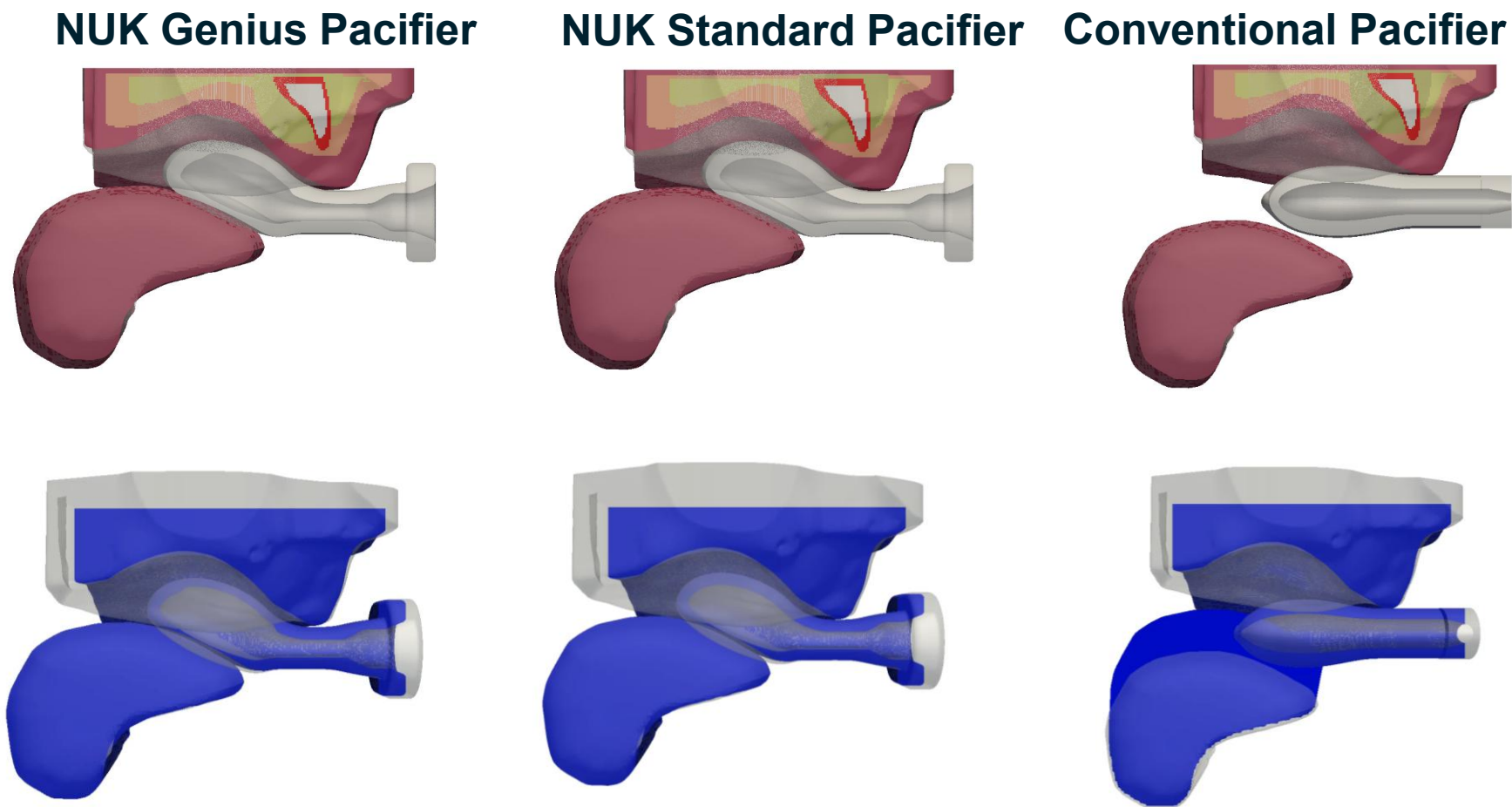


Standard Pacifier



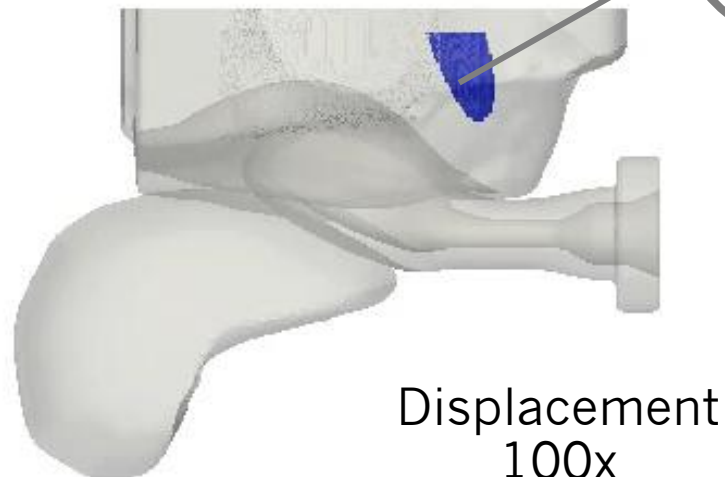
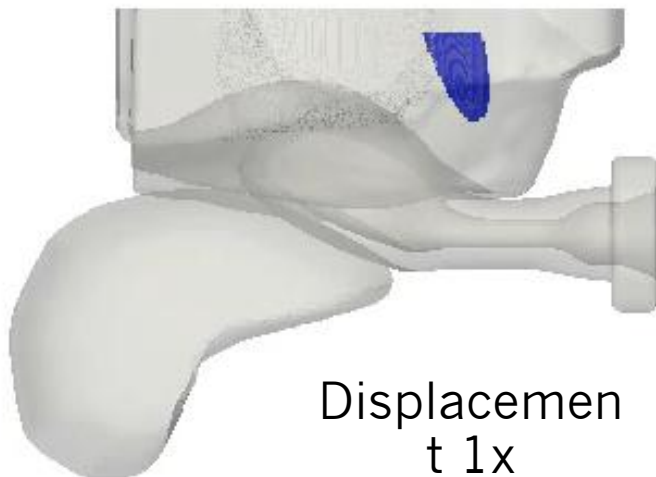
Conventional Pacifier





Pereira, R., Romero, J., Norton, A., & Nóbrega, J. M. (2024). Advancing the assessment of pacifier effects with a novel computational method. *BMC Oral Health*, 24(1), 87.

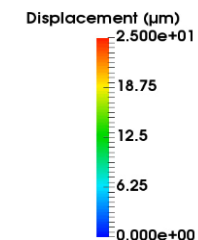
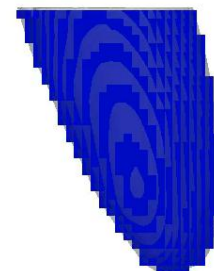
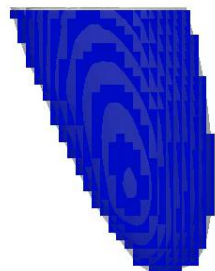
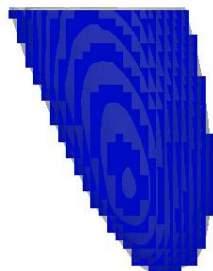




Orthodontic Pacifier

Standard Pacifier

Conventional Pacifier



Beruhigungssauger: Die richtige Form ist entscheidend

Soother: The right shape is crucial

WORKSHOP

Springer Medizin
Experten-Roundtable

„Beruhigungssauger –
aktuelle Erkenntnisse aus der
Wissenschaft und Implikationen
für die Praxis“, online, 2. Mai 2022

Referierende:

Mathilde Furtenbach, Logopädin,
Innsbruck, Österreich

Dr. Isabell von Gymnich,
Kinderzahnärztin, Regensburg

Dr. Matthias Kiefl,
Kieferorthopäde, Straubing

Dipl. Med. Suzanne Knauer-Schiefer,
Pädiaterin und Neonatologin,
Wolfsburg

Ingrid Lohmann, Hebamme
und Stillberaterin, BSc.,
Bad Gandersheim

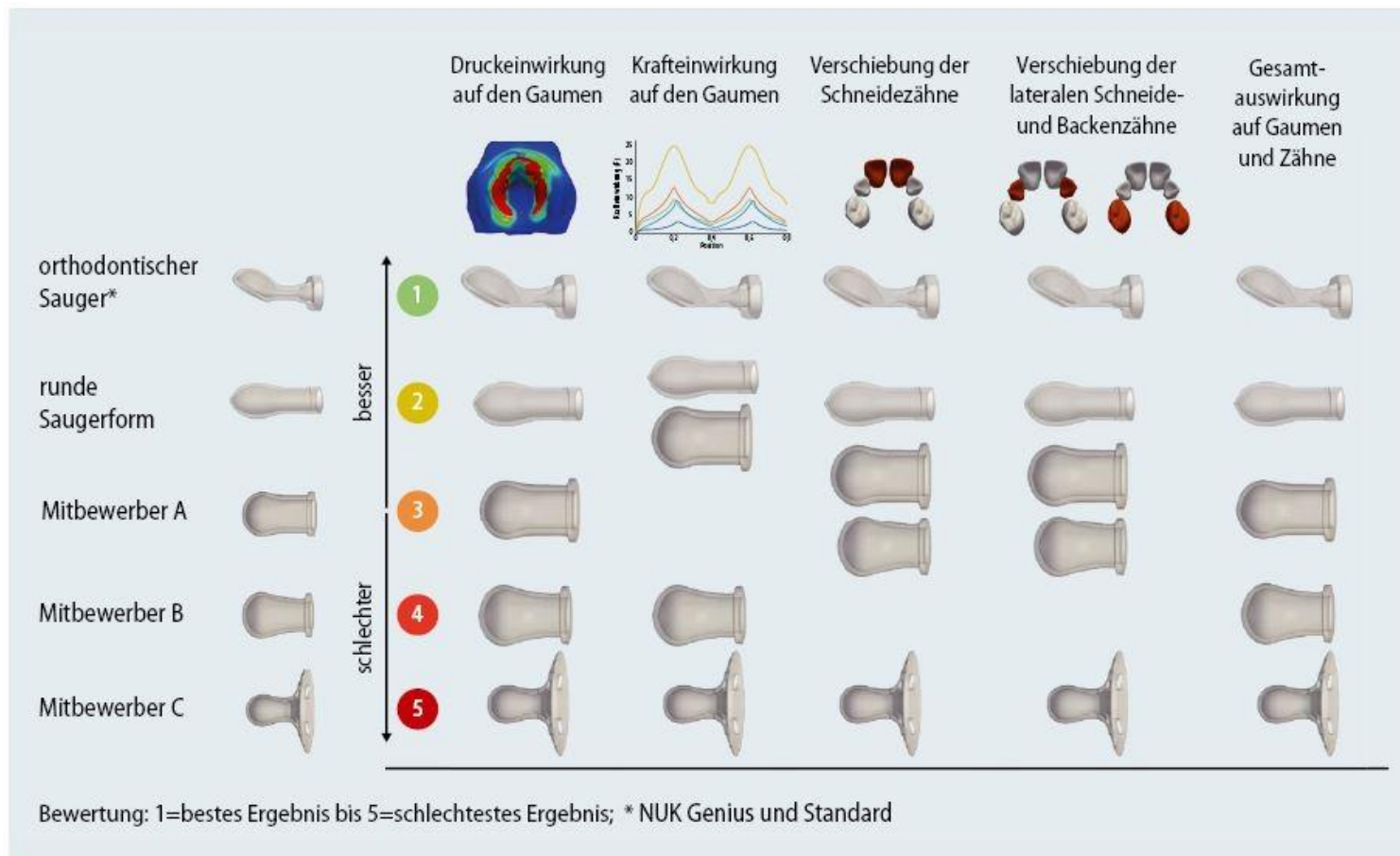
Dr. Christof Metzler, Pädiater,
Langenargen

Prof. Dr. João Miguel Nóbrega, De-
partment of Polymer Engineering,
University of Minho, Campus de
Azurém, Guimarães, Portugal

Prof. Dr. Ana Norton, Dental
Medicine School, University of
Porto, Portugal

Moderation:

Dr. Erik Heintz, Springer Medizin
Verlag GmbH, München



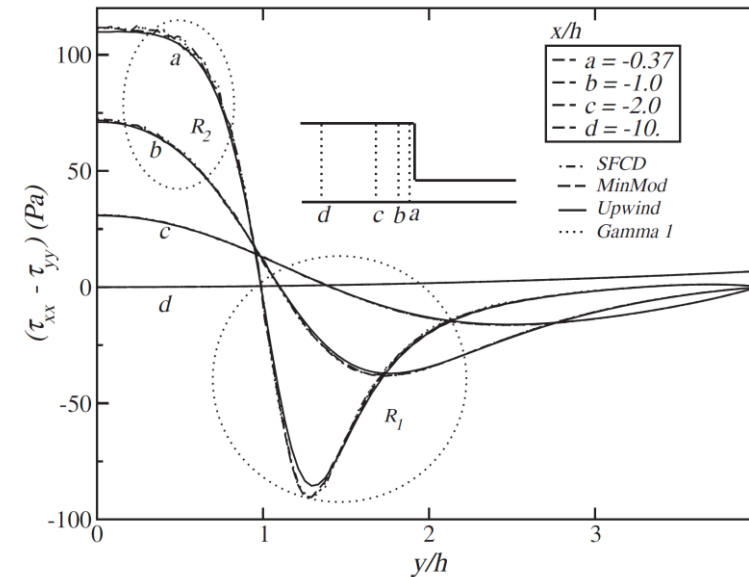
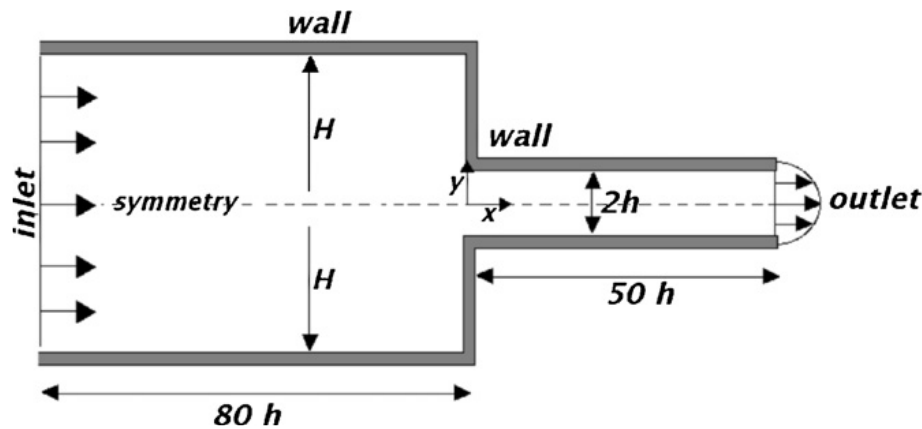
Solvers/Numerical Development (SND)



Differential viscoelastic flow solvers in OpenFOAM

Multi mode constitutive models

Maxwell	(L,E, Feta) PTT	FENE-(P,CR)
Oldroyd-B	Giesekus	(S,D) XPP
White Metzner	Leonov	DCPP



JL Favero et al. (Computer Aided Chemical Engineering, 2009, 2010 / Journal of non-Newtonian Fluid Mechanics, 2010 / Computers & Chemical Engineering, 2010)

$$\boldsymbol{\tau}_p = \int_{-\infty}^t M(t-t') f(\mathbf{B}_{t'}) dt'$$

$$M(t-t') = \sum_k \frac{a_k}{\lambda_k} e^{-\frac{(t-t')}{\lambda_k}}$$

$$f(\mathbf{B}_{t'}) = \begin{cases} \mathbf{B}_{t'} & \text{- UCM} \\ \frac{\alpha}{\alpha + \beta I_1 + (1-\beta) I_2} \mathbf{B}_{t'} & \text{- K-BKZ (PSM)} \end{cases}$$

Deformation Fields approach

$$\frac{\partial \mathbf{B}_i}{\partial t} + \nabla \cdot (\mathbf{U} \mathbf{B}_i) - ((\nabla \mathbf{U})^T \cdot \mathbf{B}_i + \mathbf{B}_i \cdot \nabla \mathbf{U}) = 0$$

Araujo, MSB., et al., "A stable numerical implementation of integral viscoelastic models in the OpenFOAM® computational library. Computers & Fluids, 2018



Stress Tensor Field Calculation

- Define **cutoff time** (s_{max}) and **number of deformation fields** (nf)
- At each time step t :
 1. Update velocity and pressure fields (PISO)
 2. Transport all the previously created deformation fields ($\mathbf{B}_{i=1,nf}$)

$$\frac{\partial \mathbf{B}_i}{\partial t} + \nabla \cdot (\mathbf{U} \mathbf{B}_i) - \left((\nabla \mathbf{U})^T \cdot \mathbf{B}_i + \mathbf{B}_i \cdot \nabla \mathbf{U} \right) = 0$$

3. Create a new deformation field ($\mathbf{B}_t = \mathbf{I}$)
4. If required redistribute/interpolate the deformation fields
5. Compute the stress field



Stre

```

volTensorField L = fvc::grad(U);

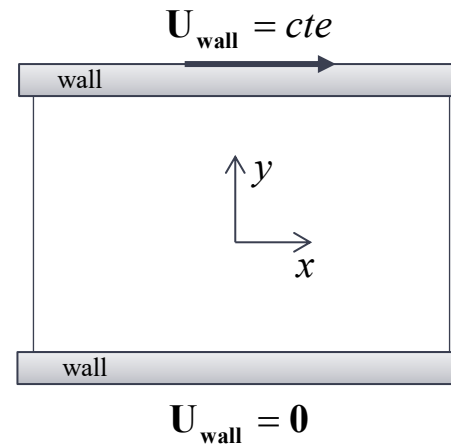
for (int fieldI = 0; fieldI <= nActFields ; fieldI++)
{
    volTensorField SB = B[fieldI] & L;
    fvSymmTensorMatrix BEqn
    (
        fvm::ddt(B[fieldI])
        + fvm::div(phi, B[fieldI], "div(phi,B)")
        ==
        twoSymm(SB)
    );
    BEqn.solve(mesh.solutionDict().solver("B"));
}

```

$$\frac{\partial \mathbf{B}_i}{\partial t} + \nabla \cdot (\mathbf{U} \mathbf{B}_i) - \left((\nabla \mathbf{U})^T \cdot \mathbf{B}_i + \mathbf{B}_i \cdot \nabla \mathbf{U} \right) = 0$$

3. Create a new deformation field ($\mathbf{B}_t = \mathbf{I}$)
4. If required redistribute/interpolate the deformation fields
5. Compute the stress field

Couette Flow – UCM – Imposed Velocity and Pressure Fields



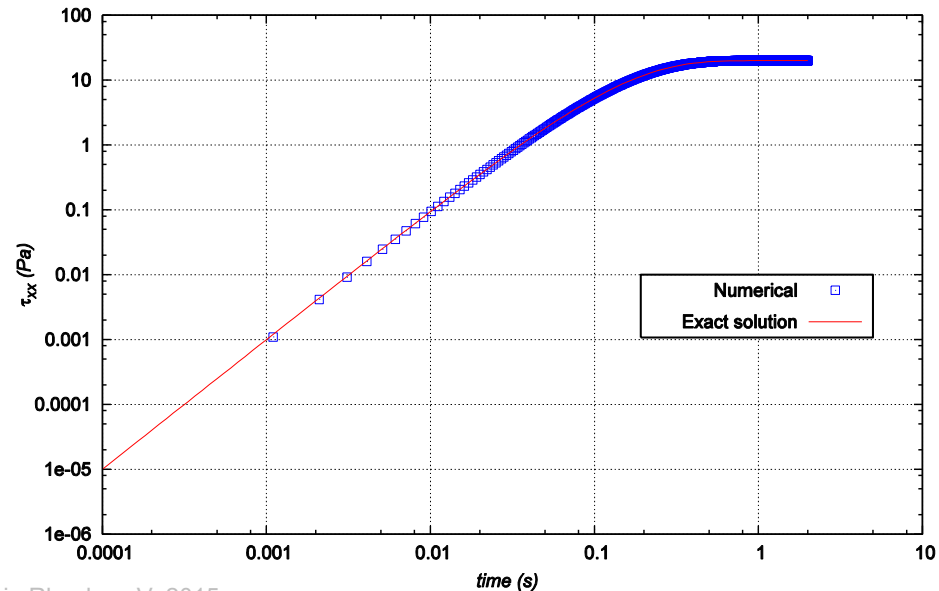
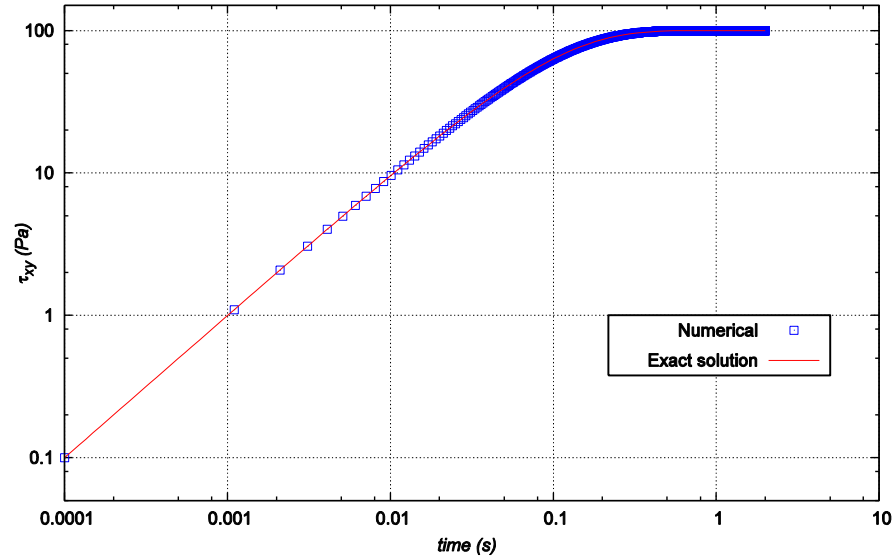
Analytical Solution

$$u_x = \begin{cases} 0 & , t < 0 \\ \dot{\gamma} y & , t \geq 0 \end{cases}$$

$$\tau_{xx} = 2a\dot{\gamma}^2 \lambda^2 \left(1 - \exp\left(-\frac{t}{\lambda}\right) \left(1 + \frac{t}{\lambda} \right) \right)$$

$$\tau_{xy} = a\lambda\dot{\gamma} \left(1 - \exp\left(-\frac{t}{\lambda}\right) \right)$$

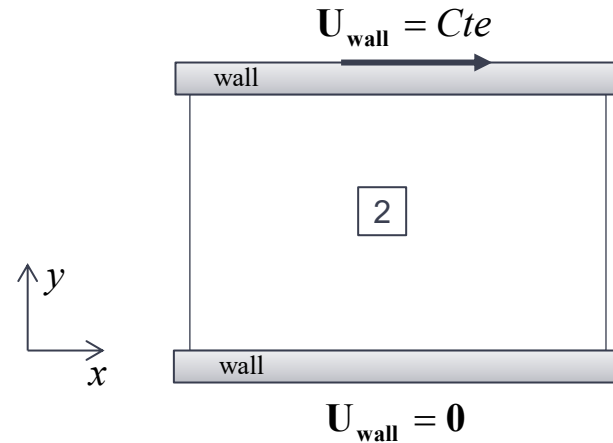
Couette Flow – UCM – Imposed Velocity and Pressure Fields



MSB Araújo, C Fernandes, LL Ferrás, Ž Tukovic, H Jasak, JM Nóbrega, Novel Trends in Rheology V, 2015



Couette Flow – UCM – Constant Wall Velocity



UCM Integral (nf=100)

UCM Integral (nf=2000)

UCM Differential

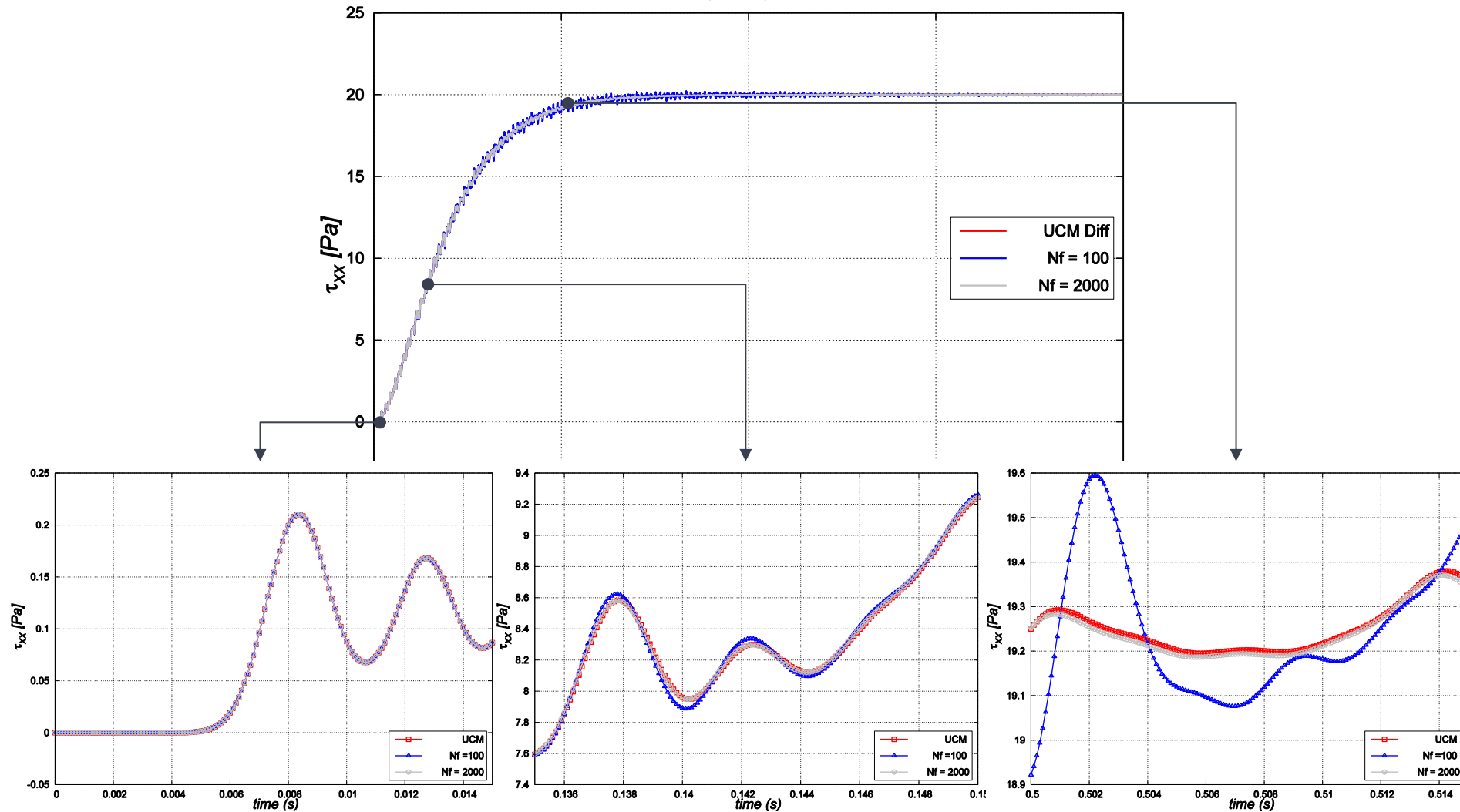


IPC



Couette Flow – UCM – Constant Wall Velocity

De = 0.1



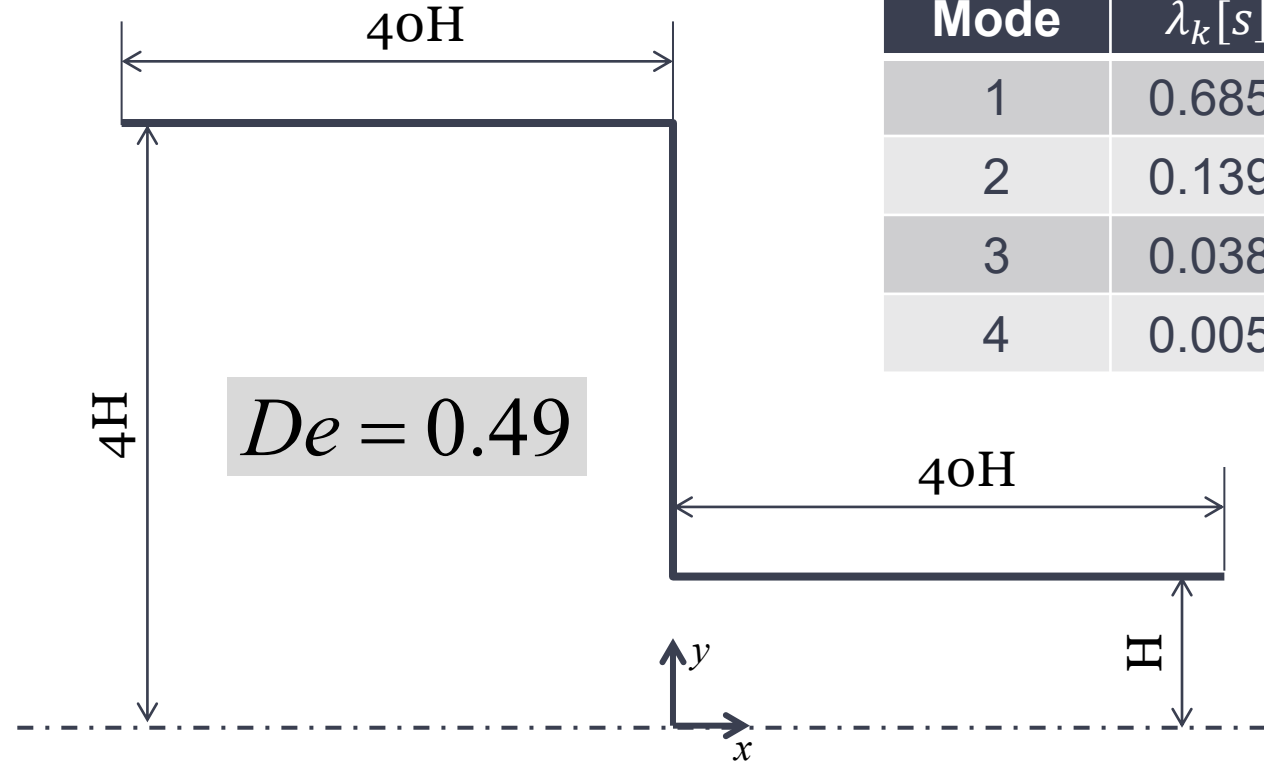
MSB Araújo, C Fernandes, LL Ferrás, Ž Tukovic, H Jasak, JM Nóbrega, Novel Trends in Rheology V, 2015



Case Study - 4:1 Abrupt Planar Contraction - K- BKZ

Solution of 5% wt. polyisobutylene (PIB) in Tetradecane(C14)

$S_{\max} = 1.5 \text{ s}$
 $n_f = 150$



Mode	$\lambda_k [s]$	$a_k [Pa]$
1	0.6855	0.0584
2	0.1396	1.6648
3	0.0389	14.5604
4	0.0059	99.1525

$\alpha = 10$

$\beta = 0.7$

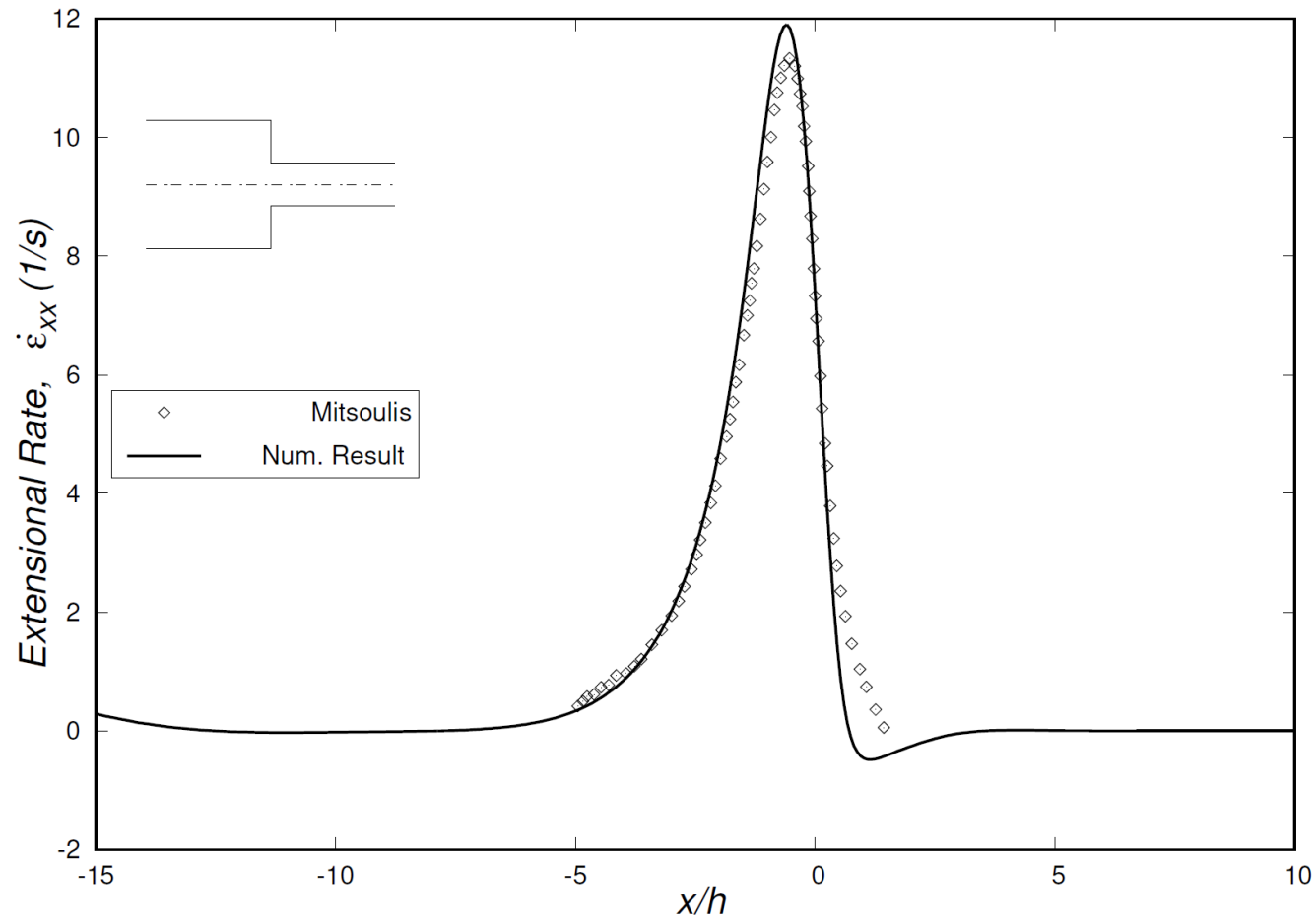
$\theta = 0$

- LM Quinzani, RC Armstrong, RA Brown, Journal non-Newtonian Fluid Mechanics, 52, 1994
- E Mitsoulis, Journal of Rheology, 37, 1993

Araujo, MSB., et al., "A stable numerical implementation of integral viscoelastic models in the OpenFOAM® computational library. Computers & Fluids, 2018



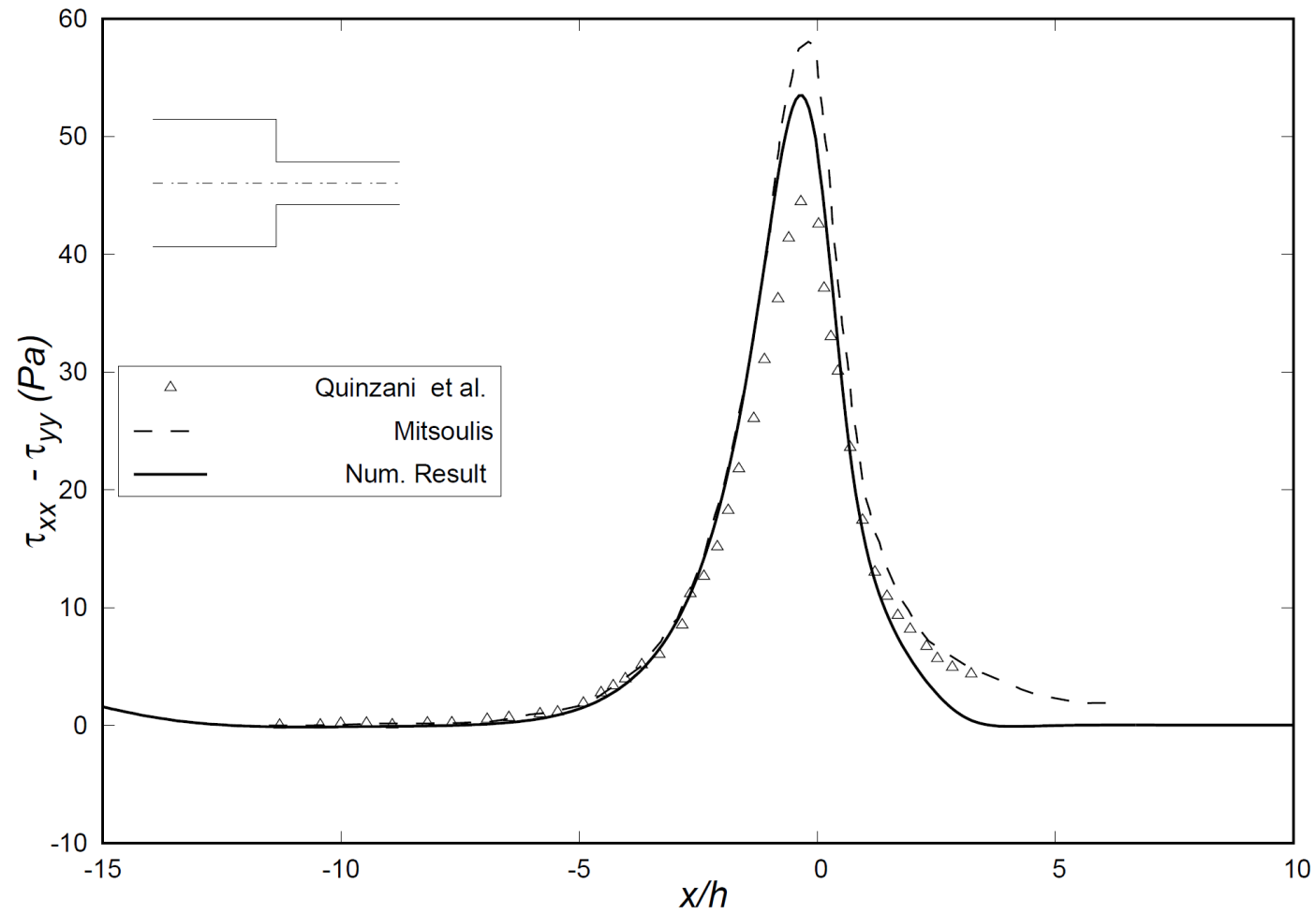
Case Study - 4:1 Abrupt Planar Contraction - K- BKZ



Araujo, MSB., et al., "A stable numerical implementation of integral viscoelastic models in the OpenFOAM® computational library. Computers & Fluids, 2018

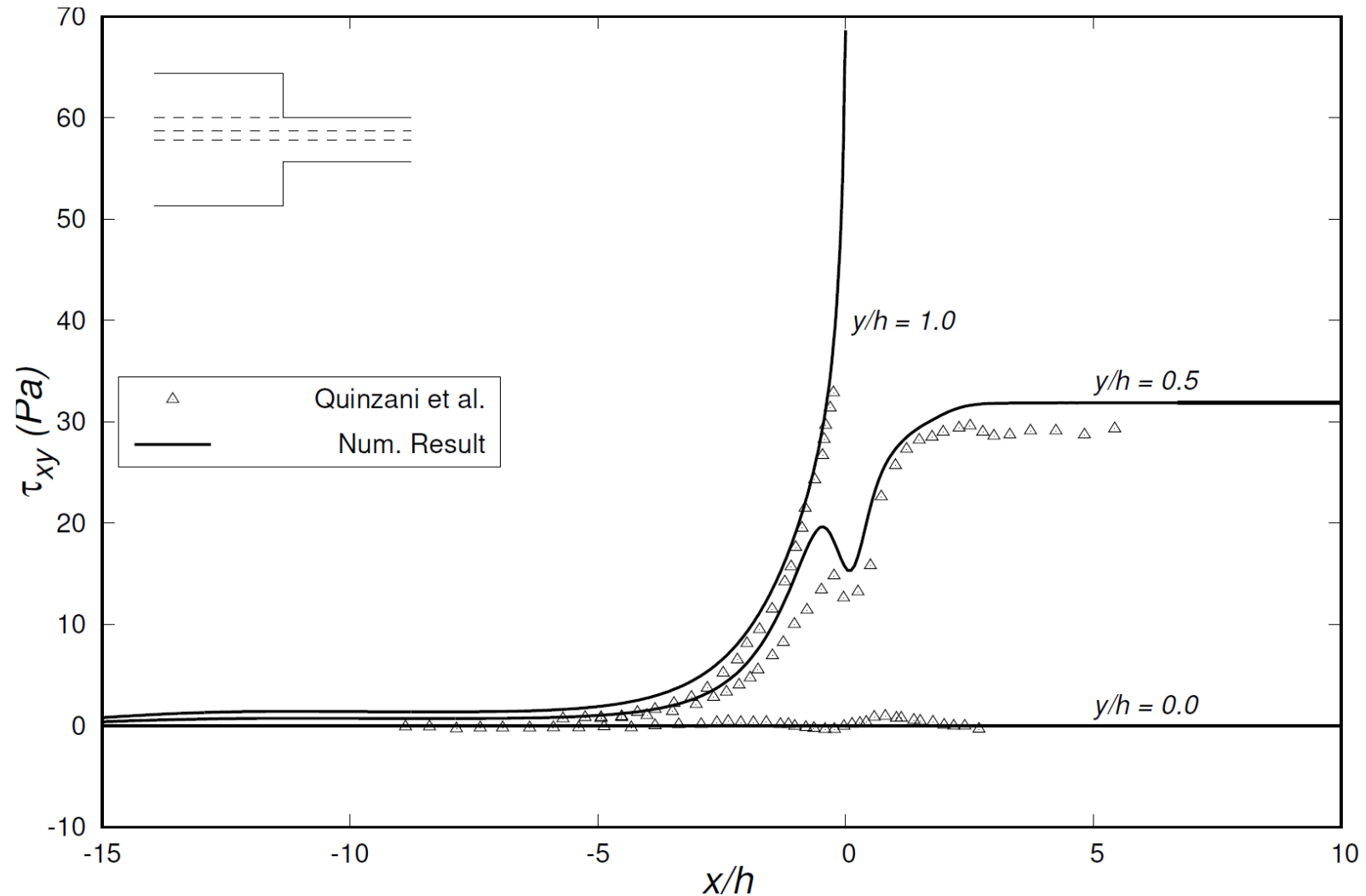


Case Study - 4:1 Abrupt Planar Contraction - K- BKZ



Araujo, MSB., et al., "A stable numerical implementation of integral viscoelastic models in the OpenFOAM® computational library. Computers & Fluids, 2018

Case Study - 4:1 Abrupt Planar Contraction - K- BKZ

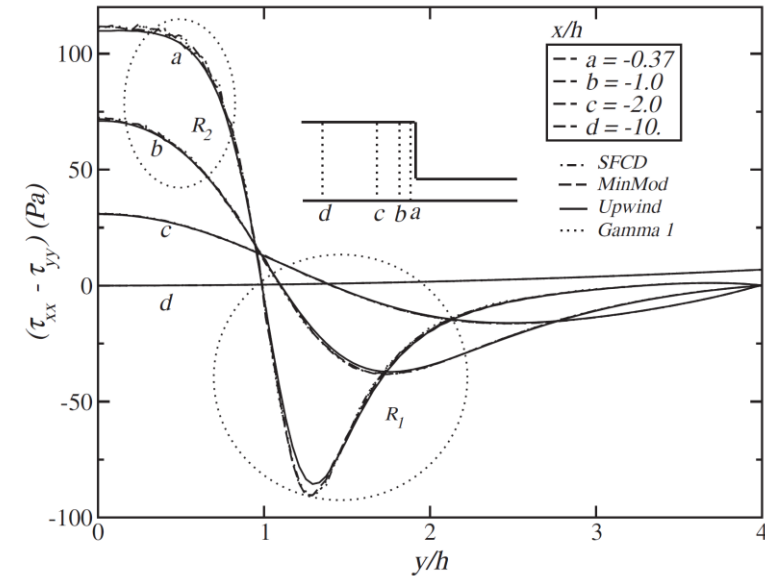
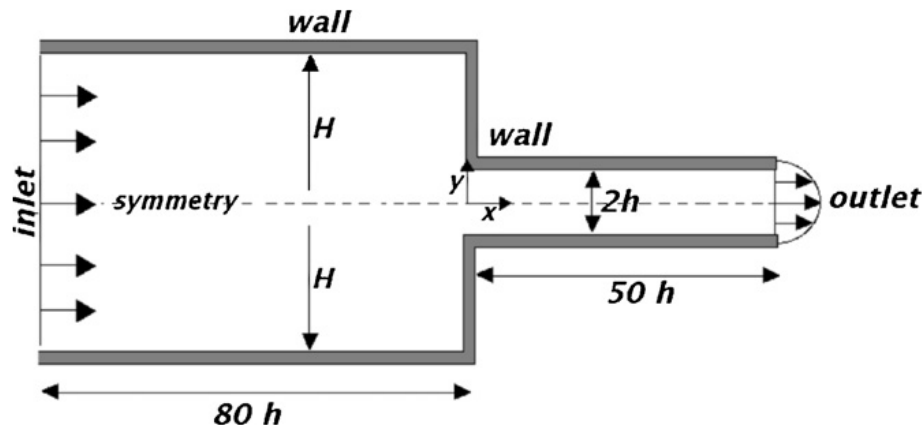


Araujo, MSB., et al., "A stable numerical implementation of integral viscoelastic models in the OpenFOAM® computational library. Computers & Fluids, 2018

Differential viscoelastic flow solvers in OpenFOAM

Multi mode constitutive models

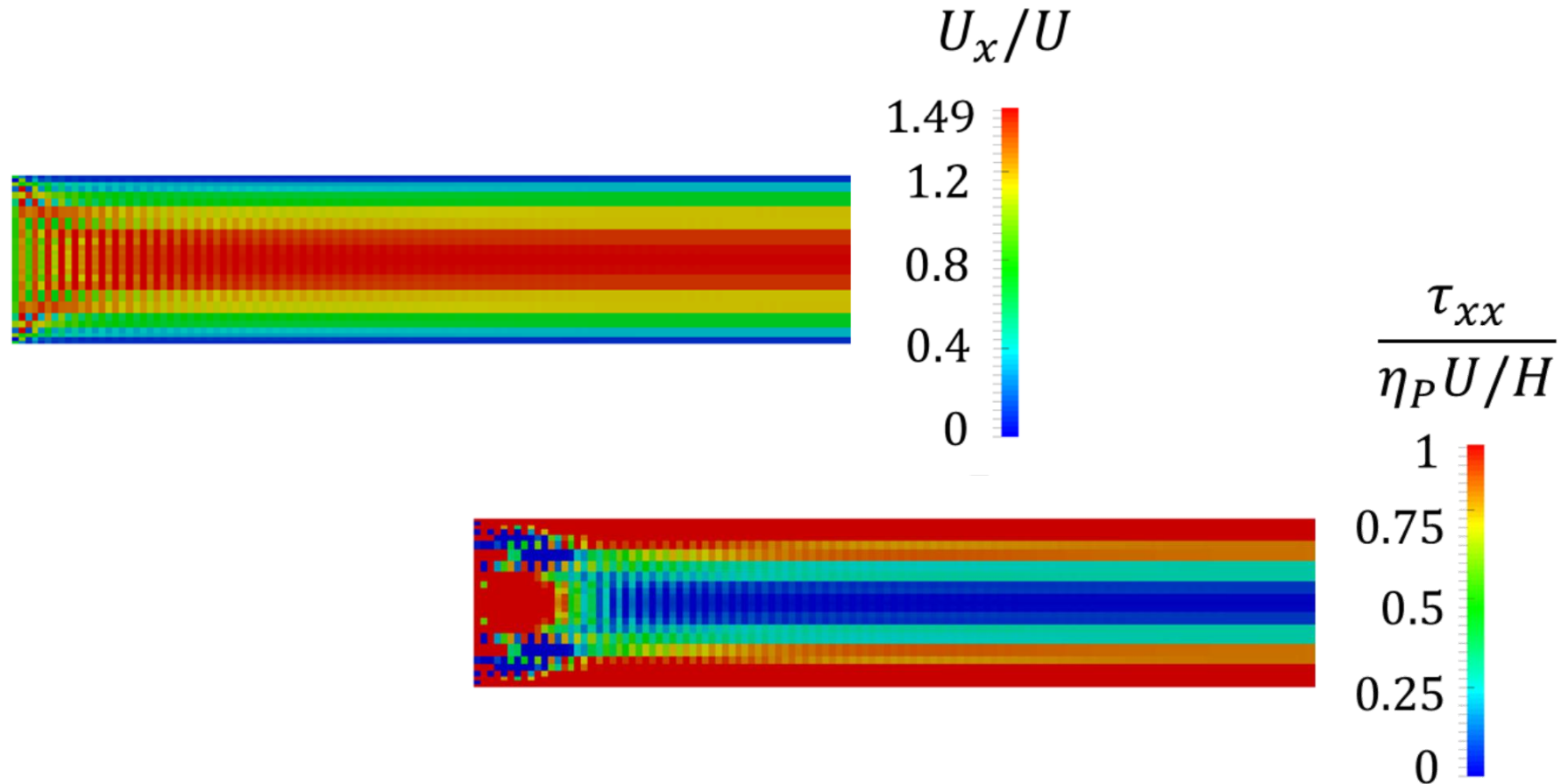
Maxwell	(L,E, Feta) PTT	FENE-(P,CR)
Oldroyd-B	Giesekus	(S,D) XPP
White Metzner	Leonov	DCPP



JL Favero et al. (Computer Aided Chemical Engineering, **2009, 2010** / Journal of non-Newtonian Fluid Mechanics, **2010** / Computers & Chemical Engineering, **2010**)

Poiseuille Flow + UCM (Oldroyd-B $\eta_s=0$)

Re=0.01, De=1



The iBSD – Improved Both-Sides-Diffusion

Conservative

```
fvm::div(phi, U)
```

Original - `fvm::laplacian(etaStr/rho, U)`

==

```
fvm::div(phi, U)
```

```
- fvm::laplacian(etaStr/rho, U)
```

BSD ==

```
- fvc::grad(p)
```

```
+ fvc::div(tau/rho)
```

iBSD

```
- fvc::div((etaStr/rho) * fvc::grad(U))
```

$$\nabla \cdot (\rho \mathbf{U}\mathbf{U}) - \eta * \nabla^2 \mathbf{U} = -\nabla p + \nabla \cdot \boldsymbol{\tau} - \nabla \cdot (\eta * \nabla \mathbf{U})$$

Larger Stencil

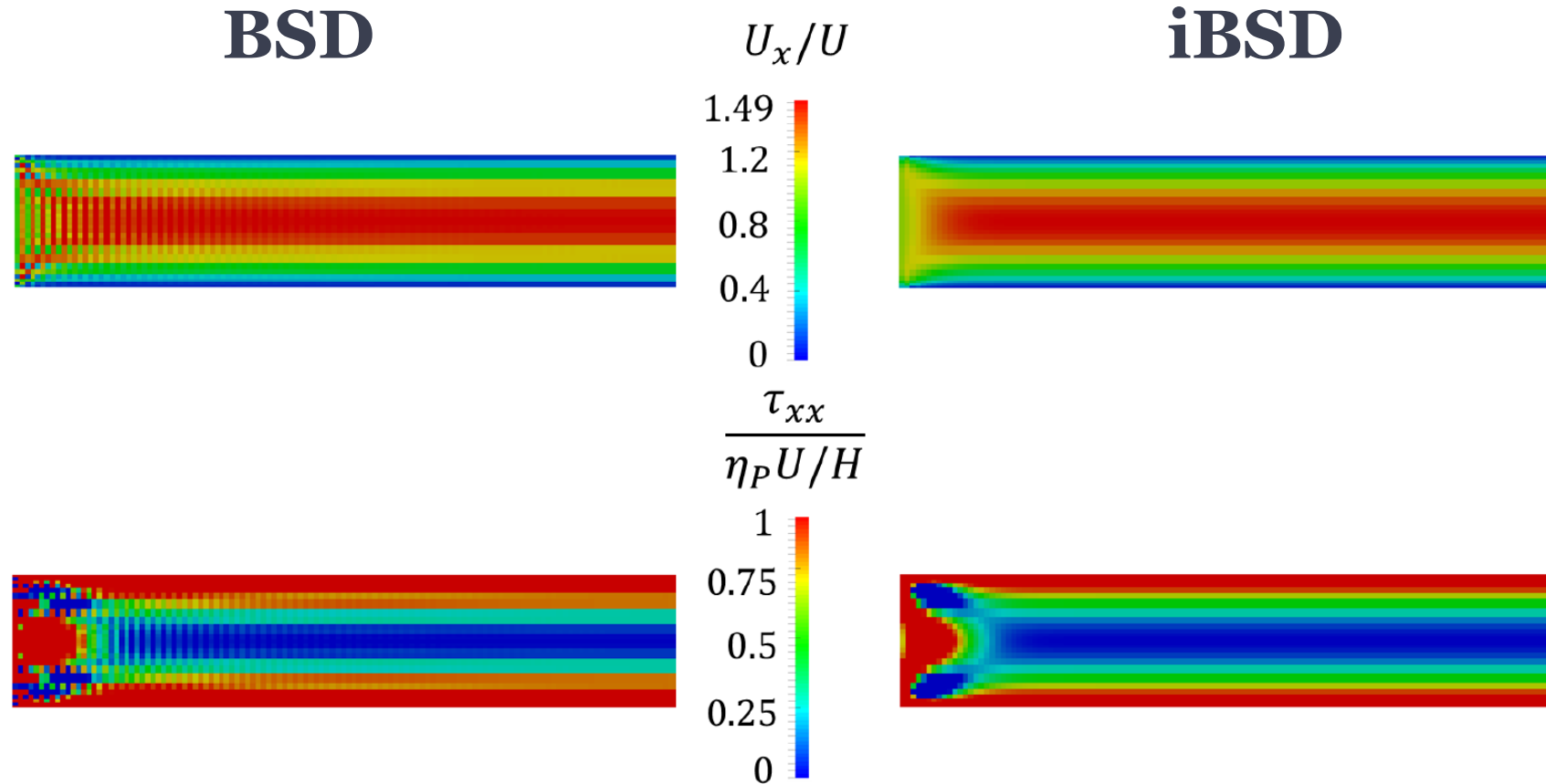


IPC

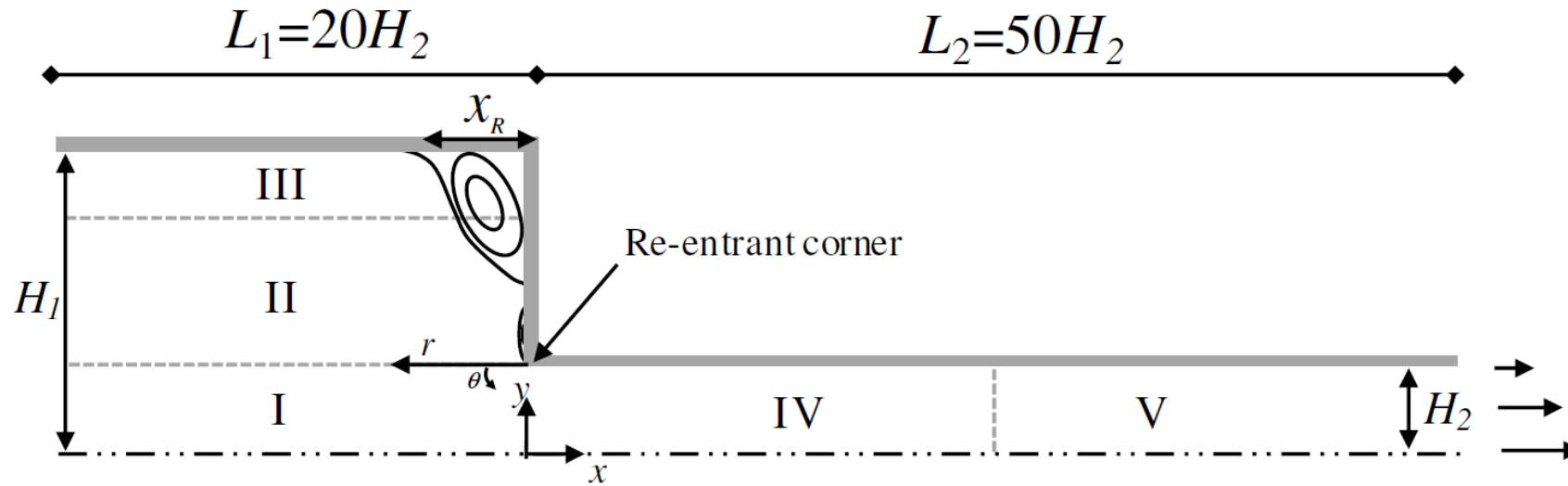


Poiseuille Flow + UCM (Oldroyd-B $h_s=0$)

Re=0.01, De=1



Case Study 1 – 4:1 Contraction (UCM)



Meshes

M1 – 228 Cells

...

M5 – 228128 Cells

Re = 0.01

De = {0,1,2,3,4,5}

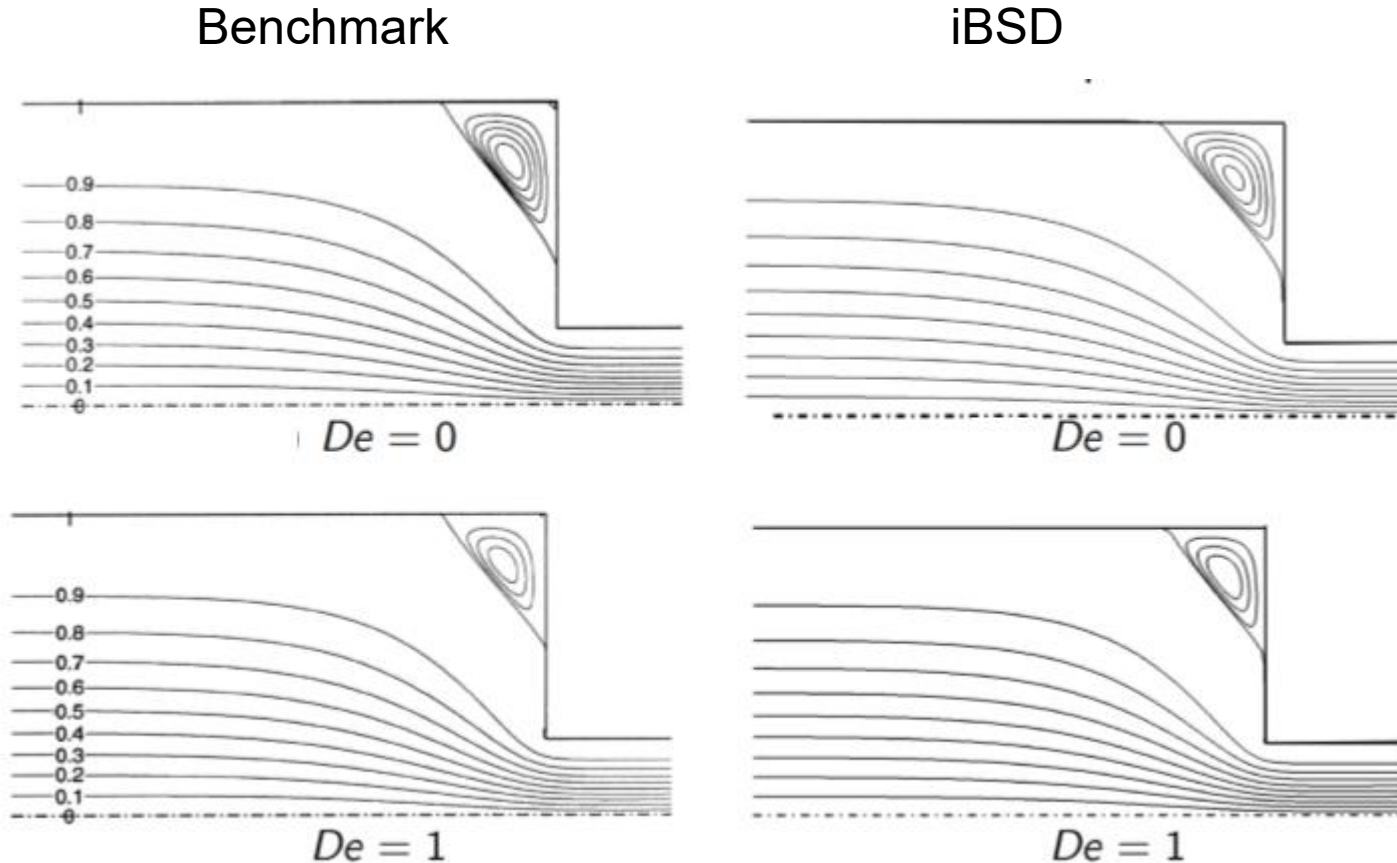


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Case Study 1 – 4:1 Contraction (UCM)

Streamlines



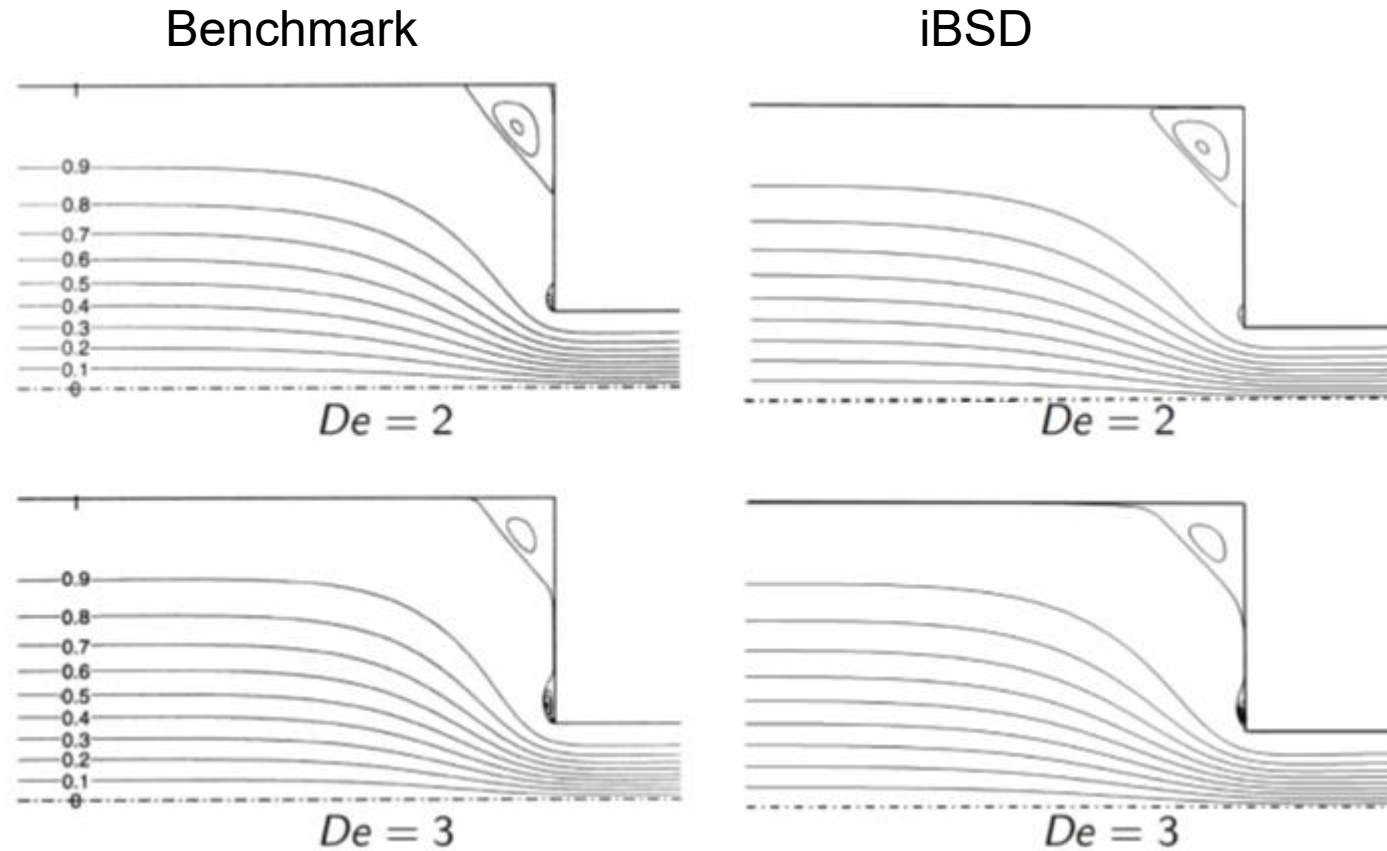
MM Alves, FT Pinho, PJ Oliveira, J. Non-Newtonian Fluid Mech., 93, 2000

C Fernandes et al., Improved Both Sides Diffusion (iBSD): a new and straightforward stabilization approach for viscoelastic fluid flows, JNNFM, 249, 63-78, 2017



Case Study 1 – 4:1 Contraction (UCM)

Streamlines



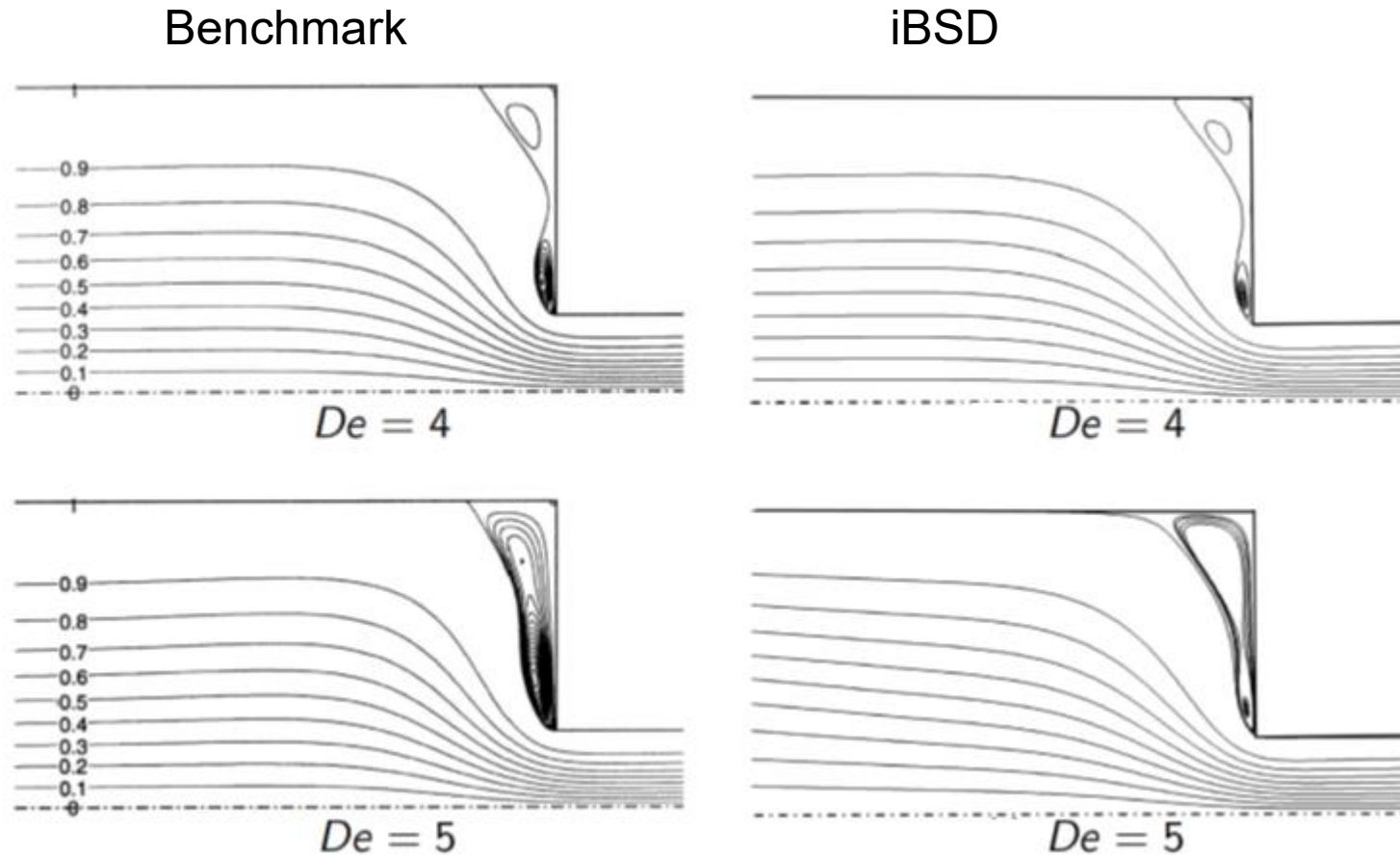
MM Alves, FT Pinho, PJ Oliveira, J. Non-Newtonian Fluid Mech., 93, 2000

C Fernandes et al., Improved Both Sides Diffusion (iBSD): a new and straightforward stabilization approach for viscoelastic fluid flows, JNNFM, 249, 63-78, 2017



Case Study 1 – 4:1 Contraction (UCM)

Streamlines



MM Alves, FT Pinho, PJ Oliveira, J. Non-Newtonian Fluid Mech., 93, 2000

C Fernandes et al., Improved Both Sides Diffusion (iBSD): a new and straightforward stabilization approach for viscoelastic fluid flows, JNNFM, 249, 63-78, 2017

Case Study 1 – 4:1 Contraction (UCM)

Primary vortex length ($X_r = x_r/H_2$)

Developed code in <i>OpenFOAM</i> [®]							
De	Mesh 1	Mesh 2	Mesh 3	Mesh 4	Mesh 5	Extrapolated	Difference (%)
0	1.438	1.479	1.492	1.495	1.496	1.4965	0.03
1	1.293	1.336	1.326	1.32711	1.32696	1.32694	0.002
2	1.207	1.200	1.130	1.101	1.091	1.0857	0.5
3	1.333	1.118	0.958	0.900	0.885	0.880	0.6
4	1.391	1.088	0.845	0.75	0.732	0.728	0.6
5	1.469	1.101	0.758	0.636	0.617	0.613	0.6

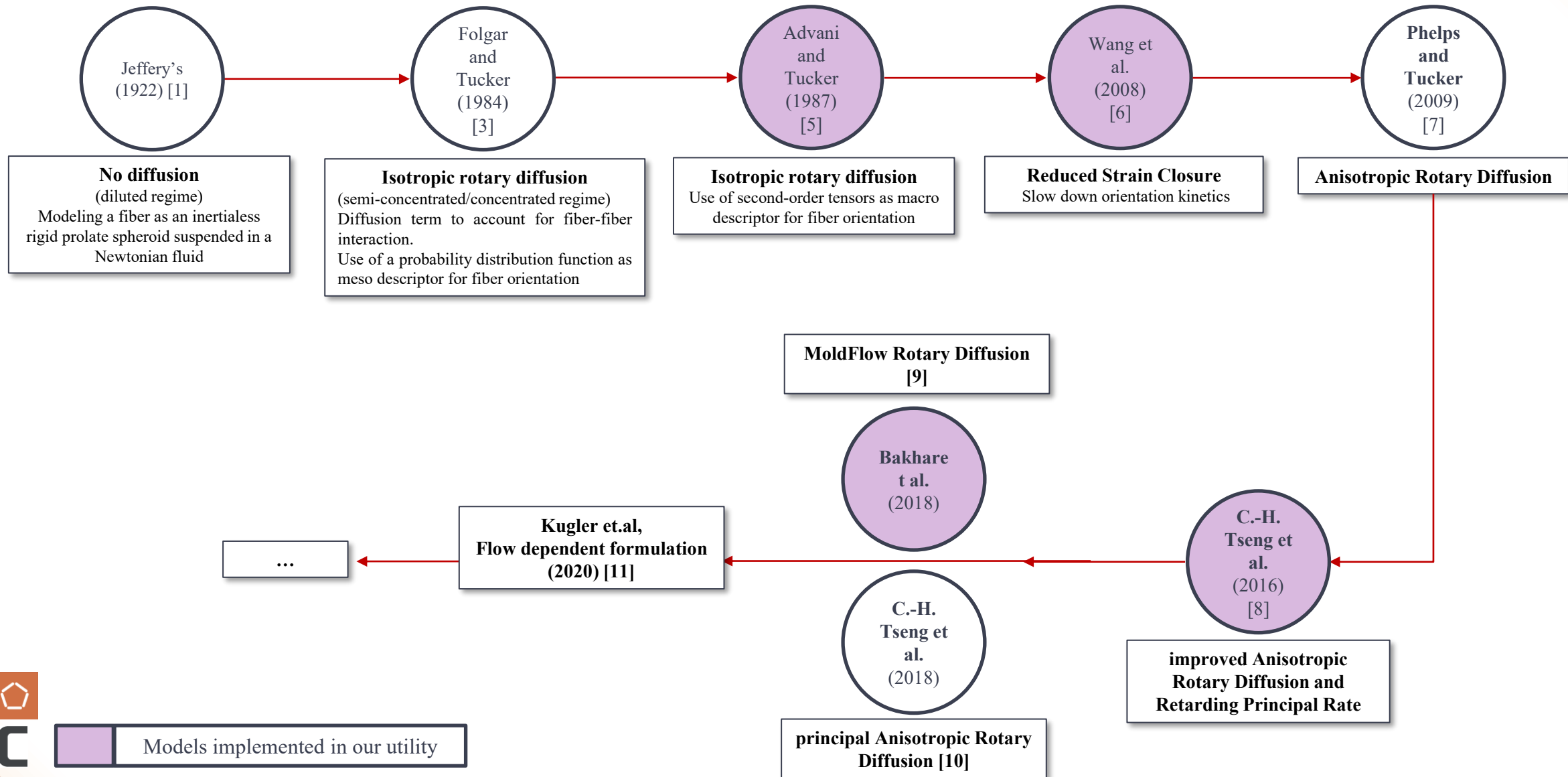
Alves et al. (2000)						
De	Mesh 1	Mesh 2	Mesh 3	Mesh 4	Extrapolated	Difference (%)
0	1.472	1.488	1.494	1.495	1.496	0.1
1	1.349	1.371	1.349	1.339	1.335	0.3
2	1.631	1.259	1.154	1.118	1.105	1.2
3	1.517	1.266	1.014	0.946	0.923	2.5
4	1.644	1.337	0.987	–	0.87	13.4
5	1.687	1.517	1.127	–	0.997	13

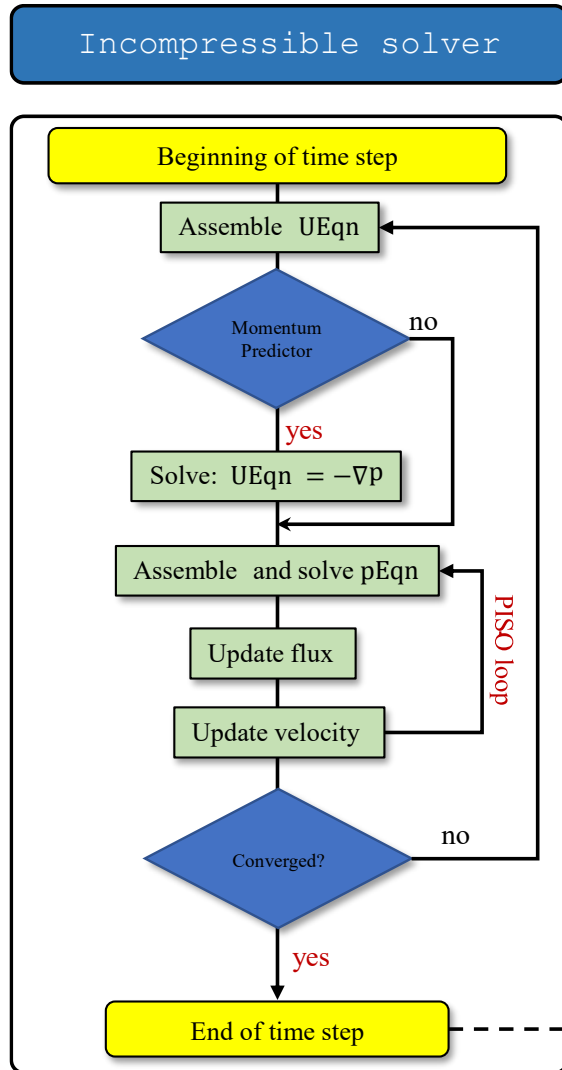
MM Alves, FT Pinho, PJ Oliveira, J. Non-Newtonian Fluid Mech., 93, 2000

C Fernandes et al., Improved Both Sides Diffusion (iBSD): a new and straightforward stabilization approach for viscoelastic fluid flows, JNNFM, 249, 63-78, 2017



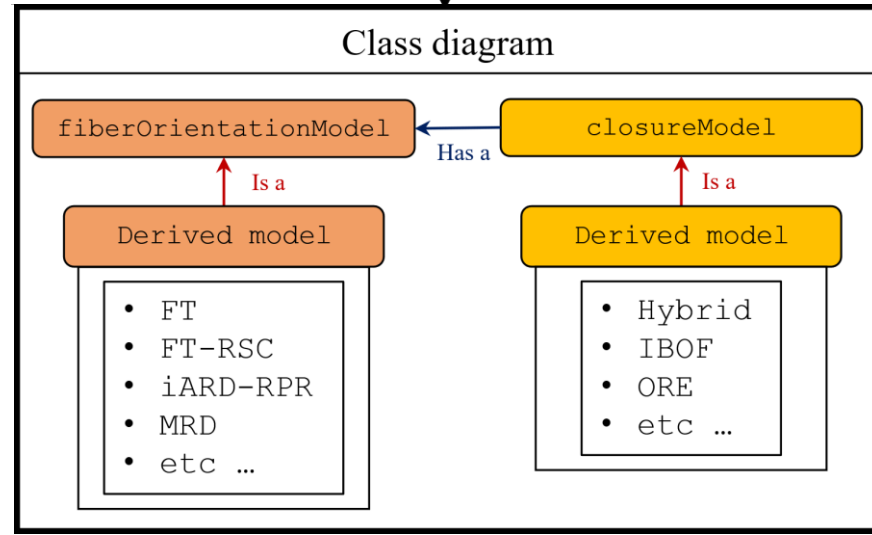
SND - Fiber Orientation





```

    fiberOrientationModeling functionObject
    {
        bool execute()
        {
            fiberOrientationModel_ -> solve();
            return true;
        }
    }
  
```



User input

```

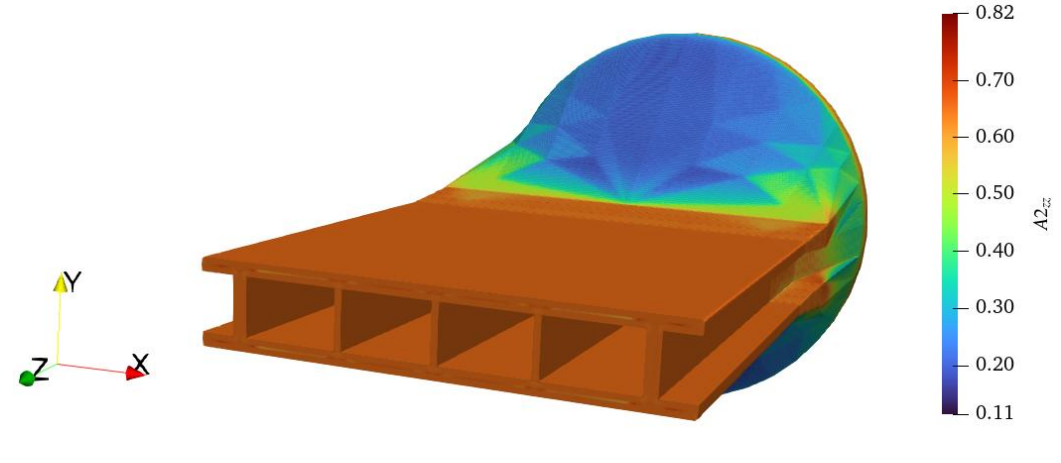
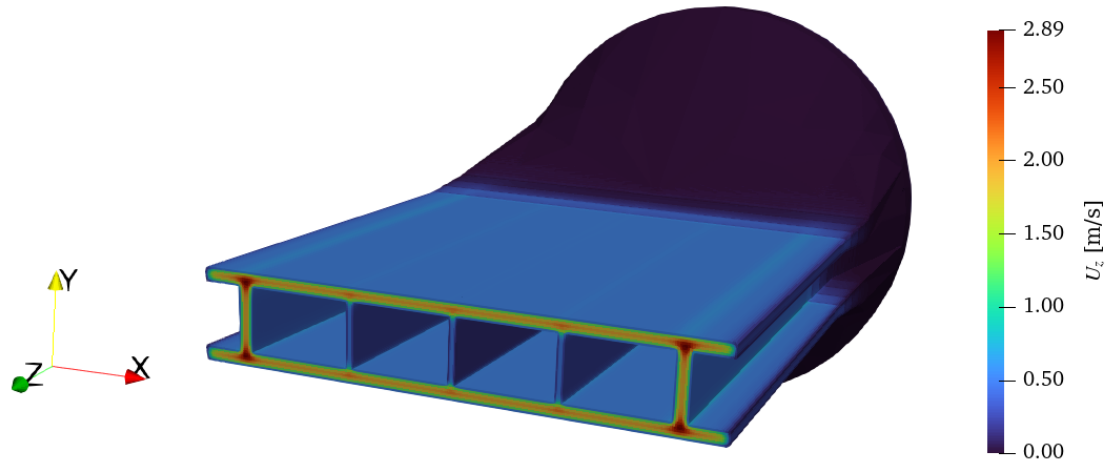
    controlDict
    {
        functions
        {
            FiberModeling
            {
                type          fiberOrientationModeling;
                libs          (libnewSolverFunctionObjects);
                errors strict;
                executeControl    timeStep;
                executeInterval  1;
            }
        }

        fiberOrientationProperties
        {
            model          <fiberModel>;
            xi             1;
            closureModel  <closureModel>;

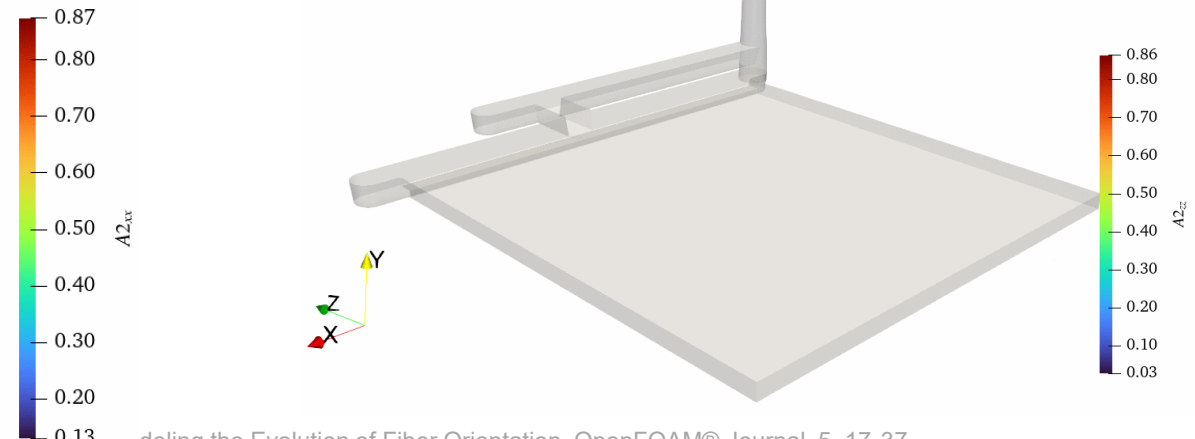
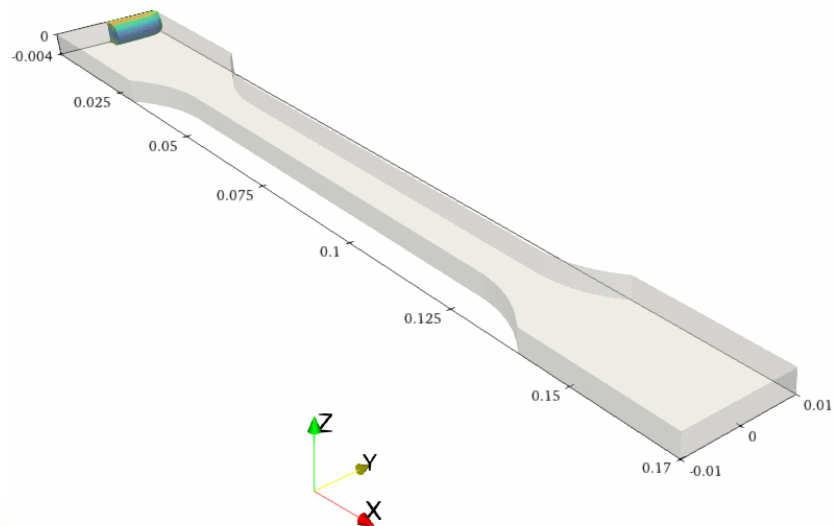
            <fiberModel>Properties
            {
                CI          0.01;
            }
        }
    }
  
```



Single Phase - Steady state

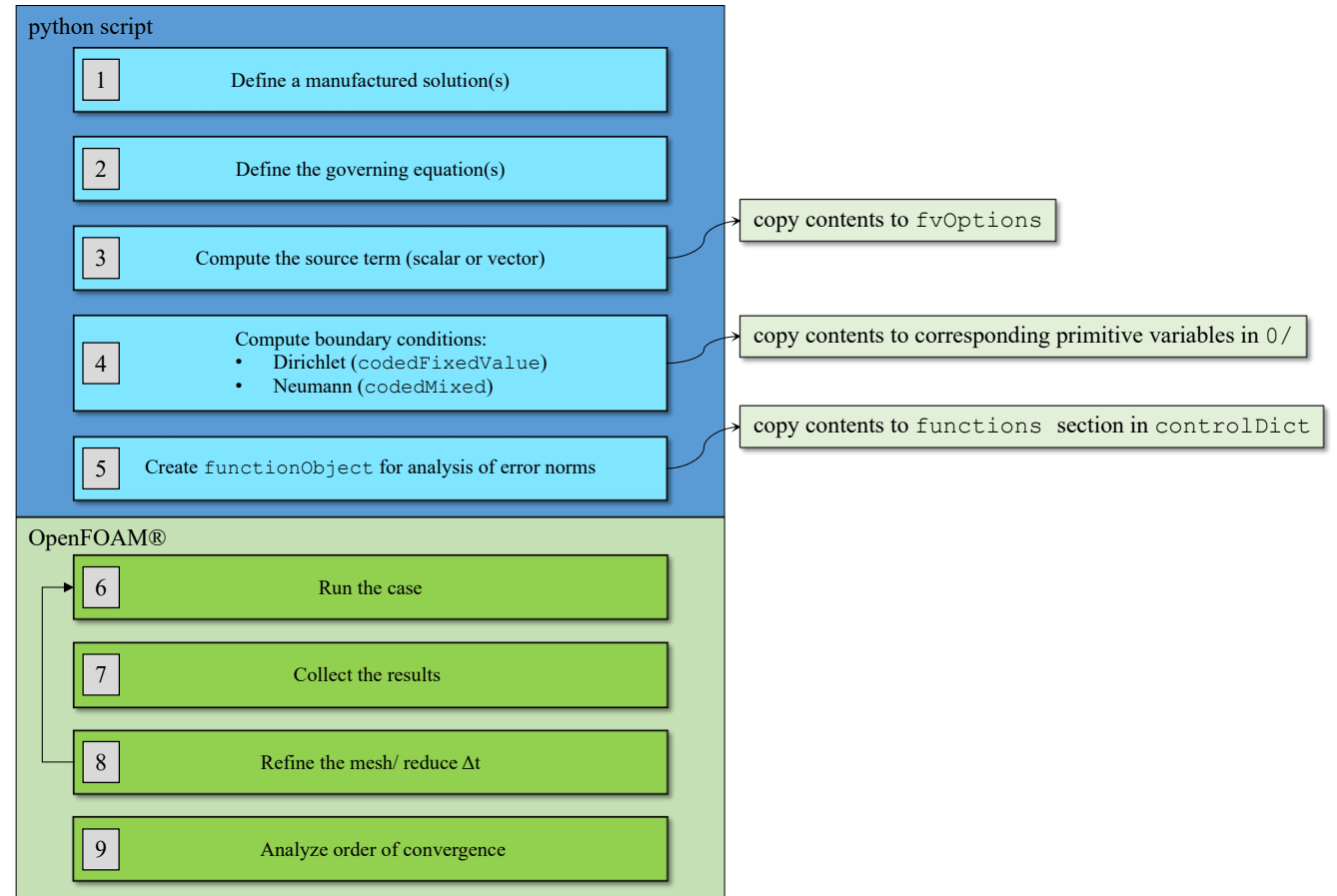
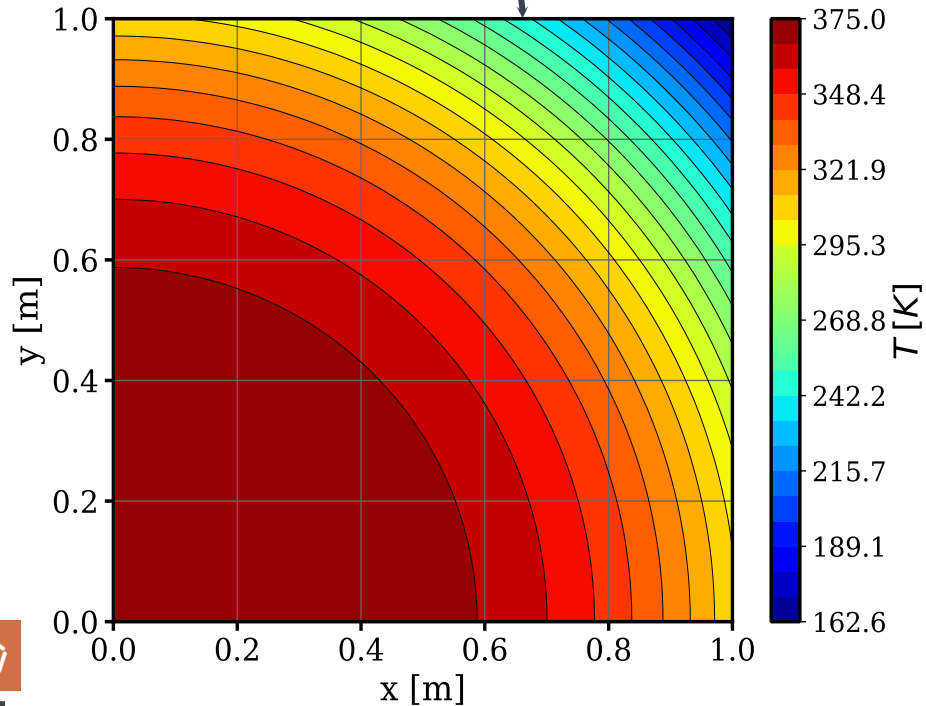


Two phase - Unsteady



Code Verification

$$T_{\text{ex}}(x, y, t) = 150 (\cos(x^2 + y^2 + \omega t) + 1.5)$$

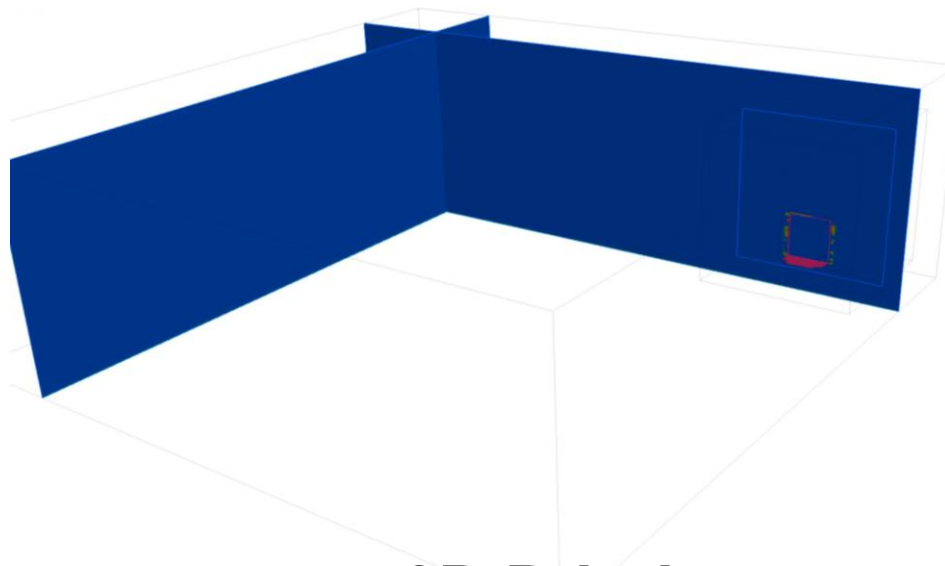
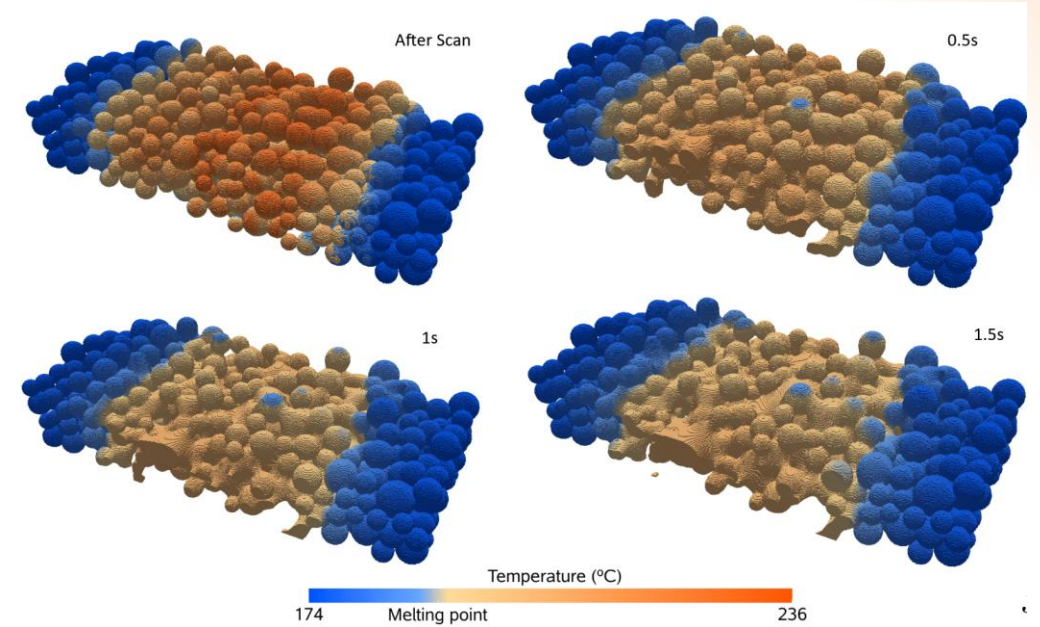
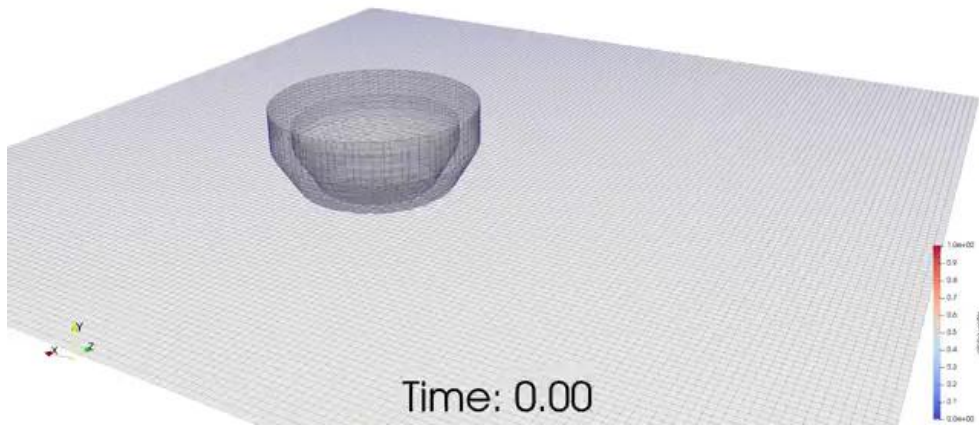


Ramôa et al. (2022). A Semi-Automatic Approach Based on the Method of Manufactured Solutions to Assess the Convergence Order in OpenFOAM. OpenFOAM® Journal



Recent Works





3D Printing

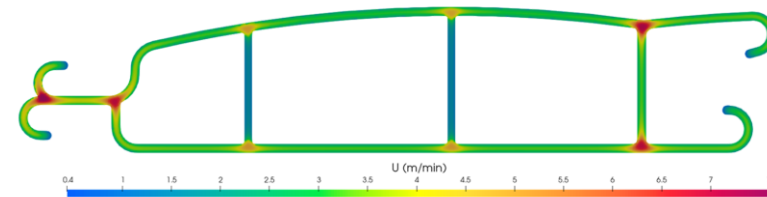
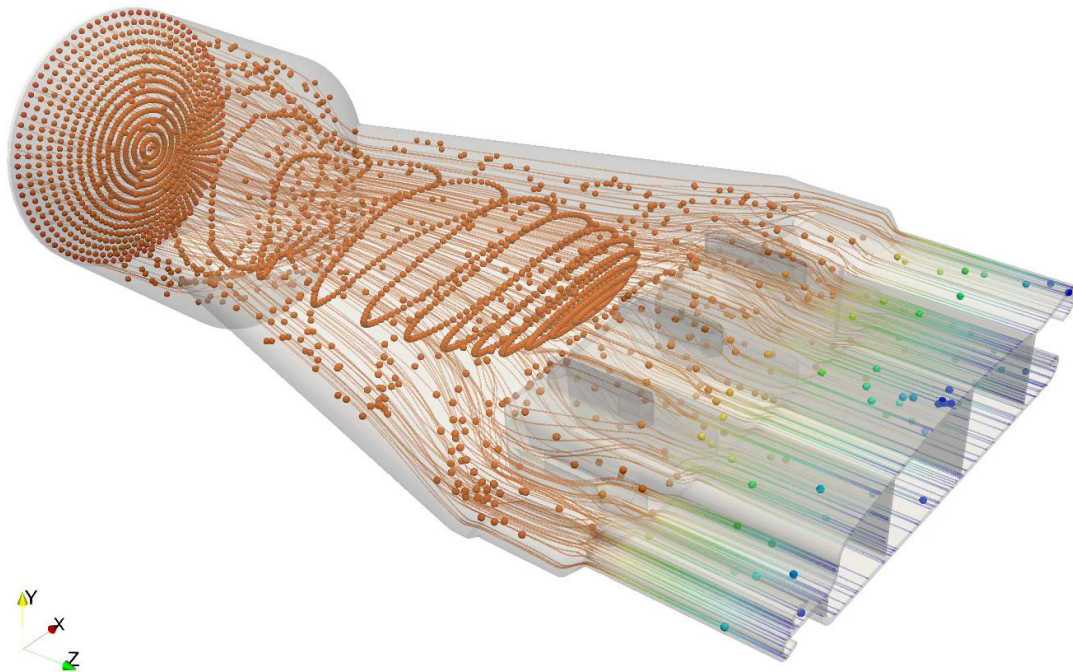
SLS



IPC



exaFOAM



Coupled solver

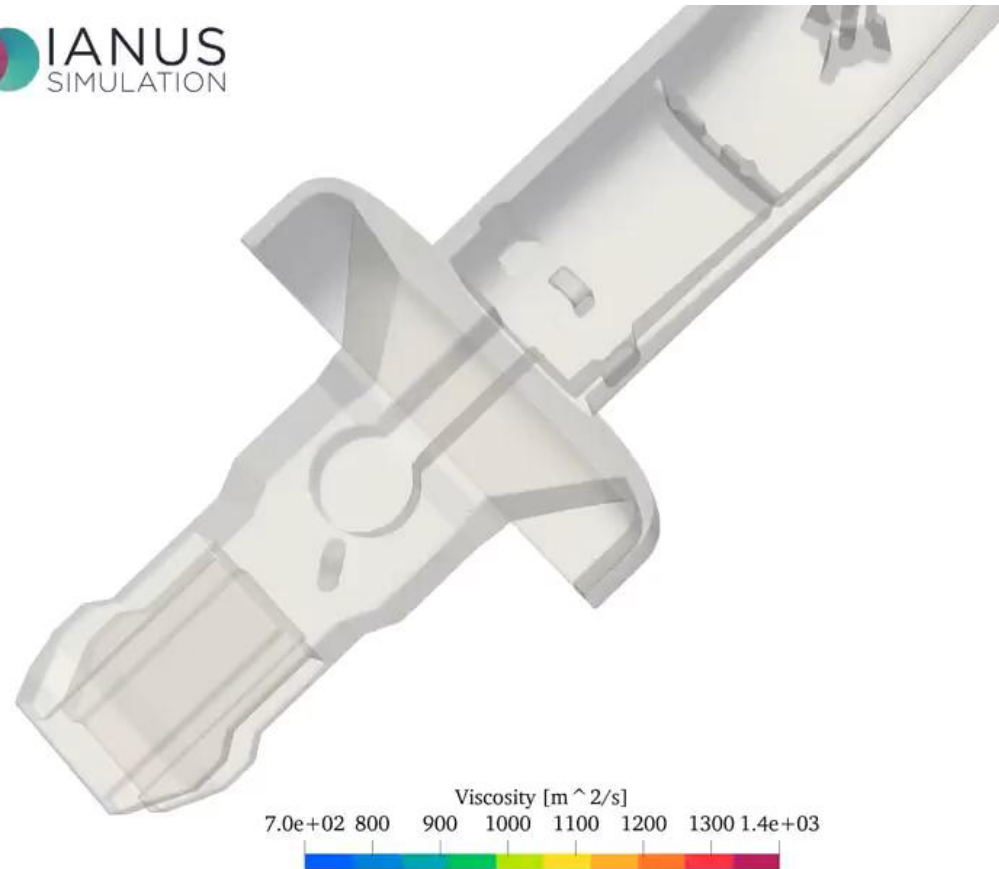
$$\begin{pmatrix} \mathbf{A}_u & \nabla & \nabla \cdot \\ \nabla \cdot & -\nabla \cdot [\mathbf{\Gamma}_u^{-1} \nabla] & 0 \\ \nabla \cdot (\boldsymbol{\tau}^{*0}) & 0 & \mathbf{A}_\tau \end{pmatrix} \begin{bmatrix} \mathbf{u} \\ p \\ \boldsymbol{\tau}^* \end{bmatrix} = \begin{bmatrix} b_u \\ b_p \\ b_{\boldsymbol{\tau}^*} \end{bmatrix}$$

20M cells / 1536 cores / 15 k core*h

Speedup
3x

www.exafoam.eu

New Injection Molding Solver



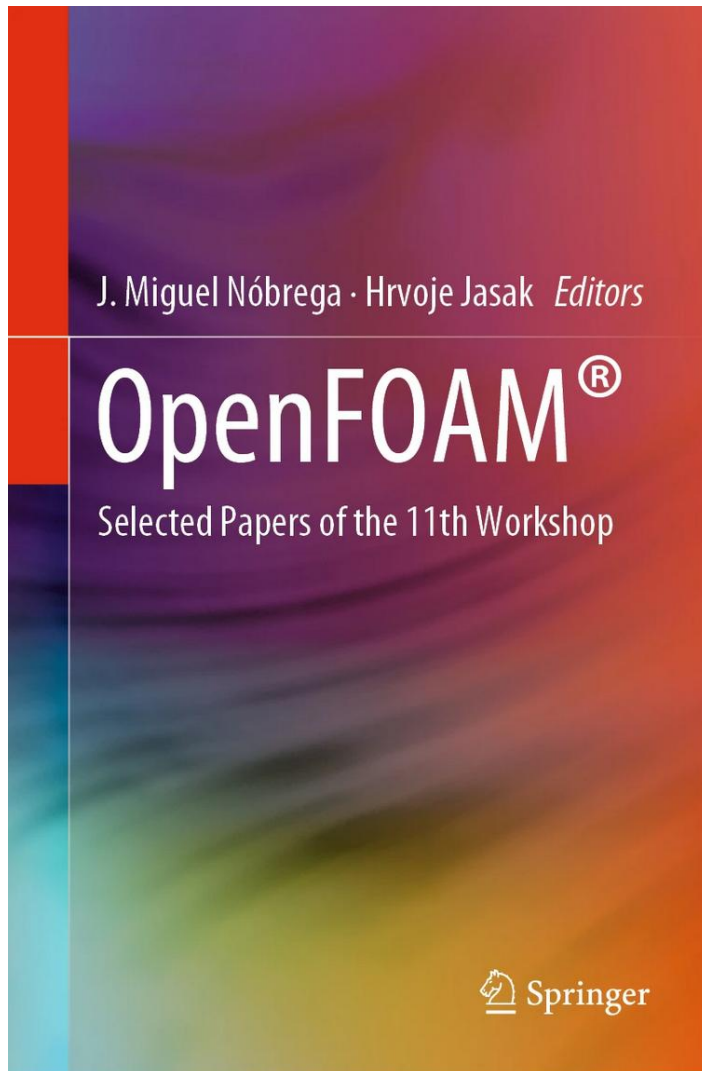
Time: 0 s

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



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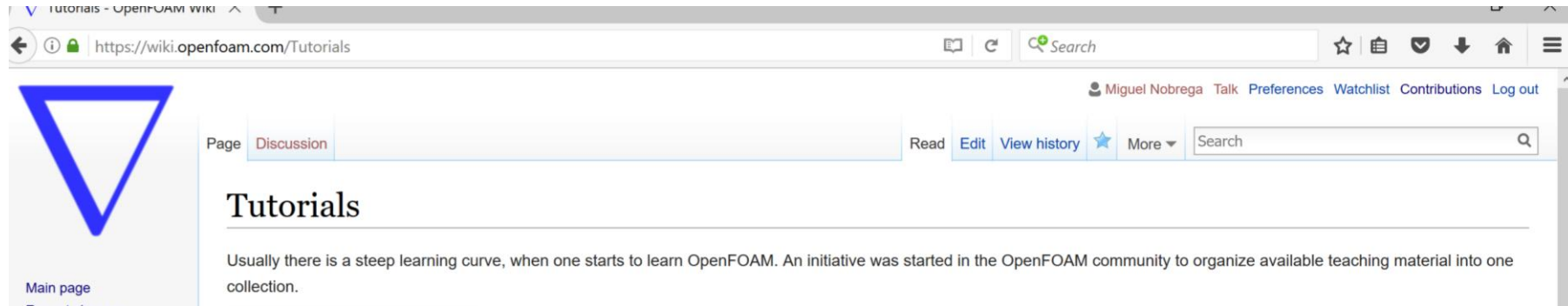
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OpenFOAM-preCICE: Coupling OpenFOAM with External Solvers for Multi-Physics Simulations

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David Schneider
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University of Stuttgart
<https://orcid.org/0000-0002-1314-9989>

DOI: <https://doi.org/10.51560/ofj.v3.88>

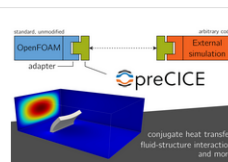
Keywords: Fluid Structure Interaction, conjugate heat transfer, multiphysics simulation

Abstract

Multi-physics simulations, such as conjugate heat transfer or fluid-structure interaction, are often constructed completely in OpenFOAM. However, they can also be formed by coupling OpenFOAM to third-party simulation software via a coupling tool. This approach indirectly adds to the capabilities of OpenFOAM those of other simulation tools (such as physical models or discretization methods more fitting for specific applications), and allows building complex multi-physics simulations by connecting specialized single-physics codes. We present the OpenFOAM-preCICE adapter, a function object that enables standard OpenFOAM solvers to use the open-source, massively parallel coupling library preCICE, without requiring any code modifications. We review alternative coupling approaches, analyze our design decisions, peek into key implementation details, validate the adapter, study the effect on runtime, and give an overview of the growing community of users and contributors.

Author Biography

Gerasimos Chourdakis, Technical University of Munich
Doctoral candidate at the Chair of Scientific Computing, Department of



PDF Discussion Forum
Abstract Video

Case files and source code

Published
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Comments and questions are welcomed on the article Chourdakis et al, OpenFOAM-preCICE: Coupling OpenFOAM with external solvers, OpenFOAM Journal, February 2023, <https://doi.org/10.51560/ofj.v3.88>.

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February 28, 2023, 07:49 #2

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The article is now online! Thank you very much to the editors and all five reviewers for their hard work and extensive feedback. We would be very happy for further questions and feedback here.

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March 7, 2023, 16:36 #3

ancolli
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I have read your article and it is really interesting. I have two minor questions:

a) In the partitioned and conjugated heat transfer examples, you have used a Dirichlet-Neuman coupling. A few years ago, for a similar problem, I found that this was a faster method than the harmonic averaging already implemented in the chtMultiregionFoam. However, with the Dirichlet-Neuman coupling, I found some convergence problems depending on the relative difference of the conductivities on each side (electrical problems



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Thank you!!