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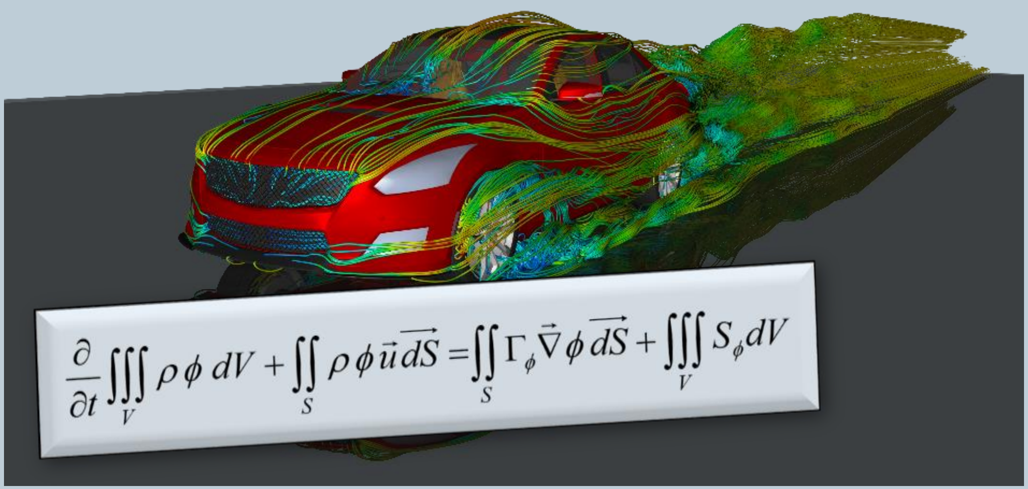
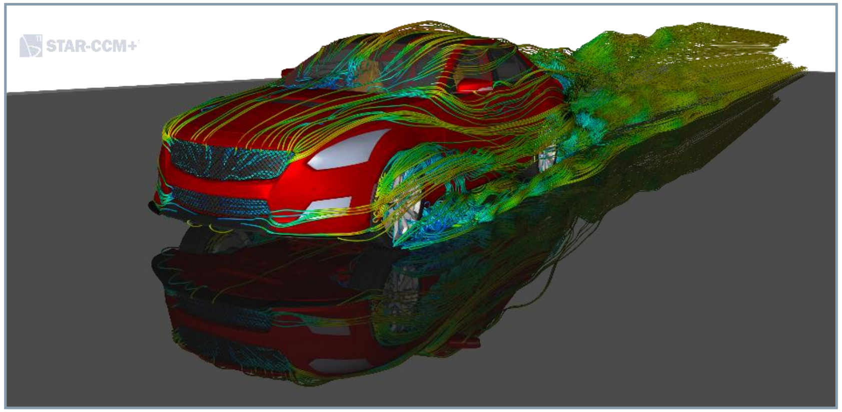
Ingenuity for life



Introduction to CFD

 CT09105_CM13_1

Section 1: Introduction



- What is CFD?
- CFD in the context of a company
- Historical development of CFD
- CFD Workflow
- Introduction to Siemens PLM Software

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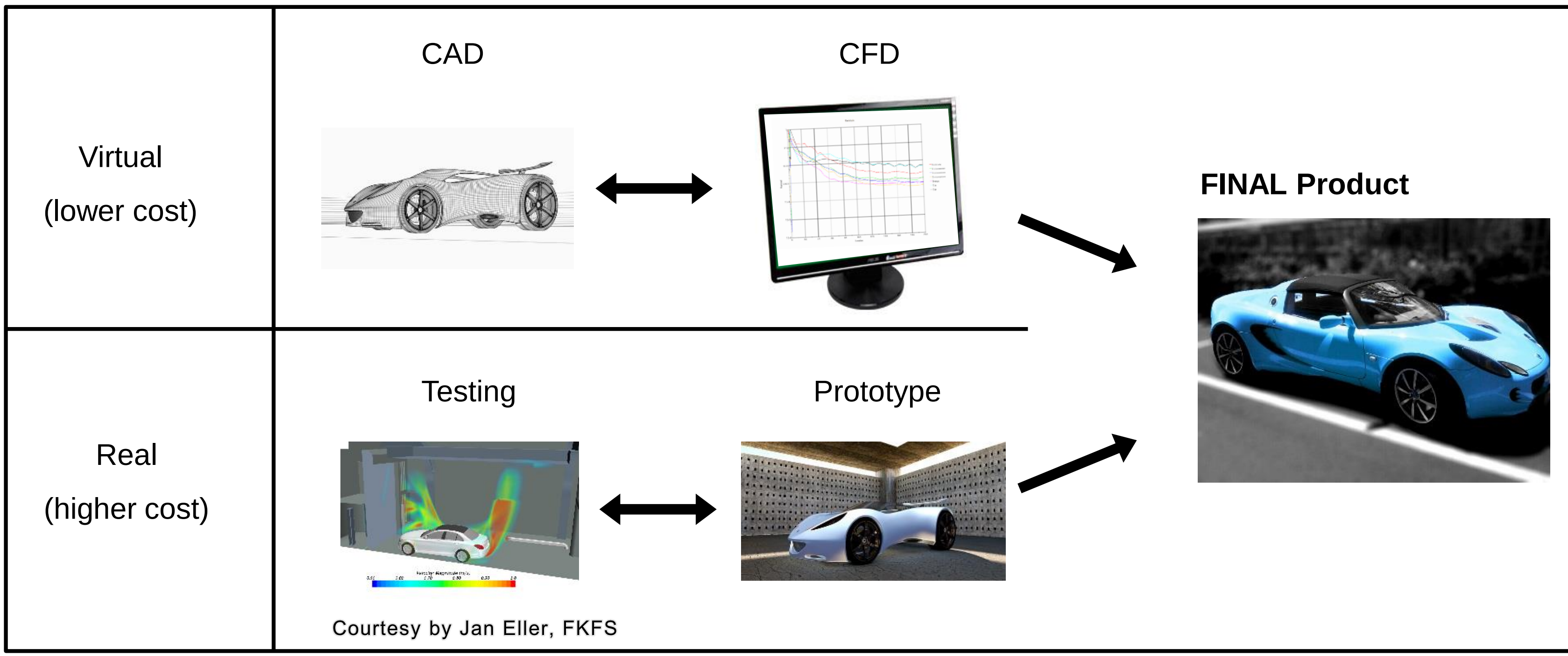
Why do CFD?

Economical and technical motivations

Obtain results comparable to prototyping / experiments, but with a **reduction of time and cost.**

Obtain more in-depth results, **better understanding of physical phenomena.**



Lyophilization process is currently:

Time consuming… *days and weeks*

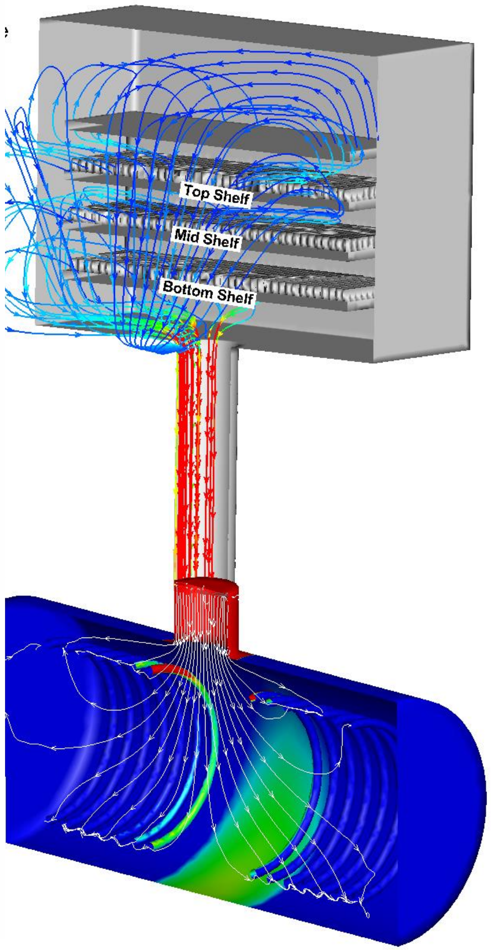
Expensive to Run…

Energy inefficient… *<5%*

Advances in freeze-drying technology are required to meet the growing demand for high-capacity ad efficient freeze-dryers.

Lyophilizer: A Closer Look

Lab-scale Lyostar/SP Scientific



Sublimation Rate:

- heat transfer
  - •Radiation
  - •Contact conduction
  - •Gas Conduction
  - •Convection
- •Intrabatch position
- •Suspended *vs* on-shelf

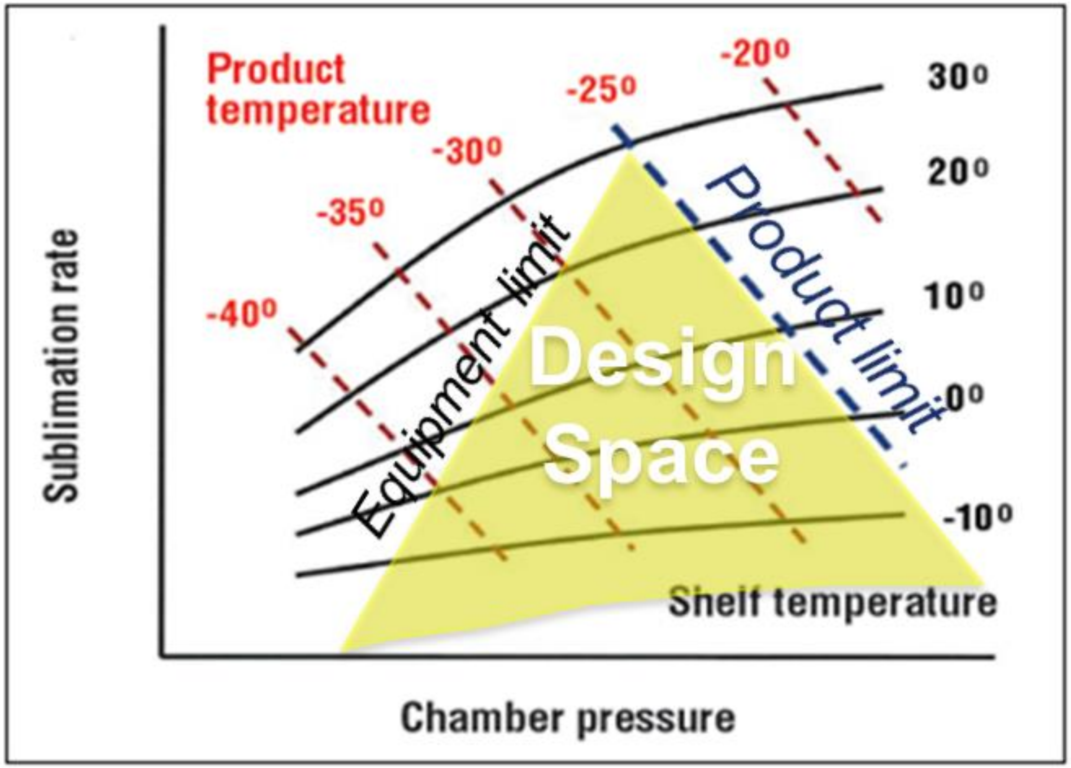
Vapor Removal Rate:

- Duct length, diameter
- CIP/SIP
- Isolation valve

Condensation Rate:

- Coil/plate topology
- Coil/plate temperature
- Non-condensable pump

Equipment Limit

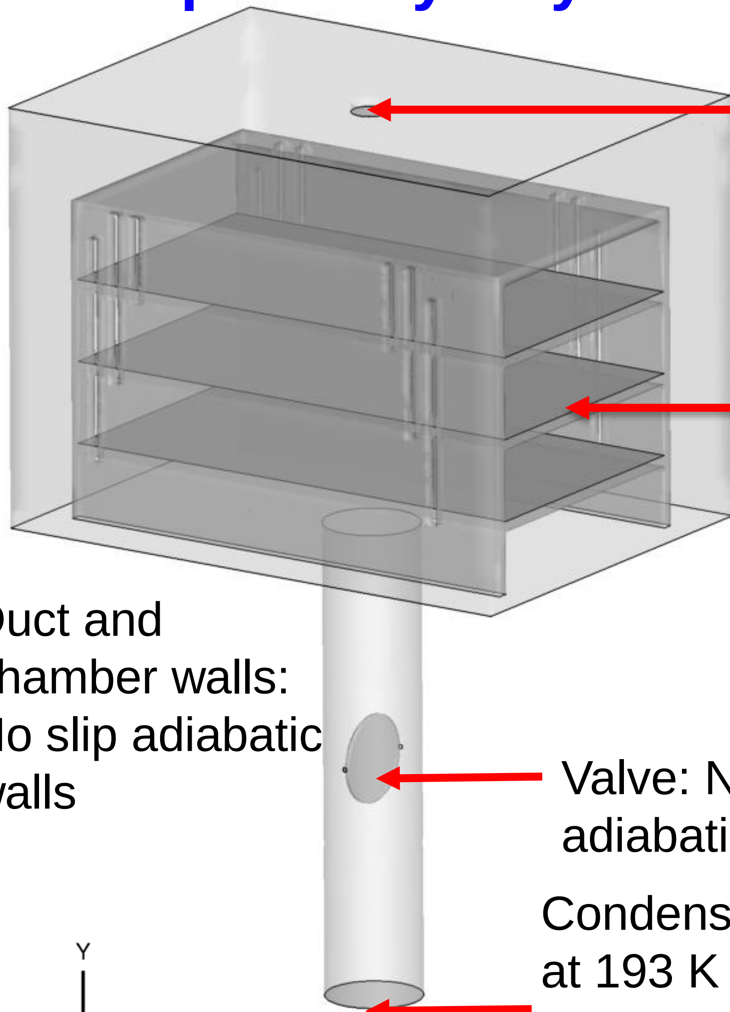


S. Nail, J. Searles, "Elements of QbD in Development and Scale-Up of Freeze-Dried Parenterals", *InterPharm*, 2007.

- ❖ Equipment Capability curve is accurately predicted by CFD
- ❖ A CFD case takes just minutes-hour of CPU time

CFD Setup: Lyostar 2 Simulations

Prepared by Gayathri Shivkumar & Vaibhav Kshirsagar



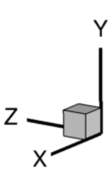
Nitrogen inlet: No slip adiabatic wall

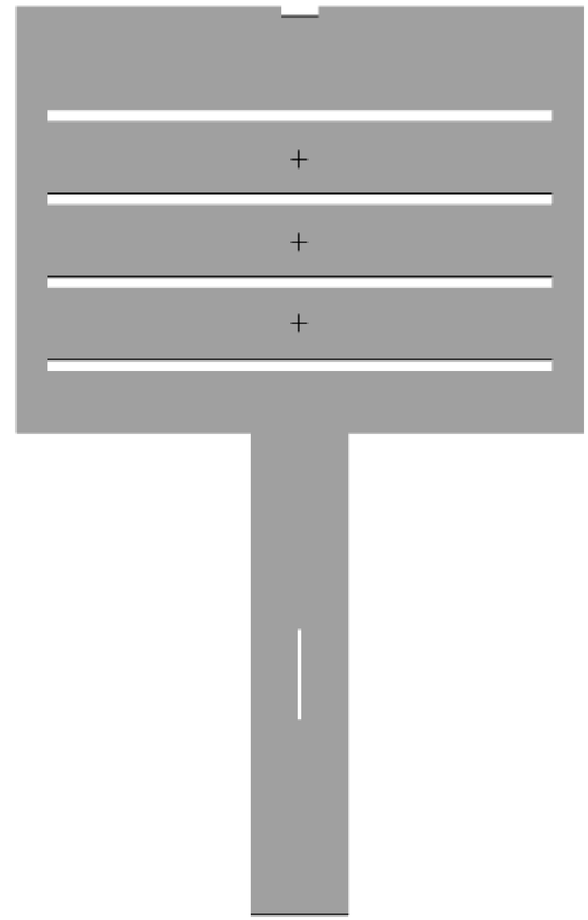
Shelves and vial pack: Mass flow inlet at shelf temperature (specified from experimental data)

Duct and chamber walls: No slip adiabatic walls

Valve: No slip adiabatic wall

Condenser: Pressure outlet at 193 K (from experiments)





Boundary conditions

Experimental Validation of CFD

Parameters	Conditions
❖ Test method	Ice sublimation using deionized water in ‘bottomless trays’
❖ Test conditions	Chamber pressure and shelf temperature set to achieve maximum sublimation rate
❖ Shelf temperature measurement	Thermocouple
❖ Condenser pressure measurement	Capacitance manometer in foreline connecting condenser chamber and vacuum pump
❖ Chamber pressure measurement	Capacitance manometer mounted on product chamber
❖ Mass flow rate measurement	Tunable Diode Laser Absorption Spectroscopy (TDLAS)

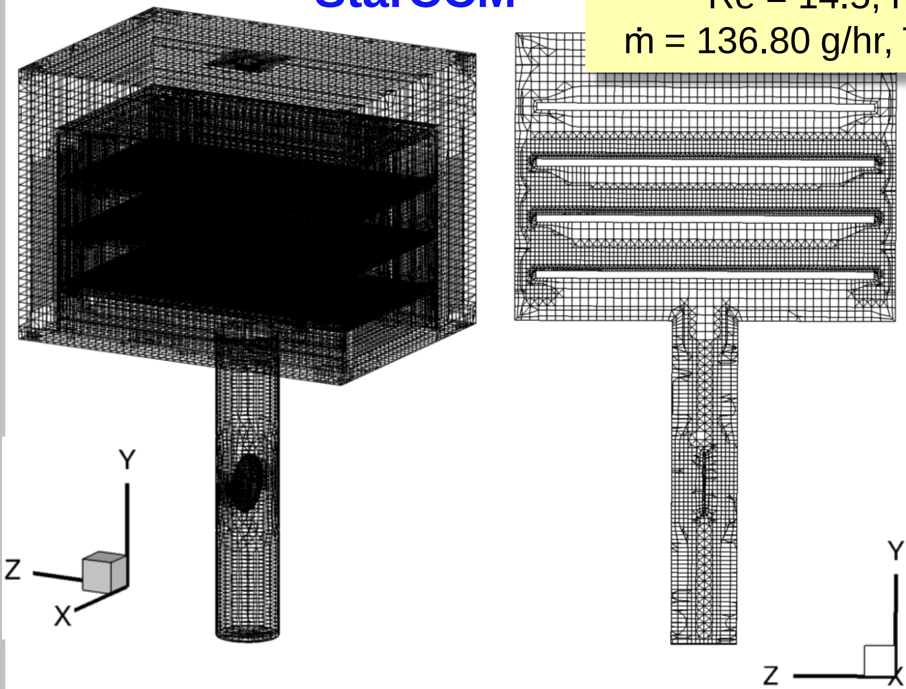
CFD Simulation Settings

Parameters	Star CCM Conditions	Fluent Conditions
❖ Space	3D	3D
❖ Time	Steady	Steady
❖ Density	Ideal gas	Ideal gas
❖ Flow	Laminar	Laminar
❖ P-V Coupling	Segregated (SIMPLE scheme)	SIMPLE
❖ Spatial discretization scheme (Convection / Pressure & Velocity)	2^{nd} order	2^{nd} order

Grid Convergence

Re = 14.5, P_{ch} (exp) = 55 mTorr:
$\dot{m}$ = 136.80 g/hr, T_s = -22 ºC, P_{cd} = 6 mTorr

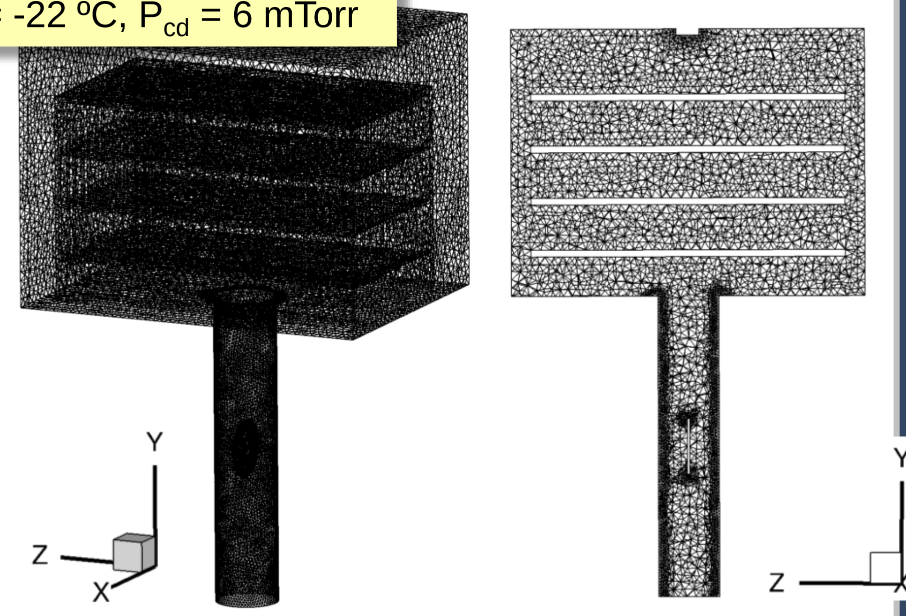
StarCCM



Number of cells	Chamber pressure, P_{ch} (mTorr)	% Change in chamber pressure
6,311	60.37	-
69,248	56.06	-7.14 %
275,967	58.51	4.37 %
340,577	59.59	1.84 %
1,626,971	59.57	-0.03 %

< 3%

Fluent



Number of cells	Chamber pressure, P_{ch} (mTorr)	% Change in chamber pressure
158,124	58.59	-
365,740	59.47	1.50 %
480,372	59.64	0.28 %
1,216,644	59.87	0.38 %

< 3%

Simulation Parameters

Property	StarCCM Simulations	Fluent Simulations
Number of cells	275,967	480,372
Relaxation factors	Pressure = 0.3 Velocity = 0.7 Energy = 0.9	Pressure = 0.3 Density = 1 Momentum = 0.7 Energy = 1
Pressure-velocity coupling	SIMPLE	SIMPLE
Number of iterations	3,500	3,500
Residuals	Continuity ~ 10^{-11} Momentum ~ 10^{-7} Energy ~ 10^{-5}	Continuity ~ 10^{-4} Velocity ~ 10^{-5} Energy ~ 10^{-7}
Physical parameter (Chamber pressure) convergence	< 0.01 % variation for >1000 iterations	< 0.01 % variation for >1000 iterations
Processor (serial)	Intel Xeon CPU E5-2670	Intel Xeon CPU E5-2670
CPU time	2.1 hrs	6.2 hrs

Minimum Controllable Pressure

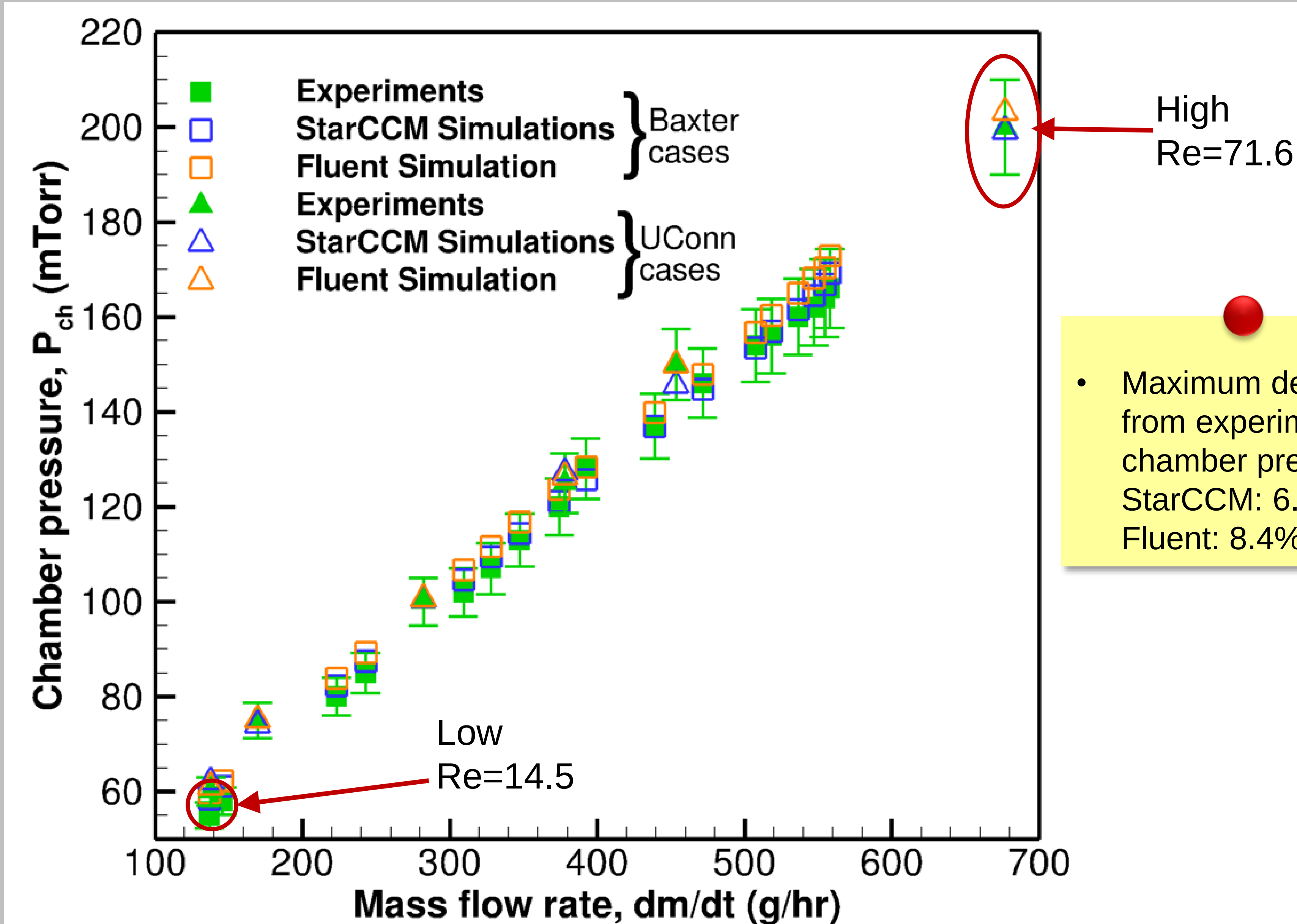
Mass flow rate, dm/dt (g/hr)	Shelf temperature, Ts (°C)	Condenser pressure, Pcd (mTorr)	Chamber pressure, Pch (mTorr)			Percentage deviation from experiments	
Inputs for simulations			Experiments	StarCCM	Fluent	Star CCM	Fluent
Baxter cases							
136.8	-22	6	55	58.51	59.64	6.4%	8.4%
145.44	-20	6	58	61.09	62.27	5.3%	7.4%
223.2	-12	10	80	82.31	83.95	2.9%	4.9%
243	-10	11	85	87.54	89.31	3.0%	5.1%
309.24	-4	10	102	104.58	106.74	2.5%	4.7%
327.96	-2	10	107	109.40	111.68	2.2%	4.4%
347.4	0	10	113	114.38	116.77	1.2%	3.3%
374.4	2	9	120	121.12	123.65	0.9%	3.0%
392.4	4	9	128	125.74	128.38	-1.8%	0.3%
439.2	6	5	137	136.96	139.85	0.0%	2.1%
471.6	8	4	146	144.82	147.90	-0.8%	1.3%
507.6	10	4	154	153.47	156.74	-0.3%	1.8%
518.4	14	5.5	156	156.98	160.38	0.6%	2.8%
536.4	16	3	160	161.57	165.06	1.0%	3.2%
547.2	18	3	162	164.58	168.13	1.6%	3.8%
554.4	20	3	164	166.80	170.38	1.7%	3.9%
558	26	3	166	169.31	172.94	2.0%	4.2%
UConn cases							
137.88	-23	27	60	62.04	60.97	3.4%	1.6%
169.56	-18	38	75	73.98	75.08	-1.4%	0.1%
282.24	-7	40	100	100.58	100.66	0.6%	0.7%
378	8	53	125	127.20	126.31	1.8%	1.0%
453.6	13	59	150	145.68	149.91	-2.9%	-0.1%
676.8	30	67	200	199.17	203.17	-0.4%	1.6%

Low Re (14.5) case

High Re (71.6) case

* Patel, Chaudhuri, & Pikal, *Chemical Engineering Science*, 2010

Minimum Controllable Pressure

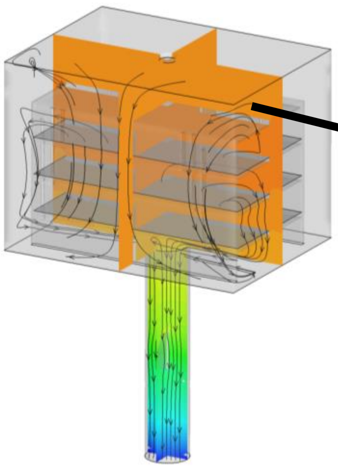


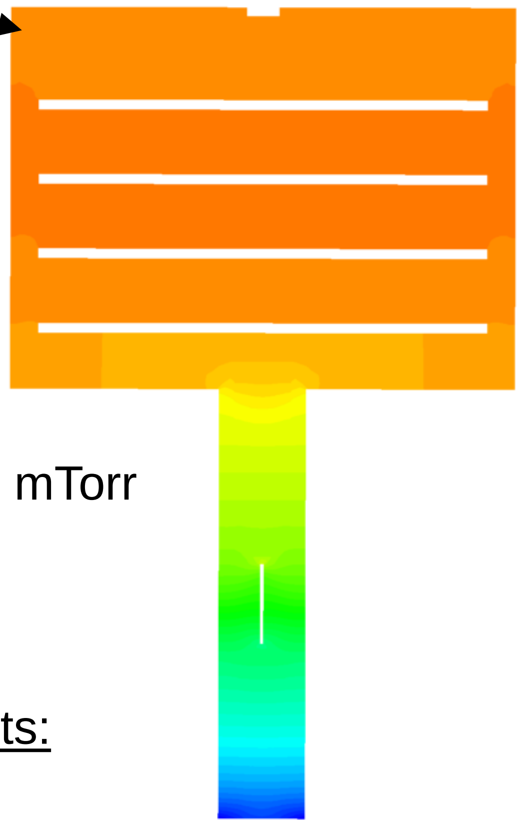
- Maximum deviation from experimental chamber pressure: StarCCM: 6.4%, Fluent: 8.4%

CFD Solvers: Pressure

Re = 14.5, P_{ch} (exp) = 55 mTorr

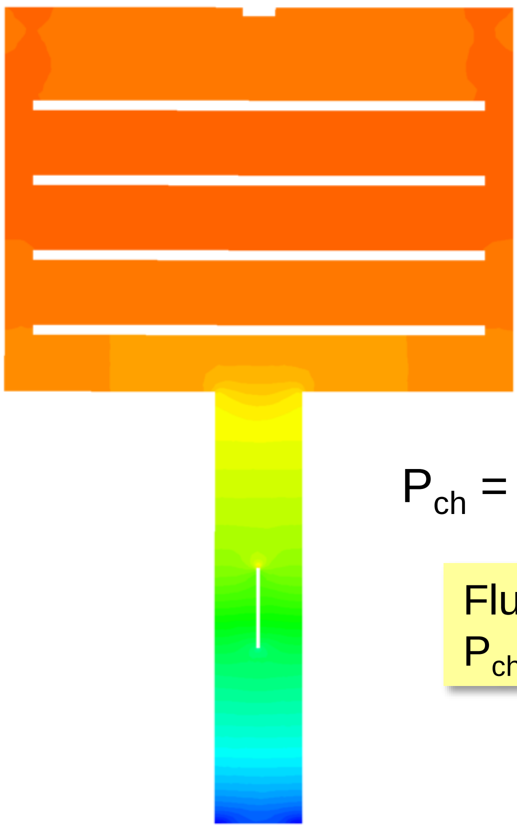
StarCCM Results

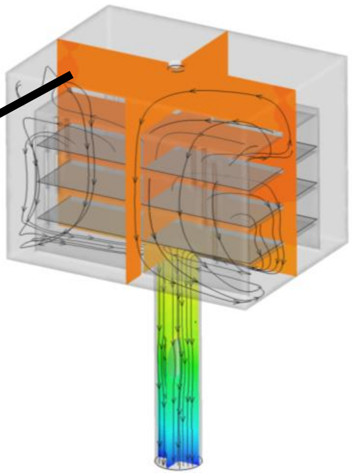




P_{ch} = 58.51 mTorr

Fluent Results





P_{ch} = 59.64 mTorr

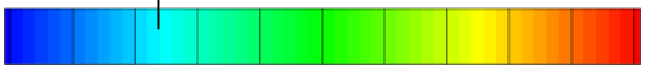
Fluent P_{ch} > StarCCM P_{ch} by 1.93%.

<u>Baxter case inputs:</u>

$\dot{m}$ = 136.80 g/hr

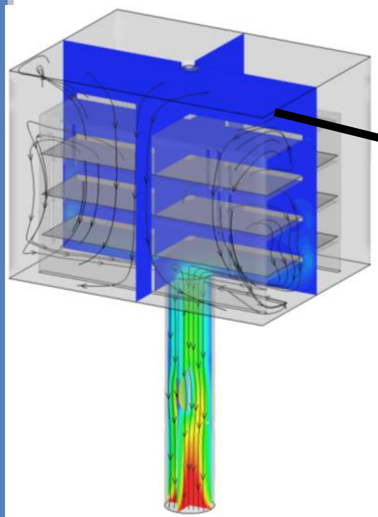
T_s = -22 °C

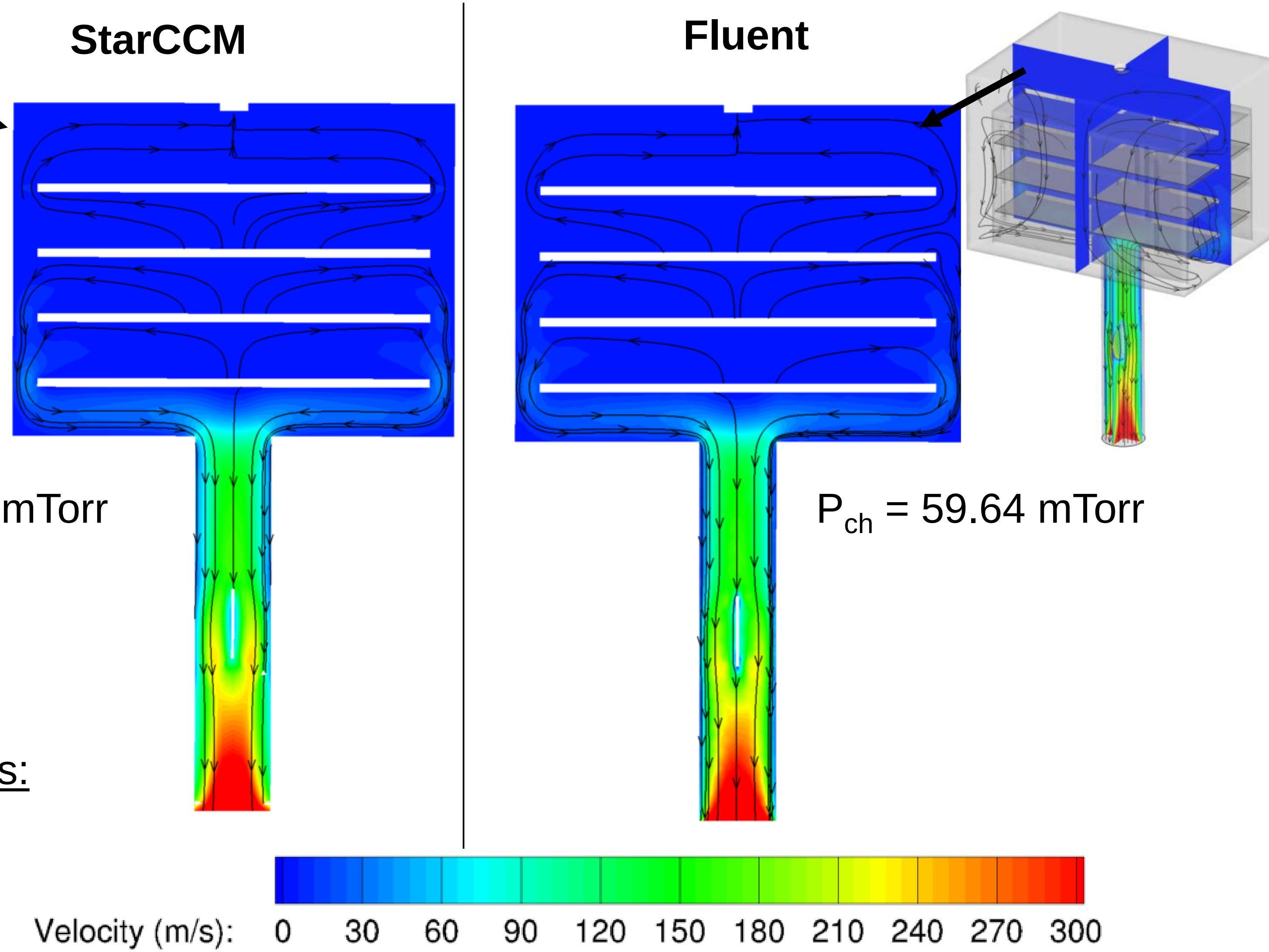
P_{cd} = 6 mTorr



CFD Solvers: Velocity

Re = 14.5, P_{ch} (exp) = 55 mTorr





P_{ch} = 58.51 mTorr

P_{ch} = 59.64 mTorr

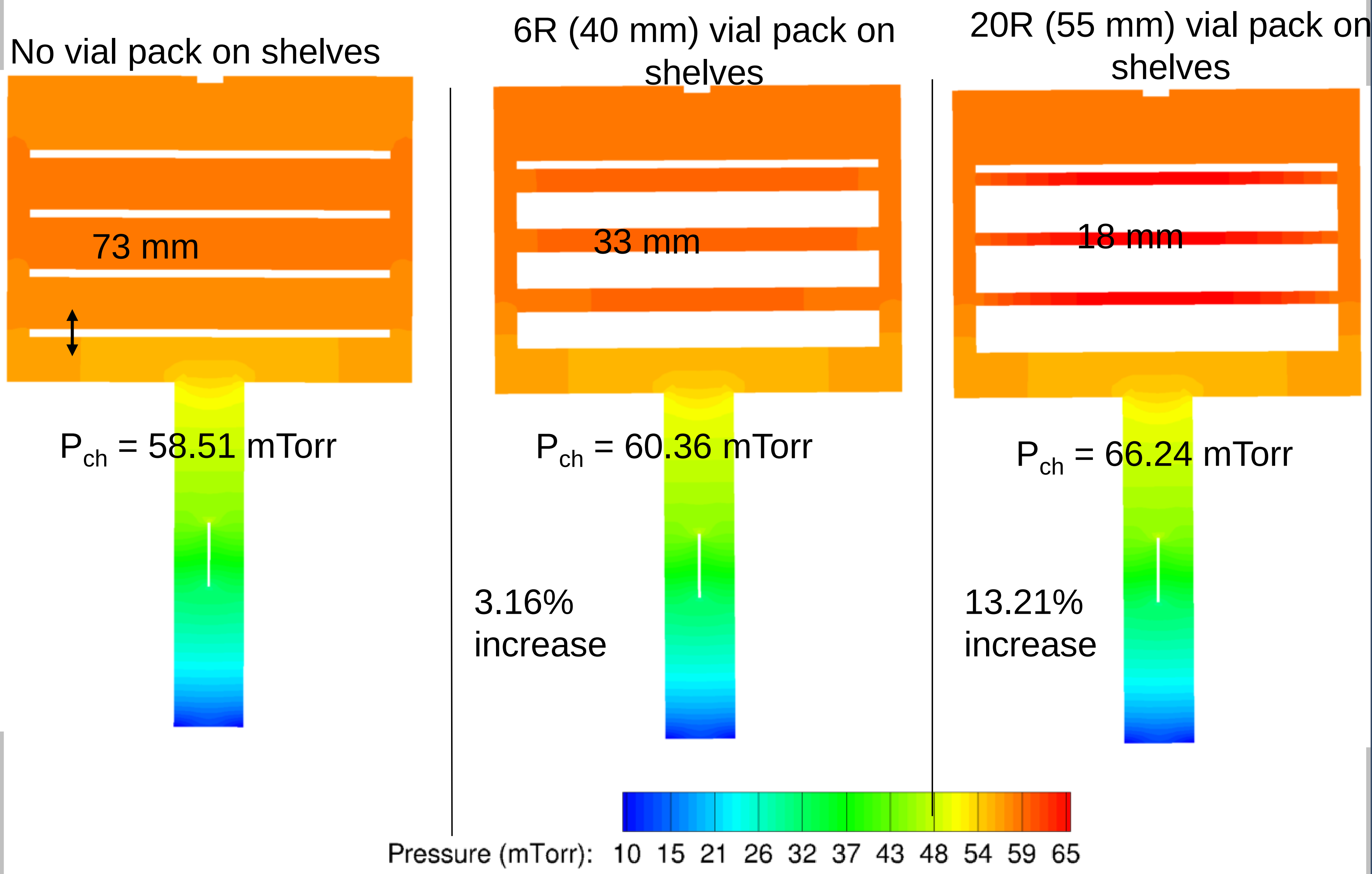
<u>Baxter case inputs:</u>

$\dot{m}$ = 136.80 g/hr

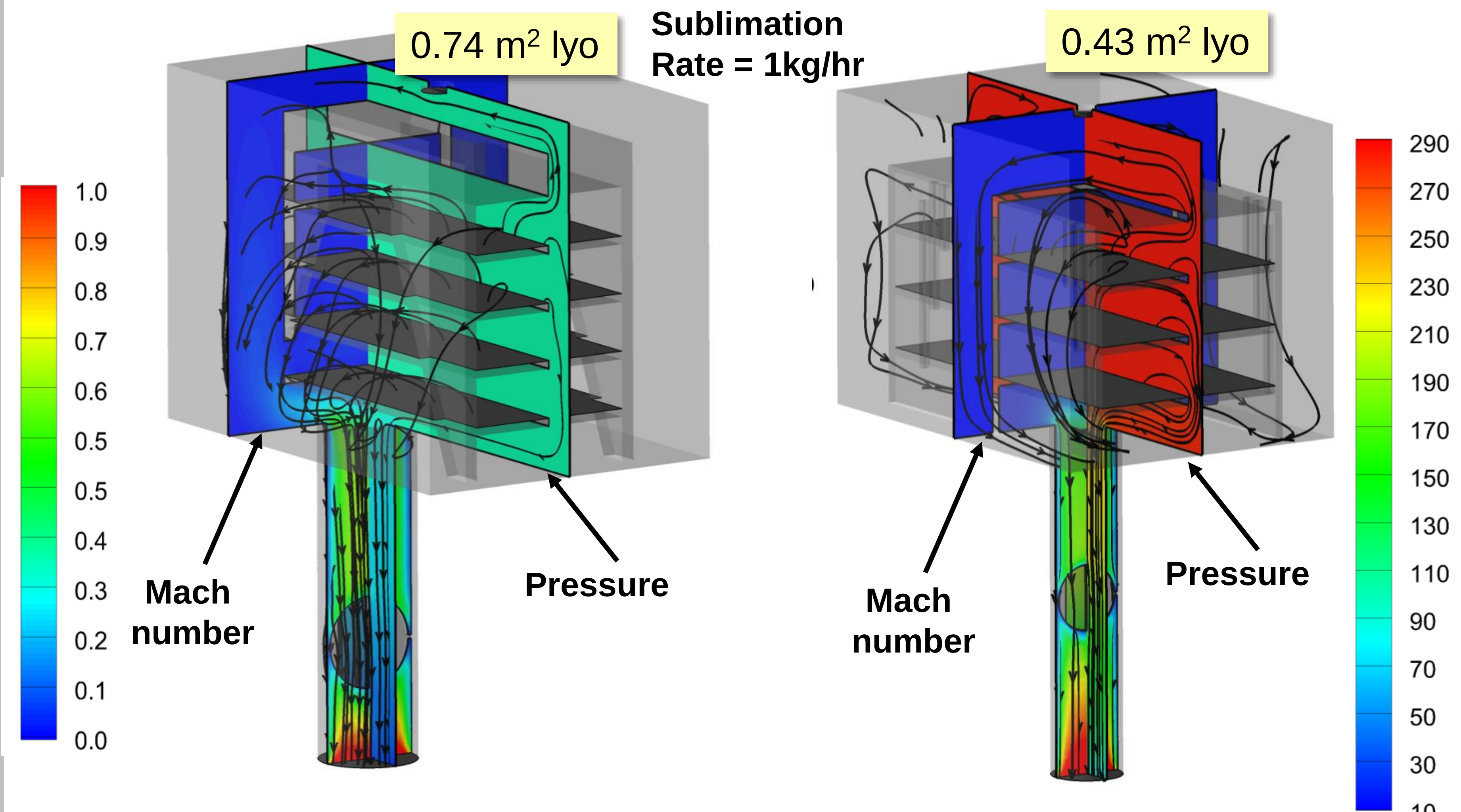
T_s = -22 ^{o}C

P_{cd} = 6 mTorr

Effect of Shelf Gap



CFD: *Equipment Differences*

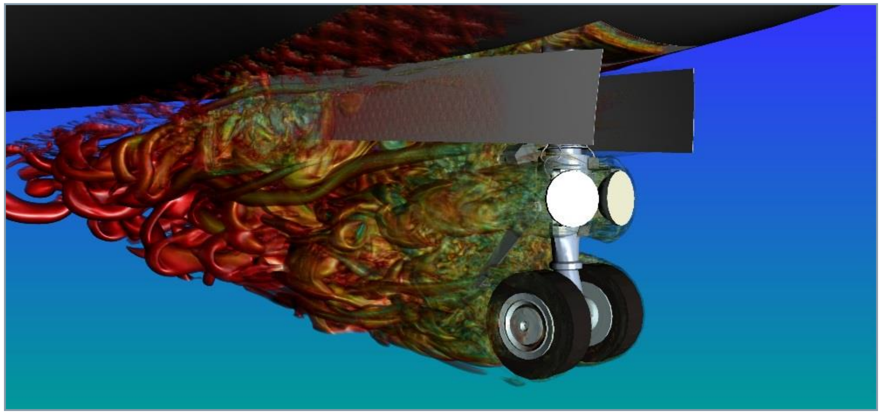


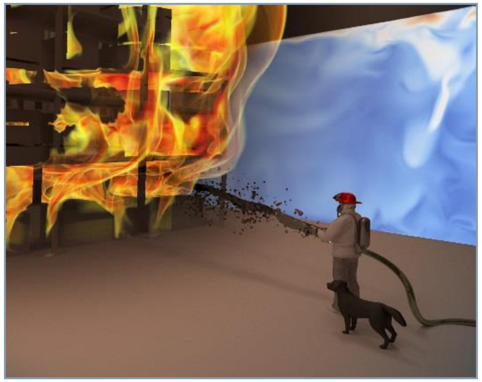
Min P_{ch} = 102 mTorr

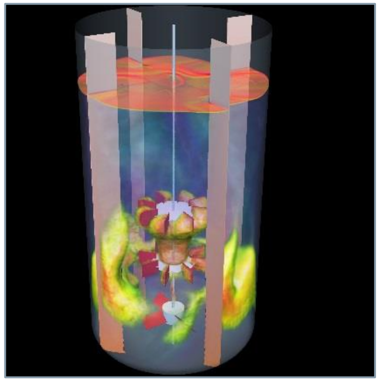
Min P_{ch} = 287 mTorr

What are some industrial applications of CFD?

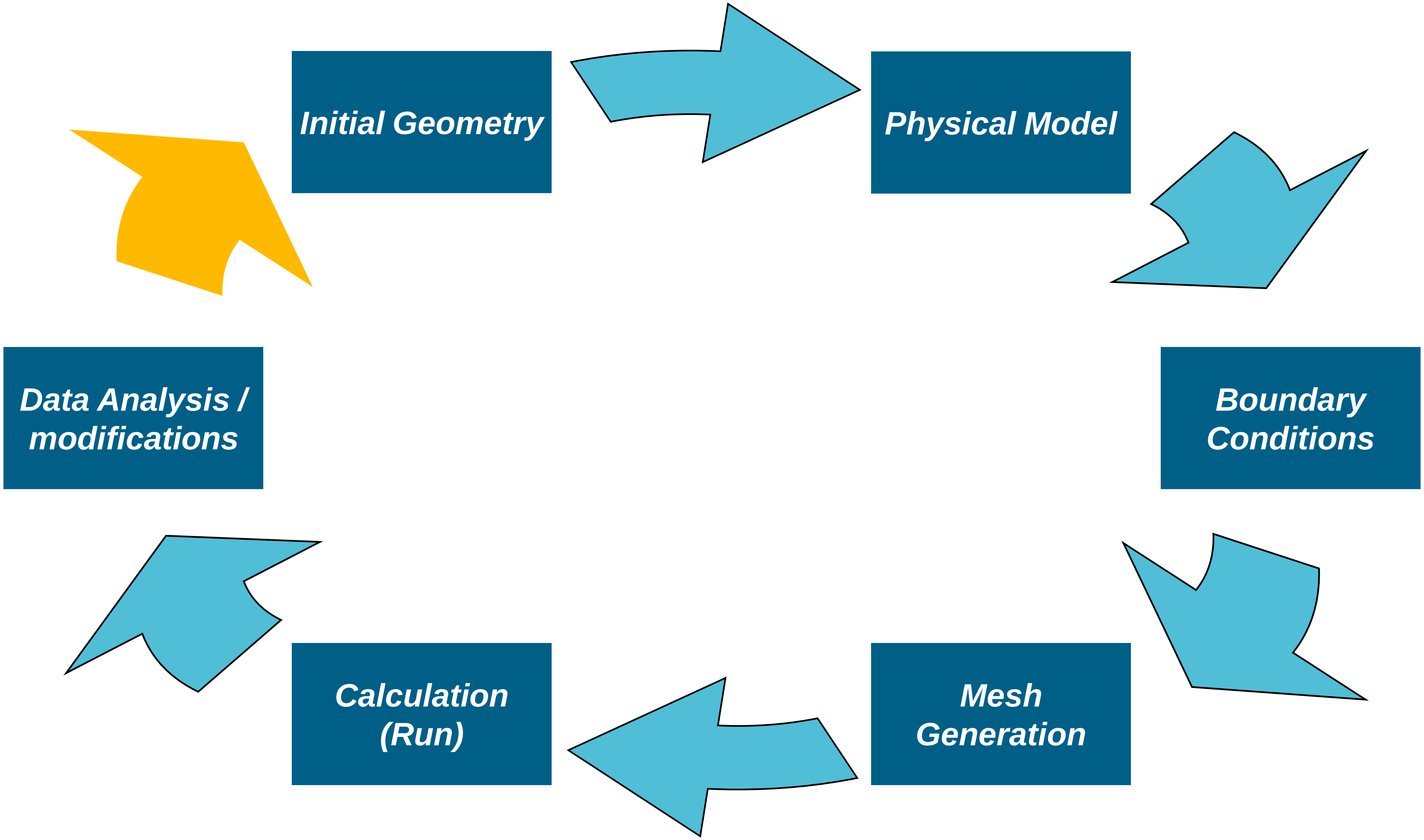
- Aerospace
- Automotive
- Chemical
- Home Appliances
- Marine / Naval
- Offshore
- Building / Architecture
- Bio-engineering
- Medicine
- Turbomachinery







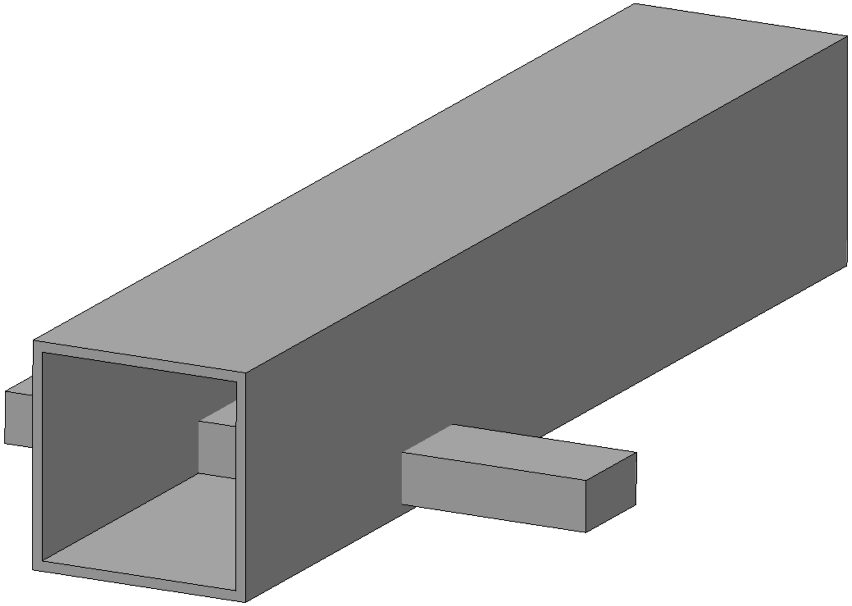
CFD workflow



Workflow – available CAD

2 CAD parts:

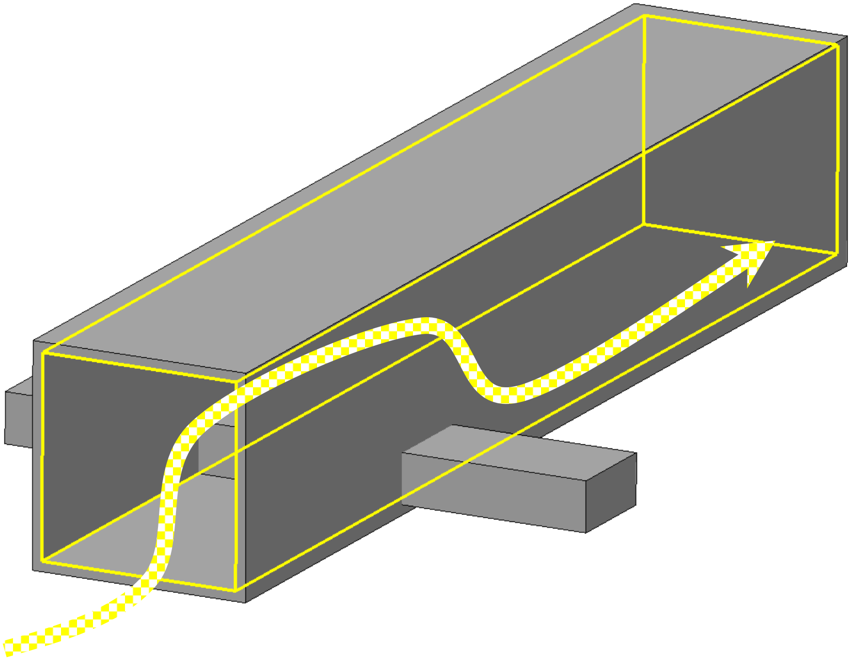
- Channel (wall thickness),
- Obstacle (full solid).



Workflow – fluid dynamics definition

Channel with an obstacle: wall at prescribed temperature.

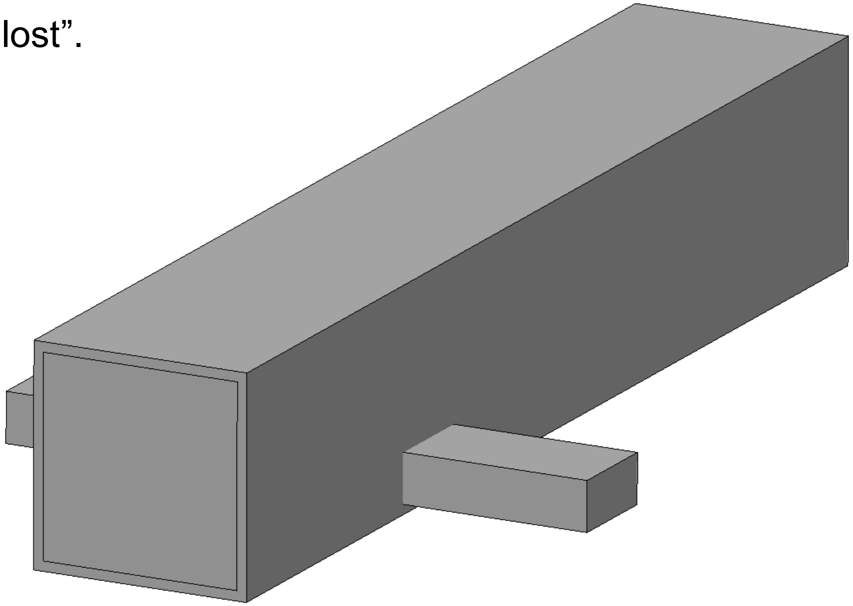
- Analysis of fluid motion,
- Analysis of temperature field.



Workflow – identification of fluid part

The channel volume is rebuilt by selecting the internal faces of the "wall", plus adding inlet and outlet sections.

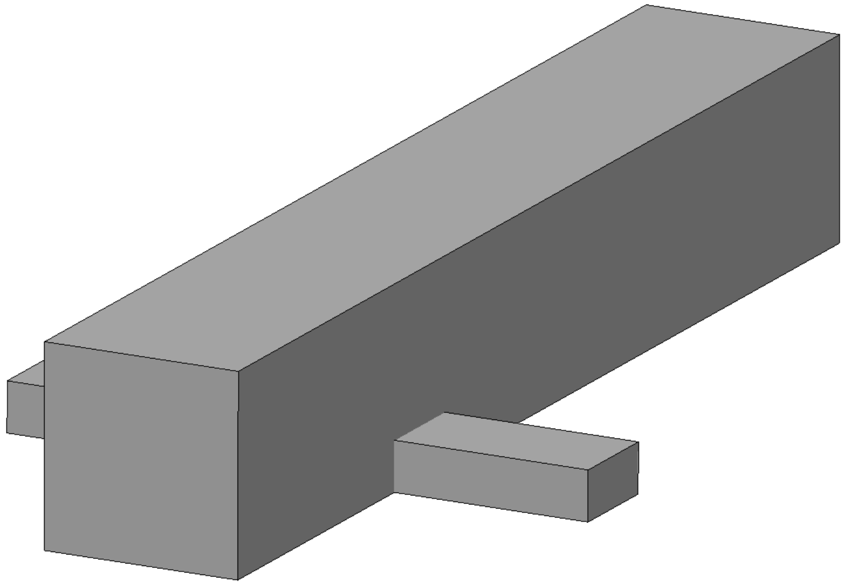
Wall thickness is not relevant and will be "lost".



Workflow – extraction of fluid part

Boolean operation:

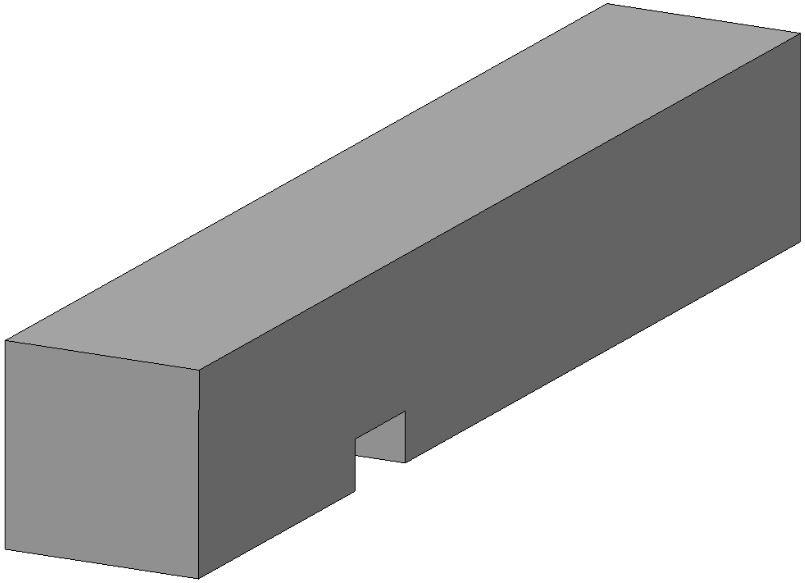
- Subtraction between solid bodies.



Workflow – definition of fluid domain

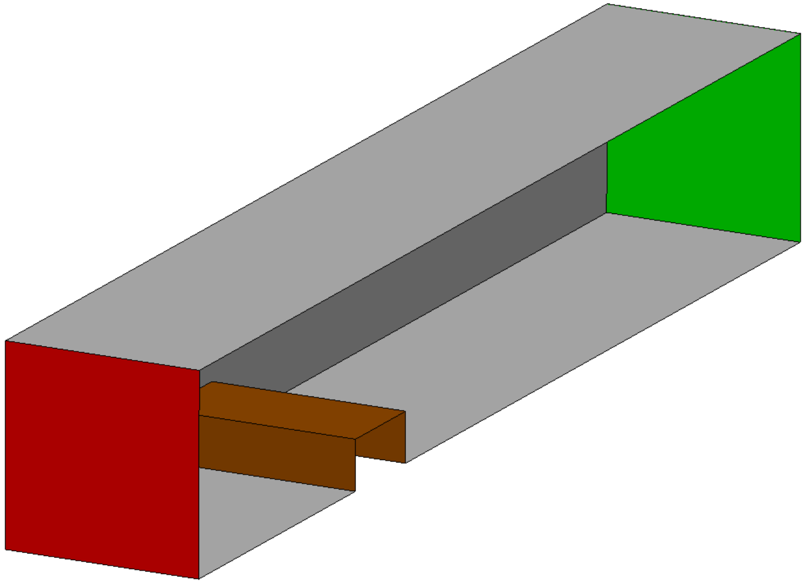
Domain where the actual calculation will take place.

- CAD suitable for CFD.



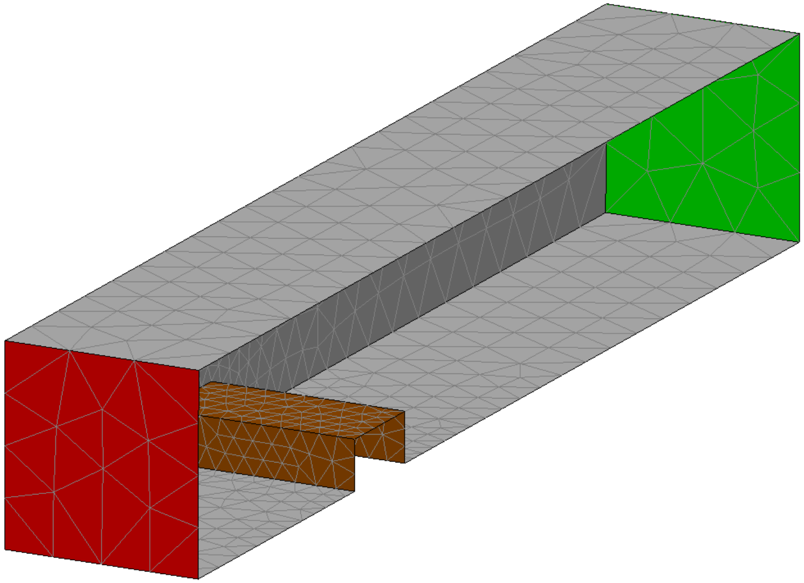
Workflow – boundary conditions

- Inlet condition,
- Wall + Temperature condition,
- Outlet condition.



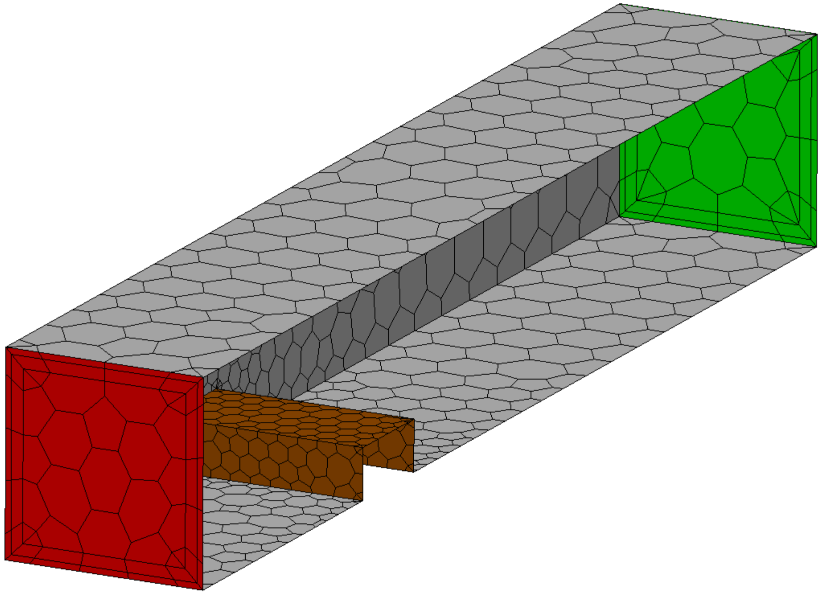
Workflow – surface mesh generation

The surface mesh represents the boundary of the fluid domain and its discretization influences the discretization of the volume mesh.

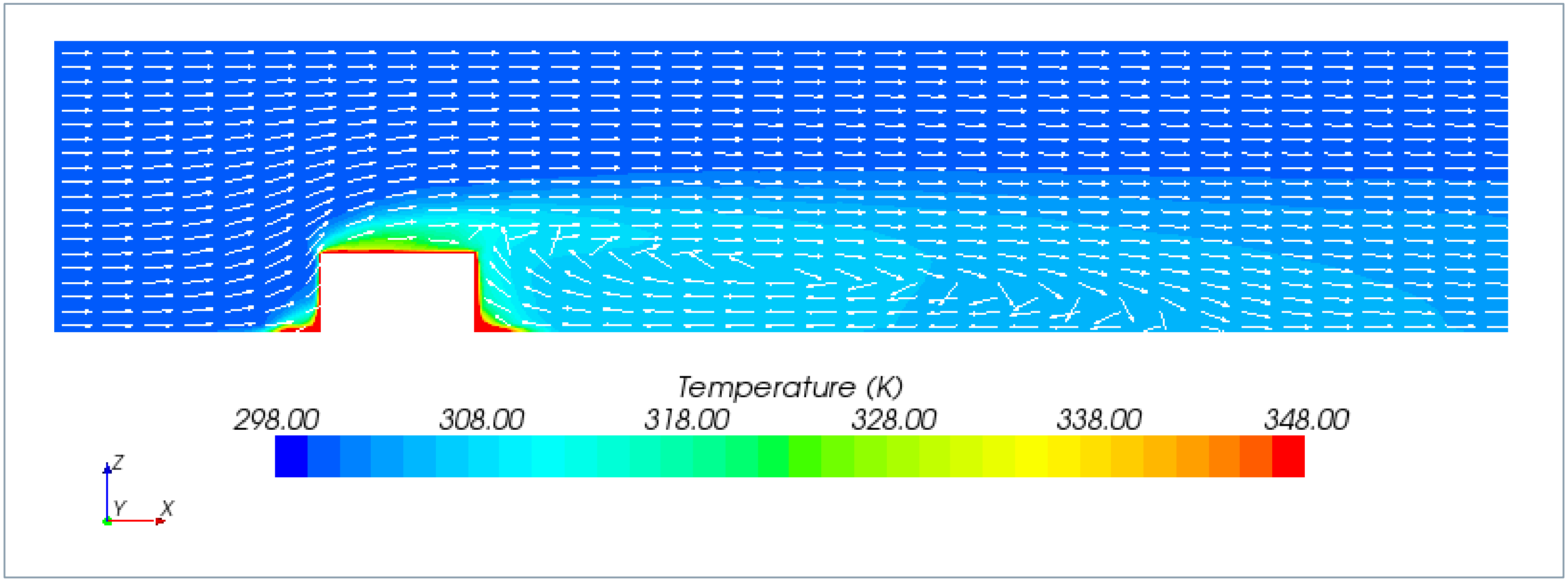


Workflow – volume mesh generation

The volume mesh represents the object of the CFD calculation.



Workflow – data analysis



- Temperature field: scalar T = T(x,z) at y = constant.
- Flow-field: flow direction shown with arrows.

Workflow – summary

Geometry preparation

- Volume extraction

Boundary conditions

- Data are applied at inflow and outflow, e.g. mass flow, pressure, temperature.

Meshing strategy

- Grid independent solutions are ideal
- Characteristic cell sizes are dependent on time available, accuracy needed

Modeling

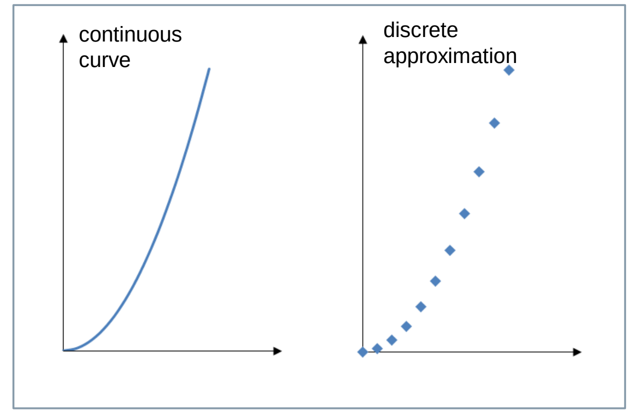
- Flow type: laminar or turbulent
- Heat exchange on or off

Data analysis

Any CFD software solves the governing equations of fluid dynamics.

They need to be discretized:

- The approximation of a continuously-varying quantity in terms of values at a finite number of points is called **discretization.**



These are the fundamental elements of all CFD simulations:

Flow field is discretized	Field variables (*r, u,v,w, P,* ...) are approximated by their values at a finite number of nodes or faces.
Equations of motion are discretized	Approximated in terms of values at nodes or faces.
System of algebraic equations is solved	Cell gradients are monitored as system of equations is solved iteratively.

control-volume or differential equations
(*continuous*)

↓

algebraic equations
(*discrete*)

The basic equations will be discussed in the next section.

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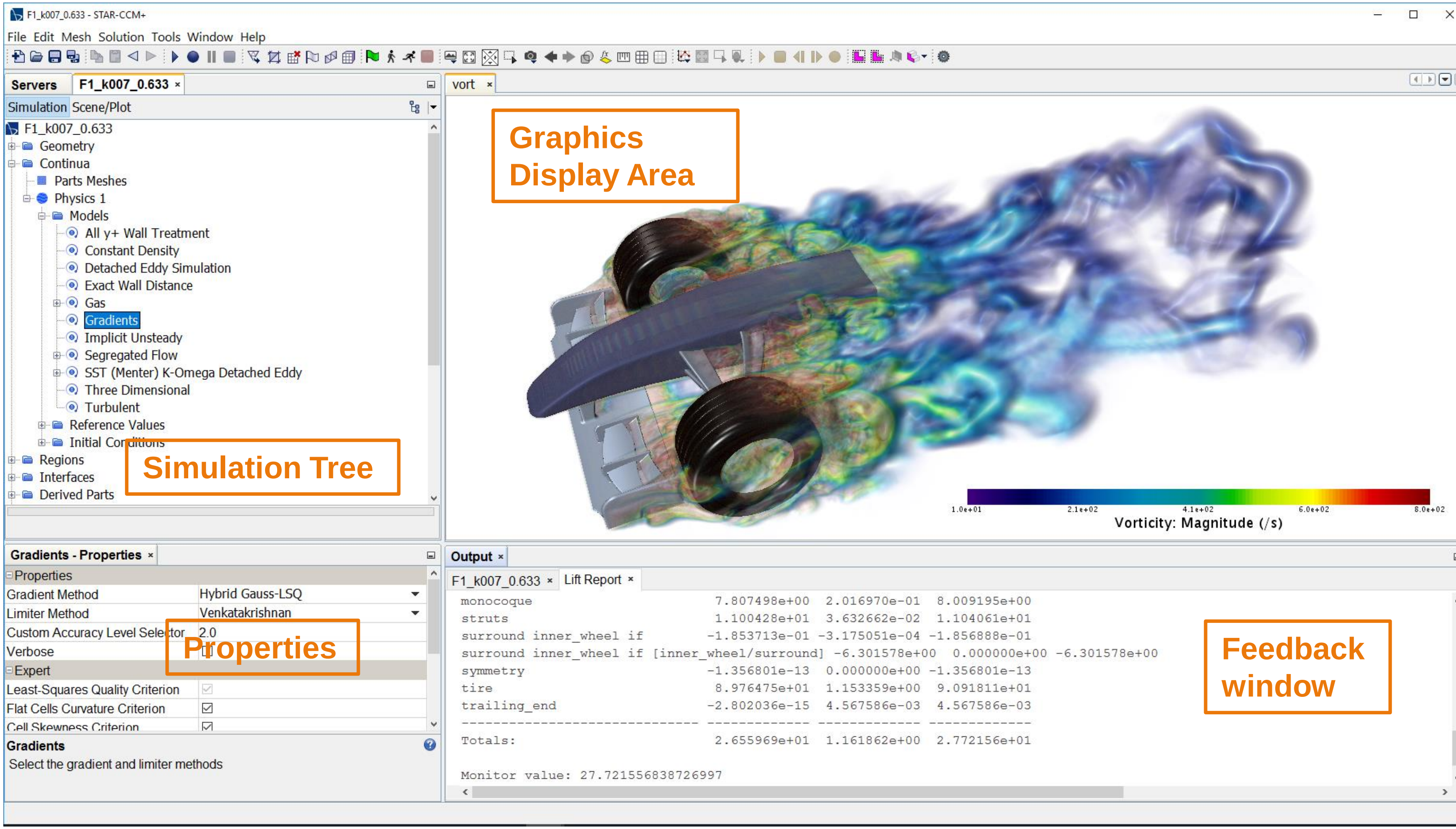
Look and feel of the CFD software STAR-CCM+



Section 2: Basic Equations

$$\frac{\partial}{\partial t}\iiint_V \rho\phi dV + \iint_S \rho\phi\vec{u}\overrightarrow{dS} = \iint_S \Gamma_\phi\vec{\nabla}\phi\,\overrightarrow{dS} + \iiint_V S_\phi dV$$

Governing equations of fluid dynamics

The following equations are the basis of CFD:

Conservation of Mass

Continuity

Conservation of Momentum

Conservation of Energy

1st law of thermodynamics

These equations take the form of non-linear differential equations with partial derivatives.

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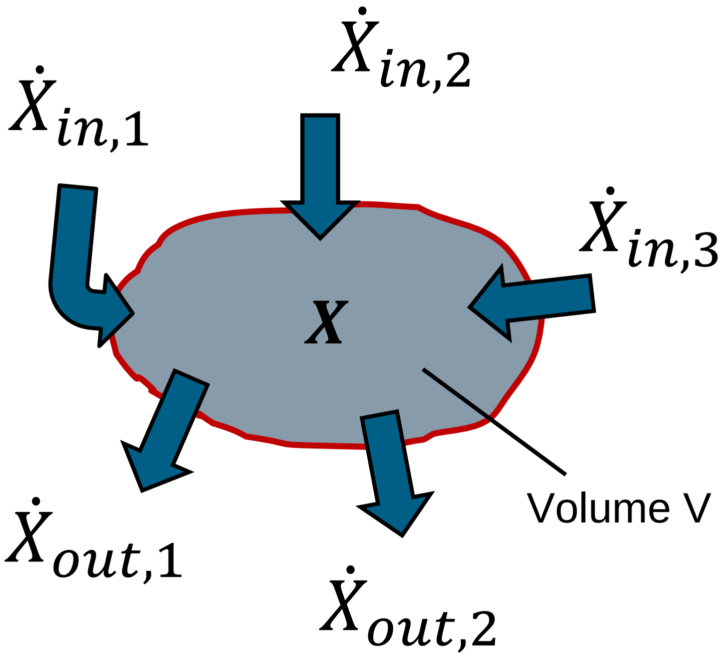


Conservation of X in Volume V

X ... mass, momentum, energy, etc.

temporal variation of X in volume V **=** **flows of X entering V** **-** **flows of X leaving V**

in our example: $$\frac{\partial X}{\partial t} = \sum_{i=1}^{3} \dot{X}_{in,i} - \sum_{j=1}^{2} \dot{X}_{out,j}$$

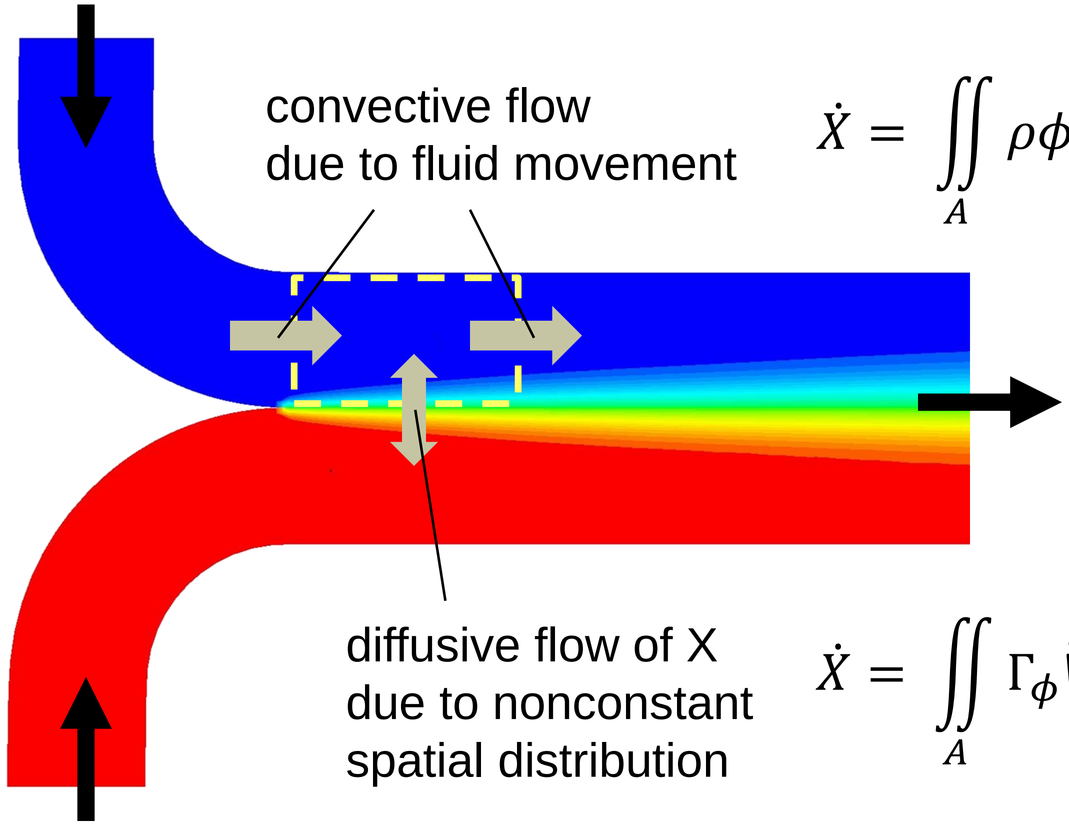
Flows of X over the boundaries of a control volume

X = mass
(mass transport)
$\Rightarrow \phi = 1$

X = momentum
(momentum transport)
$\Rightarrow \phi = u, v, w$

X = energy
(energy transport)

$$\Rightarrow \phi = \rho\left(U + \frac{1}{2}u^2\right)$$



convective flow
due to fluid movement

$$\dot{X} = \iint_A \rho\phi\vec{u}\overrightarrow{dA}$$

diffusive flow of X
due to nonconstant
spatial distribution

$$\dot{X} = \iint_A \Gamma_\phi \vec{\nabla}\phi\overrightarrow{dA}$$

If necessary a source term has to be taken into account:
(of course never in the mass balance)

$$\dot{X} = \iiint_V S_\phi dV$$

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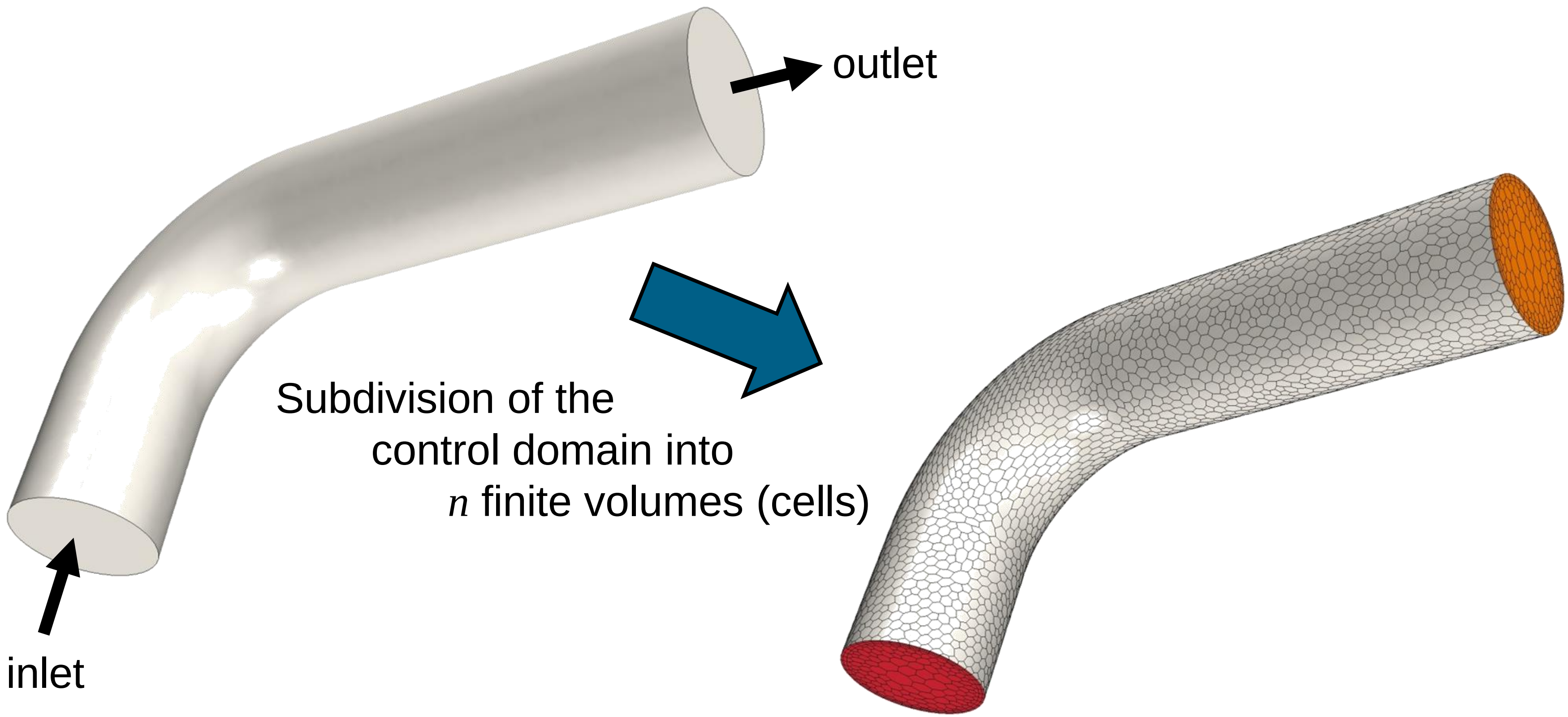
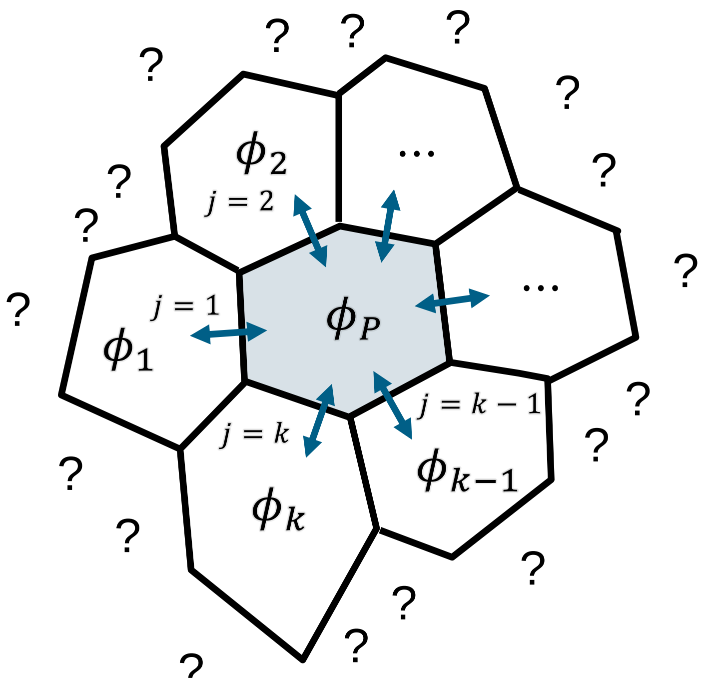
How are these equations used?



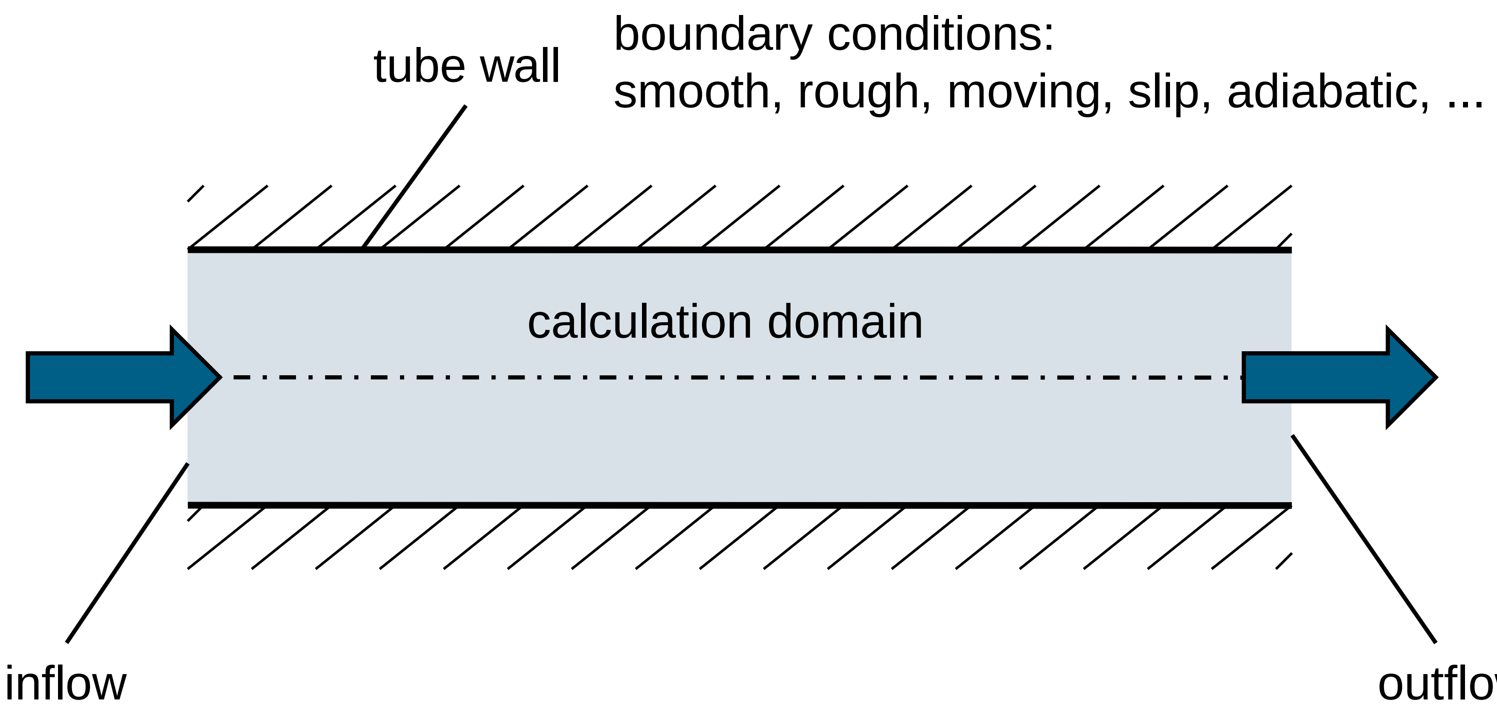
Equations have to be solved for every single cell within the control domain

Section 3: Boundary Conditions



The boundary conditions represent in a mathematical way how the calculation domain interacts with the rest of the universe

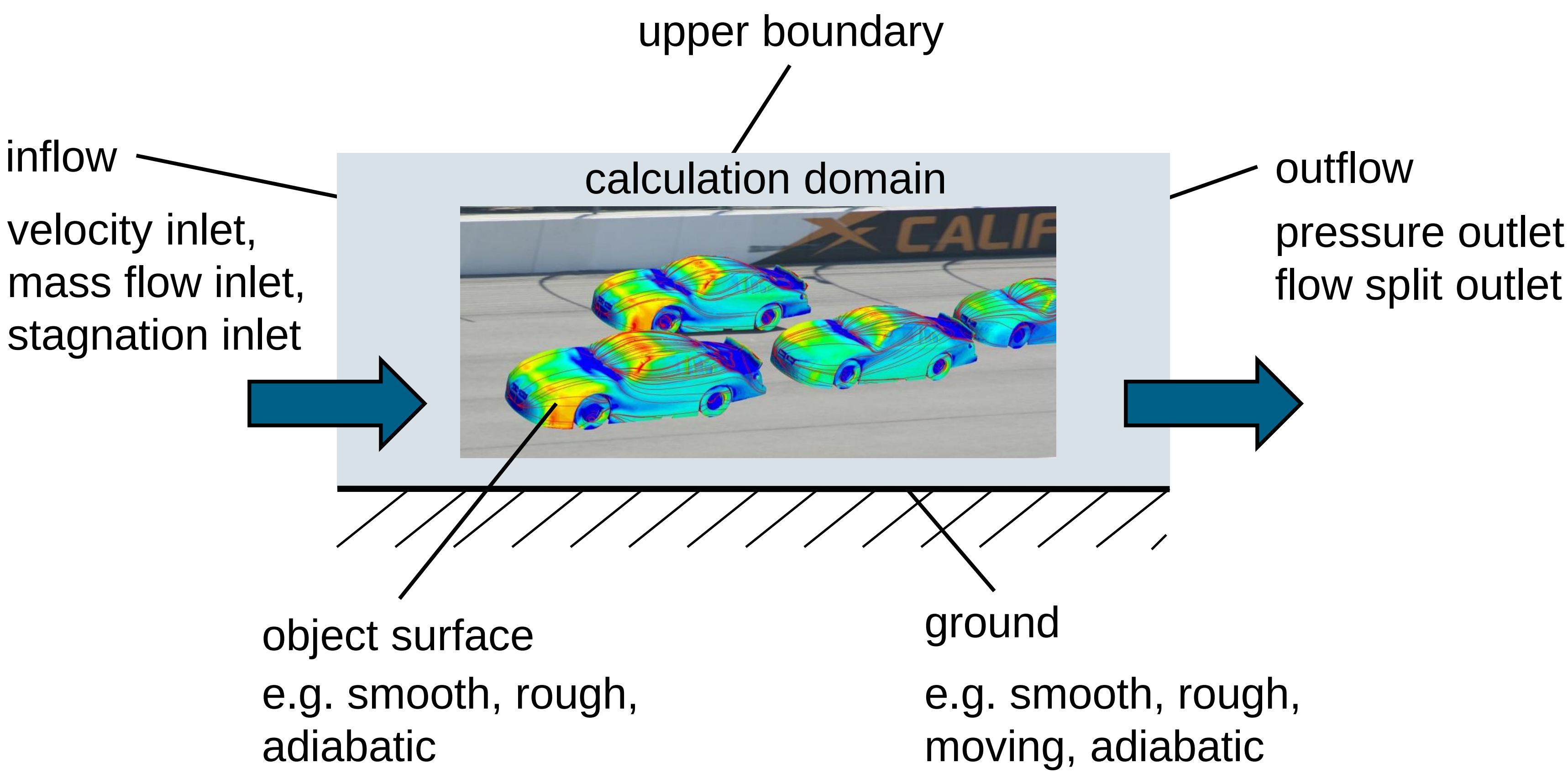
Boundary types: internal flow



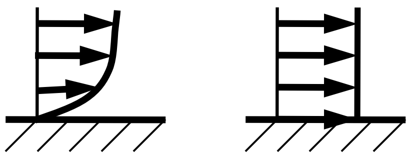
boundary types in STAR-CCM+:
velocity inlet, mass flow inlet, stagnation inlet

boundary types in STAR-CCM+:
pressure outlet, flow split outlet

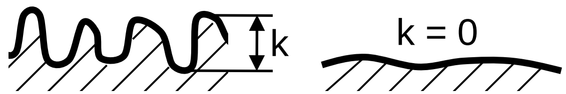
Boundary types: external flow



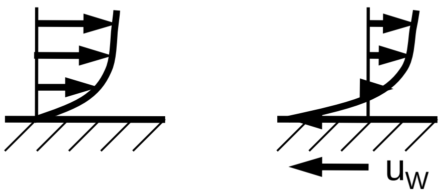
shear stress specification	wall surface specification	wall velocity specification



no-slip | slip



rough | smooth



wall with $u_W = 0$ | wall with $u_W \neq 0$

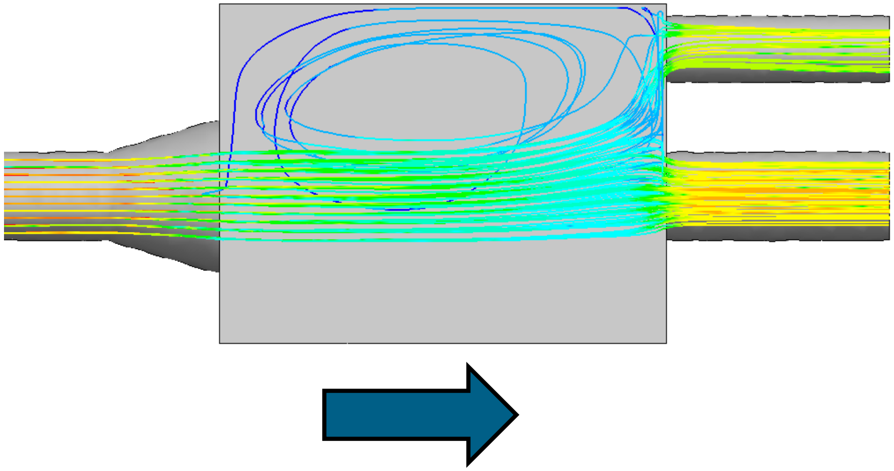
additional specification when thermal exchange is taken into account:

adiabatic	predefined heat flux	predefined temperature	predefined heat transfer coefficient
$\dot{q}=0$	$\dot{q}=\text{constant}$	$\dot{q}=-\lambda\frac{\partial T}{\partial x}$	$\dot{q}=\alpha\left(T_{wall}-T_{fluid}\right)$

Boundary type *wall* - example

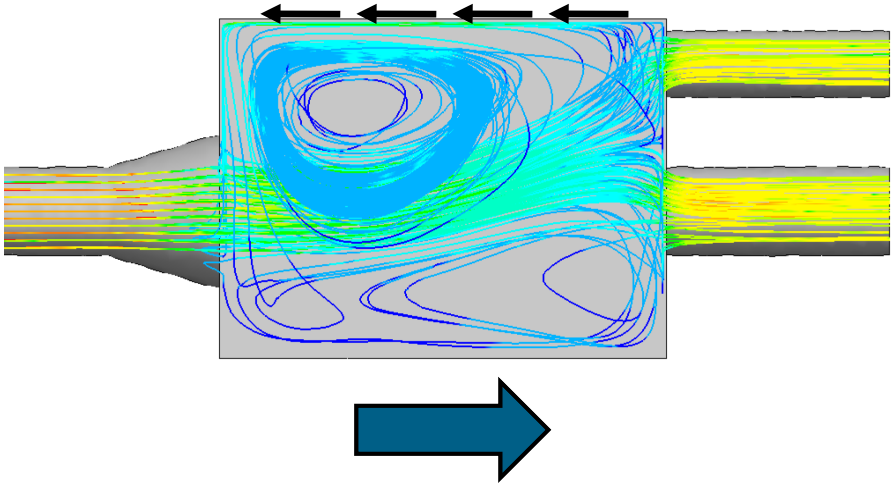
immobile wall

Inlet: u = 10, v = 0, w = 0
Wall: u = 0, v = 0, w = 0



moving wall

Inlet: u = 10, v = 0, w = 0
Wall: u = -10, v = 0, w = 0

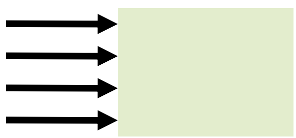


Conditions of inlet boundary types

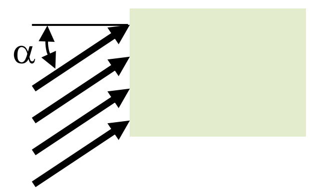
velocity inlet, mass flow inlet, stagnation inlet

boundary conditions to be specified:

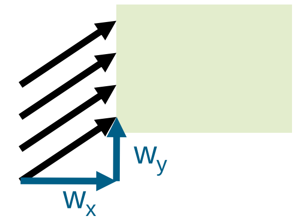
flow direction



normal to boundary



angle to reference



defined by components

turbulence specification

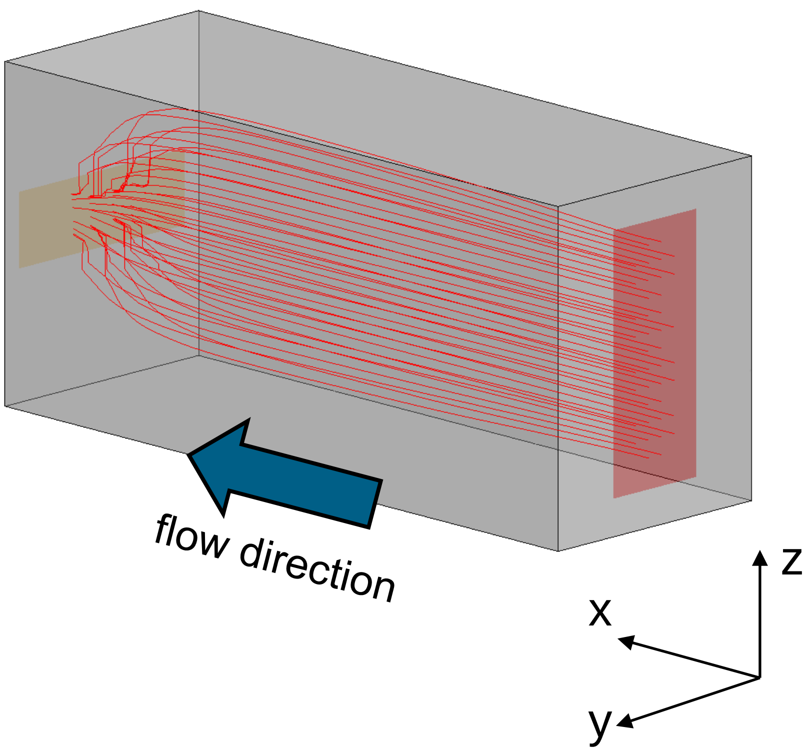
Reynolds Averaged, Detached Eddy Simulation, Large Eddy Simulation

physical values

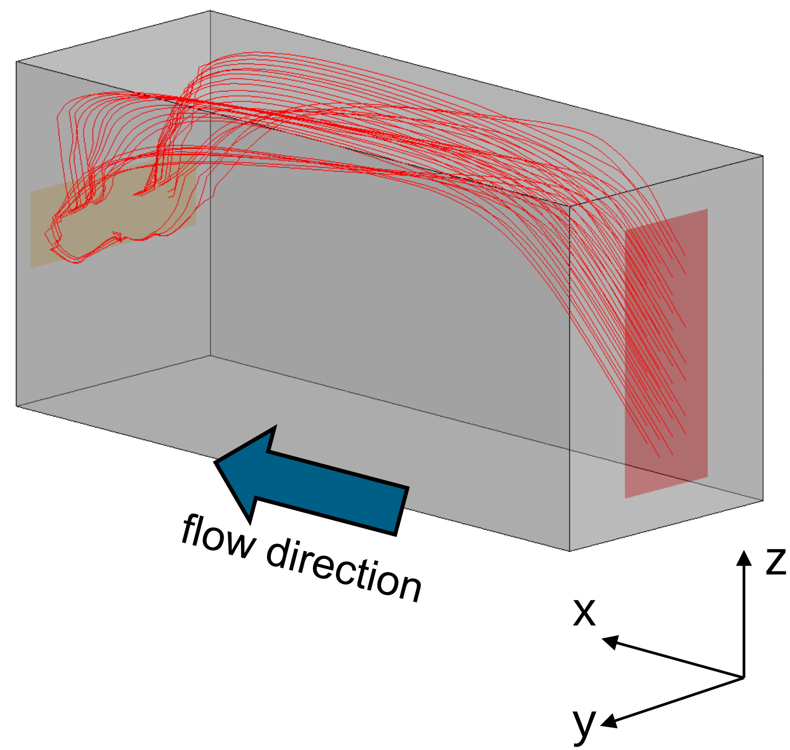
	velocity inlet	mass flow inlet	stagnation inlet
velocity	X		
mass flow rate		X	
temperature	X	X	X
pressure			X

Boundary type velocity inlet – example

$(u,v,w)_{in} = (u,0,0)$

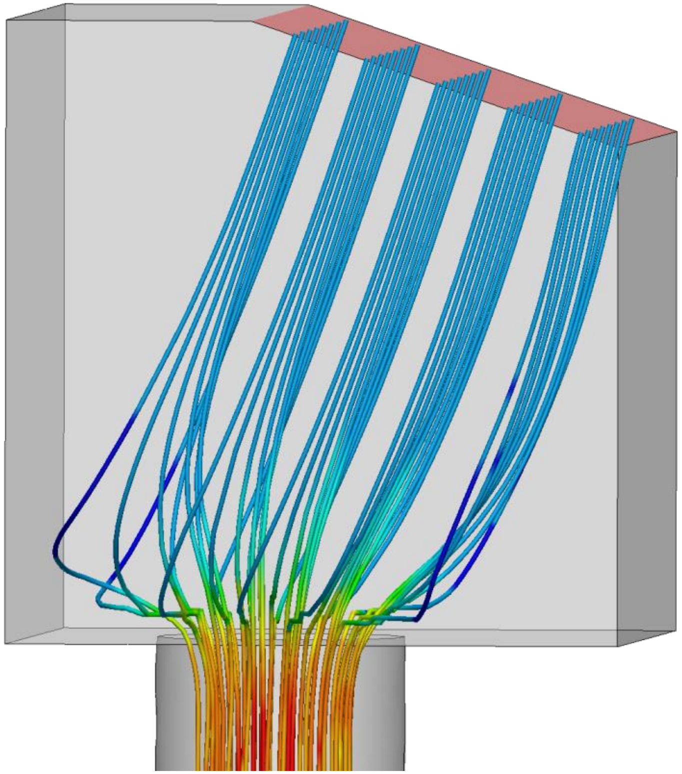


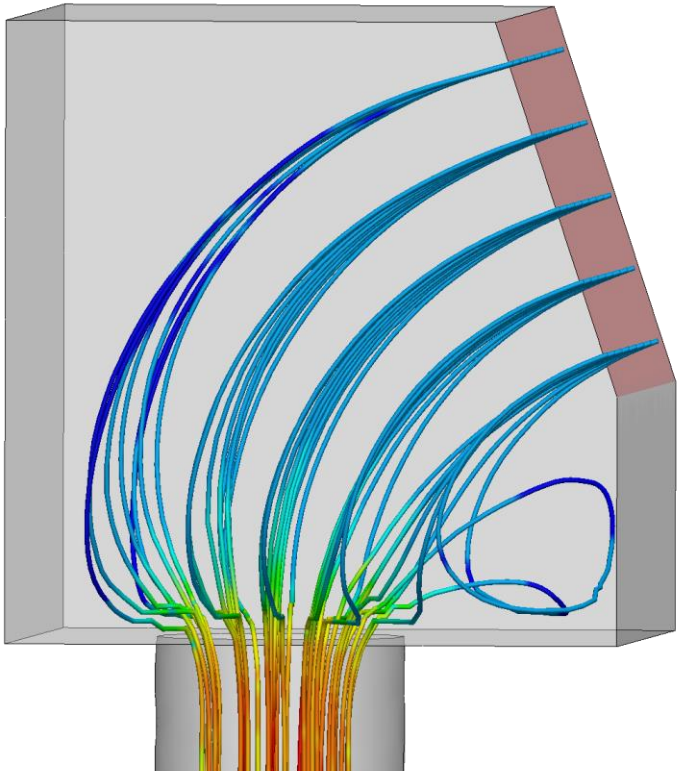
$(u,v,w)_{in} = (u,0,w)$



Boundary type velocity inlet – example

inlet flow direction specification: normal to boundary



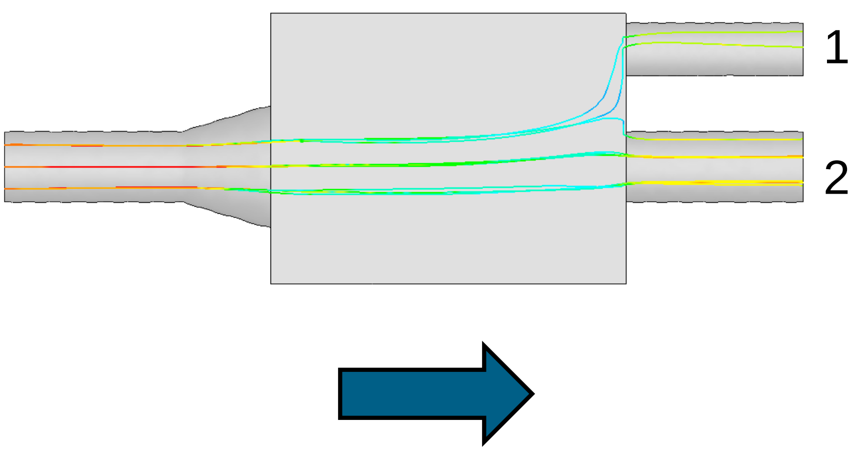


Conditions of outlet boundary types

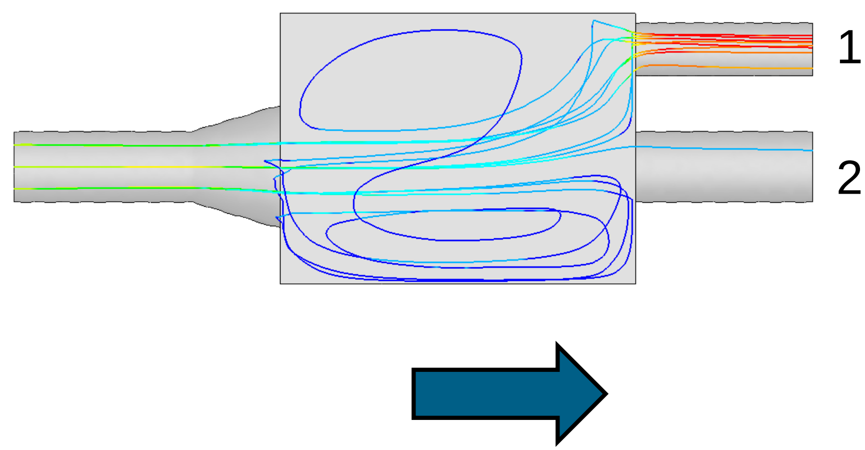
flow split outlet, pressure outlet

	pressure outlet	flow split outlet
value to be specified	pressure in outlet area	percentage of flow in the considered outlet in relation to the total outflow
application	fluid leaving a domain through one or several outlets into a surrounding with known pressure	hydraulic systems with multiple outlets whose flow rates are known
backflow through individual faces of the outlet area	permitted	not permitted

Outlet boundary type "pressure outlet"	Outlet boundary type "flow split outlet"
specification: pressure 1 = pressure 2	specification, for example: flow split 1 = 80%, flow split 2 = 20%



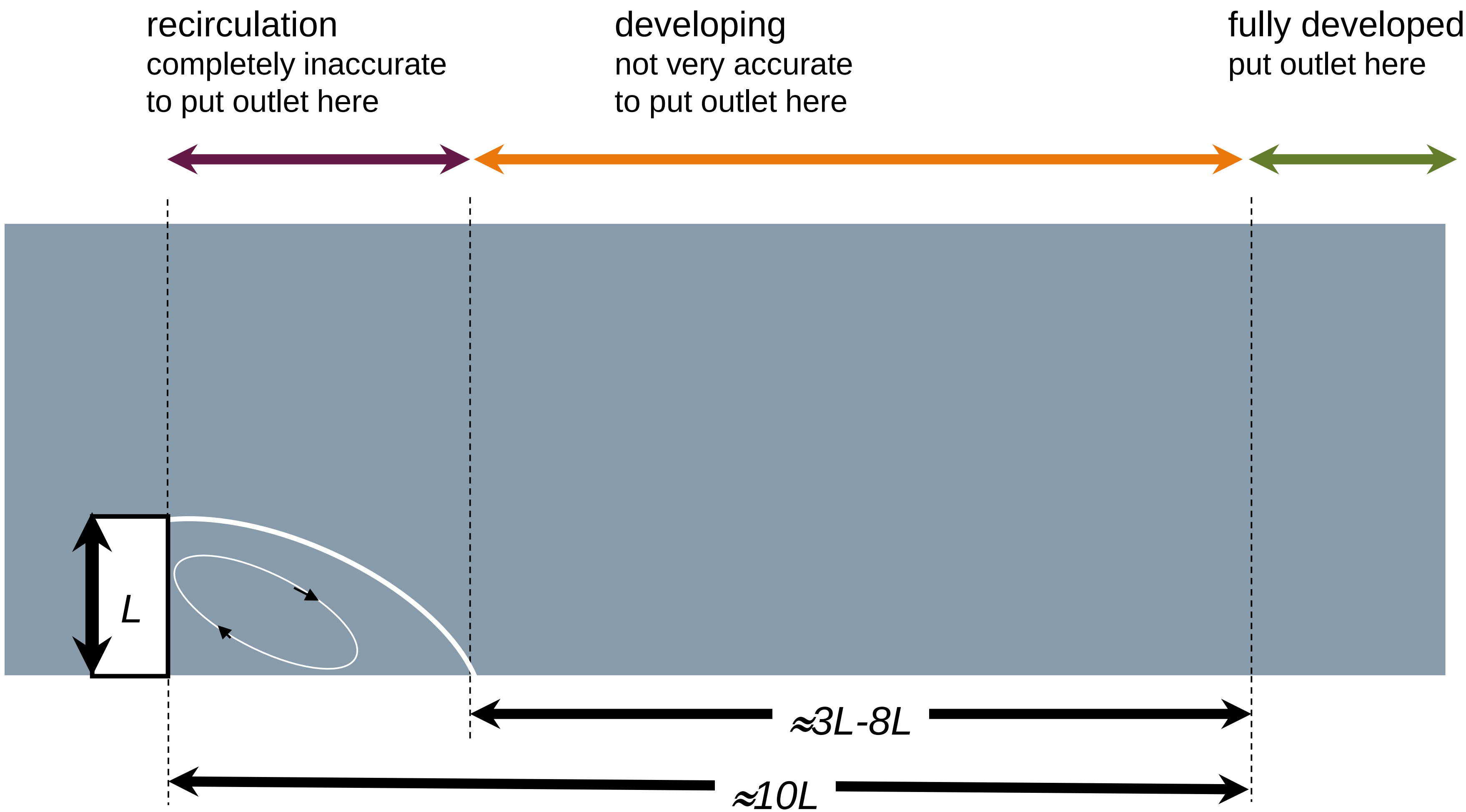
flow direction



flow direction

Outlet boundary – backward facing step

Importance of choosing the right location



Symmetry boundary condition

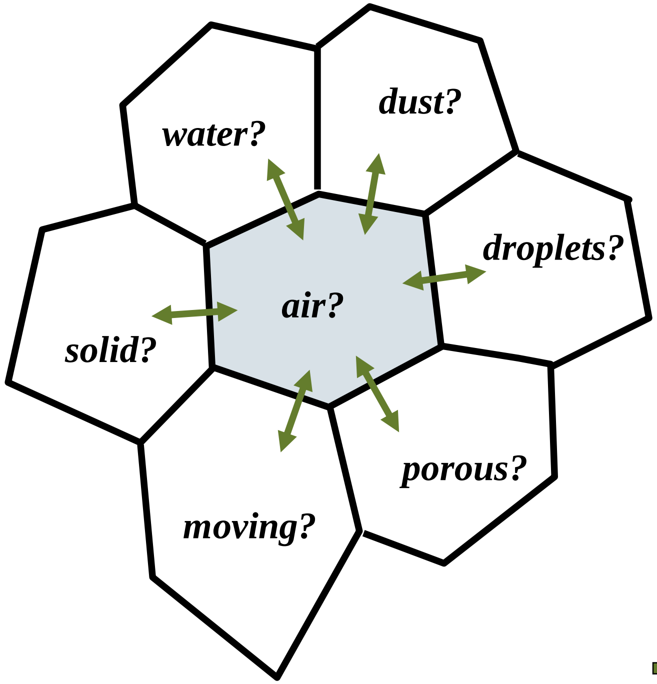
Symmetry boundary can be applied if,

- the determined geometry is symmetric to a plane,
- the velocity field can be assumed to be symmetric to the plane.

Advantages:

- less computational time required,
- less disk space required,
- results can be post-processed in the whole region (on both sides of the symmetry plane).

Section 4: Flow Physics



- 2D or 3D ?
- steady-state or transient ?
- compressible or incompressible fluid ?
- fluid, porous, or solid ?
- influence of temperature (free convection) ?
- stationary or rotating ?
- single-phase or multiphase ?

Several different physical models exist

→ Choose the most suitable ones for your application

2D or 3D? incompressible or compressible?

3D flow: variation in quantities in all three directions

2D flow: variation in one direction can be ignored (under certain conditions)

- Solution only in the two other directions
- Reduction of computation time

incompressible fluid: constant density

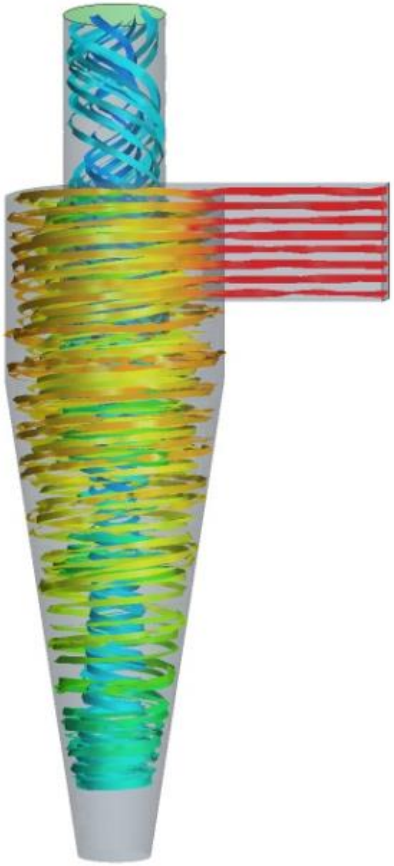
$$\rho = constant$$

compressible fluid: density varies

- Fluid can be treated as an ideal gas $\rho = p/(RT)$
- Density is only function of temperature $\rho = f(T)$ (e.g. polynomial function)

Steady-state or transient?

velocity field in a cyclone
can be considered as steady-state to study major effects



Video: ship movement in waves

Fluid, porous, or solid?

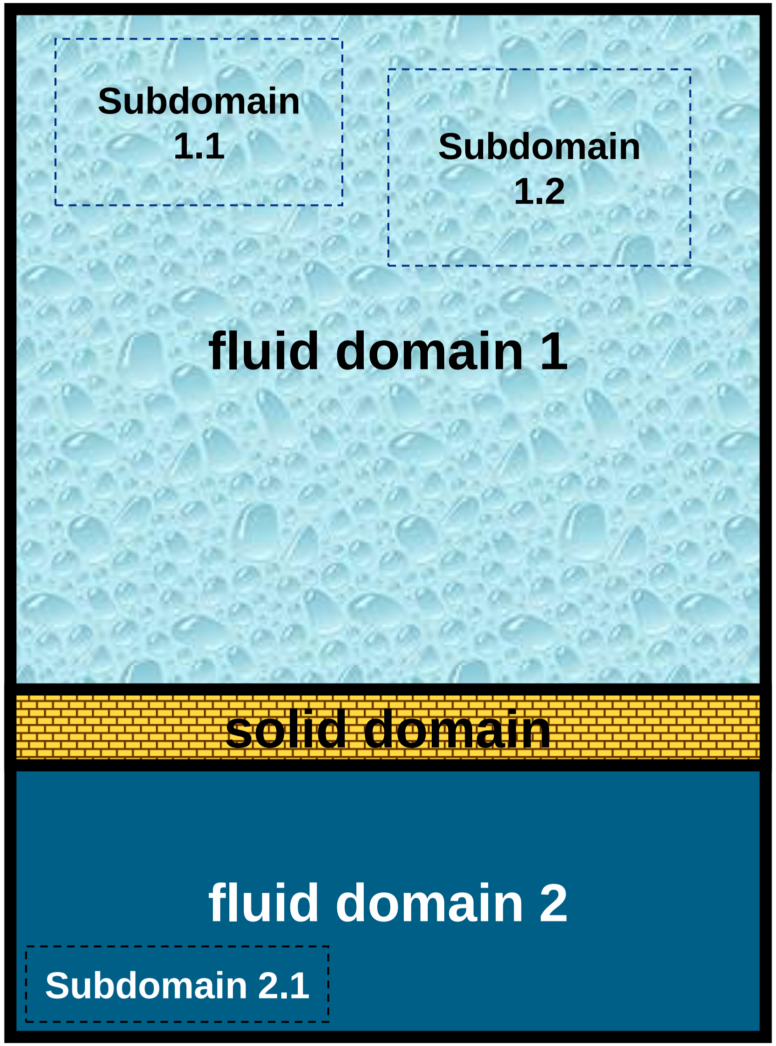
Multi-region modeling

Neighboring domains

- gas
- liquid
- solid

Subdomains

- contain fluid cells with specific resistance (porosity)
- contain fluid cells with spin



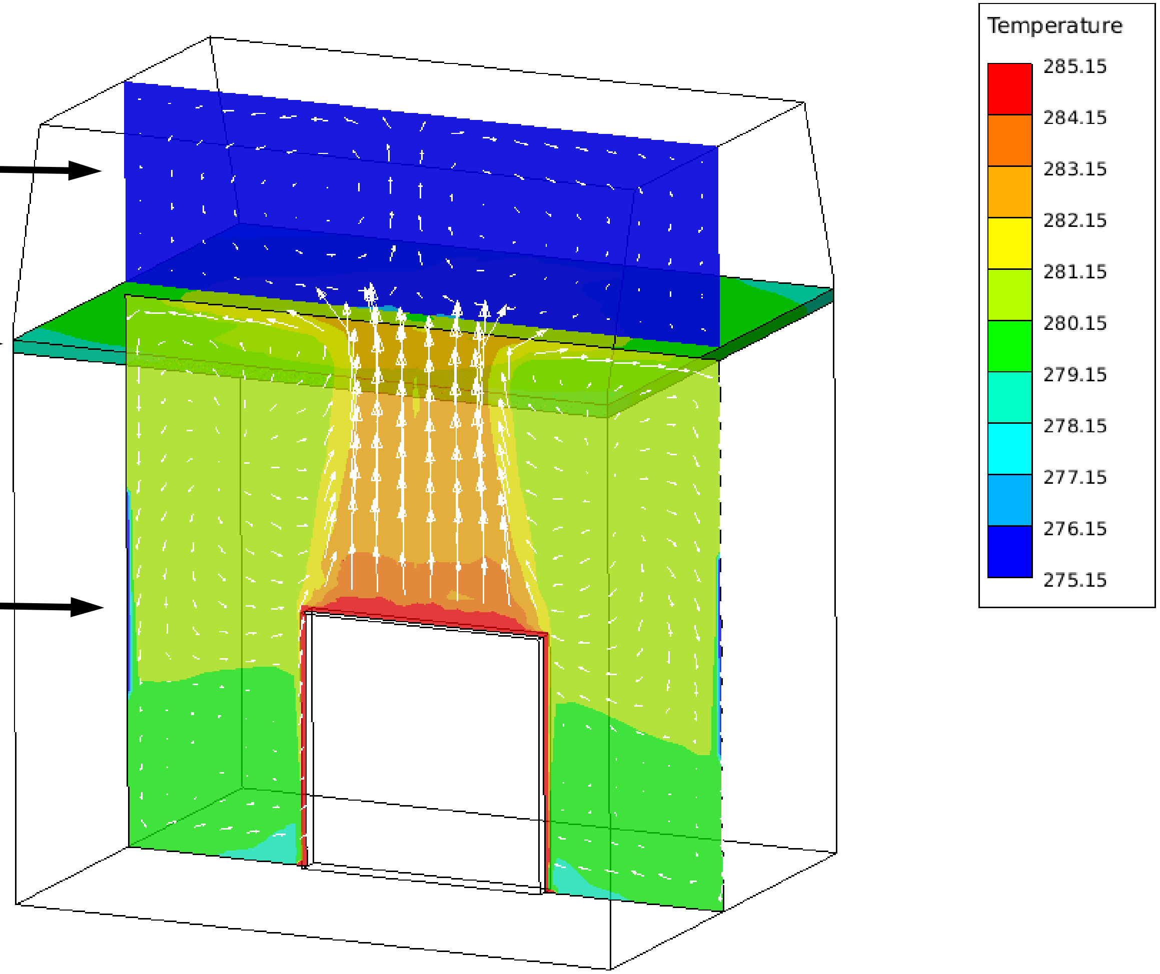
Example of multi-domain calculation

3 domains: fluid1 + solid + fluid2

fluid1
properties = water

solid
properties = brick

fluid2
properties = air



Example of multi-domain calculation

2 domains: fluid + solid

Conjugate heat transfer:

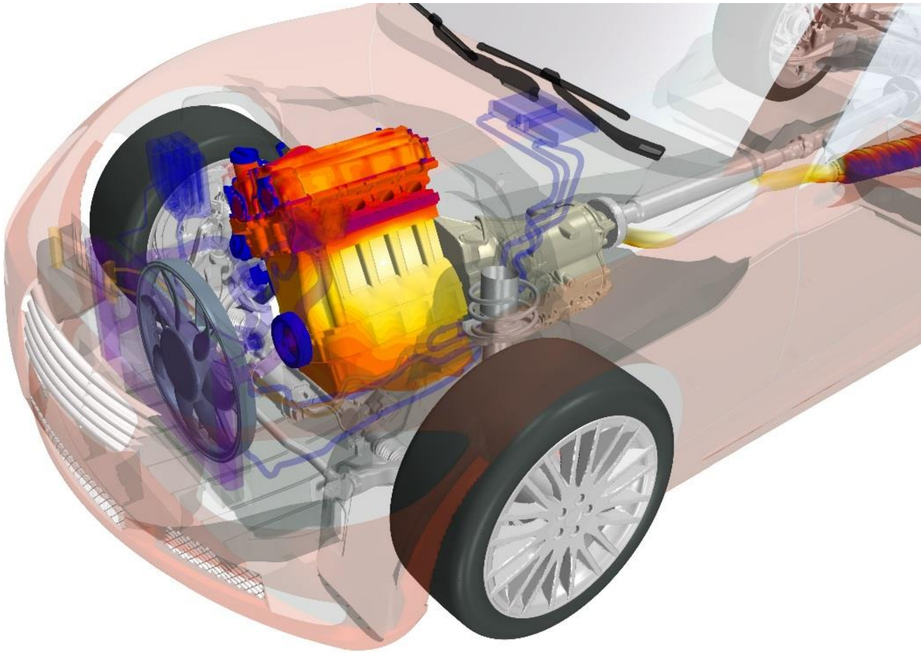
- fluid movement and enthalpy transport in fluid phase
- heat transport by conduction in solid phase
- heat exchange between both phases

Examples of applications

- food industry
- chemical processing industry
- power generation
- automotive powertrain
- building and in-vehicle climate studies

Examples of heat transfer processes

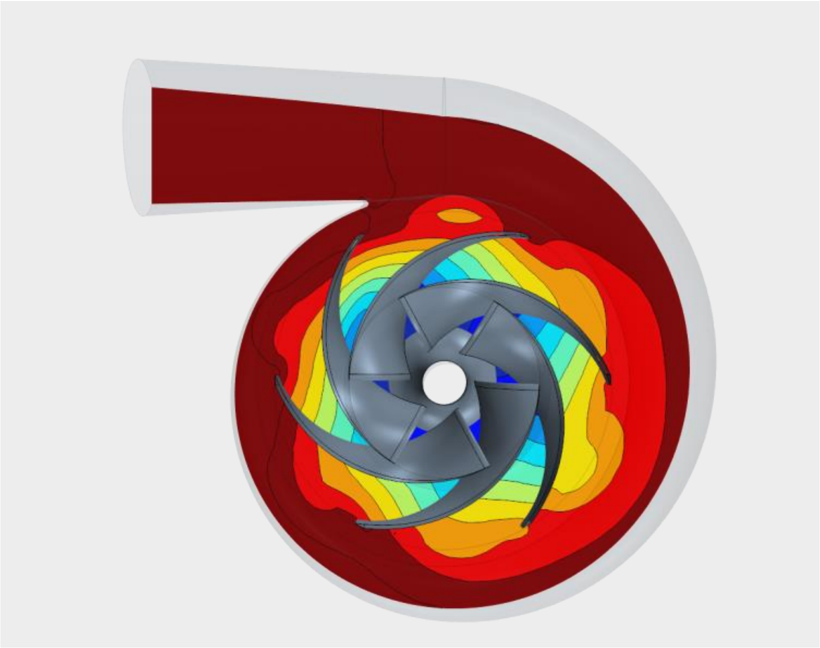
- single phase heat exchange
- condensation
- boiling, evaporation

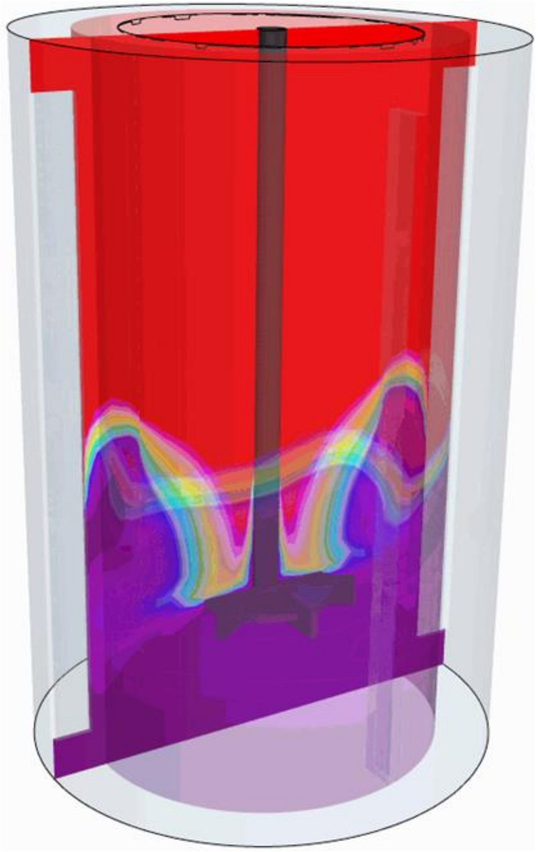


When to use rotational regions?

Examples of application:

- Turbomachinery
  - Torque converters
  - Fans
- Mixers
- Axial flow centrifugal pumps





Single phase or multiphase?

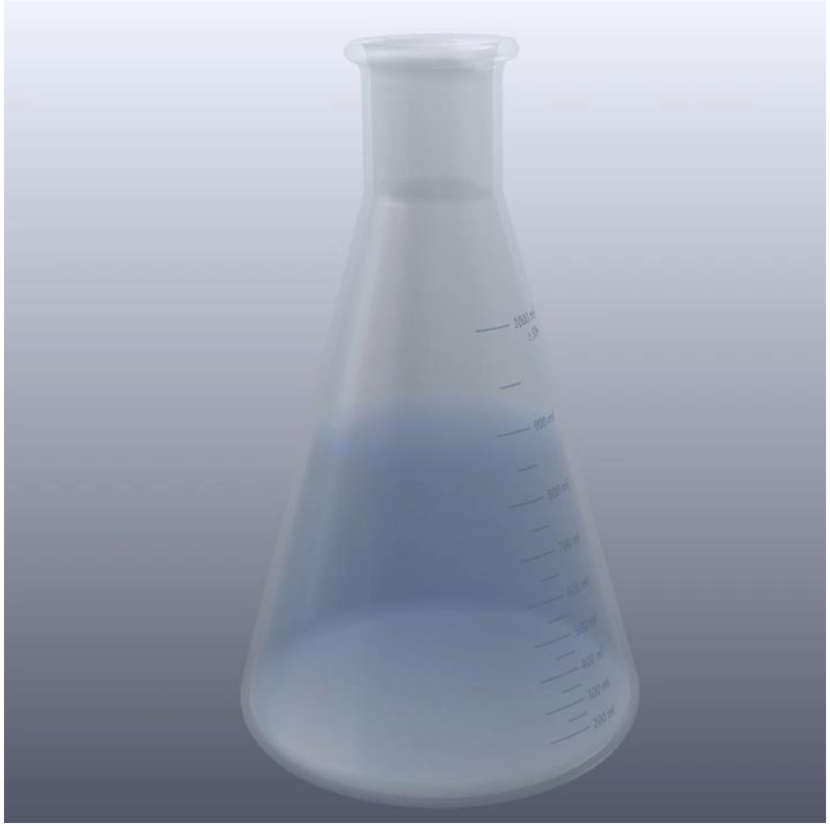
Lagrangian

- Fluid – Solid
- Fluid – Fluid (liquid – liquid, gas – liquid)

Eulerian

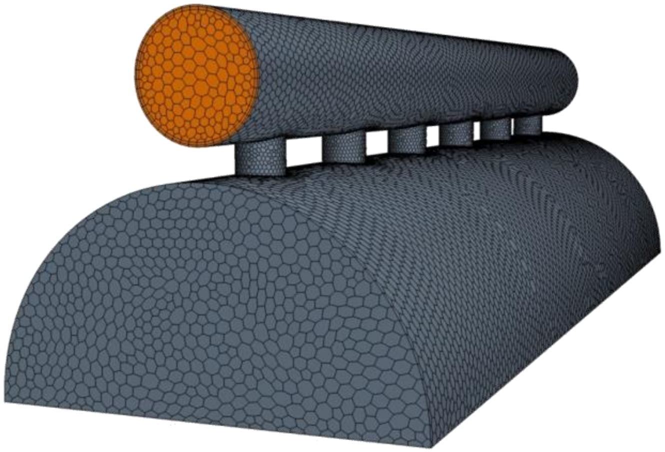
- Volume of Fluid

Multi-component



Video

Section 5: Meshes for CFD

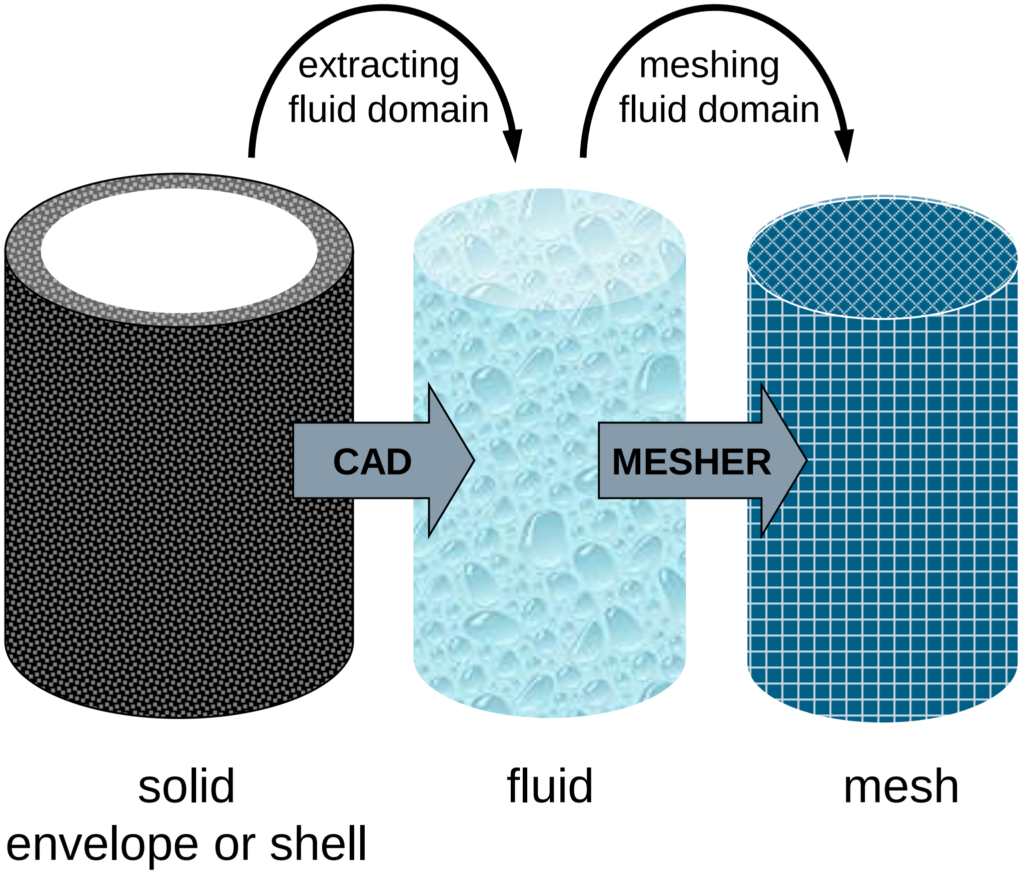


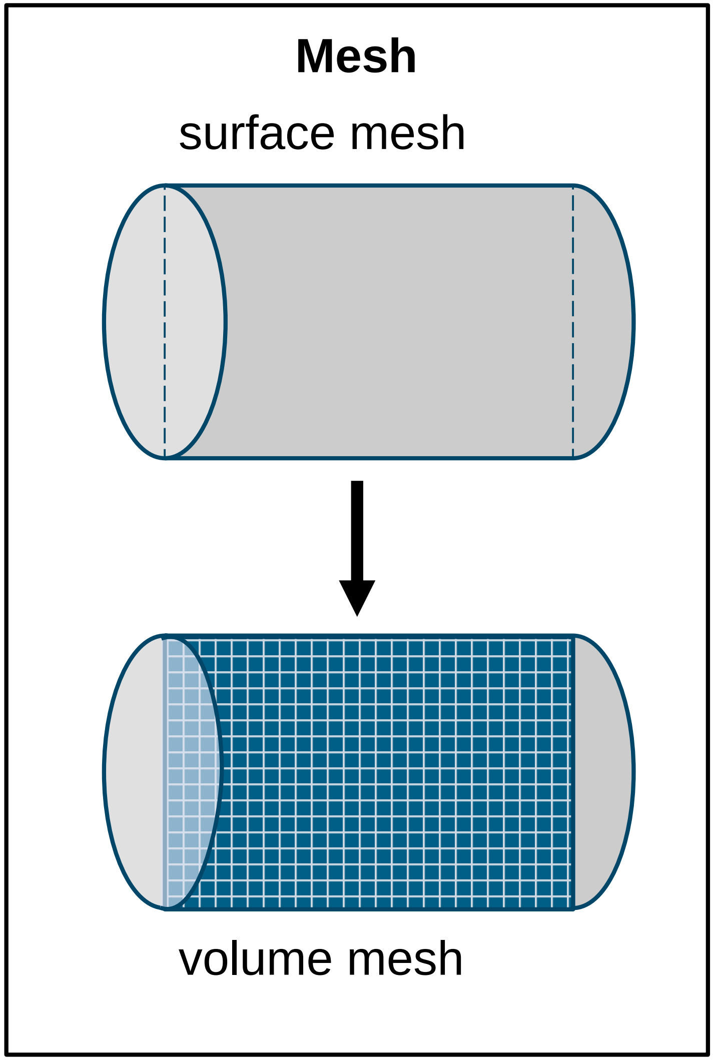
- Meshing workflow
- Parameters and quality of surface meshes
- Parameters and quality of volume meshes
- Types of volume meshes

Control domain

Fluid domain must be specified

Fluid domain must be meshed





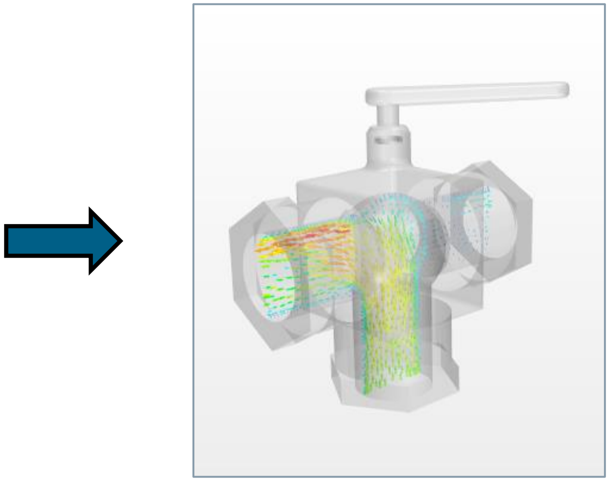
Extraction of fluid domain

The extraction of the fluid from the solid CAD model can be done in several ways:

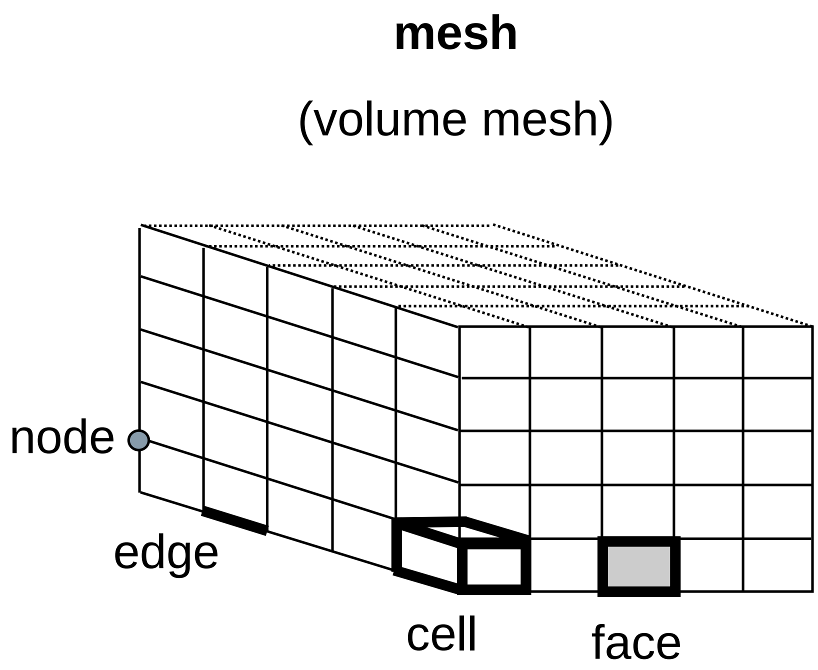
- External CAD software
- Internal CAD tool in the CFD software (e.g. 3D-CAD modeler)
- Simple operations in the CFD software
- Surface Wrapper

Solid CAD

Extracted Fluid



SIEMENS



mesh
calculation mesh defining the computational domain

cell
basic unit of the calculation mesh
collection of all cells = volume mesh

face
face of a cell
collection of all external faces = surface mesh

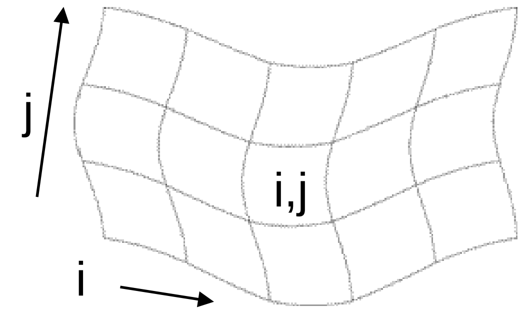
edge
side of a face

node
vertex / node of the mesh

Structured / unstructured meshes

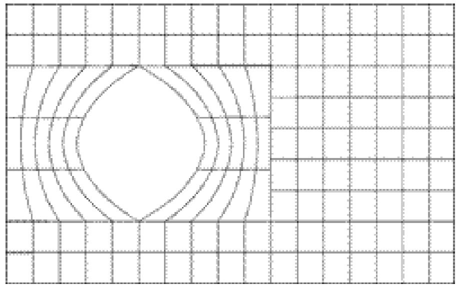
structured meshes

- cells can be identified by a matrix with indexes i,j (2-dimensional) or indexes i,j,k (3-dimensional)



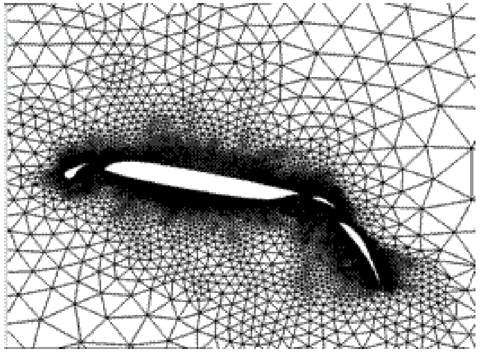
block-structured meshes

- mesh is block-wise structured



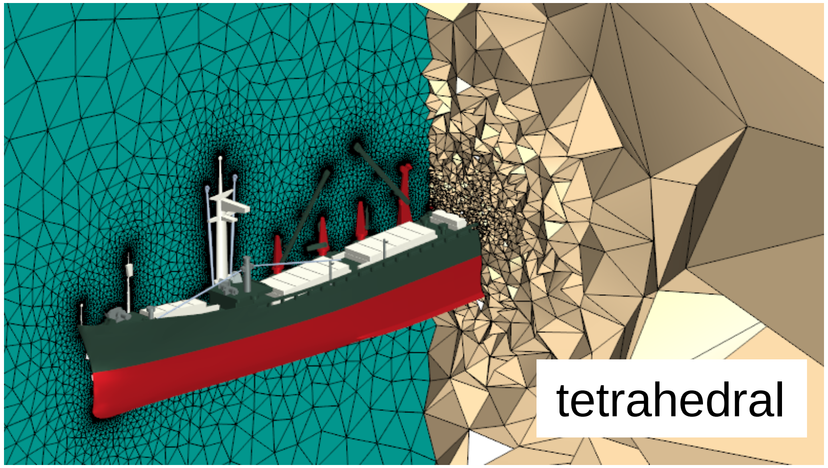
unstructured meshes

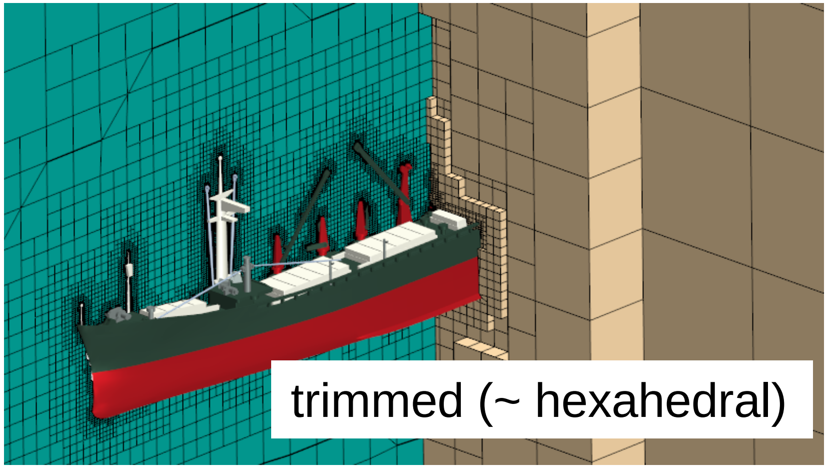
- irregular mesh structure

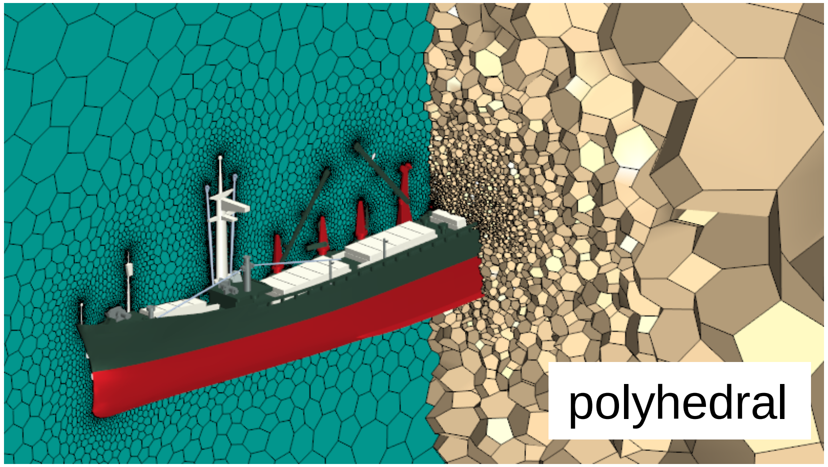


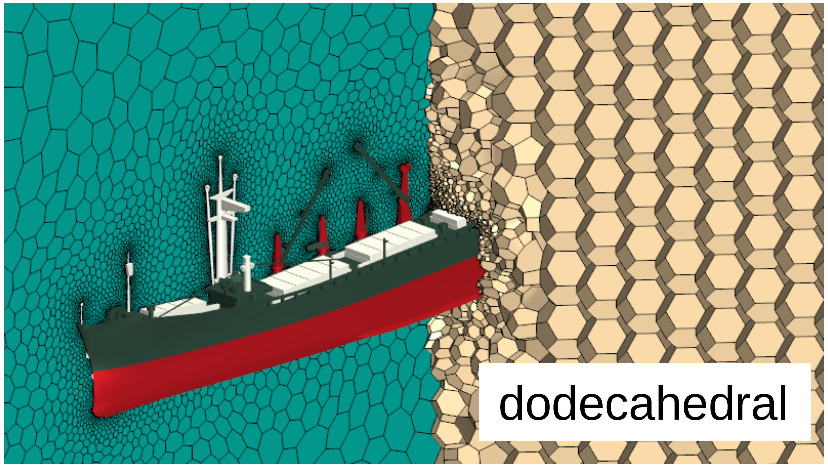
Types of unstructured meshes

Example: volume mesh around a ship

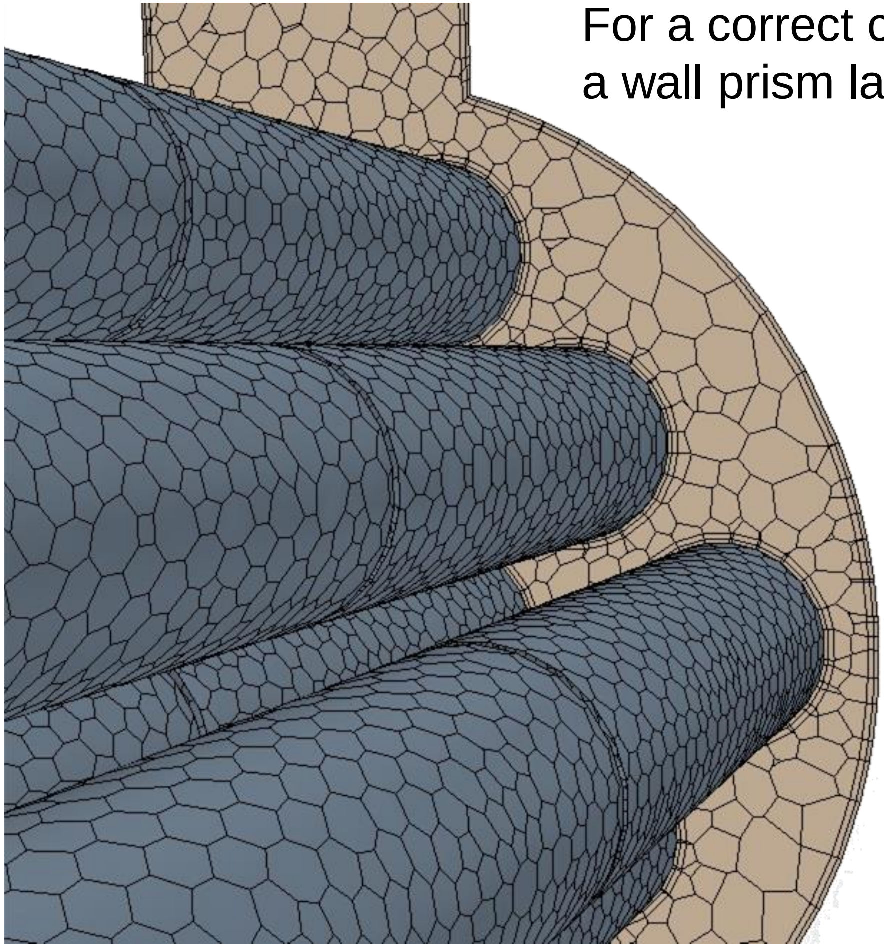




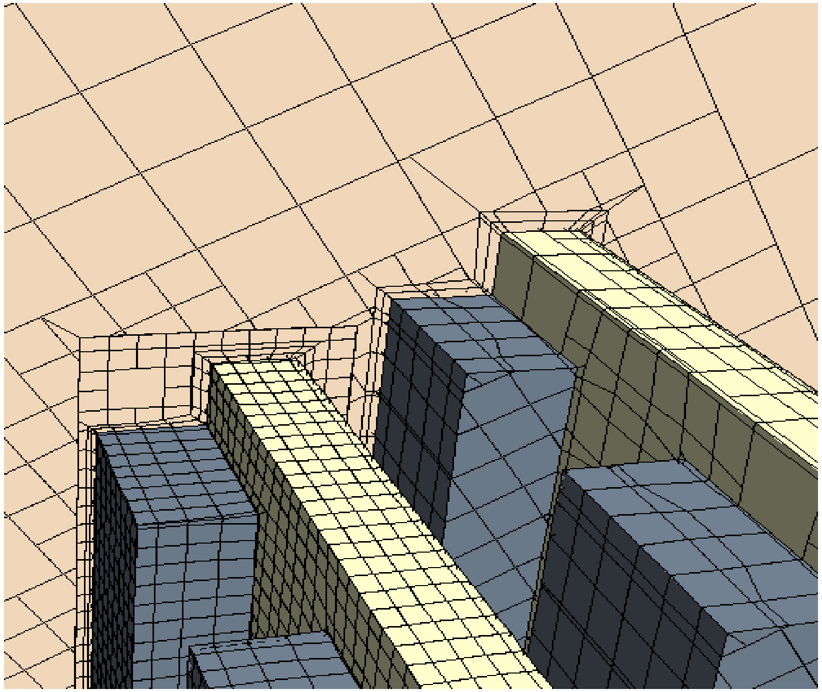




Wall prism layers



For a correct calculation of the velocity boundary layer, a wall prism layer is added to the mesh



Section 7: Data Analysis

The solver returns a vast amount of that need to be transformed into a form a human mind can quickly assess.

This is called Data Analysis, commonly also referred to as “Post-Processing”.

- Data Analysis can be prepared before or after a CFD solution is obtained.
- Preparing the Data Analysis before the start of the computation offers the advantage of watching the solution develop.

A visual representation of the flow field is the most common interpretation of the data, but graphs are also important tools.

STAR-CCM+ contains a full suite of powerful Data Analysis tools:

- 3D flow visualization,
- Animation,
- Graphing of data,
- User defined calculations.

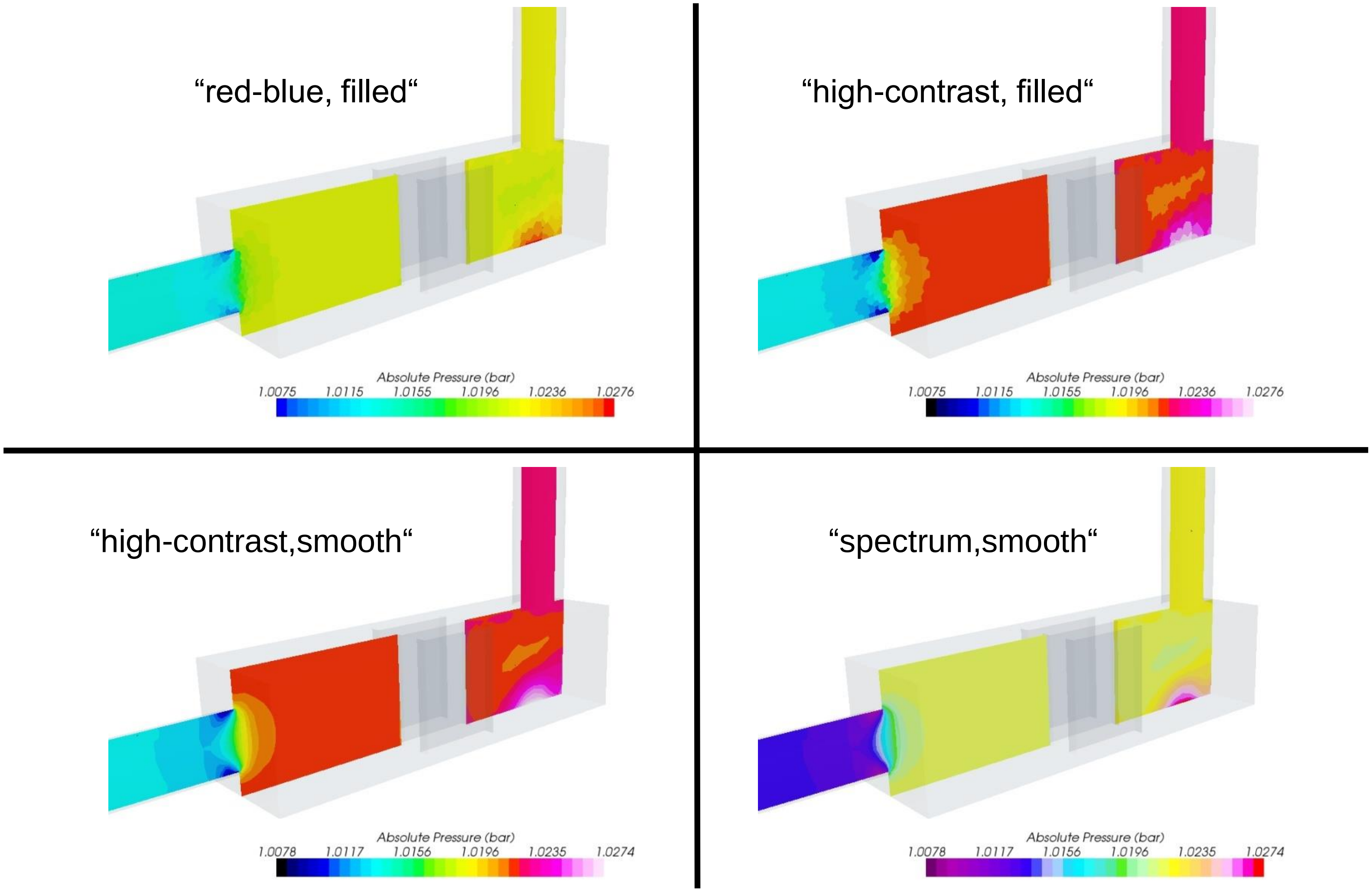
SIEMENS

Data Analysis

- **Visualization**
  - **Visualization of field data**
    - Scalars, Vectors
  - **Flow lines**
    - Streamlines
  - **Iso-Surfaces**
- **Reporting**
  - **System**
    - CPU time, elapsed time
  - **Statistical**
    - Sum
    - Minimum, Maximum
    - Area and Volume Averaged
    - Uniformity Index
    - Mass Flow
  - **Expression**

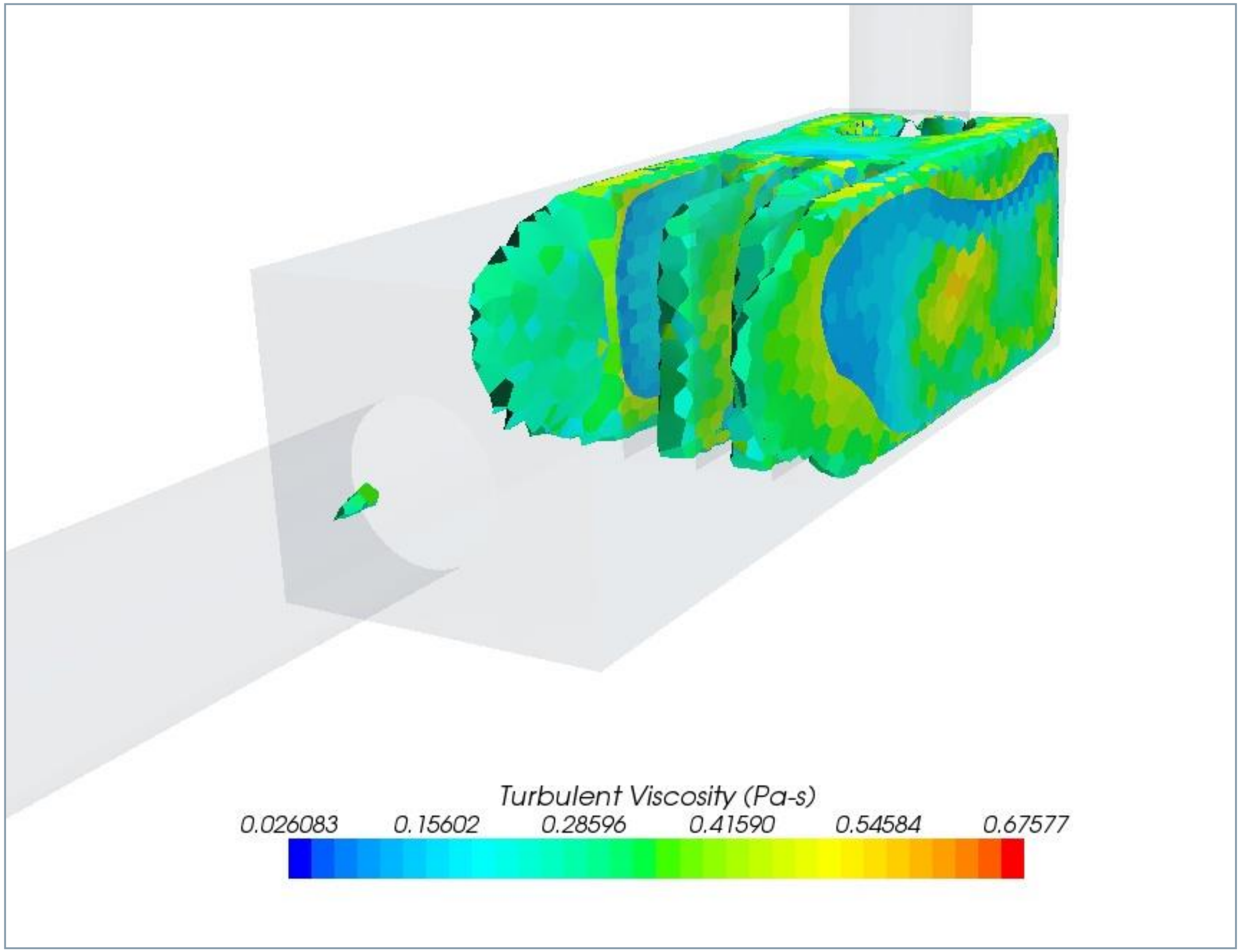
Examples of data analysis

Scalars: color legend variants



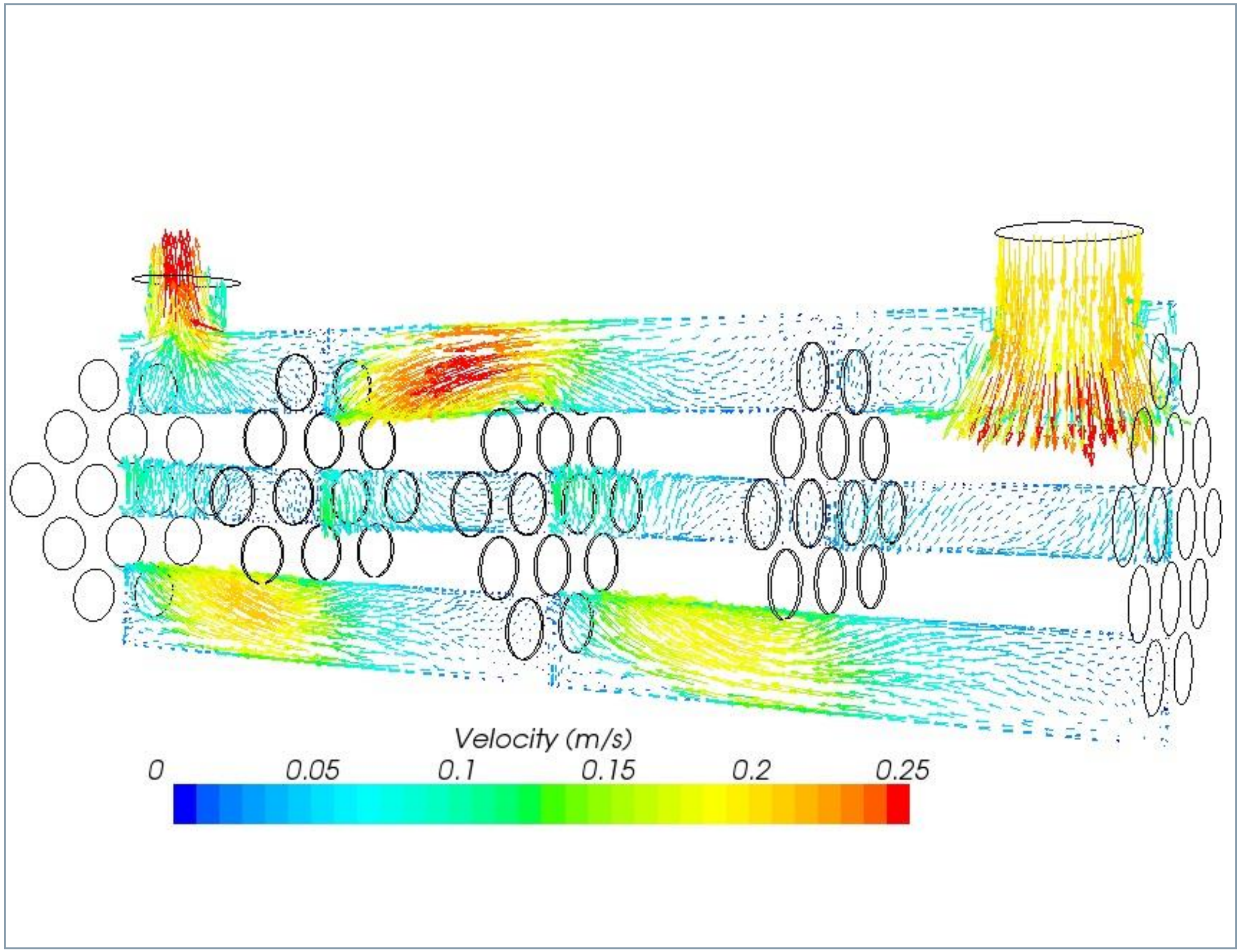
Examples of data analysis

Iso-surfaces



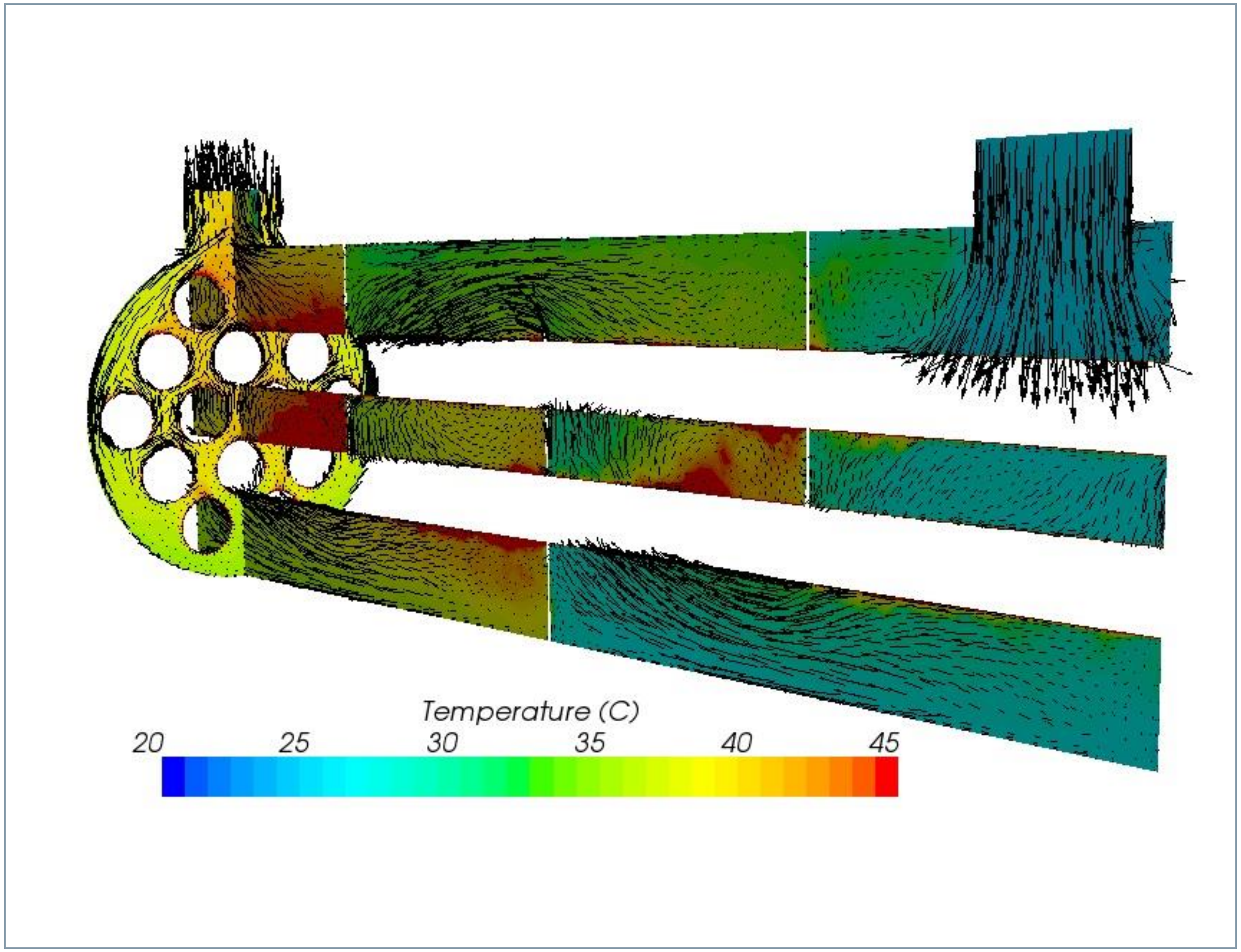
Examples of data analysis

Vectors



Examples of data analysis

Scalars + Vectors



Examples of data analysis

Streamlines