

Case study: Fuel cell

Numerical Flow Simulation

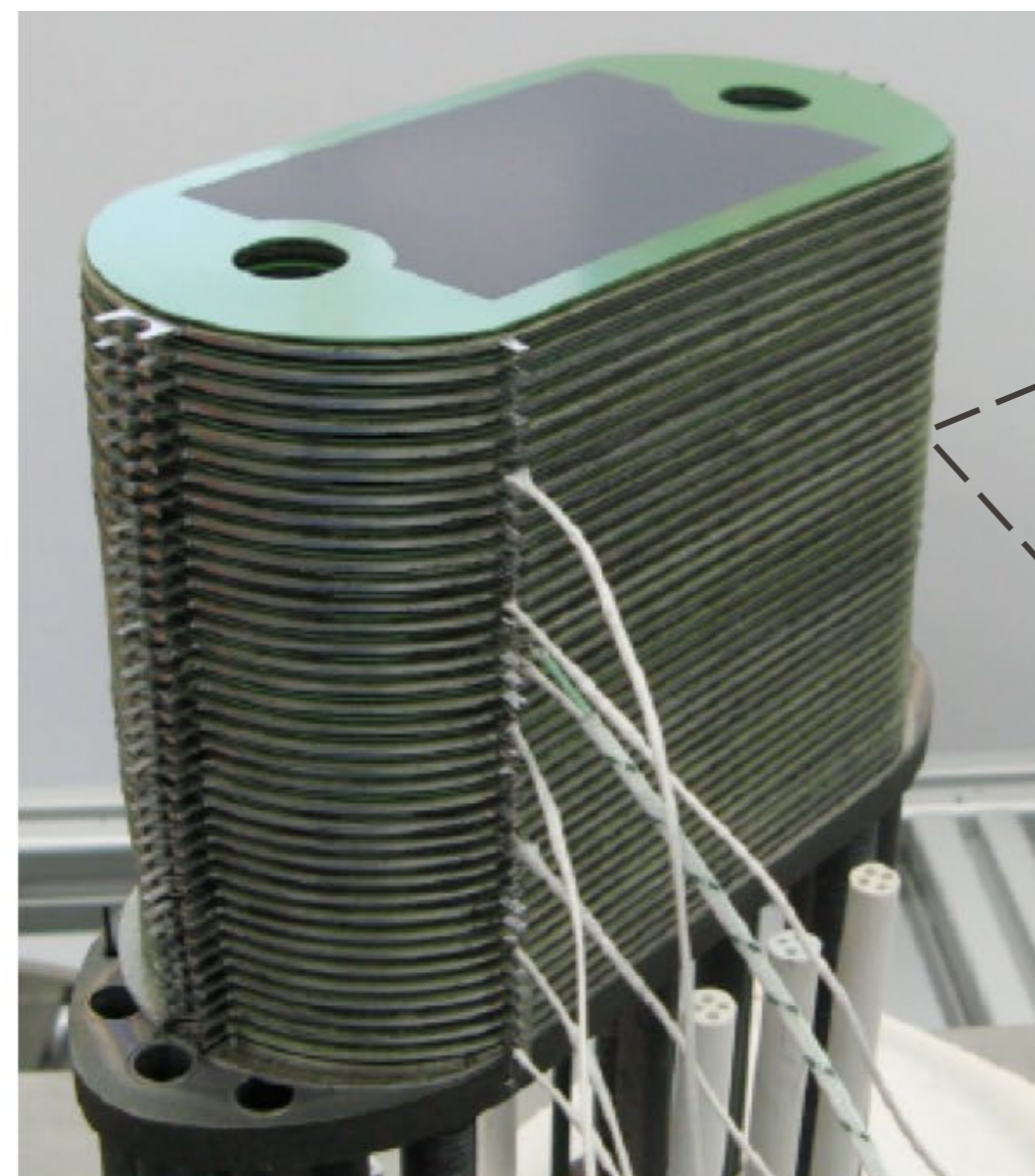
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Fall 2021

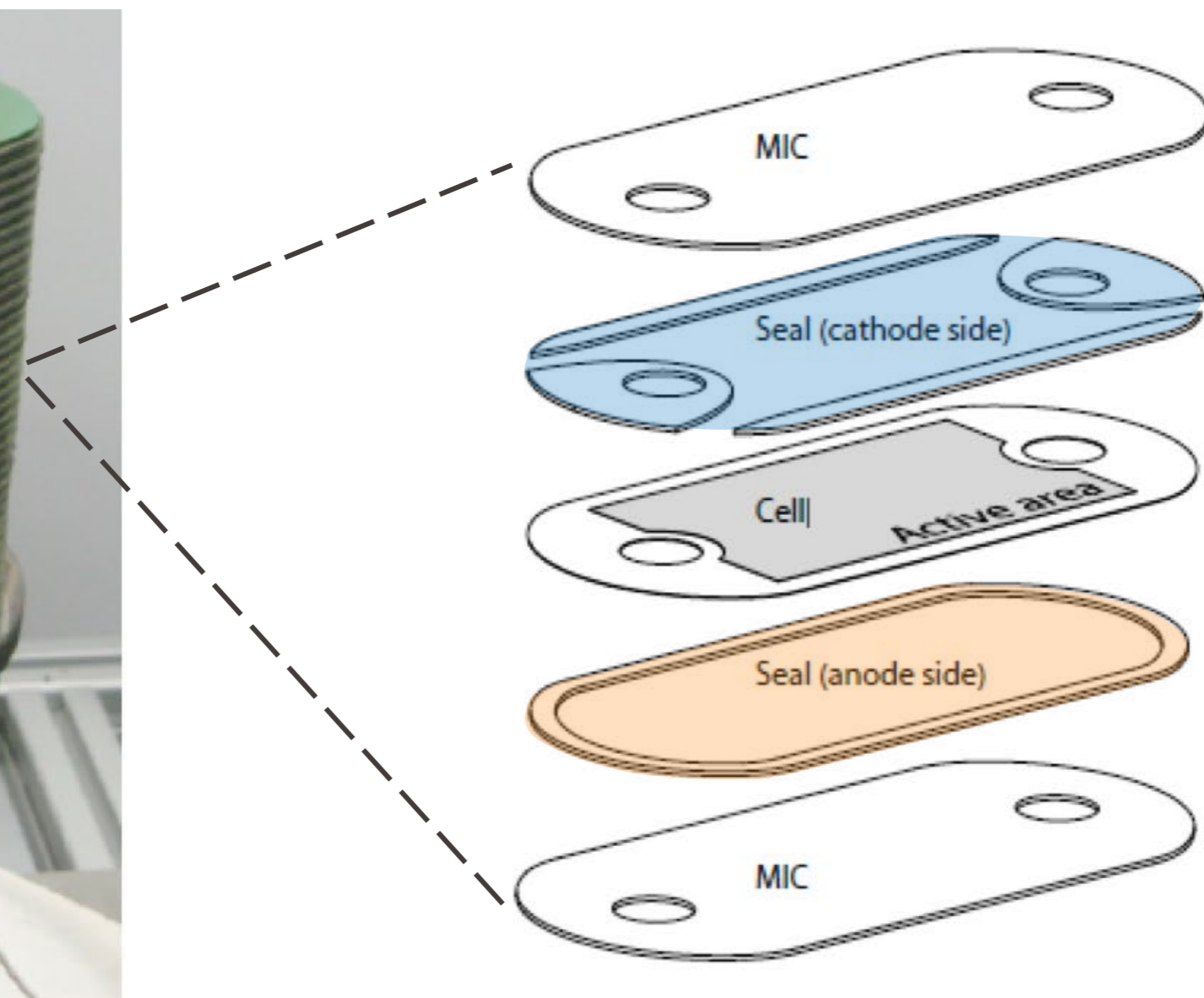
Physical problem

- A solid-oxide fuel cell is used to generate electrical power through the reaction of fuel (containing H_2) and air (containing O_2)
- Air is circulated across the cell to:
 - provide oxygen for the electrochemical reaction
 - dissipate the heat generated

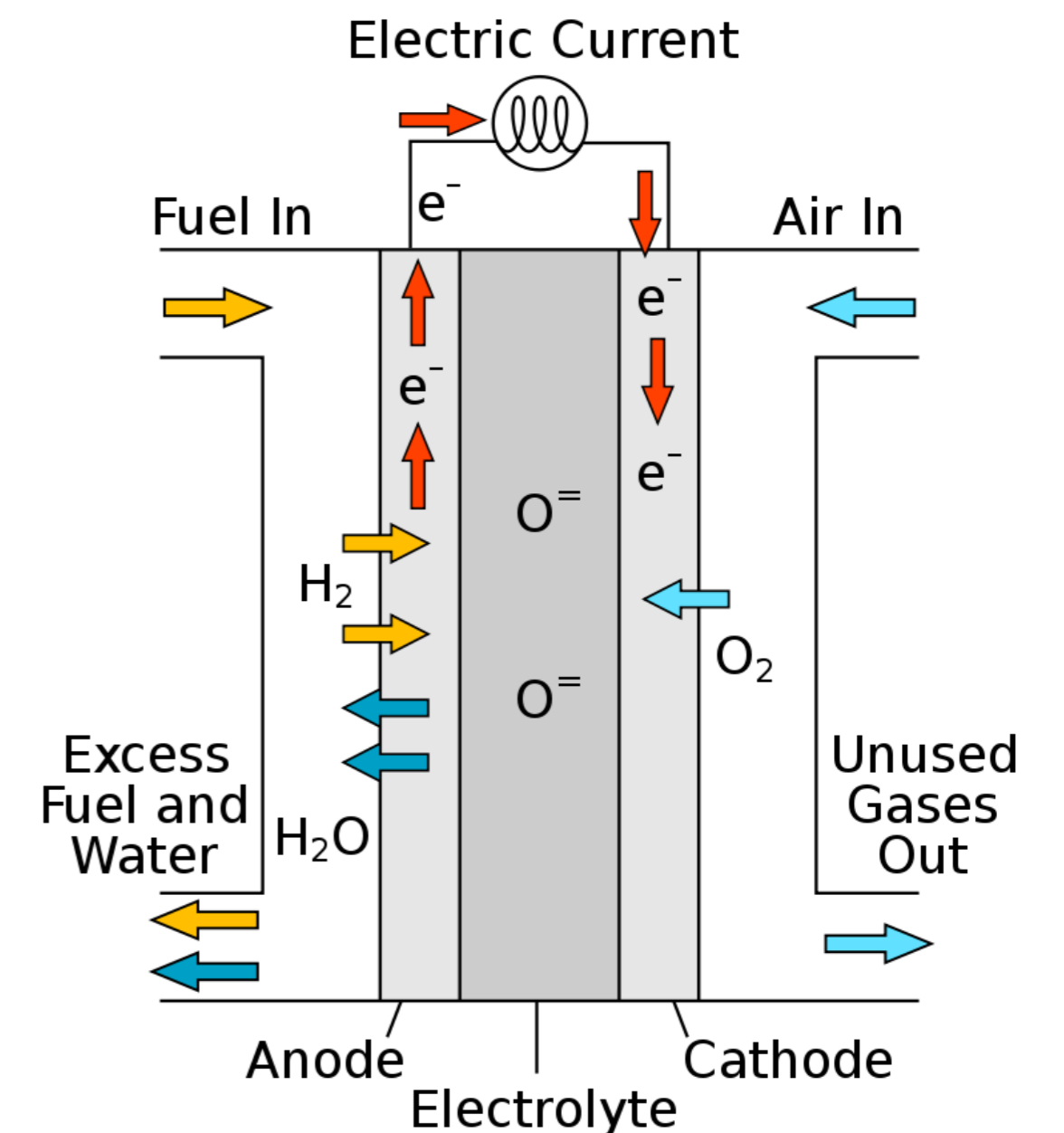
Numerical Flow Simulation



Fuel cell stack



One cell module

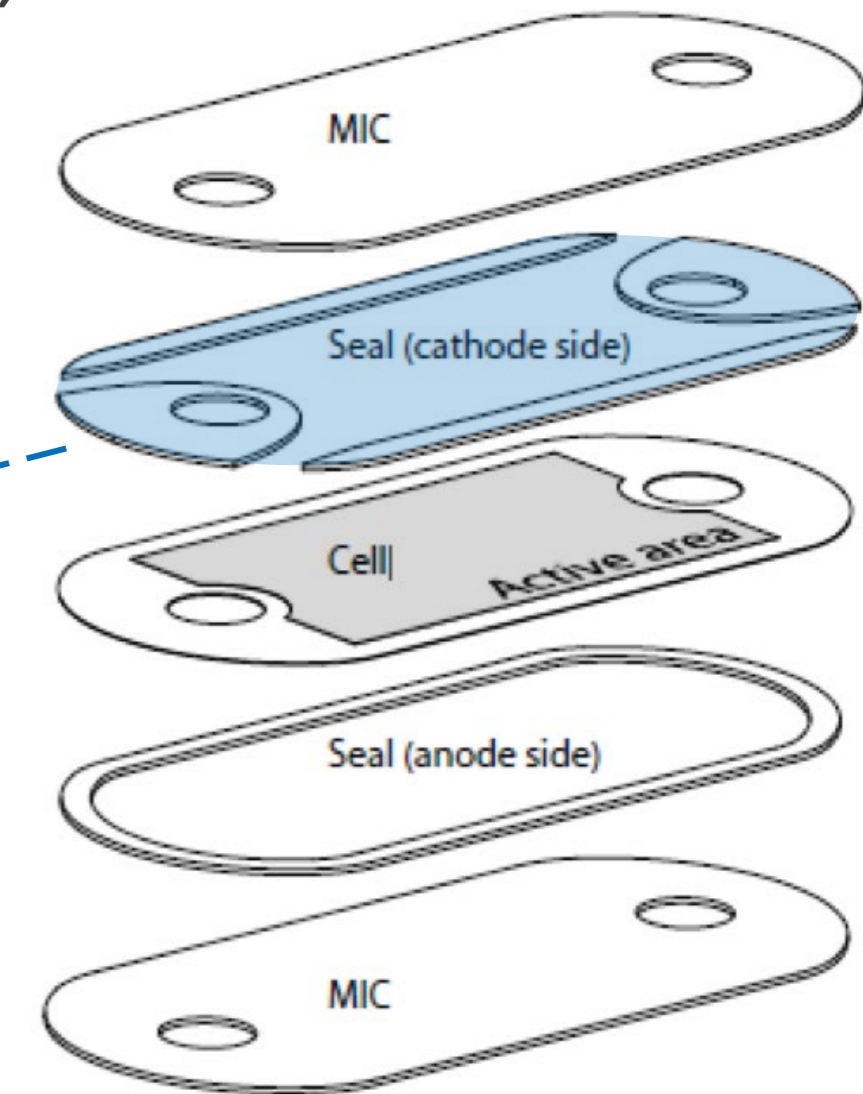
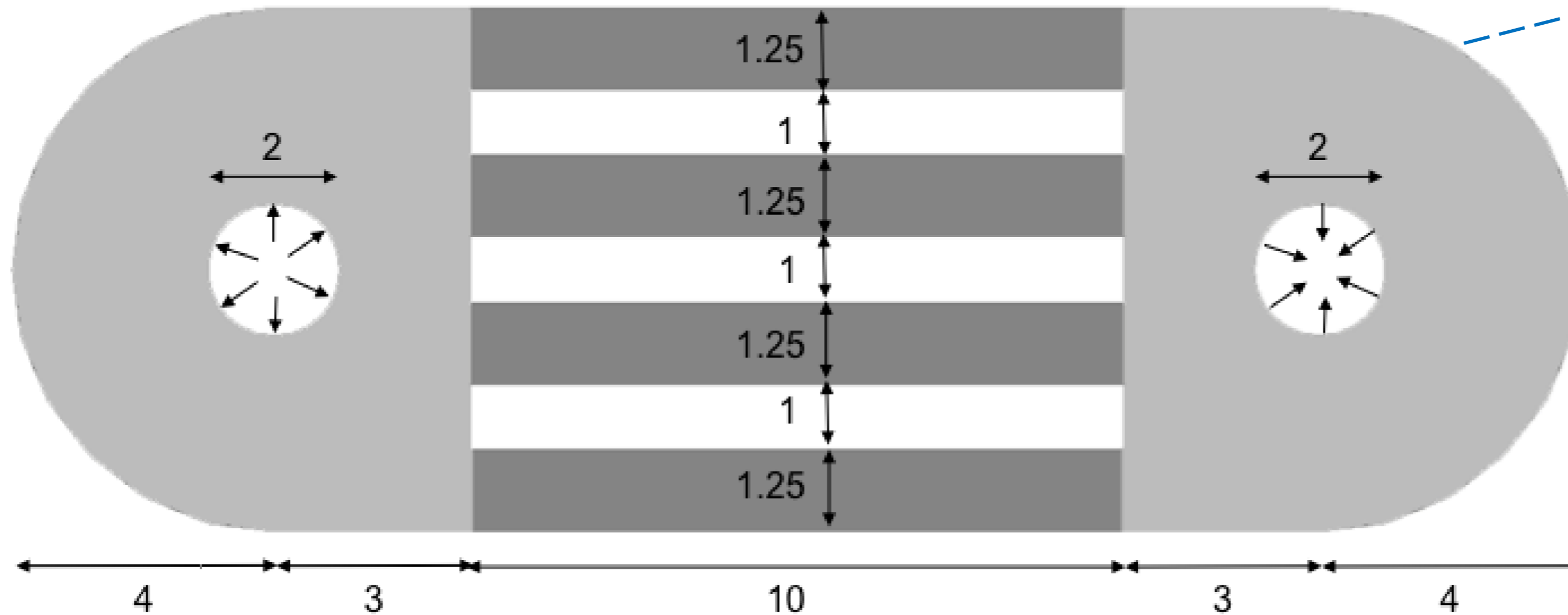


Physical problem

- Goals of present numerical simulation study:
 1. Compute 2D solution for a simplified version of the problem
 - Neglect details of electrical power generation process
 - Simplify heat generation by imposing fixed surface heating rate
 - Simplify geometry by considering 2D problem
 2. Questions to resolve:
 - Are these approximations valid? Do they influence the flow?
 - How can they be improved to make the simulation results more realistic?

Fuel cell geometry

- Simplified geometry:
 - 2D horizontal cross-section through one cell module (ignore vertical flow)
 - Oblong section with circular end sections (total length $L = 24$ cm)
 - Circular inflow & outflow sections (diameter 2 cm)
 - 3 inserts (each of width 1 cm)
 - 4 flow channels (each of width 1.25 cm)



Numerical Flow Simulation

Flow conditions

- Flow and thermal conditions:

- uniform inflow velocity $V = 4 \text{ m/s}$,
- inflow turbulence intensity 10%,
- inflow temperature $T = 1000 \text{ K}$,
- uniform heat generation rate in the 4 flow channels 1 MW/m^3 ,
- outer cell wall and sidewalls of 3 rectangular inserts assumed adiabatic.

- Material properties (high-temperature air):

- air density, $\rho = 0.34 \text{ kg/m}^3$,
- dynamic viscosity, $\mu = 4.30 \times 10^{-5} \text{ Pa s}$,
- specific heat capacity at constant pressure, $C_p = 1145 \text{ J/kg K}$,
- thermal conductivity, $k = 0.068 \text{ W/m K}$.

Gravitation and associated buoyancy effects, as well as radiation, are to be neglected.

Flow conditions

- Dimensionless numbers

- Reynolds number

- $Re = \rho VL/\mu = 7'600$

- Slightly turbulent flow

- Relatively thick velocity boundary layer

- choice of boundary-layer mesh, and wall treatment for turbulence model

- Mach number

- $M_\infty = V/c = V/(\gamma RT/M_{\text{air}})^{1/2} = 0.006 \ll 1$ ($\gamma = 1.4$, $R = 8.314 \text{ J}/(\text{mol}\cdot\text{K})$, $M_{\text{air}} = 0.029 \text{ kg}/\text{mol}$)

- Flow can be considered as incompressible

- choice of physical model for fluid, and numerical method

Flow conditions

- Dimensionless numbers

- Prandtl number (depends only on material)

- $Pr = \text{momentum diffusivity} / \text{thermal diffusivity} = \mu / (k / C_p) = 0.74$
 - Thermal boundary layer, $\delta_t \sim \delta / Pr^{-1/3} \sim 1.1 \delta$ (with δ the velocity BL thickness)
→ thermal BL and velocity BL have similar thicknesses

- Brinkman number

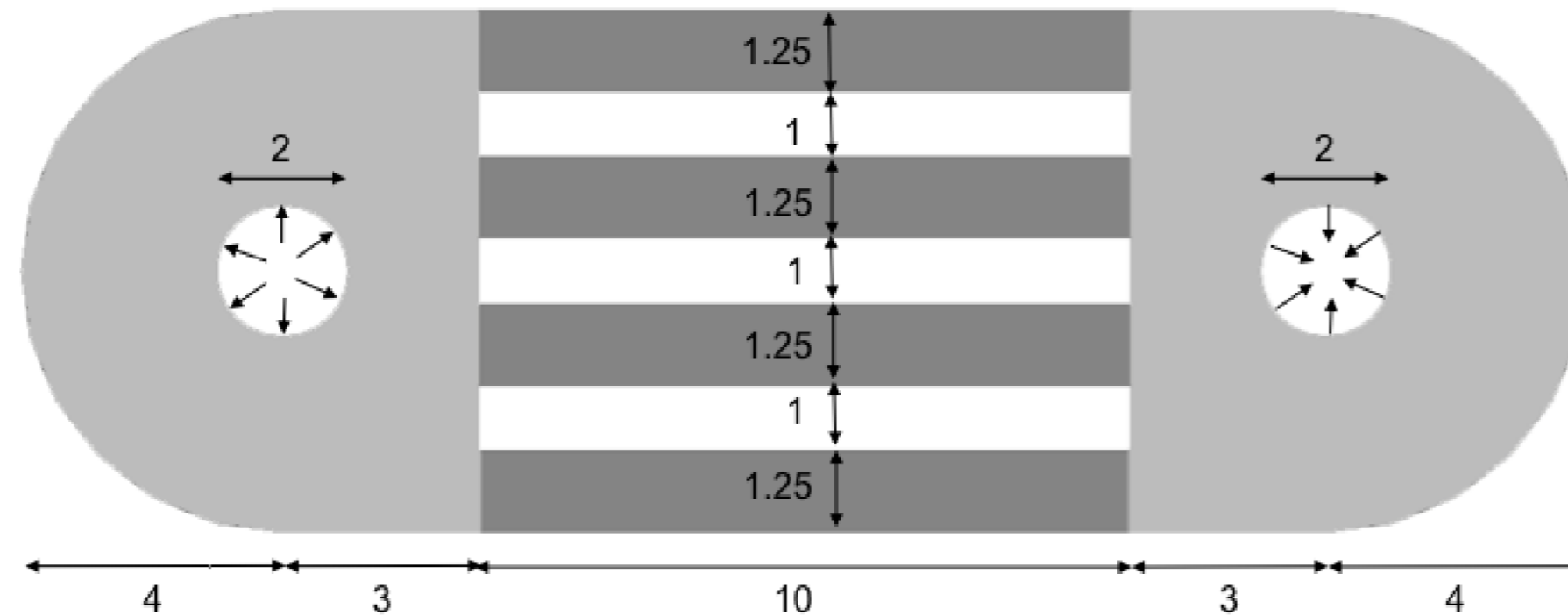
- $Br = \text{heat produced by viscous dissipation} / \text{heat transported by conduction}$
 $= \mu V^2 / k (T_w - T_f) \ll 1$ for air in general
→ viscous heating effects can be neglected (in turbulence model)

- Nusselt number

- $Nu = \text{convective heat transfer} / \text{conductive heat transfer}$
 $= h / (k / L)$ (with $h = Q / \Delta T$ the heat transfer coefficient) $\gg 1$
→ heat produced will be much more transported than conducted

Flow conditions

- Other geometrical / physical considerations
 - Flow in 4 channels:
 - Decide which boundary layers are important
 - Heat generation in channels
 - Flow around 3 inserts:
 - Possible boundary-layer separation and recirculation
→ choice of mesh and turbulence model

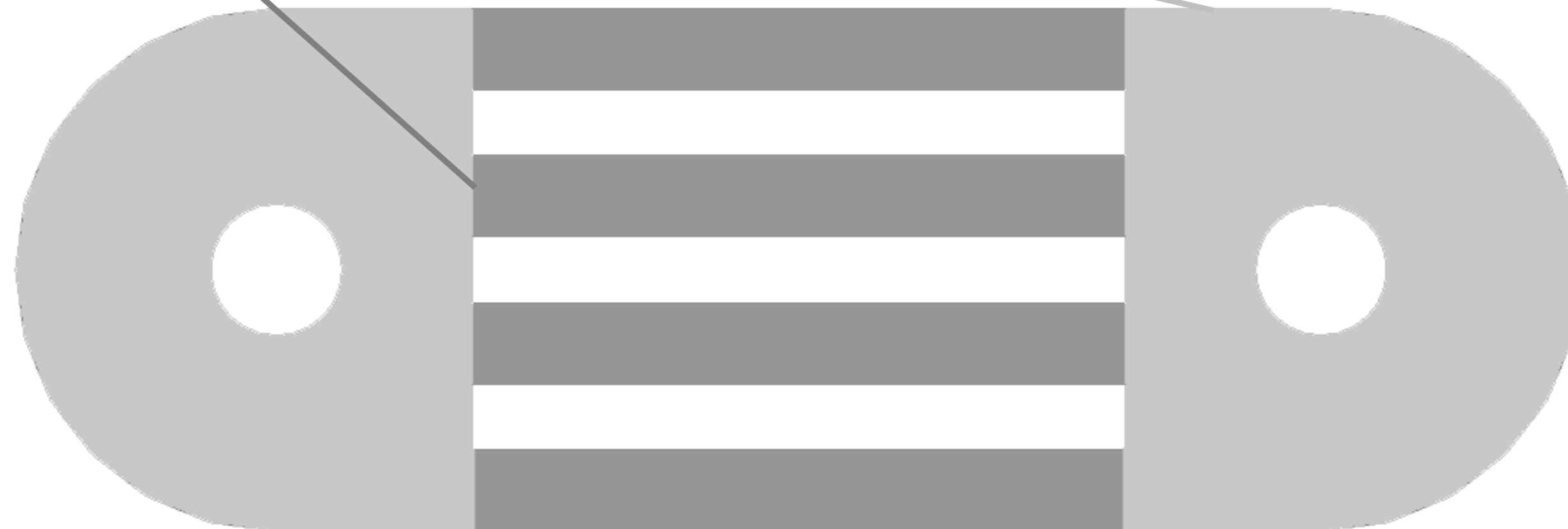


Pre-processing

- Mesh

- Two main regions:

- Inflow and outflow regions
 - 4 channels

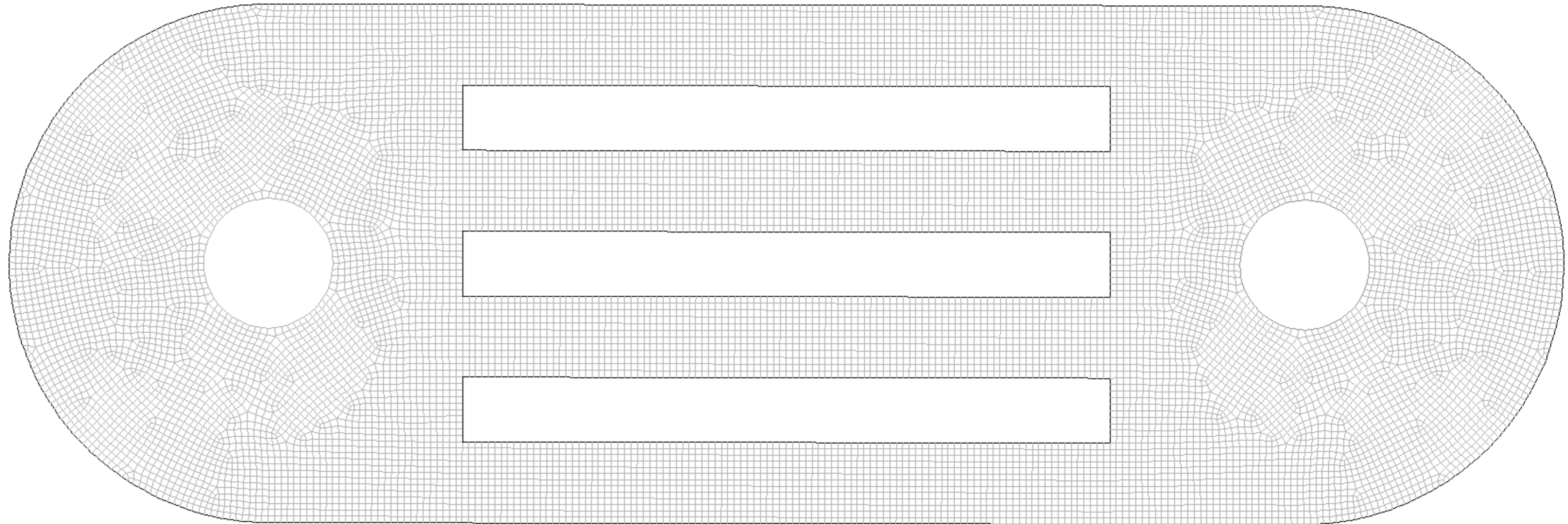


- Type of mesh?

- structured / unstructured / block-structured / hybrid
 - triangular / quadrilateral / mixed

Pre-processing

- Mesh:



- Properties:

- Hybrid: unstructured (quad) + structured (quad) in 4 channels
- 14'561 cells
- Minimum orthogonal quality = 0.87 (1 represents high-quality cells)
- Maximum orthogonal skew = 0.13 (0 represents high-quality cells)
- Other suitable types exist

Solver set-up

- Physical models
 - Ideal gas law, high-temperature air properties
 - k - ε turbulence model
 - RNG k - ε (realizable also possible; RNG may be suitable)
 - Enhanced wall treatment (two-layer model) (thick boundary layer \rightarrow can afford $y^+=O(1)$)
 - Neglect viscous heating (Brinkman number $\ll 1$)
 - k - ω models are also appropriate
- Numerical methods
 - Pressure-based segregated solver, SIMPLE scheme, 2nd-order discretization
 - Default under-relaxation factors
 - Monitor average temperature on channel walls

Solver set-up

- Boundary conditions (flow + thermal):

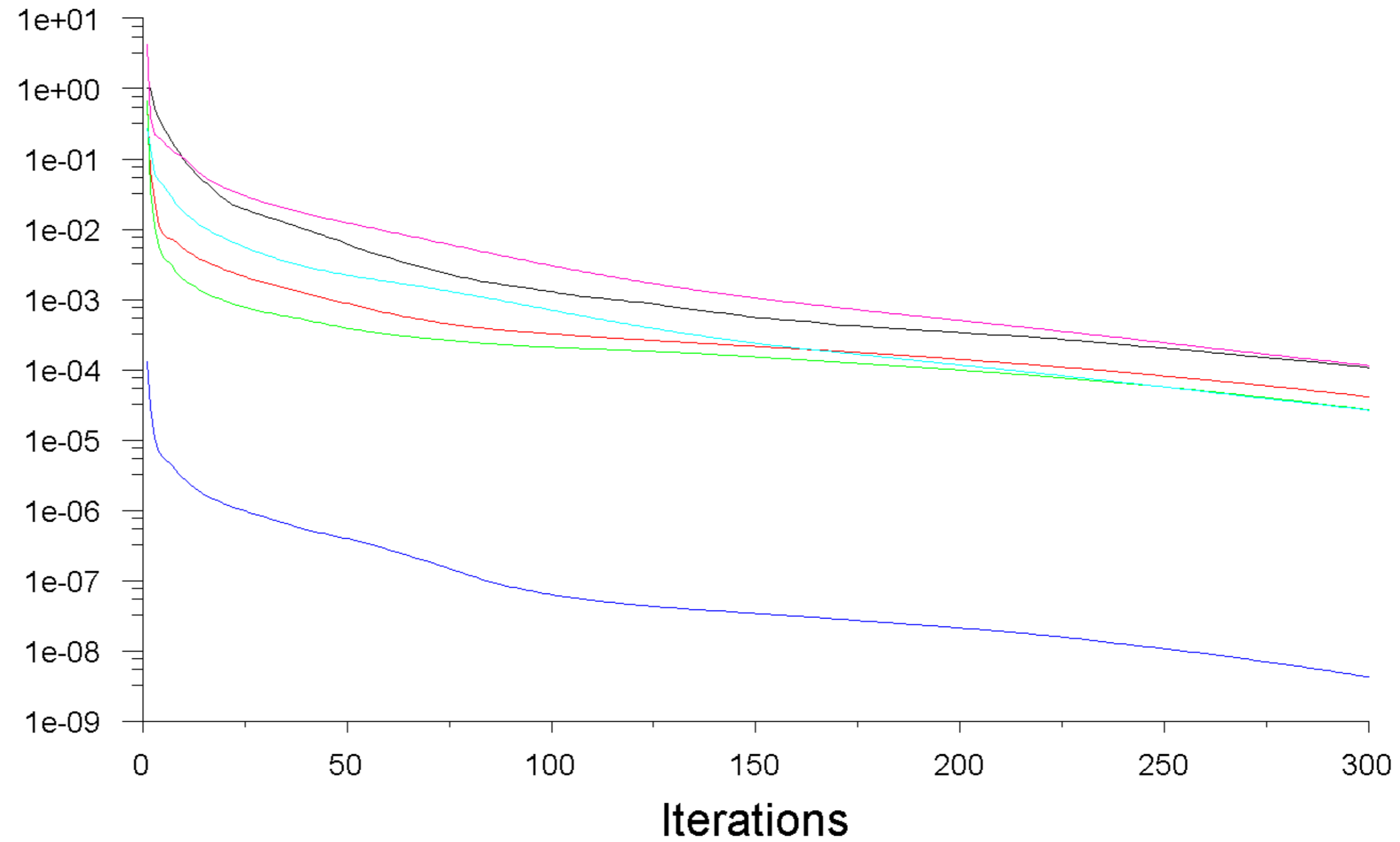
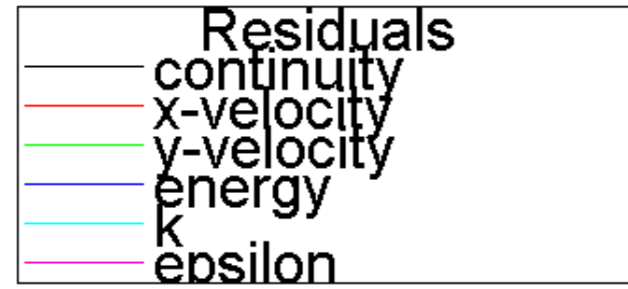
Outer wall and channel walls: no-slip $V_w = 0$, adiabatic



Volumic heat flux Q in 4 channels

Solver procedure

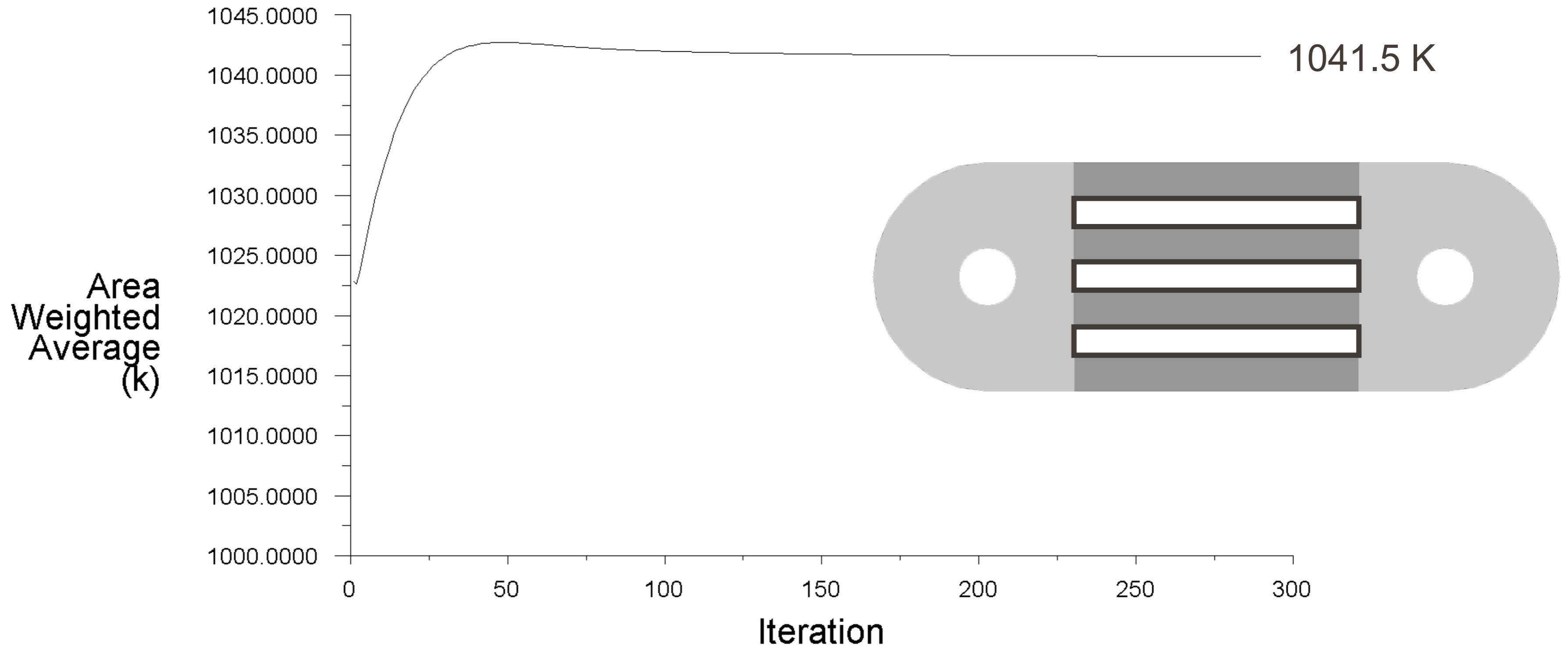
- Convergence: residuals



Solver procedure

- Convergence: average temperature on channel walls

— <temp>



Solver procedure

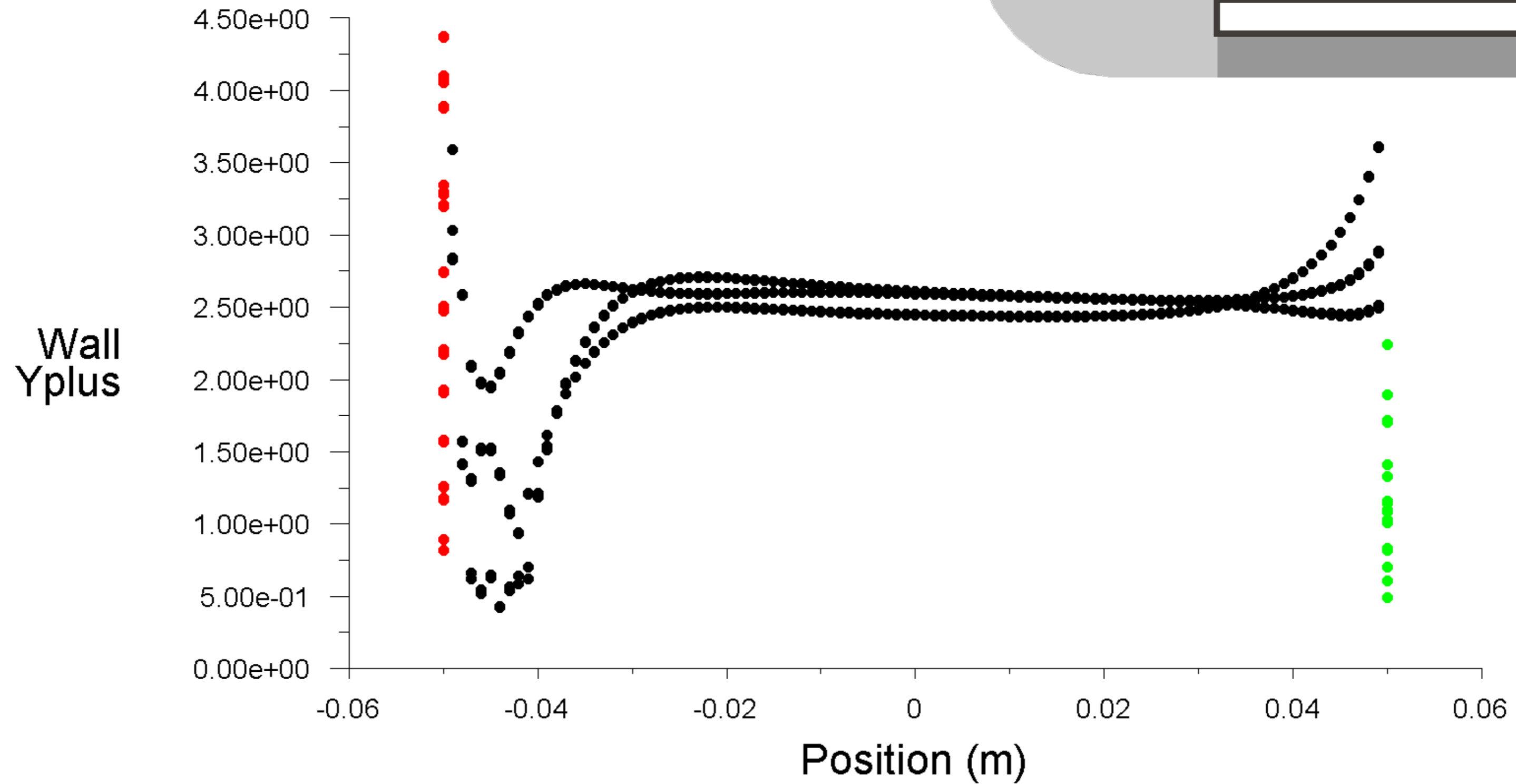
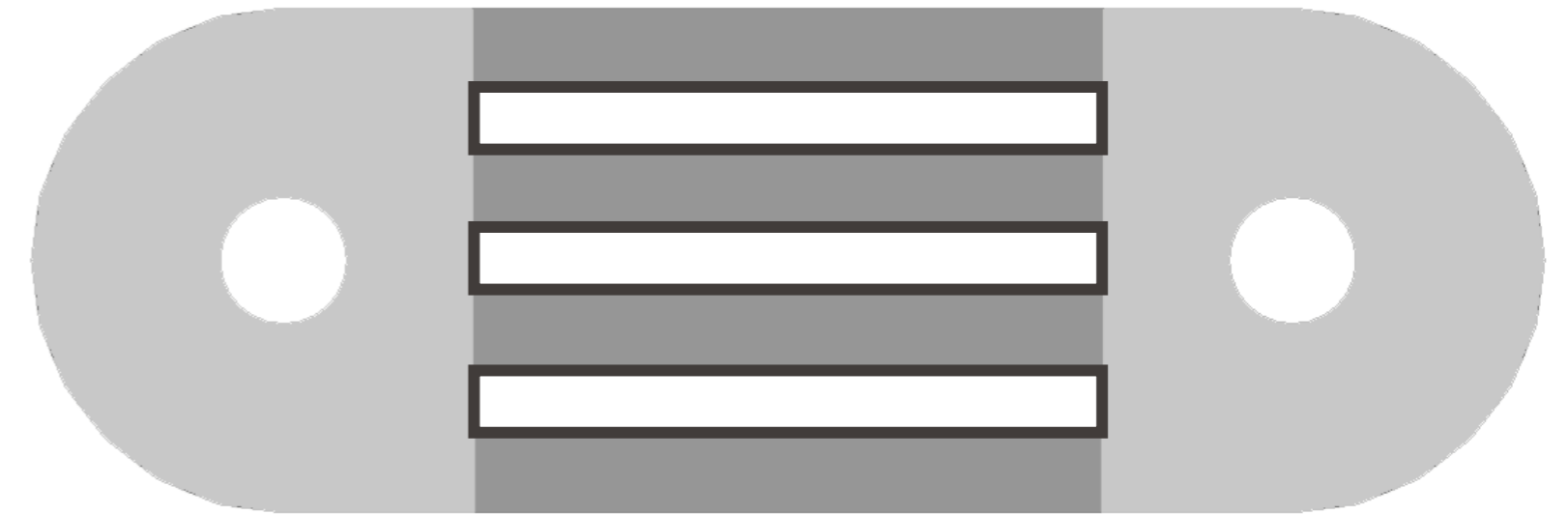
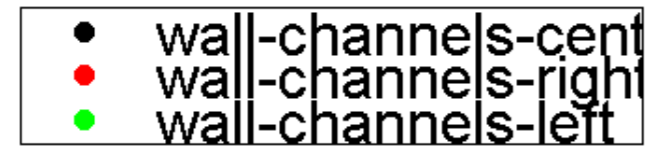
- Convergence: mass conservation
 - Require net mass flux between inlet and outlet to be conserved to $< 0.2\%$

Mass flow rate [kg/s]	
Inlet	0.0854170
Outlet	-0.0854169
Net imbalance	5.2×10^{-8} ($6 \times 10^{-5}\%$)

- Mass conservation satisfied for this solution.

Post-processing

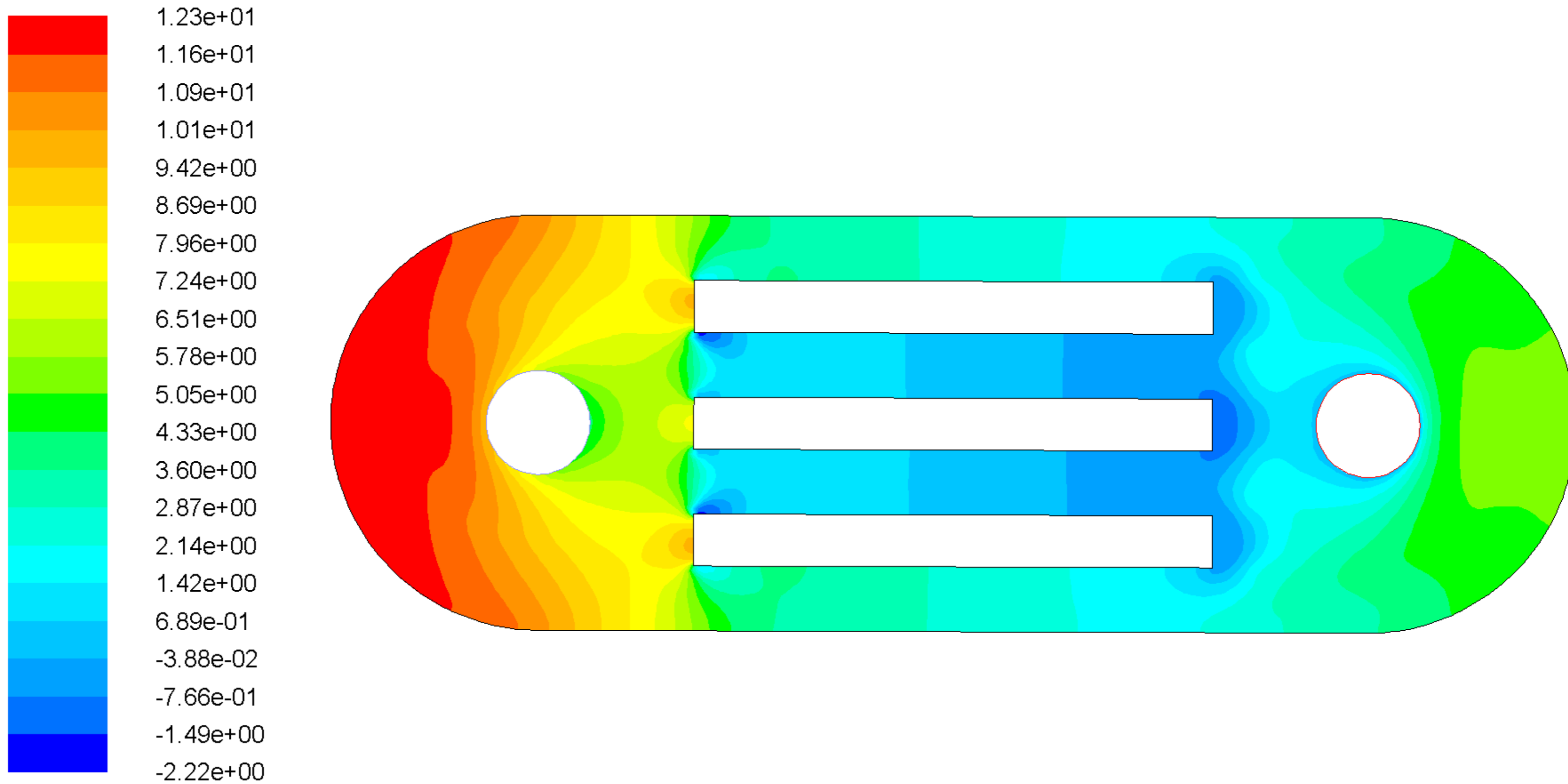
- Control: first-cell y^+ along channels



Post-processing

- Contours: pressure

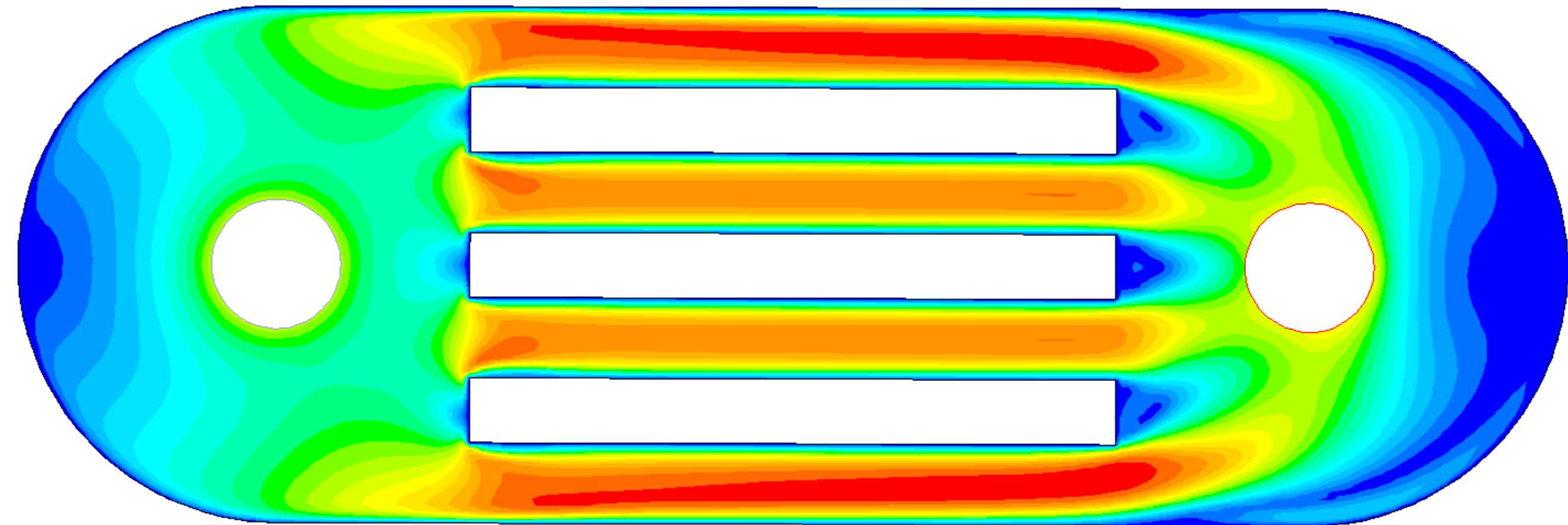
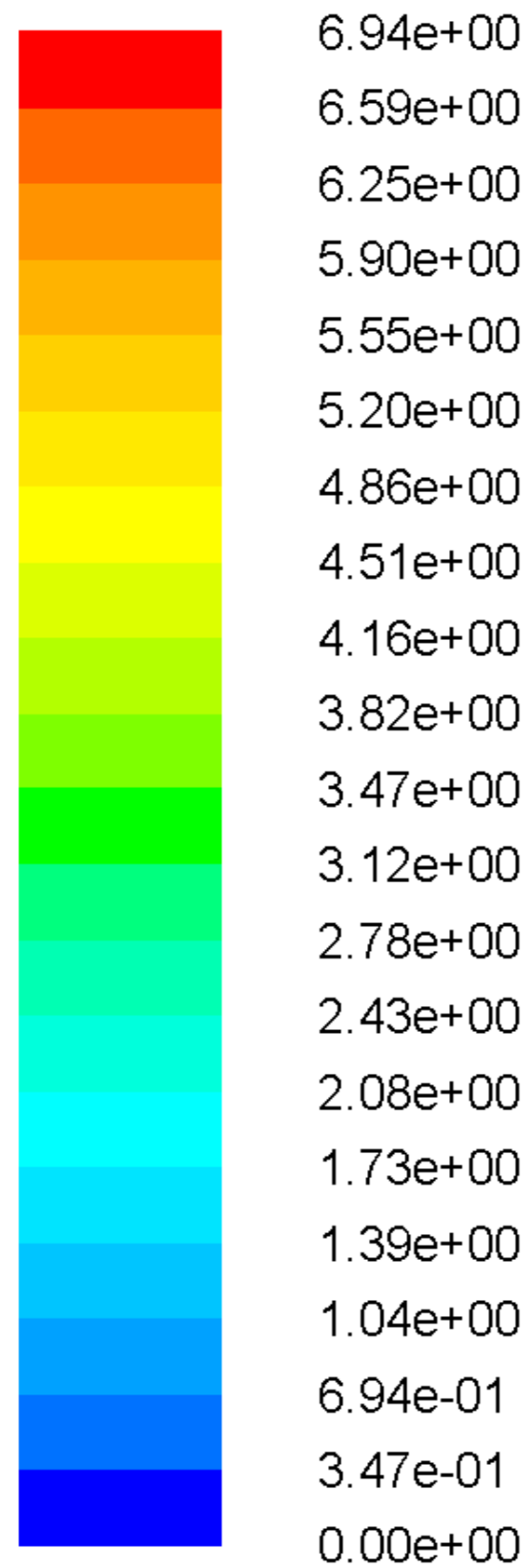
Numerical Flow Simulation



Post-processing

- Contours: velocity magnitude

Numerical Flow Simulation

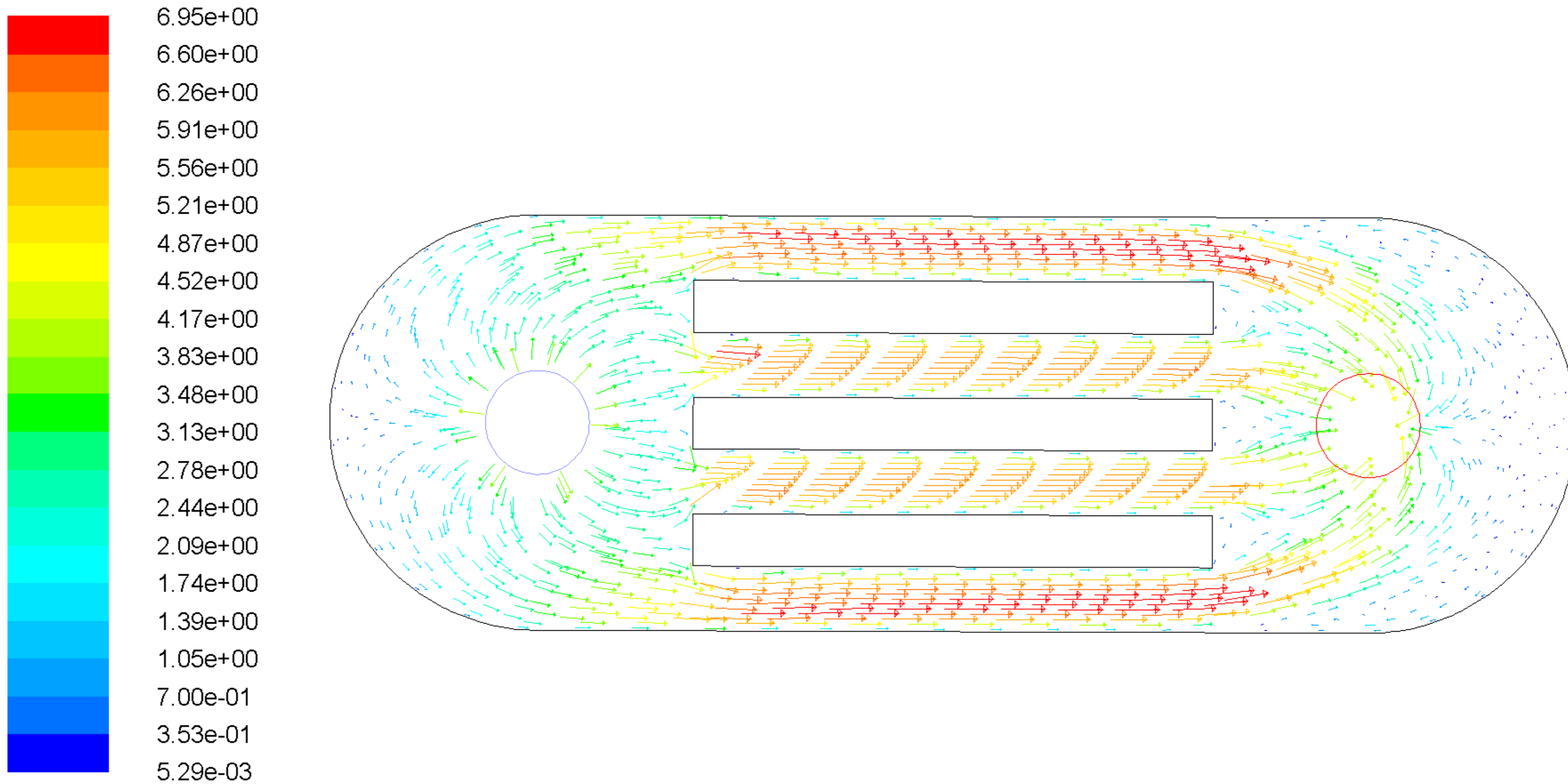


Note: effective Reynolds number in channels: 500~700 (laminar)

Post-processing

- Velocity vectors

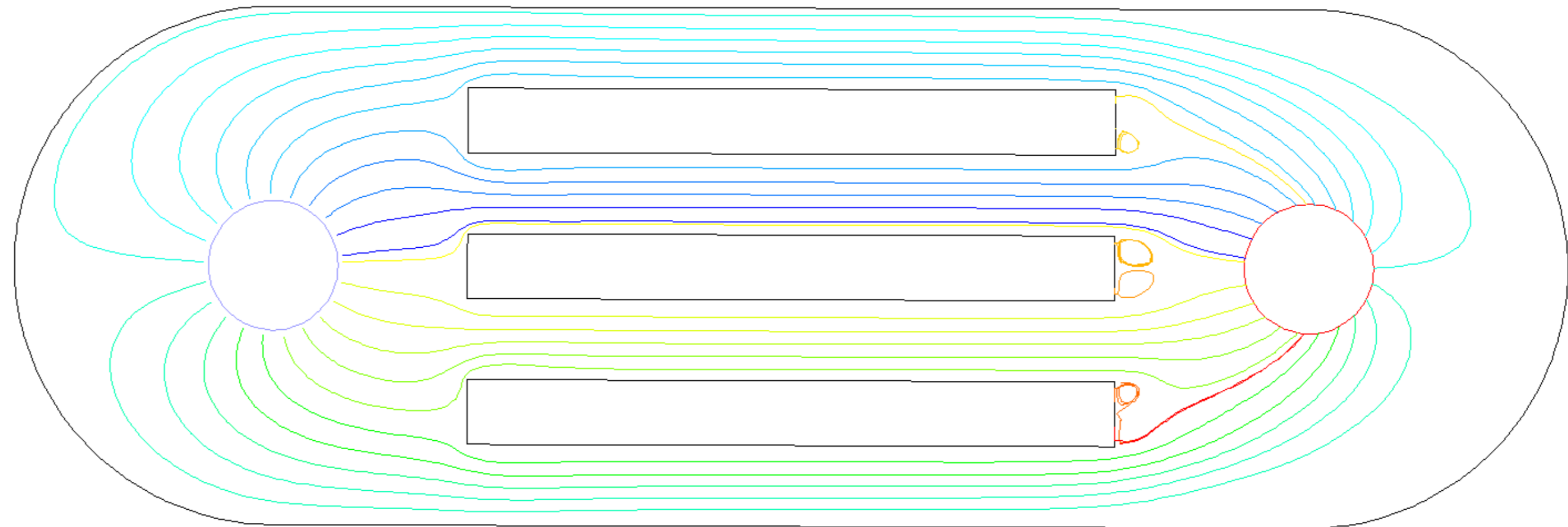
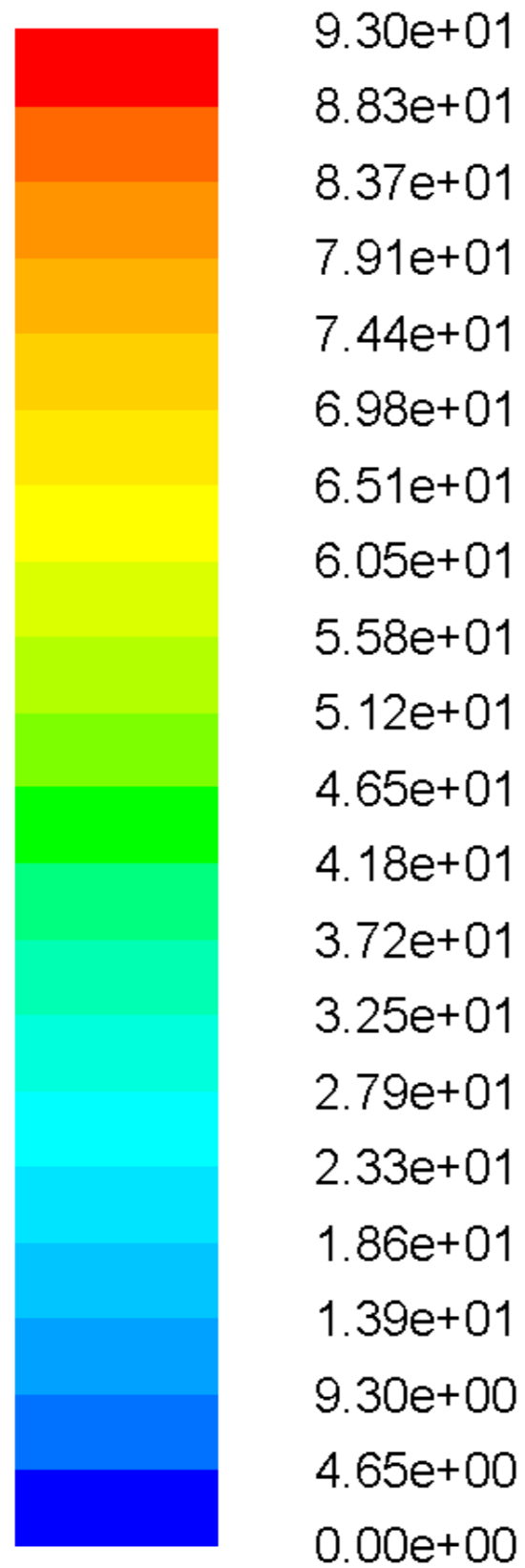
Numerical Flow Simulation



Post-processing

- Streamlines

Numerical Flow Simulation

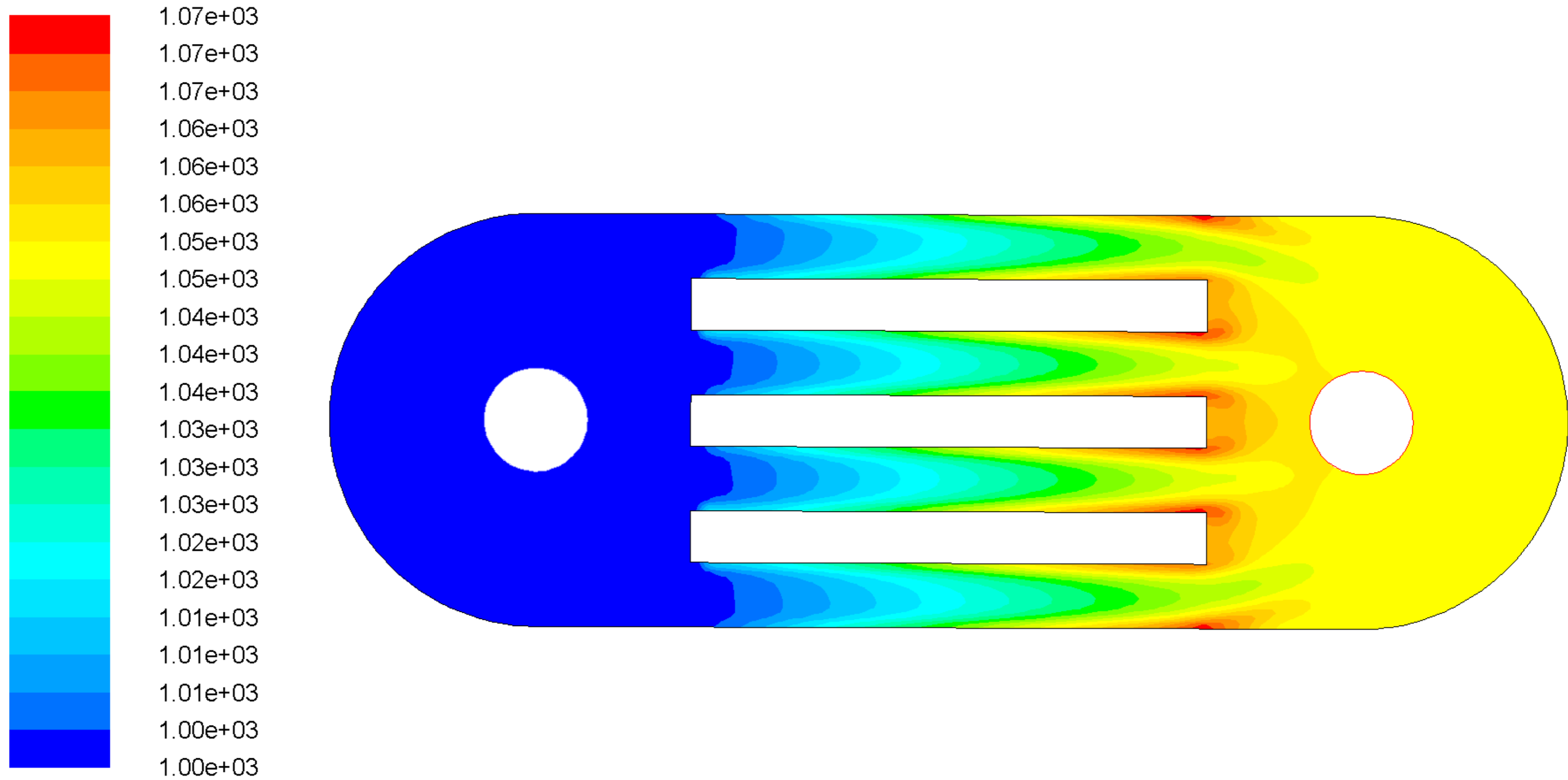


Flow attached in channels; separation at sharp edge downstream

Post-processing

- Contours: temperature

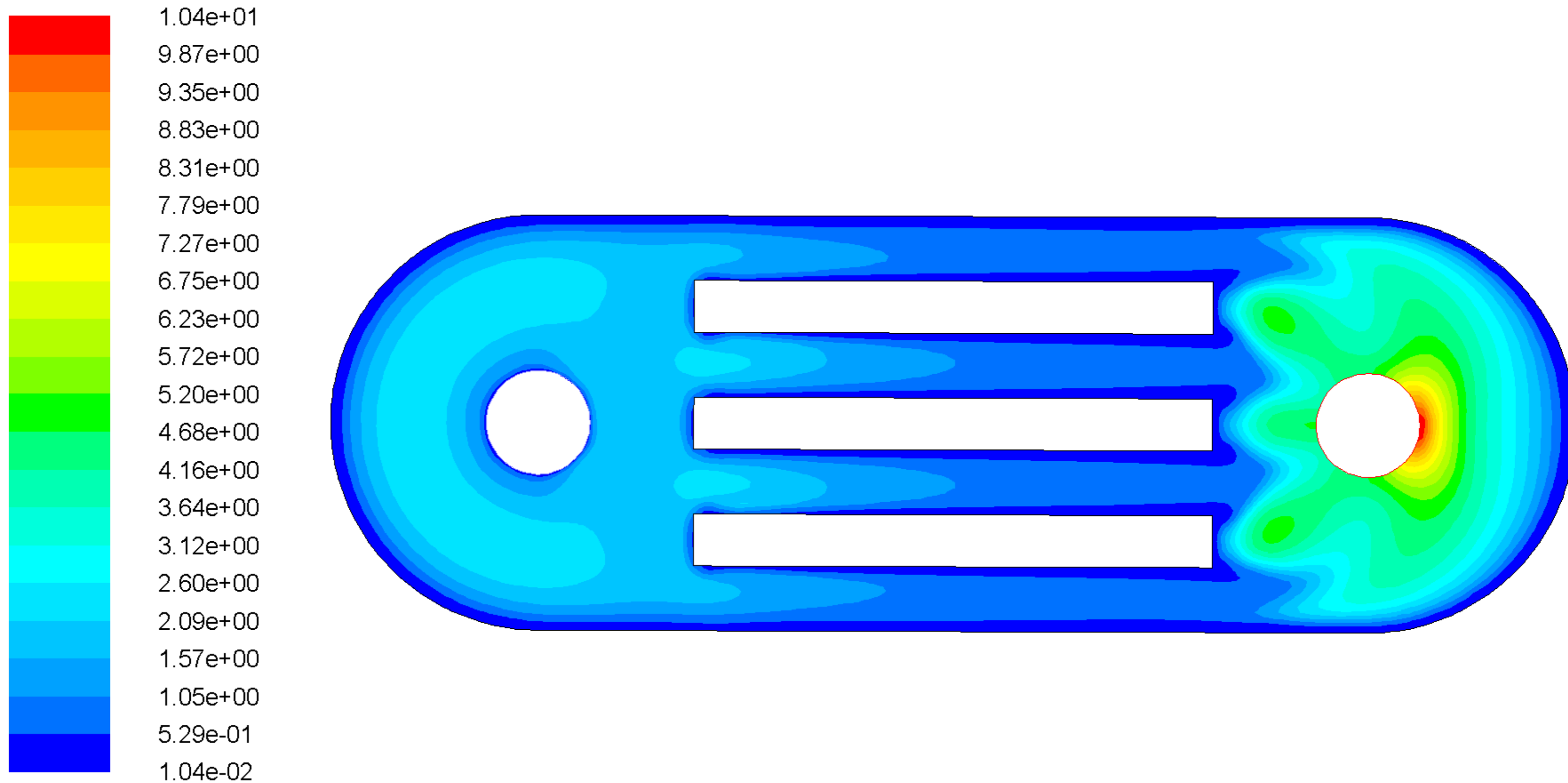
Numerical Flow Simulation



Post-processing

- Contours: turbulent kinetic energy k

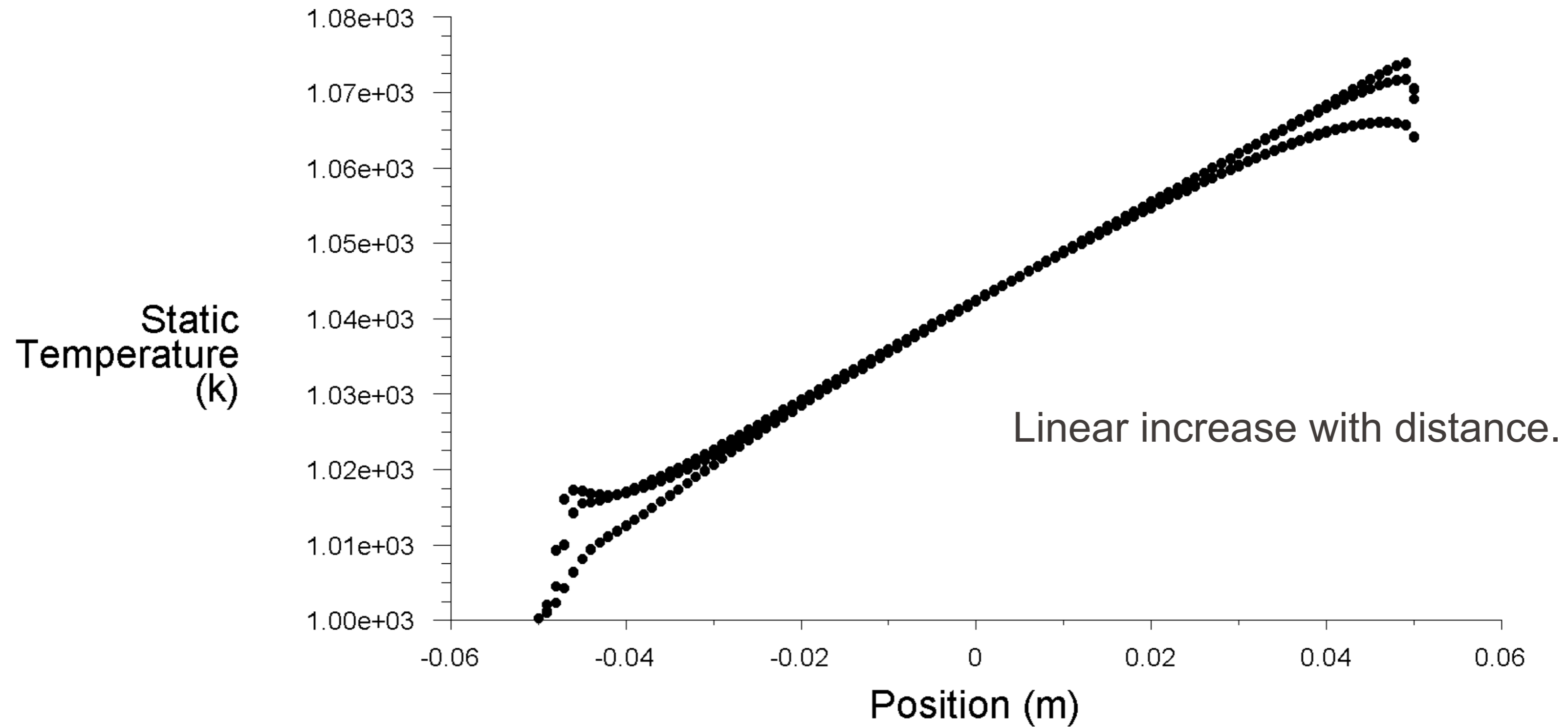
Numerical Flow Simulation



Post-processing

- Temperature on channel surfaces

• wall-channels-cent

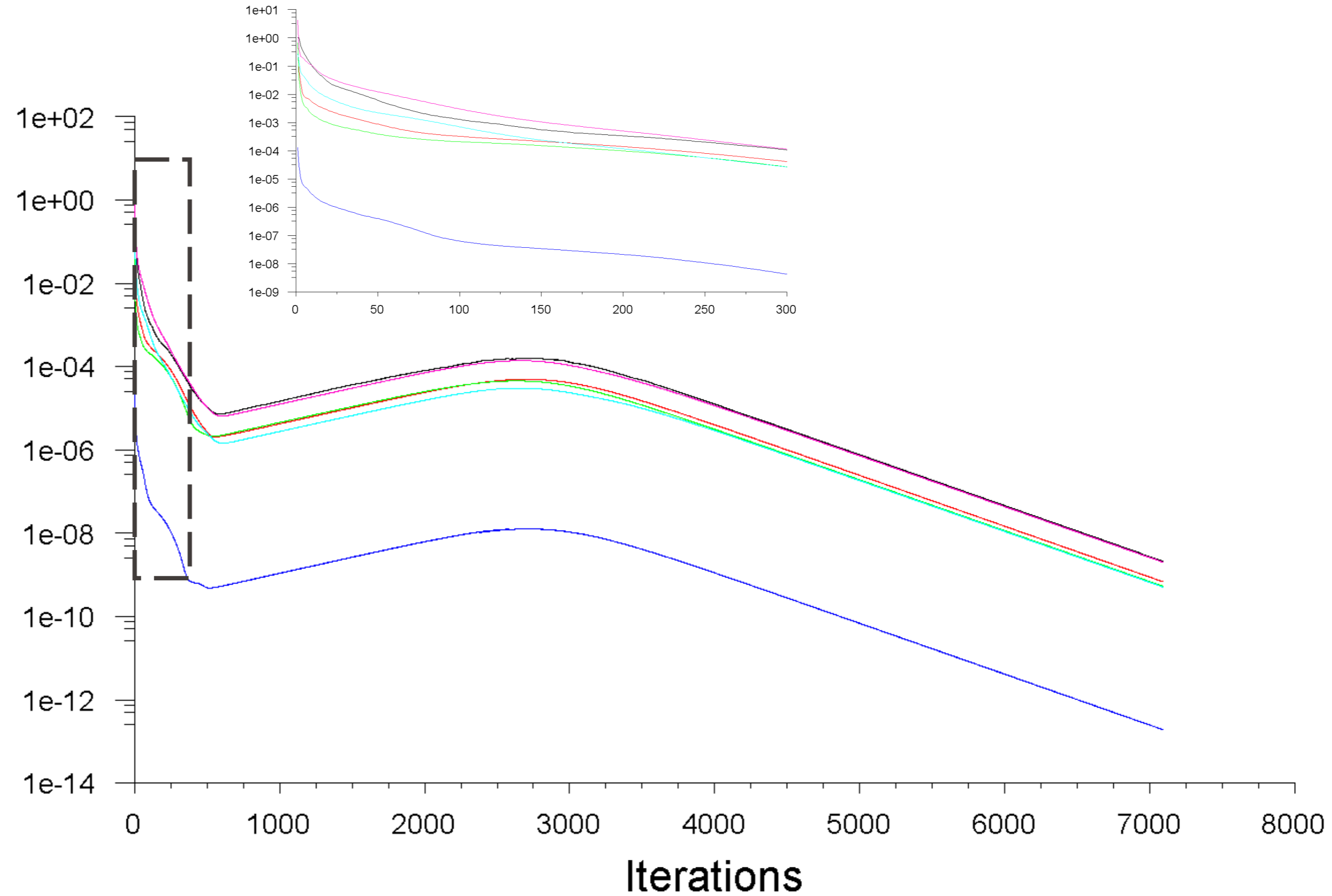
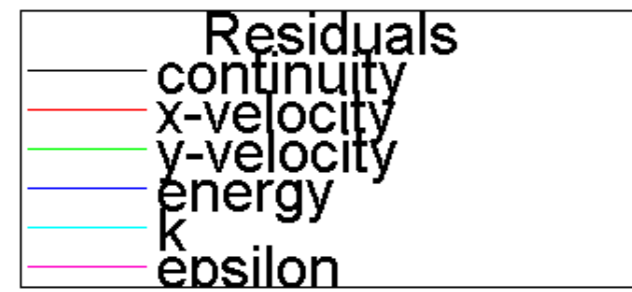


Global observations (1/2)

- Physical analysis of the numerical solution:
 - The flow field has the same top-bottom symmetry as the geometry and boundary conditions.
 - Within the channels, flow aligned with geometry (and mesh).
 - Flow attached in channels; separation at the sharp edge downstream.
 - Turbulence generation highest in outflow region (recirculation, large gradients of mean velocity).
 - Relatively thick boundary layer, justifying the use of a near wall (two-layer) treatment of the turbulence (with y^+ confirmed to be $O(1)$).
 - Air temperature increases linearly in the channels; same temperature in the central region of all channels.
- However...

Solver procedure

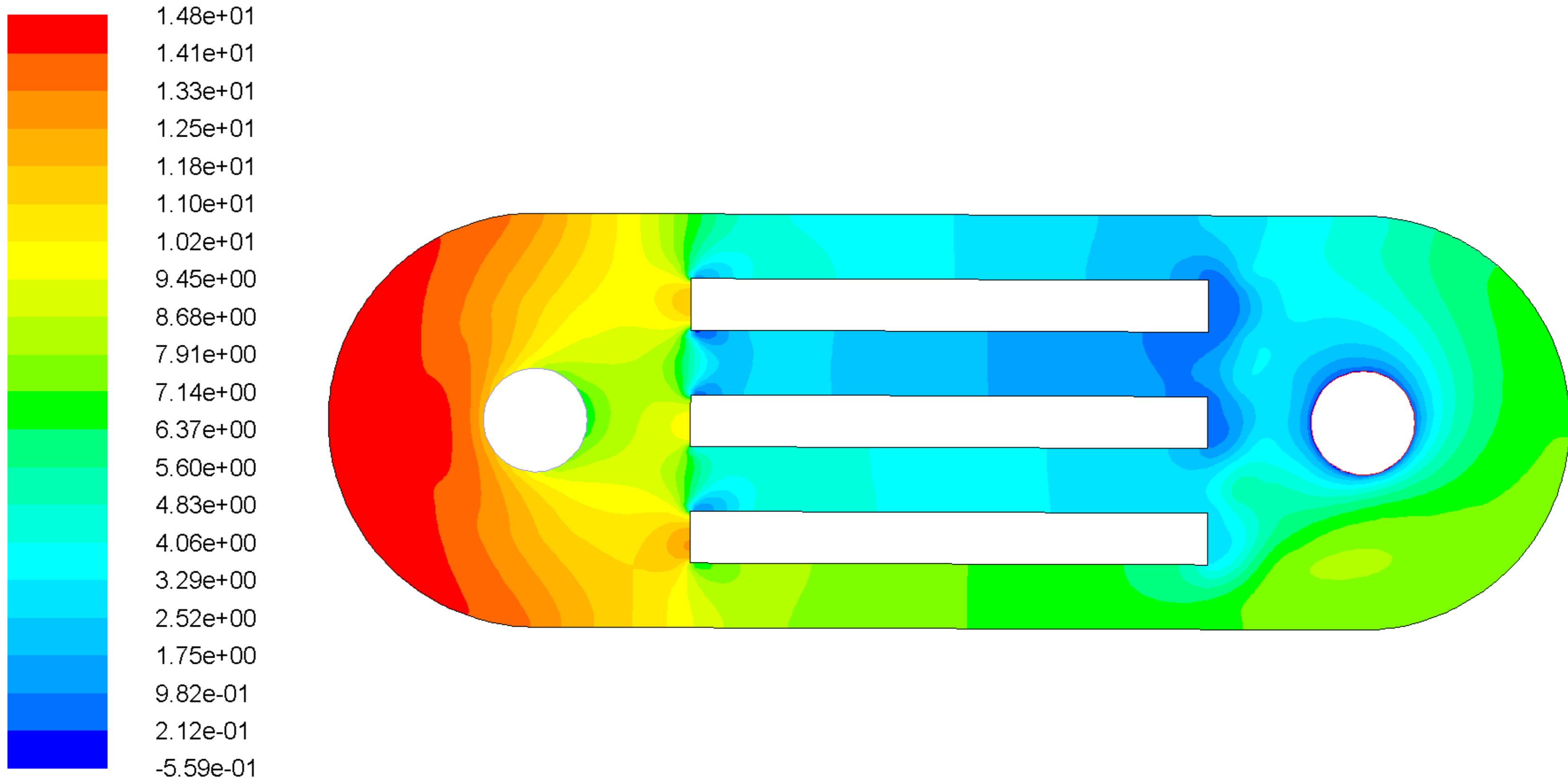
- Convergence: further iterations reveal a second solution



Post-processing

- Contours: pressure

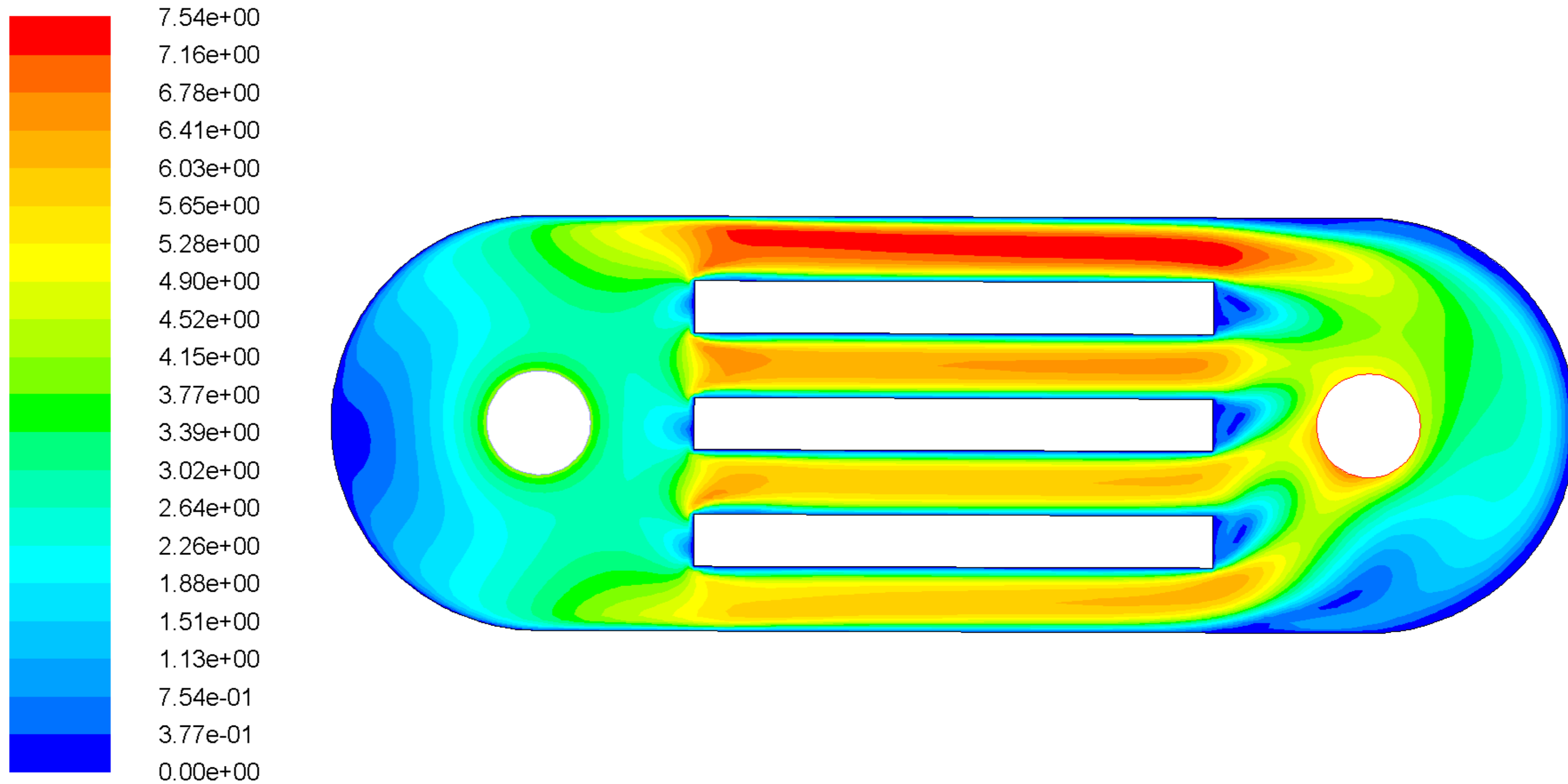
Numerical Flow Simulation



Post-processing

- Contours: velocity magnitude

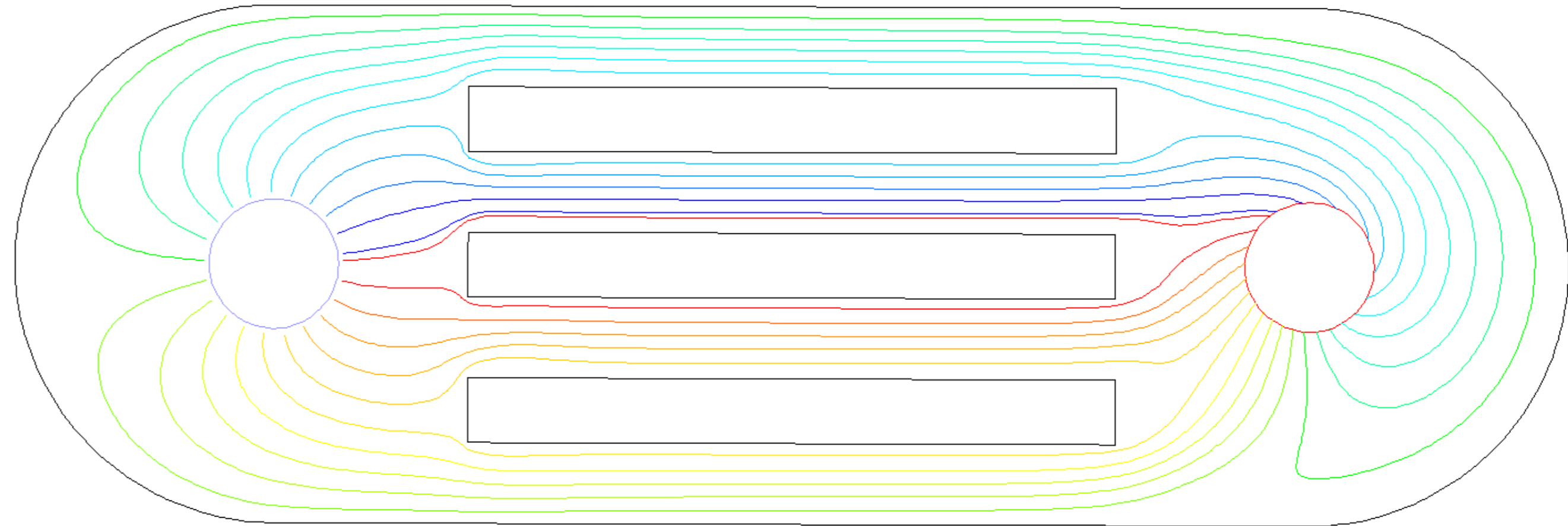
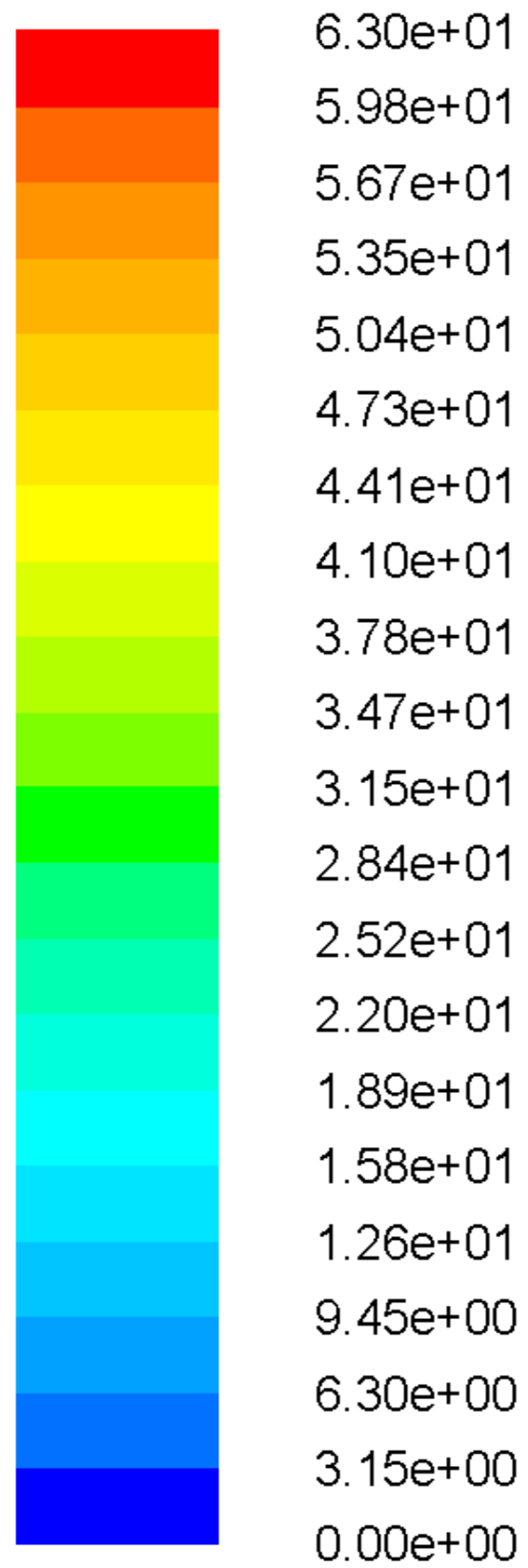
Numerical Flow Simulation



Post-processing

- Streamlines

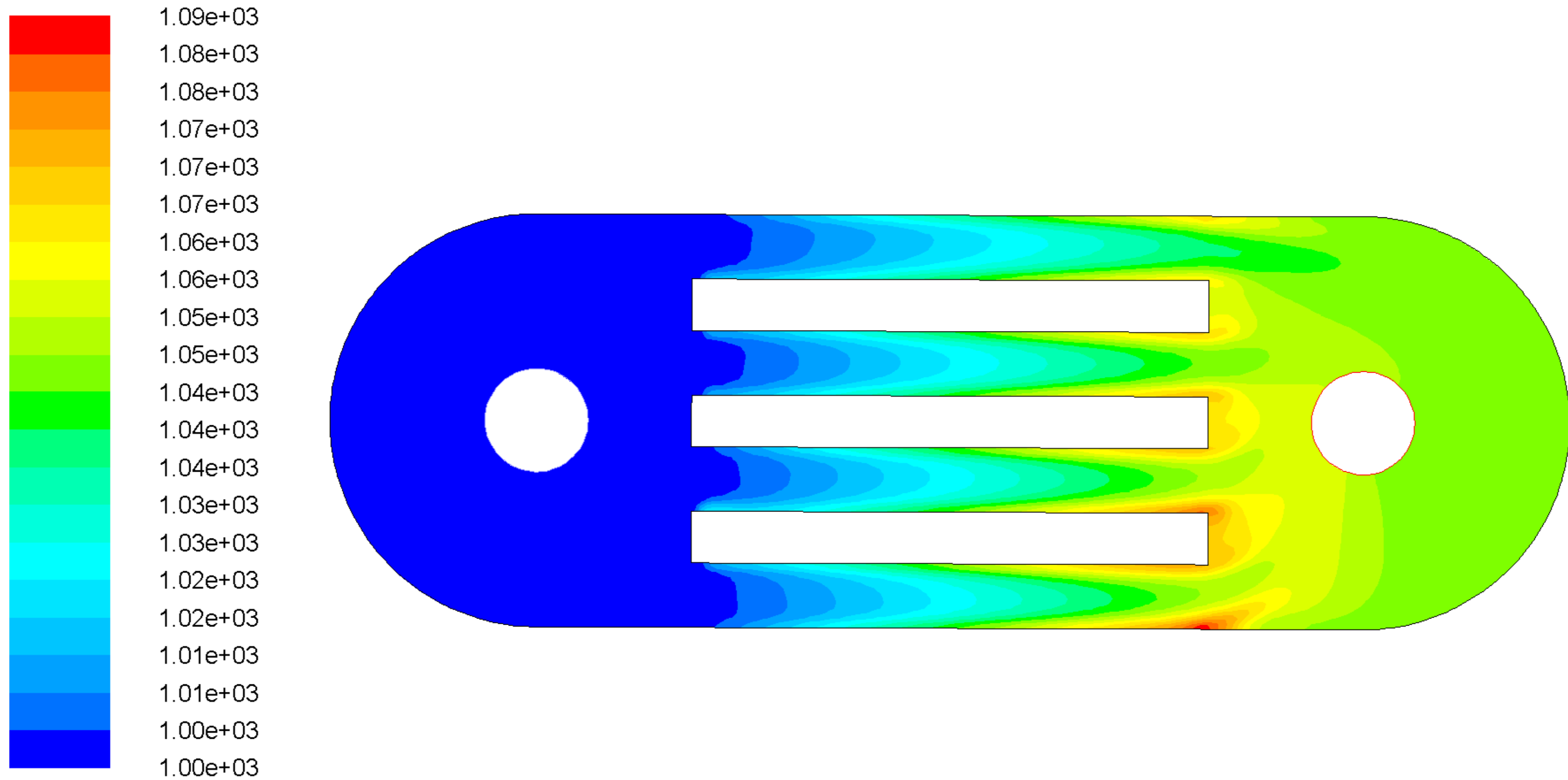
Numerical Flow Simulation



Post-processing

- Contours: temperature

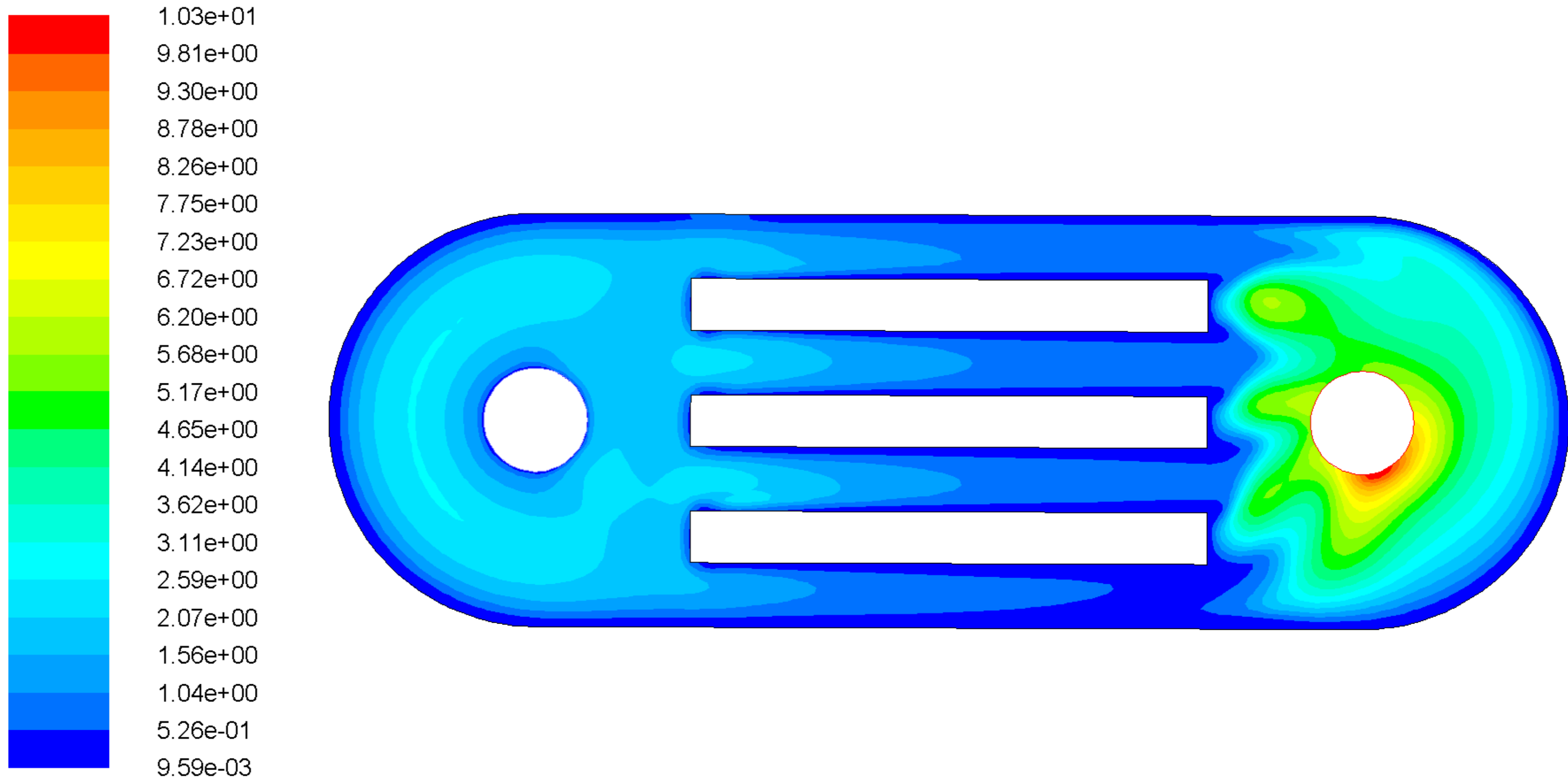
Numerical Flow Simulation



Post-processing

- Contours: turbulent kinetic energy k

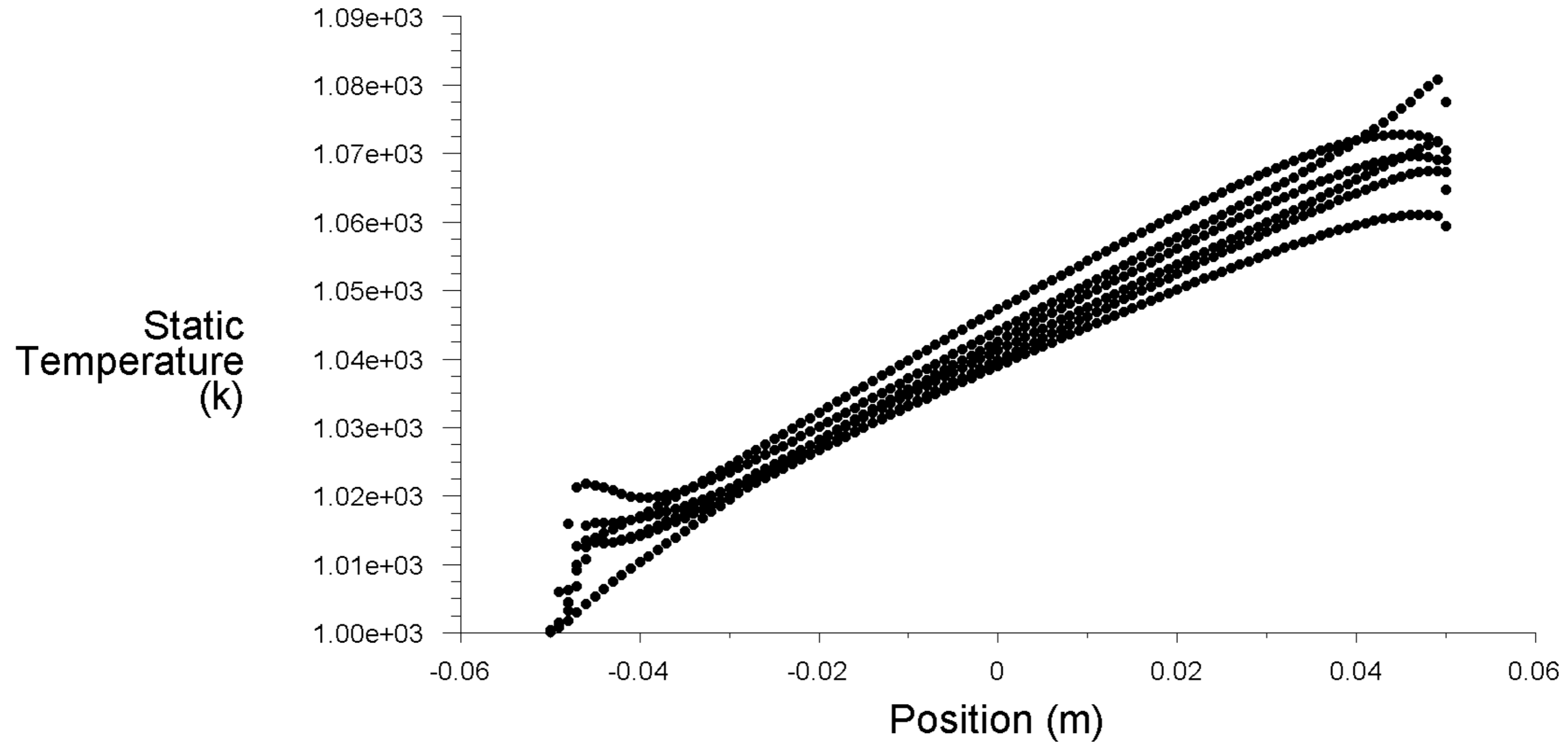
Numerical Flow Simulation



Post-processing

- Temperature on channel surfaces

• wall-channels-cent

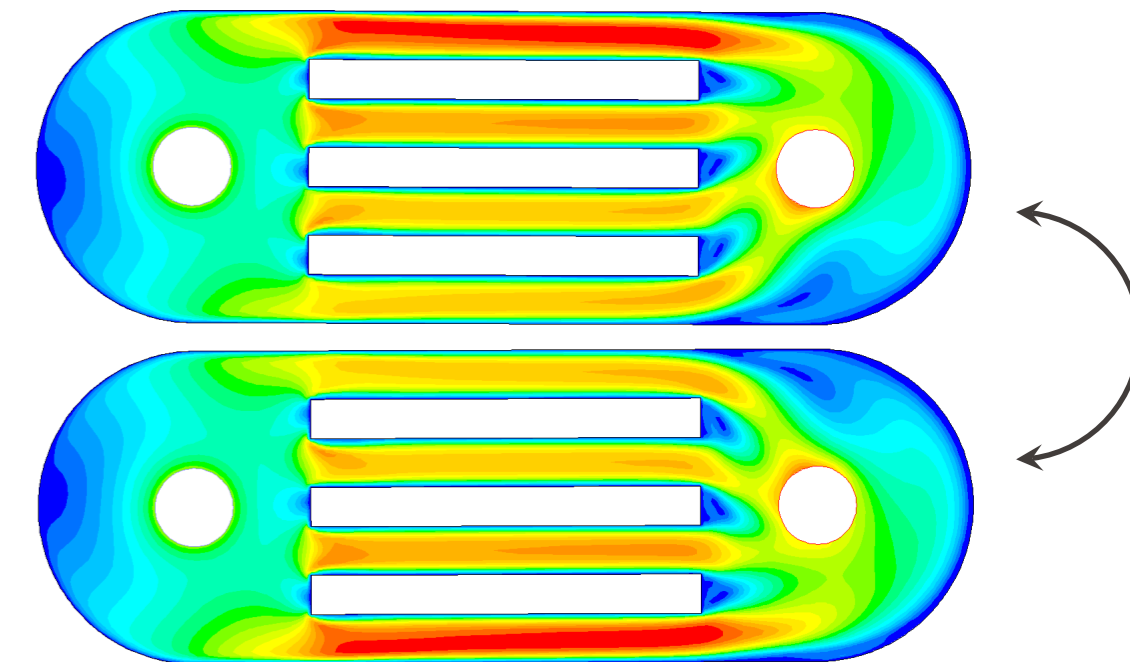


Post-processing

- Estimation of the inlet-outlet temperature difference from $Q = M C_p \Delta T$:
 - Mass flow rate (measured): $M = 0.085 \text{ kg/s}$
 - Specific heat capacity (given): $C_p = 1145 \text{ J/kg K}$
 - Area of 4 flow channels (given): $A = 4 * 1.25 \text{ cm} * 10 \text{ cm} = 50 \text{ cm}^2$
 - Heat generation rate (given): $1 \text{e}6 \text{ W/m}^3 = 1 \text{e}6 \text{ W/m}^2$ per unit depth
 - \rightarrow Total heat input $Q = \text{heat generation rate} * \text{flow channels area}$
 $= 1 \text{e}6 \text{ W/m}^2 * 50 \text{e-}4 \text{ m}^2 = 5000 \text{ W}$
 - $\rightarrow \Delta T = Q / (M C_p) = 5000 \text{ J/s} / (0.085 \text{ kg/s} * 1145 \text{ J/kg K})$
 $= 51.4 \text{ K}$
 - Good agreement with average outlet temperature (1050.4 K).

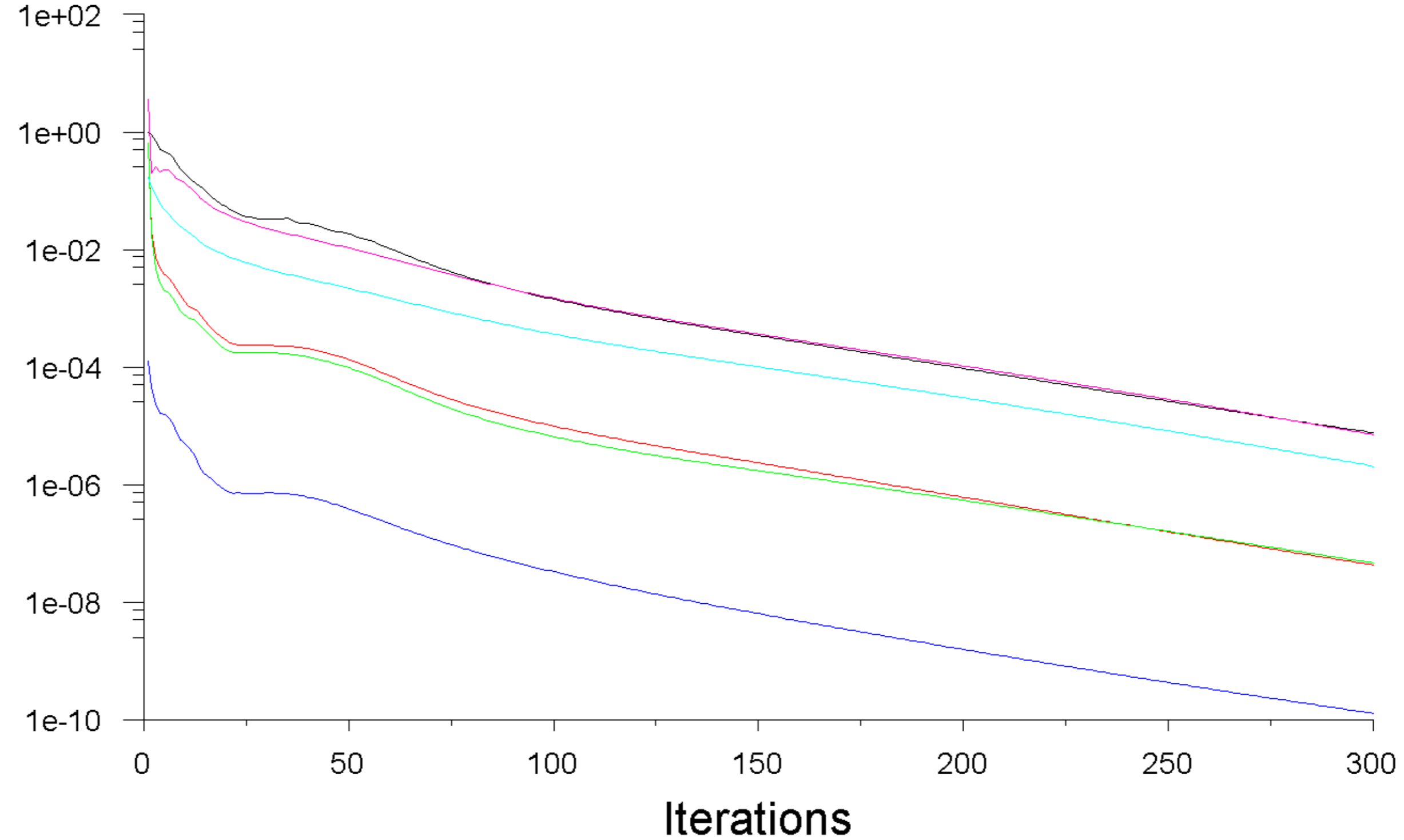
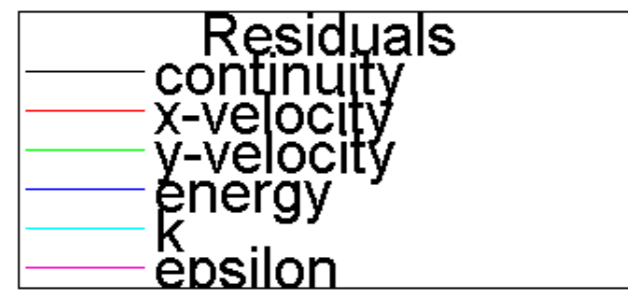
Global observations (2/2)

- Physical analysis of the numerical solution:
 - Residuals increase and then decrease until they reach machine precision.
 - The 2nd solution breaks the top-bottom symmetry.
 - Within the channels, flow still aligned with geometry (and mesh), and still attached; separation at the sharp edge downstream.
 - Temperature still increases linearly, but different value in each channel.
 - 1st (symmetric) solution not stable, therefore not physically observable. Obtained solution depends on initialization, numerical method, physical model...
 - Due to turbulence, actual physical flow may switch between the two symmetry-breaking solutions, and restore symmetry on average. Need experiments or long time-dependent simulations to investigate this point.



Solver procedure

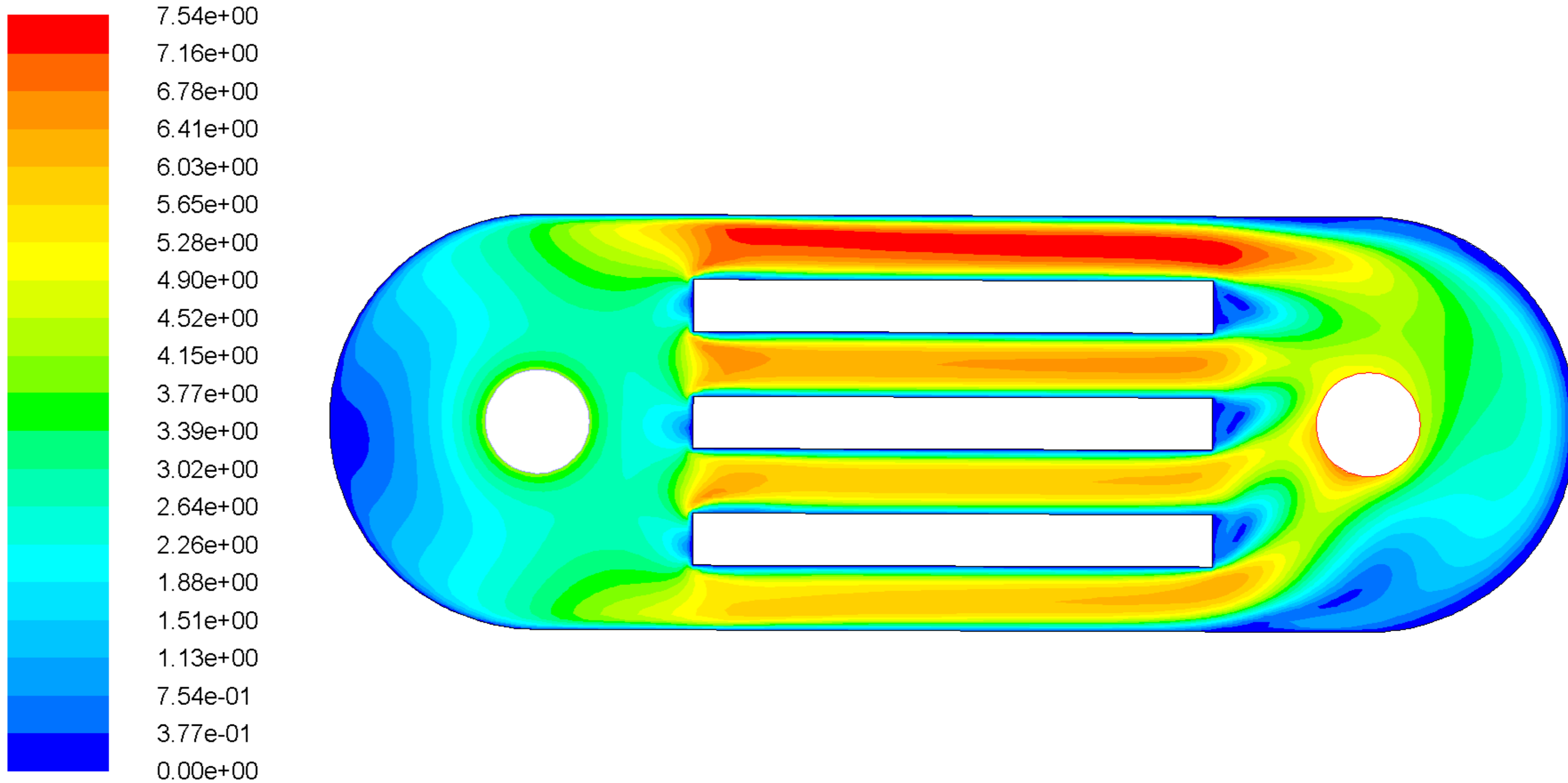
- Convergence: same computation with coupled solver. Obtain the same asymmetric solution much faster.



Post-processing

- Contours: velocity magnitude

Numerical Flow Simulation



Your work (optional):

- Perform the flow simulation using Fluent, varying the numerical method, physical model etc.
- Perform a detailed post-processing analysis of the solution.
- Analyze whether the initial assumptions are justified.
- Suggest improvements in fuel cell design.