Flow case 3: Fuel cell

Numerical Flow Simulation

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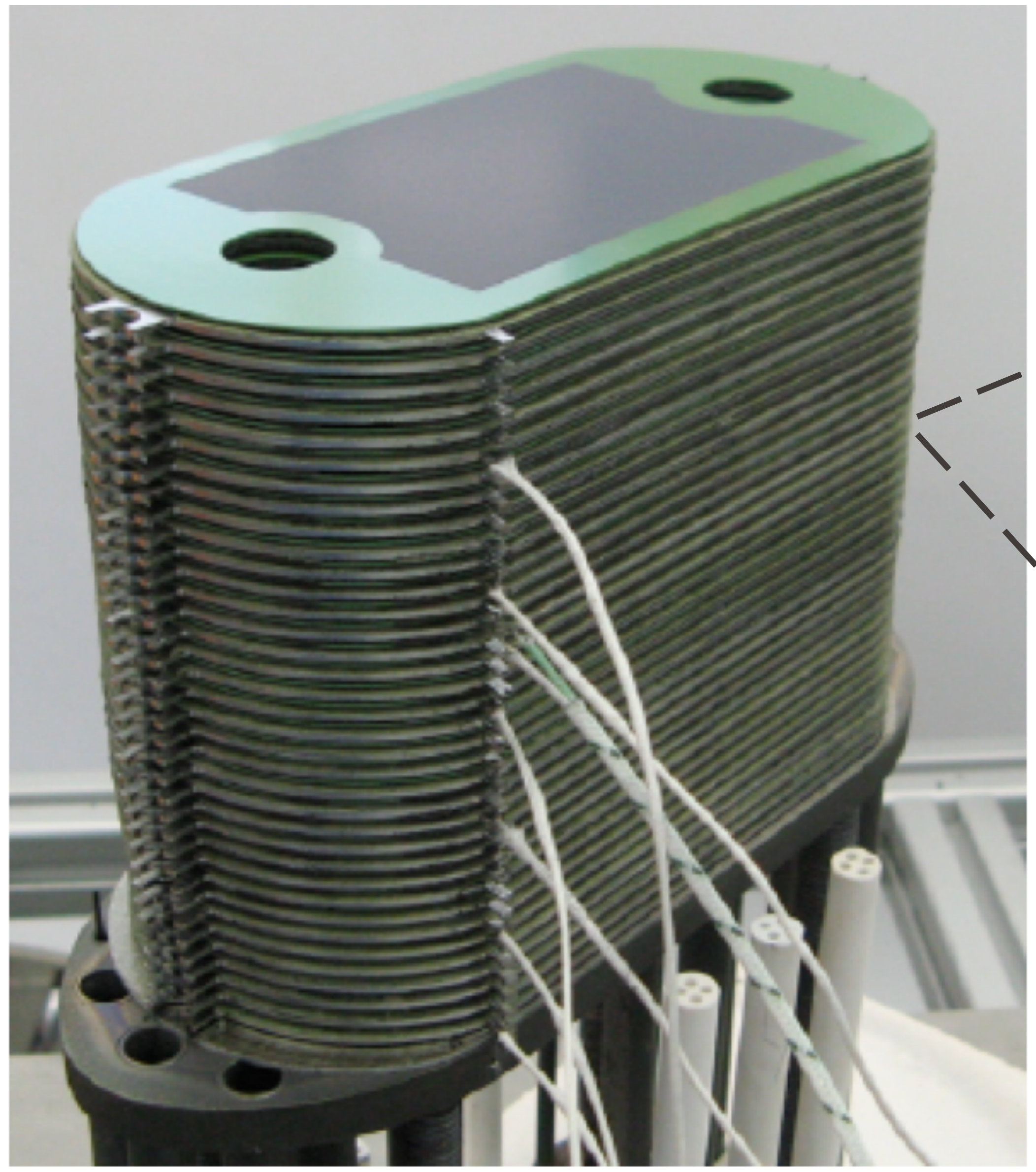
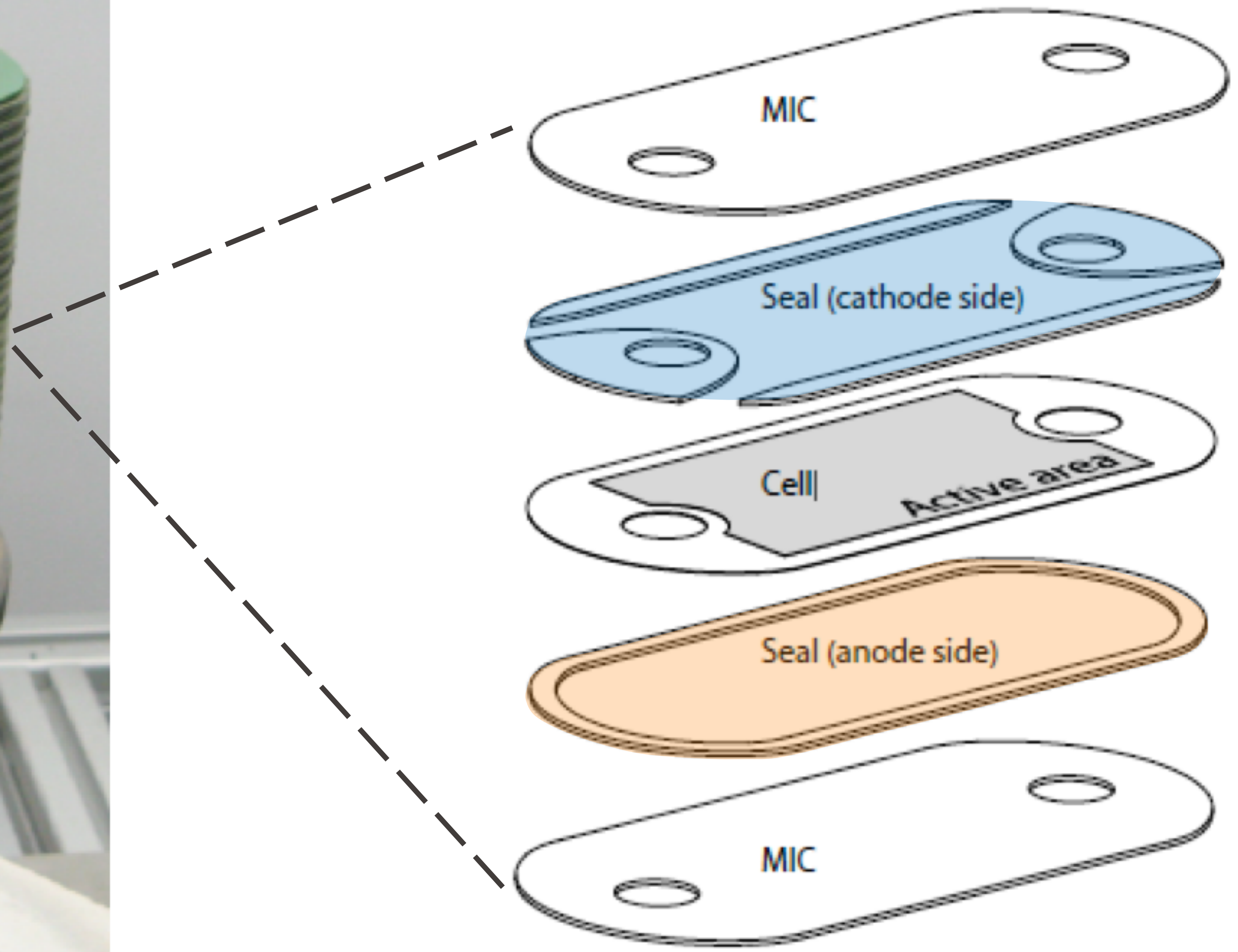
Physical problem

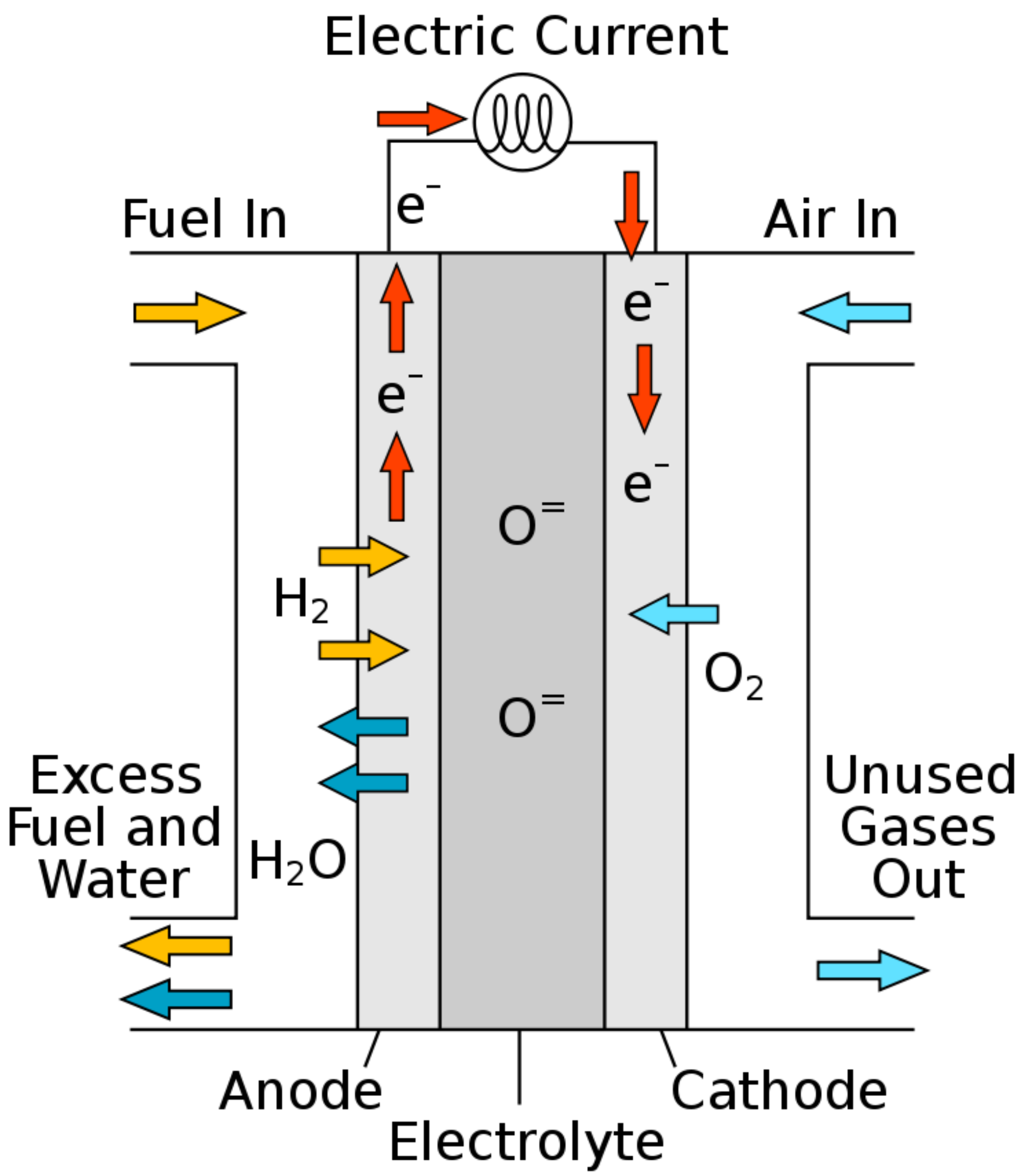
- A solid-oxide fuel cell is used to generate electrical power through the reaction of fuel (containing H_2) and air (containing O_2)
- Air is circulated across the cell to:
  - provide oxygen for the electrochemical reaction
  - dissipate the heat generated



Fuel cell stack



One cell module

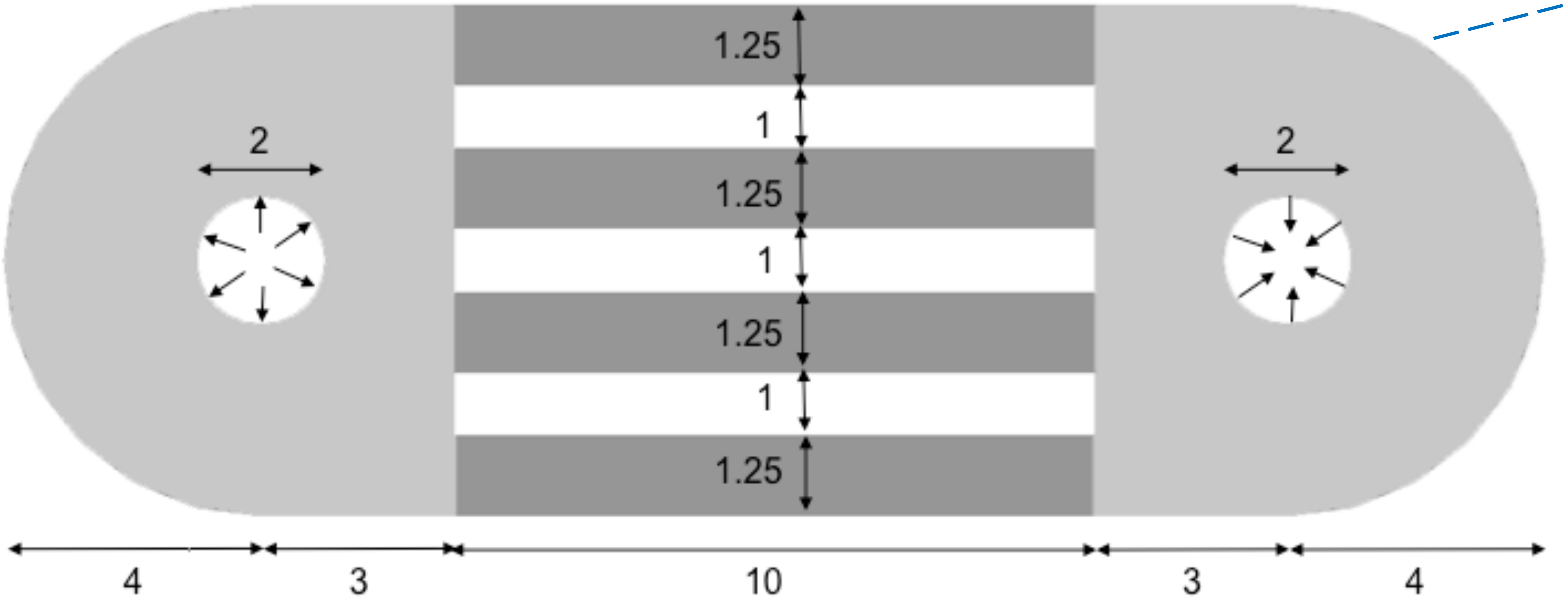


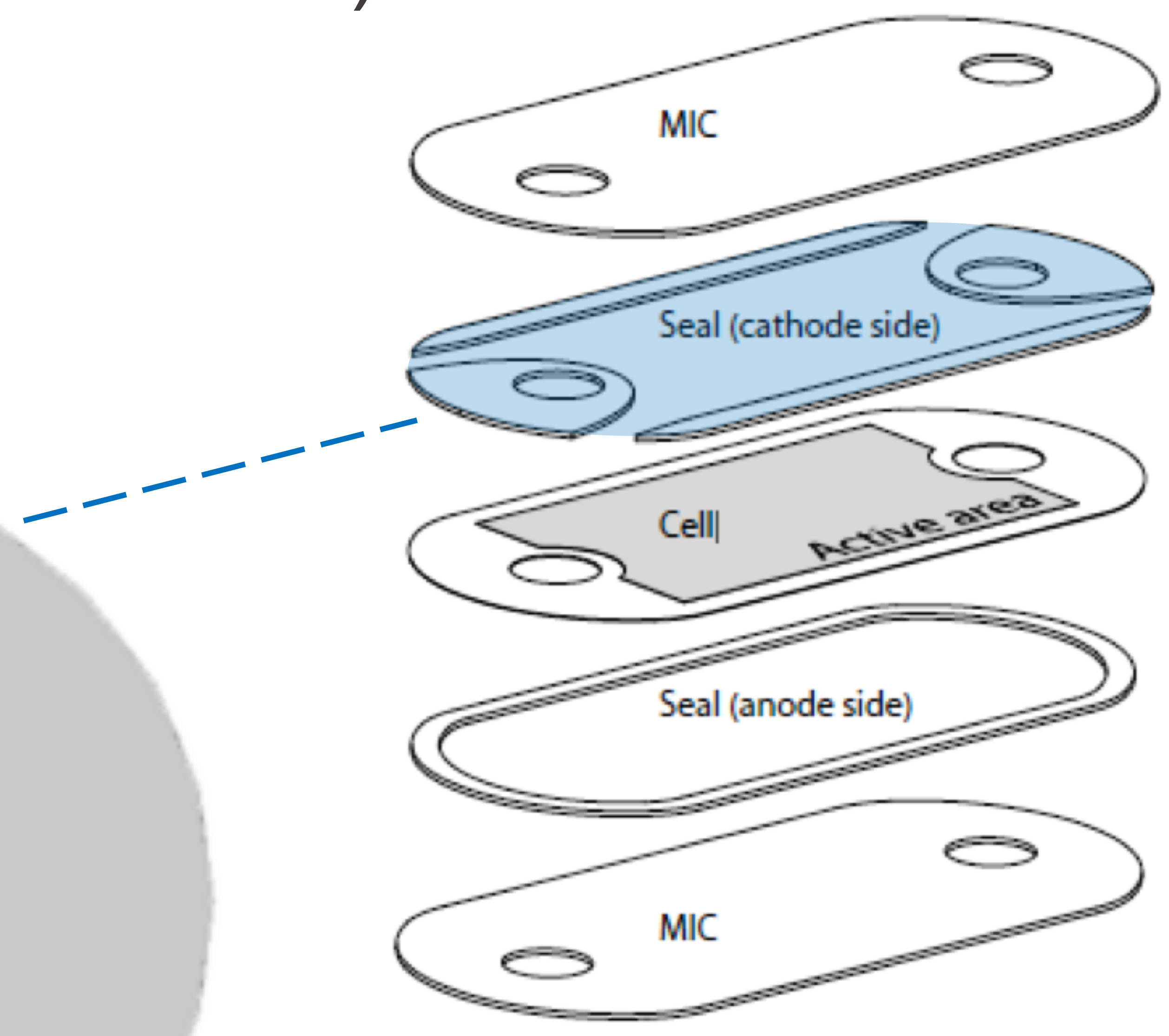
Physical problem

- 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)





Flow conditions

- Flow and thermal conditions:
  - uniform inflow velocity V = 4 m/s
  - inflow turbulence intensity 10%
  - inflow temperature T = 1000 K
  - uniform heat generation rate in 4 flow channels Q = 10 MW/m3
  - outer cell wall and sidewalls of 3 rectangular inserts assumed adiabatic

- Material properties (high-temperature air):
  - air density, $\rho = 0.34\ kg/m^3$
  - dynamic viscosity, $\mu = 4.30 \times 10^{-5}$ Pa s
  - specific heat capacity at constant pressure, $C_p = 1145$ J/kg K
  - thermal conductivity, $k = 0.068$ 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 (thickness $\delta \sim x/Re^{1/2}$)

      → choice of boundary-layer mesh, and wall treatment for turbulence model
  - Mach number
    - $M_\infty = V/c = V/(\gamma RT/M_{air})^{1/2} = 0.006 \ll 1$ (γ = 1.4, R = 8.314 J/(mol.K), M_{air} = 0.029 kg/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 = momentum diffusivity / thermal diffusivity = $\mu/(k/C_p)$ = 0.74
    - Thermal boundary layer, $\delta_t \sim \delta/Pr^{-1/3} \sim 1.1\delta$

      → thermal boundary layer as thin as velocity boundary layer

  - Brinkman number
    - Br = heat produced by viscous dissipation / 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 = convective heat transfer / conductive heat transfer

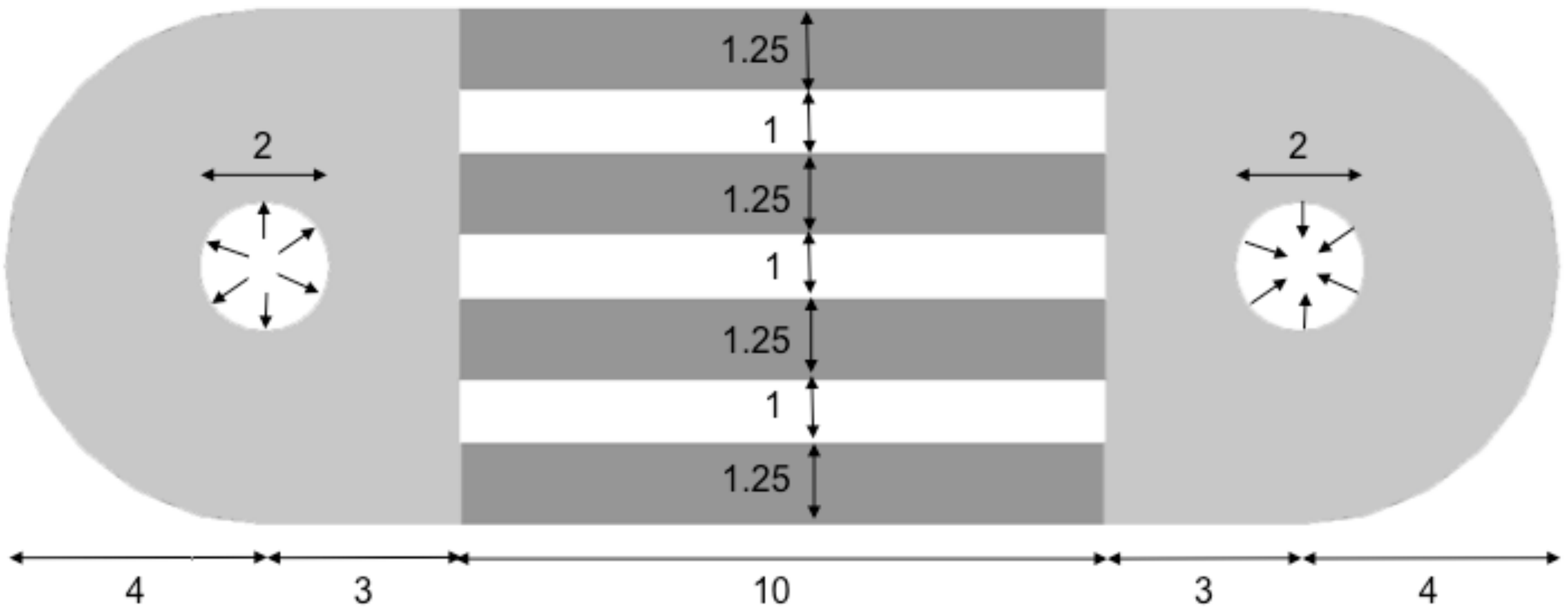
      = $h/(k/L)$ (with $h = Q/\Delta T$ the heat transfer coefficient) >> 1

      → 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



Numerical Flow Simulation

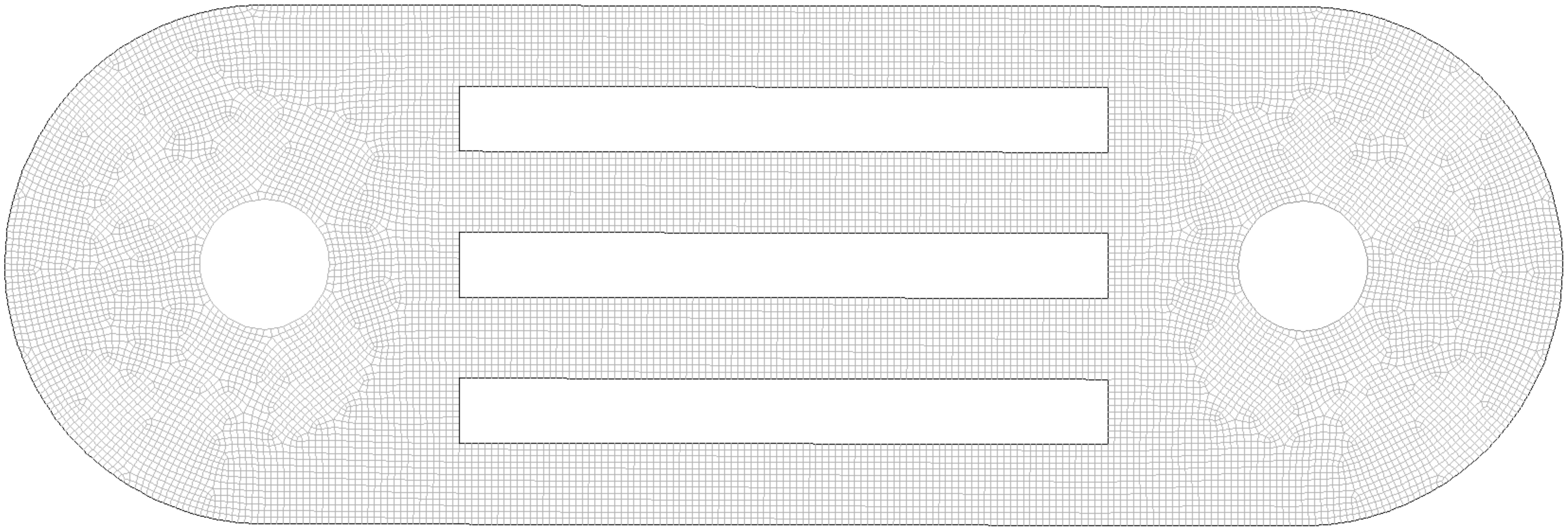
Pre-processing

- 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

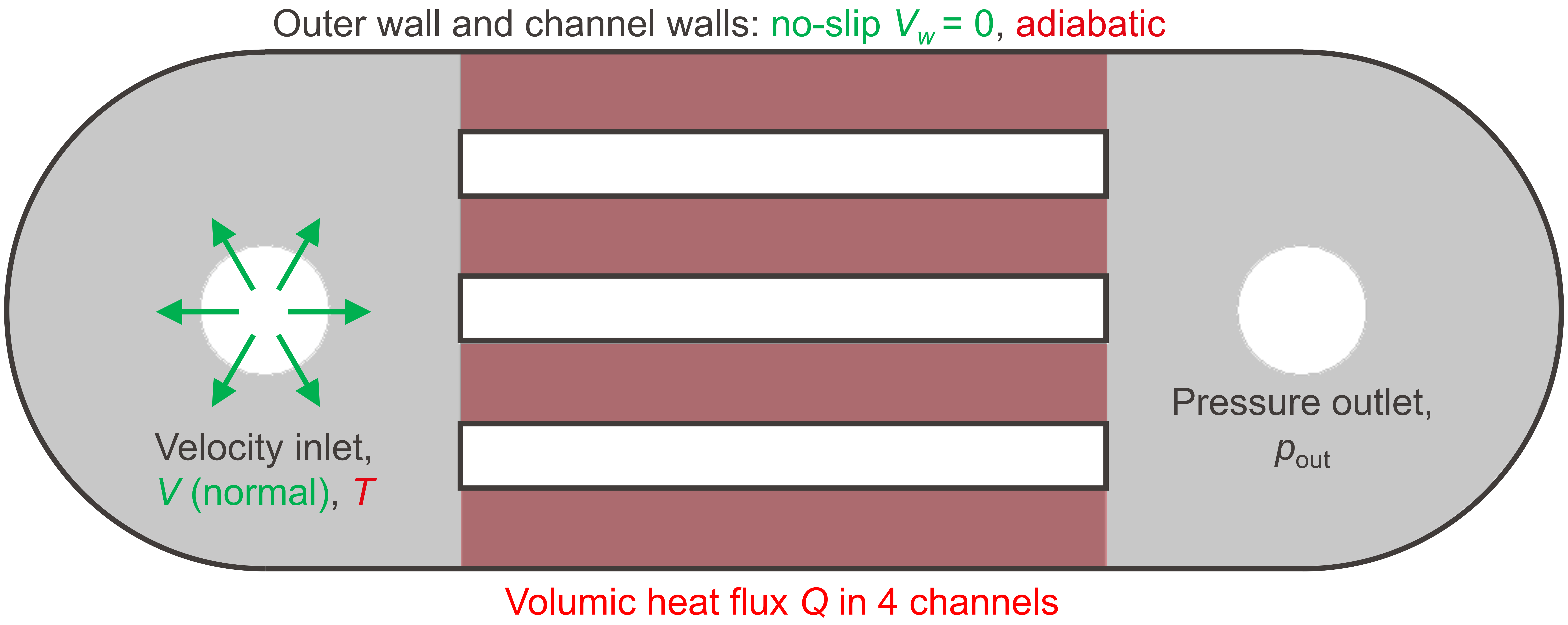
- Physical models
  - Ideal gas law, high-temperature air properties

  - k-ε turbulence model
    - RNG k-ε (realizable also possible; RNG may be suitable)
    - Enhanced wall treatment (two-layer model) (thick boundary layer → can afford $y^+ = O(1)$)
    - Neglect viscous heating (Brinkman number << 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

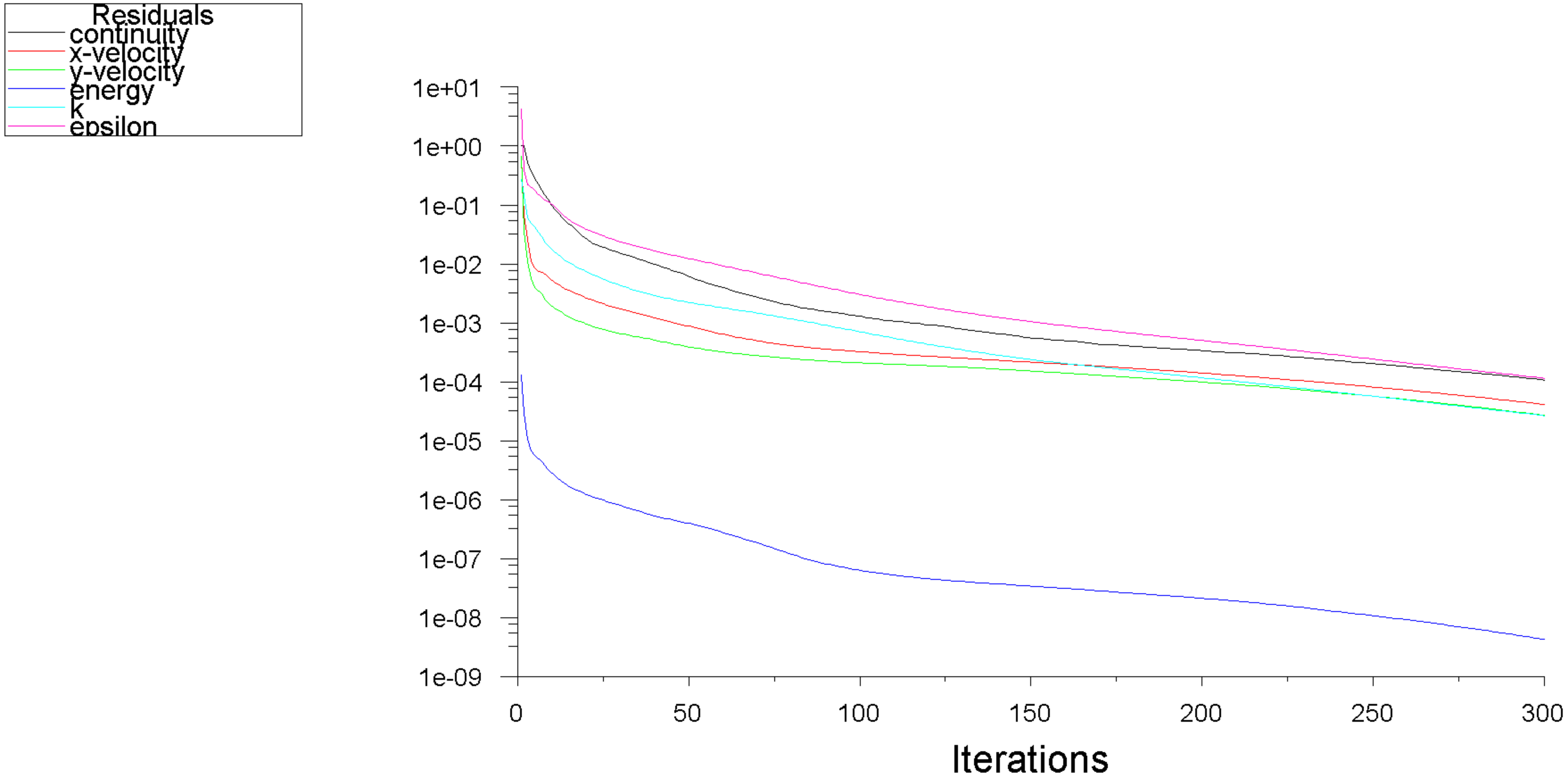
Solver set-up

- Boundary conditions (flow + thermal):



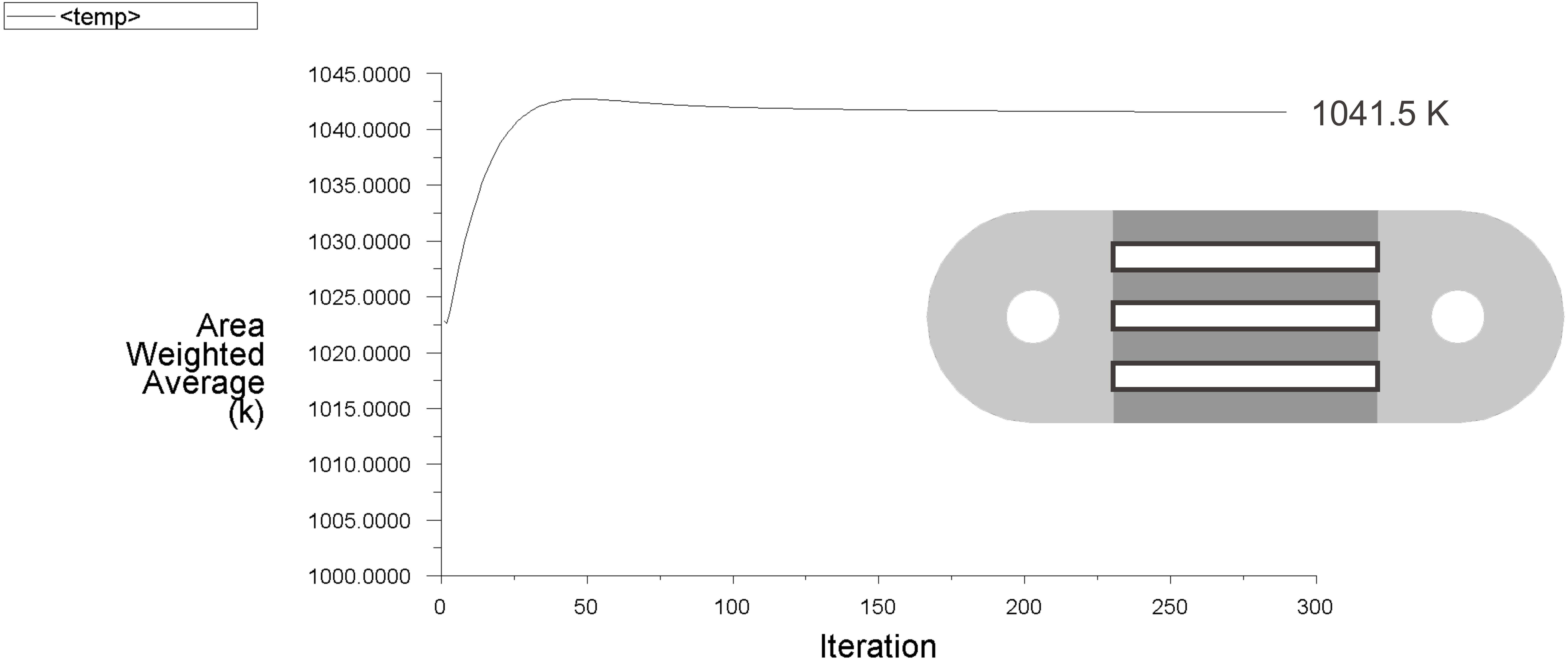
Solver procedure

- Convergence: residuals



Solver procedure

- Convergence: average temperature on channel walls



Solver procedure

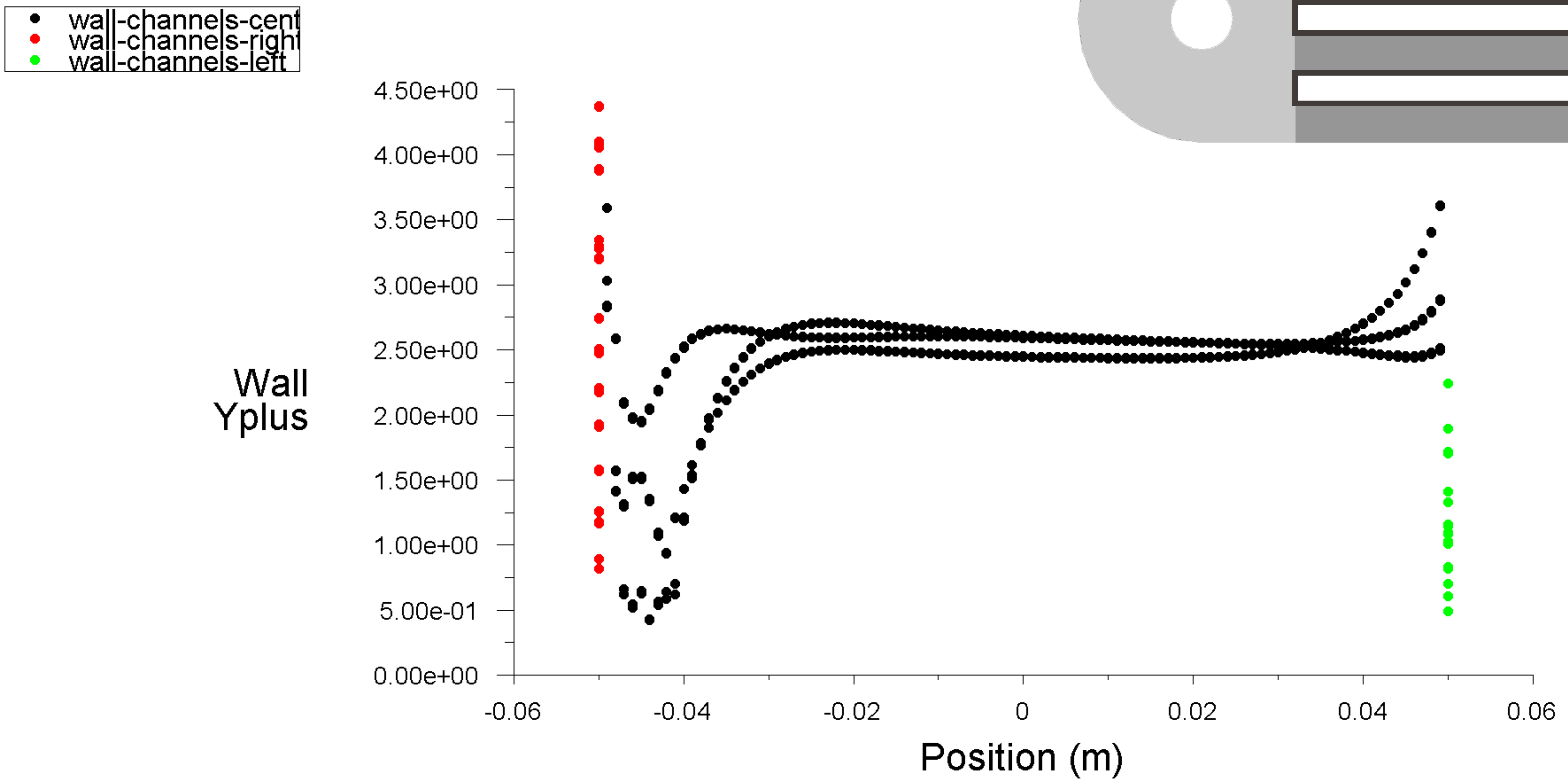
- Convergence: mass conservation
  - Require net mass flux between inlet and outlet to be conserved to < 0.2 %

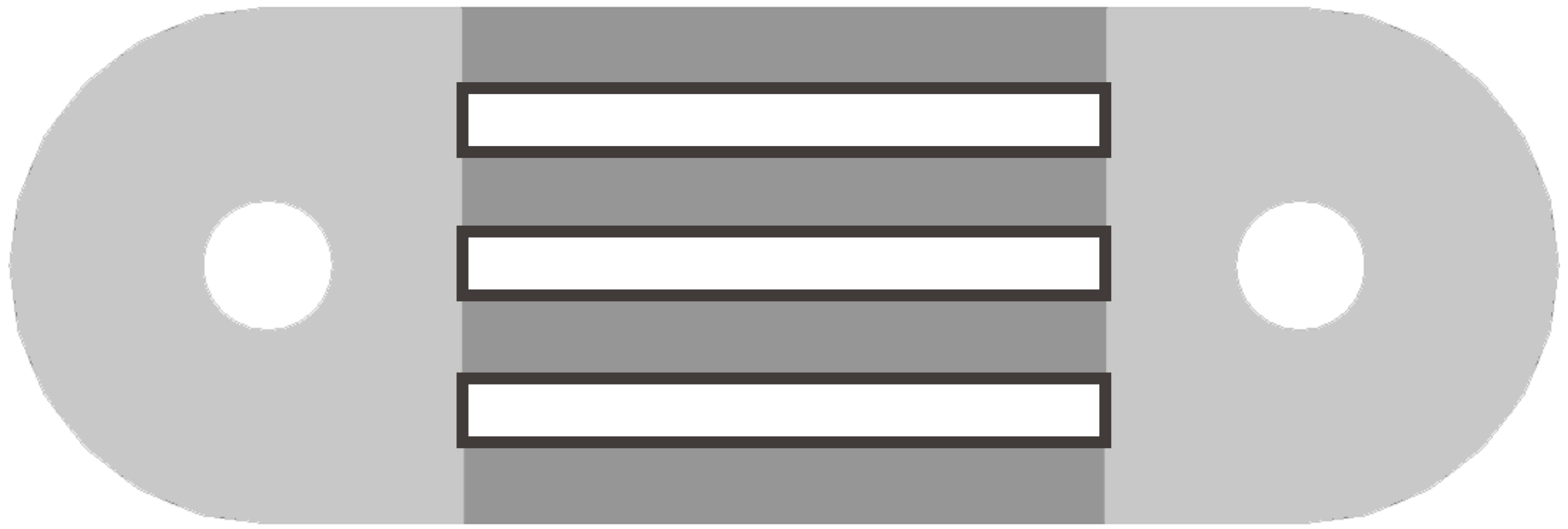
Mass flow rate [kg/s]	
Inlet	0.0854170
Outlet	-0.0854169
Net imbalance	**5.2×10^{-8} (6×10^{-5} %)**

  - Mass conservation satisfied for this solution.

Post-processing

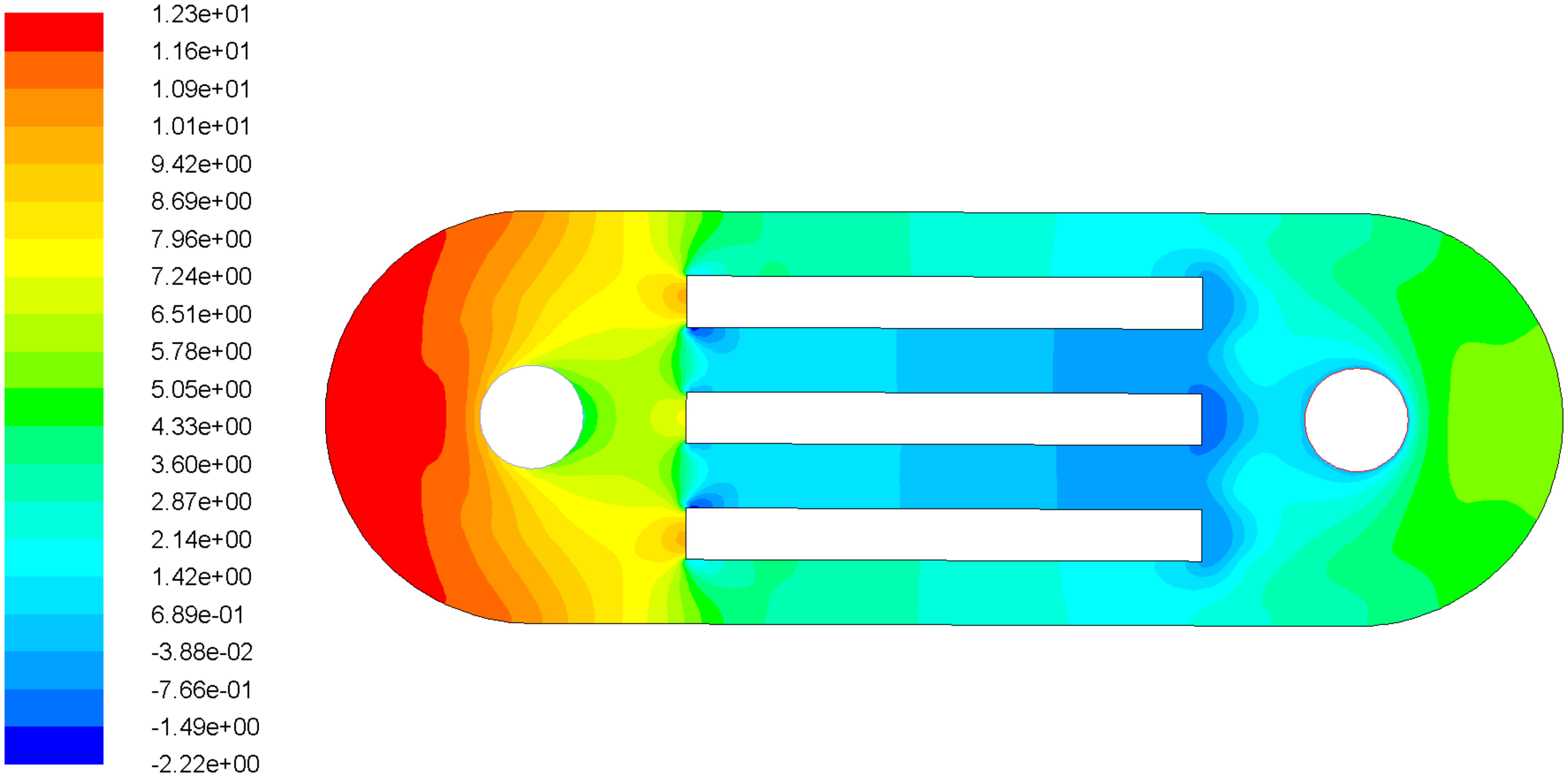
- Control: first-cell y^+ along channels





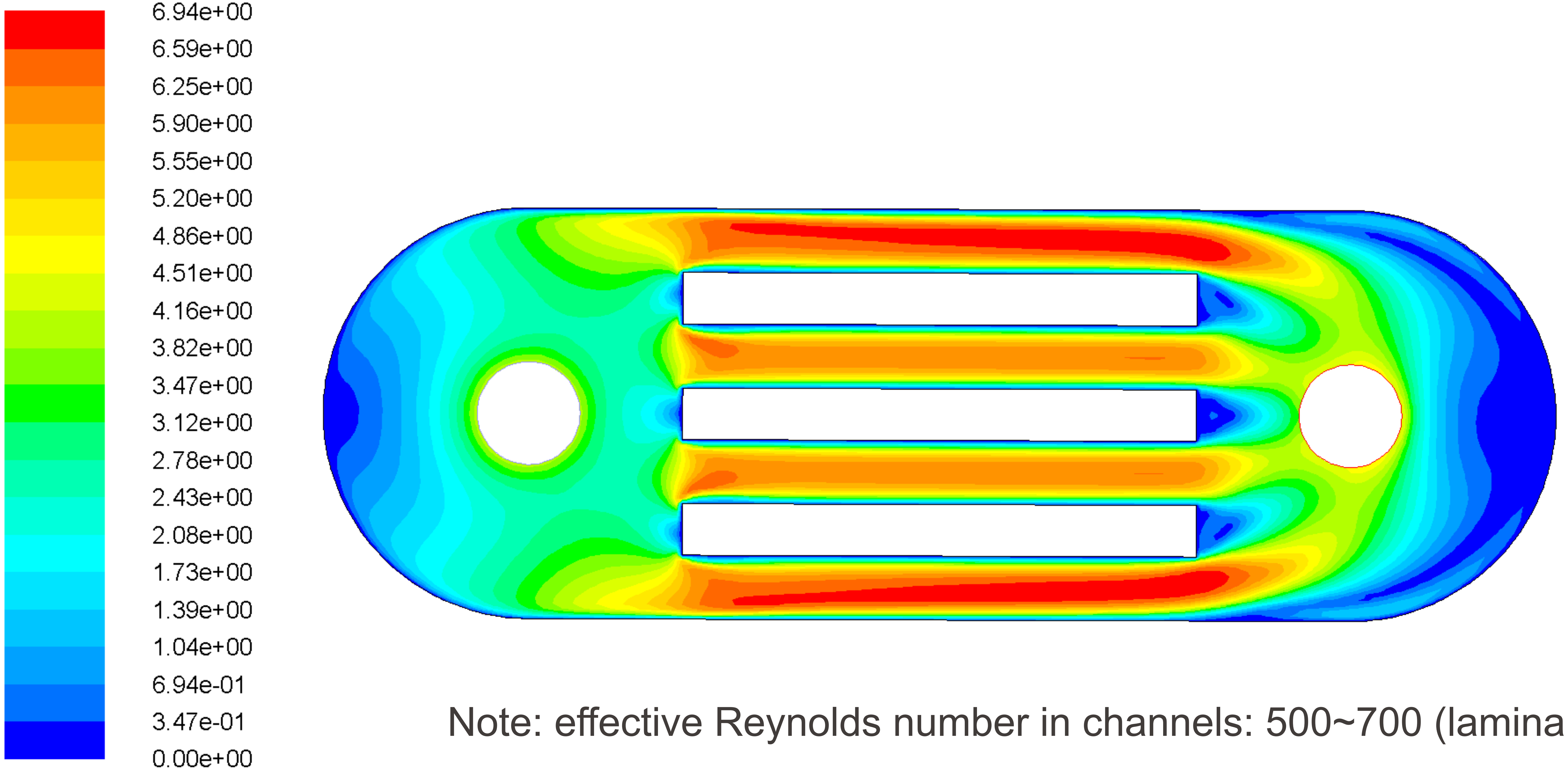
Post-processing

- Contours: pressure



Post-processing

- Contours: velocity magnitude

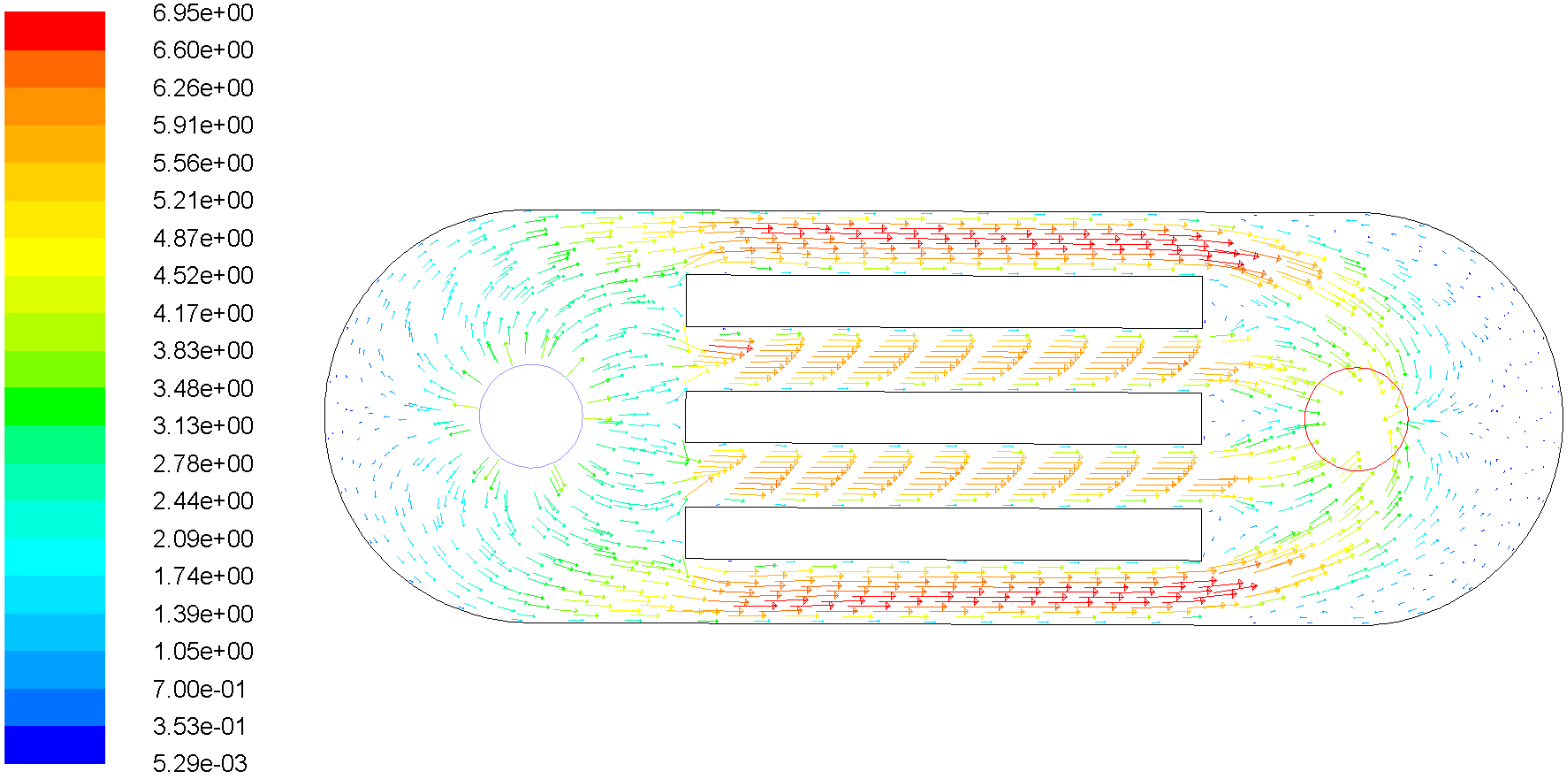


Note: effective Reynolds number in channels: 500~700 (laminar)

Numerical Flow Simulation

Post-processing

- Velocity vectors

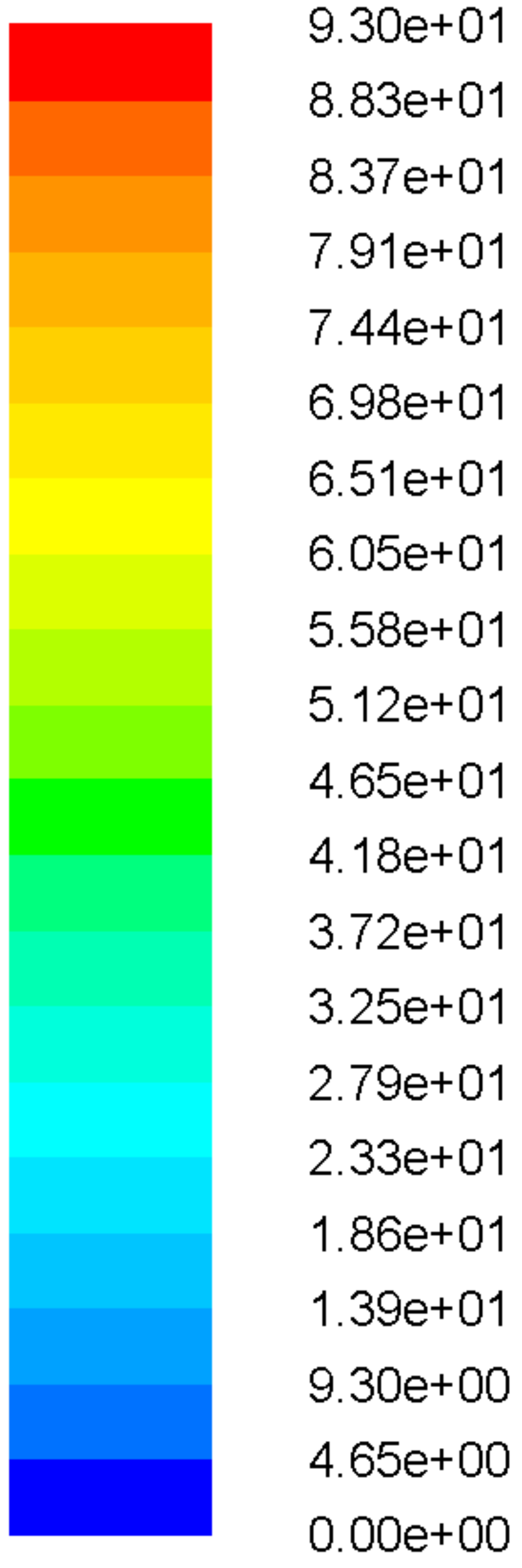


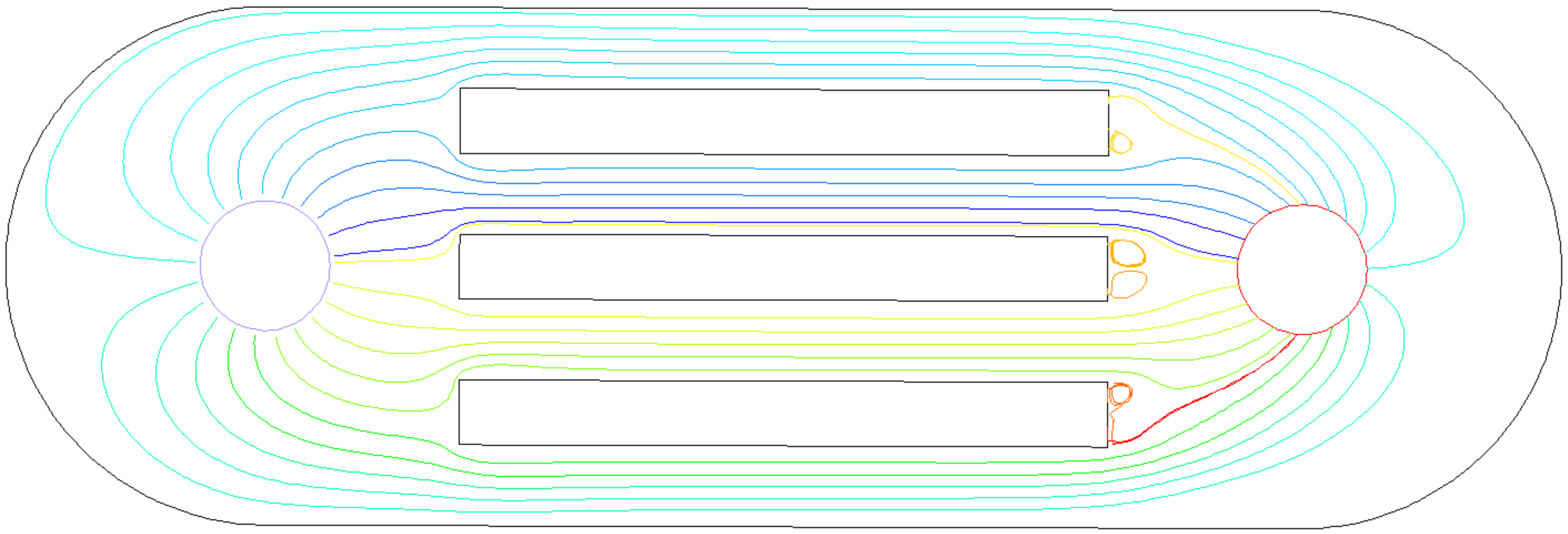
Numerical Flow Simulation

Post-processing

- Streamlines

Numerical Flow Simulation

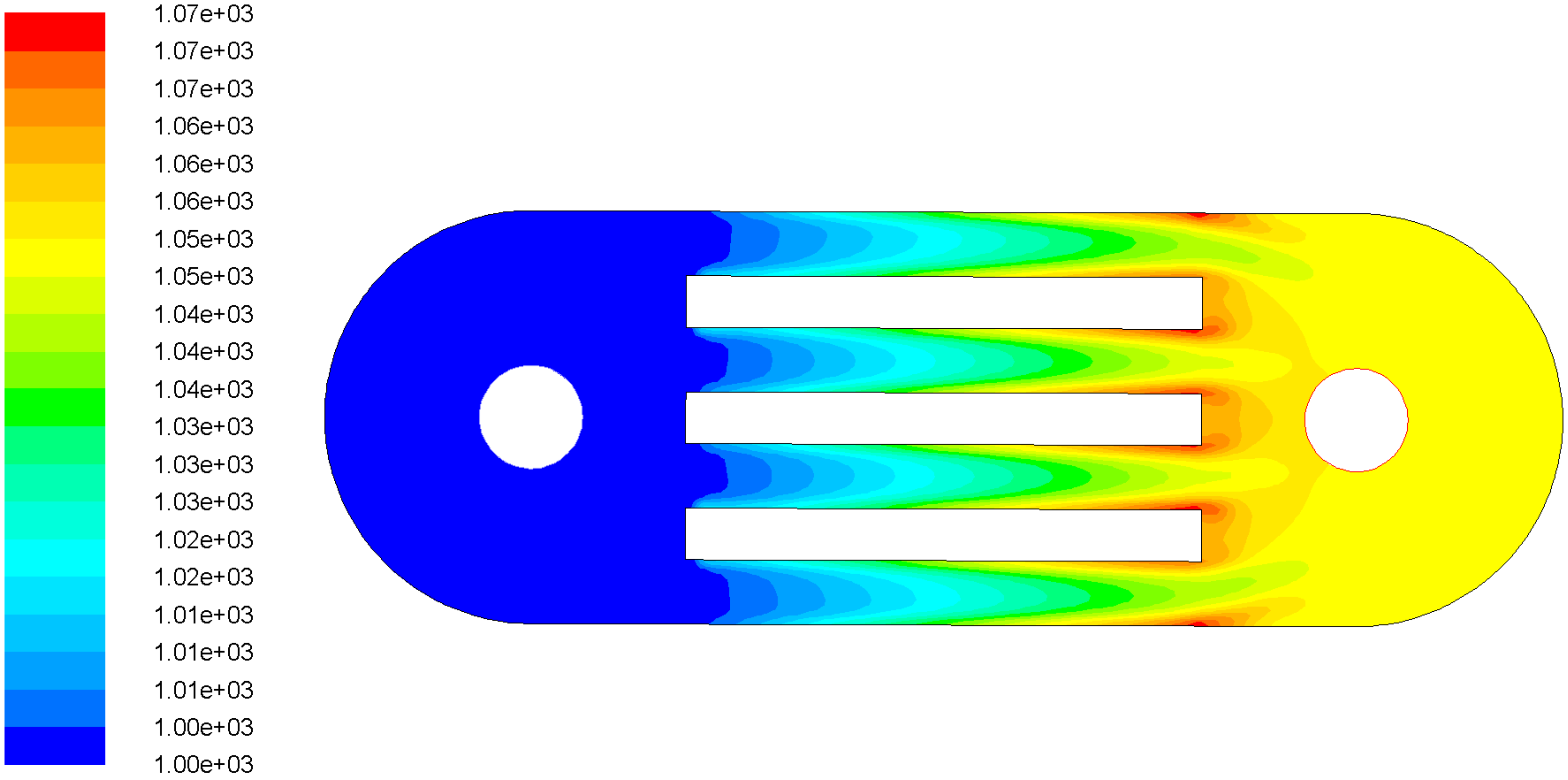




Flow attached in channels; separation at sharp edge downstream

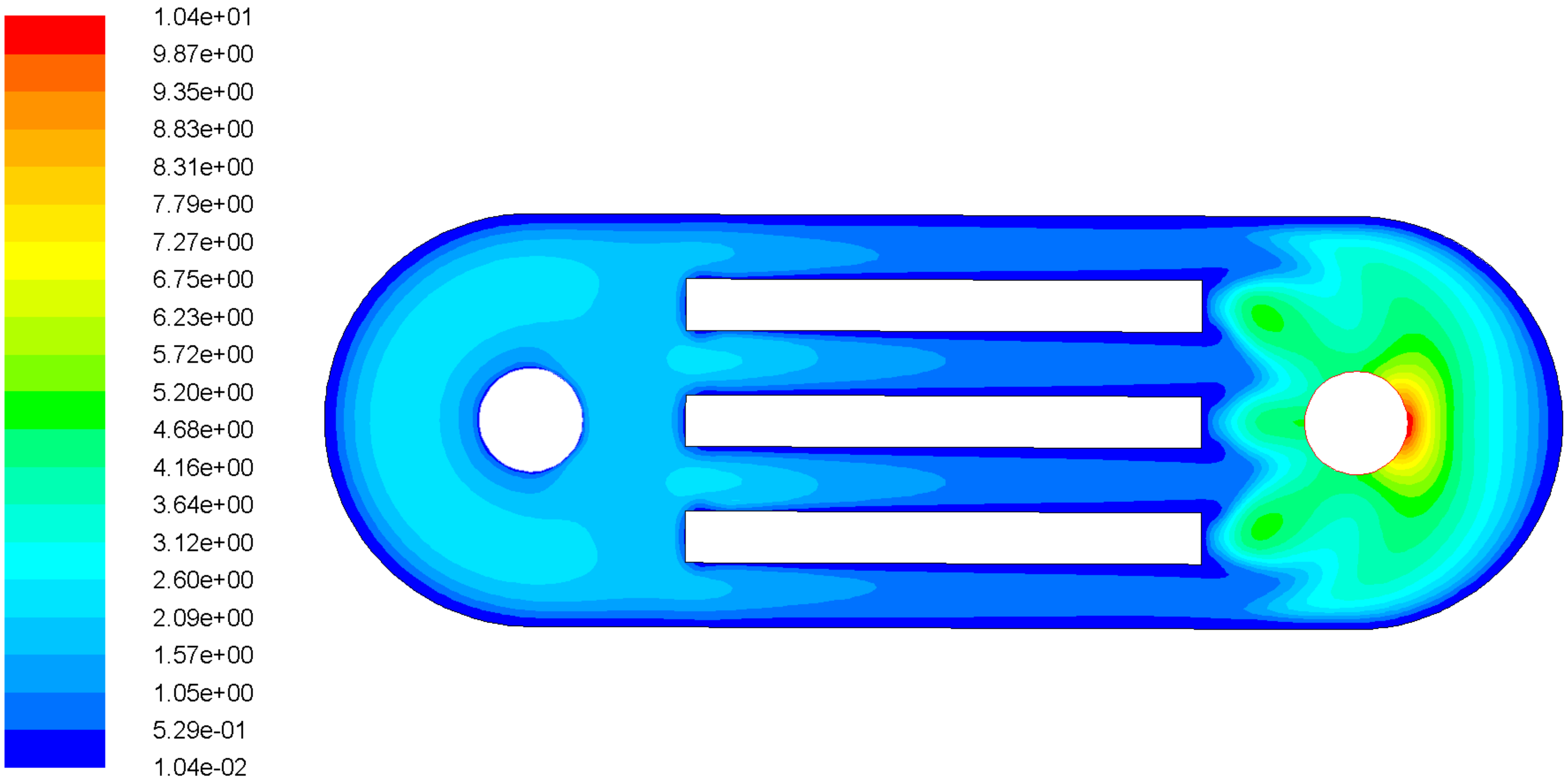
Post-processing

- Contours: temperature



Post-processing

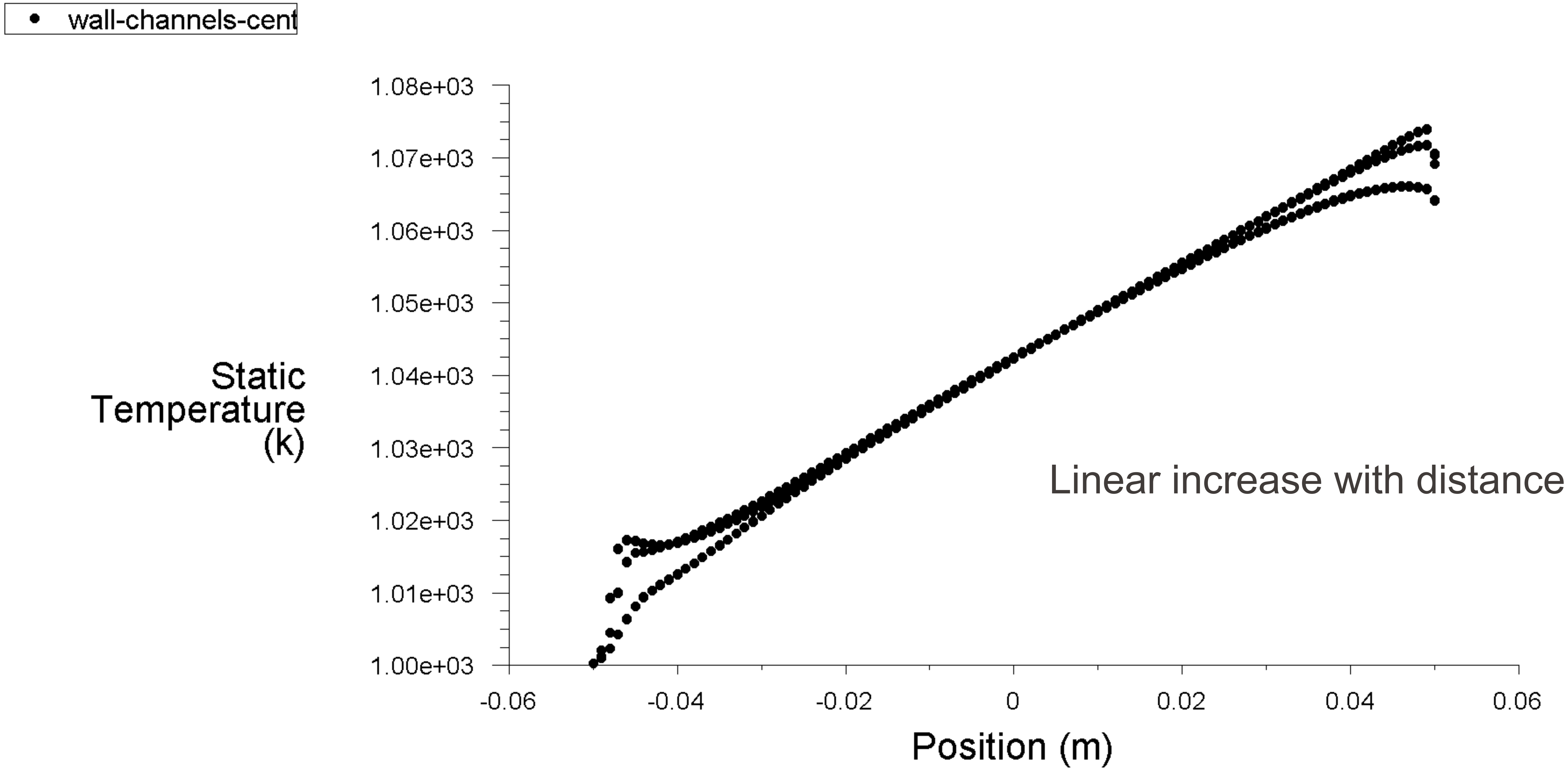
- Contours: turbulent kinetic energy *k*



Numerical Flow Simulation

Post-processing

- Temperature on channel surfaces



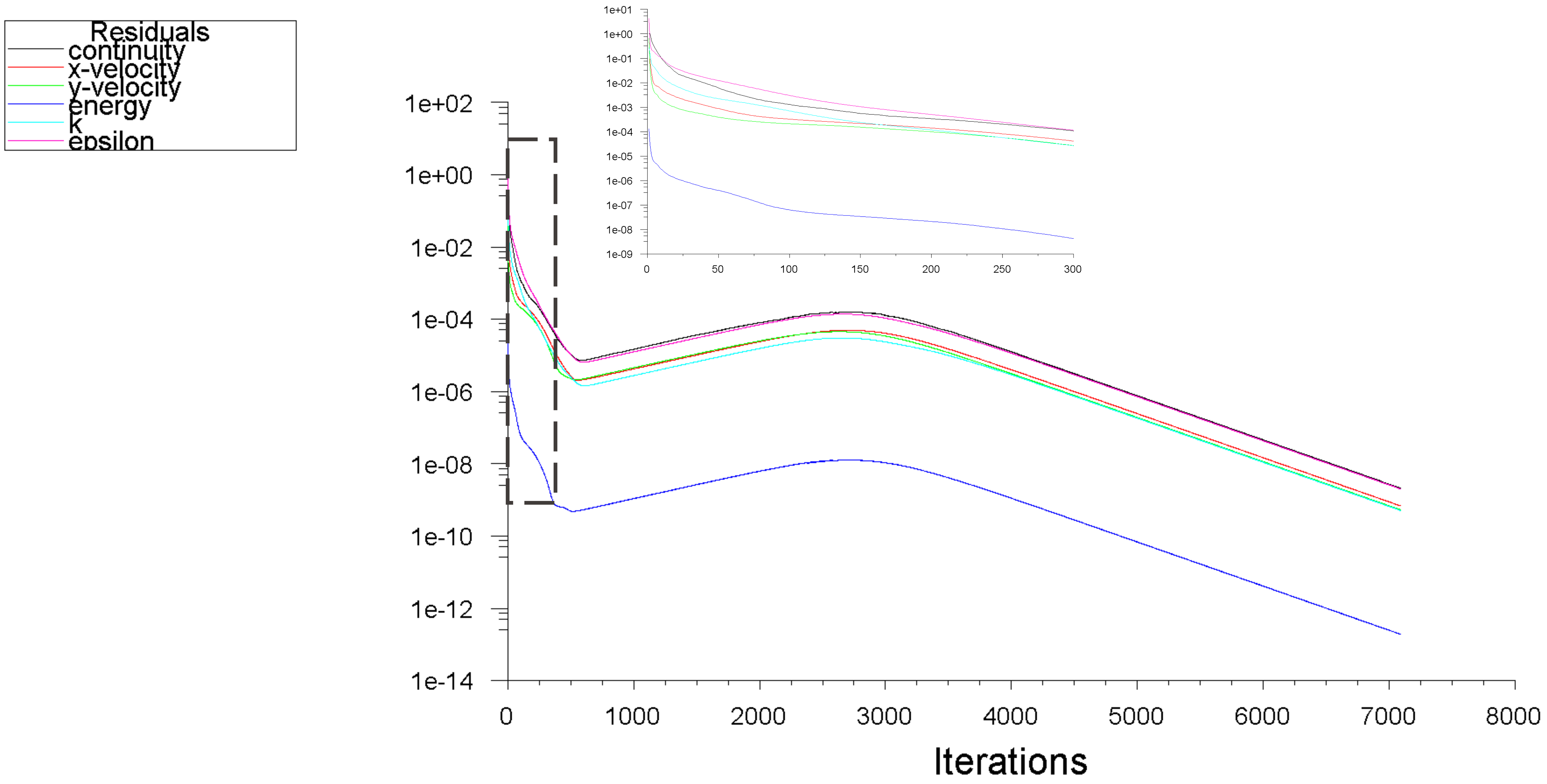
Linear increase with distance.

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…

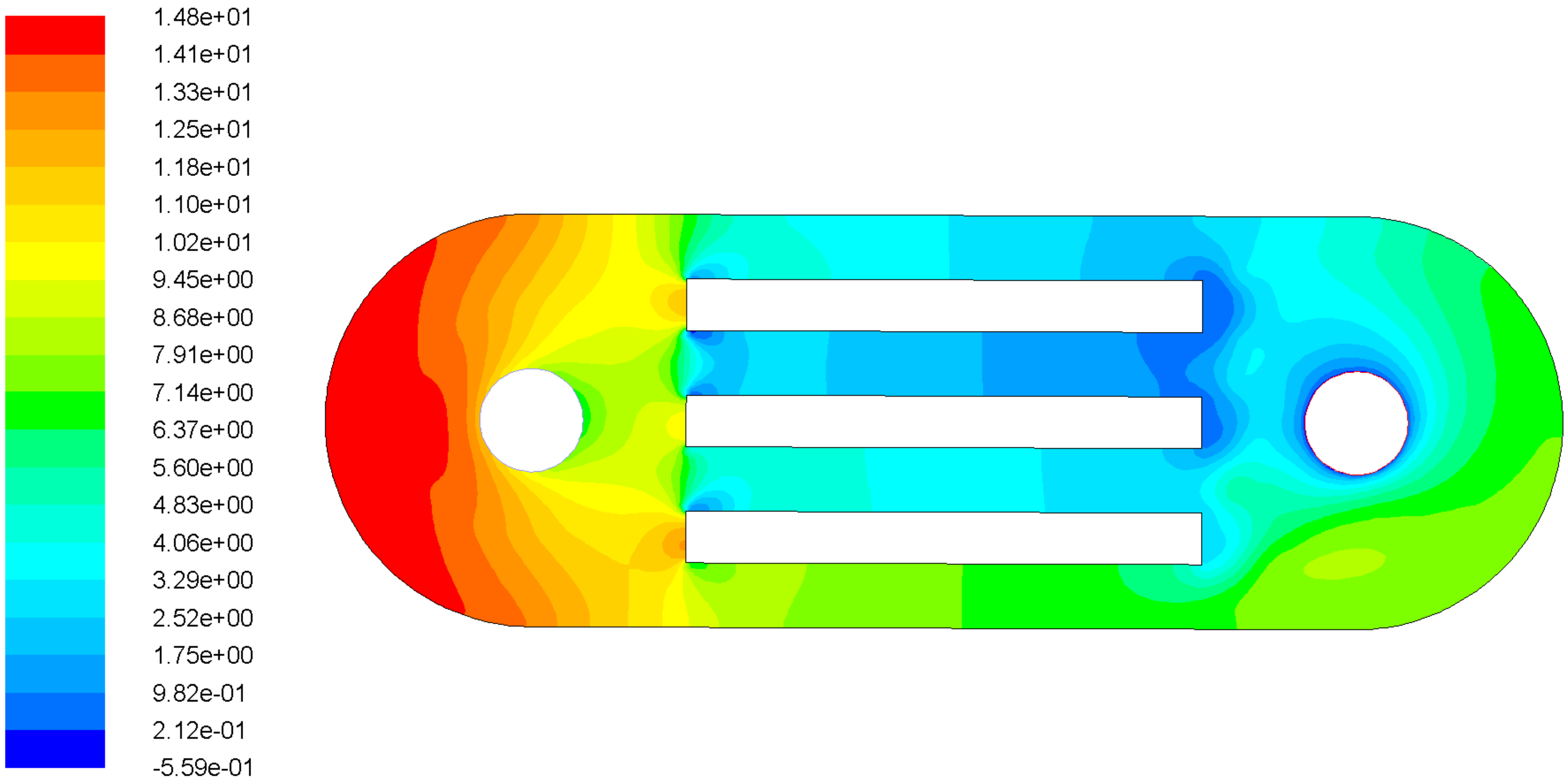
Solver procedure

- Convergence: further iterations reveal a second solution



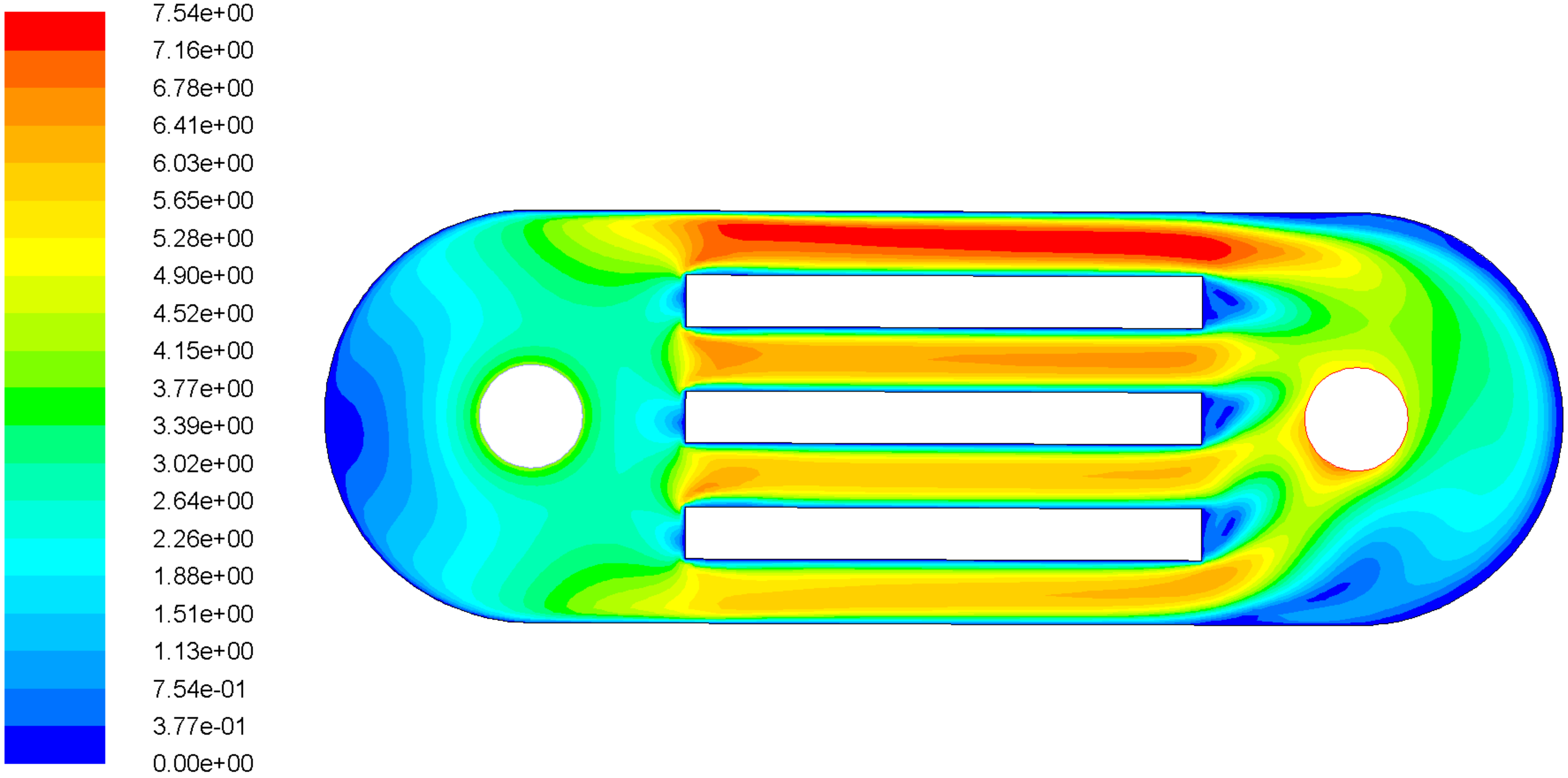
Post-processing

- Contours: pressure



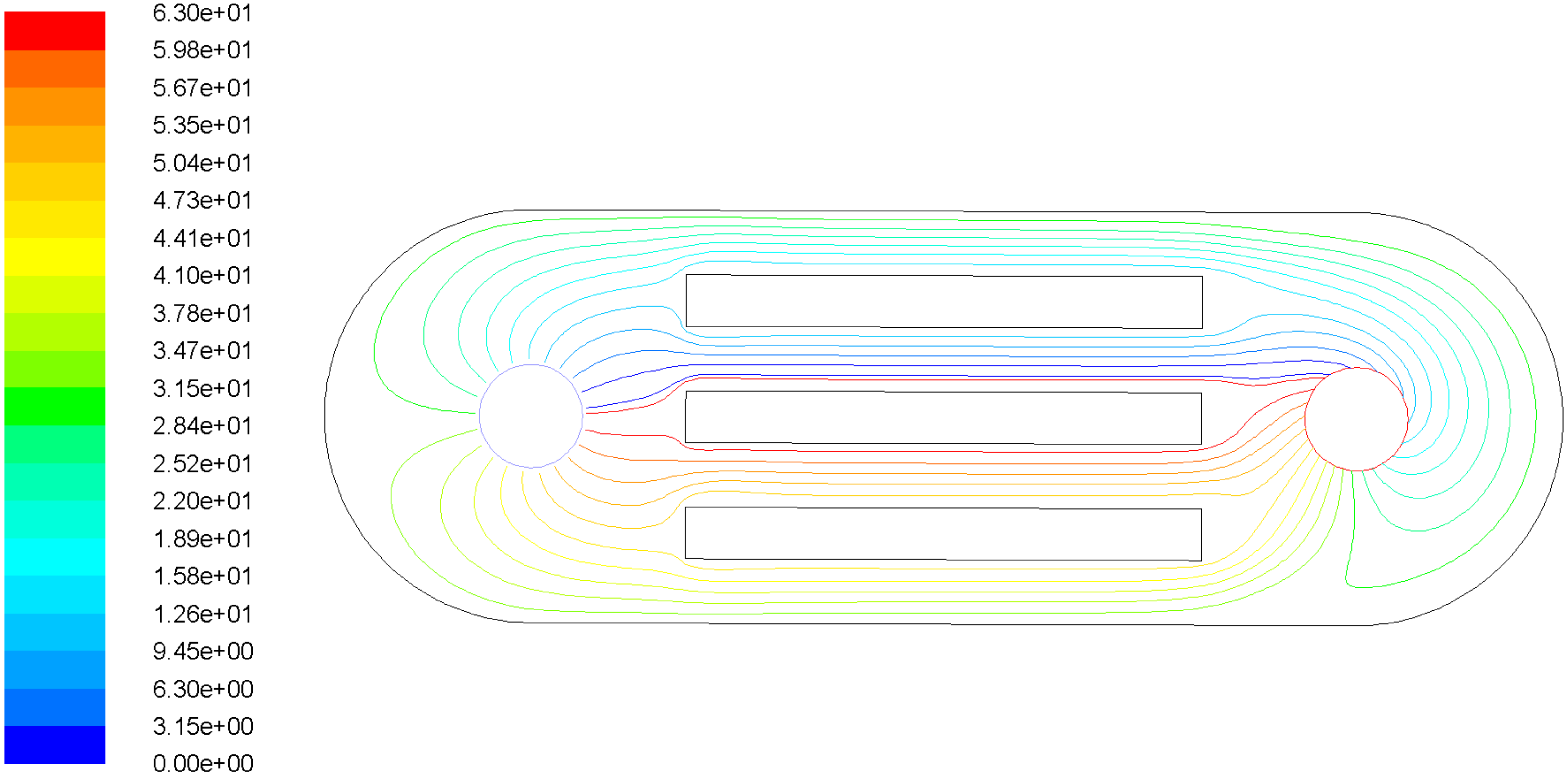
Post-processing

- Contours: velocity magnitude



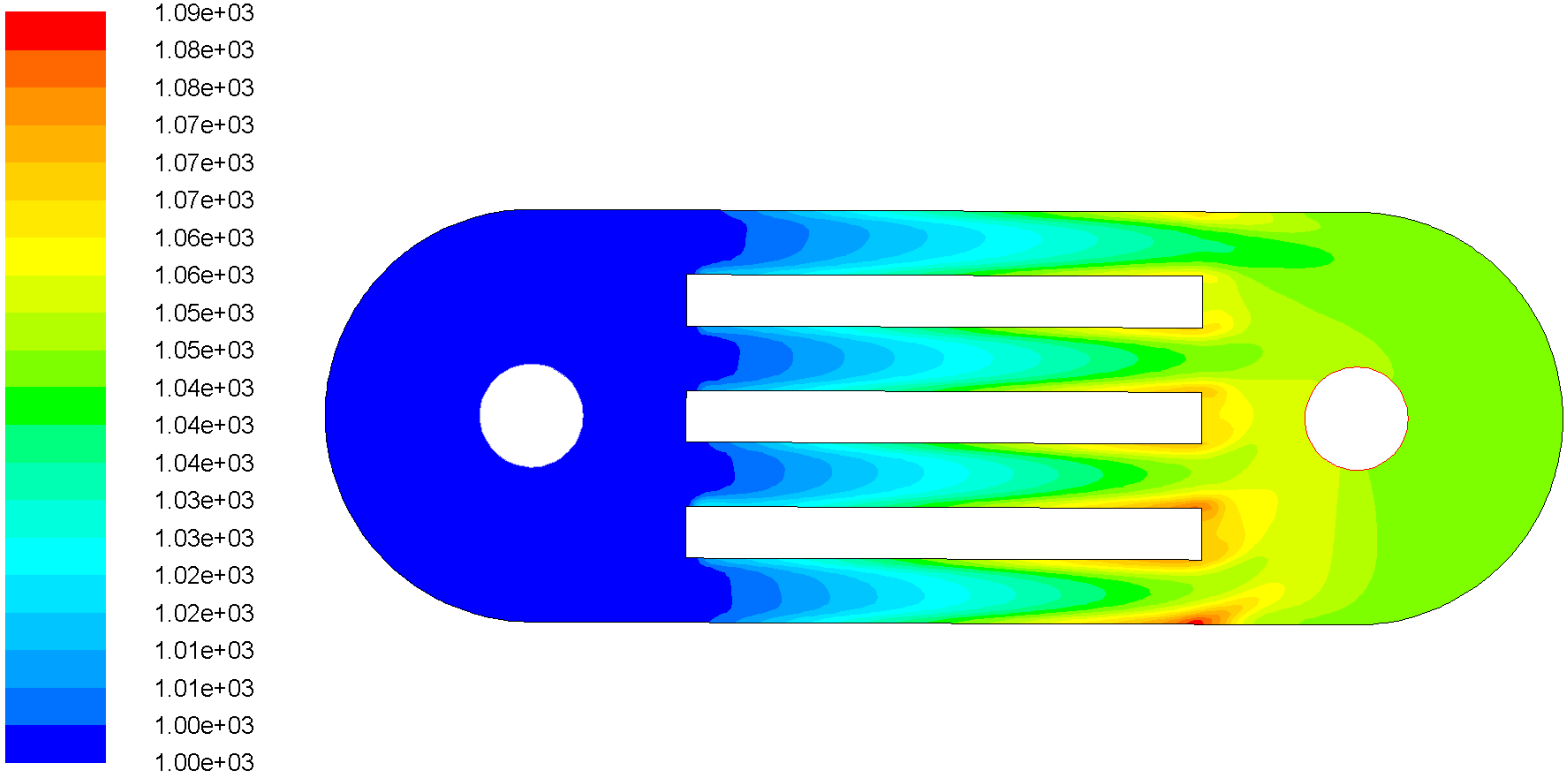
Post-processing

- Streamlines



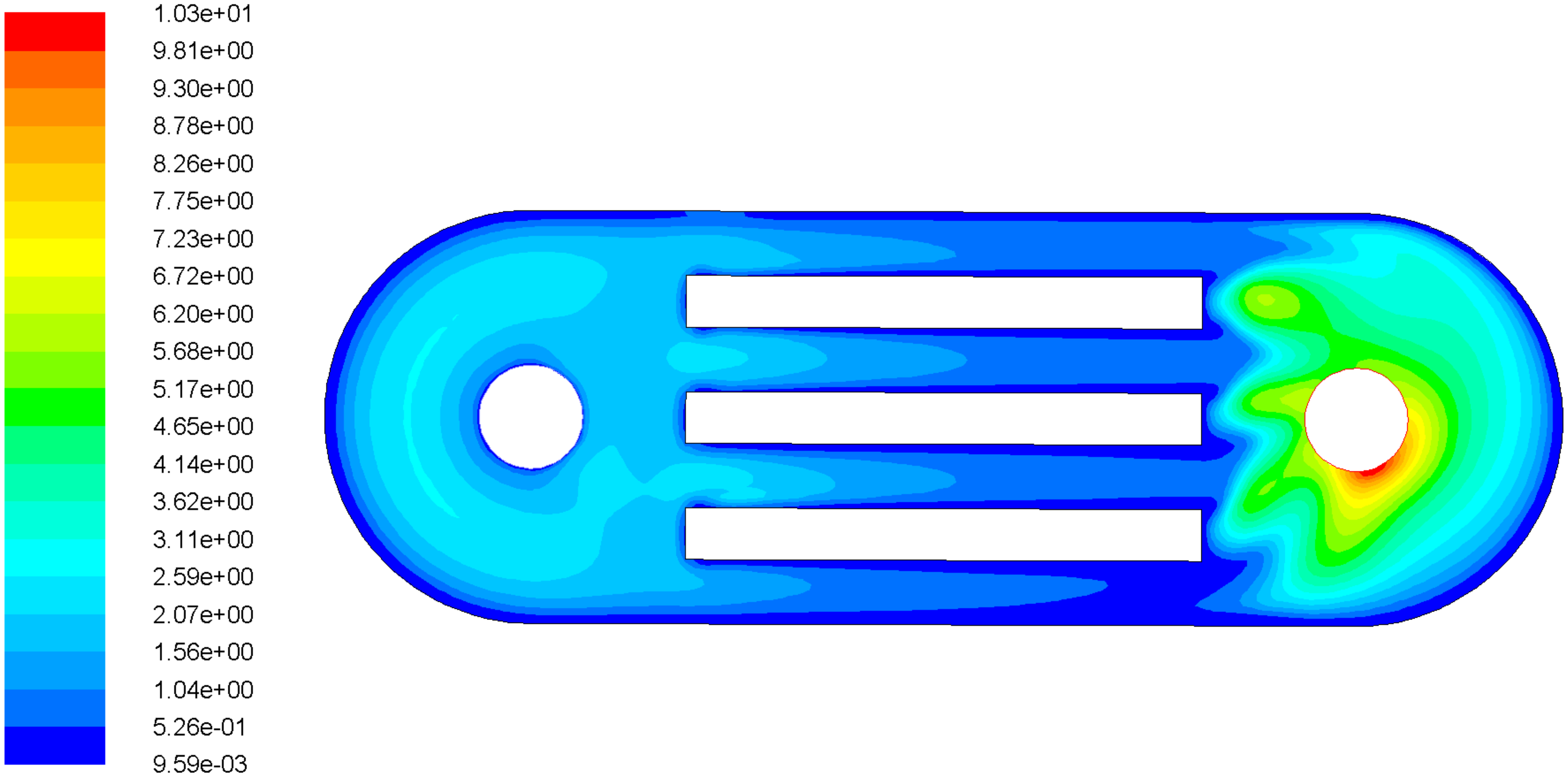
Post-processing

- Contours: temperature



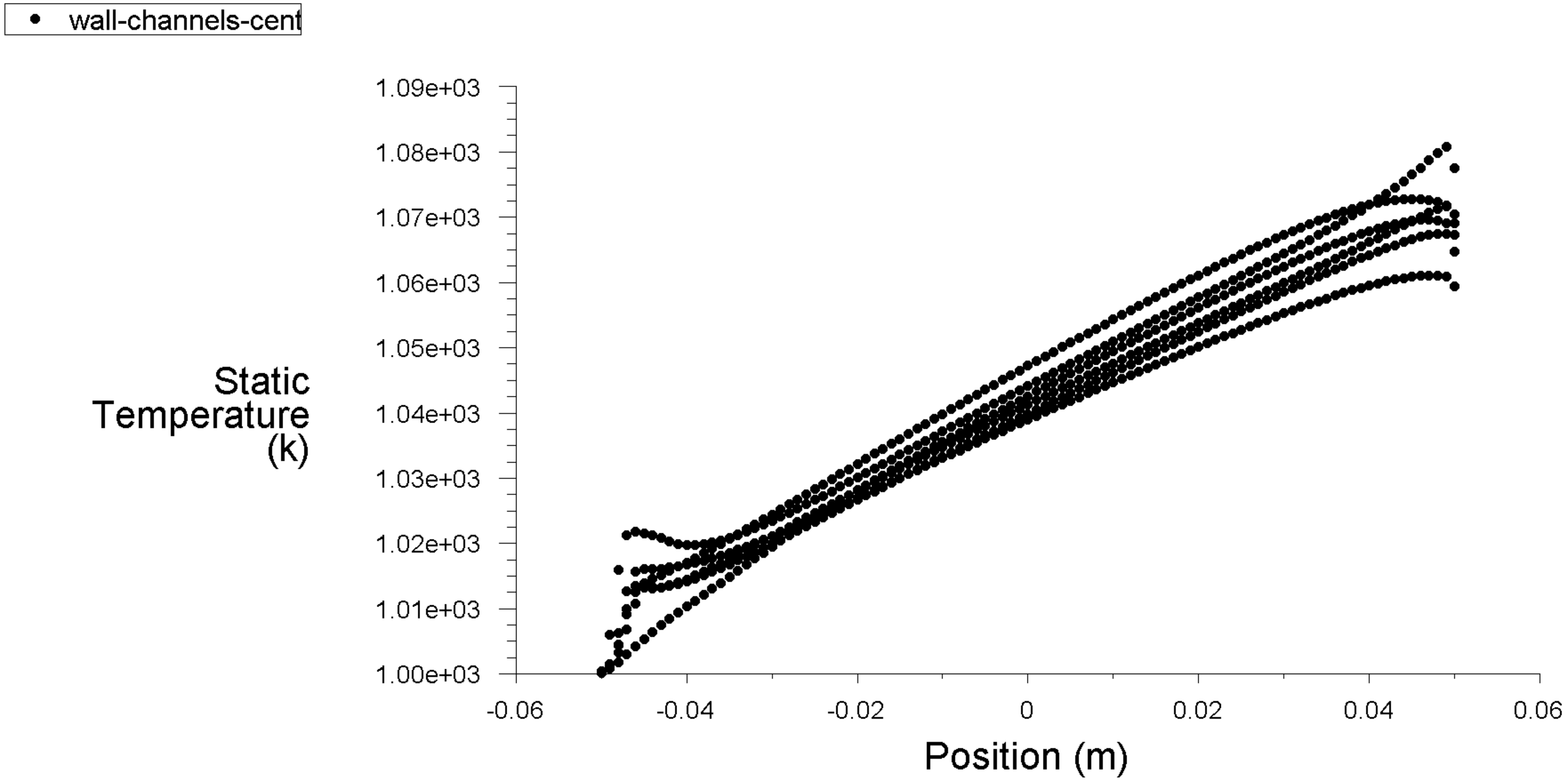
Post-processing

- Contours: turbulent kinetic energy *k*



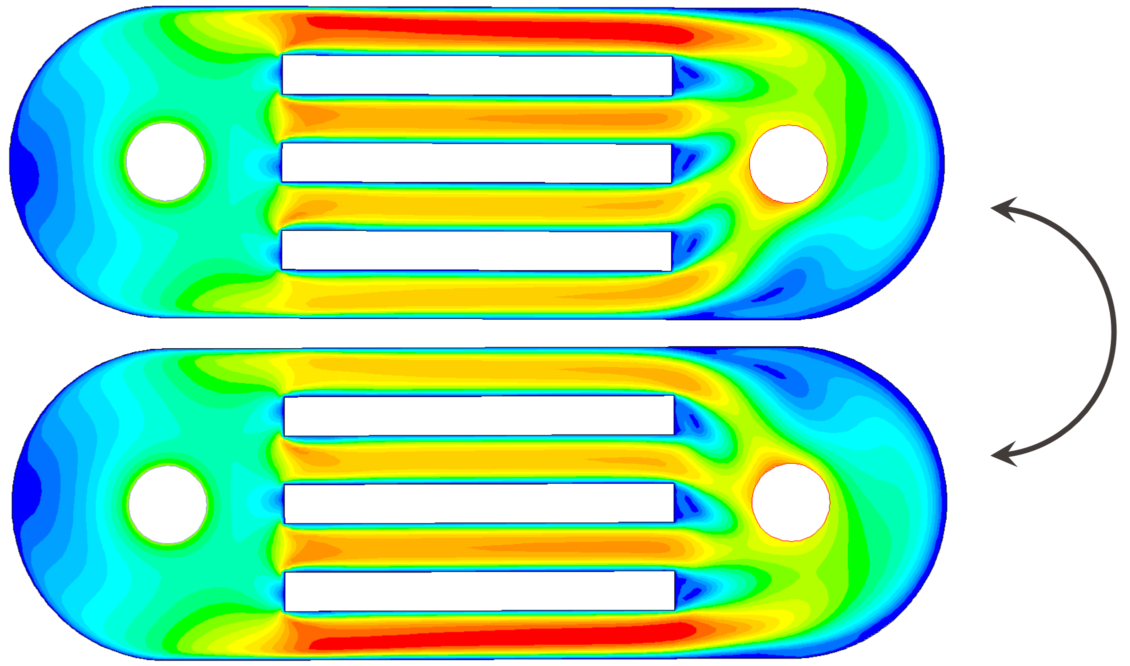
Post-processing

- Temperature on channel surfaces



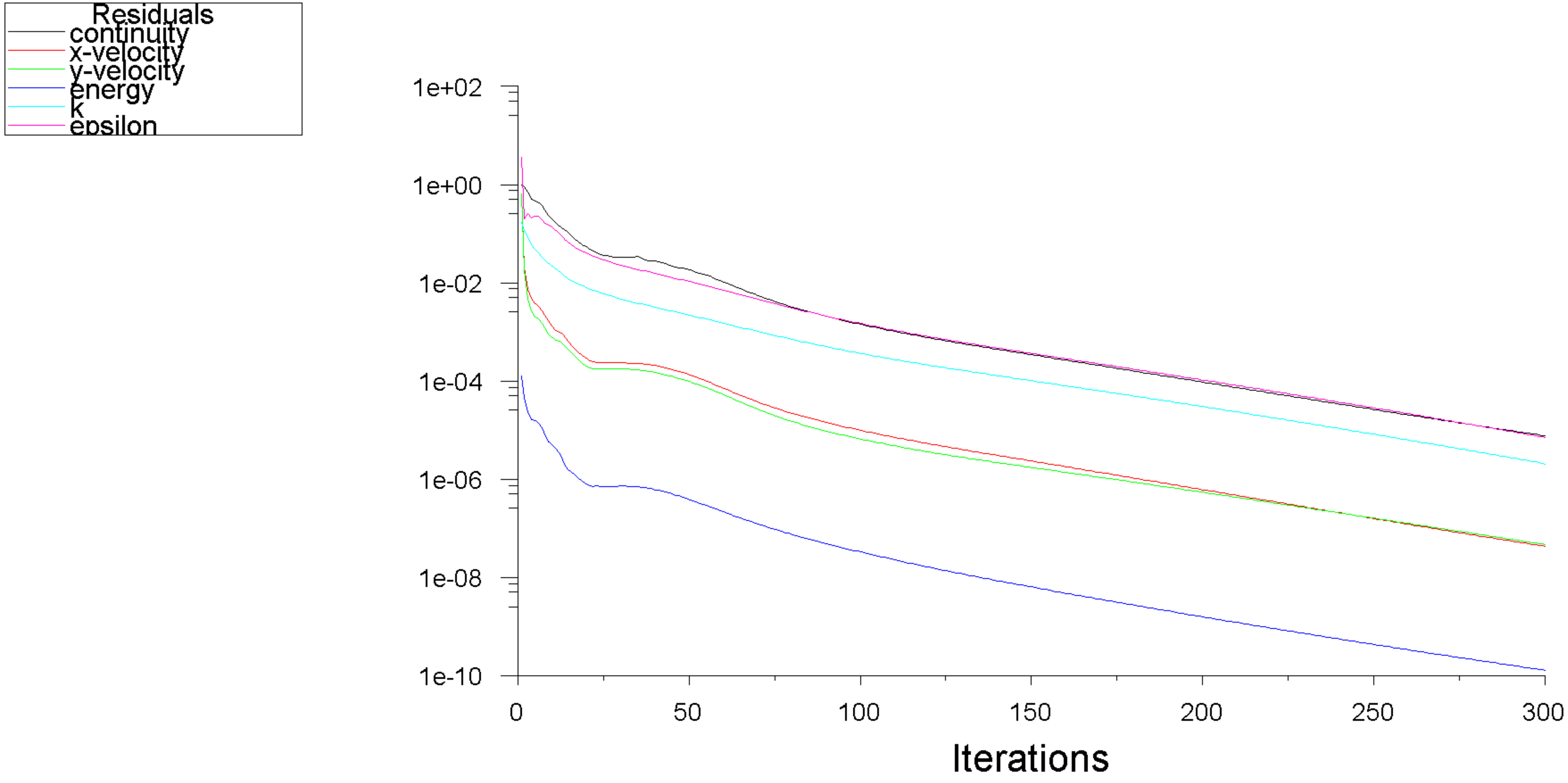
Global observations (2/2)

- 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

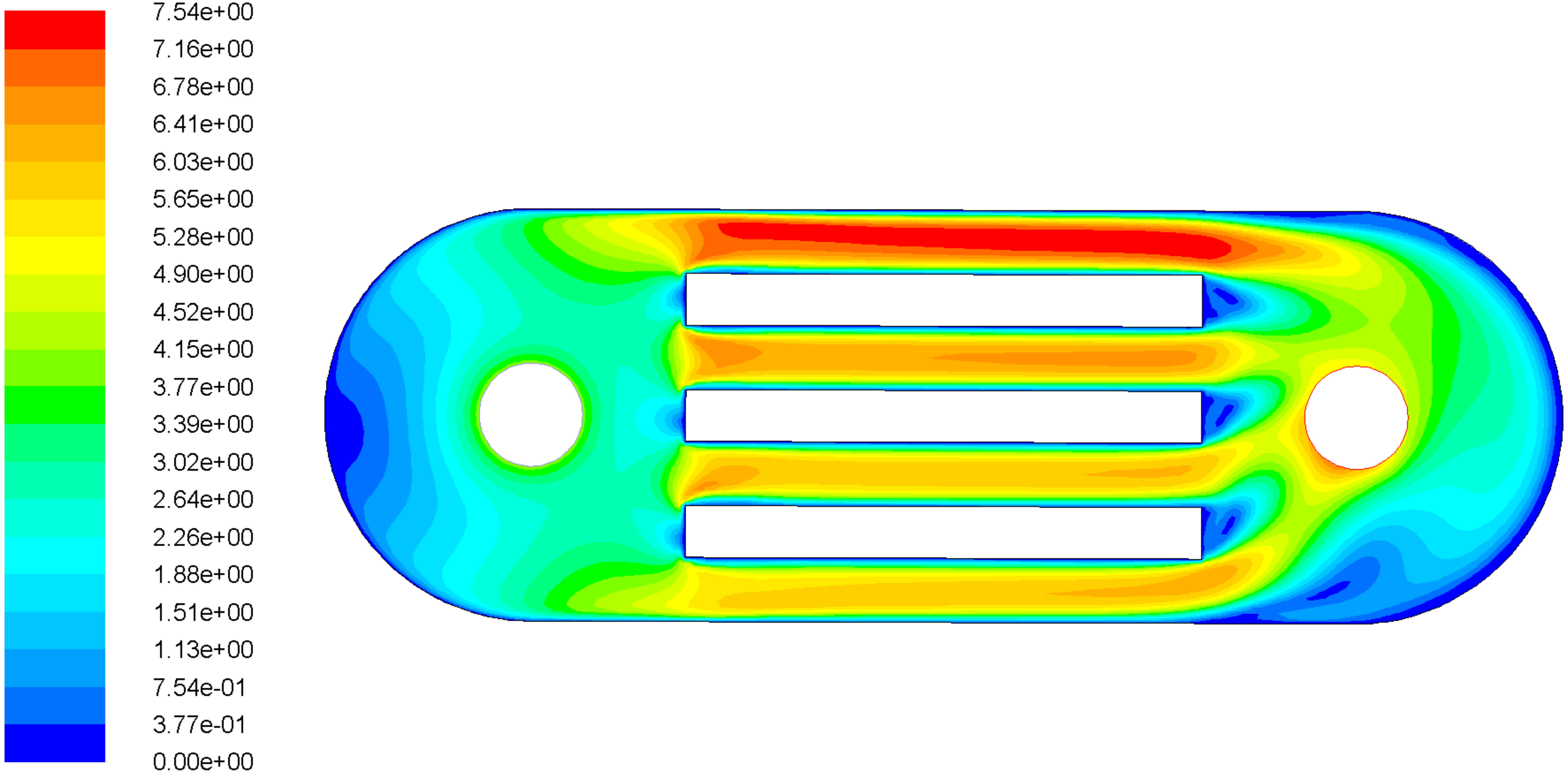
- Convergence: same computation with coupled solver. Obtain the same asymmetric solution much faster.



Numerical Flow Simulation

Post-processing

- Contours: velocity magnitude



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.