Verification & Validation

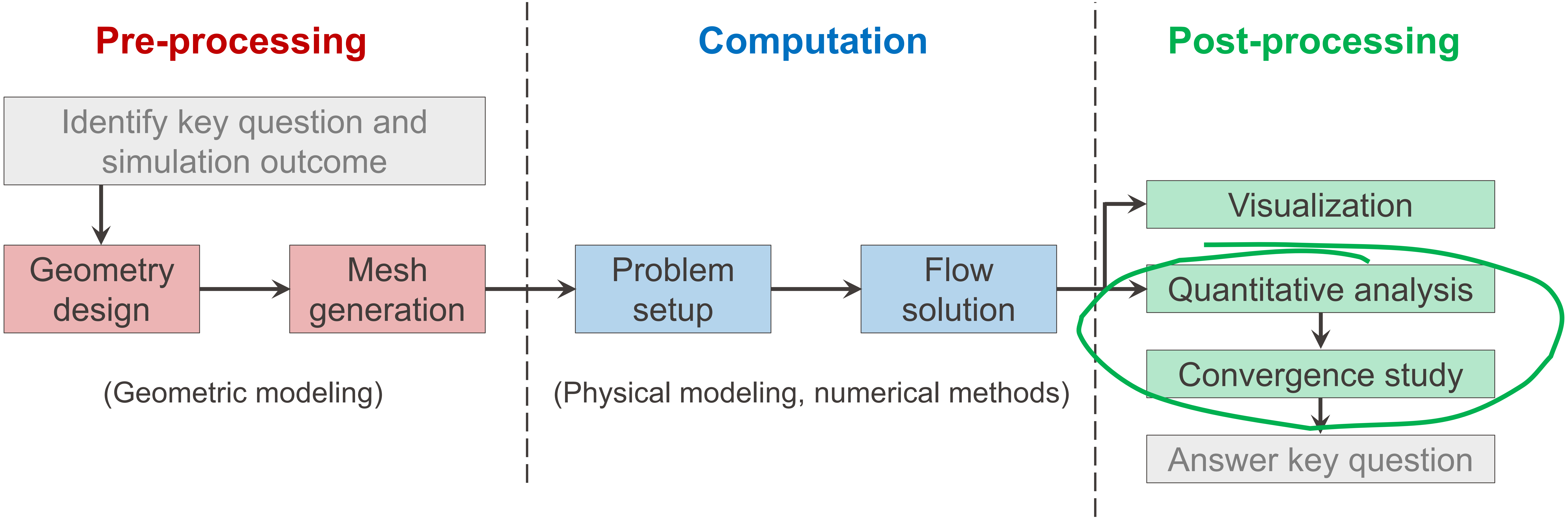
Numerical Flow Simulation

Edouard Boujo

Fall 2024

École
polytechnique
fédérale
de Lausanne

Numerical simulation workflow



Numerical Flow Simulation

Verification and validation

- Various sources of **error**:
  - Numerical errors: roundoff, iterative convergence, discretization.
  - Coding errors: mistakes.
  - User errors: incorrect use of software.

- Various sources of **uncertainty**:
  - Input uncertainty: limited information / approximation of material properties, geometry, boundary conditions.
  - Physical model uncertainty:
    - inadequate representation of physical processes (e.g. turbulence, combustion),
    - simplifying modelling assumptions (e.g. incompressible vs. compressible, steady vs. unsteady, 2D or symmetric vs. fully 3D).

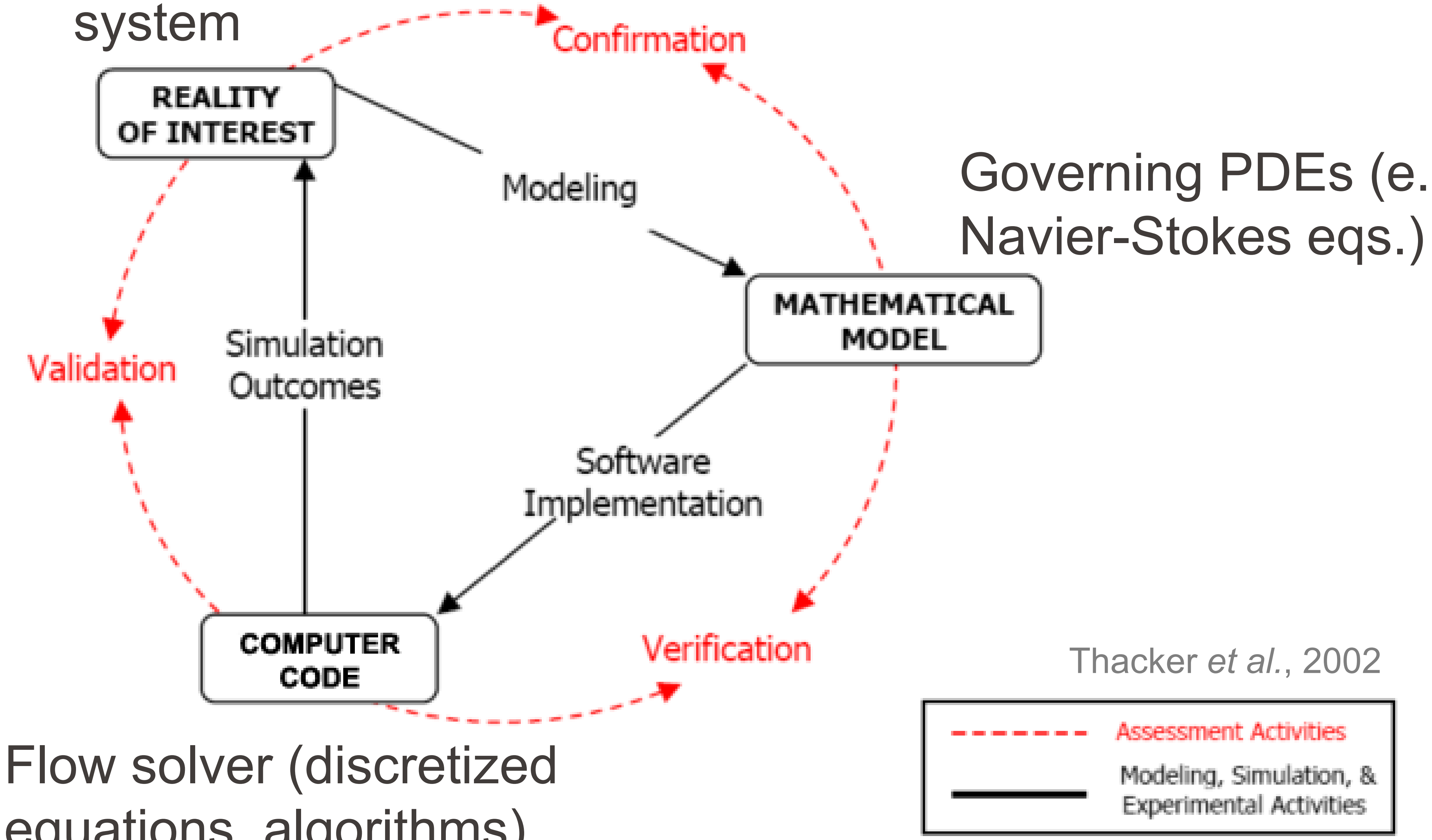
Verification and validation

- V&V examine the credibility of the code and simulation results by demonstrating acceptable levels of error and uncertainty.

- Two processes:
  - **Verification**: are we solving the equations correctly? (Are the math and the code correct? Is the mesh fine enough?)
  - **Validation**: are we solving the correct equations? (Are the physics and the BCs correct?)

Physical system

Governing PDEs (e.g. Navier-Stokes eqs.)



Thacker *et al.*, 2002

Flow solver (discretized equations, algorithms)

Numerical Flow Simulation

Verification and validation

- **Verification** (are we solving the equations correctly?)
  - Motivation: verify that computer code can be used to obtain correct solution to given model / PDEs.
  - Goal: identify / eliminate mathematical-based errors (e.g. coding mistakes, poor discretization, coarse mesh, insufficient convergence).
  - Method: compare numerical results with exact (analytical) or highly accurate (numerical) results.

- **Validation** (are we solving the correct equations?)
  - Motivation: increase confidence in the predictive capacity of the model / PDEs / BCs.
  - Goal: identify/eliminate errors in the model / PDEs / BCs.
  - Method: compare numerical results with validation experiment results.

Verification

- **Qualitative** analysis: numerical solution should be **physically realistic**.
  - Smooth solution (except if shock), with no evidence of the underlying mesh.
  - All important fine flow structures are resolved.

- **Quantitative** analysis: numerical solution should be independent of computational mesh → **mesh convergence study** is essential.
  - Numerical solution should become more accurate when the mesh is refined.
  - The mesh must be refined until the desired accuracy is obtained.
  - Refining further has no significant influence on computed flow solution.
  - Different quantities of interest may exhibit different convergence behaviors.
  - Mesh-to-mesh interpolation convenient to speed up the process.

Verification: mesh convergence study

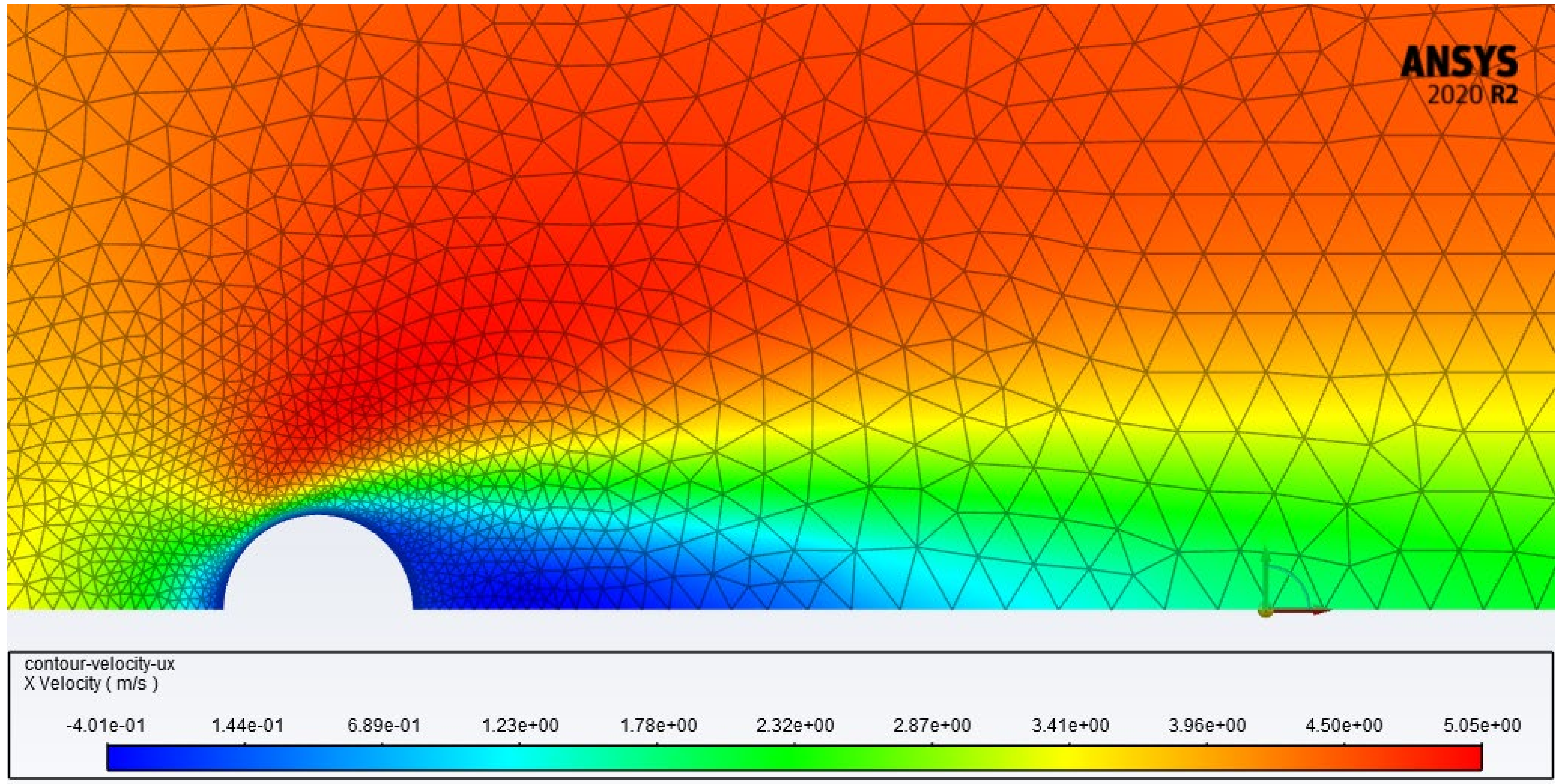
- **Theoretical** study:
  - Compare with **exact** (analytical) solution and analyze how the error decreases.
  - Useful when developing a new CFD code. Impossible for practical problems.

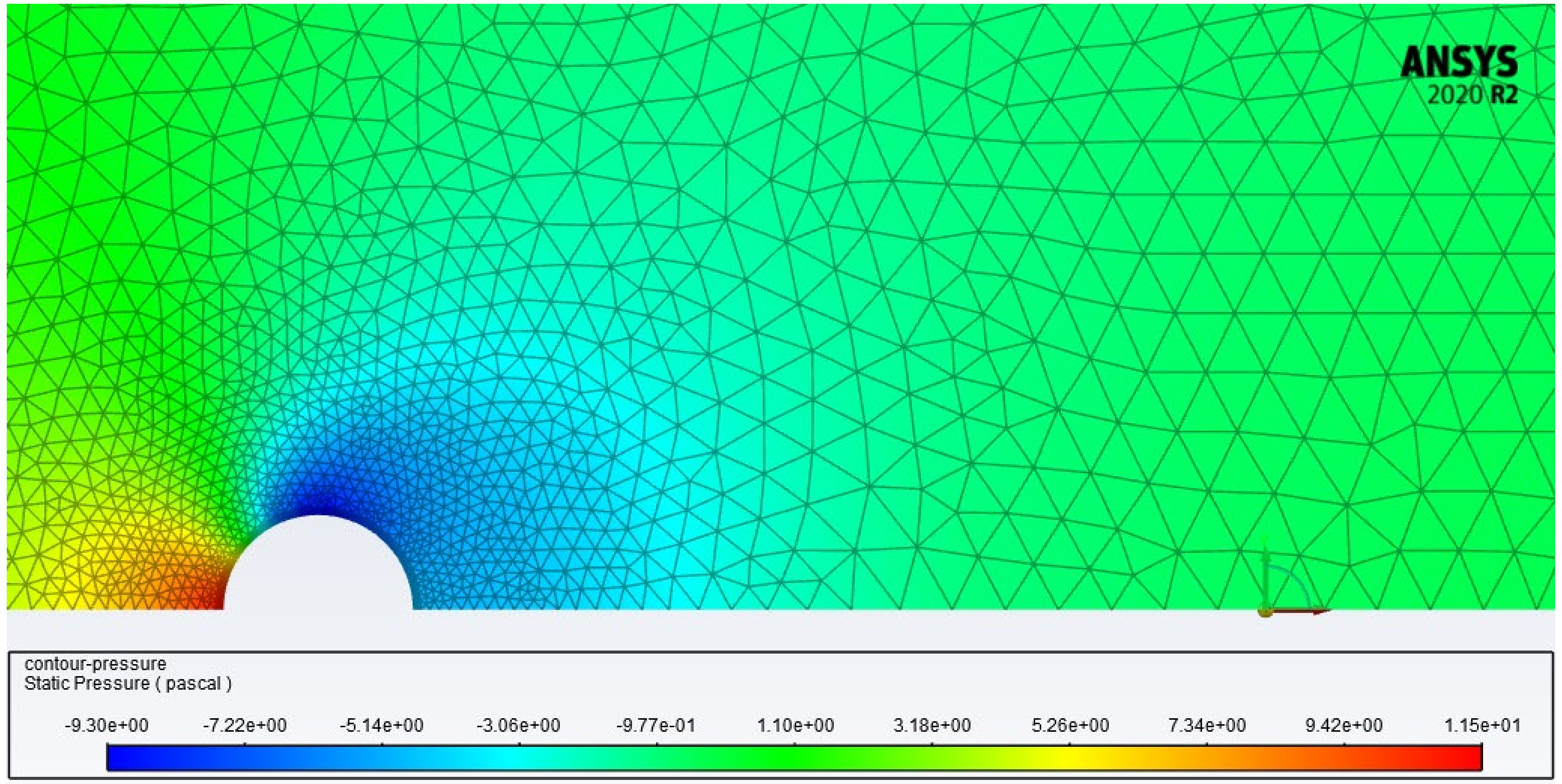
- **Practical** study:
  - Use numerical solution on the **finest** mesh as a **reference**;
  - Or analyze **relative variation** from one mesh to the next.

Mesh convergence study: cylinder flow example

- 2D laminar, *Re*=40 (*U*=4 m/s, *D*=10 mm, ν=1e-3 m^2/s)
- Probe: pressure *p* and velocity u_x at (*x*,*y*)=(5*D*,0)
- Drag force F_d on the cylinder → drag force coefficient $$C_d = \frac{F_d}{\frac{1}{2}\rho_\infty U_\infty^2 D}$$
- No analytical solution available

Numerical Flow Simulation

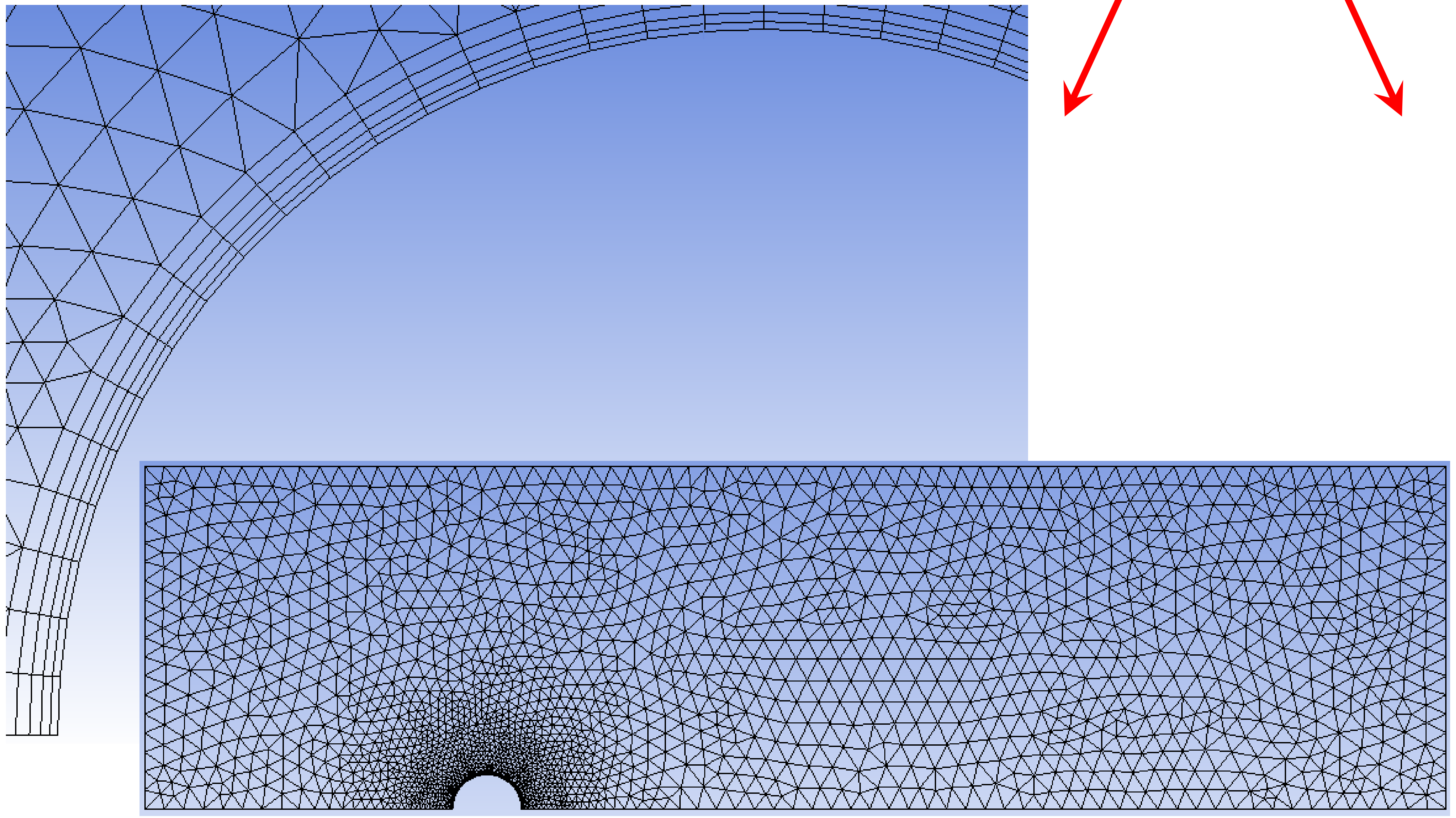


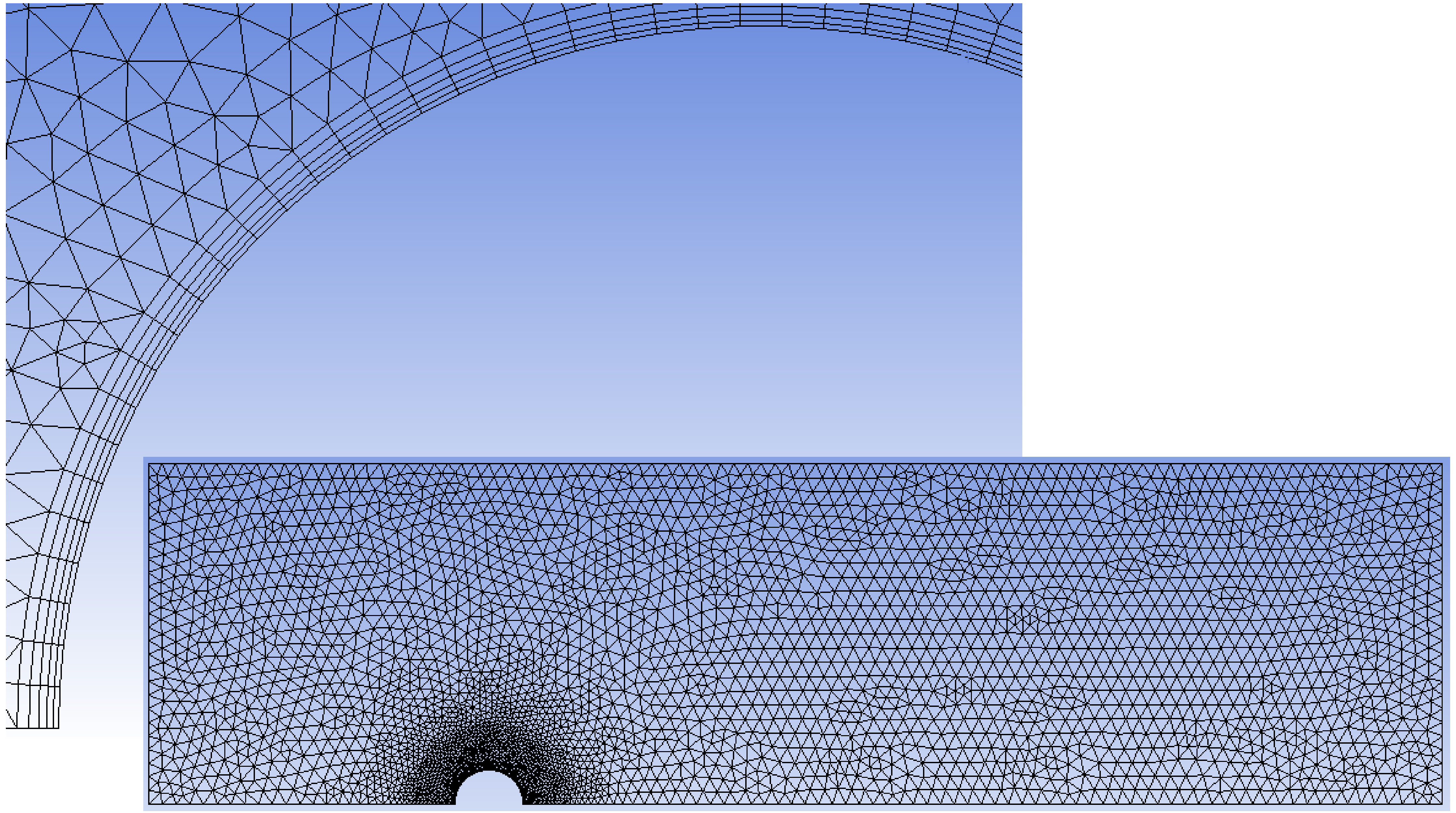


Mesh convergence study: cylinder flow example

- Uniform refinement: at each iteration, divide size *h* by approx. $\sqrt{2}$ in the whole domain.
- 2D → at each iteration, number of elements *N* multiplied by approximately 2.

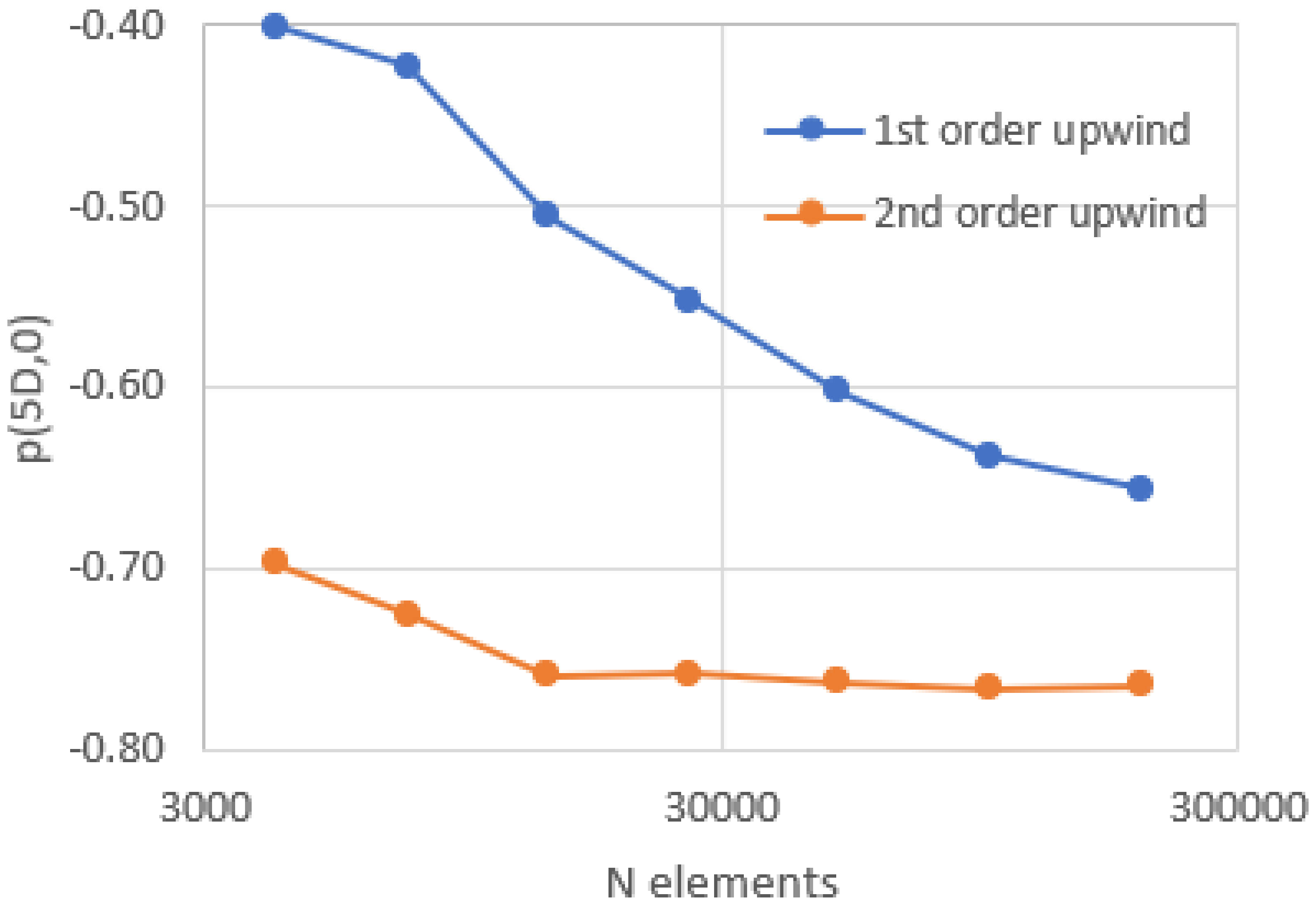
Mesh	1	2	3	4	5	6	7
h max (mm)	2.820	2.000	1.400	1.000	0.710	0.500	0.350
h cyl (mm)	0.420	0.300	0.210	0.150	0.110	0.075	0.053
Nb of elements	4106	7385	13808	26083	50495	98620	193551

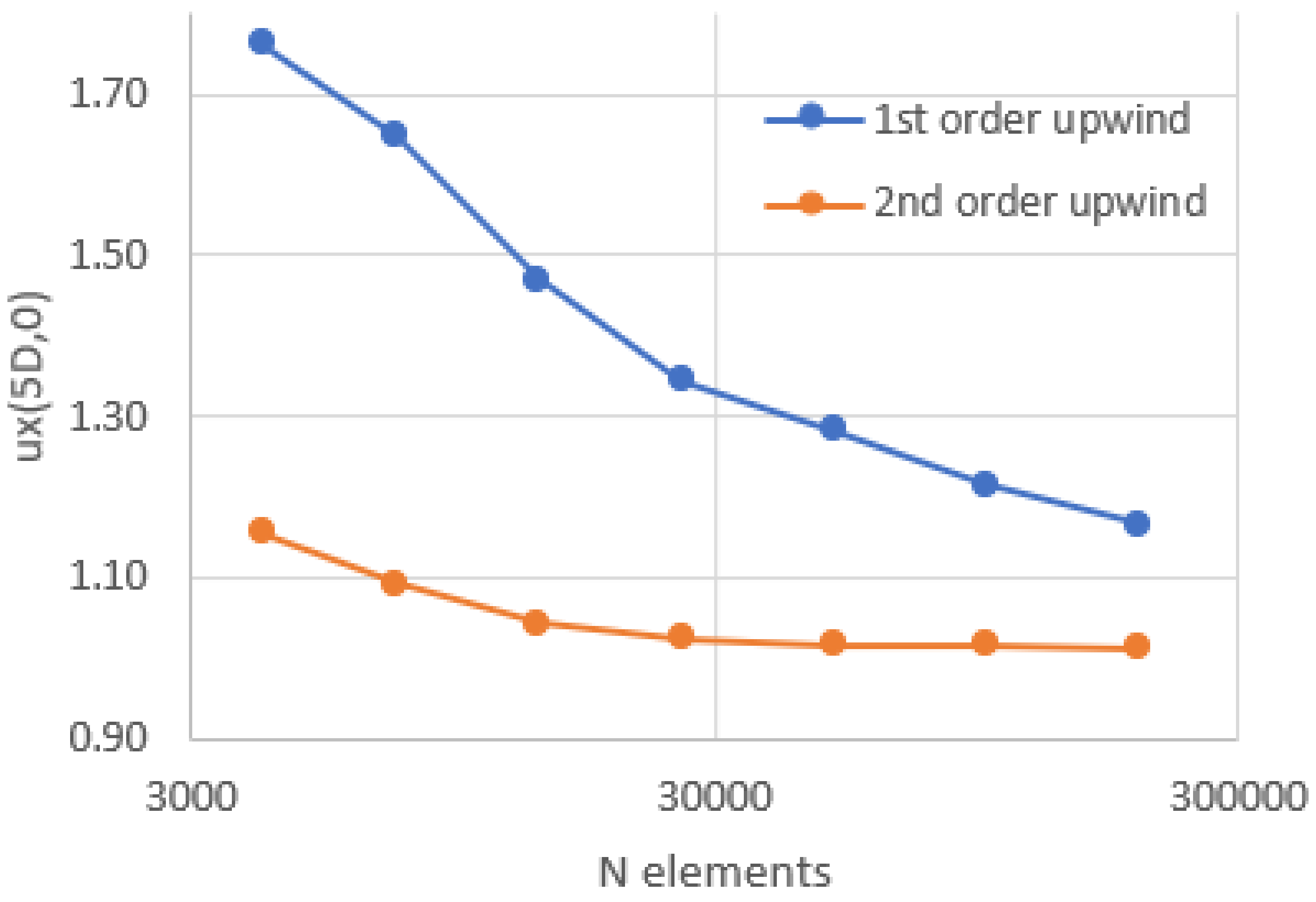




Mesh convergence study: cylinder flow example

- Plot data against *h* or 1/*h* or *N* etc. (May be clearer in log scale.)

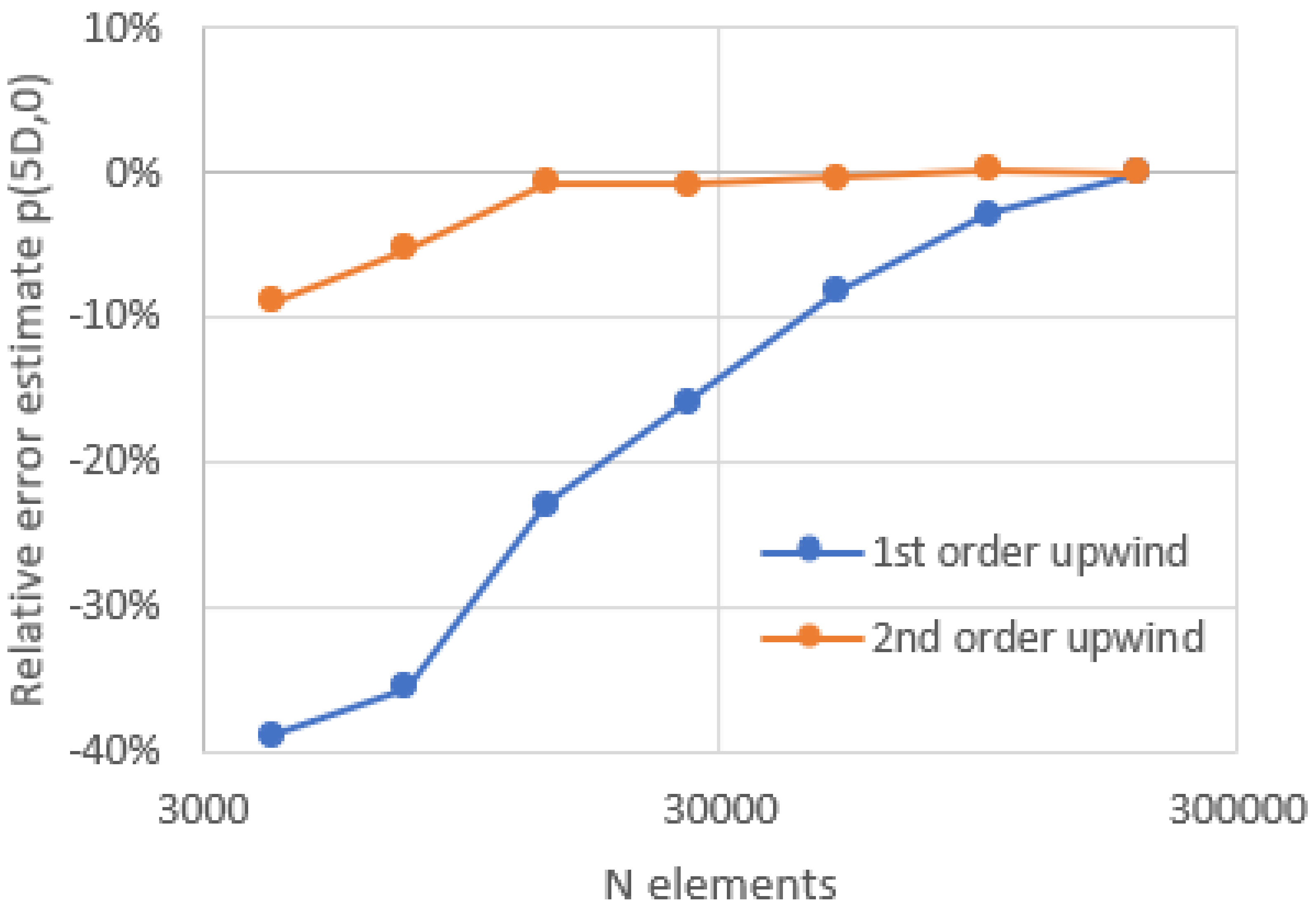


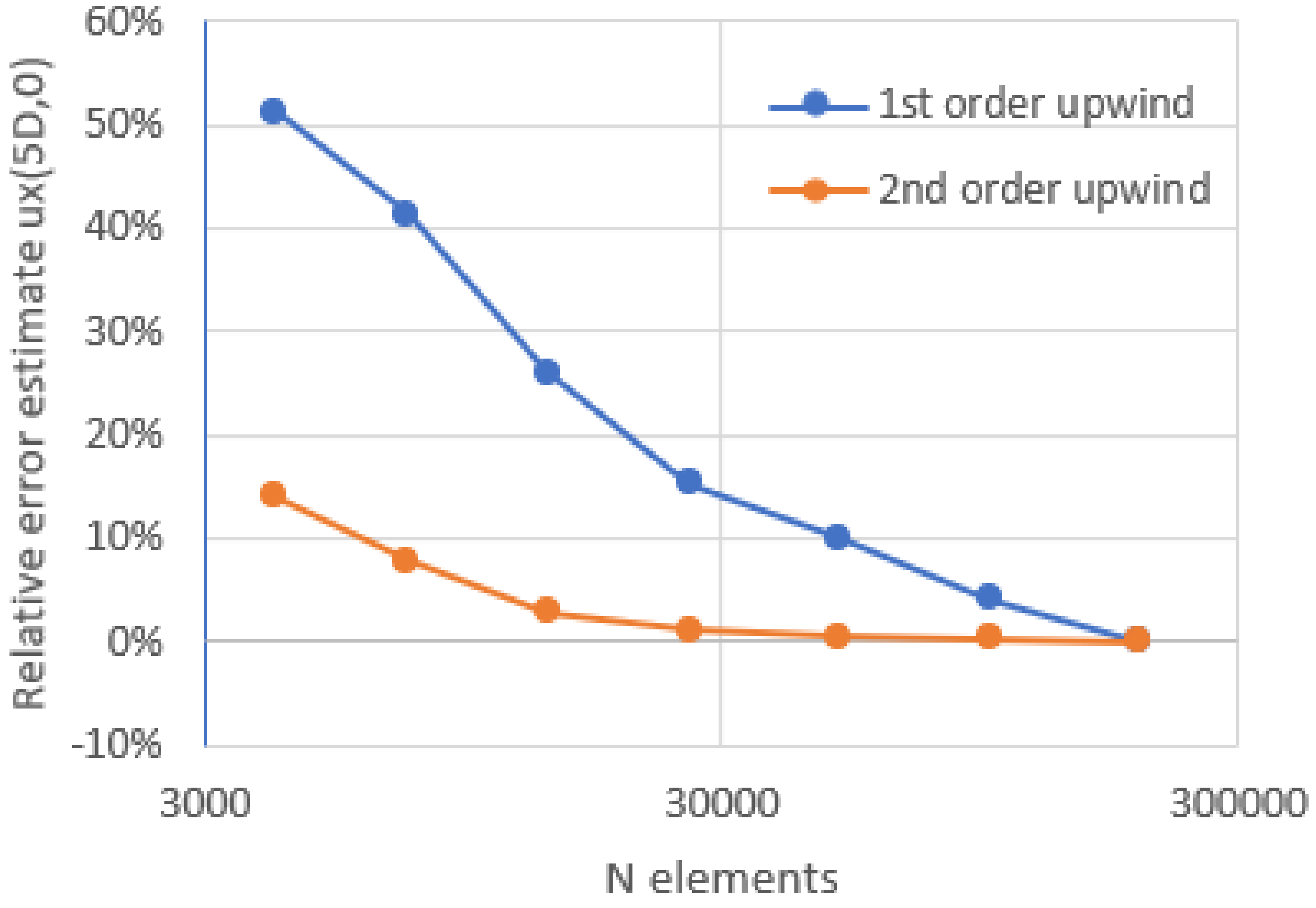


- Check that 2nd-order spatial scheme converges faster than 1st-order scheme.
- Convergence is not necessarily monotonic.

Mesh convergence study: cylinder flow example

- Error estimate with respect to finest mesh:

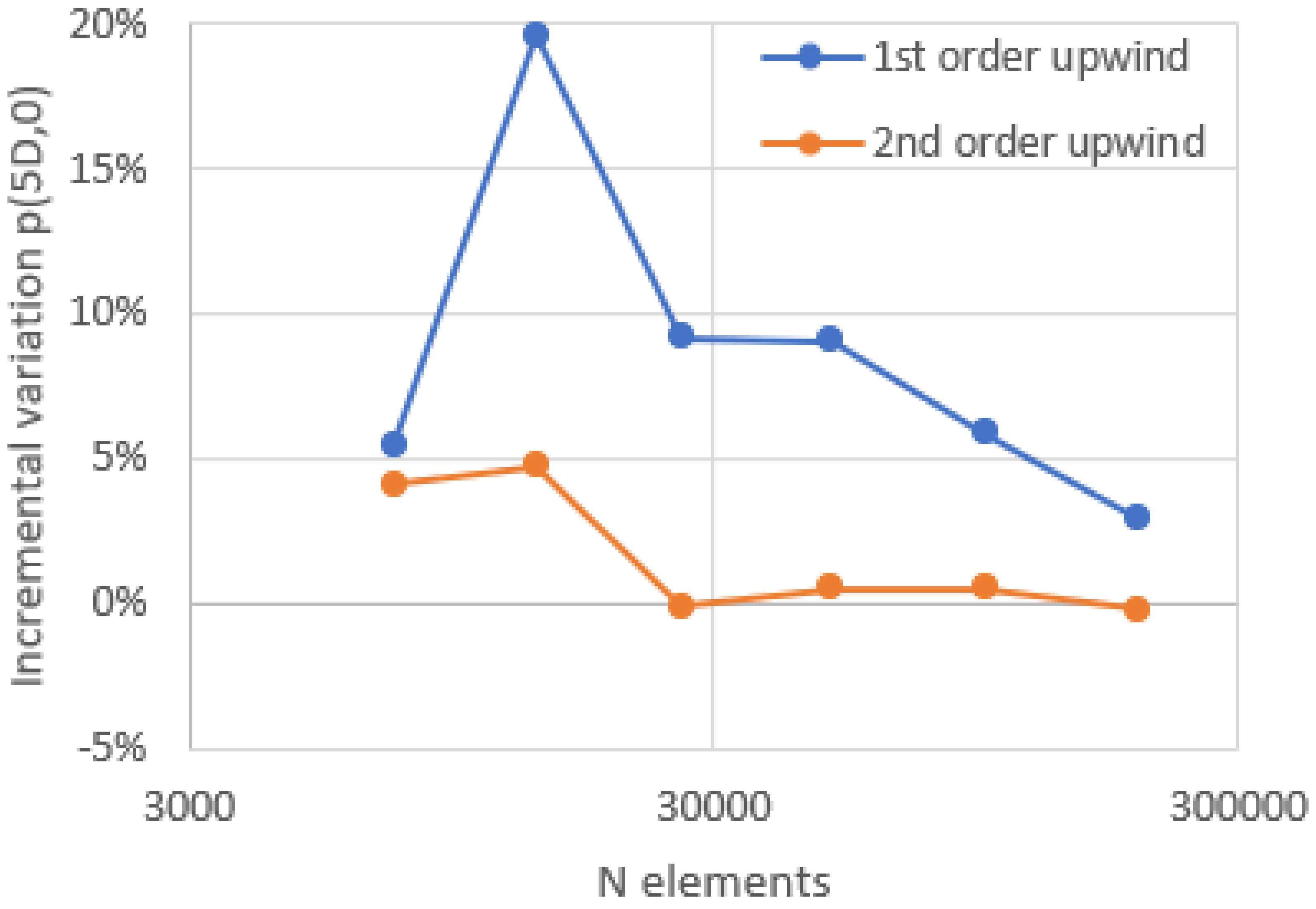


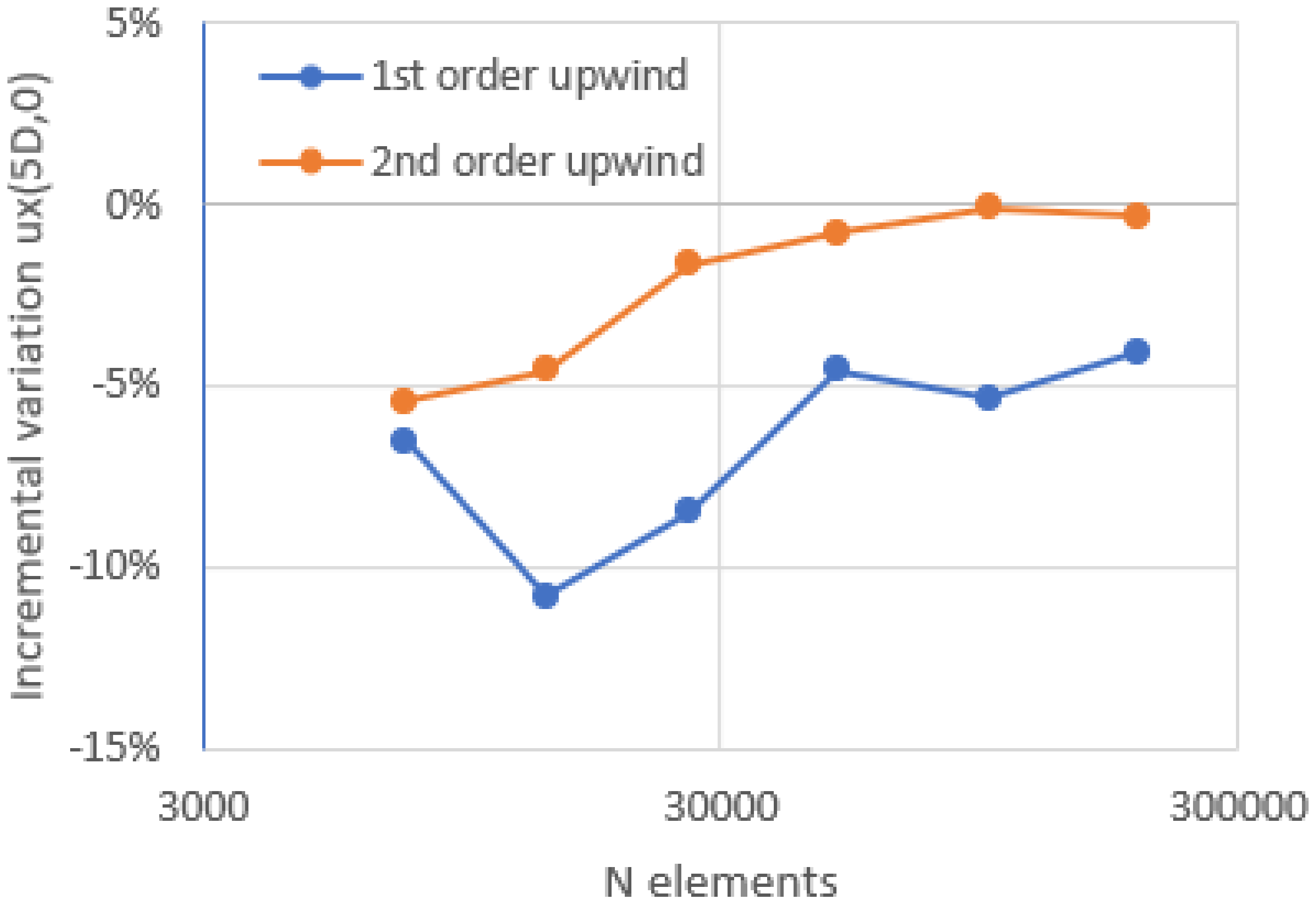


- Can choose the coarsest mesh such that the relative error remains smaller than a chosen threshold (depends on the required accuracy).
- For ex., would choose mesh 3 for an error threshold of 5%, and mesh 4 for an error threshold of 2%.

Mesh convergence study: cylinder flow example

- Incremental variation from one mesh to the next:

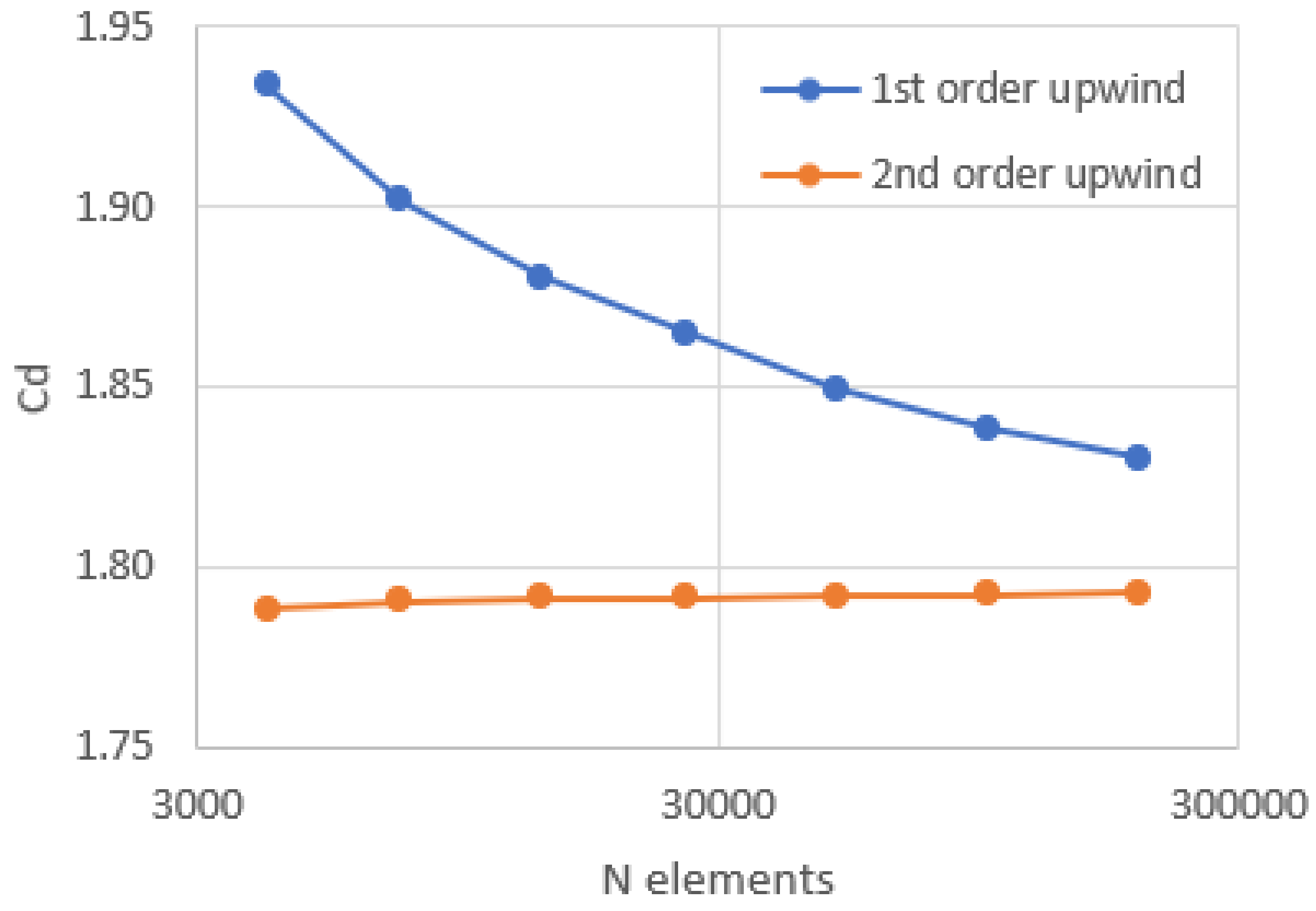


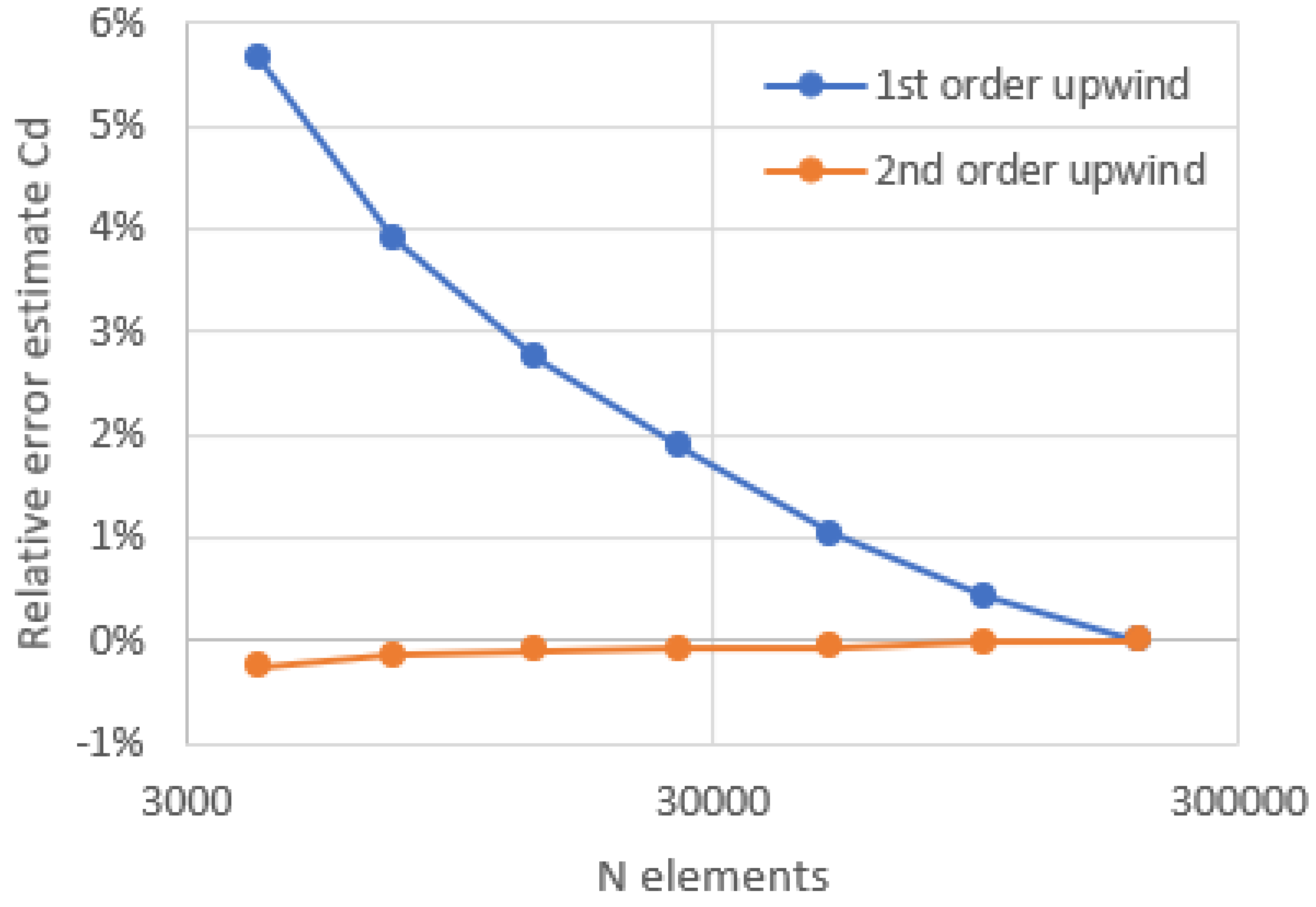


- Meaningful only if significant decrease in *h* from one mesh to the next.
- May be safer to use a smaller threshold in this case.
- In this example, would also choose mesh 3 for a threshold of 5%, and mesh 4 for a threshold of 2%.

Mesh convergence study: cylinder flow example

- Note: convergence may depend on the quantity of interest and on the region.
- In this example, C_d turns out to converge faster than p and u_x measured in $(5D,0)$:





Numerical Flow Simulation

Richardson extrapolation

- Objective: estimate the **discretization error** and the **exact solution**, using numerical solutions computed on different meshes.

- Assumptions:
  - Smooth solution;
  - **Discretization order = *p*** (not the formal order known *a priori* - in general 1st or 2nd order - but the actual order observed *a posteriori*);
  - **Monotonic convergence** (achieved only on fine meshes; can only be checked with at least 3 solutions, 2 is not enough).

Richardson extrapolation

- On 3 grids of sizes h, rh, r^2h, write the calculated numerical solution as:

$$\text{Numerical solutions}\left\{\begin{aligned} f_h &\approx \underbrace{f_e}_{\text{Exact solution}} + \underbrace{\alpha}_{\text{Coefficient (independent of } h\text{)}} h^{\overbrace{p}^{\text{Discretization order}}} \\ f_{rh} &\approx f_e + \alpha(rh)^p \\ f_{r^2h} &\approx f_e + \alpha(r^2h)^p \end{aligned}\right.$$

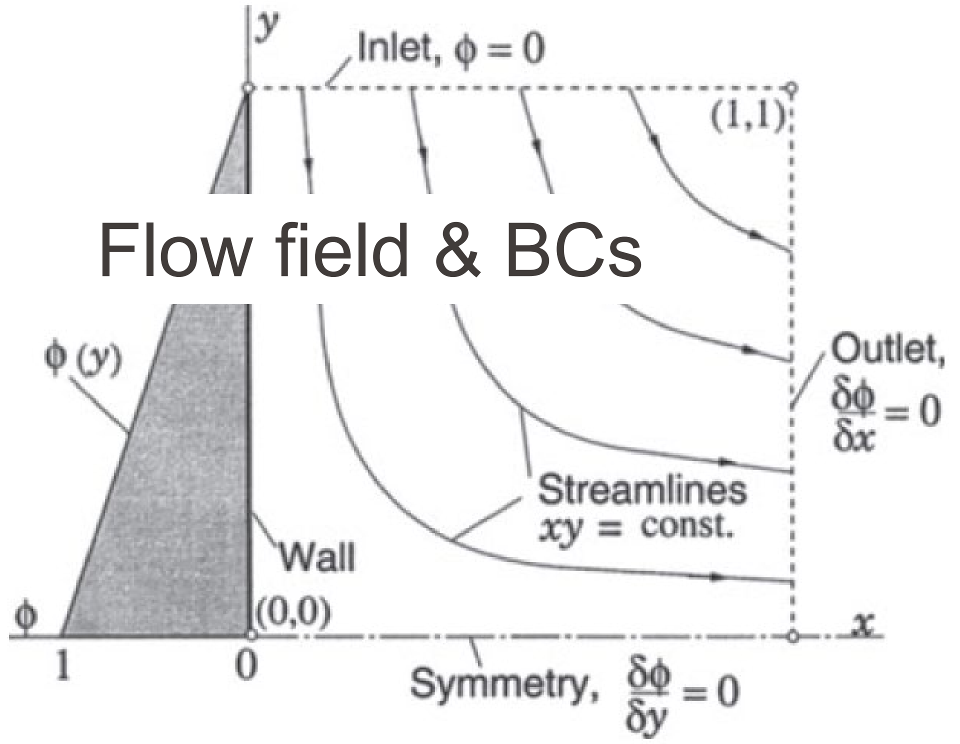
- Discretization order: $p \approx \dfrac{\log\left(\frac{f_{rh}-f_{r^2h}}{f_h-f_{rh}}\right)}{\log(r)}$

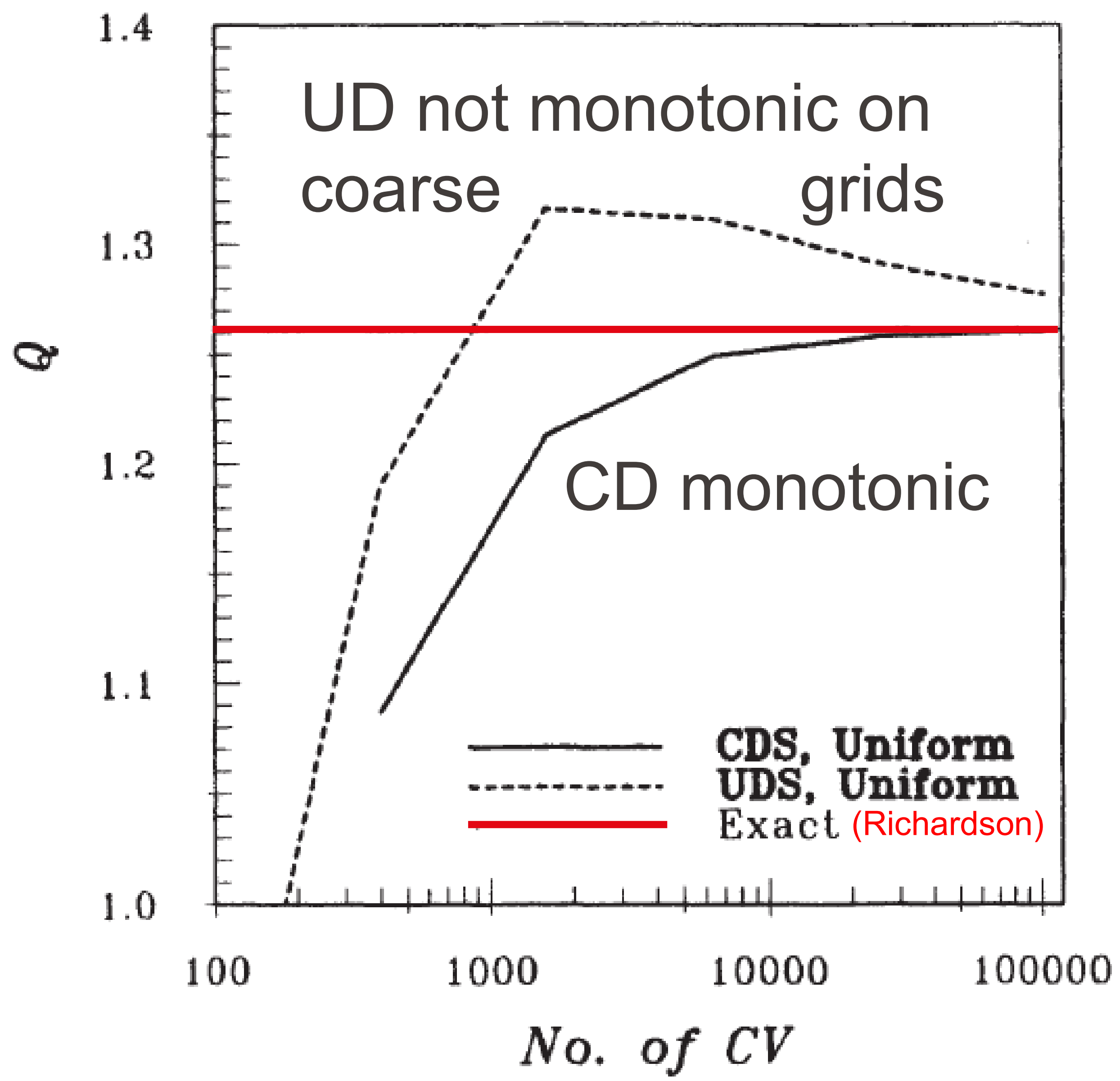
- Discretization error: $f_h - f_e \approx \dfrac{f_h - f_{rh}}{r^p - 1}$

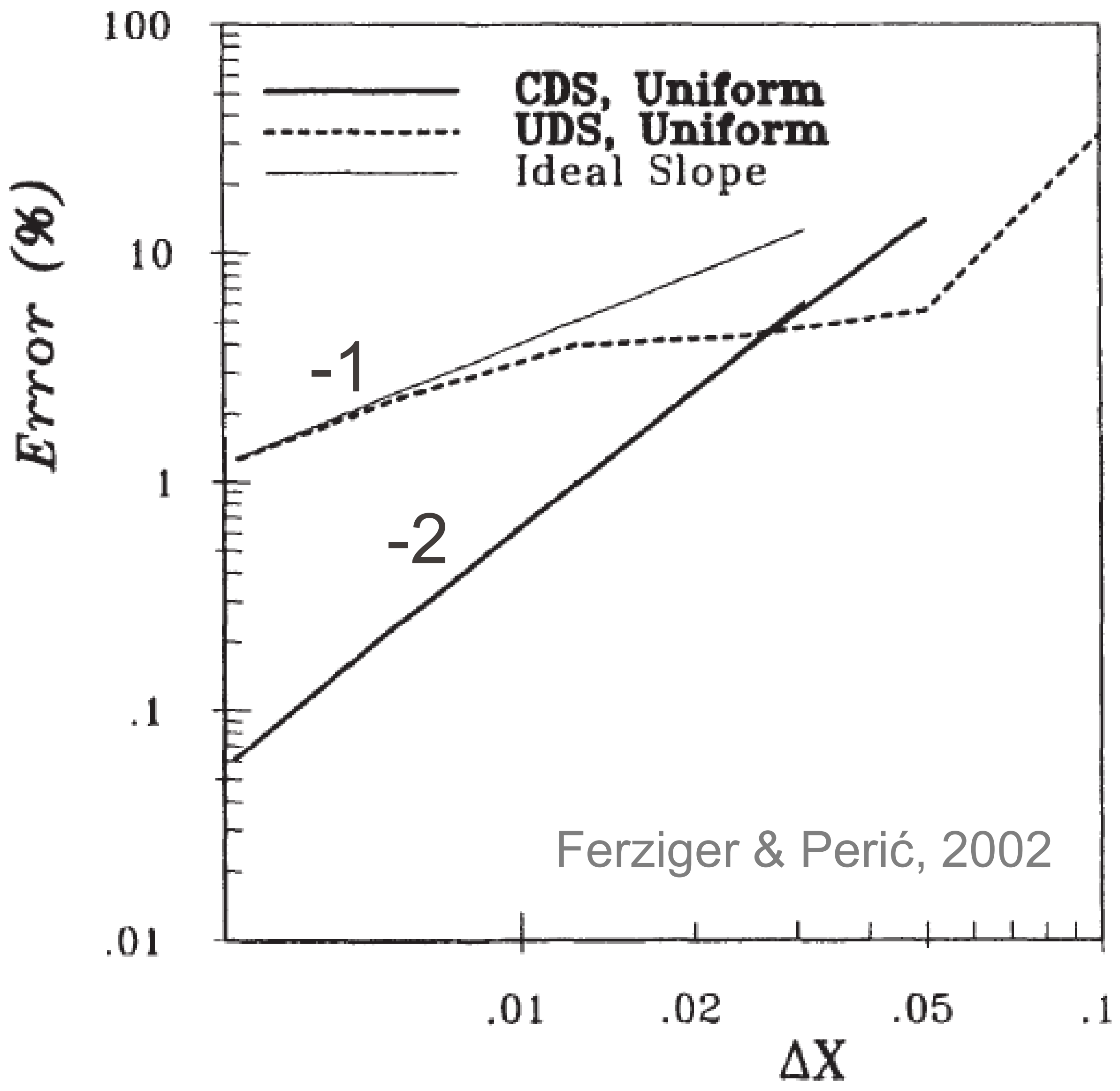
Richardson extrapolation

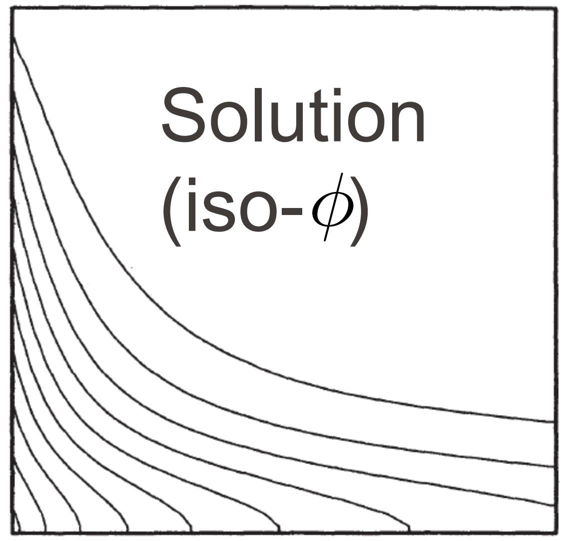
- Valid for **global** solution (and thus pointwise values) → useful to compute error.
  (Can also approximate exact solution f_e, but this approximation does not satisfy governing eqs.)
- Valid for **integrated** quantities too (if integration scheme has same discretization order p): fluxes, forces etc.

- Example: transport of a scalar ϕ in a known 2D velocity field (stagnation point). Monitor total flux Q through west boundary.





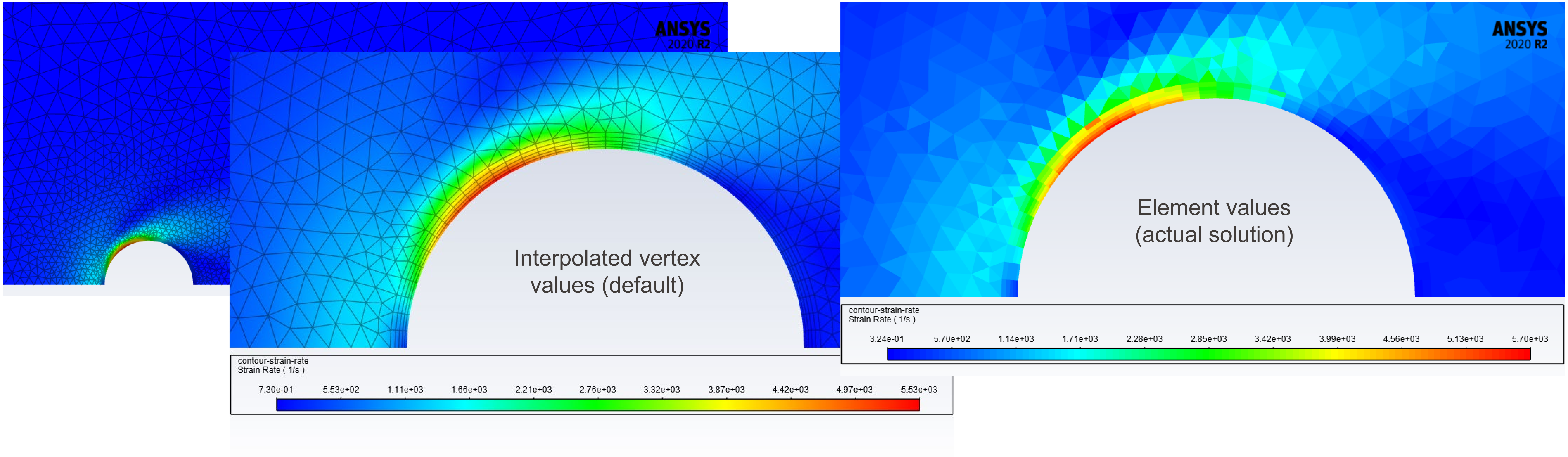




Numerical Flow Simulation

Local refinement

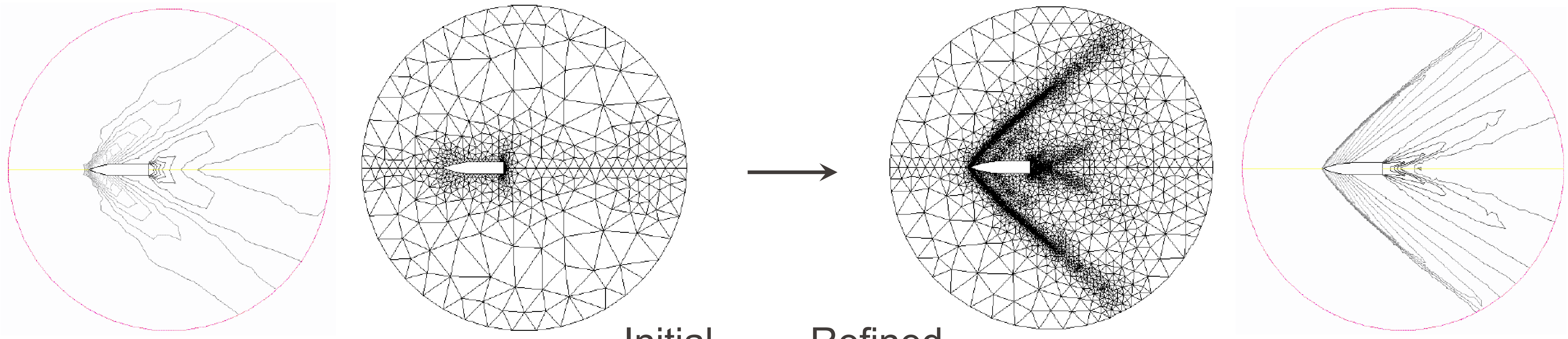
- Refinement need not be uniform. **Local** refinement in well-chosen regions (e.g. regions of large gradients) can help reach desired level of convergence with less mesh elements.
- Example: strain rate $(2S_{ij}S_{ij})^{1/2}$, where $S_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$:



- But be careful to retain a good **mesh quality**. For instance, should avoid sudden variations in element size.

Adaptive mesh refinement

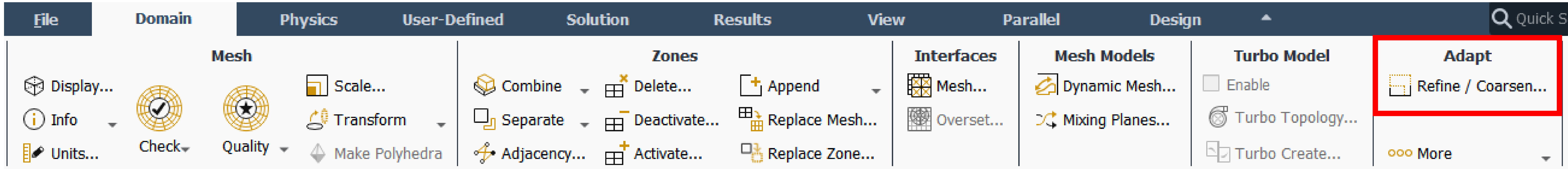
- Mesh adaption adds more cells where needed to better resolve the flow field.
- Cells to be adapted are listed in a register, based on a variety of criteria:
  - Gradient (velocity for shear layers, pressure for shocks…)
  - Iso-value (high-velocity jets, low-pressure wakes, reaction rate for combustion…)
  - Region
  - Element size or size change
  - Wall y^+ or y^* (turbulent flows)
  - Volume fraction (multiphase flows with Volume of Fluid method)
- Example: 2D supersonic flow around a projectile, 5 refinement cycles



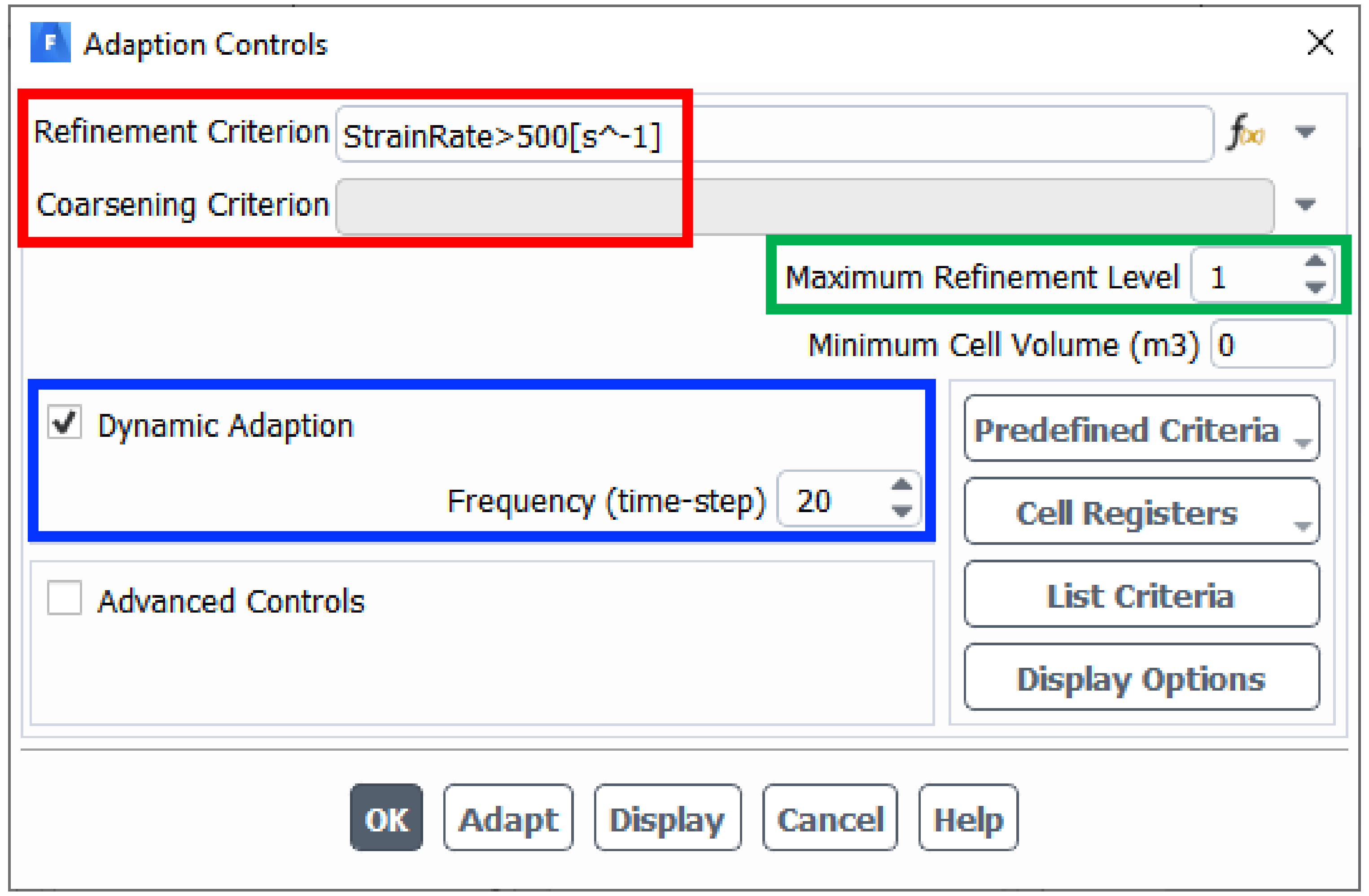
Initial Refined

Adaptive mesh refinement

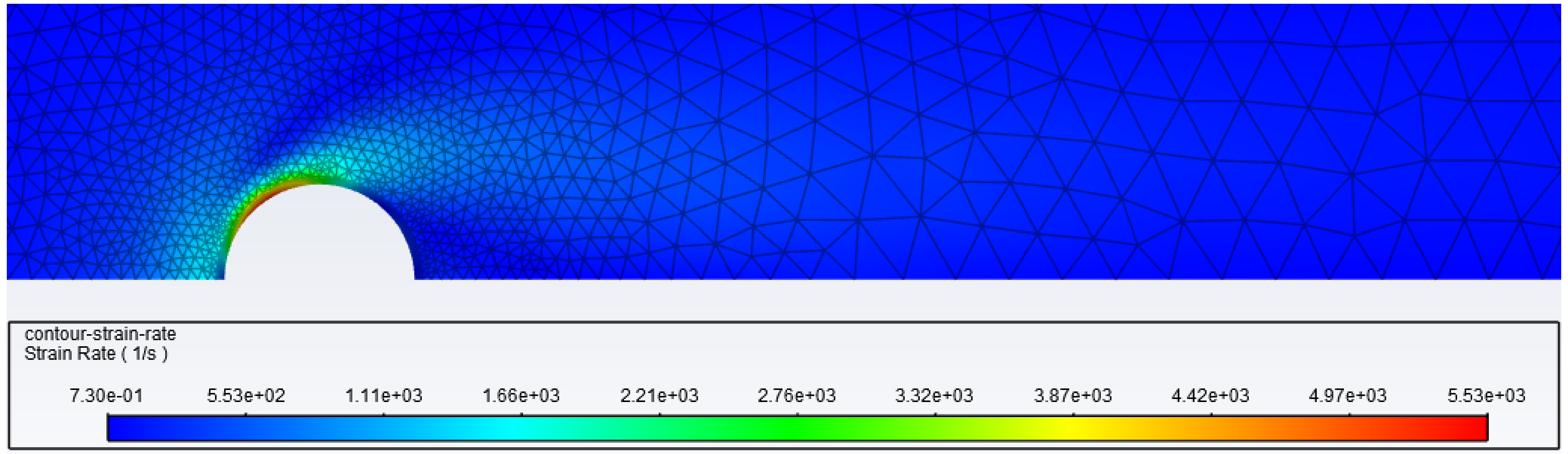
- In Fluent:

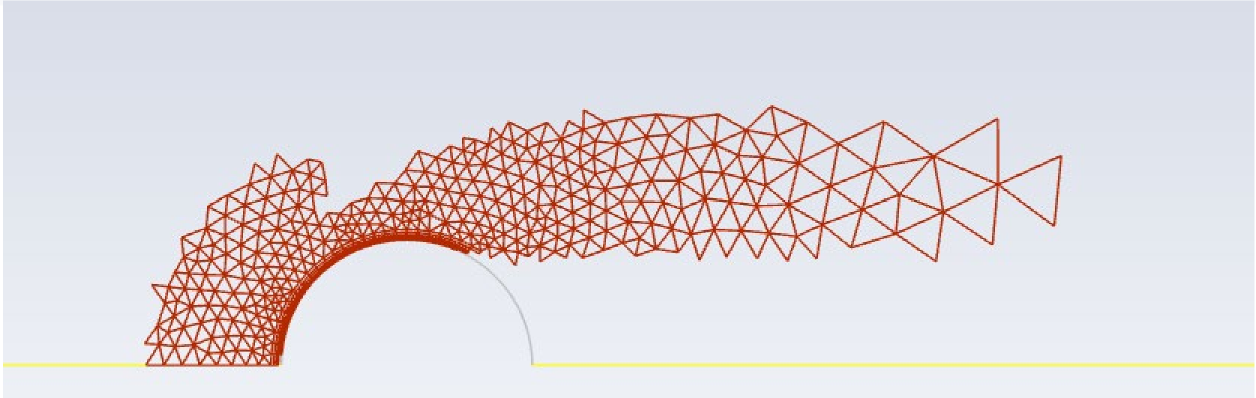


- Define refinement and/or coarsening criteria with an expression or with a “cell register”.
- Choose the maximum number of refinements (mesh size divided by 2, 2^2, 2^3 etc.).
- For unsteady problems: set the dynamic adaption frequency (every *n* time steps).



Example: refine elements where strain rate is larger than 500 s^{-1} (only once, steady problem).

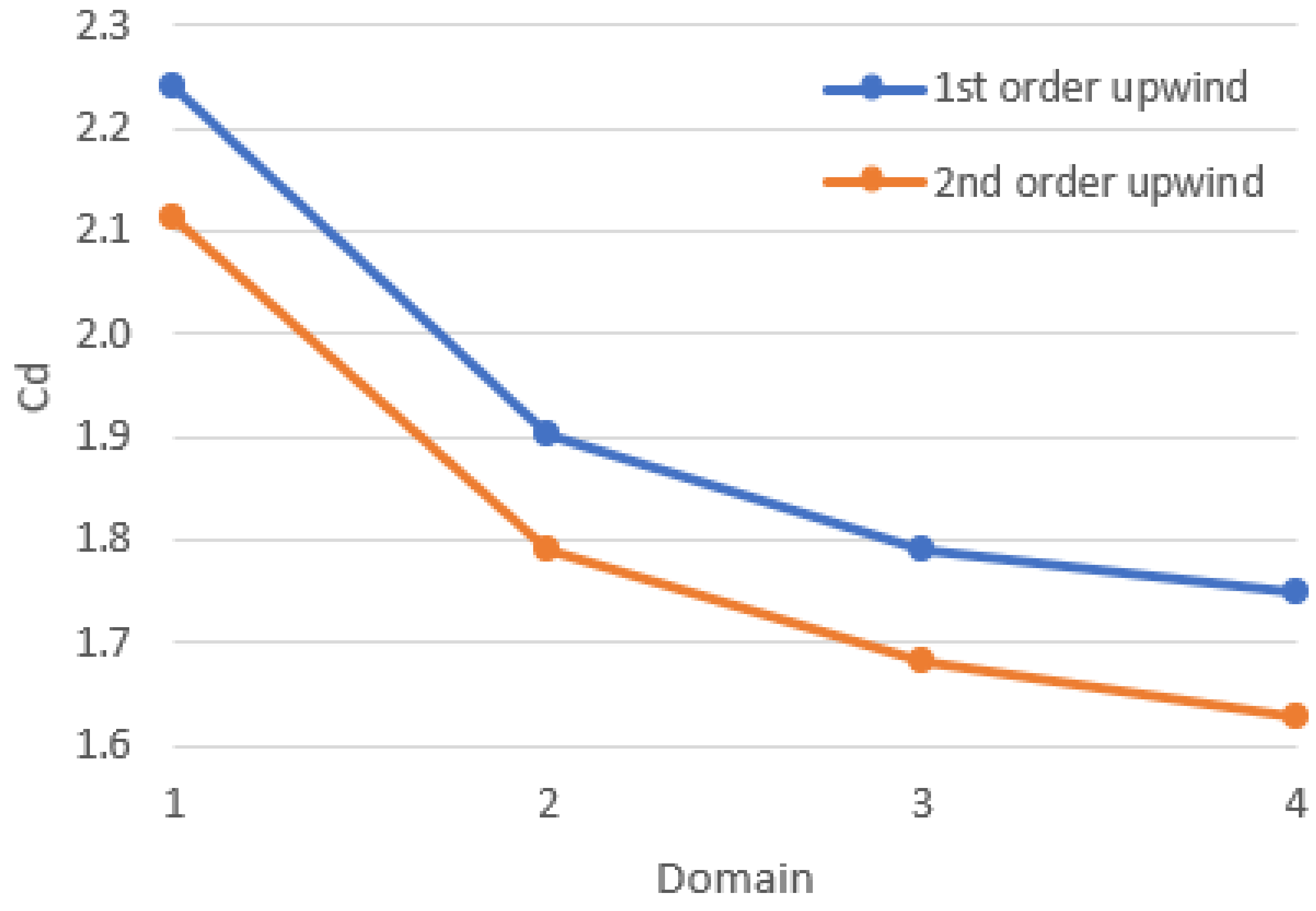




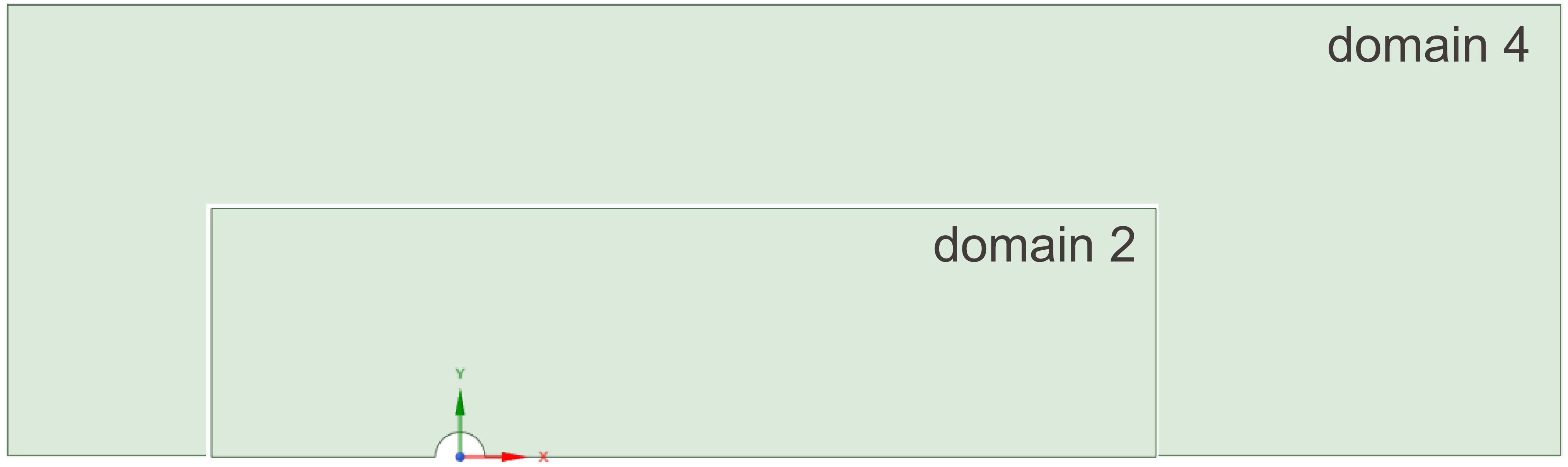
- “Display”: visualize elements to be adapted.
  “Adapt”: actually refine/coarsen.

Influence of domain size

- For external flows, domain size (location of boundaries) is also important:



Domain	1	2	3	4
Inlet x (D)	-3	-5	-7	-9
Top y (D)	3	5	7	9
Outlet x (D)	10	14	18	22



- Previous slides (cylinder flow): convergence study performed on domain 2, found well-converged C_d value of 1.8, but actual value close to 1.5. Domain 4 may still be too small.

Summary

- CFD results need to be checked for accuracy:
  - Verification: the eqs. are solved correctly (check against independent solutions).
  - Validation: the correct eqs. are solved (check against experimental measurements).

References

- General guidelines for best practices in CFD
  - AIAA: *Guide for the Verification and Validation of Computational Fluid Dynamics Simulations,* AIAA Guide G-077-1998 (1998)
  - ERCOFTAC: *Best Practice Guidelines*, Version 1.0, M. Casey and T. Wintergerste (eds), ERCOFTAC Special Interest Group on Quality and Trust Industrial CFD (2000)
- Verification and validation
  - *Quantification of Uncertainty in Computational Fluid Dynamics,* P.J. Roache, Annual Review of Fluid Mechanics, 29 (1997)
  - *Verification and Validation in Computational Fluid Dynamics*, W.L. Oberkampf and T.G. Trucano, Progress in Aerospace Sciences, 38-3 (2002)