ME-474 Numerical Flow Simulation

Checklist / report template

- This document can be used as a **checklist** when performing a numerical flow study.
- The structure of this document can be used as a **report template**. It is somewhat closer to an engineering report than to a scientific article. It can of course be adapted. Not all sections of this template are relevant to all studies; conversely, some studies may require additional sections.
- A report has several **objectives**, including:
  1. **answering** one or several well-identified initial **questions**,
  2. **explaining and justifying the method** (geometric and physical modeling hypotheses, choice of mesh and numerical method, etc.),
  3. providing enough information for the reader to perform independently a numerical study and reproduce the results.
- A report should be **complete**, but also **clear** and **concise**.

Study report: title

Date, names, email addresses, Sciper numbers etc.

1. Introduction

1.1 Context and goals of the study

Initial engineering / research question(s): What do we want to study? Why? What for?

Literature review: previous numerical or experimental studies for the same problem or a similar one?

1.2 Type of analysis, Methodology

General overview of the method.

What are the data available? If applicable, put relevant documents (numerical data, technical / engineering drawings, scope statement etc.) in appendix, or cite them in the references.

2. Geometric modeling and hypotheses

2.1 Presentation of the geometry

Text + images

Justify any simplifications

2.2 Unit system

2.3 Characteristic dimensions

Length, velocity…

Relevant dimensionless numbers?

2.4 Symmetry / periodicity of the problem?

Not only geometry but also boundary conditions, external forces etc.

2.5 Geometrical space

2D? 2D axisymmetric? 3D?

3. Physical modeling and hypotheses

3.1 Physical behavior

Newtonian? Non-Newtonian? Temperature-dependent viscosity?...

Compressible? Incompressible? Ideal gas?...

Physical models: Heat transfer? Multi-phase? Chemistry? Combustion?…

3.2 Fluid properties

Values + units

3.3 If applicable: turbulent flow calculation

Turbulence model? Near-wall treatment?

4. Boundary conditions, external forces, initial conditions

4.1 Boundary conditions

Type, location, orientation, values + units…

4.2 External forces

Gravity, magnetic force, centrifugal / Coriolis forces…

4.3 Initial conditions

If applicable (i.e. for unsteady simulations).

5. Computational mesh

5.1 Mesh type

Structured / unstructured / block-structured / hybrid

5.2 Cell type

2D: triangles, quadrilaterals, or mixed?

3D: tetrahedra, hexahedra, prisms, pyramids… or mixed?

5.3 Size / number of cells

Which size in which region? Local refinements?

Details of boundary-layer mesh, if any.

Total number of cells and nodes

5.4 Final mesh

Present here the final mesh: images, characteristics, quality metrics…

Other meshes are presented in the section "Mesh size / domain size convergence study"

6. Numerical methods

6.1 Spatial discretization method

Finite volume? Finite element? Finite difference? Spectral method? Spectral elements? Lattice-Boltzmann? Particle-based method?... (Fluent: always FVM)

First-order / second-order spatial discretization?

6.2 Type of simulation/solver

Steady? Unsteady?

Pressure-based / density-based solver? Segregated / coupled?

Variables solved for? Velocity, pressure? Density? Temperature? Turbulent quantities? Chemical species?... In some cases, it may be useful to write down the governing equations.

6.3 Solution options

Initialization: Constant? Piecewise constant? Hybrid? From another solution? From experimental measurements?...

If steady: Stop after convergence (what convergence criteria?) or after number of iterations?

If unsteady: Temporal discretization scheme? Time step size? Time interval?

6.4 Computed quantities?

What, where, when, why?

For example: Spatial derivatives? Surface / volume integrals? Forces? Fluxes? Average / min / max values? Standard deviation?... If unsteady: time-average, fluctuations, standard deviation, frequency?...

7. Mesh size / domain size convergence study

7.1 Criterion

What quantity (quantities) of interest is (are) used to assess convergence?

7.2 Presentation of the different meshes

Relevant images of (some of) the different meshes / domains

Type and location of refinement / coarsening, global / local cell sizes, etc.

Table with values of the number of cells and nodes for each mesh / domain

7.3 Results on the coarsest mesh / smallest domain

Values of the quantities of interest, images of relevant fields

Possibly: identify regions to be refined (large gradients, discontinuities etc.) or boundaries to be moved farther away (solution varying significantly, backflow at the outlet etc.)

7.4 Results on the finest mesh / largest domain

Values of the quantities of interest, images of relevant contours or 1D plots

7.5 Estimation of the relative error

Calculation of the relative error. Is it acceptable?

7.6 Choice of the mesh / domain

Which mesh / domain will be used for the rest of the study?

8. Results

For each result, one section with: Type of results? Type of representation? Location?

If unsteady: Snapshot (at what time)? Time-average? Standard deviation?...

9. Analysis & conclusions

9.1 Summary of calculated results

9.2 Relevance / accuracy of the results?

Major causes of uncertainty / error?

When possible: verification and validation (compare with high-accuracy numerical simulation or experimental measurements).

9.3 Criteria and analysis

If the initial question is a quantitative question: Type of evaluation criteria? Details: limit values, formulas…? How do the results compare with the criteria?

If applicable: compare the different designs investigated.

9.4 Conclusion

Answer the initial question(s)!

9.5 Recommendations

Possibly give recommendations, suggest improvements. Both for the numerical simulation and for the physical system investigated.

10. Appendix

Any document that can be useful to set up the numerical simulation: numerical data, list of material properties, technical / engineering drawings, scope statement, results from experimental tests or other numerical studies etc., but also spreadsheet or formula with calculation details (for instance for boundary conditions), etc.