Optimal Shape Design of Air Ducts in Combustion Engines

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FG8

July 5, 2020

ROMSOC Project 11

General Information.

- Within the *European Innovative Training Network* (ITN): Reduced Order Modeling, Simulation and Optimization of Coupled Systems (ROMSOC).
- *Project 11*: Optimal Shape Design of Air Ducts in Combustion Engines.
- *Project Partners*: WIAS, Germany; Math.Tec GmbH, Austria.
- *Starting Date*: Mar 16, 2020. *Contract*: 17.5 months, extension in the network is potentially possible (6 months); some additional months.
- To be discussed: Total 8 months in Austria (Date not yet specified); Ethics.
- Next Delivery: D5.3 - Software with benchmark problems.

Training Process.

- *Canceled*: Jyväskylä Summer School, Finland; SAMM 2020 in Graz, Austria.
- *Waiting*: Student Compact course, Thematic Einstein Semester, TU Berlin.
- *On going*: Stephan Schmidt's Shape Optimization Course, HU.
- *Winter term*: Topology Optimization.

Up to Now

Theory.

- Gather literature on: Shape Optimization, NSEs, (not yet on Turbulence).
- Get familiar with:
  - *NSEs* [Temam2000, Maz'ya-Rossmann2009];
  - *Shape Optimization* [Schmidt2020, Sokolowski-Zolésio1992];
  - *Turbulence Models* k-ϵ [Mohammadi-Pironneau1994].
- Read [Temam2000]: NSEs with Dirichlet BCs in Lipschitz domains.
- Read [Maz'ya-Rossmann2009] for polygonal domains and general mixed BCs, existence (fixed-point argument).

Numerics.

- Martin Kanitsar's code runs ≈ 2 days for 6 gradient descent steps.
- Installation of software: OpenFOAM (latest), additionally: FEniCS, Fireshape (on Firedrake, AD)[Paganini-Wechsung], AD, ROL.
- Started 2 Documentations: Understand Kanitsar's codes + Relevant parts of OpenFOAM.

Next Steps

Theory.

- Learn Shape and Adjoint Calculus.
- Literature on: turbulence/turbulent + adjoint
  - Hartmann, Ralf; Held, Joachim; Leicht, Tobias. *Adjoint-based error estimation and adaptive mesh refinement for the RANS and k-ω turbulence model equations*. J. Comput. Phys. 230 (2011), no. 11, 4268-4284.
  - Vishnampet, Ramanathan; Bodony, Daniel J.; Freund, Jonathan B. *A practical discrete-adjoint method for high-fidelity compressible turbulence simulations*. J. Comput. Phys. 285 (2015), 173–192.
  - Marta, Andre C.; Shankaran, Sriram. *On the handling of turbulence equations in RANS adjoint solvers*. Comput. & Fluids 74 (2013), 102–113.
  - Kavvadias, I. S.; Papoutsis-Kiachagias, E. M.; Dimitrakopoulos, G.; Giannakoglou, K. C. The continuous adjoint approach to the k-ω SST turbulence model with applications in shape optimization. Eng. Optim. 47 (2015), no. 11, 1523–1542. . . .
- Analyze the existence of optimization problems.
- Learn Turbulence (k-ϵ).
- Topology Optimization (TO).

Numerics.

- Learn OpenFOAM; Upgrade Martin Kanitsar's Code (2012) to latest version of OpenFOAM (considerable difference before/after 2016).

Targets

Theory.

- *1st Target*: Implementation of Shape Optimization on Semi-discrete NSEs in 3D + Turbulence.

$$\frac{\mathbf{v}^{n+1}-\mathbf{v}^{n}}{\Delta t}-\nu\Delta\mathbf{v}^{n+1}+(\mathbf{v}^{n+1}\cdot\nabla)\mathbf{v}^{n+1}+\nabla p^{n+1}=\mathbf{f}^{n+1} \text{ in } \Omega,\ n=1,\ldots,N.$$

- Continuous adjoint + Theoretical framework.
- Implementation of continuous adjoint and turbulence.

Software.

- Upgrade Software (e.g. OpenFOAM) to latest version.
- 2D version of codes.
- Replace Star-CCM+.
- Time-dependent case.

Mathematical Theory: A Roadmap

- In order to model the flow in the considered shape, use the stationary NSEs for the *velocity* $\mathbf{v}$ and the *kinematic pressure* p:

$$\begin{cases} -\nu\Delta\mathbf{v} + (\mathbf{v}\cdot\nabla)\mathbf{v} + \nabla p = \mathbf{f} \text{ in } \Omega, \\ \nabla\cdot\mathbf{v} = 0 \text{ in } \Omega, \\ \mathbf{v} = \mathbf{f}_{\mathrm{i}} \text{ on } \Gamma_{\mathrm{i}}, \\ \mathbf{v} = \mathbf{0} \text{ on } \Gamma_{\mathrm{w}}, \\ -\nu\partial_{\mathbf{n}}\mathbf{v} + p\mathbf{n} = \mathbf{0} \text{ on } \Gamma_{\mathrm{o}}, \end{cases} \tag{NSEs1}$$

  where $\mathbf{f}_{\mathrm{i}}$ is the *inflow profile*, ν is the *viscosity*, and $\mathbf{n}$ is the outer normal vector.

- **Weak formulation.** $(\mathbf{v}, p) \in W^{1,2}(\Omega)^3 \times L^2(\Omega)$ satisfying

$$\nu\int_\Omega \nabla\mathbf{v} : \nabla\mathbf{w} + \int_\Omega (\mathbf{v}\cdot\nabla)\mathbf{v}\cdot\mathbf{w} - \int_\Omega p\nabla\cdot\mathbf{w} = \int_\Omega \mathbf{f}\cdot\mathbf{w}, \ \forall\mathbf{w}\in V,$$
$$\nabla\cdot\mathbf{v} = 0 \text{ in } \Omega, \ \mathbf{v} = \mathbf{f}_{\mathrm{i}} \text{ on } \Gamma_{\mathrm{i}}, \ \mathbf{v} = \mathbf{0} \text{ on } \Gamma_{\mathrm{w}}.$$

- (Not yet) Existence of Optimal Shape.
- (Not yet) Shape Derivative and Optimality Condition; 2 Formulations: Domain and Boundary.

2nd BVP for NSEs

- A particular relevant case of [Maz'ya-Rossman2009]:

$$\begin{cases} -\nu\Delta\mathbf{v} + (\mathbf{v}\cdot\nabla)\mathbf{v} + \nabla p = \mathbf{f} \text{ in } \Omega, \\ -\nabla\cdot\mathbf{v} = g \text{ in } \Omega, \\ \mathbf{v} = \mathbf{f}_{\mathrm{i}} \text{ on } \Gamma_{\mathrm{i}}, \\ \mathbf{v} = \mathbf{0} \text{ on } \Gamma_{\mathrm{w}}, \\ -2\nu\varepsilon_{\mathbf{n}}(\mathbf{v}) + p\mathbf{n} = \mathbf{0} \text{ on } \Gamma_{\mathrm{o}}, \end{cases} \tag{NSEs2}$$

- **Weak formulation.** $(\mathbf{v}, p) \in W^{1,2}(\Omega)^3 \times L^2(\Omega)$ satisfying

$$b(\mathbf{v},\mathbf{w}) + \int_\Omega (\mathbf{v}\cdot\nabla)\mathbf{v}\cdot\mathbf{w}\,dx - \int_\Omega p\nabla\cdot\mathbf{w}\,dx = \int_\Omega \mathbf{f}\cdot\mathbf{w}\,dx, \ \forall\mathbf{w}\in V,$$
$$\nabla\cdot\mathbf{v} = 0 \text{ in } \Omega, \ \mathbf{v} = \mathbf{f}_{\mathrm{i}} \text{ on } \Gamma_{\mathrm{i}}, \ \mathbf{v} = \mathbf{0} \text{ on } \Gamma_{\mathrm{w}},$$

where $V := \{\mathbf{v}\in W^{1,2}(\Omega)^3; \mathbf{v} = \mathbf{f}_{\mathrm{i}} \text{ on } \Gamma_{\mathrm{i}}, \ \mathbf{v} = \mathbf{0} \text{ on } \Gamma_{\mathrm{w}}\}$, and

$$b(\mathbf{v},\mathbf{w}) := 2\nu\int_\Omega \sum_{i,j=1}^{3} \varepsilon_{ij}(\mathbf{v})\varepsilon_{ij}(\mathbf{w})\,dx \text{ where } \varepsilon_{ij}(\mathbf{v}) := \frac{\partial_{x_i}v_j + \partial_{x_j}v_i}{2}.$$

Theorem (Maz'ya-Rossman2009)

Assumptions.

- $\mathbf{f}_{\mathrm{i}} \in W^{1/2,2}(\Gamma_{\mathrm{i}})^3$ *s.t.* $\exists \mathbf{w} \in W^{1,2}(\Omega)^3$ *satisfying the conditions* $\mathbf{w}|_{\Gamma_{\mathrm{i}}} = \mathbf{f}_{\mathrm{i}}$ *and* $\mathbf{w}|_{\Gamma_{\mathrm{w}}} = \mathbf{0}$.
- *Suppose that* $L_V := \{w \in V; \varepsilon(\mathbf{w}) = \mathbf{0}\} = \{\mathbf{0}\}$ *and* $\|\mathbf{f}\|_{V^\star} + \|\mathbf{f}_{\mathrm{i}}\|_{W^{1/2,2}(\Gamma_{\mathrm{i}})^3}$ *is sufficiently small.*

Existence. *Then there exists a solution* $(\mathbf{v}, p) \in W^{1,2}(\Omega)^3 \times L^2(\Omega)$ *of* (NSEs2).

Uniqueness.

- $\mathbf{v}$ *is unique on the set of all functions with norm* $<$ *a certain* $\varepsilon > 0$.
- p *is unique (due to the BC on* Γ_{o}*).*

Cost Functional

Main Problem. Find an $\Omega \in \mathcal{O}_{\mathrm{ad}}$ s.t. 2 criteria are considered:

- **Uniform Outflow Criteria.** The normal component of the outflow $\mathbf{v} \cdot \mathbf{n}|_{\Gamma_{\mathrm{o}}}$ should be close to uniform on entire Γ_{o}.

  By conservation of mass, the average outflow is $\overline{v} = \frac{1}{|\Gamma_o|} \int_{\Gamma_i} -\mathbf{f}_i \cdot \mathbf{n}$. Consider:

$$\mathcal{J}_1(\mathbf{v}(\Omega)) := \frac{1}{2} \int_{\Gamma_o} (\mathbf{v} \cdot \mathbf{n} - \overline{v})^2.$$

- **Total Pressure Loss Criteria.** Bernoulli principle: The total pressure $p + \frac{1}{2}|\mathbf{v}|^2$ is a quantity that remains constant along the streamlines.

  Minimize the drop of pressure from $(p + \frac{1}{2}|\mathbf{v}|^2)|_{\Gamma_{\mathrm{i}}} > (p + \frac{1}{2}|\mathbf{v}|^2)|_{\Gamma_{\mathrm{o}}}$. Consider:

$$\mathcal{J}_2((\mathbf{v}, p)(\Omega)) := -\frac{|\Gamma_i|}{|\Gamma_i^{\varepsilon}|} \int_{\Gamma_i^{\epsilon}} \left(p + \frac{1}{2}|\mathbf{v}|^2\right) \mathbf{v} \cdot \mathbf{n} - \frac{|\Gamma_o|}{|\Gamma_o^{\varepsilon}|} \int_{\Gamma_o^{\varepsilon}} \left(p + \frac{1}{2}|\mathbf{v}|^2\right) \mathbf{v} \cdot \mathbf{n}.$$

Mixed Cost Functional

$$\mathcal{J}_{12}(\mathbf{v}(\Omega)) := (1-\gamma)\mathcal{J}_1(\mathbf{v}(\Omega)) + \gamma\rho\mathcal{J}_2(\mathbf{v}(\Omega)), \tag{$\mathcal{J}_{12}$}$$

with the *weighting parameter* $\gamma \in [0,1]$ and (not yet considered)

$$\rho := \begin{cases} \dfrac{\|\partial\mathcal{J}_1(\mathbf{v}(\Omega^0))\|_{L^2(\Gamma_w^0)}}{\|\partial\mathcal{J}_2(\mathbf{v}(\Omega^0))\|_{L^2(\Gamma_w^0)}} & \text{if } \gamma \in (0,1), \\ 1 & \text{if } \gamma \in \{0,1\}. \end{cases}$$

OpenFOAM's Structure

OpenFOAM layout constitutes of 2 main directories:

- `OpenFOAM-<version>`: OpenFOAM libraries
- `ThirdParty`: A set of third-party libraries.

OpenFoam Cases. configured by several plain text input files in 3 directories:

- `0/`: initial time directory including field files.
- `system/`: `controlDict, fvSchemes, fvSolution`
- `constant/`: `polyMesh/`, and files declaring constant values.

OpenFOAM Solvers.

- `Make/`: `files` (declare the main C++ file and its location to generate dependencies), `options` (include OpenFOAM libraries).
- `createFields.H`: Declare types of all variables needed.
- `<Solver-Name>.C`: Main script declared in `Make/`.

Outputs of Martin Kanitsar's Codes

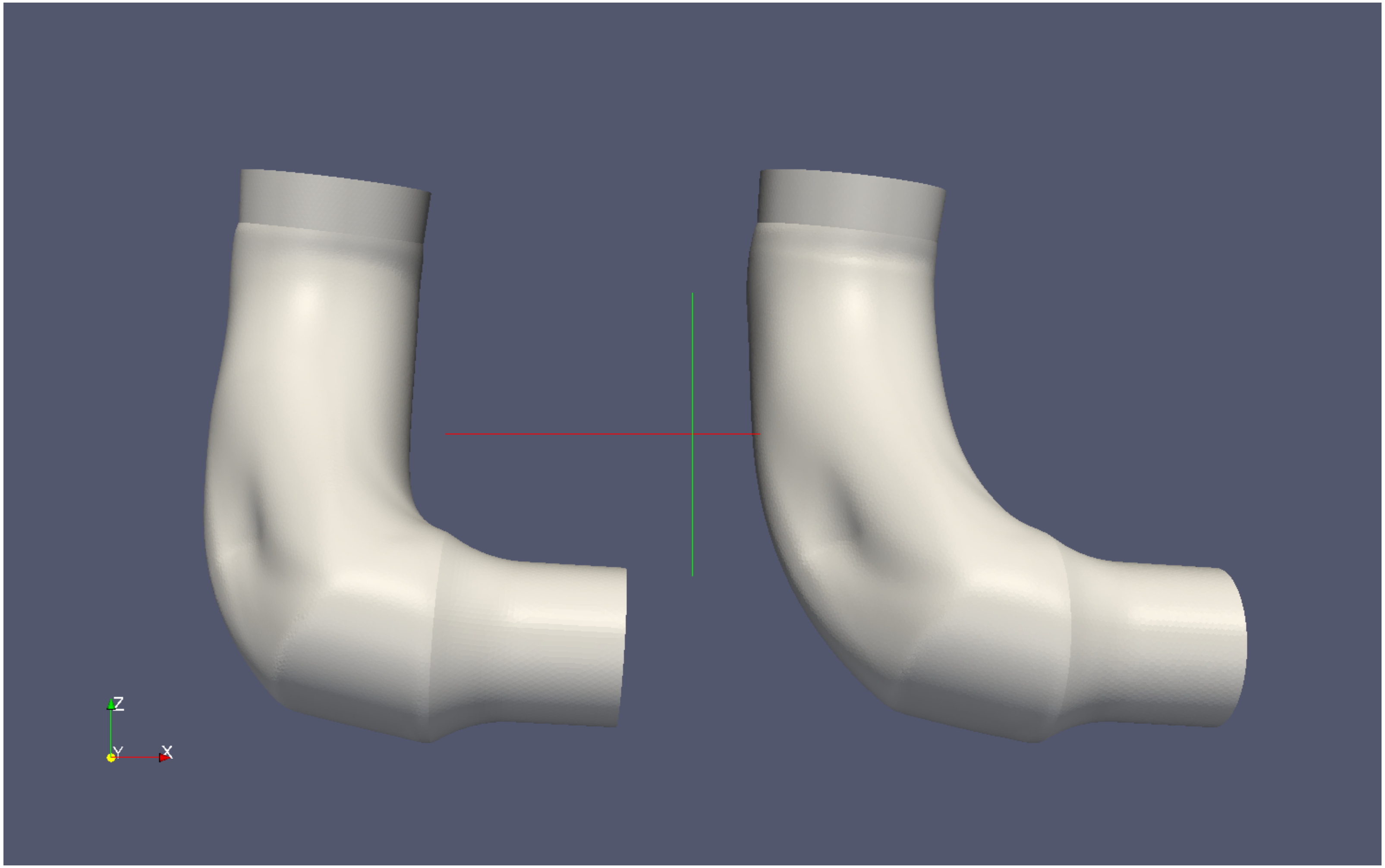


Figure: Left: Initial Tube. Right: Optimized Tube after 6 Gradient-Descent Iterations.

Values of Cost Functional $\mathcal{J}_{12}$

Choose the weighting parameter $\gamma = 1$ (`dp_J12` in Martin Kanitsar's code), so $\rho = 1$:

Iteration	$(1-\gamma)\mathcal{J}_1$	$\gamma\mathcal{J}_2$	$\mathcal{J}_{12}$
0	0	181.731920964434	182.07227883754
1	0	180.335741264281	180.929940529294
2	0	179.204741499965	180.136772627044
3	0	178.618996623167	179.571215644196
4	0	177.72661280195	179.091345594335
5	0	176.968052608864	178.804927417778
6	0	176.187919434572	178.048912220916

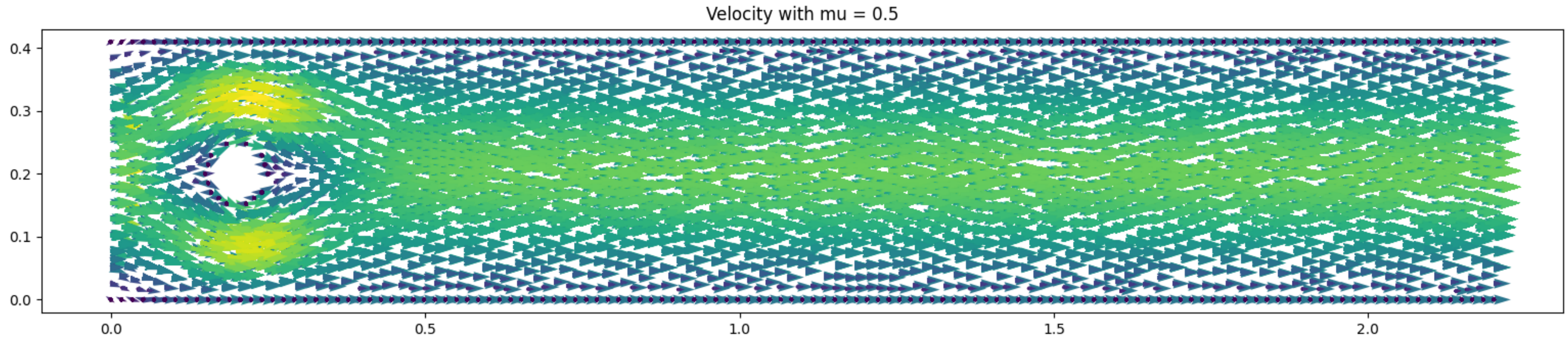
Q: *Why* $\mathcal{J}_{12} \neq (1-\gamma)\mathcal{J}_1 + \gamma\rho\mathcal{J}_2$*?*

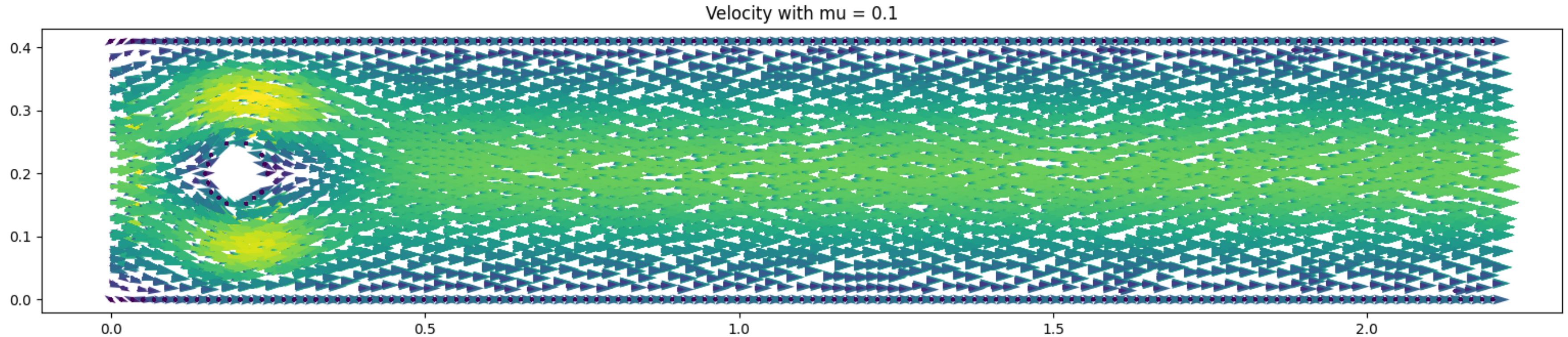
FEniCS

Example. Incompressible NSEs for flow around a cylinder:

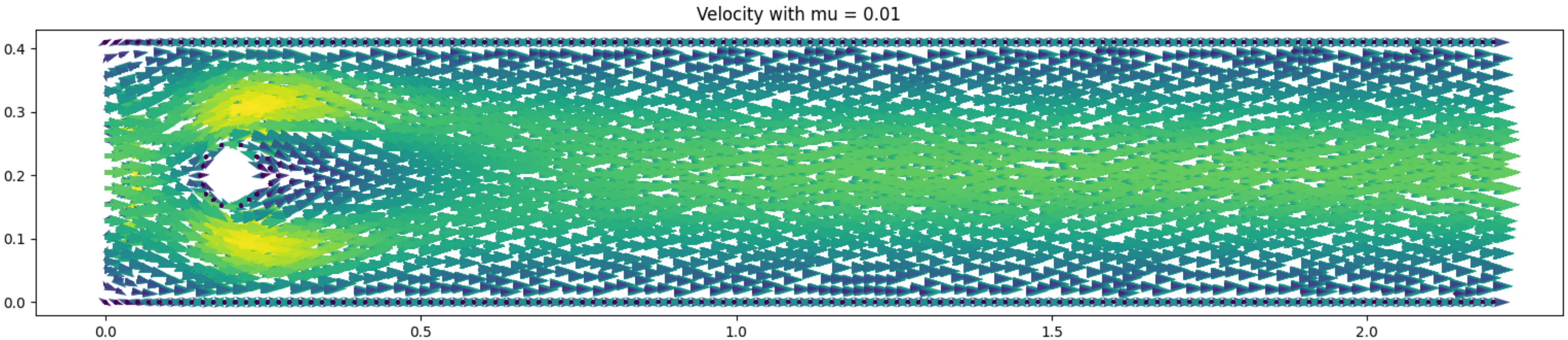
$$\mathbf{v}_t + (\mathbf{v} \cdot \nabla)\mathbf{v} - \nabla \cdot (\sigma(\mathbf{v}, p)) = \mathbf{f}, \ \nabla \cdot \mathbf{v} = 0,$$

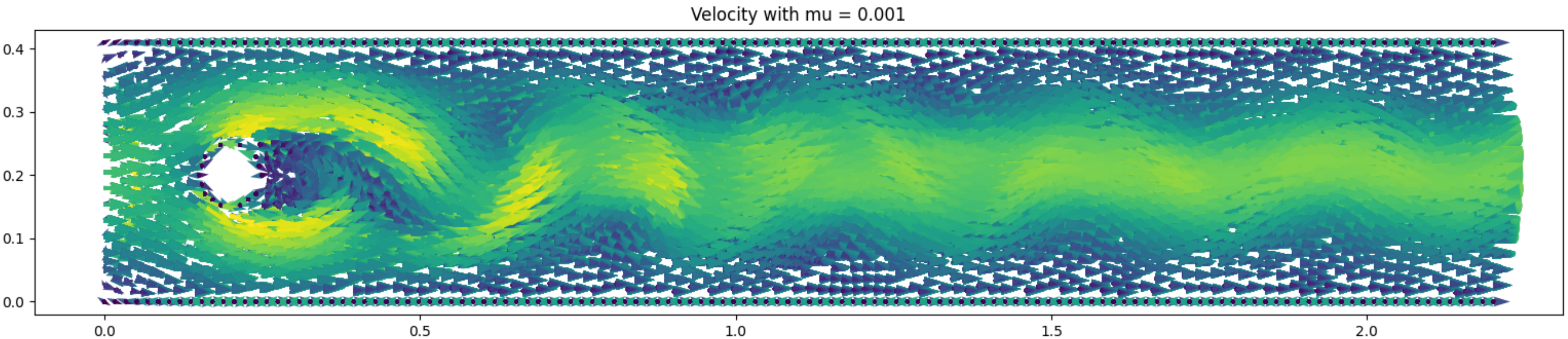
with $T = 5$, $dt = 10^{-3}$, $\mu = 0.5$, $\rho = 1$.





Velocities with Different Viscosities





Discussion

Mathematics.

- **Software for Fluids + Turbulence**: OpenFOAM, Star-CCM+ (SU2, ParMooN may be later).
- **Turbulence**: Which turbulence models are best?
- Realization in the code: Topology Optimization.
- Need to check its physical derivation + mathematical definition of functional $\mathcal{J}_2$.

Project.

- How frequently to spend 8 months in Austria?
- ROMSOC - Ethical Monitoring - 3rd Assignment.

Ethical Issues

Short description of issue.

- **ESR.** In this project, mathematical methods and software are developed for the purpose of improving combustion engines. The results could be used to improve the engine of a military vehicle after adjustments that require mathematical expert knowledge.
- **PI.** The developed tools can be applied to cases, where necessary conditions for a reliable output are not satisfied. This can cause misleading results, and then, wrong decisions with unintended implications.

Strategy used to cope with it.

- **ESR.** We will include a disclaimer, that excludes military use of the software.
- **PI.** Publications, preprints, technical reports are written in the course of this project. In this way, the results are explained, documented, and tested. Software tools should be well documented. The staff connected to the project is educated to understand the limits of applicability.

Ethics: 7. Ongoing Monitoring. Question 1

Could you successfully implement your strategy in order to cope with the issue? (implementation of strategy)

- **ESR.** A disclaimer excluding military use of the software will be stated in both the licence and the documentation of the software.
- **PI.** The implementation of the strategy can be monitored and evaluated by checking the licence and the documentation of the software. Software will be only available after contacting WIAS and signing the licence agreement.

Ethics: 7. Ongoing Monitoring. Question 2

In your and your PI's opinion, is the chosen strategy working and satisfying? (evaluation of strategy: efficacy and efficiency)

- **ESR.** Including a disclaimer in the licence and controlled access to the software are working and satisfying to prevent military use of the software.
- **PI.** A signed statement is an effective and efficient method and give the legal option against violators.

Ethics: 7. Ongoing Monitoring. Question 3

Which are good markers, indicators and/or hints that the strategy is working a) effectively and b) efficently?

- **ESR.** Controlled access to the software and feedback from the community by users.
- **PI.** Controlled access to the software and feedback from the community by users.

Ethics: 7. Ongoing Monitoring. Question 4

Is there a sub-project and issue specific written and documented agreement between ESR and PI on:

a) **how, when and by whom the strategy will be monitored until the end of the project?**

ESR. a) The ESR writes the licence and the PI will monitor the strategy frequently during ESR's work at WIAS.

PI. a) The ESR writes the licence and the PI will monitor the strategy frequently during ESR's work at WIAS.

b) **how the monitoring will be documented?**

ESR. b) The PI will monitor in exchange with the ESR the documentation of the process.

PI. b) The PI will monitor in exchange with the ESR the documentation of the process.

c) **how ethical monitoring after the end of the project should be assured?**

ESR. c) The monitoring will be done by the Institute where the ESR is affiliated.

PI. c) The monitoring will be done by the Institute where the ESR is affiliated.

References

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