Handbook for Software
Shape- and Topology Optimization

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Software-Version: 1612.

Contents

1 Installation

1.1 Folder structuring and compilation of the applications

To use the shape and topology optimizations, the standard installation of OpenFOAM `$FOAM_APP/solvers/incompressible/` must be extended by the following applications:

- `generateFieldsFoam`
- `shapeGradientWall`
- `shapeGradientCCM`
- `setupShapeGradientCCM`
- `shapeGradientAddSTL`
- `shapeGradientCloseAll`
- `topoOpt`
- `topoOptCloseAll`
- `topoExtractSTL`

The folder `InitialSGccm` must be copied into the `$FOAM_RUN/tutorials/` directory. The console commands for installation can be found in the shell-script `installShapeGradient.sh`.

2 Geometry Data

2.1 Storage structure of the data in STL format

The geometry data must be created in the `initial_stl` folder. In addition to the installation space geometry (`bds.stl`), the surfaces are saved in 4 files in STL format (`inlet.stl`, `fixed.stl`, `wall.stl`, `outlet.stl`).

The test geometry *M23* with 2 inlets, 3 outlets and an additional fixed geometry (see Table 1) serves as an illustration.

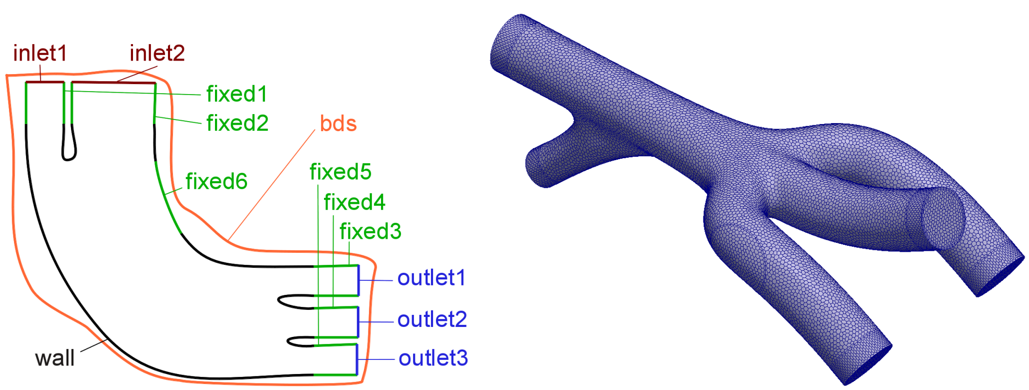


Figure 2.1: Left: Sketch geometry data, right: test geometry M23.

Each inlet and outlet area has a fixed geometry that describes the connection to the geometry to be optimized. Additionally, the user can define fixed geometries which are only connected to the geometry to be optimized (e.g.: `fixed6` in test geometry *M23*).

The fixed geometries are numbered consecutively, starting with the connections to the inlet geometry, continuing with the connections to the outlet geometry and ending with the fixed geometries that are only connected to the geometry to be shape optimized.

When selecting the installation space geometry, care should be taken to ensure that the start geometry is completely within the allowed range and extends beyond the `inti_freegeom_fixed-inlet` and `into_free-geom_fixed-outlet` interfaces (see Fig. 2.1).

Table 2. Geometric data in STL format.

`File name`: **Designation**: **Description**

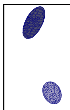
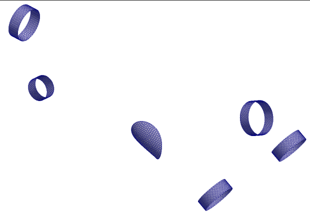
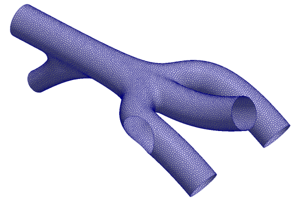
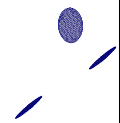
			
inlet.stl	fixed.stl	wall.stl	outlet.stl
inlet1 inlet2	fixed1 [inlet1] , fixed2 [inlet2] fixed3 [outlet1] , fixed4 [out-let2] fixed5 [outlet3] , fixed6	wall.stl	outlet.stl

Table 1: Geometric data in STL format.

File name	Designation	Description
inlet.stl	inlet1, inlet2, inlet3	Inflow geometries.
outlet.stl	outlet1, outlet2, outlet3	Outflow geometries.
fixed.stl	fixed1, fixed2, fixed3, fixed4, fixed5, fixed6, fixed7, fixed8, fixed9	Geometric data of the fixed areas.
wall.stl	wall	Geometric data of the area to be optimized.
bds.stl	bds	Geometric data of the installation space.

Table 2: Geometric data in STL format.

- `inlet.stl`: inlet1, inlet2, inlet 3: Inflow geometries.
- `outlet.stl`: outlet1, outlet2, outlet3: Outlet geometries.
- `fixed.stl`: fixed1, fixed2, fixed3, fixed4, fixed5, fixed6, fixed7, fixed8, fixed9: Geometric data of the fixed areas.
- `wall.stl`: wall: Geometric data of the area to be optimized.
- `bds.stl`: bds: Geometric data of the installation space.

2.2 Modeling of the inflow/outflow areas

The following preparation serves to represent the modeling of an application with regard to the surface geometries of the inflow areas and the outflow areas.

2.2.1 Inflow areas

Any number of inlet flow ranges can be defined. An inflow area can also consist of several unconnected geometries. The characteristic of an inlet flow area is not the shape/topology but the physical properties, e.g: face velocity.

- Therefore an application with the same inflow velocity can also be modeled with an inflow area (left graph in Fig. 2.2).
- If there are different inflow velocities in the application, different inflow ranges must be defined (right graph in Fig. 2.2).

2.2.2 Outflow areas

Any number of discharge ranges can be defined. Analogous to the definition of the inlet flow ranges, the definition of the outlet flow ranges must be made on the basis of the physical properties. In the previous applications, however, the 'do nothing' boundary condition was always used uniformly. The division into different discharge ranges is also relevant if different discharge profiles are desired. Figure 2.3 illustrates the two optimization variants for a uniform flow ($\mathcal{J}_1$).

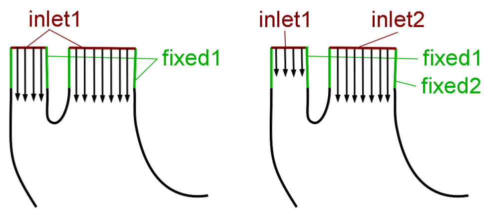


Figure 2.2: Figure 2.2: Inflow areas.

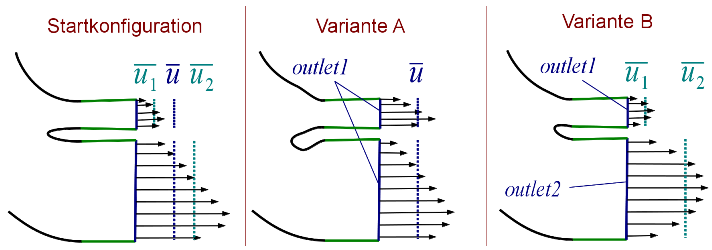


Figure 2.3: Fig. 2.3: Left: Start. Middle: Optimization $\mathcal{J}_1|_{\Gamma^1_{\mathrm{out}} \cap \Gamma^2_{\mathrm{out}}}$. Right: Optimization $\gamma_1 \mathcal{J}_1|_{\Gamma^1_{\mathrm{out}}} + \gamma_2 \mathcal{J}_1|_{\Gamma^2_{\mathrm{out}}}$.

2.3 User defined inflow profile

If an inflow profile is to be specified, the corresponding entry in the parameter `velocity_ massflow` must be set to 0 and a file `velocity_inletI.csv` with $I = \{0, 1, 2, \ldots\}$ must be specified in the order of the test calculation. If, in the example M23, a profile is to be specified at the 2nd inflow area, `velocity_massflow` $= 2(36.5, 0)$ must be set and a file `velocity_inlet2.csv` must be created.

2.4 Initial geometry Topology optimization

For topology optimization, the largest possible initial geometry should be specified. Figure 2.4 shows an initial geometry for the application example clean air tube (RLR).

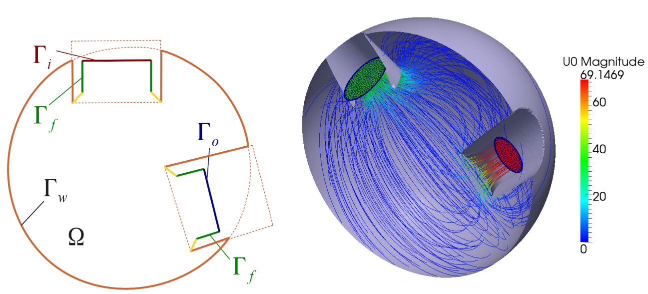


Figure 2.4: Figure 2.4: Initial geometry Topology Optimization RLR.

3 Parameters and their meaning

In addition to the geometry data, the parameter file `parameter_sg` must be created. The parameters contained in this file are explained in this chapter. The parameters are inserted in the Java scripts `mbmw3.java, solvePrimal.java` and `solveAdjoint.java`. If changes are to be made in the Star-CD CCM+ usage, these 3 files in the `initialSG` folder must be adapted. The parameters relevant for OpenFOAM are stored in `system/fvSolution` after calling the setup routine.

3.1 Grid generation

In Star-CD CCM+ a polyhedron grid is created. The grid fineness is defined by the Reference value for the cell size `base_size` adjustable. The number of inlets and outlets as well as the number of optional fixed surfaces must be specified (`numInlet, numOutlet, numFixed`). The mesh quality for mesh generation can be increased through the `mesh_opt_cycles` and `mesh_quality_treshold` parameters. Layer layers are to be used near the wall. The size and number of these layers

Parameter name	Default value	Admissibility	RLR	M23	Description
`install_location`					Path of the star CD CCM+ bin file to start CCM+.
`prozessNumber`	2	[1,100]	2	2	Number of processors with parallelization in Star-CD CCM+.

Table 3: Parameter Star-CD CCM+.

is defined by the `num_layer_wall`, `thick_layer` and `layer_stretch` parameters. To prevent backflow on the outflow geometry ('do-nothing' boundary condition), usually an additional extrusion geometry is required. The adjustment of length and discretization can be done with the parameters `extrude_...` parameters. The grid is locally refined in CCM+ on the basis of the surface condition. If this refinement is not the parameter `grid_local_refinement` is to be set to 0.

Parameter-name	Default value	Admissibili	RLR	M23	B135	Description
base_size	0.004	[1e-4,0.1]	0.004	0.03	0.04	Grid fineness: Cell size.
numInlet	1	{1,2,...1e3}	1	2	1	Number of inflow areas.
numOutlet	1	{1,2,...1e3}	1	3	1	Number of outlet areas.
numFixed	0	{0,1,...1e3}	0	1	0	Number of optional fixed geometries.
num_layer_wall	2	[0,6]	2	3	6	Number of layer layers at the edge.
thick_layer	60	[10,100]	80	60	60	Thickness of the layer layers in percent (relative to neighboring cell size).
layer_stretch	1.5	[1e-3,1e3]	1.5	1.5	1.4	Magnification factor of the layer layers.
extrude_ outlet_length	0.05	[1e-8,1e8]	0.06	0.2	1.2	Length of the extrusion geometry at the outlet.
extrude_ outlet_num	32	[1,1e5]	20	10	90	Number of cell layers in the extrusion geometry at the outlet.
extrude_ outlet_stretch	1	[1e-3,1e3]	1	1	1	Magnification factor of the layers in the extrusion geometry at the outlet.
extrude_ inlet_length	0.025	[1e-8,1e8]	0.03	0.2	0.2	Length of the extrusion geometry at the inlet.
extrude_ inlet_num	16	[1,1e5]	10	10	15	Number of cell layers in the extrusion geometry at the inlet.
extrude_ inlet_stretch	1	[1e-3,1e3]	1	1	1	Magnification factor of the layer layers in the extrusion geometry at the inlet.
mesh_opt_ cycles	8	[1,8]	8	8	8	Polyhedron mesh: Quality optimization loops.
mesh_quality _treshold	1	[0,1]	1	1	1	Polyhedron mesh: quality optimization barrier.
grid_local_ refinement	0	{0,1}	0	1	1	Local grid refinement: 0:no, 1:yes.
ext_merge	0	{0,1}	0	1	0	Combine extrusion geometry with fixed geometries: 0:no, 1:yes

Table 4: Parameters for grid generation in Star-CD CCM+.

3.2 Model selection and physical settings

To specify the flow velocity, either a constant inflow velocity in m/s or the mass flow rate in kg/s can be entered (`velocity_massflow_pa` = 0 or 1). The values are defined by the parameter `velocity_massflow` to be specified. The corresponding syntax is shown in table 5.

Beside the direct numerical simulation (`turb_model` = 0) currently 4 turbulence models can be selected with the parameter `turb_model`. If other turbulence models prove to be suitable for future software versions, the JavaScript *mbmw3.java* must be adapted accordingly. Furthermore, the following model parameters must be specified in Star-CD CCM+: `inlet_turb_intensity`, `inlet_visc_ratio`, `outlet_turb_intensity`, `outlet_visc_ratio`.

Parametername	Default value	Admissibili	RLR	M23	B135	Description
turb_model	2	[0,100]	1	0	4	0: DNS, 1: Realiz. k-ε all Y+, 2: Std. k-ε high Y+, 3: RSM all Y+, 4: Realiz. k-ε low Y+.
velocity_massflow_par	0	{0,1}	0	0	0	Inflow: 0:velocity, 1:mass flow.
velocity_massflow	1(0.1)	[1e-8,1e8]	1(36.5)	2(0.006, 0.006)	1(4.3)	Inflow (velocity or mass flow)
inlet_turb_intensity	0.1	[1e-8,1e8]	0.1		0.1	Turbulent Intensity Inlet.
inlet_turb_length	10	[1e-8,1e8]	0.1		10	Turbulent Length Scale Inlet.
outlet_turb_intensity	0.1	[1e-8,1e8]	0.1		0.1	Turbulent Intensity Outlet.
outlet_turb_length	10	[1e-8,1e8]	0.1		10	Turbulent Length Scale Outlet.

Table 5: Parameters for physical models.

3.3 Solver settings for the primary and adjoint equation

The solvers in CCM+ use a pseudo time-stepping method. The step size control is to be specified by the Courant-Friedrichs-Lewy number (`CFLpri, CFLadj`). The choice of a large number allows a faster achievement of the desired solution, but can lead to convergence problems if the choice is too large. For the adjoint equation a GMRES solver (`gmresAdj`) with the relevant settings `krylov_dim`, `krylov_accuracy` is available in addition to the standard solver.

As termination criteria the maximum number of iterations (`iterPri, iterAdj`) and a termination at desired accuracies are used. The second is achieved if the standard deviation is below the tolerance values (`stop_accuracyPri`, `stop_accuracyAdj`). If you choose `stop_sample` e.g. 100, the standard deviation of the last 100 iterations is always calculated.

The primary solver is considered to be out-converged if the desired solution accuracy is achieved before reaching the `iterPri` iteration. If the accuracy is not reached after `iterPri` steps, a smaller step size is chosen for the grid shift. It is therefore important to make sure that `iterPri` is always selected large enough!

If convergence problems of the adjoint solver occur, the parameter `adj_order` must be set to 1.

3.4 Line search

In the course of shape optimization we use a step size control based on the grid quality query and the query for a sufficiently large reduction of the function value. The rule used is called *Armijo line search* and reads

$$\mathcal{J}_{12}^{\alpha}\left(\Omega^{k+1}\right) \leq \mathcal{J}_{12}^{\alpha}\left(\Omega^{k}\right) - \mu s_k \|\mathcal{D}\mathcal{J}_{12}^{\alpha}\left(\Omega^{k}\right)\|_{L^2(\Gamma_w^k)} \tag{3.1}$$

with $0 < \mu < 1$ and $\Omega^{k+1} = \mathcal{T}_{D(s_k,\Omega^k)}(\Omega^k)$. The mapping $T_D(s_k,\Omega^k)(\Omega)(\boldsymbol{x}) : \mathbb{R}^3 \to \mathbb{R}^3$ is determined by the shape gradient.

The user must specify a start step size s_0 (`spStepLength`). In case the condition (3.1) is not fulfilled, the step length is reduced by the factor `spReduceKoeff`. The reduction of the step size is performed until the step size is smaller than the value `spLowerBound`. After that a mesh reconnection is performed. The weighting $\mu > 0$ (`linesearch weight`) ensures a sufficiently large descent, which is relevant for the mathematical consideration of the line search. For numerical applications this parameter should be set rather small. If you want to force a mesh re-connection after a certain number of iterations, you can use the parameter `remesh_iter`. Usually a mesh reconnection is not necessary if the mesh is valid. Thus this value was set higher than the maximum number of iterations in the calculations.

3.5 Termination criteria for shape optimization

Table 8 shows the parameters for completing the shape optimization. The most relevant parameters are the maximum number of iterations (`outerLoopEnd`), the number of remeshings performed (`rem_max`) and the progress in the target functional (`sigma_stop_J`).

Parameter-name	Default value	Admiss	RLR	M23	B135	Description
ccm_solver	1	{0,1}	1	1	1	1: Use of CCM+ solver, 0: Alternative solver.
gmresAdj	0	{0,1}	0	0	0	Adjoint solver: 0: without GMRES, 1: with GMRES.
krylov_dim	50	[1,1e5]				Number of Krylov spaces (adj, GMRES).
krylov_accuracy	1e-12	]0,1]				Calculation accuracy Krylov spaces.
CFLpri	4	[0.1, 1000]	4	3	4	CFL primal.
CFLadj	100	[0.1, 10000]	90	40	90	CFL adjoint.
stop_accuracyPri	1e-12	]0,1]	1e-12	1e-12	1e-8	Termination criterion standard deviation: accuracy of primary solution.
stop_accuracyAdj	1e-12	]0,1]	1e-12	1e-12	1e-12	Abbruchkriterium Standardabweichung: Genauigkeit adjungierte Lösung.
stop_sample	100	[1,1e5]	200	50	50	Termination criterion standard deviation: accuracy of adjoint solution.
iterPri	2000	[1,1e4]	4000	2500	1200	Maximum iteration count of the primary equation after a remeshing.
iterAdj	1000	[1,1e5]	3000	2000	1000	Maximum iteration number of the adjoint equation after a remeshing.
adj_order	2	{1,2}	2	2	1	Discretization Adjoint order.

Table 6: Parameters for the solvers in Star-CD CCM+.

3.6 Shape optimization: Target functionalities.

3.6.1 Uniform discharge and total pressure loss

Shape optimization can be carried out with regard to achieving a uniform outflow and minimizing the total pressure loss. The discrete objective functional with regard to uniform outflow is

$$\mathcal{J}_1 = \frac{\sqrt{\frac{1}{A}\sum\limits_{k\in\Gamma_o}\left(\boldsymbol{u}_k\cdot\boldsymbol{n}_k-\bar{u}\right)^2 A_k}}{\bar{u}} \tag{3.2}$$

with

$$\bar{u} = \frac{1}{A}\sum_{j\in\Gamma_o}\boldsymbol{u}_j\cdot\boldsymbol{n}_j A_j, \tag{3.3}$$

where $A = |\Gamma_o|$. The discrete objective functional with regard to minimizing the total pressure loss is

$$\mathcal{J}_2 = \left|\frac{\sum\limits_{k\in\Gamma_i}\left(p_k+\frac{\rho_k}{2}\left(\boldsymbol{u}_k\cdot\boldsymbol{u}_k\right)\right)\boldsymbol{u}_k\cdot\left(-\boldsymbol{n}_k\right)\ A_k}{\sum\limits_{k\in\Gamma_i}\boldsymbol{u}_k\cdot\left(-\boldsymbol{n}_k\right)A_k}\right| - \left|\frac{\sum\limits_{k\in\Gamma_o}\left(p_k+\frac{\rho_k}{2}\left(\boldsymbol{u}_k\cdot\boldsymbol{u}_k\right)\right)\boldsymbol{u}_k\cdot\boldsymbol{n}_k\ A_k}{\sum\limits_{k\in\Gamma_o}\boldsymbol{u}_k\cdot\boldsymbol{n}_k A_k}\right|. \tag{3.4}$$

With $\boldsymbol{u}_k$ we denote the velocity vector at the finite surface with index k. The pressure p_k and the density ρ_k is also evaluated at the finite surface with index k. In order to keep the notation simple, we denote the index quantity of all surface pieces at the inflow and outflow geometry with Γ_i and Γ_o respectively. The surface dimension of a finite surface is denoted with A_k. The outwardly directed unit normal vector is designated with $\boldsymbol{n}_k$. The unit normal vector $\boldsymbol{n}_k$ on Γ_i is oriented against the main flow direction. This results in the mixed objective functional:

$$\mathcal{J}_{12}\left(\boldsymbol{u}\left(\Omega\right)\right) = \left(1-\gamma\right)\mathcal{J}_1\left(\boldsymbol{u}\left(\Omega\right)\right) + \gamma\rho\mathcal{J}_2\left(\boldsymbol{u}\left(\Omega\right)\right) \tag{3.5}$$

Parameter name	Default value	Admis	RLR	M23	Description
spStepLength	2.0e-6	[0,1]	1e-4	1e-2	Start step size s_0 in the Armijo line search 3.1.
spLowerBound	1.0e-8	[0,1]	1e-6	1e-5	Lower limit of the step width.
spReduceKoeff	0.5	[0,1]	0.6	0.5	Reduction factor for step size control.
linesearchGewicht	1.0e-16	[0,1]	1e-14	0	Weighting μ in Armijo line search.
remesh_iter	1000	[1,1e5]	900	10	Remeshing in every ... 10 iterations (even if grid quality is OK).

Table 7: Parameters for line search in OpenFOAM..

Parameter name	Default value	Admissibil	RLR	M23	Description
outerLoopEnd	8	[1,1e5]	200	200	Maximum number of iterations.
rem_max	20	[1,1000]	30	30	Maximum number of remeshings performed.
rem_num_max	8	[1,1000]	30	30	Maximum number of remeshings with rem_tol distance.
rem_tol	2	[0,100]	2		Distance tolerance for remeshing.
sigma_stop_J	50	[0,100]	100	100	Termination criterion: Progress in % in target function J. Notation: σ.
sigma_stop_DJ	50	[0,100]	100	100	Abort criterion: Progress in % in the L2 norm of the shape gradient. Notation: σ_d.

Table 8: Termination criteria of shape optimization in OpenFOAM.

$$\text{with} \quad \gamma \in [0,1] \quad \text{and} \quad \rho = \begin{cases} \frac{\|\partial \mathcal{J}_1(\boldsymbol{u}(\Omega^0))\|_{L^2(\Gamma_w^0)}}{\|\partial \mathcal{J}_2(\boldsymbol{u}(\Omega^0))\|_{L^2(\Gamma_w^0)}} & \text{if } \gamma \in (0,1)\,, \\ 1 & \text{if } \gamma \in \{0,1\}, \end{cases}$$

with the weighting parameter γ (`dp_J12`). The parameters `gnu_plot_visual` and `gnu_plot_visual_i` are used for the graphical representation of the target function values.

If this option is selected, the graphics appear during shape optimization and are stored in the Test Run folder under `Function_values_J1.ps`, `Function_values_J2.ps` and `Function_values_J12.ps`.

3.6.2 Target functionalities with multiple outflow ranges

For illustration we use 3 outflow areas and call them Γ_o^a, Γ_o^b, Γ_o^c. The target functionalities for the even outflow are

$$\mathcal{J}_1 = \mathcal{J}_1|_{\Gamma_o^a \cup \Gamma_o^b \cup \Gamma_o^c}, \quad \mathcal{J}_{1a} = \mathcal{J}_1|_{\Gamma_o^a}, \quad \mathcal{J}_{1b} = \mathcal{J}_1|_{\Gamma_o^b}, \quad \mathcal{J}_{1c} = \mathcal{J}_1|_{\Gamma_o^c}. \tag{3.6}$$

The mixed objective functional is:

$$\begin{aligned} \mathcal{J}_{12} \;=\; & (1-\gamma)\,(1-\gamma_a-\gamma_b-\gamma_c)\,\rho_1\mathcal{J}_1 && (3.7) \\ & +(1-\gamma)\,\gamma_a\rho_{1a}\mathcal{J}_{1a} + (1-\gamma)\,\gamma_b\rho_{1b}\mathcal{J}_{1b} + (1-\gamma)\,\gamma_c\rho_{1c}\mathcal{J}_{1c} && (3.8) \\ & +\gamma\rho_2\mathcal{J}_2 && (3.9) \end{aligned}$$

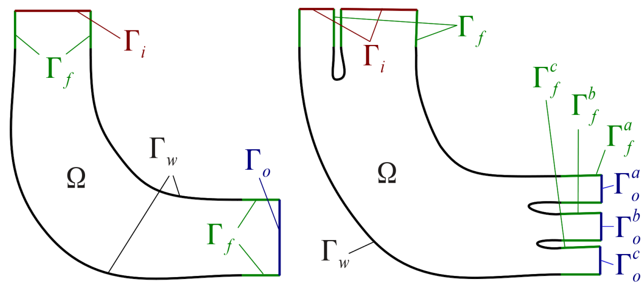


Figure 3.1: Skizze von Ω mit Bezeichnung der Teile der Oberfläche.

Parameter name	Default value	Admissibilit	RLR	M23	Description
dp_J12	0.5	[0,1]	0.5	0.5	Weighting parameter γ between $\mathcal{J}_1$ and $\mathcal{J}_2$.
dp_J1	1(0)	$\sum$ dp_J1 $\in$ [0,1]	1(0)	3(0.25, 0.25,0.25)	Weighting parameter γ_i concerning $\mathcal{J}_1$.
gnu_plot_visual	0	{0,1}	0	0	Graphic display of the target function values (1). No graphical representation (0).
gnu_plot_visual_i	3	[1,1000]	1	1	Update the graphics after ... iterations.

Table 9: Form optimization: Target functionalities

with the user-defined weighting parameters $\gamma, \gamma_a, \gamma_b, \gamma_c \in [0,1]$ (`dp_J12`, `dp_J1`) where $\gamma_a + \gamma_b + \gamma_c \leq 1$ and the scales ρ_1, ρ_2, ρ_{1a}, ρ_{1b}, ρ_{1c}, which are calculated as follows if $\gamma < 1$. We define

$$\mu_{uni} = \max\Big(\hat{\gamma}_1 \left\|\partial \mathcal{J}_1 \left(\boldsymbol{u}\left(\Omega^0\right)\right)\right\|_{L^2(\Gamma_w^0)}, \hat{\gamma}_a \left\|\partial \mathcal{J}_{1a} \left(\boldsymbol{u}\left(\Omega^0\right)\right)\right\|_{L^2(\Gamma_w^0)}, \tag{3.10}$$

$$\hat{\gamma}_b \left\|\partial \mathcal{J}_{1b} \left(\boldsymbol{u}\left(\Omega^0\right)\right)\right\|_{L^2(\Gamma_w^0)}, \hat{\gamma}_c \left\|\partial \mathcal{J}_{1c} \left(\boldsymbol{u}\left(\Omega^0\right)\right)\right\|_{L^2(\Gamma_w^0)}\Big) \tag{3.11}$$

where Ω^0 and Γ_w^0 the geometry in the area and at the edge is at the beginning of the shape optimization and

$$\hat{\gamma}_1 = \begin{cases} 0 & \text{if } \gamma_a + \gamma_b + \gamma_c = 1, \\ 1 & \text{if } \gamma_a + \gamma_b + \gamma_c < 1, \end{cases} \quad \hat{\gamma}_I = \begin{cases} 0 & \text{if } \gamma_I = 0, \\ 1 & \text{if } \gamma_I > 0, \end{cases} \text{with } I \in \{a, b, c\}. \tag{3.12}$$

The scaling parameters are

$$\rho_k = \frac{\mu_{uni}}{\left\|\partial \mathcal{J}_k \left(\boldsymbol{u}\left(\Omega^0\right)\right)\right\|_{L^2(\Gamma_w^0)}} \text{ with } k \in \{1, 2, 1a, 1b, 1c\}. \tag{3.13}$$

If $\gamma = 1$, then $\rho_1 = 1$ is set.

3.7 Geometric restrictions

The shape optimization is subject to 2 geometrical restrictions:

- Installation space restriction: An optimum geometry is sought within a fixed installation space.
- Transition restriction: At the transition between the geometry to be shape-optimized and the fixed geometry an edge should be avoided to avoid problems in the flow simulation.

3.7.1 Method 1: Fixing at the transition area

Shape gradient at the centers of the surfaces adjacent to the fixed geometry set to 0.

Numerical calculation at these locations is not trustworthy. In previous calculations the shape gradient was automatically set to zero on these areas. This is also recommended for further test calculations. The setting is done with the parameter: `uer_fix_faces` (0:do not fix, 1: fix).

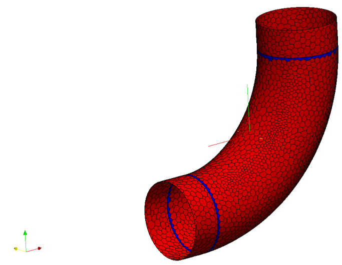


Figure 3.2: BLUE: Faces on which the shape gradient is set to 0 at the center of the surface.

3.7.2 Method 2: Use of objective functionals for installation space and transition restrictions

To take these restrictions into account in shape optimization, the previously used objective function $\mathcal{J}_12$ is extended to

$$\mathcal{J}_{12}^{\alpha,\varphi}\left(\boldsymbol{u}\left(\Omega\right)\right) = \mathcal{J}_{12}\left(\boldsymbol{u}\left(\Omega\right)\right) + \alpha\mathcal{L}\left(\Omega\right) + \varphi\mathcal{L}_F\left(\Omega\right)$$

with $\mathcal{L}\left(\Omega\right) = \int_\Omega \ell\left(x\right)$, $\mathcal{L}_F\left(\Omega\right) = \int_\Omega (d(x, K_F))^2$, the weighting parameters $\alpha \geq 0$ (`installation_weighting`), $\varphi \geq 0$ (`fixed_weighting`) and the distance function $d(x, K_F) = c_1 \min_{y\in K_F} |x-y|$. In the case of the barrier method, $l(x) = |\log d(x, K^c)|$ and in the case of the penalty method, $l(x) = c_2(d(x, K))^\beta$, with $\beta > 0$ (`bauraum_straf_potenz`). The scaling factors c_1, c_2 are discussed in section 3.7.3. The geometry K denotes the installation space geometry, $K^c = \mathbb{R}^n \backslash K$ and the geometry K_F denotes the permissible range of the geometry in the transition between the fixed parts and the parts to be optimized. The `bauraum_restriction` parameter specifies whether and/or which method is to be used for dealing with the installation space restriction. The parameters `OuterLoopCycleNr` (Table 8) and `bauraum_modification_scale` can be used to increase (in case of the penalty method) or decrease (in case of the barrier method) the installation space weighting α during the shape optimization process. Figure 3.4 shows transition curves for three different parameter settings. In order to avoid strong curvatures of the geometry, the variant in green color is recommended.

Within the area defined by the distance to the fixed geometry (`uer_bereich`) the transition restriction is applied. The user can control the restriction geometry with the parameters: `uer_pow` (degree of power function of the nonlinear portion), `uer_nonlinear`, and `uer_linear` (see Fig. 3.3).

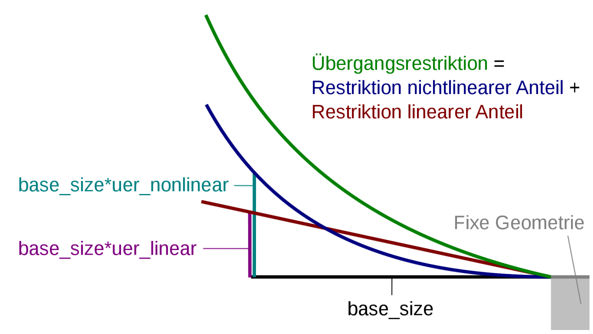


Figure 3.3: Transition geometry.

3.7.3 Heuristic scaling of the target functionals in geometrical restrictions

To achieve equal orders of magnitude of geometric objective functionals and physical objective functionals, we use a scale c_1 of the spatial coordinates and a scale c_2 of the function $l(d)$ using the starting geometry Ω^0. In the case of the **penalty method**, the parameters c_1 and c_2 are chosen so that the equations

$$\int_{\Sigma(d_{min})} \int_0^{c_1 d_{max}} c_2 d^\beta \mathrm{d}d = \mathcal{J}_{12}\left(\boldsymbol{u}\left(\Omega^0\right)\right), \tag{3.14}$$

$$c_2\left(c_1 d_{max}\right)^\beta = \|\mathcal{D}\mathcal{J}_{12}^\alpha\left(\Omega^0\right)\|_{L^\infty(\Gamma_w^0)} \tag{3.15}$$

where $d_{\min}$ and $d_{\max}$ are to be specified by selecting the `dminDS` and `dmaxDS` parameters for the installation space restriction (or analog `dminIF` and `dmaxIF` for the transition restriction). In the case of the **barrier method**, an effective installation space can be selected instead of the geometric installation space (`bds.stl`). In this case the installation space is increased

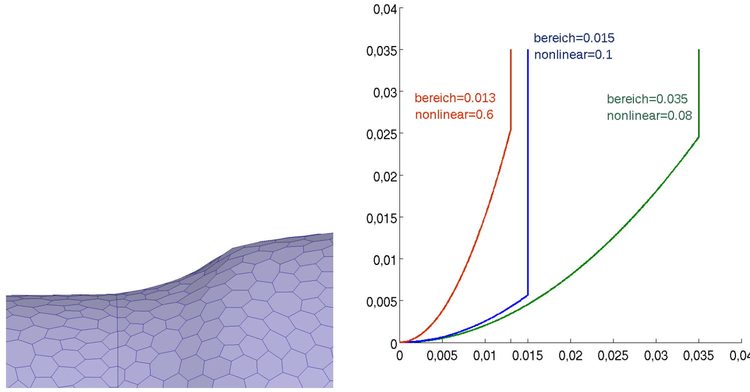


Figure 3.4: Left: Geometry at the transition. Right: different transition restrictions.

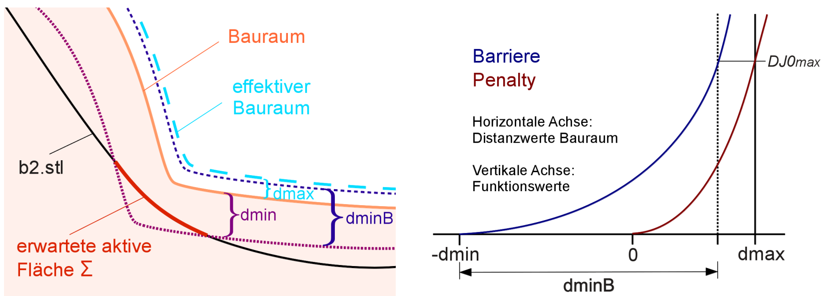


Figure 3.5: Left: Sketch installation space. Right: Functions: Penalty, Barrier.

by the length **dmaxDS** (unit in meters). If this parameter is set to 0, the effective installation space is equal to the geometric installation space. The setting of **dmaxDS** greater than 0 is intended in particular for those cases where the start geometry lies outside the geometric installation space. The scaling variables c_1 and c_2 are selected so that the equations

$$\int_{\Sigma(d_{min})} \int_0^{c_1 d_{minB}} c_2 d^\beta \mathrm{d}d = \mathcal{J}_{12}\left(\boldsymbol{u}\left(\Omega^0\right)\right), \tag{3.16}$$

$$c_2 \left(c_1 d_{minB}\right)^\beta = \|\mathcal{D}\mathcal{J}_{12}^\alpha\left(\Omega^0\right)\|_{L^\infty(\Gamma_w^0)} \tag{3.17}$$

are fulfilled, where d_{min} and d_{minB} are to be specified by selecting the **dminDS** and **dminBDS** parameters (see figure 3.5).

3.7.4 Method 3: Damping in the transition area

Damping of the shape gradient in the transition area. Properties:

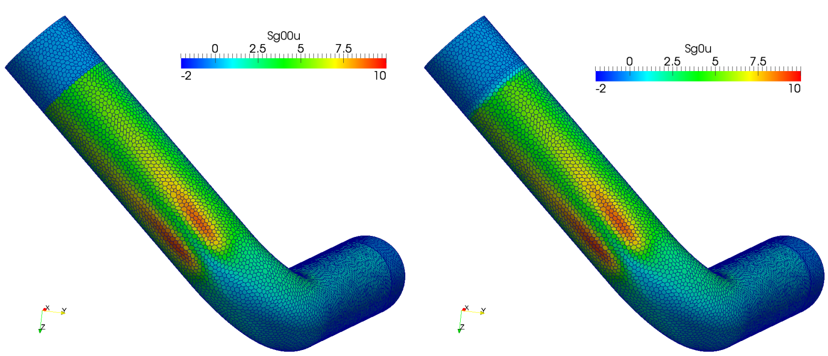


Figure 3.6: Left: Tube 3 without damping. Right: Tube 3 with damping.

- - Unfavorable with inadmissible start geometry.
- - Undesirable effects in the transition from attenuated to undamped areas.

- + Easy user handling, as no additional parameter is required.

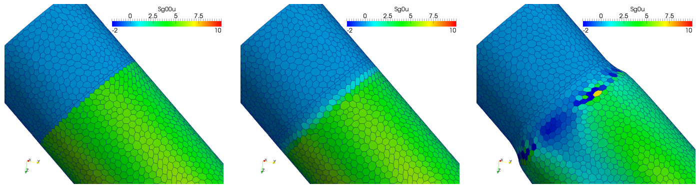


Figure 3.7: Detailed view: left: without damping, middle: with damping, right: damped shape gradient after 40 iterations.

3.7.5 Method 4: Smoothing the shape gradient

Solve the Laplace-Beltrami equation with boundary conditions equal to 0 on the transition curve.

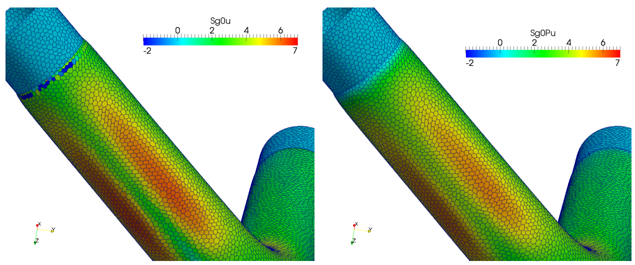


Figure 3.8: Rohr 3: links: ohne LB-Glättung, rechts: mit LB-Glättung.

$$
\begin{aligned}
-\varepsilon \Delta_\Gamma w + w &= -g_{\mathcal{J}_{12}} \qquad \text{auf} \quad \Gamma && (3.18)\\
w &= 0 \qquad\quad\;\; \text{auf} \quad \partial\Gamma && (3.19)
\end{aligned}
$$

The parameter ε in equation (3.18) corresponds to the parameter `scaleLB` in table 11. If no Laplace-Beltrami smoothing is to be performed, this parameter must be set to 0. Experience shows that the parameter should be selected in the range [1e-6, 1e-3]. Smoothing becomes stronger the larger the parameter is selected.

Parameter name	Default value	Admissib	RLR	M23	Description
uer_bereich	0.01	[0,100]	0.015	0.35	Transition restriction: Range in m.
uer_nonlinear	0.2	[0,100]	0.6	0.3	Übergang.: ¡¡1: flache, ¿¿1:steile Kurve.
uer_linear	0	[0,100]	0	10	Transition: ¡¡1: flat, ¿¿1:steep curve.
uer_pow	2	[0,10]	2	2	Transition: Potency of the transition fact.
bauraum_restriktion	1	{0,1,2}	2	0	0:without installation space, 1:barrier, 2:penalty.
bauraum_straf_potenz	2	[1,3]	2	2	Potency β in penalty proceedings.
fix_gewichtung	1	[0,100]	1	1	Weighting φ for transition restriction.
uer_fix_faces	1	{0,1}	1	1	Transition restriction: Use method 1: 0:no, 1:yes.
scaleShapeGradientFix	1	{0,1}	1	0	Transition restriction: Use method 3: 0:no, 1:yes.
scaleLB	1e-5	[0,1]	5e-5	1e-3	Transition restriction: Method 4 smoothing parameters: 0 no smoothing, 1 strong smoothing.

Table 10: Geometric restrictions 1.

Parameter name	Default value	Admissi	Description
dminIF, dmaxIF	1e-2, 5e-3	[0,10]	Transition Restriction: Scaling.
dminDS, dminDS	1e-2, 5e-3	[0,10]	Installation space restricted: Scaling.
dminBDS	(dminDS+dmaxDS)*0.8	[0,10]	Installation space restricted: Scaling.

Table 11: Geometric restrictions 2 (detail).

Parameter name	Default value	Admissi	Description
restart_opt	0	{0,1}	Use initial geometry `wall0.stl` for geometry change: 0:no, 1:yes.
damp	3(0 0 0)	[0,1e20]	Damping parameters (ρ_2, ρ_1, ρ_{1a}, ρ_{1b}, ρ_{1c}), to be optionally specified based on the entries in Test Run_Info.txt.

Table 12: Optional restart parameters.

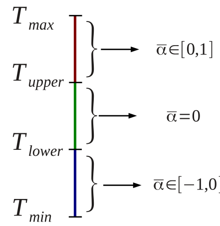
3.8 Topology optimization

If topology optimization is to be performed, the parameter `topOpt` must be set to 1. The adapted impulse equation of the flow in a porous medium is:

$$\nabla \cdot \left(\boldsymbol{u}\boldsymbol{u}^T\right) - \nu \Delta \boldsymbol{u} + \nabla p + P_V \boldsymbol{u} + P_I \left|\boldsymbol{u}\right| \boldsymbol{u} = \mathbf{0}, \tag{3.20}$$

The maximum values for P_V and P_I must be specified by the parameters `porosityV` and `porosityI`. These values are multiplied by the parameter `startPOR` to determine the initial porosity.

It seems to be numerically necessary to define limits $\mathcal{T}_{upper}$ (**thresholdTOPupper**) and $\mathcal{T}_{lower}$ (**thresholdTOPlower**) at which the porosity is increased or decreased. Theoretical determination would be $\mathcal{T}_{upper} = \mathcal{T}_{lower} = 0$.
Separate scaling of the values greater than $\mathcal{T}_{upper}$ and the smaller $\mathcal{T}_{lower}$ leads to $\overline{\alpha}$ (see right figure). If this scaling is desired, set **boundPOR** to 1.



Parameter name	Default value	Admissib	B135	Description
topOpt	0	{0,1}	1	0:shape optimization, 1: topology optimization.
startPOR	0	[0,1]	0.1	Scaling of the starting porosity.
porosityI	0	[0,1e6]	0	Porous Inertial Resistence (maximaler Wert).
porosityV	0	[0,1e6]	150	Porous Viscous Resistence (maximaler Wert).
boundPOR	1	{0,1}	1	Use of the scaling technique.
thresholdTOPupper	2	[0,10]	-1e-4	Upper limit value for porosity update.
thresholdTOPlower	1	{0,1,2}	-0.05	Lower limit for porosity update.

Table 13: Topology optimization.

3.9 Extraction of the topology-optimized geometry

The extracted geometry can be based on the porosity or the topological gradient (`grad_por`). With the parameter `extractFolder` the folder number in which the desired data set is located has to be specified. Instead of the original data T_σ can be used:

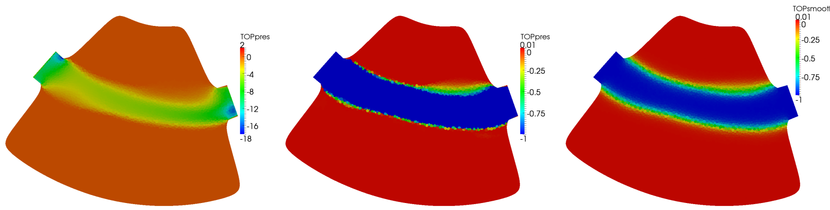


Figure 3.9: Left: $\mathcal{T}(\boldsymbol{x})$, middle: $\overline{\mathcal{T}}(\boldsymbol{x})$, right: $\mathcal{T}_\sigma(\boldsymbol{x})$.

$$\overline{\mathcal{T}}(\boldsymbol{x}) = \min\left(\max\left(\mathcal{T}(\boldsymbol{x}), \mathcal{T}_{min}\right), \mathcal{T}_{max}\right), \tag{3.21}$$

$$\begin{aligned} -\sigma\Delta\mathcal{T}_\sigma + \mathcal{T}_\sigma &= \overline{\mathcal{T}} \quad \text{in } \Omega, & (3.22)\\ \mathcal{T}_\sigma &= \mathcal{T}_{min} \quad \text{auf } \Gamma_i \cup \Gamma_o, & (3.23)\\ \partial_n \mathcal{T}_\sigma &= 0 \quad \text{auf } \Gamma_w \cup \Gamma_f. & (3.24)\end{aligned}$$

The parameters $\mathcal{T}_{\min}$ and $\mathcal{T}_{\max}$ are to be specified by the user with `cutTOP`. The smoothing parameter σ must be set with `smoothTOP`. To avoid possible overlaps with the fixed geometries, the parameter `feasibleTOP` can be used to define the allowable range (see Figure 3.10). To allow the user to change the parameters quickly, the topoExtractSTL routine lists the

Figure 3.10: Left: Inadmissibility area (red); extracted geometry: middle: *wallExtract.stl*, right: *wall.stl*

default values and provides an input option. The parameters can also be changed in `system/fvSolution/SGparameter`.

Parameter name	Default value	Admissibilit	B135	Description
grad_por	0	{0,1}	0	0: use TOPpres; 1: use PORalpha.
extractFolder	1	{0,1e4}	60	Extract geometry from folder with this number.
cutTOP	2(0 0)	{0,1}	2(-1,0.01)	Maximum and minimum value.
smoothTOP	0	[0,1e5]	0.003	Laplace smoothing the top degrees. information.
feasibleTOP	2(0 0)	[0,1e6]	2(0 0)	Range of inadmissibility at the in-/outlet in meters.
thresholdTOP	0	[-1e6,1e6]	-0.5	Level layer to achieve the surface.

Table 14: Extraction of the topology optimized surface.

4 Initialization and calculation

4.1 Executing the shape optimization

- Create a folder e.g. M23Test in `$FOAM_RUN/tutorials/incompressible/`.
- In the folder M23Test the file `parameter_sg` with the parameters and the folder `initial_stl` with the geometry data must be created.
- From the folder M23Test the commands `setupShapeGradientCCM` and then `shapeGradientCCM > outtestShape.txt`.

4.2 Executing the topology optimization

- Create a folder B135Test in `$FOAM_RUN/tutorials/incompressible/`. In folder B135Test the file `parameter_sg` with the parameters and the folder `initial_stl` with the geometry data is to be created.
- The commands `setupShapeGradientCCM` and `topoOpt > outtestTop1.txt` must be executed from the B135Test folder. This returns TOPpres and PORalpha.
- From the M23Test folder the commands `topoExtractSTL` and `topoOptCloseAll > outtestTop2.txt` must be executed. This returns the intermediate result `wallExtract.stl` and the result `wall.stl`.

4.3 Stop and restart shape optimization

At the beginning of the shape optimization the file STOP.txt is automatically created. If the shape optimization is to be stopped, the number in the file must be changed to 0. During the shape optimization the subfolder sim is created in the iteration number folders where a mesh re-connection was performed. Together with the start geometries inlet.stl, outlet.stl, fixed.stl and if necessary bds.stl, wall.stl can be used for a new test calculation.

If the geometry change with respect to the start geometry is to be calculated, it must be saved in the `wall0.stl` file in the `initial_stl` folder and the `restart_opt` parameter must be set to 1 (see Table 12). If the same scaling of the target functionals is desired, the parameter `damp` must be specified in the `parameter_sg` file. These values are always stored in the `Test Run_Info.txt` file.

5 Data evaluation and visualization

5.1 Output data

During shape and topology optimization, the relevant data (see tables 15 and 16) are stored in the corresponding folders (designation according to the number of iterations) in each iteration. The current geometry data is stored in `polyMesh`. Further data such as target function values, used step sizes, etc. can be found in the text file `Testlauf_Info.txt`.

5.2 Visualization with ParaView

For visualization of the data the use of ParaView is recommended. After installation in the course of the OpenFOAM setup paraView can be called with the command *paraFOAM* in the folder with the data to be visualized. The following possibilities of data visualization can be used in paraView (see figure 5.1 - 5.2)

- *Point Field* and *Volume Field* information on the surface (Sg0P, GeomChange), vector field with *Glyph* (U0),
- cross-section with *clip* or *Slice* or contour with *Contour* (TOPpres, PORalpha, TOPsmooth),
- STL data with *File>Open* (wallExtract.stl).

Output file	Dimension	Appearance	Description
U0	Vector	Area, boundary	Solution $\boldsymbol{u}$ the primary equation (velocity).
p0	Scalar	Area, boundary	Solution p of the primary equation (pressure).
density0	Scalar	Area, boundary	Used density in the Navier-Stokes equation.
Vunif	Vector	Area, boundary	Solution $\boldsymbol{v}$ the adjoint equation (adjoint velocity) with regard to achieving a uniform flow.
Vpres	Vector	Area, boundary	Solution $\boldsymbol{v}$ the adjoint equation (adjoint velocity) with regard to minimizing the total pressure loss.
Sg0u	Scalar	Boundary	Negative shape gradient (scaled).
Sg00u	Scalar	Boundary	Negative shape gradient (scaled): proportion of $\mathcal{J}_1$, $\mathcal{J}_2$.
Sg0Lu	Scalar	Boundary	Negative shape gradient (scaled): proportion geometric restriction.
SgVpres0	Scalar	Boundary	Negative shape gradient (scaled): portion of $\mathcal{J}_2$ (total pressure loss).
SgVunif0	Scalar	Boundary	Negative shape gradient (scaled): portion of $\mathcal{J}_1$ (uniform discharge).
GeomChange	Scalar	Boundary	Geometry change to the initial geometry (in meters).
Distance	Scalar	Boundary	Distance to the installation space geometry (in meters).
Sg0Pu	Scalar	Boundary, Point	Negative shape gradient - Laplace-Beltrami (scaled).

Table 15: Output data shape optimization.

Output file	Dimension	Appearance	Description
TOPpres	Scalar	Area	Topological sensitivity Total pressure loss.
TOPmix	Scalar	Area	Effective topological sensitivity.
PORalpha	Scalar	Area	Porosity.
1/TOPsmooth	Scalar	Area	Smoothed data $\mathcal{T}_\sigma$ (**smoothTOP**).
1/TOPfea	Scalar	Area	Admissibility range (**feasibleTOP**).

Table 16: Output data topology optimization.

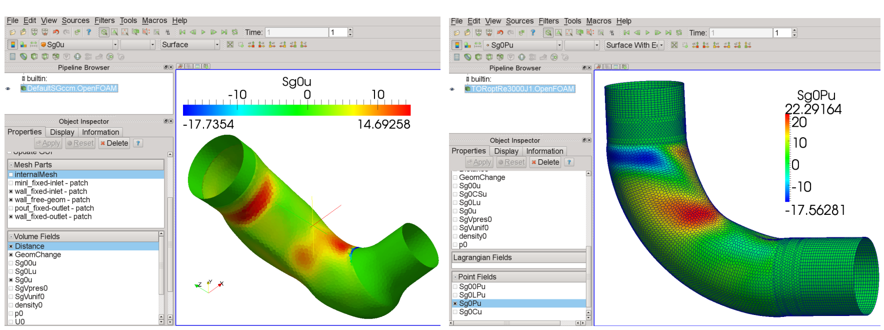


Figure 5.1: Use of ParaView: VolumeFields, PointFields.

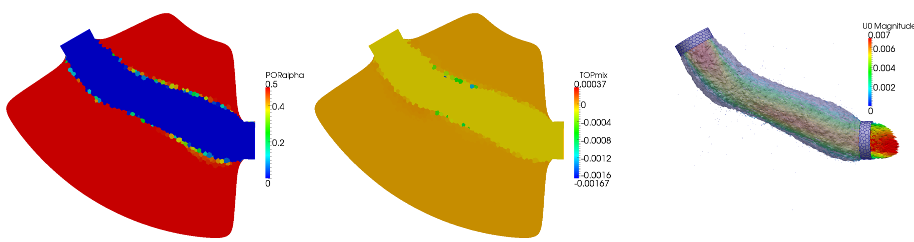


Figure 5.2: Porosity, effective top. degree and contour.

```
Einstellungen dieses Testlaufes:

  |Zielfunktional            |>  | Gewichtung Unif(0)/TotP(1): 0.5 | dp_J1a:0.33 | dp_J1b:0.34 | dp_J1c:0.33 | damp0:6796.87795898391 | damp1:0 | damp1a:1 | damp1b:1.73643100874038 | damp1c:1.00277671114272 |
  |Modellwahl                |>  | Turbulenzmodell: 0 | Einstroemgeschwindigkeit: 0.00600669109128612
  |Bauraum - Allgemein       |>  | Bauraummethode: 0 | BRaum_gew: 1 | FixGeom_gew: 1
  |Bauraum - Fixer Uebergang |>  | uer_bereich: 0.35 | uer_nonlinear: 0.3 | uer_linear: 10 | uer_pow: 2
  |Bauraum - Skalierung      |>  | dmaxDS: 0.005 | dminDS: 0.01 | dminBDS: 0.012 | dmaxIF: 0.005 | dminIF: 0.01 | areaDS: 20.59476 | areaDSall: 20.594765 | areaIF: 2.282647 | areaIFall: 4.5652955
                                 | scaleXDS: 1 | scaleYDS: 1 | scaleXIF: 0.000104271719212112 | scaleYIF: 4.10539066438754e+18 | delta12: 1115905.88359879 | jota12: 0.442671699342665
  |Liniensuche               |>  | Schrittweite start: 0.01 | Schrittweite untere Schranke: 1e-05 | Schrittweite Reduktionsfaktor: 0.5.

-----------------------------------------------------------------------------------------------------------------------------------------------

Erklaerung der Bezeichnungen:

Spalte 1  [Iter]:                 ||Anzahl der Iterationen.
Spalte 2  [Gemischtes Funkt(J12)]: ||Funktionswerte des gemischten Zielfunktionals (J12).
Spalte 3  [Gleichm Ausstr(J1)]:   ||Funktionswerte des Funktionals fuer eine gleichmaessige Ausstroemung (J1).
Spalte 4  [Totaldruckv(J2)]:      ||Funktionswerte des Funktionals zur Minimierung des Totaldruckverlustes (J2).
Spalte 5  [Gleichm Ausstr(J1a)]:  ||Funktionswerte des Funktionals fuer eine gleichmaessige Ausstroemung (J1a).
Spalte 6  [Gleichm Ausstr(J1b)]:  ||Funktionswerte des Funktionals fuer eine gleichmaessige Ausstroemung (J1b).
Spalte 7  [Gleichm Ausstr(J1c)]:  ||Funktionswerte des Funktionals fuer eine gleichmaessige Ausstroemung (J1c).
Spalte 8  [Restr Fix Uebg]:       ||Funktionswerte des Funktionals resultierend aus der Uebergangsrestriktion zur fixen Geometrie (skaliert mit Gewichtungsparameter).
Spalte 9  [Restr BauRaum]:        ||Funktionswerte des Funktionals resultierend aus der Bauraumgeometrie (skaliert mit Gewichtungsparameter).
Spalte 10 [Gleichm Ausstr(J1)]:   ||Funktionswerte des Funktionals fuer eine gleichmaessige Ausstroemung (J1) ohne Skalierung.
Spalte 11 [Gleichm Ausstr(J1a)]:  ||Funktionswerte des Funktionals fuer eine gleichmaessige Ausstroemung (J1a) ohne Skalierung.
Spalte 12 [Gleichm Ausstr(J1b)]:  ||Funktionswerte des Funktionals fuer eine gleichmaessige Ausstroemung (J1b) ohne Skalierung.
Spalte 13 [Gleichm Ausstr(J1c)]:  ||Funktionswerte des Funktionals fuer eine gleichmaessige Ausstroemung (J1c) ohne Skalierung.
Spalte 14 [J1io]:                 ||Funktionswerte des CCM Funktionals J1 auf Gamma_i und Gamma_o.
Spalte 15 [J1io_original]:        ||Funktionswerte des originalen Funktionals J1 auf Gamma_i und Gamma_o.
Spalte 16 [J2io]:                 ||Funktionswerte des CCM Funktionals J2 auf Gamma_i und Gamma_o.
Spalte 17 [L2-Norm DJ12]:         ||L2-Norm des Formgradienten.
Spalte 18 [Gewicht BauR]:         ||Gewichtung Bauraum.
Spalte 19 [Stepsize]:             ||Schrittweite des Abstiegsverfahrens, welches den neg Formgradienten als Abstiegsrichtung verwendet.
Spalte 20 [TotRemesh]:            ||Anzahl der durchgefuehrten Gitterneuvernetzungen.
Spalte 21 [RemeshNum]:            ||Anzahl der Gitterneuvernetzungen mit rem_tol(Parameter) Abstand.
Spalte 22 [RemeshNum]:            ||Anzahl der Gitterneuvernetzungen mit rem_tol(Parameter) Abstand.
-----------------------------------------------------------------------------------------------------------------------------------------------

Testlauf:

 |Iter   |Gemischtes Funkt(J12)|             |Gleichm Ausstr(J1)|                |Totaldruckv(J2)|                |Gleichm Ausstr(J1a)|               |Gleichm Ausstr(J1b)|               |Gleichm Ausstr(J1c)

     |0  |0.442671699342665    |[      0%]   |-0                  |[      0%]   |0.129180783563424    |[      0%]   |0.0858576640633667   |[      0%]   |0.141673826945094    |[      0%]   |0.0859594247707797
     |1  |0.441013054002075    |[   0.37%]   |-0                  |[  -0.08%]   |0.128108040069079    |[   0.83%]   |0.0857300945586884   |[   0.15%]   |0.14134586192583     |[   0.23%]   |0.0858290574484771
     |2  |0.440572663881268    |[   0.47%]   |-0                  |[  -0.05%]   |0.127821059625448    |[   1.05%]   |0.0856929973349942   |[   0.19%]   |0.141265171690983    |[   0.29%]   |0.0857934352298425
     |3  |0.440122162882233    |[   0.58%]   |-0                  |[  -0.01%]   |0.127531158079058    |[   1.28%]   |0.0856549846761583   |[   0.24%]   |0.141180145078611    |[   0.35%]   |0.0857558750484056
     |4  |0.43989397295804     |[   0.63%]   |-0                  |[   0.01%]   |0.127385161550478    |[   1.39%]   |0.0856363474828737   |[   0.26%]   |0.141136647825198    |[   0.38%]   |0.0857358160994897
     |5  |0.439668965648141    |[   0.68%]   |-0                  |[   0.03%]   |0.127240524514082    |[    1.5%]   |0.0856177398415695   |[   0.28%]   |0.141095088248518    |[   0.41%]   |0.0857156130439718


             |Restr Fix Uebg |          |Restr BauRaum |          |     J1      |       |     J1a     |       |     J1b     |       |     J1c     |       |    J1io    |

[      0%]  |0                    |     |0                    |     |0.6101213371273      |0.52034947917192     |0.479935827236084    |0.519523643641792    |0.6101213371273      |[      0%]
[   0.15%]  |0                    |     |0                    |     |0.610602988715077    |0.519576330658717    |0.47882480929989     |0.518735726476512    |0.610602988715077    |[  -0.08%]
[   0.19%]  |0                    |     |0                    |     |0.610434890886619    |0.519351498999965    |0.478551462165518    |0.518520432052788    |0.610434890886619    |[  -0.05%]
[   0.24%]  |0                    |     |0                    |     |0.610207746771549    |0.519121119249444    |0.478263425070552    |0.518293424922761    |0.610207746771549    |[  -0.01%]
[   0.26%]  |0                    |     |0                    |     |0.61006886390712     |0.519008166562871    |0.478116073292532    |0.518172192163745    |0.61006886390712     |[   0.01%]
[   0.28%]  |0                    |     |0                    |     |0.609919375247875    |0.518895392979209    |0.477975285609699    |0.518050088449774    |0.609919375247875    |[   0.03%]


   |  J1io_orig |                    |    J2io    |                     |L2-Norm DJ12|                          _____ |Gewicht BauR         |Stepsize                |TotRemesh ||RemeshN |CycleNr

|1.30464465454475e-06 |[      0%]   |3.80118002244478e-05 |[      0%]   |54772.184722058      |[      0%]   |0.747593803721546   |                      |                        |0      |0      |1
|1.30670622320529e-06 |[  -0.16%]   |3.76961425060604e-05 |[   0.83%]   |49747.2769886953     |[   9.17%]   |0.802640573784492   |1                     |0.005                   |0      |0      |1 [2,0]
|1.30598702443564e-06 |[   -0.1%]   |3.7611697722628e-05  |[   1.05%]   |48737.1726285706     |[  11.02%]   |0.814686221706336   |1                     |0.00125                 |0      |0      |1 [2,2,0]
|1.30501548159787e-06 |[  -0.03%]   |3.75263933966892e-05 |[   1.28%]   |47922.2473472471     |[  12.51%]   |0.823981548305418   |1                     |0.00125                 |0      |0      |1 [0]
|1.3044216102252e-06  |[   0.02%]   |3.74834335173267e-05 |[   1.39%]   |47568.3901392243     |[  13.15%]   |0.827813257682541   |1                     |0.000625                |0      |0      |1 [2,0]
|1.30378252160933e-06 |[   0.07%]   |3.74408736722717e-05 |[    1.5%]   |47311.0966826674     |[  13.62%]   |0.829968366333142   |1                     |0.000625                |0      |0      |1 [0]
```

5.3 Structure diagram

A software structure chart is shown in figure 5.3. Calculation steps are shown in square fields and queries in rounded fields. The essential software parts are shown in grey letters for the respective calculation steps. In the output file *test run_Info.txt*, a numerical code is located in square brackets at the end of the line of each iteration. This numerical code indicates the progress of the step size control within the respective iteration.
The digits can be found in the structure diagram in figure 5.3, their meaning is given in table 17.

Digit	Meaning
0	Step accepted/end of iteration.
1	Grid Networking.
2	Grid quality criteria not fulfilled for entire geometry .
3	Installation space exceeded when using the barrier method.
33	Installation space overrun of the start geometry when using barrier method.
4	Target functional does not fall according to Armijo - rule.
6	Primary solver does not converge.
66	Primary solver does not converge at startup configuration.
7	Grid quality criteria not met for geometry *wall*.
8	Surface quality insufficient.
9	User enforced reconnection.

Table 17: Number code line search shape optimization.

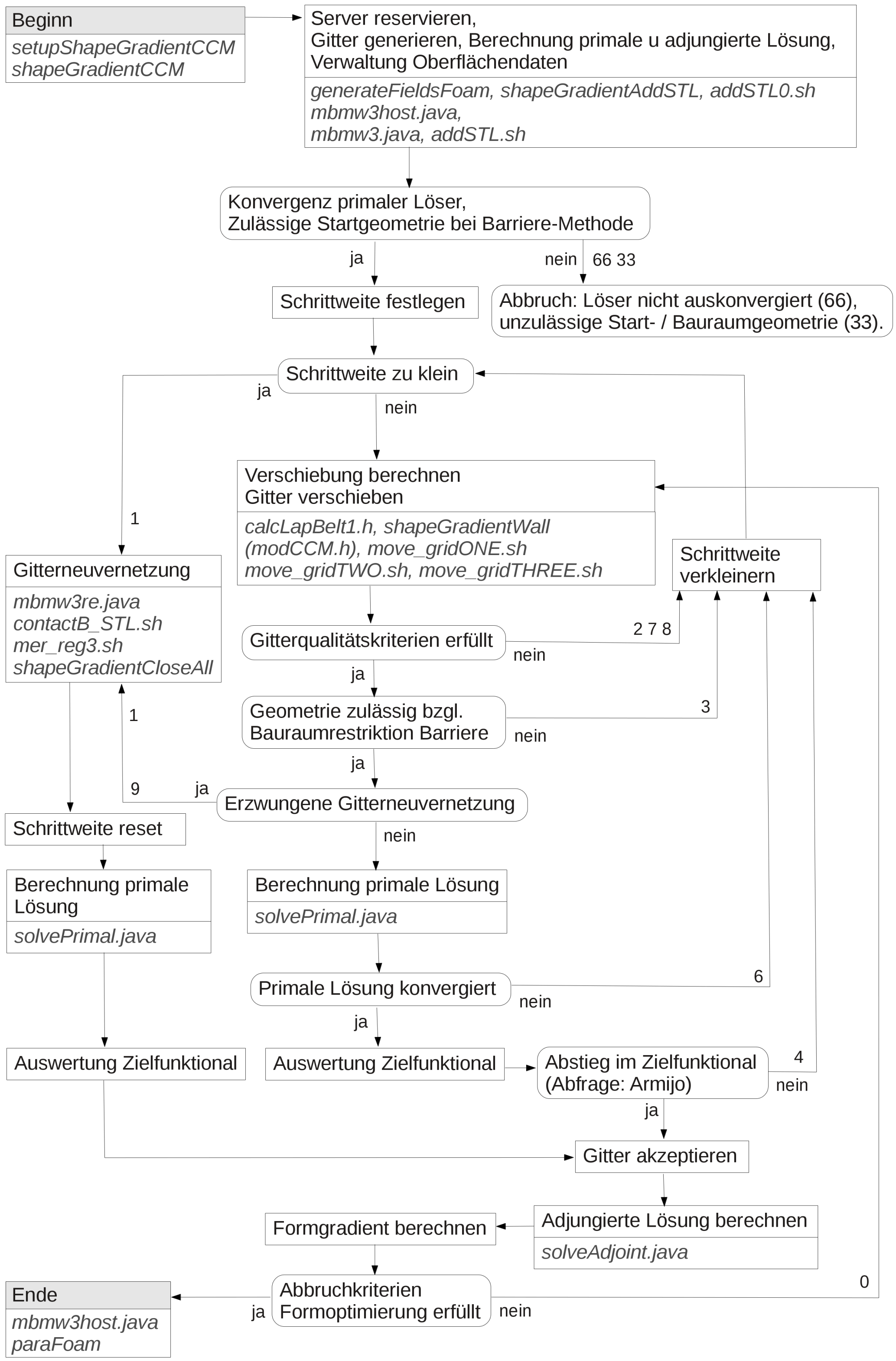


Figure 5.3: Structogram shape optimization.