EURO Greece

HPC Training Series

Setting up and running an optimization case in OpenFOAM.

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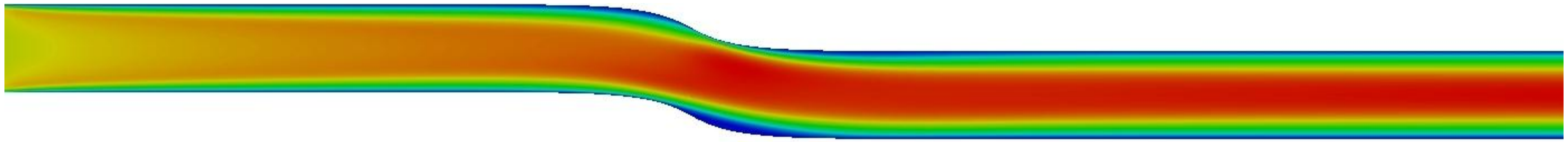
The tutorial case

- **Case is derived from**
  `$FOAM_TUTORIALS/incompressible/adjointOptimisationFoam/shapeOptimisation/sbend/laminar/opt/\`
  `unconstrained/BFGS/`
  but with a smaller mesh to get results faster

- **Laminar flow within an S-bend 2D duct, mesh is provided**

- $Re = 1000$

- **Objective: minimize volume-weighted total pressure losses** $J = -\int_{S_{I,O}} \left(p + \frac{1}{2} v_k^2\right) v_i n_i dS$



Gradient-based Shape Optimisation Loop

- Define design variables b_n ⇨ Need to define variables controlling the aerodynamic shape
- Solve flow equations $\rightarrow U$
- Compute J ⇨ Quantity to be optimized (forces, moments, losses, etc)
- Solve adjoint equations $\rightarrow \Psi$
- Compute $\delta J/\delta b_n \ (U, \Psi)$ ⇨ Drives the optimisation loop
- Update design variables ⇨ Steepest descent, CG, BFGS …
- Update mesh ⇨ PDE-based, Algebraic models …

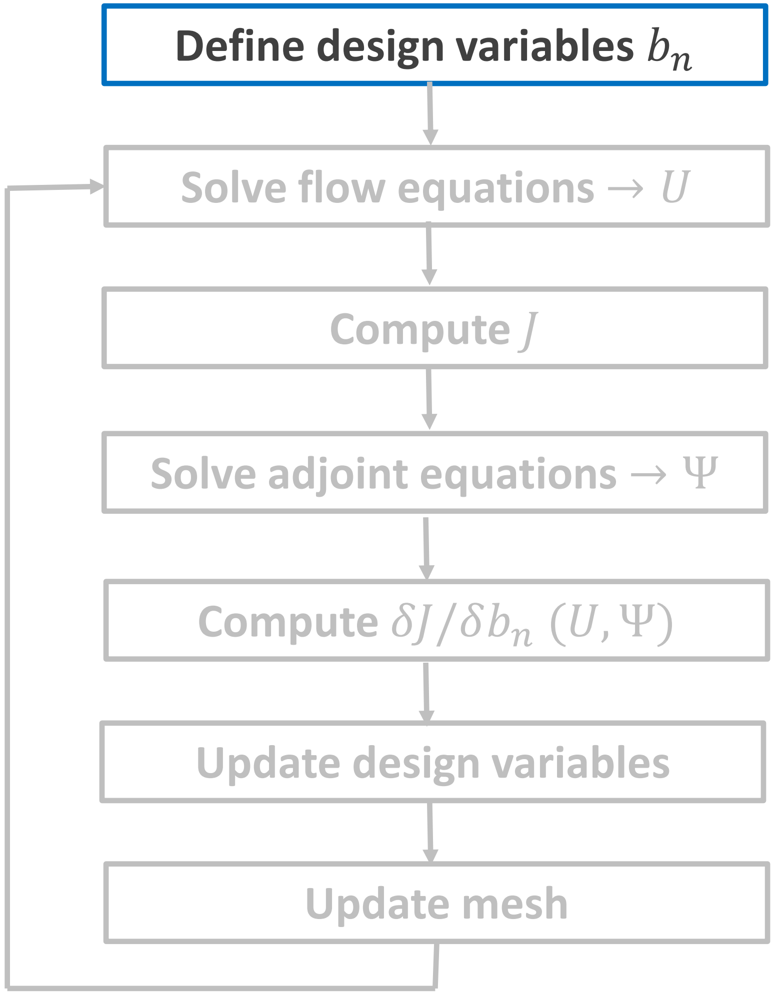
(loop back from "Update mesh" to "Solve flow equations")

Everything is implemented within OpenFOAM:
No need for third-party software, external scripts, etc

Gradient-based Shape Optimisation Loop

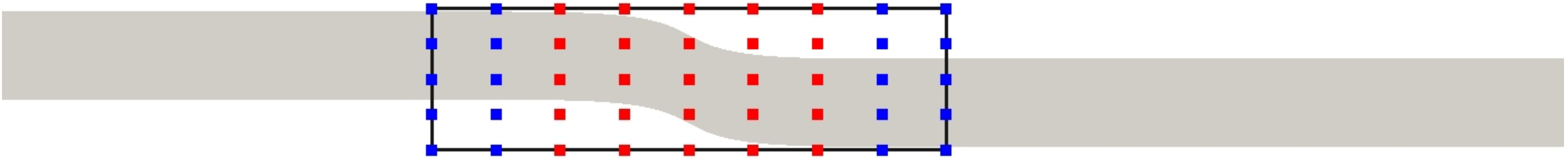
Define design variables b_n	⇨ *system/optimisationDict.optimisation.designVariables*
Solve flow equations $\rightarrow U$	⇨ *system/optimisationDict.primalSolvers*
Compute J	⇨ *system/optimisationDict.adjointManagers,* **within each adjoint solver**
Solve adjoint equations $\rightarrow \Psi$	⇨ **Discretization in** *system/fvSchemes,* **Relaxation in** *system/fvSolution*
Compute $\delta J/\delta b_n\ (U, \Psi)$	⇨ **Definition in:** *system/optimisationDict.optimisation.designVariables*
Update design variables	⇨ **Definition in:** *system/optimisationDict.optimisation.updateMethod*
Update mesh	⇨ **Definition in:** *constant/dynamicMeshDict*

Gradient-based Shape optimisation Loop



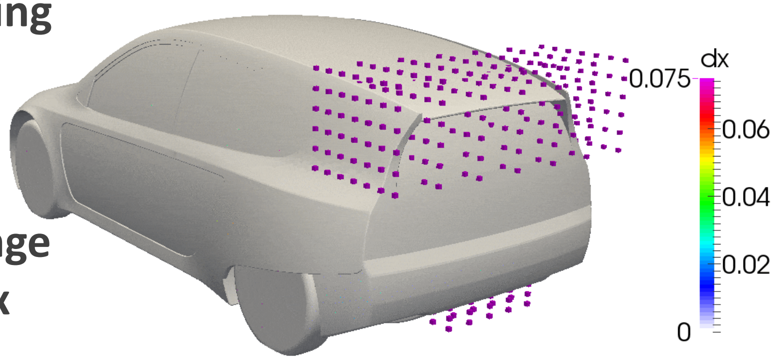
Parameterization for shape optimisation:

- **NURBS Curves (2D) and Surfaces (3D)**
- **All of the wall nodes**
- **Volumetric B-Splines (Free Form Deformation, FFD)**



Volumetric B-Splines:

- **Maps all CFD grid points within the morphing boxes from the Cartesian to a parametric space $(x, y, z) \rightarrow (u, v, w)$**
- **Mapping has to be done only once**
- **Then, changing the control points will change all CFD grid nodes within the morphing box (boundary and internal)**
- **Update is done through an algebraic relation: very fast!**



Gradient-based Shape optimisation Loop

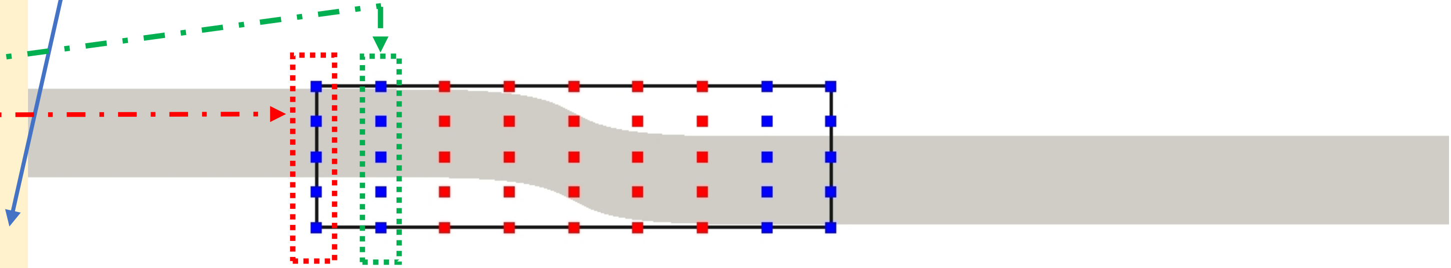
Define design variables b_n

Defined in: *constant/dynamicMeshDict*

```
solver volumetricBSplinesMotionSolver;

volumetricBSplinesMotionSolverCoeffs
{
 duct
 {
  type    cartesian;
  nCPsU   9;
  nCPsV   5;
  nCPsW   3;
  degreeU 3; // max: nCPsU - 1
  degreeV 3; // max: nCPsV - 1
  degreeW 2; // max: nCPsW - 1

  controlPointsDefinition axisAligned;
  lowerCpBounds (-1.1 -0.21 -0.05);
  upperCpBounds ( 1.1  0.39  0.15);

  confineUMovement false;
  confineVMovement false;
  confineWMovement true;
  confineBoundaryControlPoints false;


  confineUMinCPs ( (true true true) (true true true) );
  confineUMaxCPs ( (true true true) (true true true) );
  confineWMinCPs ( (true true true) );
  confineWMaxCPs ( (true true true) );
 }
}
```

Basic entries:

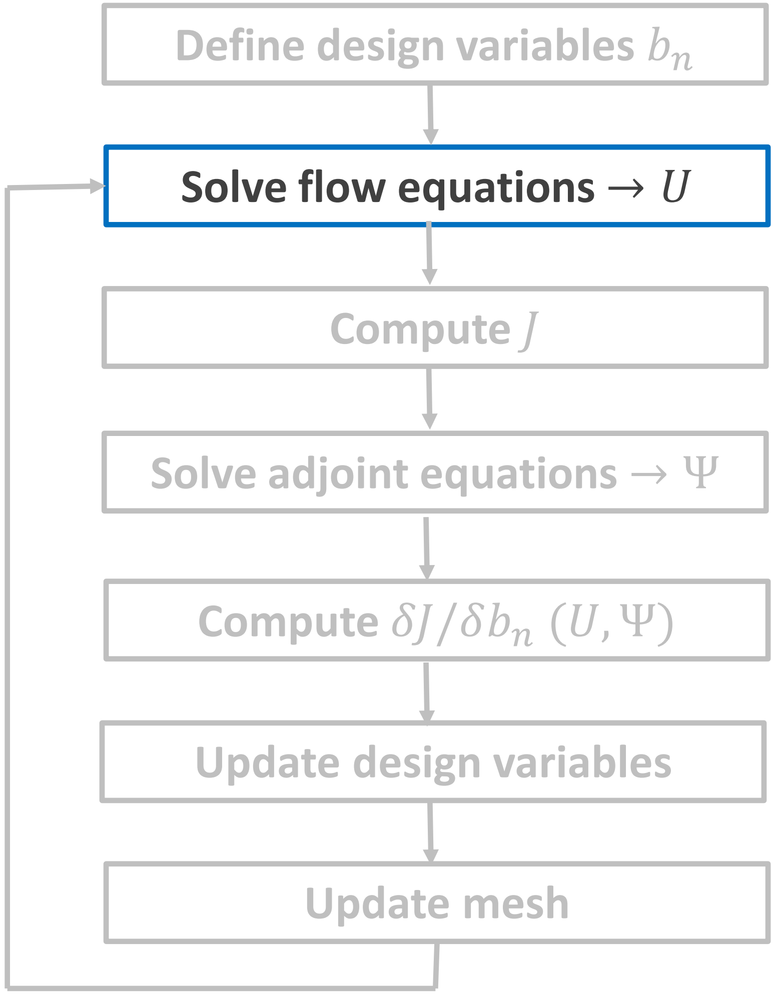
- Number of control points (CPs) per box direction
- Degree per direction (smaller degree → more local support)
- CPs defined either aligned with a coordinate system (Cartesian, cylindrical) or given manually through a dictionary
- Possible to confine the movement of (some of) the CPs in certain directions
- Continuity with the stationary part of the mesh must be preserved! Keeping the boundary CPs constant



>> writeMorpherCps

Writes the control points in a Paraview-readable format

Gradient-based Shape optimisation Loop



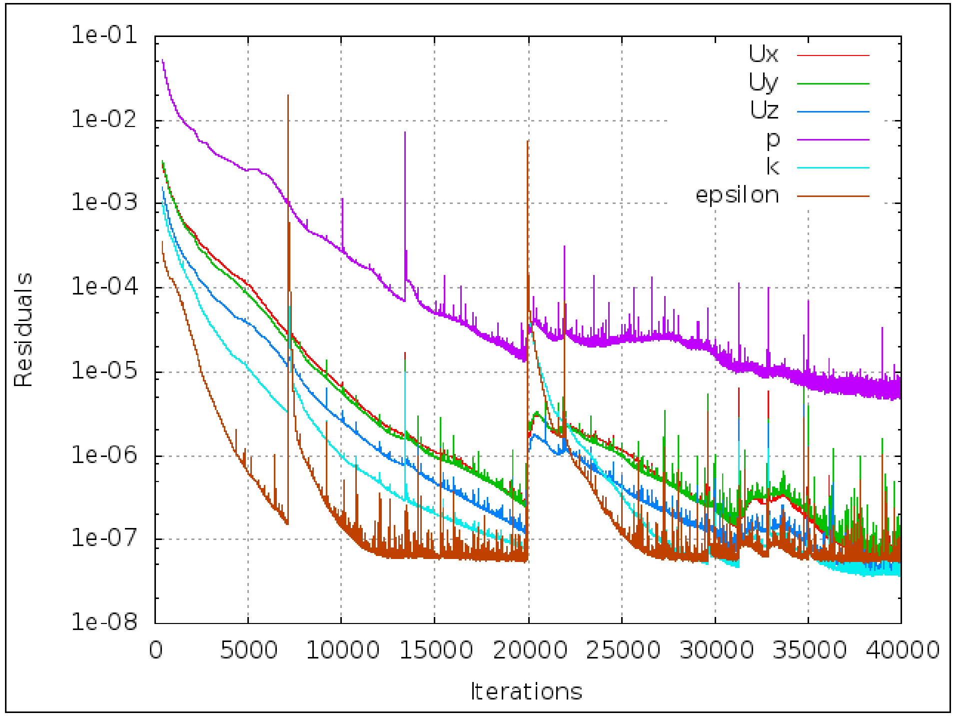
Defined in ***system/optimisationDict.primalSolvers***

Incompressible, steady-state flows

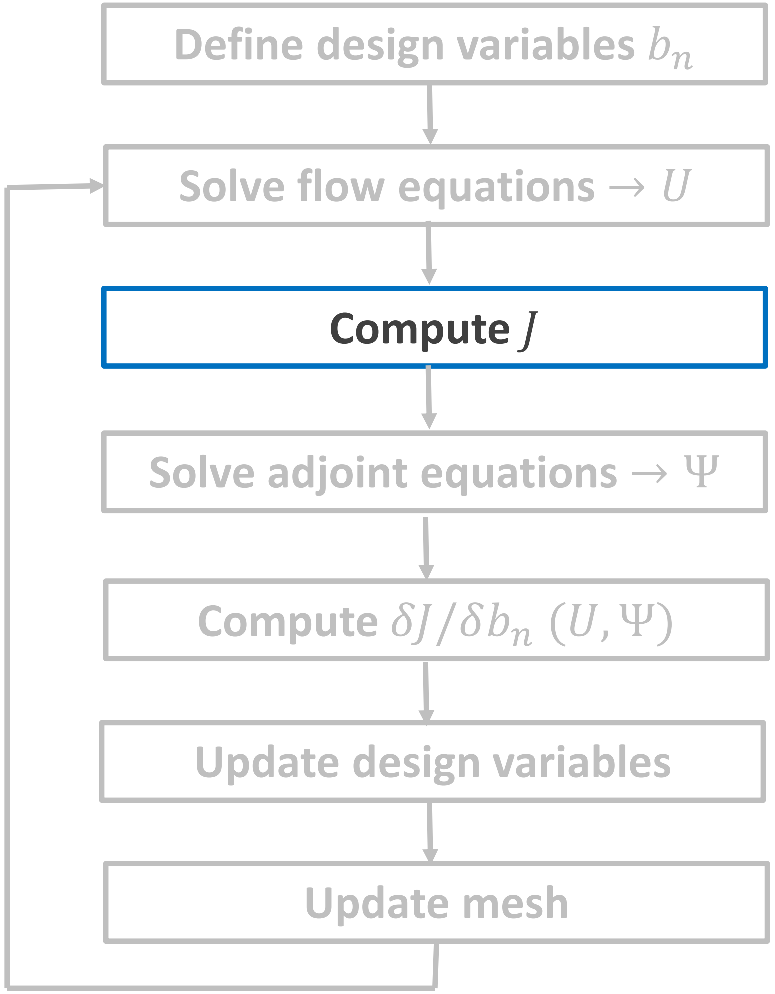
- **SIMPLE is incorporated into** ***adjointOptimisationFoam***
- **Multi-point optimisation supported; can define more than one primal solvers**

Desired for optimisation, if possible

- **Well converged solution (e.g. residuals of ∼1.e−05, 1.e−06)**
- **Non-oscillating residuals**



Gradient-based Shape optimisation Loop



Defined in system/optimisationDict.adjointManagers, within each adjoint solver

Quantity to be optimised

- ***adjointOptimisationFoam*** **always assumes minimization**
- **Objectives can be defined as (surface or volume) integral quantities**
- **A number of objective functions are available:**
  Forces, moments, total pressure losses etc …
- **Multiple objective functions can be tackled by concatenating them into a single one using appropriate weights**

$$J = w_1 J_1 + w_2 J_2$$

Gradient-based Shape optimisation Loop

- Define design variables b_n
- Solve flow equations $\rightarrow U$
- Compute J
- **Solve adjoint equations $\rightarrow \Psi$**
- Compute $\delta J/\delta b_n\ (U,\Psi)$
- Update design variables
- Update mesh

Discretization in system/fvSchemes, Relaxation in system/fvSolution

$$R^q = -\frac{\partial u_j}{\partial x_j} + \boxed{\frac{\partial J_{\Omega'}}{\partial p}} = 0$$

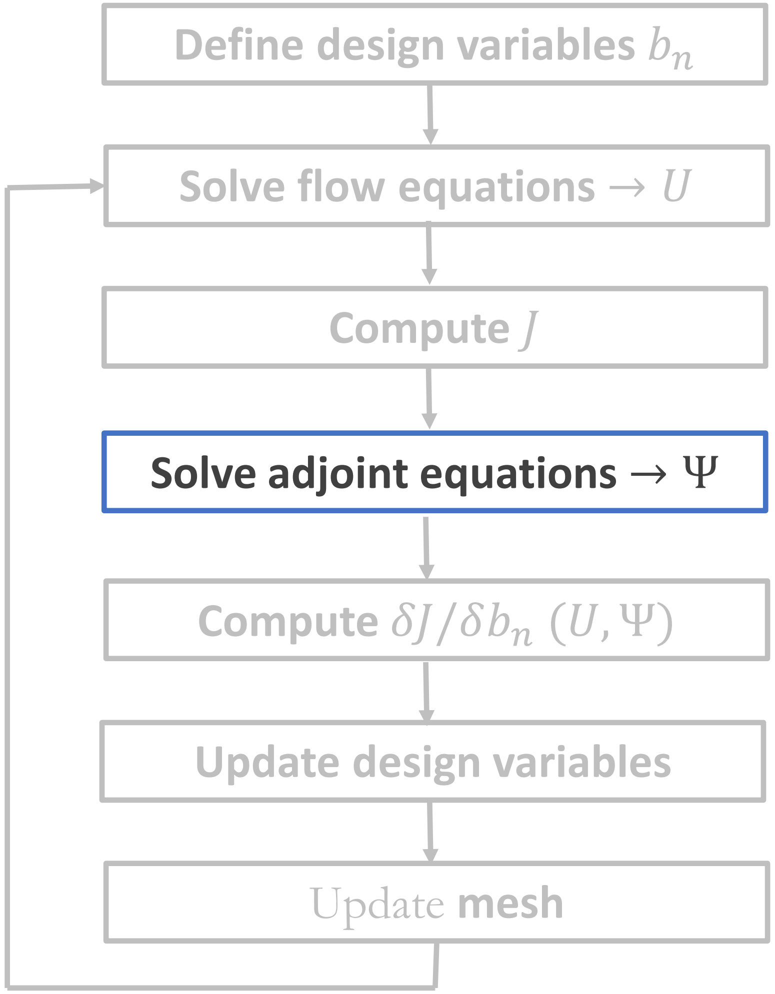
$$R_i^u = \underbrace{\boxed{u_j \frac{\partial v_j}{\partial x_i}}}_{\text{ATC}} \underbrace{\boxed{- \frac{\partial (u_i v_j)}{\partial x_j}}}_{\text{AC}} - \frac{\partial \tau_{ij}^a}{\partial x_j} + \frac{\partial q}{\partial x_i} + \boxed{\frac{\partial J_{\Omega'}}{\partial v_i}} = 0\ ,\ \ i=1,2(,3)$$

Adjoint PDEs (laminar flows):

- **Similar form with the Navier-Stokes equations. A few noticeable differences**
- **Adjoint convection (AC): adjoint velocity is convected by the (minus) primal velocity. Linear equations!**
- **Adjoint Transpose Convection (ATC): Non-conservative term. Numerically tricky in real-word applications.**
- **Source terms if the objective function includes volume integrals containing p or v_i**

Additional terms and equations when dealing with turbulent flows

Gradient-based Shape optimisation Loop



Defined in 0/pa and 0/Ua

$$u_{\langle n\rangle} = u_j n_j = -\frac{\partial J_{S_{I-W},i}}{\partial p} n_i$$

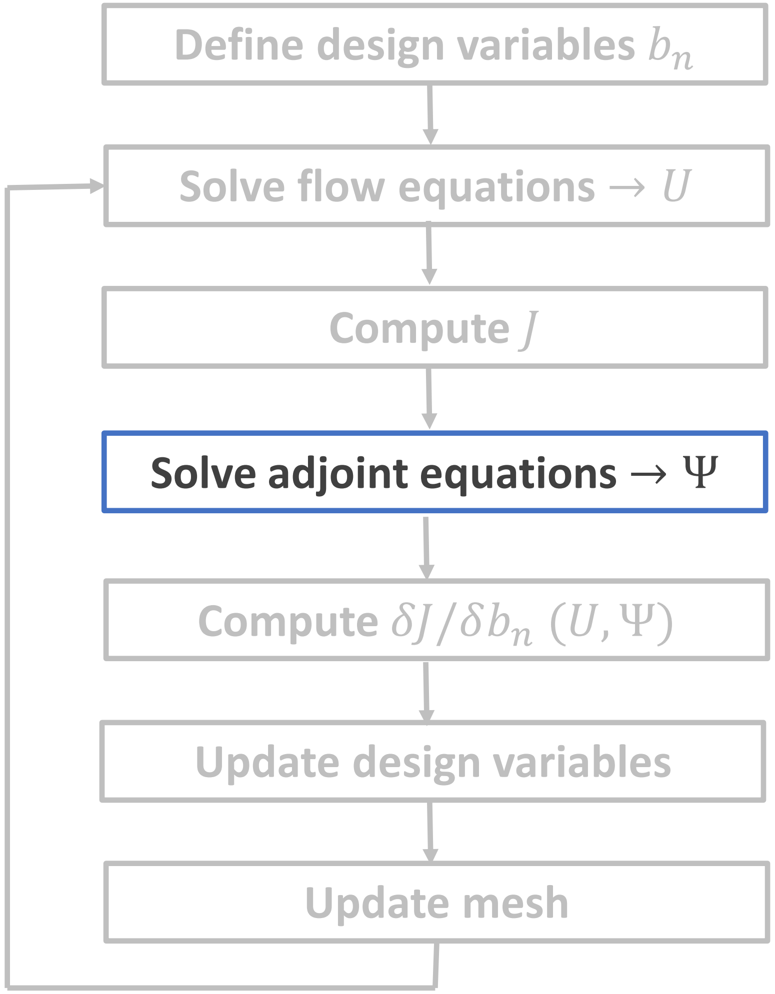
$$u^{I}_{\langle t\rangle} = u_i t^{I}_i = \frac{\partial J_{S_{I-W},k}}{\partial \tau_{ij}} n_k t^{I}_i n_j + \frac{\partial J_{S_{I-W},k}}{\partial \tau_{ij}} n_k t^{I}_j n_i$$

$$u^{II}_{\langle t\rangle} = u_i t^{II}_i = \frac{\partial J_{S_{I-W},k}}{\partial \tau_{ij}} n_k t^{II}_i n_j + \frac{\partial J_{S_{I-W},k}}{\partial \tau_{ij}} n_k t^{II}_j n_i$$

Adjoint Boundary conditions:

- **Depend on the type (not value!) of primal boundary conditions!**
- **Most common for incompressible flows: Dirichlet Inlet $\vec{v}$, Dirichlet Outlet p**
- **Depend on the derivatives of J w.r.t. the pressure, velocity and stress tensor**

Gradient-based Shape optimisation Loop



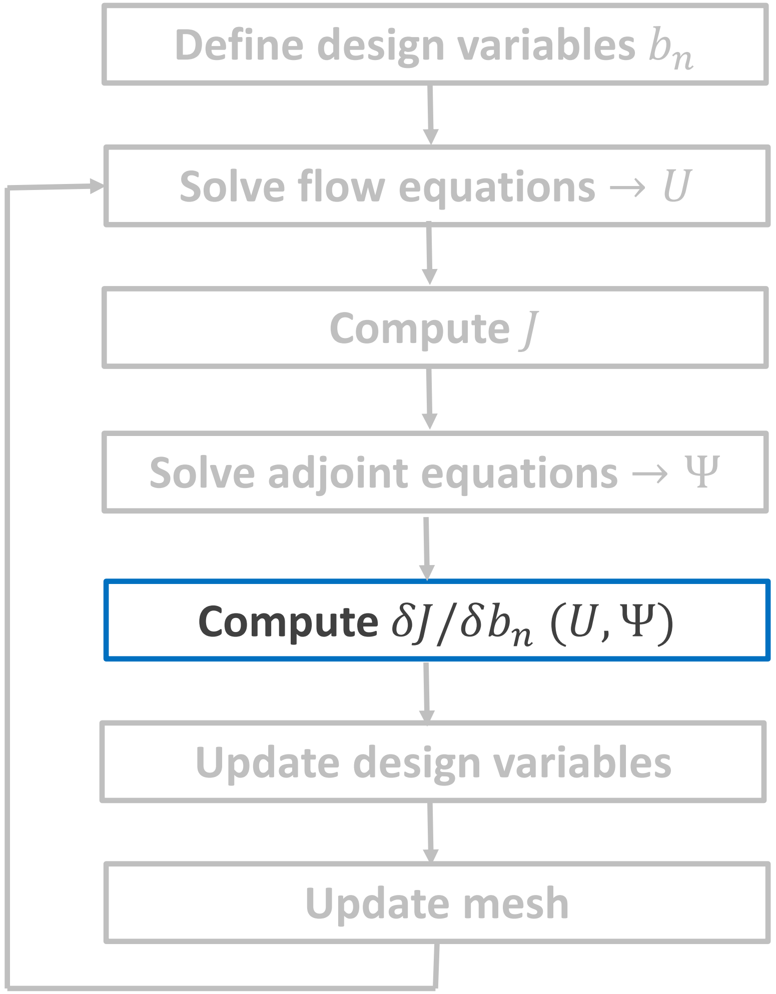
Defined in ***system/optimisationDict.adjointManagers***

How many adjoint equations do we have to solve?

- **One for each objective for which we need the gradient**
  - **Gradients of linear combinations of functions defined at a single operating point can be computed with one adjoint solution!**
  - **Advanced methods dealing with constraints (e.g. SQP, constraint projection) need the gradient of the constraint function separately**

- **(At least) One for each operating point solved**

Gradient-based Shape optimisation Loop



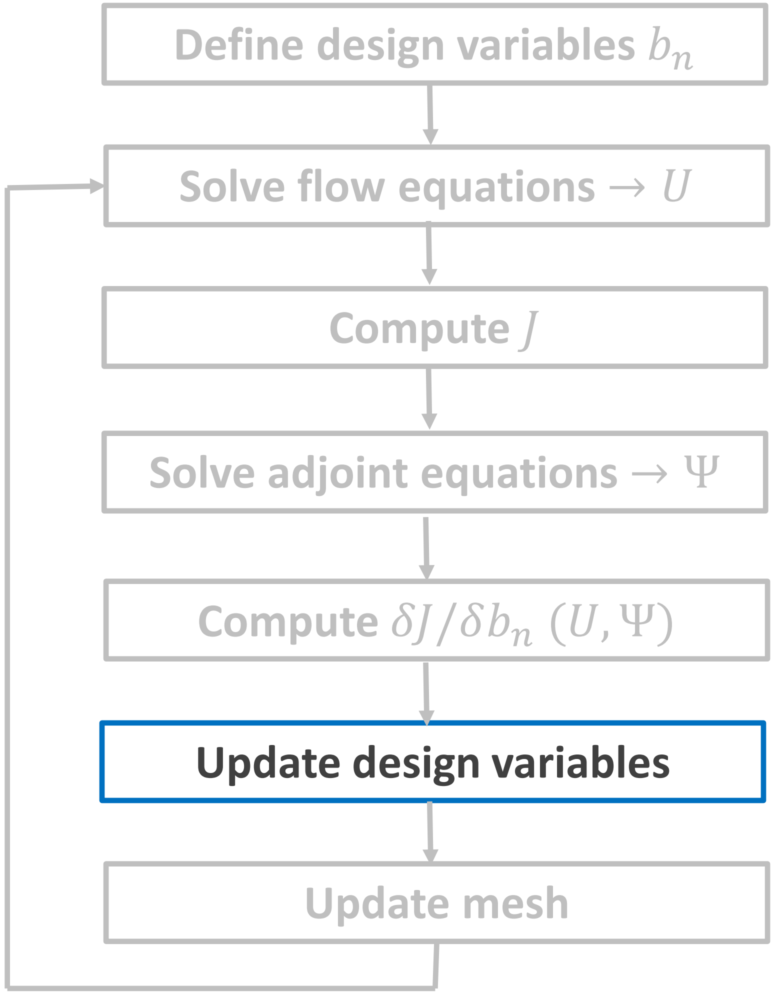
Defined in *system/optimisationDict.optimisation.designVariables*

Two mathematical formulations for shape optimisation

- **Based on Surface Integrals, (E)-SI**
  - **Need to solve an additional adjoint grid displacement PDE for m_i^a**
    - **Boundary conditions are created automatically**
    - **Need to define a linear solver in *fvSolution***
    - **No relaxation is required**
    - **Solved at a post-processing level, i.e. after the solution of the adjoint mean flow equations**

- **Based on Field Integrals, FI**
  - **Need to compute the grid sensitivities fields, i.e. $\frac{\delta x_k}{\delta b_n}$**
  - **Depending on the grid displacement model this might be computed by**
    - **solving additional PDEs (e.g. PDE-based grid displacement)**
    - **Analytically (e.g. Volumetric B-Splines)**

Gradient-based Shape optimisation Loop



Defined in
system/optimisationDict.optimisation.updateMethod

Compute the update of the design variables based on $\frac{\delta J}{\delta b_n}$ through

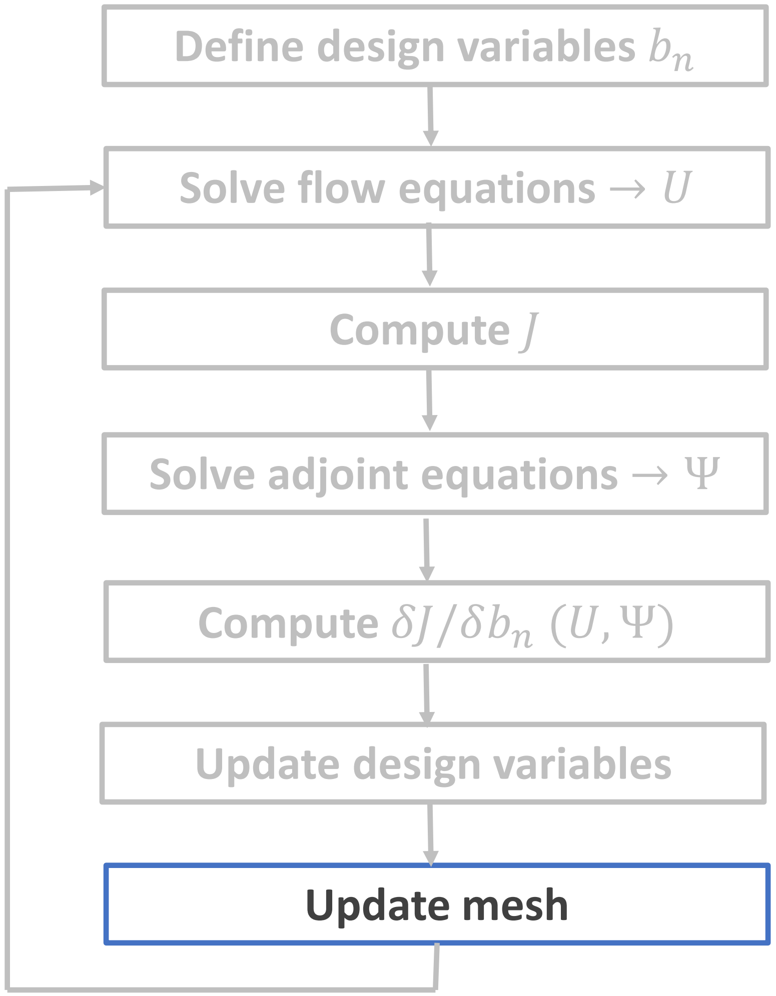
$$b_n^{new} = b_n^{old} + \eta s_n$$

- Unconstrained optimisation
  - Steepest descent
  - Conjugate Gradient
  - Quasi-Newton methods: BFGS, SR1

- Constrained optimisation
  - Constraint projection (exceptional for linear constraints)
  - SQP

- Step (η) definition
  - Direct (usually not practical)
  - Through a max. desired deformation in the initial opt. cycle

Gradient-based Shape optimisation Loop



Defined in
constant/dynamicMeshDict

- **Need to translate $\Delta \mathrm{b}_\mathrm{n}$ into a new geometry and computational mesh**
- **Remeshing can be costly and possibly result to inconsistent sensitivity derivatives. Grid displacement is preferable**
- **Depends on the parameterization and chosen grid displacement method**
  - **Usually, one tool for parameterization (e.g. NURBS), a different one for grid displacement (e.g. Laplace PDEs)**
  - **Volumetric B-Splines handles both simultaneously**
- **checkMesh ran after each update to check mesh quality**

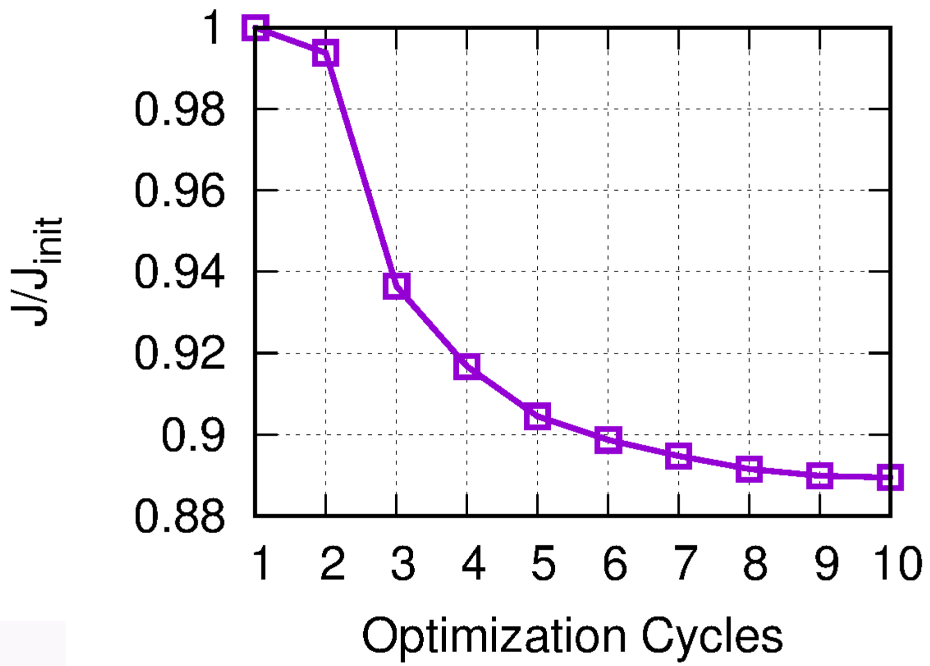
S-bend: optimisation results

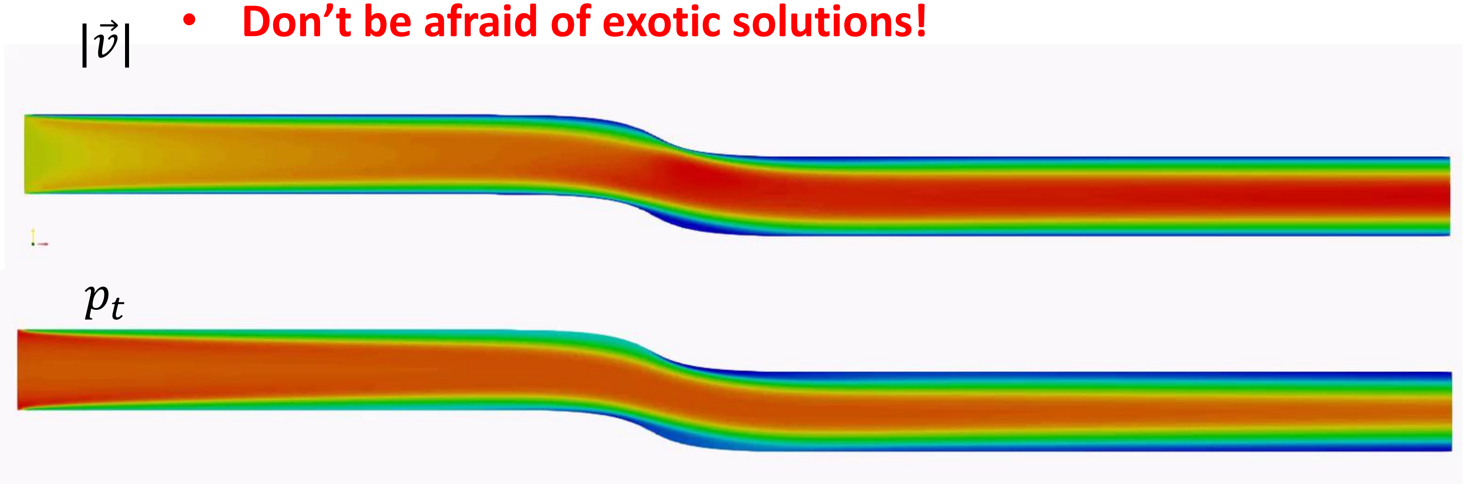
Run the optimization loop

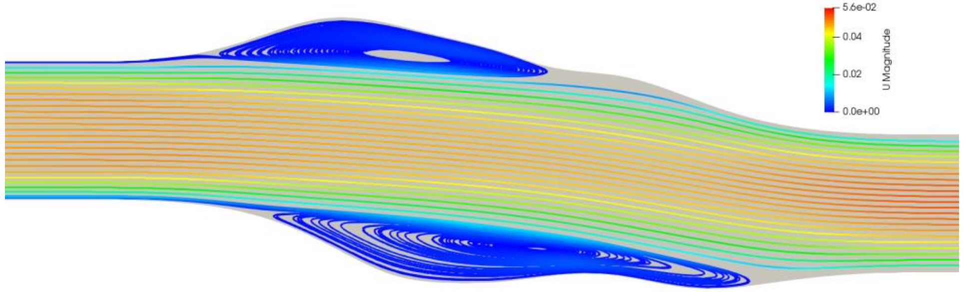
```
>> ./Allrun.parallel > log 2> err & (~2.5
min/4 procs)
```

What to examine:

- **Is J reduced?**
- **Is J converged? (history in *optimisation/objective* folder)**
- **Have the flow equations converged? (check log file)**
- **Is the mesh valid at the optimised solutions? (check log file or checkMesh)**
- **What is the mechanism behind the reduction in J?**
- **Don't be afraid of exotic solutions!**

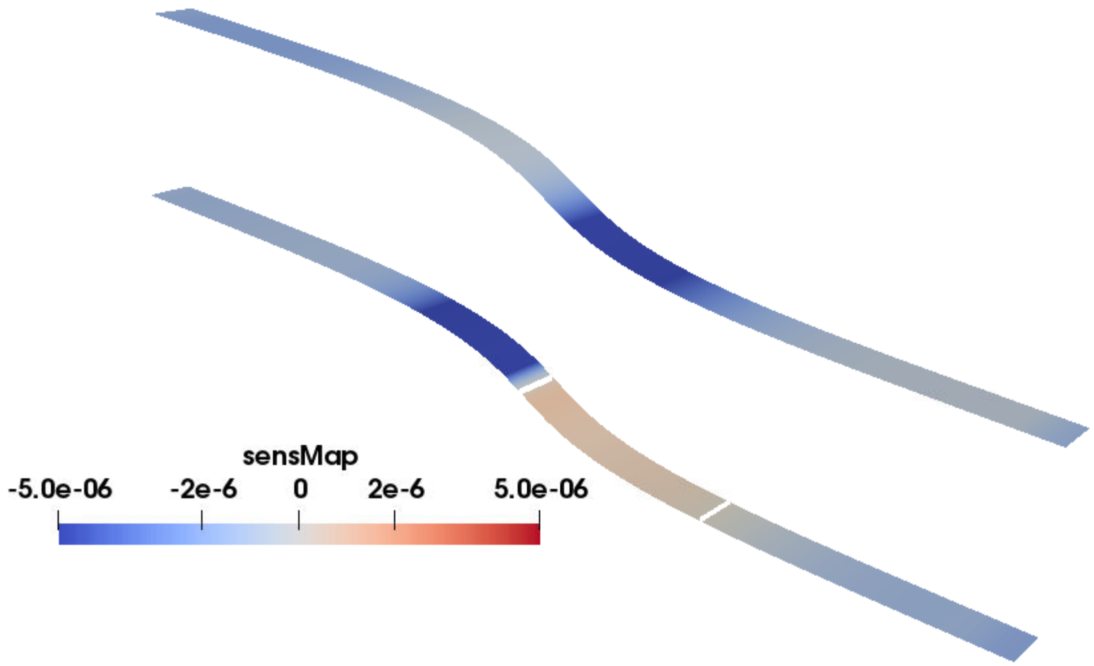






S-bend: Computing sensitivity maps

- Compute $\frac{\delta J}{\delta x_i} n_i$
- A few changes in *optimisationDict and controlDict*
- Tells us how each boundary node has to move to reduce J
    - Red: move against the surface normal (inwards)
    - Blue: move towards the surface normal (outwards)
    - White-ish: insignificant
- Computed on the initial geometry: does not mean that the optimised geometry will follow this ! …
- Good feedback towards the designer
- Useful in placing morhing boxes

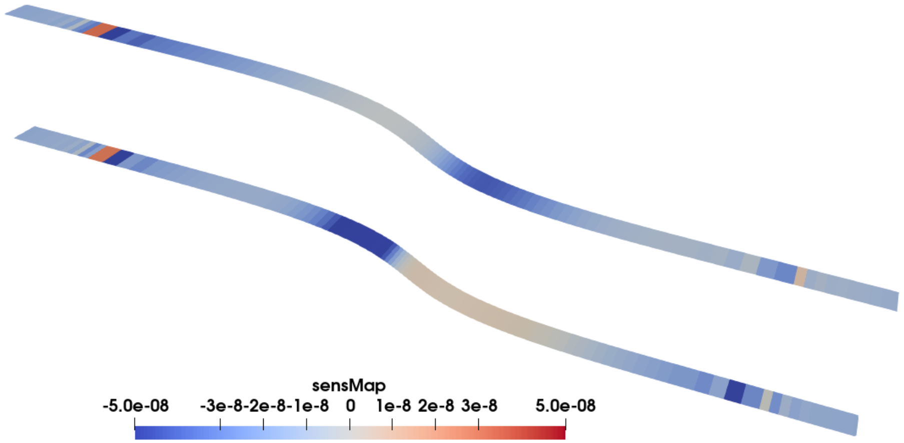


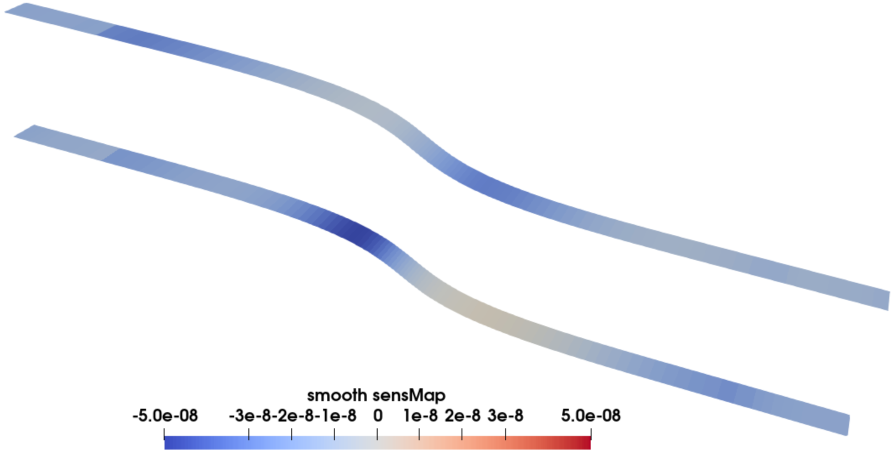
S-bend: Smoothing the sensitivity map

- **In more complex/industrial cases, checkerboards occur in the computed sensitivity maps.**
- **This problem becomes pronounced in meshes built with snappyHexMesh!**
- **The direction of favorable surface displacement becomes ambiguous...**
- **Smooth the sensitivity-map, G, by solving**

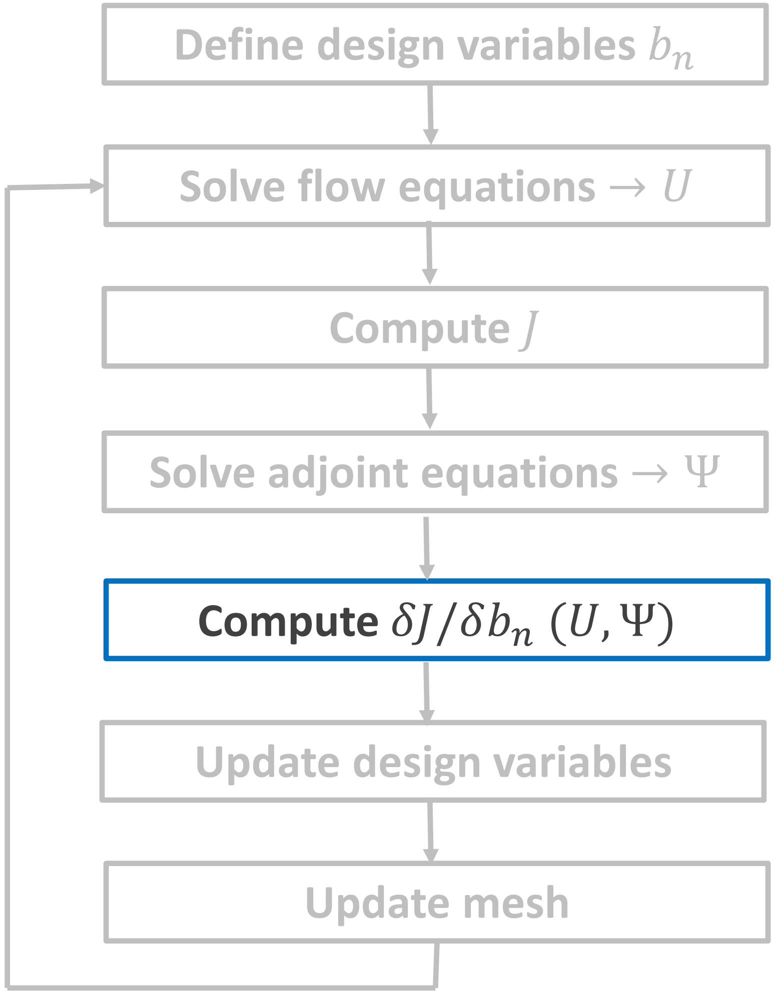
$$-R^2 \frac{\partial^2 \hat{G}}{\partial x_j^2} + \hat{G} = G$$

on a *finiteArea* mesh.





S-bend: Smoothing the sensitivity map – Additional Entries



- **Additional entries in *system/optimisationDict.optimisation.designVariables* related to the Laplace-Beltrami equation**

$$-R^2\frac{\partial^2 \hat{G}}{\partial x_j^2}+\hat{G}=G$$

  - **The smoothing radius is either specified explicitly, or computed as a multiple of the average surface edges' length.**
  - **Boundary conditions for the smooth sensitivity field are created automatically.**

- **For the creation of the *faMesh*, an *faMeshDefinition* dictionary can be optionally provided in the *system* folder.**

- ***faSchemes* & *faSolution* should be present in the *system* directory.**

Takeaway messages:

- **Adjoint supports optimisation loops at a small CPU cost ($\sim$20 cycles $\rightarrow$ ~ 40 flow solutions)**

- **Ideal for both early-stage development and refinement**

- **More optimisation types available**
  - **Active flow control (jet-based optimisation)**
  - **A Posteriori Error Analysis (optimally refine your mesh to compute an accurate objective)**
  - **Design under uncertainties**

- **Optimisation (like CFD) is not magic. Take care when defining your problem**

- **Before accepting (or discarding) an optimised geometry**
  - **Check the convergence of the flow equations**
  - **Check the mesh quality**

- **Try to understand the mechanisms behind the objective reduction**
  - **Often leads to better designs and/or better-defined optimisation problems!**

Additional topics covered through the tutorials under `$FOAM_TUTORIALS/incompressible/adjointOptimisationFoam`

- **Effect of the update method**
  `shapeOptimisation/sbend/laminar/opt/unconstrained`
- **Constrained optimisation**
  `shapeOptimisation/naca0012/lift/opt/constraintProjection`
- **3D, industrial-like cases**
  `shapeOptimisation/motorbike`

When in doubt about the case settings, you can consult the manual