



Analytical and Numerical Approaches for the Computation of Aeroelastic Sensitivities Using the Direct and Adjoint Methods

Lukas Scheucher, B.Sc.

Master Thesis



SUPERVISOR:
Dr.-Ing. Alexander Popp, Dr.-Ing. Georg Hammerl
popp@lnm.mw.tum.de

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Abstract

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Zusammenfassung

german version of your abstract.

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Nomenclature

Operators

Algebraic operations

A^T	Transpose of a tensor	T
A^{-1}	Inverse of a tensor	inv
\bar{a}	Average component of a quantity	av
a'	Fluctuating component of a qunatity	fluc
a	Norm of a quatntity	norm

Analytic operations

\ddot{A}	Second time derivative at a fixed refrence position	dderivtime
\dot{A}	First time derivative at a fixed reference position	derivtime
$ \frac{\partial A}{\partial B} \\ \frac{\partial^2 A}{\partial B^2} \\ \underline{\frac{\partial A}{\partial B^2}} \\ \underline{\frac{DA}{DB}} \\ \underline{\frac{dA}{dB}} $	partial derivative of one argument with respect to the other	pdfrac
$\frac{\partial^2 A}{\partial B^2}$	Second partial derivative of one argument with respect to the other	ppdfrac
$\frac{DA}{DB}$	Material time derivative	mfrac
$\frac{d\widetilde{A}}{dB}$	First total derivative of one argument with respect to the other	tfrac

Representation of scalars, tensors and other quantities

a	Scalar quantity	s
\boldsymbol{a}	Vector quantity	V
\boldsymbol{A}	Matrix quantity	m
A, a	continuous quantity	С
A, a	discrete quantity	d
$a^{(k)}$	Iteration index in the optimization loop	it
$a^{(k)}$	Iteration index in the optimization loop	ito
$a^{(n)}$	Iteration index in the staggered algorithm	its
\bar{A}	Fictious entity	fic
$\mathcal{O}(A)$	Order of magnitude	order

Symbols

3-field formulations

T_p	Interface projection matrix from fluid to structure mesh	ifaceprojFt
$oldsymbol{H}_2$	Second order Jacobian	jactwo
S	Turbulence term	turbmat
T_u	Interface projection matrix from structure to fluid mesh	ifaceprojSt
F	Convective part of the flux matrix	fluxmatconv
w	Discrete fsluid state vector	dfstate
\mathcal{D}_{EOS}	State equation of the mesh	EOSmesh
\boldsymbol{P}	Fluid load TODO	load
a_u	Adjoint structure displacement	structdispa
$oldsymbol{w}$	Fluid state vector	fstate
\boldsymbol{P}_F	Fluid load	fload
\mathcal{S}_{EOS}	State equation of the structure	EOSstruct
a_w	Adjoint fluid state vector	fstatead
$ ilde{m{w}}$	Primitive fluid state vector	fstateprim
$oldsymbol{x}$	Fluid mesh motion	mms
G	diffusive part of the flux matrix	fluxmatdifi
\mathcal{F}_{EOS}	State equation of the fluid	EOSfluid
S	Source term in the Reynolds Averaged Navier-Stokes (RANS) equations	turbulences
a_x	Adjoint fluid mesh motion	mmsad
$oldsymbol{w}_{RANS}$	Augumentes fluid state vector in the RANS formulation	fstaterans
\boldsymbol{P}_T	Structure load	sload
$oldsymbol{u}$	Structure displacement	structdisp
Α	Diagonal matrix with vell volumes	${\tt cellvolmat}$
χ	Additional fluid state variable introduced by the turbulence model	turbparamve

Fluid Structure Interaction

${\mathcal P}$	State equation of the structure	strucstateq
\mathcal{D}	State equation of the mesh motion	${\tt mmsstateeq}$
\mathcal{F}	State equation of the fluid	fluidstateg

Sturctural Analysis

K	Finite Elements (FE) stiffness matrix	stiffmat
u	Displacement vector	disp
d	Interface displacement	ifacedispvec
u	Discrete displacement vector	dispvec
\boldsymbol{x}	Mesh motion	motion

Optimization

s	Abstract optimazation variable	absvar
q	Optimization criterium	optcrit
ϵ^{SA}	Specified tolerance in the Sensitivity analysis	tolsa
η	Lagrange multipliers of the equality constraints	lagmultseq
L	Lagrangian function of the optimization problem	Lagfunc
$oldsymbol{s}$	Vector of abstract optimization variables	absvars
$oldsymbol{g}$	Non-equality constraints	neqctr
γ	Lagrange multipliers of the inequality constraints	lagmultsneq
$oldsymbol{q}$	Vector of optimization criteria	optcrits
$oldsymbol{d}$	Physical design parameters	physvars
z	Target cost function	costfunc
$n_{\boldsymbol{g}}$	Number of non-equality constraints	numneqctr
\boldsymbol{h}	Equality constraints	eqctr
\boldsymbol{a}	Adjoint solutions	adjoints
$n_{\boldsymbol{h}}$	Number of equality constraints	numeqctr

Fluid Mechanics

	D	
p	Pressure	pres
\mathcal{F}	Convective fluxes	fluxesconv
\boldsymbol{P}	Matrix that contains the eigenvectors of the jacobian matrix of F	jaceigvecs
T	Fluid temperature	temp
v_3	Fluid velocity in z-direction	fluidvelz
$oldsymbol{\Lambda}$	Diagonal matrix that contains the eigenvalues of the jacobian matrix of ${f F}$	jaceigvals
${\cal H}$	Jacoian matrix	jac
ρ	Density	dens
μ	Dynamic viscosity	viscosdyn
I	Identity matrix	eye
ν	Kinematic viscosity	viscoskin
$\mathcal A$	Flux Jacobian	fluxjac
au	Deviatoric fluid stress tensor	fluidstressc
${\cal G}$	Diffusive fluxes	fluxesdiff
q	Heat flux comopnement	heatfluxcomp
k	Thermal conductivity of the fluid	thermcond
E	Total energies	energytot
RE	Reynolds number	reynolds
$oldsymbol{q}$	Heat flux vector	heatflux
γ	Specific heat ratio	specheatrati
v_2	Fluid velocity in y-direction	fluidvely
e	Internal energy	energyint
v	Fluid velocity vector	fluidvelcomp
v_1	Fluid velocity in x-direction	fluidvelx
M	Averaging function associated with the Roe flux	roeavgfunc

Abbrevations

SQP Sequential Quadratic Programming

GSE Global Sensitivity Equations

SA Sensitivity Analysis

VOF Volume of Fluid Method

GFM Ghost Fluid Method

GFMP Ghost Fluid Method of the Poor

EOS Equation of State

JWL Jones-Wilkins-Lee

PG Perfect Gas

SG Stiffened Gas

MUSCL Monotonic Upwind scheme for Conservation Laws

FIVER Finite Volume Method with exact two-phase Riemann Integrals

RANS Reynolds Averaged Navier-Stokes

FV Finite Volumes

FD Finite Differences

FE Finite Elements

SA Sensitivity Analysis

LNM Lehrstuhl für Numerische Mechanik(Institute for Computational Mechanics)

TUM Technical University of Munich

CFD Computational Fluid Dynamics

ALE Arbitrary Lagrangian Eulerian

VOF Volume of Fluid Methods

DFP Davidon-Fletcher Powell formula

BFGS Broyden-Fletcher-Goldfarb-Shanno algorithm

LDR Lift over Drag Ratio

NSE Navier Stokes Equations

NSME Momentum Equation of the Navier Stokes Equations

NSCE Continuity Equation of the Navier Stokes Equations

NSEE Energy Equation of the Navier Stokes Equations

PDE Partial Differential Equation

CG Conjugate Gradient

PCG Preconditioned Conjugate Gradient

SA Sensitivity Analysis

CFD Computational Fluid Dynamics

FSI Fluid Structure Interaction

FRG Farhat Research Group

1 About this template

The purpose of this document is two-fold:

Firstly, this is a plain and simple template with the most basic LATEX-commands and structures introduced that are needed for writing a thesis in LATEX. It should be sufficient for 95% of the theses submitted at LNM - this means that completeness is not claimed. It is recommended to stick to these basic suggestions, knowing that other - possibly better - philosophies or styles exist. In case a more complex structure is needed, refer to literature or the web, although you should think twice about introducing a much more complex structure.

Secondly, this report gives some basic suggestions on what the structure of the report should look like and also some brief description about typically expected content.

Figure 1: aaa bbb

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2 Fluid mechanics

2.1 Eulerian and Lagrangian view

In time dependent analytical physics there are two basic concepts of how to view a system of interest: the Eulerian and the Lagrangian approach. It shall be stressed here, that Eulerian view and Euler equations are two totally separate things. One view this issue from different perspectives, but what the difference points down to is the interpretation of the time derivative. Since we will be using the different derivatives frequently in this thesis, a short introduction shall be provided.

2.1.1 Material derivative

The material derivative of a property, is a derivative (rate of change), that follows a specific particle 'p'. That means that at every time instance the material derivative gives as the current value of the property of a specific particle. Since in general, a particle will move its position in time quite a lot, some mean is required to track the particles motion. The material derivative is also known as the Lagrangian concept, and is commonly used in Solid mechanics, since the motion of the solid particles is typically little, or at least nearly uniform over the body, which makes position tracking easy.

2.1.2 Eulerian derivative

The Eulerian derivative takes a different approach. It refers to a fixed frame of reference in the domain, and gives the rate of change at that specific position. Due to the particle movement, it typically refers to different particles at different times. Material and Eulerian derivatives can be linked via the so-called convective rate of change as:

$$\underbrace{\frac{D\mathbf{G}}{Dt}}_{\text{Lagrangian rate of change}} = \underbrace{\frac{\partial \mathbf{G}}{\partial t}}_{\text{Eulerian rate of change}} + \underbrace{\mathbf{v} \cdot \nabla \mathbf{G}}_{\text{Convective rate of change}} \tag{1}$$

In fluid mechanics the Eulerian concept is typically prefered.

However, when looking at fluid-structure interaction problems, the interface is typically moving. To account for that motion in the fluid, one either has to come up with some cell-intersection approach, or the fluid-mesh has to be deformed to. An appealing and straightforward approach to do so, is the so called Arbitrary Lagrangian Eulerian (ALE) approach. As the name suggest, it is a hybrid between Eulerian and Lagrangian point of view. The ALE approach allows to utilize the best of both approaches. The mesh can either be fixed, moved with the continuum in an Eulerian manner, or be moved in some arbitrarily specified manner in between. The ALE method can handle larger distortions than a pure Eulerian would, while still allowing to keep interface continuity between the structure and the fluid, such that no intersection of fluid cells is necessary.

In this thesis, both Eulerian and ALE methods will be covered. In general, no

recommendation on to prefer one or the other method can be given. Instead, one should always be aware of the strength and weaknesses of either method and choose the appropriate one for a specific problem accordingly.

2.2 Basic equations of fluid mechanics

The physics of fluid motion are governed by the so-called Navier Stokes Equations (NSE). These equations were derived independently of one another by Claude-Louis Navier and George Gabriel Stokes as a generalization of the Euler-equations that now includes viscosity effects. In general one distinguishes the incompressible and the compressible NSE. The validity of their application depends on the problem setup. As a rule of thumb, flows with Mach-numbers lower than 0.3 can usually be safely approximated by the incompressible NSE.

The Navier stokes equation consist of the Momentum Equation of the Navier Stokes Equations (NSME), the Continuity Equation of the Navier Stokes Equations (NSCE) and, if the compressible equations are solved, the Energy Equation of the Navier Stokes Equations (NSEE). In the literature, the term NSE is often synonymously used for the NSCE, in this thesis however, with NSE we will always refer to the full set of equations and will explicitly name the momentum, continuity or energy equation otherwise.

2.2.1 Incompressible Navier Stokes Equations

The incompressible NSE are derived by putting a few assumptions on the Cauchy stress tensor:

- Galilean invariance of the fluid stress tensor
- Isotropy of the fluid
- The stokes stress constitutive equation applies: $\tau = 2\mu\epsilon$ with $\epsilon = \frac{1}{2}(\nabla v + (\nabla v)^T)$

In convective form, the incompressible NSME can be written as

$$\underbrace{\frac{\partial \boldsymbol{v}}{\partial t} + (\boldsymbol{v} \cdot \nabla)\boldsymbol{v}}_{\text{Variation}} + \underbrace{\frac{\partial \boldsymbol{v}}{\partial t} + (\boldsymbol{v} \cdot \nabla)\boldsymbol{v}}_{\text{Convection}} - \underbrace{\frac{\partial \boldsymbol{v}}{\nu \nabla^2 \boldsymbol{v}} = -\underbrace{\nabla \boldsymbol{w}}_{\text{Internal source}} + \underbrace{\frac{\operatorname{eq:nsg_incompressible}}{g}}_{\text{External source}}$$

where \boldsymbol{w} is the specific thermodynamic work, whiuch statisfies

$$\nabla \boldsymbol{w} = \frac{1}{\rho} \nabla p \tag{3}$$

And the incompressible NSCE can be written as

$$\nabla \cdot \boldsymbol{v} = 0 \tag{4}$$

It shall be noted, that the in the incompressible NSE, the pressure can only be solved up to a certain constant. The pressure at a certain point therefore has to be fixed, or the system will be singular.

2.2.2 Compressible Navier Stokes Equations

Compared to the incompressible NSE, the compressible NSE introduce one additional unknown, since the density can now vary. To close the system, one additional equation is required, the energy equation.

The compressible NSE are derived by making the following assumptions:

- Galilean invariance of the stress tensor
- Linearity of the stress in the velocity gradient: $\tau(\nabla v) = C : (\nabla v)$, where C is called the viscosity or elasticity tensor.
- Isotopy of the fluid

The compressible NSME can be written as

$$\frac{\partial \boldsymbol{v}}{\partial t} + \boldsymbol{v} \cdot \nabla \boldsymbol{v} = -\frac{\partial 1}{\partial \rho} \nabla p + \nu \nabla^2 \boldsymbol{v} + \frac{1}{3} \nu \nabla (\nabla \cdot \boldsymbol{v}) + g$$
(5)

where it shall be noted that for the special case of an incompressible flow, the volume of the fluid elements is constant, resulting in a solenoidal velocity field. Thus $\nabla \cdot \mathbf{v} = \mathbf{0}$ and $\nabla p = 0$, which gives equation 2.

The NSCE now takes into accounts for the variable density

$$\frac{\partial \rho}{\partial t} = \nabla \cdot (\rho \mathbf{v}) = 0 \tag{6}$$

And finally the NSEE writes

$$\frac{\partial s}{\partial t} = -\boldsymbol{v} \cdot \boldsymbol{s} + \frac{Q}{T} \tag{7}$$

where s is the entropy per unit mass, Q is the heat transferred, and T is the temperature.

2.2.3 Euler equations

The Euler equations can be regarded as a special case of the Navies stokes equations where the diffusive(viscous) contributions are neglected. Dimension analysis [?] reveals that this is usually justified for high Mach numbers and distant from walls. In fact, boundary Layer theory suggests that a lot of problems can be well approximated by solving the full, diffusive equations only near the wall boundary and using the Euler equations everywhere else. Although the Euler equations can be derived for both incompressible and compressible flows, the statement above suggests that only the compressible ones give actual, physically correct results. We therefore restrict our considerations to the compressible Euler equations.

Summing up, these equations can be written in convective form as

$$\begin{cases} \frac{\partial \rho}{\partial t} + \boldsymbol{v} \cdot \nabla \rho + \rho \nabla \cdot \boldsymbol{v} = 0 & \text{Continuity equation} \\ \frac{\partial \boldsymbol{v}}{\partial t} + \boldsymbol{v} \cdot \nabla \boldsymbol{v} + \frac{p}{\rho} = \boldsymbol{g} & \text{Momentum equation} \\ \frac{\partial e}{\partial t} + \boldsymbol{v} \cdot \nabla e + \frac{p}{\rho} \nabla \cdot \boldsymbol{v} = 0 & \text{Energy equation} \end{cases}$$
(8)

2.2.4 Conservative Form

For the purpose of FV discretization one usually brings the equations into the socalled conservative form, which can be written generally as

$$\frac{\mathrm{d}\boldsymbol{\xi}}{\mathrm{d}t} + \nabla \cdot f(\boldsymbol{\xi}) = \mathbf{0} \quad \text{eq:conservative_form_general} \tag{9}$$

where $\boldsymbol{\xi}$ is the conserved qunatity of interest and $f(\boldsymbol{\xi})$ is denoted as "flux function". This equation can then be transformed into an integral form using the divergence theorem

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_{V} \boldsymbol{\xi} dV + \int_{\partial V} f(\boldsymbol{\xi}) \cdot \overset{\text{eq:conservation_form_integral}}{dS}$$
(11)

This equations states that the rate of change of the integral of the quantity ξ over an arbitrary control volume V is equal to the negative of the "flux" through the boundary of the control volume ∂V .

A simple choice for f would be $f(\xi) = \xi v$, which means that the quantity ξ follows the fluid field and gives the so-called "advection equation".

Although one form is derived from the other, these two are not equivalent. Particularly, it is possible to find solutions to the integral equations that are non-differentiable and therefore not a solutions to the differential form. This leads to so called "weak solutions" and is the cause for many numerical difficulties in the finite volume simulation of such problems.

This thesis focuses on the compressible NSE only. They can be brought to conservative form as:

$$\frac{\partial w}{\partial t} + \nabla \cdot \mathcal{F}(w) + \nabla \cdot \mathcal{G}(w) = 0$$
 eq:nsg_conservative_form (12)

where, comparing to the general conservative form, one can see that $\boldsymbol{\xi} = \boldsymbol{w}$ and $f(\boldsymbol{\xi}) = \mathcal{F}(\boldsymbol{w}) + \mathcal{G}(\boldsymbol{w})$

In the conservative form of the NSE the so-called "fluid state vector" \boldsymbol{w} is defined as

$$m{w} = \begin{bmatrix}
ho \\
ho \mbox{v} \\ E \end{bmatrix}$$
 eq:fstate_definition (13)

with

$$m{v} = egin{bmatrix} v_1 \\ v_2 \\ v_3 \end{bmatrix}$$
 eq:fluidvel_definition (14)

denoting the fluid velocity vector.

The total energy E can be computed as a sum of the so called internal energy and the kinematic energy due to fluid velocity as

$$E_{\text{total energy}} = \underbrace{\rho e}_{\text{internal energy}} + \underbrace{\frac{1}{2} \mathbf{v}^T \mathbf{v}}_{\text{kinematic energy}}$$
eq:energytot

Bringing the convective form of the compressible NSE (5) into the conservative form (??), one can derive \mathcal{F} and \mathcal{G} as

$$\mathcal{F} = \boldsymbol{w}\boldsymbol{v}^{T} + p \begin{bmatrix} 0 \\ \mathbf{I} \\ \boldsymbol{v}^{T} \end{bmatrix}$$
 eq:fluxesconv (16)
$$= \begin{bmatrix} \rho \boldsymbol{v}^{T} \\ \rho(\boldsymbol{v}\boldsymbol{v}^{T}) + p \mathbf{I} \\ (E+p)\boldsymbol{v}^{T} \end{bmatrix}$$

$$= \begin{bmatrix} \rho v_{1} & \rho v_{2} & \rho v_{3} \\ p + \rho v_{1}^{2} & \rho v_{1}v_{2} & \rho v_{1}v_{3} \\ \rho v_{2}v_{1} & p + \rho v_{2}^{2} & \rho v_{2}v_{3} \\ \rho v_{3}v_{1} & \rho v_{3}v_{2} & p + \rho v_{3}^{2} \\ v_{1}(E+p) & v_{1}(E+p) & v_{1}(E+p) \end{bmatrix}$$

$$(17)$$

depending on the algorithm, one or another form can be advantageous.

The diffusive fluxes can be written as

$$\mathcal{G} = \begin{bmatrix} 0 \\ \tau \\ \tau v + q \end{bmatrix}$$
 eq:fluxes_diff (19)|
$$= \begin{bmatrix} 0 & 0 & 0 & 0 \\ -\tau_{xx} & -\tau_{yx} & -\tau_{zx} \\ -\tau_{xy} & -\tau_{yy} & -\tau_{zy} \\ -\tau_{xz} & -\tau_{yz} & -\tau_{zz} \\ -q_x - v_1 \tau_{xx} - v_1 \tau_{yx} - v_1 \tau_{zx} & -q_y - v_1 \tau_{xy} - v_1 \tau_{yy} - v_1 \tau_{zy} & -q_z - v_1 \tau_{xz} - v_1 \tau_{yz} - v_1 \tau_{zz} \end{bmatrix}^T$$
(20)

The definition of the stress tensor depends of the fluid model used. For the simple case of a Newtonian fluid, it can be written as

$$oldsymbol{ au} = \mu(\nabla oldsymbol{v} + (\nabla oldsymbol{v})^T) + \lambda(\nabla \cdot oldsymbol{v}) oldsymbol{\mathsf{I}}$$
 eq:fluidstress (21)

For the relation between Temperature and heat flux an assumption has to be made. Most often, a simple Fourier's law is assumed

$$\mathbf{q} = -k\nabla T$$
 eq:heatflux (22)

2.2.5 Euler equations

The euler equations are a simplified form of the Navier-Stokes Equations (2)(5), where the viscous effects are neglected by setting $\mathcal{G} = \mathbf{0}$.

$$\frac{\partial \boldsymbol{w}}{\partial t} + \nabla \cdot \boldsymbol{\mathcal{F}}(\boldsymbol{w}) = \boldsymbol{0}$$
 eq:euler (23)

The Euler equations are appropriate for a wide range of applications. A typical indicator is the Reynolds number, which describes the ratio between inertial forces and viscous forces:

$$RE = \frac{\rho vL}{\mu} = \frac{vL}{\nu}$$
 eq:reynolds (24)

where L describes a characteristic length.

A high Reynolds number thus indicates that the flow is dominated by inertial forces, thus the Euler Equations should give satisfying results. However, an Euler flow lacks the ability to represent stick wall boundary conditions, thus it is unable to represent boundary layers.

2.2.6 Equations of State

Looking at the above Equations, one might notice that the number of unknowns is greater than the number of equations. Particularly, the pressure only appears in Equation (16) and is not linked to the other formulas. This problem is solved by introducing an Equation of State (EOS) that relates pressure, internal energy and density. The EOS depends on the fluid model, some well-known ones are: Perfect Gas (PG), Stiffened Gas (SG), Jones-Wilkins-Lee (JWL).

For the simplest one, PG, the EOS can be written as

$$p = (\gamma - 1)\rho e$$
 eq: eqs. pg
(25)

2.2.7 Reynolds Averaged Navier-Stokes Equations

The Reynolds Averaged Navier-Stokes (RANS) Equations are time-averaged equations of motion for the fluid.

$$m{w}
ightarrow ar{m{w}} = \lim_{T
ightarrow \infty} rac{1}{T} \int_{t^0}^{t^0 + T} m{w} dt$$
 eq:rans_averaging (26)

The main idea of the approach is to decompose an instantaneous quantity into time-averaged and fluctuating components

$$m{w} = \underbrace{ar{w}}_{time-average} + \underbrace{m{w}'}_{fluctuation}$$
 eq:rans_decomposition (27)

When substituting this decomposition back into the NSE(and injecting several other approximations), a closure problem induced by the arising non-linear Reynolds

stress term $RE_{ij} = -v_i \bar{v}_j'$ arises. Additional modeling is therefore requires to close the RANS equations, which has led to many different turbulence models.

Whatever turbulence model is chosen, the fluid-state vector is augmented by the m parameters of the turbulence model

$$\boldsymbol{w}_{RANS} \leftarrow \begin{bmatrix} \boldsymbol{w} \\ \chi_1 \\ \vdots \\ \chi_m \end{bmatrix} = \begin{bmatrix} \rho \\ \rho \boldsymbol{v}^T \\ E \\ \chi_1 \\ \vdots \\ \chi_m \end{bmatrix}$$
(28)

The RANS equation can then be written as

$$\frac{\partial \bar{\boldsymbol{w}}}{\partial t} + \nabla \cdot \mathcal{F}(\bar{\boldsymbol{w}}) + \nabla \cdot \mathcal{G}(\bar{\boldsymbol{w}}) = \mathsf{S}(\bar{\boldsymbol{w}}, \chi_1, \cdots, \chi_m) \overset{\text{eq:rans_eqautions}}{(29)}$$

3 The Finite Volume methodaaa

3.1 General

Like Finite Differences (FD) or FE, the FV method is a mean to solving a Partial Differential Equation (PDE) by transforming it into a discrete algebraic form. In the field of fluid mechanics, the finite volume method is the most popular approach. Other than FD or FE, the finite volume is conservative by construction. Other than FD it can easily be implemented for unstructured grids. Compared to the FE method, where boundary conditions come naturally from the formulation, this causes some difficulties in FV.

It shall also be mentioned that the introduction of stabilization schemes(like stream-line upwinding), is much easier in an FV formulation. Overall, for Computational Fluid Dynamics (CFD), FV has so far shown to be the best compromise between accuracy, stability and efficiency.

Finite volume methods are typically derived from the so called conservative form of a PDE. It is shown in Section 2.2.4, that the NSE equation can be brought to the same form. In general, the conservative form can be written as:

$$\frac{\mathrm{d}\boldsymbol{\xi}}{\mathrm{d}t} + \nabla \cdot f(\boldsymbol{\xi}) = \mathbf{0} \tag{30}$$

(31)

where ξ represents a vector of states and f is the so-called flux tensor. After subdividing the domain into finite volumes, also called cells, on car

After subdividing the domain into finite volumes, also called cells, on can write for each particular cell i

$$\int_{V_i} \frac{\mathrm{d}\boldsymbol{\xi}}{\mathrm{d}t} dV_i + \int_{V_i} \nabla \cdot f(\boldsymbol{\xi}) dV_i$$
(32)

After applying the divergence theorem to the second term this gives:

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_{V_i} \boldsymbol{\xi} dV_i + \int_{\partial V_i} f(\boldsymbol{\xi}) \cdot \boldsymbol{n} \ dS_i$$
 (33)

And after integration the first term to get the volume average

$$V_i \frac{\mathrm{d}\bar{\boldsymbol{\xi}}}{\mathrm{d}t} + \int_{\partial V_i} f(\boldsymbol{\xi}) \cdot \boldsymbol{n} \ dS_i \tag{34}$$

So that finally, the equation can be written as

$$\frac{\mathrm{d}\bar{\boldsymbol{\xi}}}{\mathrm{d}t} + \frac{1}{V_i} \int_{\partial V_i} f(\boldsymbol{\xi}) \cdot \boldsymbol{n} \ dS_i \tag{35}$$

which can easily be interpreted. The cell average of the conserved properties changes according to the total flux through the cells surface. Of course, the conservative

value is defined as being constant within one cell, so there will be different values on faces or edges, depending on which side one is looking at. There are different approaches on how to choose an appropriate value. And the choice may greatly effect the numerical properties. In a FV solver, the numerical flux at the interface is typically constructed such, that upwinding is achieved.

3.2 Finite Volume method for fluid mechanics

It has already been shown in Section 2.2.4, that the NSE can be brought into the conservative form (12). The flux has been shown to consist of a convective and a diffusive part(16)(19). For this thesis, a Monotonic Upwind scheme for Conservation Laws (MUSCL) type FV framework for unstructured three-dimensional grids, as described in [8] has been used.

The formulation is derived by re-writing equation 12 in variational form by multiplying with a test function:

$$\int_{\Omega} \frac{\partial \boldsymbol{w}}{\partial t} \phi_i d\Omega + \int_{\Omega} \nabla \cdot \mathcal{F}(\boldsymbol{w}) \phi_i d\Omega + \int_{\Omega} \nabla \cdot \mathcal{G}(\boldsymbol{w}) \phi_i d\Omega = \mathbf{0}$$
 (36)

where $\phi_i \in C^0(\Omega)$. For this formulation ϕ_i is chosen to be piecewise linear. Particularly, the test functions fulfill

$$\phi_i(\boldsymbol{X}_j) = \delta_{ij} \tag{37}$$

Now, Gauss divergence theorem is applied to the last part, giving

$$\int_{\Omega} \frac{\partial \boldsymbol{w}}{\partial t} \phi_i \ d\Omega + \int_{\Omega} \nabla \cdot \mathcal{F}(\boldsymbol{w}) \phi_i \ d\Omega + \left(\int_{\Gamma} \mathcal{G}(\boldsymbol{w}) \cdot \boldsymbol{n} \ d\Gamma - \int_{\Omega} \mathcal{G}(\boldsymbol{w}) \cdot \nabla \phi_i \ d\Omega \right) = \mathbf{0}$$
(38)

In contrast to a real FE formulation, the contribution of the viscous flux at the far field boundary is now neglected, as explained in [6]. How the boundary conditions at the far fields are taken care of will be explained at a proper place. We finally get the mixed FV-FE form by mass lumping the first two terms. Since we are using a vertex-centered approach here, mass lumping is equivalent to using a constant test function of ϕ_i on the dual cell. We therefore get:

$$\int_{\Omega_i} \frac{\partial \boldsymbol{w}}{\partial t} \ d\Omega + \int_{\Omega_i} \nabla \cdot \mathcal{F}(\boldsymbol{w}) \ d\Omega - \int_{\Omega} \mathcal{G}(\boldsymbol{w}) \cdot \nabla \phi_i \ d\Omega = \boldsymbol{0}$$
 (39)

Please note that we have switched from an integral over the whole domain to an integral across the dual cells here. Finally by averaging \boldsymbol{w} over the cell in the first term, we can derive the FV formulation as

$$\frac{\partial \boldsymbol{w}_{i}}{\partial t} + \frac{1}{\|\Omega_{i}\|} \int_{\Omega_{i}} \nabla \cdot \mathcal{F}(\boldsymbol{w}) \ d\Omega_{i} - \frac{1}{\|\Omega_{i}\|} \int_{\Omega} \mathcal{G}(\boldsymbol{w}) \cdot \nabla \phi_{i} \ d\Omega = \boldsymbol{0}$$
(40)

Where now, \boldsymbol{w}_i denotes the average of \boldsymbol{w} in the dual cell Ω_i , which is by construction the value of \boldsymbol{w} at vertex i. The volume of cell Ω_i is denoted as $\|\Omega_i\|$ here. Finally, gauss divergence theorem is applied to the convective term, resulting in

$$\frac{\partial \boldsymbol{w}_i}{\partial t} + \frac{1}{\|\Omega_i\|} \int_{\partial \Omega_i} \mathcal{F}(\boldsymbol{w}) \cdot dS - \frac{1}{\|\Omega_i\|} \int_{\Omega} \mathcal{G}(\boldsymbol{w}) \cdot \nabla \phi_i^{\texttt{eq:nsg_basic_fv-form}} \tag{41}$$

As can be seen from figure 2, the dual cells themselves can have very random shapes. This makes the integration over the boundary of the second term in Equation (41) more cumbersome than in a primal approach. Also, the volume integral in the FE-like expression has to be splitted into regular shaped subdomains, e.g. tetrahedra, such that standard integration rules, like gauss rule, can be applied.

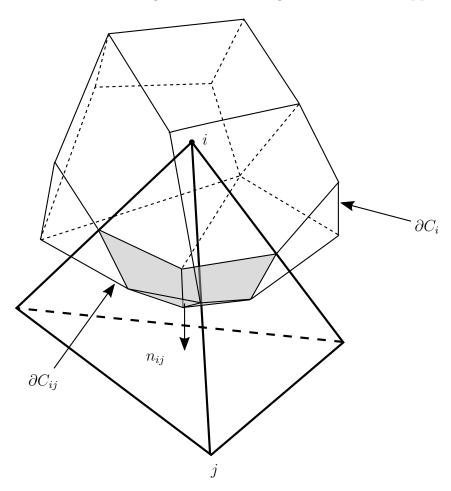


Figure 2: FV semi-discretization of an unstructured mesh. Vertex i is the center of dual cell C_i . The boundary of the dual cell is denoted as ∂C_{ij}

For a closer look into the convective fluxes integral, we decompose the boundary as $\partial \Omega_i = \sum_{i \in \kappa(i)} \partial \Omega_{ij}$, where $\kappa(i)$ denotes the set of vertices connected by an edge to vertex i.

In this thesis, the surface integral in equation (41) is than approximated using a

Riemann solver and a MUSCL [14] technique. This approximation can be written as

$$\int_{\partial\Omega_i} \mathcal{F}(\boldsymbol{w}) \cdot dS \approx \sum_{j \in \kappa(i)} \boldsymbol{\phi}_{ij}(\boldsymbol{w}_{ij}, \boldsymbol{w}_{ji}, \boldsymbol{n}_{ij})$$
(42)

where ϕ_{ij} denotes the chosen numerical flux function along the edge i-j and the two extrapolated fluid states at the i and the j-side of the the intersection of the cell boundary $\partial\Omega_{ij}$ and edge i-j are denoted by \boldsymbol{w}_{ij} and \boldsymbol{w}_{ji} respectively. The area-weighted normal of edge i-j is denoted as \boldsymbol{n}_{ij} .

As for the volume integral of the diffusive term in Equation (41), it shall be noted that the shape function is still denoted in the primal cell. Since the gradient of the test function is constant, as is the diffusive flux itself, the integral becomes a summation of the primal sub-tetrahedral contributions.

3.3 Treatment of the viscous term

The equivalence of the finite volume representation of the viscous term, with the finite element-like representation provided in Equation **TODO** might not be obvious to the reader. This section is therefore denoted to a FE discretiation of the governing equations, that can then be reformulated such that the mixed FV-FE formulation is obtained.

First, we start with the full NSE in conservative form, as provided in Equation **TODO12**. Next, a test function is defined. We chose the function $(\chi_i)_{i \in \mathcal{P}_h}$ where \mathcal{P}_h represents the primal mesh, as step functions over the dual cells of \mathcal{D}_h . A multiplication with the test-functions and subsequent integration thus gives the following weak form

$$\int_{\Omega} \frac{\partial \boldsymbol{w}}{\partial t} \chi_i dx + \int_{\Omega} \nabla \cdot \mathcal{F}(\boldsymbol{w}) \chi_i dx + \int_{\Omega} \nabla \cdot \mathcal{G}(\boldsymbol{w}, \nabla \boldsymbol{w}) \chi_i dx = \mathbf{0}^{\text{form_felike}} \tag{43}$$

where by using the divergence theorem, we obtain

$$\int_{\Omega} \nabla \cdot \mathcal{F}(\boldsymbol{w}) \chi_i dx = \int_{\partial C_i} \mathcal{F}(\boldsymbol{w}) \cdot \boldsymbol{n} ds \stackrel{\text{eq:divtheorem_felike}}{(45)}$$

$$\int_{\Omega} \nabla \cdot \mathcal{G}(\boldsymbol{w}, \nabla \boldsymbol{w}) \chi_i dx = \underbrace{\int_{\partial C_i} \mathbb{K} \nabla \boldsymbol{w} \cdot \boldsymbol{n} ds}_{II}$$
(46)

Where the first term is already equivalent to what we have derived by the FV approach in **TODO**.

It the diffusive tensor \mathbb{K} is approximated to be constant over the triangle, which is justified in **TODO**, th product $\mathbb{K}w$ is constant on can now write the above integral as

$$II = \sum_{T \in \mathcal{D}_i} \mathbb{K} \nabla \boldsymbol{w} \int_{\partial C_i \cap T} \boldsymbol{n}_C ds$$
 (47)

Now, we use a particular geometric relation, that holds for primitive elements like triangles and tetrahedra, and will be derived in Section 3.3.1

$$\int_{C_i \cap T} \mathbf{n} ds = \frac{\mathbf{n}_i^T}{2} \tag{48}$$

where n_i^T is the normal to the primal mesh triangle T on the edge opposite of node i. This is where the geometric considerations of section 3.3.1 come int place. As shown in equations (57), the integral over the dual face edge can be written via the normal of the primal mesh triangle as

$$-\sum_{T\in\mathcal{D}_i} \mathbb{K}\nabla \boldsymbol{w} \frac{\boldsymbol{n}_i^T}{2} \tag{49}$$

Also, we have shown in Section 3.3.1, that for the case of a simple triangle (but equally applicable to tetrahedra), the last term of the above equation can be written as

$$-\sum_{T\in\mathcal{D}_i} \mathbb{K} \nabla \boldsymbol{w} \int_T \nabla \phi_i dx \tag{50}$$

where ϕ_i is the P1 shape-function defined in (52). Finally we can go the opposite way, and join the summations over integrals over triangular contributions back to an overall integral over the whole dual cell. Doing this finally leads to

$$II = -\int_{\mathcal{D}_i} \mathbb{K} \nabla \boldsymbol{w} \cdot \nabla \phi_i dx \tag{51}$$

which is exactly the term provided in equation **TODO**. Since we used the same step-function based test-functions for all terms in equation (43), this approach is not only consistent, for the special case, of linear triangles we have shown that our finite element term is equivalent to a FV approximation.

3.3.1 Geometric considerations

This section is dedicated to the the derivation of a particular link between the shapefuntion of a linear triangle/tetrahedra and its outward facing normals that we use in chapter ?? to proof the equivalence of the FE-formulation of the finite volume term with the FV formulation.

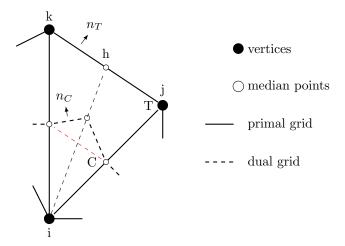


Figure 3: One Triangle T out of the set of triangles \sum_{T} , that are connected to vertex i. C denotes the dual cell related to vertex i.

We first look at one triangle of the set of triangles \sum_{T} that belong to node *i*. The setup is visualized in Figure 3.

The reader can easily verify, that a linear shape-function of node i can be written as:

$$\phi_i(m{x}) = rac{m{h}m{x}\cdotm{h}m{i}}{\|m{h}m{i}\|^2}$$
 eq:p1_triangle_eq1 (52)

where hx is the vector from point h to any point x in the triangle, and hi is the vector from point h to point i. For this particular representation of the shape function, the gradient can be elegantly written as

$$abla \phi_i(m{x}) = rac{m{h} m{i}}{\|m{h} m{i}\|^2} = rac{\hat{m{h}} m{i}}{\|m{h} m{i}\|}$$
 eq:p1_triangle_eq2 (53)

where $\hat{\boldsymbol{h}}\boldsymbol{i}$ is the normalized vector in h-i direction. Moreover, simple geometry tells us that

$$\|\mathbf{h}\mathbf{i}\| \|\mathbf{k}\mathbf{j}\| = 2|T|$$
 eq:p1_triangle_eq3 (54)

where |T| is the area of the triangle T

Substituting equation 54 into equation 53 therefore leads to

$$abla \phi_i(m{x}) = m{h} m{i} \cdot \frac{\|m{k} m{j}\|}{2|T|} = -\frac{m{\nu}}{2|T|}$$
 eq:p1_triangle_eq4 (55)

where ν is the weighted outward facing normal to edge jk.

$$\boldsymbol{\nu} = -\hat{\boldsymbol{h}}\boldsymbol{i} \|k\boldsymbol{j}\| = -\int_{[jk]} \boldsymbol{n}_T d\Gamma$$
 (56)

Referring to previous chapter we remind the reader that in the vertex based FV approach, and integration over the dual face interface (dashed line in Figure 3) via the weighted interface normal is typically performed.

By simple geometrical considerations we can now determine, that the following relation holds

$$\int_{\Gamma_C \cap T} const. \ \boldsymbol{n}_c = \frac{1}{2} \int_{\Gamma_T} const. \ \boldsymbol{n}_T \qquad \qquad = \frac{e \boldsymbol{\varphi}_t^T \text{inal_relation}}{2} \tag{57}$$

4 Fluid structure interaction

Fluid Structure Interaction (FSI) describes the aeroelastic response of a mechanical system under fluid load, as well as the interaction between fluid and structure itself. Synonymously the term "Aeroelasticity" is often used.

For this thesis, we first will focus on an ALE formulation, a closer look into this topic in the context of en Embedded formulation will follow.

4.1 Coupled three-field formulation

In an aeroelastic ALE problem, three solution fields have to be considered. Firstly, the usual fluid problem has to be solved. Over the FSI interface, the fluid now interacts with the structure, imposing a Neumann problem on it. Finally, since we are considering ALE here, a governing equation for the fluid mesh motion has to be introduced, which closes the system.

Generally speaking, there exist two main approaches for solving this problem. Firstly, one can solve all three problems in one joint system, leading to a so-called monolithic algorithm. The advantage is, that the formulation is consistent and compared to the subsequently introduced staggered algorithm it does not introduce errors in the coupling. However, the solution of the monolithic system is cumbersome, since completely different physics are involved. In practice, using a so-called "staggered algorithm" has shown to be a more robust choice. In a staggered algorithm, fluid-and structure problem are updated from time step n to n+1 one after the other. Therefore, consistency is lost, and (if no correction is applied) accuracy drops to first order. On the other hand each problem by itself can be treated by well established, optimized, existing solvers so the solution procedure is more robust.

This thesis utilizes the staggered approach. We have coupled a three-dimensional second order finite volume code [4] with a second order accurate finite element code [5] according to the popular three-field formulation of [2].

The three-field formulation of ALE aeroelasticity can be written as:

```
state equation of the structure: \mathcal{S}_{EOS}(s, \boldsymbol{u}, \boldsymbol{x}, \boldsymbol{w}) = \boldsymbol{0} \quad (58)
governing equation of meshmotion: \mathcal{D}_{EOS}(s, \boldsymbol{u}, \boldsymbol{x}, \boldsymbol{w}) = \boldsymbol{0} \quad (59)
state equation of the fluid: \mathcal{F}_{EOS}(s, \boldsymbol{x}, \boldsymbol{w}) = \boldsymbol{0} \quad (60)
```

State equation of the structure: For a simple linear case, that is assumed in this thesis, the structure state equation can be written as

$$\mathcal{S}_{EOS} = \mathbf{K} oldsymbol{u} - oldsymbol{P}(oldsymbol{x}, oldsymbol{w})$$
 eq:eos_struct

where **K** represents the finite element stiffness matrix and P denotes the external load vector that combines aerodynamic loads P_F that are inflected to the structure

by the fluid, and gravity loads P_0

$$\boldsymbol{P} = \boldsymbol{P}_0 + \boldsymbol{P}_F \tag{63}$$

Governing equation of the mesh motion: In an Arbitrary Lagrangian Eulerian formulation, the fluid mesh deforms with the structure. A governing equation is thus required to describe that deformation; Typically a simple linear pseudo finite element approach or a spring analogy method [1] is used to do so. A Dirichlet problem is solved to move the mesh.

$$\mathcal{D}_{EOS} = \bar{\mathbf{K}} oldsymbol{x} \quad ext{with} \quad oldsymbol{x} = oldsymbol{u} \quad ext{on } \Gamma_{F|S} \qquad \qquad ext{eq:eos_mesh} \ (64)$$

State equation of the fluid: The state equation of the fluid depends on the flow model used, as well as ton whether a Eulerian or Lagrangian approach is used. A quick overview is provided in Section 2.2.

Please note, that the frame of reference (Eulerian, Lagrangian, Arbitrary Lagrangian Eulerian) has nothing to do with the fluid equation type.

The state equation of the fluid (Equation three in (??) for can be expressed as

$$\mathcal{F}_{EOS} = \begin{bmatrix} & \text{EULER} & \mathbf{F}_{2}(\boldsymbol{x}, \boldsymbol{w}) \\ & \text{NSG} & \mathbf{F}_{2}(\boldsymbol{x}, \boldsymbol{w}) + \mathbf{G}_{2}(\boldsymbol{x}, \boldsymbol{w}) \\ & \text{RANS} & \mathbf{F}_{2}(\boldsymbol{x}, \boldsymbol{w}) + \mathbf{G}_{2}(\boldsymbol{x}, \boldsymbol{w}) - \mathbf{S}(\boldsymbol{x}, \boldsymbol{w}, \boldsymbol{\chi}) \\ & & \text{EULER} & (\mathbf{A}(\dot{\boldsymbol{x}})\boldsymbol{w}) + \mathbf{F}_{2}(\boldsymbol{x}, \boldsymbol{w}) \\ & & \text{NSG} & (\mathbf{A}(\dot{\boldsymbol{x}})\boldsymbol{w}) + \mathbf{F}_{2}(\boldsymbol{x}, \boldsymbol{w}) + \mathbf{G}_{2}(\boldsymbol{x}, \boldsymbol{w}) \\ & & \text{RANS} & (\mathbf{A}(\dot{\boldsymbol{x}})\boldsymbol{w}) + \mathbf{F}_{2}(\boldsymbol{x}, \boldsymbol{w}) + \mathbf{G}_{2}(\boldsymbol{x}, \boldsymbol{w}) - \mathbf{S}(\boldsymbol{x}, \boldsymbol{w}, \boldsymbol{\chi}) \end{bmatrix}$$
(65)

where \mathbf{F}_2 denotes the vector of Roe fluxes resulting from a second-order finite volume discretization of the convective part of the NSE 3.2, \mathbf{G}_2 likewise denotes a second-order FV discretization oft the diffusive part, \mathbf{A} denotes the matrix of cell volumes and \mathbf{S} denotes the matrix resulting from the additional turbulence closures in the RANS equations (see Section??).

The above table also gives a very nice overview over the different equation types and the used simplifications. The Euler equations are obviously obtained by neglecting the diffusive part of the NSE. One can also see that the RANS equations are more difficult than the NSE themselves. However, as explained in TODO, the advantage is that RANS can operate on much coarser meshes that do not have to resolve the small scale turbulence phenomena, which makes the more numerically efficient overall in many applications.

4.1.1 Staggered algorithm

The three-field coupled system of equations **TODO**, can be solved very efficiently with an iterative staggered procedure, such as the one proposed by by [2]. This work utilizes the second-order staggered algorithm described in Figure 4.

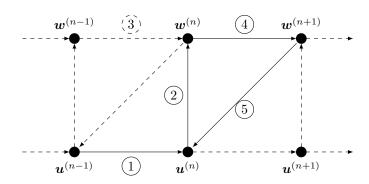


Figure 4: Scheme for the staggered algorithm. The picture depicts the sequential $structure(\mathbf{u})$ and $fluid(\mathbf{w})$ solves. First, the structure is updated to a new time step. With this information, a corresponding fluid solution is obtained. After the fluid is progressed in time, the structure solutions is being corrected with that information. A detailed description of all steps follows below.

① Determining structural response For a given external load $P^{(n)}$, the structural response $u^{(n)}$ is determined by solving the state equation of the structure **TODO**. To increase stability, and under-relaxation is typically performed:

$$\boldsymbol{u}^{(n)} = (1 - \theta)\boldsymbol{u}^{(n-1)} + \theta\tilde{\boldsymbol{u}} \tag{66}$$

$$\tilde{\boldsymbol{u}} = \mathbf{K}^{-1} \boldsymbol{P}^{(n)} \tag{67}$$

Typically, the relaxation factor is chosen as $0.5 \le \theta \le 0.9$

② Motion transfer to wet surface The motion of the wet surface of the structure has to be transformed to the fluid.

$$\boldsymbol{u}_{T}^{(n)} = \mathbf{T}_{u} \boldsymbol{u}^{(n)} \tag{68}$$

where \mathbf{T}_u is a transfer matrix that also accounts for potentially non-matching meshes [9].

③ Fluid mesh motion update The fluid mesh motion is then updated by solving an auxiliary pseudo Dirichlet problem on the fluid mesh. This step is the very heart of the ALE algorithm.

$$\bar{\mathbf{K}} \boldsymbol{x}^{(n)} = 0 \qquad \boldsymbol{x}^{(n)} = \boldsymbol{u}_T^{(n)} \text{ on } \Gamma_{F|S}$$
 (69)

where the Dirichlet conditions are introduced into the system via a decomposition:

$$\bar{\mathbf{K}} = \begin{bmatrix} \bar{\mathbf{K}}_{\Omega\Omega} & \bar{\mathbf{K}}_{\Omega\Gamma} \\ \bar{\mathbf{K}}_{\Gamma\Omega} & \bar{\mathbf{K}}_{\Gamma\Gamma} \end{bmatrix}, \quad \boldsymbol{x} = \begin{bmatrix} \boldsymbol{x}_{\Omega} \\ \boldsymbol{x}_{\Gamma} \end{bmatrix}$$
(70)

Here, the subscript Γ denotes the fluid grid points at the FSI interface and the subscript Ω denotes the remainder. Hence, the fluid mesh is updated in two steps,

by first transferring the structure motion to the fluid interface, and then solving the auxiliary pseudo Dirichlet problem:

$$oldsymbol{x}_{\Gamma}^{(n)} = oldsymbol{\mathsf{T}}_{u} oldsymbol{u}^{(n)} \hspace{1.5cm} egin{array}{ll} & \operatorname{eq:mms_update_1} \\ ar{\mathsf{K}}_{\Omega\Omega} oldsymbol{x}_{\Omega}^{(n)} = -ar{\mathsf{K}}_{\Omega\Gamma} oldsymbol{x}^{(n)} \end{array} \hspace{0.5cm} egin{array}{ll} & \operatorname{eq:mms_update_2} \\ \operatorname{eq:mms_update_2} \\ & \operatorname{eq:mms_update_2} \end{array}$$

It shall be noted that an exact solution of the preceding equation is not required. In fact it is an arbitrarily chosen auxiliary pseudo-problem anyway. Therefor, a valid update of the mesh motion, that does not produce crossovers is enough. Such an update can be obtained at low cost by allying a few Preconditioned Conjugate Gradient (PCG) iterations to Equation (72).

④ Update fluid state vector After the mesh has been deformed, the fluid state **w** vector can be updated accordingly.

an	EULER	$oldsymbol{F}_2(oldsymbol{w}^{(n)}) + rac{\partial F_2}{\partial oldsymbol{w}}(oldsymbol{w}^{(n+1)} - oldsymbol{w}^{(n)})$		
Eulerian	NSG	1		
<u>5</u>	RANS	1	=0 (73)	3)
	EULER	1		3)
ALE	NSG	1		
	RANS	1		

t

⑤ Determining structural responses TODO a lot of stuff is missing here!

5 Optimization

A generic, aeroelastic optimization problem can be written as

$$q(oldsymbol{s}, oldsymbol{u}, oldsymbol{w}) \left\{egin{array}{ll} \min & z(oldsymbol{s}) \ & oldsymbol{s} & ext{eq:generic_optimization_problem_1} \ & oldsymbol{h}(s) = oldsymbol{0}, & oldsymbol{h} \in \mathbb{R}^{n_h} \ & oldsymbol{g}(s) > oldsymbol{0}, & oldsymbol{g} \in \mathbb{R}^{n_g} \ & oldsymbol{s} = \{oldsymbol{s} \in \mathbb{R}^{n_s} | oldsymbol{s}_L \leq oldsymbol{s} \leq oldsymbol{s}_U \} \end{array}
ight.$$

Here, z is an arbitrary cost function that should be minimized. Note that a maximization problem can easily be obtained by multiplying the cost function by a factor of -1. In aerodynamics, a typical example for a cost function would be the Lift over Drag Ratio (LDR) ratio of an airfoil. The cost-function is described in terms of so-called abstract variables. These can have some physical interpretation, but don't necessarily have to(see Section 5.2). Since typically, these optimization problems have no finite solution on an unbounded domain, some restrictions/conditions are introduced. In the airfoil example, we would probably specify a minimum lift that is required to support the configuration. Also a maximum stress for the structure will likely have be specified. These are classical examples of non-equality constraints, denoted by g(s) in the above formulation. Constraints can also be formulated in an equality sense, for instance geometrical restrictions due to the turbine suspensions. Furthermore, the abstract optimization variables s themselves are typically restricted by lower(s_L) and upper(s_U) bounds.

The combinations of objective function z and constraints \boldsymbol{h} and \boldsymbol{g} is typically denoted as optimization criteria q.

$$q = q(s, u, w)$$
 $u = u(s), \quad w = w(s)$ eq:optimization_criteria (76)

This thesis follows the *nested analysis and design approach*, meaning that we assume that u and w always satisfy the aeroelastic state equations. This means that the state equations are not included in the set of constraints, but the structural displacements u and the fluid state variables w are determined in each iteration.

As [9] write, the aeroelastic optimization problem can typically be solved by combining three different numerical approaches:

- Optimization Model
- Design Model
- Analysis Model

The optimization model describes the solution of the generic optimization problem(74)-(75). For this thesis, a Sequential Quadratic Programming (SQP) has been chosen [3].

The design model links abstract optimization variables s to actual shapes, structures, geometries or aerodynamics design parameters. For this purpose SDESIGN,

a programm specifically written for Sensitivity Analysis (SA) purpose in the Farhat Research Group (FRG), has been used during this thesis. Its basic concepts an ideas are described in [10].

Finally, the analysis model provides concepts of evaluation the optimization criteria. Typically, the optimization criteria depend on \boldsymbol{u} and \boldsymbol{w} which is why a coupled system of equations has to be solved in every design optimization process. The Sensitivity Analysis (SA) is also part of this model. Aeroelastic analysis and Sensitivity analysis are discussed in Section 7.

5.1 Optimization Model

Optimization problems are typically solved by gradient-based methods. The methods are divided into

- Primal
- Dual
- Penalty-barrier and
- Lagrange approaches

This thesis focuses on Lagrange approaches. For a thorough analysis and comparison of the different approaches, the interested reader is referred to [12].

The Lagrangian approach formulates the optimization problem(74)(75) as an extreme value problem of the Lagrangian:

$$L(\boldsymbol{s}, \boldsymbol{\eta}, \boldsymbol{\gamma}) = z(\boldsymbol{s})) = \boldsymbol{\eta}^T \boldsymbol{h}(\boldsymbol{s}) + \boldsymbol{\gamma}^T \boldsymbol{g}(\boldsymbol{s}) \tag{77}$$

Here, η denote the Lagrange multipliers for the equality constraints and γ the Lagrange multipliers for the non-equality constraints. In fact, one can easily see that the original optimization problem can be obtained as saddle point of the Lagrangian:

$$\frac{\partial L}{\partial s} = \frac{\partial z}{\partial s} = \boldsymbol{\eta}^T \frac{\partial \boldsymbol{h}}{\partial s} + \boldsymbol{\gamma}^T \frac{\partial \boldsymbol{g}}{\partial s} : \text{saddlepoint_optimization}$$
(79)

$$\frac{\partial L}{\partial \boldsymbol{\eta}} = \boldsymbol{h} = \boldsymbol{0} \tag{80}$$

$$\frac{\partial L}{\partial \gamma} = \gamma^T \mathbf{g} = \mathbf{0} \tag{81}$$

The SQP method, mention before uses a Newton-Rhapsodon algorithm to solve the above system.

$$\begin{bmatrix} \frac{\partial^{2}L^{(k)}}{\partial \boldsymbol{s}^{2}} & \frac{\partial \boldsymbol{g}^{(k)}}{\partial s} & \frac{\partial \boldsymbol{h}^{(k)}}{\partial s} \\ \boldsymbol{\gamma}^{(k)} \frac{\partial \boldsymbol{g}^{(k)}}{\partial s} & \boldsymbol{h}^{(k)} & \boldsymbol{0} \\ \frac{\partial \boldsymbol{h}^{(k)}}{\partial s} & \boldsymbol{0} & \boldsymbol{0} \end{bmatrix} \begin{bmatrix} \Delta \boldsymbol{s} \\ \Delta \boldsymbol{\gamma} \end{bmatrix} = -\begin{bmatrix} \frac{\partial L^{(k)}}{\partial \boldsymbol{s}} \\ \boldsymbol{\gamma}^{(k)} \boldsymbol{g}^{(k)} \\ \boldsymbol{h}^{(k)} \end{bmatrix} = -\begin{bmatrix} \frac{\partial L^{(k)}}{\partial s} \\ \boldsymbol{\gamma}^{(k)} \boldsymbol{g}^{(k)} \\ \boldsymbol{h}^{(k)} \end{bmatrix}$$

Here $(\cdot)^{(k)}$ denotes the iteration index of the optimization loop.

The linear Equations (82) can also be formulated as an equivalent quadratic minimization problem:

In the above formulation, the evaluation of the second derivative of the Lagrangian (Hessian of L) is the numerically most expensive part. Usually it is preferred to approximate it by a first-order information, for example by the Davidon-Fletcher Powell formula (DFP) or by the Broyden-Fletcher-Goldfarb-Shanno algorithm (BFGS) method. However, this simplification introduces an error that one should be aware of. Some correction methods have been proposed trying to minimize the error. In this thesis we adapt the one proposed by [9]:

$$egin{bmatrix} oldsymbol{s}^{(k+1)} \ oldsymbol{\eta}^{(k+1)} \ oldsymbol{\gamma}^{(k+1)} \ \end{pmatrix} = egin{bmatrix} oldsymbol{s}^{(k)} \ oldsymbol{\eta}^{(k)} \ \end{pmatrix} + lpha^{(k)} egin{bmatrix} \Delta oldsymbol{s}^{(k)} \ \Delta oldsymbol{\eta}^{(k)} \ \end{pmatrix} & ext{eq:correction_step} \ \otimes oldsymbol{s}^{(k)} \ \end{pmatrix}$$

The appropriate step size $\alpha^{(k)}$ is determined by a line search. AS [9] write, due to this insufficiencies, the Lagrangian can not be used to measure an improvement. Instead, a merit function is introduced that is minimized by the line-search. A local minimum is reached by following a sequence of decreasing merit function values. Convergence of the process can be measured via the \mathcal{L}_2 -norm of the residual of the Kuhn-Tucker conditions(79).

By construction, the constraints are satisfied only when the optimum point is reached.

5.2 Design Model

The design model represent the essential link between the described optimization model and the analysis model. Generally speaking, it relates physical design parameters to abstract ones.

$$oldsymbol{d} = oldsymbol{d}(oldsymbol{s}), \quad oldsymbol{d} \in \mathbb{R}^{n_{oldsymbol{d}}}$$
eq:physvarsTOabsvars

Here, n_d denotes the number of physical design parameters. To define a relation between the abstract optimization variables and the motion of the nodes, the following design model is introduced:

$$\boldsymbol{x} = \boldsymbol{x}(\boldsymbol{s}) \tag{88}$$

As [9] explain, it is unpractical to identify an abstract variable directly with an increment of the coordinate of a grid point. Instead, two approaches, namely geometrical and mechanical can be adopted for constructing the generic design model.

Mechanical approach In the mechanical approach, the shape variation is identified with a superposition of fictitious structural deformations $\bar{\boldsymbol{u}}_j$ due to fictitious loads $\mu \bar{\boldsymbol{P}}_j$ and fictions support conditions

$$oldsymbol{x} = \sum_j ar{oldsymbol{\mathsf{K}}}_j^{-1} \mu_j ar{oldsymbol{P}}_j \qquad ext{eq:mechanical_approach} \tag{89}$$

where $\bar{\mathbf{K}}_j$ is a fictitious pseudo structure stiffness matrix representing the fluid domain compatible to the current fictions support conditions.

Geometrical approach The geometrical approach describes the geometry of the structure or the fluid boundary the design element concept. Here, the shape of a body X is approximated by so-called design elements as follows:

$$\boldsymbol{X} = \sum_{j} \phi_{j}(\xi) \hat{\boldsymbol{X}}_{j}$$
 eq:geometrical_approach (90)

Here, $\phi_j(\xi)$ is a shape function, $\hat{\boldsymbol{X}}_j$ is the vector of control nodes and ξ represents the reference coordinate. In the design element concept, the variation of the control nodes of the design element is used to vary the shape of the body. The variation of the control nodes position denoted as "mesh-motion" is given as $\boldsymbol{x} = \Delta \hat{\boldsymbol{X}}$

$$m{x} = \sum_j \phi_j(\xi) \hat{m{x}}_j$$
 eq:mms (91)

Just as in Finite Elements, where the shape-functions can not only be used to describe the solution field, but also the body's geometry and material parameters, the design element concept can be applied to prescribe parameter distributions and their variations in the optimization process. A simple sketch of the concept is provided in Figure 5

Both approaches have pros and cons, that are quickly discussed in [10], this thesis utilizes the geometrical approach solemnly.

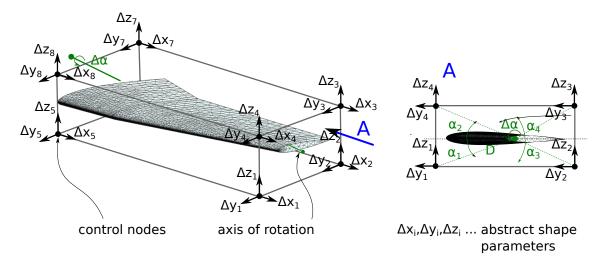


Figure 5: Geometrical approach for the design model as explained in Section 5.2. A NACA type airfoil is exemplarily considered here. The airfoil is embedded in a bounding box defined by eight so-called control nodes. The position of these control nodes can be varied, which alternates the shape of the airfoil according to some interpolation functions defined on the nodes. The 24 displacement unknowns are denoted as "abstract shape parameters". Abstract shape variables can be arbitrarily defined. As an example, a rotation axis is defined through the wing. **REFORMOLATE:** With only one independent abstract variable(α) the whole wing can now be rotated, e.g. to find the optimum angle of attack

5.3 Analysis Model

The Saddle point formulation of the Lagrangian

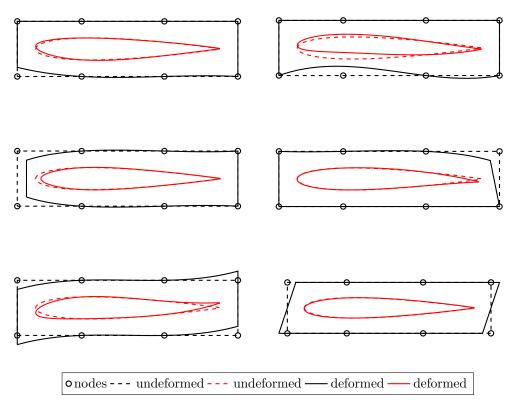


Figure 6: Visualization of the design element concept, exemplarily shown on a NACA0012 airfoil. For simplicity, a single design element (cubic in the horizontal direction and linear in the vertical direction) is used. Both the initial configuration (dashed lines) and the deformed configuration (full lines) are plotted. Although only eight design element nodes are provided, the function space of the design element allows for a great variation of the airfoil shape. Also, the size of the parameter space is now independent of the airfoil mesh size. From this perspective, the design element concept can be regarded as an model reduction for the shape variation.

6 Fluid Sensitivity Analysis

As explained in section 5, optimization is based on the calculations of gradients, also denoted as Sensitivity Analysis (SA). When it comes to calculating the gradients of a solution of a PDE, there are two fundamentally different approaches one could take.

Firstly one could think of first deriving the continuous equation and then applying the discretization scheme. On the other hand its equaly legitimate to first apply the discretization and compute the gradients of that, approximated solution. This thesis focuses uses the latter one, the reasons being explained in Figure 7.

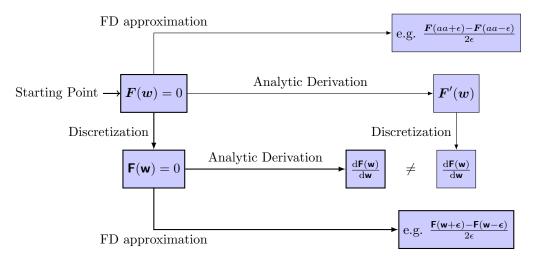


Figure 7: Two different approaches of SA. The question here is whether on discretized the system of equations first and then computes the derivative of the approximate solution, or whether the continuous system of equation is first derived and discretized afterwards. Both approaches are valid, the final result however will generally not be the same. We have solemnly focused on the case of derivation after discretization in this thesis(thick lines). There are several reason to this. Firstly, if one chose to first derive and then compute a discretized solution, one would solve a completely different equation. If on the other hand the discretization(e.g. Finite Volumes) is done first, standard solvers can be utilized. What is more, approximating the derivative by a Finite difference becomes much easier, since the finite difference evaluation involved only a evaluation of **F**, which a standard fluid solver is perfectly capable of, whereas the FD approximation in the other case would involve evaluations of the continuous function and the discretization of the obtained expression which would be much more cumbersome. **REF**Think about whether this is correct

When it comes to SA within the context of CFD, one also has to distinguish between SA of the non-coupled fluid problem and the SA in the fully coupled aeroelastic case. The latter case is much more involved, since it requires additional terms from the Structure and mesh motion equations. In the following we will therefore begin with the SA of a regular fluid problem. A generalization to a coupled FSI problem will follow.

As mentioned in Section 5, we typically deal with an optimization criteria q_j , that is in this case dependent on the fluid state variables \boldsymbol{w} that themselves may depend on abstract variables s_i

$$q_j = q_j(\boldsymbol{w}(s_i)) \tag{92}$$

$$\frac{dq_{j}}{ds_{i}}\Big|_{\boldsymbol{w}_{0}} = \underbrace{\frac{\partial q_{j}}{\partial s_{i}}\Big|_{\boldsymbol{w}_{0}}}_{\text{directy derived from the definition of } q} + \underbrace{\frac{\partial q_{j}}{\partial \boldsymbol{w}}\Big|_{\boldsymbol{w}_{0}}}_{\text{derived analytically or the definition of } q} \underbrace{\frac{d\boldsymbol{w}}{ds_{i}}\Big|_{\boldsymbol{w}_{0}}}_{\text{derived from dynamic fluid equilibrium}}$$
(93)

Also, we keep in mind, that the state equation of the fluid can be expressed as

$$\mathcal{F}_{EOS}(\boldsymbol{w}(s_i), \boldsymbol{x}(s_i), s_i) = \frac{\partial \boldsymbol{w}(s_i)}{\partial t} + \nabla \cdot \mathcal{F}(\boldsymbol{w}(s_i)) + \nabla \mathcal{G}(\boldsymbol{w}(s_i)) + S = \boldsymbol{0}$$
(94)

TODO how does the mesh motion come into the right hand side?

Therefore, deriving the fluid EOS gives:

$$\frac{\mathrm{d}\mathcal{F}_{EOS}}{\mathrm{d}s_i} = \mathbf{0} = \frac{\partial \mathcal{F}_{EOS}}{\partial s_i} + \frac{\partial \mathcal{F}_{EOS}}{\partial \boldsymbol{w}} \frac{d\boldsymbol{w}}{ds_i} + \frac{\partial \mathcal{F}_{EOS}}{\partial \boldsymbol{x}} \frac{d\boldsymbol{x}}{ds_i}$$
(95)

Therefore the total derivative of the fluid state with respect to the shape variable, needed in equation REF, can be obtained by solving

$$\frac{\partial \mathcal{F}_{EOS}}{\partial \boldsymbol{w}} \frac{d\boldsymbol{w}}{ds_i} = -\frac{\partial \mathcal{F}_{EOS}}{\partial s_i} - \frac{\partial \mathcal{F}_{EOS}}{\partial \boldsymbol{x}} \frac{d\boldsymbol{x}}{ds_i}$$
(96)

In this equation, $\frac{\partial \mathcal{F}_{EOS}}{\partial s_i}$ can be computed analytically or by FD. The derivative of the mesh motion with respect to the abstract variables is often denoted as "shape gradient". It can be divided into two components:

- The interface component $\frac{\mathrm{d}\mathbf{x}_{\Gamma}}{\mathrm{d}s_{i}}$, which is associated with the grid points lying on the fluid boundary
- The interior component $\frac{\mathrm{d}x_{\Omega}}{\mathrm{d}s_i}$, which is associated with the grid points located in the interior Ω of the computational domain.

The interface component is determined by the structure. Having obtained this one, the interior component can be computed by solving an auxiliary, fictitious Dirichlet problem:

$$\frac{\mathrm{d}\boldsymbol{x}_{\Omega}}{\mathrm{d}s_{i}} = -\left[\bar{\mathbf{K}}_{\Omega\Omega}^{-1}\bar{\mathbf{K}}_{\Omega\Gamma}\right]\frac{\mathrm{d}\boldsymbol{x}_{\Gamma}}{\mathrm{d}s_{i}} \tag{97}$$

where $\bar{\mathbf{K}}$ is a pseudo stiffness matrix that can be obtained by a simple spring analogy or similar approaches. For the later introduced Embedded framework, $\frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}s_i}$ is the position vector of the embedded discrete surface

In summary, the derivative of an optimization criteria with respect to an abstract variable can be computed as

$$\frac{\mathrm{d}q_{j}}{\mathrm{d}s_{i}}\Big|_{\boldsymbol{w}_{0}} = -\frac{\mathrm{d}q_{j}}{\mathrm{d}\boldsymbol{w}}\Big|_{\boldsymbol{w}_{0}} \left[\frac{\partial \mathcal{F}_{EOS}}{\partial \boldsymbol{w}}\Big|_{\boldsymbol{w}_{0}}\right]^{-1} \left(\frac{\partial \mathcal{F}_{EOS}}{\partial s_{i}}\Big|_{\boldsymbol{w}_{0}} + \left[\alpha \frac{\partial \mathcal{F}_{EOS}}{\partial \boldsymbol{x}_{\Omega}}\Big|_{\boldsymbol{w}_{0}} \frac{\partial \mathcal{F}_{EOS}}{\partial \boldsymbol{x}_{\Gamma}}\Big|_{\boldsymbol{w}_{0}}\right] \left[\alpha \mathbf{\bar{K}}_{\Omega\Omega}^{-1} \mathbf{\bar{K}}_{\Omega\Gamma}\right] \frac{\mathrm{d}\boldsymbol{x}_{\Gamma}}{\mathrm{d}s_{i}}\right]$$

$$\boldsymbol{\alpha} = \begin{cases} 1 \text{ in ALE framework} \\ 0 \text{ in Embedded framework} \end{cases} \tag{99}$$

7 Aero-elastic Sensitivity Analysis

The SA approach applied in this thesis is based on the work of [13], for deriving the Global Sensitivity Equations (GSE) of coupled systems. As introduced by the authors of [9], we utilize the three-field formulation of [2].

The derivative of the optimization criterion q_j , as introduced in Equation (76), with respect to the optimization variable s_i gives:

$$\frac{dq_j}{ds_i} = \frac{\partial q_j}{\partial s_i} + \frac{\partial q_j}{\partial \boldsymbol{u}} \frac{d\boldsymbol{u}}{ds_i} + \frac{\partial q_j}{\partial \boldsymbol{x}} \frac{d\boldsymbol{x}}{ds_i} + \frac{\partial q_j}{\partial \boldsymbol{w}} \frac{d\boldsymbol{w}}{ds_i}$$
(100)

$$= \frac{\partial q_{j}}{\partial s_{i}} + \begin{bmatrix} \frac{\partial q_{j}}{\partial \boldsymbol{u}} \\ \frac{\partial q_{j}}{\partial \boldsymbol{x}} \\ \frac{\partial q_{j}}{\partial \boldsymbol{w}} \end{bmatrix} \cdot \begin{bmatrix} \frac{d\boldsymbol{u}}{ds_{i}} \\ \frac{d\boldsymbol{x}}{ds_{i}} \\ \frac{d\boldsymbol{w}}{ds_{i}} \end{bmatrix}$$

$$(101)$$

where the partial derivatives, $\frac{\partial q_j}{\partial \boldsymbol{u}}$, $\frac{\partial q_j}{\partial \boldsymbol{x}}$ and $\frac{\partial q_j}{\partial \boldsymbol{w}}$ can be directly evaluated within the discretized structure and fluid model through the relation between structural, aero-dynamic design and abstract optimization parameters defied in the design model 5.2. The cumbersome part are the derivatives $\frac{d\boldsymbol{u}}{ds_i}$, $\frac{d\boldsymbol{x}}{ds_i}$ and $\frac{d\boldsymbol{w}}{ds_i}$ To obtain them, the governing equations (??)TODO write down governing equations have to be derived:

$$\begin{bmatrix} \frac{\partial \mathcal{S}_{EOS}}{\partial s_i} \\ \frac{\partial \mathcal{D}_{EOS}}{\partial s_i} \\ \frac{\partial \mathcal{F}_{EOS}}{\partial s_i} \end{bmatrix} + \underbrace{\begin{bmatrix} \frac{\partial \mathcal{S}_{EOS}}{\partial \boldsymbol{u}} & \frac{\partial \mathcal{S}_{EOS}}{\partial \boldsymbol{x}} & \frac{\partial \mathcal{S}_{EOS}}{\partial \boldsymbol{w}} \\ \frac{\partial \mathcal{D}_{EOS}}{\partial \boldsymbol{x}} & \frac{\partial \mathcal{D}_{EOS}}{\partial \boldsymbol{x}} & \frac{\partial \mathcal{F}_{EOS}}{\partial \boldsymbol{w}} \end{bmatrix}}_{\boldsymbol{A}} \underbrace{\begin{bmatrix} \frac{\partial \boldsymbol{u}}{\partial s_i} \\ \frac{\partial \boldsymbol{u}}{\partial s_i} \\ \frac{\partial \boldsymbol{w}}{\partial s_i} \end{bmatrix}}_{\boldsymbol{A}} = 0$$

$$\underbrace{\begin{bmatrix} \frac{\partial \boldsymbol{u}}{\partial s_i} \\ \frac{\partial \boldsymbol{w}}{\partial s_i} \\ \frac{\partial \boldsymbol{w}}{\partial s_i} \end{bmatrix}}_{\boldsymbol{A}} \underbrace{\begin{bmatrix} \frac{\partial \boldsymbol{u}}{\partial s_i} \\ \frac{\partial \boldsymbol{w}}{\partial s_i} \\ \frac{\partial \boldsymbol{w}}{\partial s_i} \end{bmatrix}}_{\boldsymbol{A}} \underbrace{\begin{bmatrix} \frac{\partial \boldsymbol{u}}{\partial s_i} \\ \frac{\partial \boldsymbol{w}}{\partial s_i} \\ \frac{\partial \boldsymbol{w}}{\partial s_i} \end{bmatrix}}_{\boldsymbol{A}} \underbrace{\begin{bmatrix} \frac{\partial \boldsymbol{u}}{\partial s_i} \\ \frac{\partial \boldsymbol{w}}{\partial s_i} \\ \frac{\partial \boldsymbol{w}}{\partial s_i} \end{bmatrix}}_{\boldsymbol{A}} \underbrace{\begin{bmatrix} \frac{\partial \boldsymbol{u}}{\partial s_i} \\ \frac{\partial \boldsymbol{w}}{\partial s_i} \\ \frac{\partial \boldsymbol{w}}{\partial s_i} 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s_i} \end{bmatrix}}_{\boldsymbol{A}} \underbrace{\begin{bmatrix} \frac{\partial \boldsymbol{u}}{\partial s_i} \\ \frac{\partial \boldsymbol{u}}{\partial s_i} \\ \frac{\partial \boldsymbol{u}}{\partial s_i} \end{bmatrix}}_{\boldsymbol{A}} \underbrace{\begin{bmatrix} \frac{\partial \boldsymbol{u}}{\partial s_i} \\ \frac{\partial \boldsymbol{u}}{\partial s_i} \\ \frac{\partial \boldsymbol{u}}{\partial s_i} \end{bmatrix}}_{\boldsymbol{A}} \underbrace{\begin{bmatrix} \frac{\partial \boldsymbol{u}}{\partial s_i} \\ \frac{\partial \boldsymbol{u}}{\partial s_i} \\ \frac{\partial \boldsymbol{u}}{\partial s_i} \end{bmatrix}}_{\boldsymbol{A}} \underbrace{\begin{bmatrix} \frac{\partial \boldsymbol{u}}{\partial s_i} \\ \frac{\partial \boldsymbol{u}}{\partial s_i} \\ \frac{\partial \boldsymbol{u}}{\partial s_i} \end{bmatrix}}_{\boldsymbol{A}} \underbrace{\begin{bmatrix} \frac{\partial \boldsymbol{u}}{\partial s_i} \\ \frac{\partial \boldsymbol{u}}{\partial s_i} \\ \frac{\partial \boldsymbol{u}}{\partial s_i} \end{bmatrix}}_{\boldsymbol{A}} \underbrace{\begin{bmatrix} \frac{\partial \boldsymbol{u}}{\partial s_i} \\ \frac{\partial \boldsymbol{u}}{\partial s_i} \\ \frac{\partial \boldsymbol{u}}{\partial s_i} \end{bmatrix}}_{\boldsymbol{A}} \underbrace{\begin{bmatrix} \frac{\partial \boldsymbol{u}}{\partial s_i} \\ \frac{\partial \boldsymbol{u}}{\partial s_i} \\ \frac{\partial \boldsymbol{u}}{\partial s_i} \end{bmatrix}}_{\boldsymbol{A}} \underbrace{\begin{bmatrix} \frac{\partial \boldsymbol{u}}{\partial s_i} \\ \frac{\partial \boldsymbol{u}}{\partial s_i} \\ \frac{\partial \boldsymbol{u}}{\partial s_i} \end{bmatrix}}_{\boldsymbol{A}} \underbrace{\begin{bmatrix} \frac{\partial \boldsymbol{u}}{\partial s_i} \\ \frac{\partial \boldsymbol{u}}{\partial s_i} \\ \frac{\partial \boldsymbol{u}}{\partial s_i} \end{bmatrix}}_{\boldsymbol{A}} \underbrace{\begin{bmatrix} \frac{\partial \boldsymbol{u}}{\partial s_i} \\ \frac{\partial \boldsymbol{u}}{\partial s_i} \\ \frac{\partial \boldsymbol{u}}{\partial s_i} \end{bmatrix}}_{\boldsymbol{A}} \underbrace{\begin{bmatrix} \frac{\partial \boldsymbol{u}}{\partial s_i} \\ \frac{\partial \boldsymbol{u}}{\partial s_i} \\ \frac{\partial \boldsymbol{u}}{\partial s_i} \end{bmatrix}}_{\boldsymbol{A}} \underbrace{\begin{bmatrix} \frac{\partial \boldsymbol{u}}{\partial s_i} \\ \frac{\partial \boldsymbol{u}}{\partial s_i} \\ \frac{\partial \boldsymbol{u}}{\partial s_i} \end{bmatrix}}_{\boldsymbol{A}} \underbrace{\begin{bmatrix} \frac{\partial \boldsymbol{u}}{\partial s_i} \\ \frac{\partial \boldsymbol{u}}{\partial s_i} \\ \frac{\partial \boldsymbol{u}}{\partial s_i} \end{bmatrix}}_{\boldsymbol{A}} \underbrace{\begin{bmatrix} \frac{\partial \boldsymbol{u}}{\partial s_i} \\ \frac{\partial \boldsymbol{u}}{\partial s_i} \\ \frac{\partial \boldsymbol{u}}{\partial s_i} \end{bmatrix}}_{\boldsymbol{A}} \underbrace{\begin{bmatrix} \frac{\partial \boldsymbol{u}}{\partial s_i} \\ \frac{\partial \boldsymbol{u}}{\partial s_i} \\ \frac{\partial \boldsymbol{u}}{\partial s_i} \end{bmatrix}}_{\boldsymbol{A$$

In this equations $\frac{\partial \mathcal{S}_{EOS}}{\partial s_i}$ and $\frac{\partial \mathcal{F}_{EOS}}{\partial s_i}$ can be again directly evaluated using the relation specified in the design model. The matrix of first derivatives \boldsymbol{A} is from now on denoted as the "Jacobian of the optimization problem".

Combining the previous two equations, it follows that the total derivative of the

optimization criterion with respect to the abstract variables can be expressed as:

$$\frac{dq_{j}}{ds_{i}} = \frac{\partial q_{j}}{\partial s_{i}} - \underbrace{\begin{bmatrix} \frac{\partial q_{j}}{\partial \boldsymbol{u}} \\ \frac{\partial q_{j}}{\partial \boldsymbol{x}} \\ \frac{\partial q_{j}}{\partial \boldsymbol{w}} \end{bmatrix}}_{n_{eq} \times n_{eq}} \underbrace{\begin{bmatrix} \frac{\partial \mathcal{S}_{EOS}}{\partial s_{i}} \\ \frac{\partial \mathcal{P}_{EOS}}{\partial s_{i}} \\ \frac{\partial \mathcal{F}_{EOS}}{\partial s_{i}} \end{bmatrix}}_{n_{eq} \times n_{s}} \underbrace{\begin{bmatrix} \frac{\partial \mathcal{S}_{EOS}}{\partial s_{i}} \\ \frac{\partial \mathcal{F}_{EOS}}{\partial s_{i}} \end{bmatrix}}_{n_{eq} \times n_{s}}$$

Where n_{eq} is the total number of equations (e.g. five fluid state equations for the compressible NSG in 3D, three equations of the mesh motions and another three equations for the structure motion), n_q is the number of optimization criteria and n_s is the number of abstract variables.

7.1 Direct vs. adjoint approach

Equation 103 suggests, that there are two alternatives to compute vector-matrix-vector product above.

Direct approach Firstly, one could first compute the derivatives of the aeroelastic response for each abstract variable and perform the matrix product with A:

$$\begin{bmatrix} \frac{d\boldsymbol{u}}{ds_i} \\ \frac{d\boldsymbol{x}}{ds_i} \\ \frac{d\boldsymbol{w}}{ds_i} \end{bmatrix} = -\boldsymbol{A}^{-1} \begin{bmatrix} \frac{\partial \mathcal{S}_{EOS}}{\partial s_i} \\ \frac{\partial \mathcal{D}_{EOS}}{\partial s_i} \\ \frac{\partial \mathcal{F}_{EOS}}{\partial s_i} \end{bmatrix} \quad \text{and then} \quad \stackrel{\text{eq:direct_approach}}{\text{(104)}}$$

$$\frac{dq_{j}}{ds_{i}} = \frac{\partial q_{j}}{\partial s_{i}} - \begin{bmatrix} \frac{\partial q_{j}}{\partial \mathbf{u}} \\ \frac{\partial q_{j}}{\partial \mathbf{x}} \end{bmatrix}^{T} \begin{bmatrix} \frac{d\mathbf{u}}{ds_{i}} \\ \frac{d\mathbf{x}}{ds_{i}} \\ \frac{\partial q_{j}}{\partial \mathbf{w}} \end{bmatrix} \begin{bmatrix} \frac{d\mathbf{v}}{ds_{i}} \\ \frac{d\mathbf{w}}{ds_{i}} \end{bmatrix} \tag{105}$$

Where the total complexity can be approximated as $\mathcal{O}(n_{eq}^2 n_s + n_q n_{eq} n_s)$

Adjoint approach Secondly, one could also first compute the derivatives of the optimization criteria and multiply with the Jacobian before substituting this into Equation (103):

$$\begin{bmatrix} \boldsymbol{a}_{\boldsymbol{u}} \\ \boldsymbol{a}_{\boldsymbol{x}} \\ \boldsymbol{a}_{\boldsymbol{w}} \end{bmatrix} = \boldsymbol{A}^{-T} \begin{bmatrix} \frac{\partial q_{j}}{\partial \boldsymbol{u}} \\ \frac{\partial q_{j}}{\partial \boldsymbol{x}} \\ \frac{\partial q_{j}}{\partial \boldsymbol{w}} \end{bmatrix} \qquad \text{eq:firststep_adjoint}$$

$$\frac{dq_{j}}{ds_{i}} = \frac{\partial q_{j}}{\partial s_{i}} - \begin{bmatrix} \boldsymbol{a}_{\boldsymbol{u}} \\ \boldsymbol{a}_{\boldsymbol{x}} \\ \boldsymbol{a}_{\boldsymbol{w}} \end{bmatrix}^{T} \begin{bmatrix} \frac{\partial \mathcal{S}_{EOS}}{\partial s_{i}} \\ \frac{\partial \mathcal{D}_{EOS}}{\partial s_{i}} \\ \frac{\partial \mathcal{F}_{EOS}}{\partial s_{i}} \end{bmatrix}$$

$$(107)$$

Where the total complexity can be approximated as $\mathcal{O}(n_{eq}^2 n_{\mathbf{q}} + n_{\mathbf{q}} n_{eq} n_{\mathbf{s}})$

If one or the other approach is to be preferred depends in on the optimization setup, particularly the number of optimization criteria and the number of optimization variables. Looking at the orders above, one can conclude that if the number of abstract parameters n_s is smaller than the number of optimization criteria, the direct approach is more efficient, otherwise the adjoint approach is to be preferred. Additionally the on can argue, that the relevant term in the orders above is the one with n_{eq}^2 since it dominates the sum. Therefore, depending on whether n_s or n_q is bigger, the direct or the adjoint method is to be preferred.

7.1.1 Direct Sensitivity Analysis for the Euler equations

The A matrix for the direct approach in ALE formulation looks like

$$\boldsymbol{A} = \begin{bmatrix} \frac{\partial \mathcal{S}_{EOS}}{\partial \boldsymbol{u}} & \frac{\partial \mathcal{S}_{EOS}}{\partial \boldsymbol{x}} & \frac{\partial \mathcal{S}_{EOS}}{\partial \boldsymbol{w}} \\ \frac{\partial \mathcal{D}_{EOS}}{\partial \boldsymbol{u}} & \frac{\partial \mathcal{D}_{EOS}}{\partial \boldsymbol{x}} & \boldsymbol{0} \\ \boldsymbol{0} & \frac{\partial \mathcal{F}_{EOS}}{\partial \boldsymbol{x}} & \frac{\partial \mathcal{F}_{EOS}}{\partial \boldsymbol{w}} \end{bmatrix} = \begin{bmatrix} \boldsymbol{K} & \frac{\partial \boldsymbol{P}_T}{\partial \boldsymbol{x}} & \frac{\partial \boldsymbol{P}_T}{\partial \boldsymbol{w}} \\ \boldsymbol{K}_{\Omega\Gamma} \boldsymbol{\mathsf{T}}_u \\ \boldsymbol{\mathsf{T}}_u \end{bmatrix} & \begin{bmatrix} \boldsymbol{K}_{\Omega\Omega} & \boldsymbol{0} \\ \boldsymbol{\mathsf{K}}_{\Omega\Omega} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{\mathsf{I}} \end{bmatrix} & \begin{array}{c} \boldsymbol{\mathsf{eq:Amatrix}} & \boldsymbol{\mathsf{ALE}} \\ \boldsymbol{\mathsf{0}} & \boldsymbol{\mathsf{I}} & \boldsymbol{\mathsf{Imparting}} \\ \boldsymbol{\mathsf{O}} & \boldsymbol{\mathsf{Imparting}} & \boldsymbol{\mathsf{Imparting}} & \boldsymbol{\mathsf{Imparting}} \\ \boldsymbol{\mathsf{O}} & \frac{\partial \boldsymbol{\mathsf{F}}_2}{\partial \boldsymbol{x}_{\Omega}} & \boldsymbol{H}_2 \end{bmatrix} & \boldsymbol{\mathsf{Imparting}} & \boldsymbol{\mathsf{$$

Where, \mathbf{H}_2 is the Jacobian of the second order row flux. It shall be noted that constructing this Jacobian is not a trivial issue and takes up a lot of computational resources, especially for FV, as described in [2]. Investigation into whether this term can be approximated at first order were carried out in [9] and [10].

Furthermore, [11] considered replacing the two mesh motion related matrices $\frac{\partial \mathbf{P}_T}{\partial \mathbf{x}}$

and $\frac{\partial \mathbf{F}_2}{\partial \mathbf{x}_{\Omega}}$ by a transpirational boundary condition. The consequences of this approach are also investigated in [9] and [10].

This thesis, however, does not use any of this simplifications.

The derivation of the sensitivities, can be achieved in a staggered scheme, very similar to the one, described in ??TODO. It consists of five steps.

1) Update the structural displacement sensitivity to a new time step BY differentiating equations (58) and (62) and applying an under relaxation, we can obtain

$$\frac{\mathrm{d}\boldsymbol{u}^{(n)}}{\mathrm{d}s_i} = (1 - \theta) \frac{\mathrm{d}\boldsymbol{u}^{(n)}}{\mathrm{d}s_i} + \theta \frac{\mathrm{d}\bar{\boldsymbol{u}}}{\mathrm{d}s_i}$$
eq:underrelax_structdisp (109)

where $\bar{\boldsymbol{u}}$ is obtained from:

$$\mathbf{K} \frac{\mathrm{d} \bar{\boldsymbol{u}}}{\mathrm{d} s_i} = \frac{\partial TODO}{\partial s_i} + \frac{\partial \mathbf{T}_u^{(n)}}{\partial s_i} - \frac{\partial \mathbf{K}}{\partial s_i} \boldsymbol{u}^{\mathrm{eq:fictious_structdisp}}$$
(110)

2) Transfer sensitivity of structure motion to the interface

$$rac{\mathrm{d} oldsymbol{u}_T^{(n)}}{\mathrm{d} s_i} = oldsymbol{\mathsf{T}}_u rac{\mathrm{d} oldsymbol{u}^{(n)}}{\mathrm{d} s_i}$$
 eq:interface_projections

3) Compute derivative of fluid mesh motion The fluid mesh motion is computed by solving the pseudo Dirichlet problem as described in [2]. By design, the fictions stiffness matrix $\bar{\mathbf{K}}$ does not depend on the abstract optimization variables s

$$\bar{\mathbf{K}}_{\Omega\Omega} \frac{\mathrm{d} \boldsymbol{x}_{\Omega}^{(n)}}{\mathrm{d} s_i} = -\bar{\mathbf{K}}_{\Omega\Gamma} \frac{\mathrm{d} \boldsymbol{x}_{\Gamma}^{(n)}}{\mathrm{d} s_i}$$
 eq:mms_domain (112)

with

$$\frac{\mathrm{d}\boldsymbol{x}_{\Gamma}^{(n)}}{\mathrm{d}s_i} = \frac{\mathrm{d}\boldsymbol{x}_{\Gamma}^{(n)}}{\mathrm{d}s_i} \tag{113}$$

4) Compute the sensitivity of the fluid state variables The derivatives of the fluid state variables are computed by

$$\boldsymbol{H}_{2} \frac{\mathrm{d}\boldsymbol{w}^{(n+1)}}{\mathrm{d}s_{i}} = \frac{\partial \boldsymbol{F}_{2}}{\partial s_{i}} - \frac{\partial \boldsymbol{F}_{2}}{\partial \boldsymbol{x}} \frac{\mathrm{d}\boldsymbol{x}^{(n)}}{\mathrm{d}s_{i}}$$
(114)

5) Compute the sensitivity of the structure load vector The derivative of the fluid load with respect to the abstract variables can be computed by the third of Equations (104) with the definition of A as specified in (108).

$$\frac{\partial \boldsymbol{P_F}^{(n+1)}}{\partial s_i} = \frac{\partial \boldsymbol{P_F}^{(n+1)}}{\partial \boldsymbol{x}} \frac{\mathrm{d}\boldsymbol{x}^{(n)}}{\mathrm{d}s_i} + \frac{\partial \boldsymbol{P_F}^{(n+1)}}{\partial \boldsymbol{w}} \frac{\mathrm{d}\boldsymbol{w}^{(n)}}{\mathrm{d}s_i} \text{ respective floadBYabsyar (115)}$$

and compute project it onto the structure via

$$\frac{\partial \mathbf{P}_{T}^{(n+1)}}{\partial s_{i}} = \mathbf{T}_{p} \frac{\partial \mathbf{P}_{F}^{(n+1)}}{\partial s_{i}}$$
(116)

The convergence of the staggered algorithm can be monitored via

$$\left\| \mathbf{K} \frac{\mathrm{d}\bar{\boldsymbol{u}}^{(n+1)}}{\mathrm{d}s_{i}} - \frac{\partial TODO}{\partial s_{i}} - \frac{\partial \boldsymbol{P}_{T}^{(n+1)}}{\partial s_{i}} + \frac{\partial \mathbf{K}}{\partial s_{i}} \right\|_{2} \leq$$

$$\epsilon^{SA} \left\| \mathbf{K} \frac{\mathrm{d}\bar{\boldsymbol{u}}^{(0)}}{\mathrm{d}s_{i}} - \frac{\partial TODO}{\partial s_{i}} - \frac{\partial \boldsymbol{P}_{T}^{(0)}}{\partial s_{i}} + \frac{\partial \mathbf{K}}{\partial s_{i}} \right\|_{2}$$

$$\left\| \boldsymbol{H}_{2} \frac{\mathrm{d}\boldsymbol{w}^{(n+1)}}{\mathrm{d}s_{i}} + \frac{\partial \boldsymbol{F}_{2}}{\partial s_{i}} + \frac{\partial \boldsymbol{F}_{2}}{\partial \boldsymbol{x}} \frac{\mathrm{d}\boldsymbol{x}^{(n+1)}}{\mathrm{d}s_{i}} \right\|_{2} \leq$$

$$\epsilon^{SA} \left\| \boldsymbol{H}_{2} \frac{\mathrm{d}\boldsymbol{w}^{(0)}}{\mathrm{d}s_{i}} + \frac{\partial \boldsymbol{F}_{2}}{\partial s_{i}} + \frac{\partial \boldsymbol{F}_{2}}{\partial \boldsymbol{x}} \frac{\mathrm{d}\boldsymbol{x}^{(0)}}{\mathrm{d}s_{i}} \right\|_{2}$$

$$(118)$$

7.1.2 Adjoint Sensitivity Analysis for the Euler equations

The adjoint SA follows the same scheme as the direct one Equation (106) can be written as:

$$\begin{bmatrix} \mathbf{K} & \begin{bmatrix} \frac{\partial \mathbf{P}_T}{\partial \boldsymbol{x}_{\Omega}} \frac{\partial \mathbf{P}_T}{\partial \boldsymbol{x}_{\Gamma}} \end{bmatrix} & \frac{\partial \mathbf{P}_T}{\partial \boldsymbol{w}} \end{bmatrix}^T \begin{bmatrix} \mathbf{a}_{\boldsymbol{u}} \\ \begin{bmatrix} \mathbf{K}_{\Omega \Gamma} \mathbf{T}_{\boldsymbol{u}} \\ \mathbf{T}_{\boldsymbol{u}} \end{bmatrix} & \begin{bmatrix} \mathbf{K}_{\Omega \Omega} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{bmatrix} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{bmatrix} & \mathbf{0} \\ \mathbf{0} & \begin{bmatrix} \frac{\partial \mathbf{F}_2}{\partial \boldsymbol{x}_{\Omega}} \frac{\partial \mathbf{F}_2}{\partial \boldsymbol{x}_{\Gamma}} \end{bmatrix} & \mathbf{H}_2 \end{bmatrix} \begin{bmatrix} \mathbf{a}_{\boldsymbol{u}} \\ \begin{bmatrix} \mathbf{a}_{\boldsymbol{x}_{\Omega}} \\ \mathbf{a}_{\boldsymbol{x}_{\Gamma}} \end{bmatrix} \end{bmatrix} = \begin{bmatrix} \frac{\partial q_j}{\partial \boldsymbol{u}} \\ \frac{\partial q}{\partial \boldsymbol{x}_{\Omega}} \\ \frac{\partial q}{\partial \boldsymbol{x}_{\Gamma}} \end{bmatrix} & \mathbf{H}_2 \end{bmatrix}$$

TODO check if the index j is really required here! A stated earlier, the matrices $\frac{\partial \boldsymbol{q}}{\partial \boldsymbol{x}}$ and $\frac{\partial \boldsymbol{q}}{\partial \boldsymbol{w}}$ can be computed analytically. As for \boldsymbol{H}_2 , we follow the methodology outlined in [7] for evaluating ans storing it efficiently as the product of flux operators. Again the staggered procedure for solving the adjoint state problem shares the same computational kernels with the partitioned aeroelastic scheme described in [2]

1) Update the adjoint structure displacement to the new time step

$$a_{u}^{(n+1)} = (1-\theta)a_{u}^{(n)} + \theta \bar{a_{u}}^{(n+1)}$$
 (120)

(121)

where $\bar{a_u}^{(n+1)}$ is obtained from

$$\mathbf{K}\bar{a_{u}}^{(n+1)} = \frac{\partial \mathbf{q}}{\partial u} - \mathbf{K}_{\Omega\Gamma} \mathbf{T}_{u} \mathbf{a_{x\Omega}}^{(n)} + \mathbf{T}_{u} \mathbf{a_{x\Gamma}}^{(n)}$$
(122)

TODO derive this equation

2) Compute the adjoint fluid state by solving

$$\boldsymbol{H}_{2}^{T}\boldsymbol{a}_{\boldsymbol{w}}^{(n+1)} = \frac{\partial \boldsymbol{x}}{\partial \boldsymbol{w}} + \frac{\partial \boldsymbol{P}_{T}}{\partial \boldsymbol{w}^{T}}\boldsymbol{a}_{\boldsymbol{u}}^{(n+1)}$$
(123)

TODO derive this equation Again, $\frac{\partial \mathbf{q}}{\partial \mathbf{w}}$ is computed analytically from the relations defined in the design and aeroelastic model.

3) Compute adjoint mesh motion in domain and on the interface

$$\bar{\mathbf{K}}_{\Omega\Omega} \mathbf{a}_{\boldsymbol{x}\Omega}^{(n+1)} = \frac{\partial \boldsymbol{q}}{\partial \boldsymbol{x}_{\Omega}} - \frac{\partial \boldsymbol{P}_{T}}{\partial \boldsymbol{x}_{\Omega}} \mathbf{a}_{\boldsymbol{u}}^{(n+1)} - \frac{\partial \bar{\mathbf{F}}_{1}^{T}}{\partial \boldsymbol{x}_{\Omega}} \mathbf{a}_{\boldsymbol{x}}^{(n+1)} \text{ in } \Omega$$
(124)

TODO check equations And the adjoint mesh motion on the interface is computed as $a_{x\Gamma}^{(n+1)}$

$$\boldsymbol{a_{x\Gamma}}^{(n+1)} = \frac{\partial \boldsymbol{q}}{\partial \boldsymbol{x}_{Gamma}} + \frac{\partial \boldsymbol{P}_{T}}{\partial \boldsymbol{x}_{\Gamma}} \boldsymbol{a_{u}}^{(n+1)} - \frac{\partial \boldsymbol{F}_{2}}{\partial \boldsymbol{x}_{\Gamma}}^{T} \text{ on } \Gamma$$
(125)

where $\frac{\partial \mathbf{q}}{\partial \mathbf{w}}$ is computed analytically.

The convergence of the staggered adjoint optimization algorithm can be monitored via

$$\left\| \mathbf{R}_{q} - \mathbf{A}^{T} \mathbf{a}^{(n+1)} \right\| \leq \epsilon^{SA} \left\| \mathbf{R}_{q} \right\|$$
 (126)

8 Fiver

It was already outlined in Section REF, that using an Eulerian approach int the context of an thermoelastic simulations leads to a so-called embedded formulation, where the interface of the structure mesh no longer coincides with the fluid mesh. This was appealing, since it allowed for the usage of fixed meshes and an Eulerian formulation, on the other hand as explained in Section REF, an error of the order $\mathcal{O}(()\frac{h}{2})$ is introduced.

A possible solution to this problem is the Finite Volume Method with exact two-phase Riemann Integrals (FIVER) method.

8.1 Level-set method

Since the interface in an embedded stimulation typically moves, an appropriate interface tracking approach is required.

For FIVER, the popular level set method was chosen.

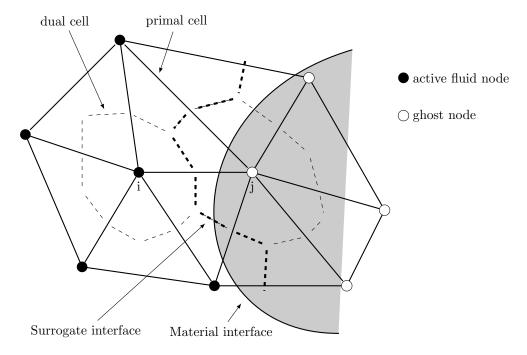


Figure 8: TODO

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