Report
Simulation Sciences Laboratory

Minimal Surfaces

add your matriculation numbers here!
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1. Introduction

A Minimal Surface is defined as a surface that has zero mean curvature. A minimal surface is characterized as surface of minimal surface area for the given boundary conditions.For example, a plane is a trivial minimal surface.

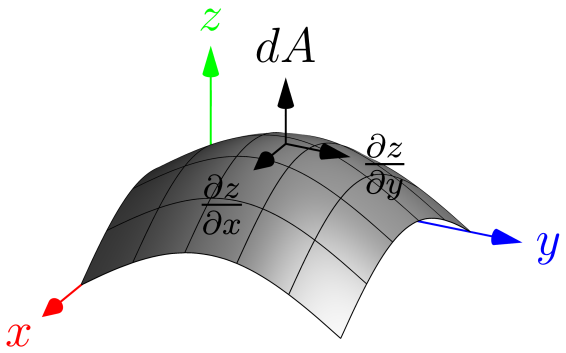

Figure 1: A *Minimal Surface* with the local area vector that is to be minimized.

The minimal surface is obtained as a solution to the Lagrange's equation (also known as the *Minimal-Surface Equation* (MSE)) given by:

$$\begin{aligned} (1+z_y^2)z_{xx} - 2z_x z_y z_{xy} + (1+z_x^2)z_{yy} = \mathcal{F}[z] = 0 \qquad & \text{in } \Omega \\ z(x,y) = g(x,y) \qquad & \text{on } \partial\Omega \end{aligned} \tag{1}$$

MSE is a Nonlinear Elliptic PDE that has a combination of first and second order differential terms in both x and y. Being a nonlinear PDE, we do not readily obtain an analytical solution necessitating the use of numerical methods, such as linearization of MSE using Newton-Raphson iterations, to solve the problem. It is also important to bear in mind that as z has second order derivative terms, we need $z \in \mathcal{C}^2$ which means that we need to provide smooth enough boundary conditions on $\partial\Omega$ in order to be able to compute the derivative terms in MSE.

MSE is used in designing structures that have great tensile strength and also to minimize the cost of construction as structural designs resulting from MSE require less material. MSE is also used to provide a relativistic description on the formation of Black Holes. Material lattice structures of biological organisms such as butterfly wings are minimal surface structures (Butterfly wings have a Gyroidal minimal surface). Hydrophobic co-polymer structures also take the shape of a minimal surface in order to reduce the energy of the structure arising due to surface tension.

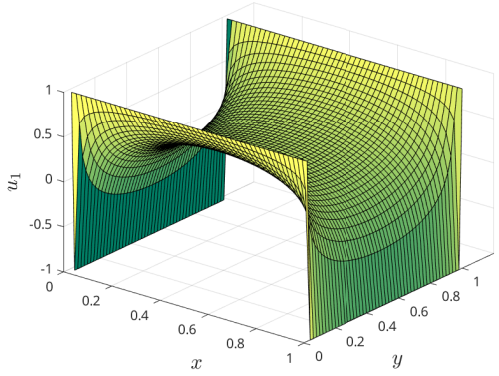

Figure 2: Scherk's first surface on $[0, 1]^2$

2. Background

2.1. General background (don't like this title)

We look at surfaces in $\mathbb{R}^3$, defined over an open set $\Omega \subset \mathbb{R}^2$. The surface of desire should contain the least possible area among all possible surfaces, that assume given values on the boundary of Ω, denoted by $\partial\Omega$. [1]

Lagrange showed in 1760, that such a surface is characterized by the graphic of a function $z(x, y)$, $z : \mathbb{R}^2 \to \mathbb{R}$, which is twice continuously differentiable on a twodimensional domain, particularly in a subset of $\mathbb{R}^2$. This function z has to fulfill the so called *Minimal-Surface Equation* (MSE) stated below.

$$\begin{aligned} (1 + z_y^2)z_{xx} - 2z_x z_y z_{xy} + (1 + z_x^2)z_{yy} = \mathcal{F}[z] = 0 \qquad & \text{in } \Omega \\ z(x, y) = g(x, y) \qquad & \text{on } \partial\Omega \end{aligned} \tag{2}$$

Clearly, this formulation satisfies the prescribed boundary values given by $g(x, y)$ due to the Dirichlet boundary condition on $\partial\Omega$. As to why the graphic of functions solving this equation describes a minimal surface, we refer to the literature. For example [1] gives a very straightforward proof.

In the following, we will call the differential operator $\mathcal{F}[\cdot]$ the Minimal-Surface Operator (MSO). The resulting partial differential equation (PDE) in eq. (2) turns out to be an elliptic PDE of second order, which is in particular *non-linear*. The solution of such a PDE is not trivial, and typically requires numerical treatment. For certain cases, analytical descriptions are available, such as for Scherk's surface.

As an example, Scherk's first surface (compare to figure 2) Σ rescaled on $\Omega = [0,1]^2$ is given by

$$\Sigma = \left\{ \left(x, y, \log\left(\frac{\cos(\pi(x-\frac{1}{2}))}{\cos(\pi(y-\frac{1}{2}))} \right) \right) \in \mathbb{R}^3 \middle| \, 0 < x, y < 1 \right\}. \tag{3}$$

which is the limit $n \to \infty$ of

$$\Sigma_n = \left\{ (x, y, u_n(x,y)) \in \mathbb{R}^3 \middle| \, 0 < x, y < 1 \right\}, \tag{4}$$

$$\lim_{y \to \pm 1} \to n \quad , 0 \leq x \leq 1 \tag{5}$$

$$\lim_{x \to \pm 1} \to -n \quad , 0 \leq y \leq 1. \tag{6}$$

The numerical solution of the MSE will require setting approbiate boundary conditions. Since $\log\left(\frac{\cos(\pi(x-\frac{1}{2}))}{\cos(\pi(y-\frac{1}{2}))}\right) \to \pm\infty$ on $\partial\Omega$, this is numerically not very practical.

We thus introduce $\beta_x, \beta_y \in (0,1)$ s.th.

$$\Sigma_{\text{trunc}} = \left\{ \left(x, y, \log\left(\frac{\cos(\pi\beta_x(x-\frac{1}{2}))}{\cos(\pi\beta_y(y-\frac{1}{2}))} \right) \right) \in \mathbb{R}^3 \middle| \, 0 < x, y < 1 \right\}. \tag{7}$$

By these means, we solve the MSE on $\Omega_{\text{trunc}} = [0,1]^2 \subset \Omega$ with $\Omega = [0, \frac{1}{\beta_x}] \times [0, \frac{1}{\beta_y}]$. Exact boundary values on $\partial\Omega_{\text{trunc}}$ ensure the correctness of the results. We choose $\beta_x = \beta_y = \beta$, as we restrict ourselves to solving on a square domain.

Later on, we will use this surface as a test-case to verify our numerical results.

2.2. Numerical solution

2.2.1. Discretization

In this project, we are supposed to solve the MSE numerically on $\Omega \equiv (0,1) \times (0,1)$. In the following, discretized quantities are indicated by a superscript h. The spatial domain is to be discretized using a structured mesh with equidistant grid spacing both in x, y, i.e. we have the same number of grid points in both directions, $N = N_x = N_y$. Thus, we define $\Omega^h := \{(x,y) \in \mathbb{R}^2 : \ (x,y) = (ih, jh),\ 0 \leq i,j < N,\ hN = 1\}$.

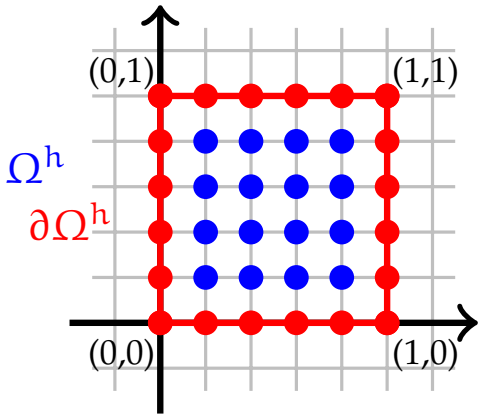

Figure 3: Depiction of Ω^h with $N = 5$, $hN = 1$. Blue: inner nodes, red: boundary nodes

We choose to discretize the MSO on Ω^h by Finite Differences, since this is usually the easiest way to go, and on a structured grid, would anyways yield similar discrete equation as in Finite Volume or Finite Element methods.

To obtain a second order consistent discrete MSO ($F^h[\cdot]$), we use central difference stencils on the first, second and mixed derivative. Since all these stencils have make only use of immediate neighours, there is no need to treat nodes close to the boundary differently, since the boundary is given by $g(\cdot)$.

This way, we obtain a discrete version of (2):

$$\begin{aligned} \left(1 + d_x[z^h]^2\right) d_{yy}[z^h] - d_x[z^h] d_y[z^h] d_{xy}[z^h] + \left(1 + d_y[z^h]^2\right) d_{xx}[z^h] = F^h\left[z^h\right] = 0 \quad &\text{in } \Omega^h \\ z^h = g \quad &\text{on } \partial\Omega^h, \end{aligned} \tag{8}$$

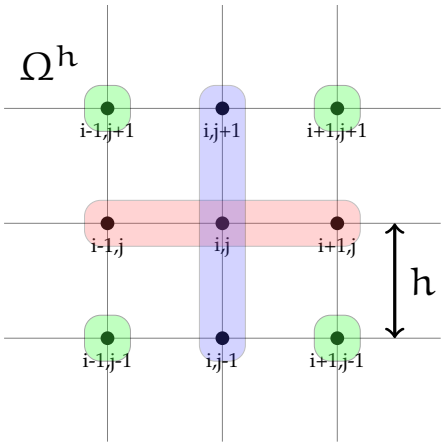

Figure 4: Snippet of the mesh with Finite Differences stencils
red/blue: first and second order stencils in x, y
green: mixed stencil

while the stencils defined on the inner nodes are given as follows ($1 \leq i, j \leq N-1$):

$$d_x[z] = \frac{z_{i+1,j} - z_{i-1,j}}{2h} \tag{9}$$

$$d_y[z] = \frac{z_{i,j+1} - z_{i,j-1}}{2h} \tag{10}$$

$$d_{xx}[z] = \frac{z_{i+1,j} - 2z_{i,j} + z_{i-1,j}}{h^2} \tag{11}$$

$$d_{yy}[z] = \frac{z_{i,j+1} - 2z_{i,j} + z_{i,j-1}}{h^2} \tag{12}$$

$$d_{xy}[z] = \frac{z_{i+1,j+1} + z_{i-1,j-1} - z_{i-1,j+1} - z_{i+1,j-1}}{4h^2}. \tag{13}$$

Figure 4 depicts the stencils on a segment of Ω^h. Since the stencils have only support to the nearest neighbors, there is no need tho treat nodes close to the boundary any different. Furthermore, this gives already rise to the conclusion, that the associated matrix will be sparse (for each of the N gridpoints, only 9 instead of N partners contribute).

2.2.2. Solution

The main difficulty in solving the MSE lies in the non-linearity of $F^h[\cdot]$. Since it is not possible, to directly invert for $z^h = \left(F^h\right)^{-1} 0$, one needs to use a procedure such as Newton-Raphson iterations. The main idea is to use some initial guess z_0^h, while in general, $F^h\left[z_0^h\right] = r_k^h \neq 0$. The goal is then to generate a sequence of z_k^h such that $r_k^h \to 0$ for increasing, but reasonably small k. Algorithm 1 shows the standard Newton-Raphson procedure, that takes as input a specific initial guess (here: 0), a tolerance for convergence TOL and the nonlinear operator $F^h[\cdot]$, outputting an approximate solution to the MSE $z_{k_{fin}}^h$.

Algorithm 1 Newton's method applied on the discrete MSE

$k \leftarrow 0$
$z_k^h \leftarrow 0$
$r_k^h \leftarrow F^h\left[z_k^h\right]$
while $\|r_k^h\| > \text{TOL}$ **do** ▷ We choose $\|\cdot\| = \|\cdot\|_2$
  $z_{k+1}^h \leftarrow z_k^h - \left(\nabla F^h\left[z_k^h\right]\right)^{-1} r_k^h$
  $k \leftarrow k + 1$
  $r_k^h \leftarrow F^h\left[z_k^h\right]$
end while

This algorithm involves the computation of the inverse of the gradient of $F^h\left[z_k^h\right]$ for each iteration k. Later, we will present and compare two different ways on how to contrive this.

It is well known, that the Newton-Raphson procedure yields fast convergence, but the success of this convergence is highly dependent on the initial guess z_0^h. Furthermore, convergence can be improved by choosing an initial guess that is closer to the solution. One possible initial guess is to take the average boundary value,
$z_{0,ave}^h = \frac{1}{|\partial\Omega^h|} \sum_{(x_i,y_j)\in\partial\Omega^h} \left(g(x_i, y_j)\right)$. While this might help convergence for surfaces, that have a certain offset with respect to the x, y-plane, it does not provide any additional information (such as preshaping the correct curvature).

To obtain a more educated initial guess, recall the MSE, equation (2). Considering only linear terms, we get

$$\begin{aligned} \mathcal{L}[z] = z_{xx} + z_{yy} = 0 \qquad & \text{in } \Omega \\ z(x, y) = g(x, y) \qquad & \text{on } \partial\Omega \end{aligned} \tag{14}$$

This linear, second order PDE is well known as the Laplace-equation, and can be solved by discretizing the second derivatives using the definitions for $d_{xx}[\cdot], d_{yy}[\cdot]$ introduced before, yielding $L[z^h] = 0$ with the usual boundary conditions. Since Laplace's equation can be regarded as a linearization of the MSE, we suspect to get a better initial guess (and thus faster and a more robust convergence behaviour) by first solving for $z_0^h = L^{-1}0$. This way, we obtain a slightly modified version of Algorithm 1, stated in Algorithm 2.

Algorithm 2 Newton's method using Laplace's Equ. as initial guess

$k \leftarrow 0$
$z_k^h \leftarrow L^{-1}0$ ▷ Solve Laplace's Equ. as initial guess
$r_k^h \leftarrow F^h\left[z_k^h\right]$
while $\|r_k^h\| > \text{TOL}$ **do**
  $z_{k+1}^h \leftarrow z_k^h - \left(\nabla F^h\left[z_k^h\right]\right)^{-1} r_k^h$
  $k \leftarrow k + 1$
  $r_k^h \leftarrow F^h\left[z_k^h\right]$
end while

2.3. Consequences for a implementation

So far we discussed the abstract numerical setting to solve the MSE. But when implementing this as a software solution, one has to consider several additional points, which especially involve the interface to the user.

We provide an overview of requirements for a potential implementation in figure 5.

We can divide communication with the user into user input and output to the user. A input interface can be realized e.g. as a GUI (graphical user interface) or as a input file (text file, that is parsed before/while running the simulations). Either realization serves the purpose to give the user a convenient possibility to set the main simulation parameters such as grid size and boundary conditions, as well as to set several tuning parameters like number of threads for parallel execution, initial guess.

The output to the user further is crucial in the sense that without giving the user any opportunity to perceive the result of the computation, there is no point in even computing anything. In terms of our application, it is required to provide the result in a form that can easily be visualized as a 3D-object. Additionally, one might want to offer a convenient validity-check and information about convergence.

Last but not least, a software implementation also needs to be able to perform all of the key steps to solve the MSE: It must allow for a discretizaion of the computational domain, and for setting the desired values on its boundary. Apart from implementing a suitable initial guess, inside a loop such as Algorithms 1, 2 there are a few important tasks missing that require special consideration: Both computing the Jacobian $\nabla \mathbf{F}^h[\cdot]$ and solving the resulting linear systems are non-trivial necessities whose treatment will be discussed in more detail in the next chapter.

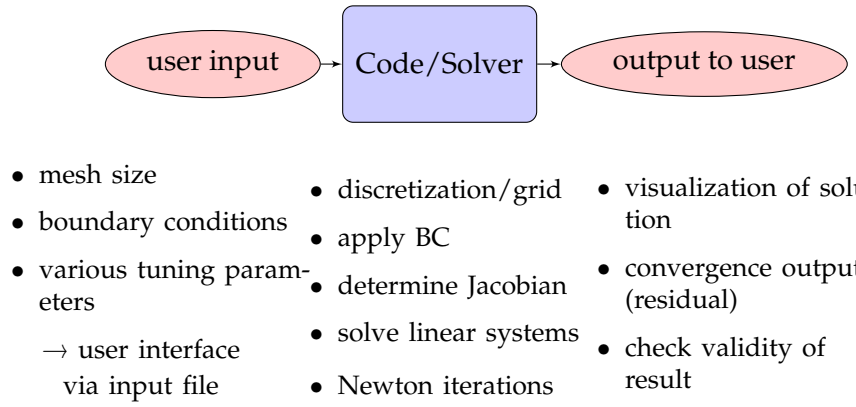

Figure 5: Requirements on a potential implementation

3. Implementation

3.1. Software/Solver Design

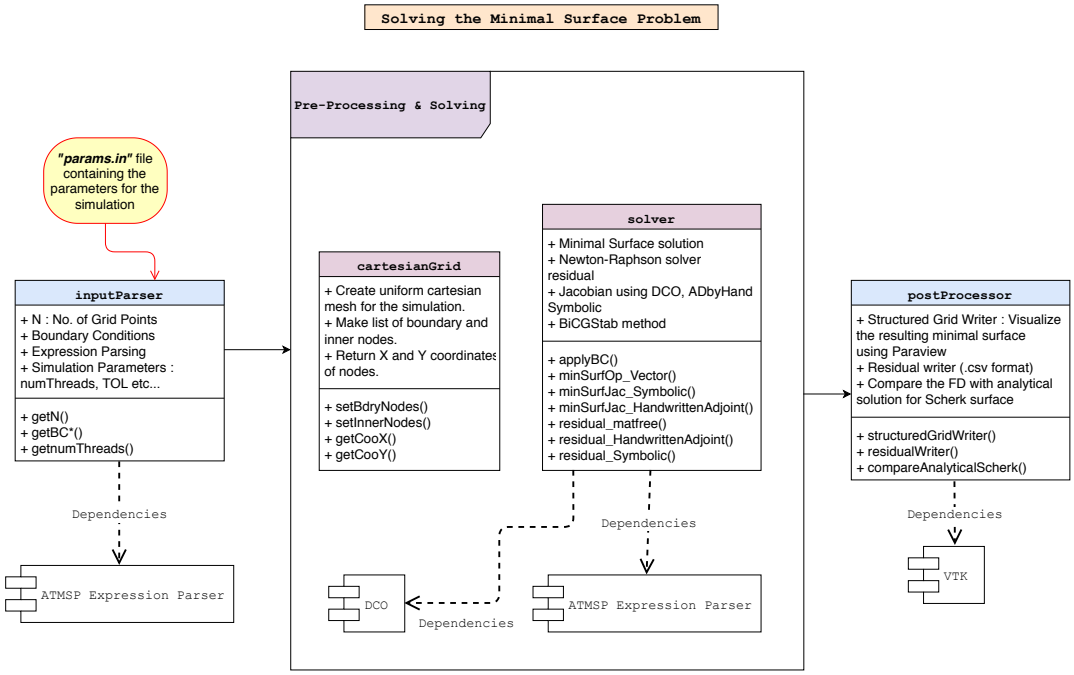

Figure 6: UML Diagram showing the strucuture of the *Minimal Surface* software.

Figure 6 shows the structure of the software, the classes and their associated functions, developed in order to solve the minimal surface problem.

- **inputParser:** This class consists of functions necessary to read all the parameters required to control and execute the minimal surface software. This class takes in `params.in` which contains all the necessary parameters such as the # of mesh elements, boundary conditions, option for the method of Jacobian computation etc... as an input to be parsed and processed. This class also depends on an external library, `ATMSP Expression Parser`, to parse the boundary conditions.

- **cartesianGrid:** This class consists of functions that help in the generation of a uniform cartesian mesh required for solving the FD problem. It also has functions required to return the `x` and `y` coordinates of a node required to apply the

boundary conditions. It also provides function calls to allocate separate storage of boundary and inner node indices.

- **solver:** This class consists of functions required to solve the minimal surface problem using Newton-Raphson method. The function to apply the boundary conditions is specified inside this class. `ATMSP Expression Parser` library is again required for this as the library provides methods to parse the boundary condition given as a string expression inside `params.in` into an executable byte code. It also uses `DCO` library to compute the Jacobian required for the Newton Raphson iterations. Separate function definitions are created to run the solver for different options of Jacobian such as Symbolic differentiation, AD by Hand and Matrix-free methods based on the option provided inside `params.in`

- **postProcessor:** This class consists of functions designed to write the solver residual as a CSV file and the resulting minimal surface as a VTS file to be visualized inside *Paraview*. To write the VTS file, the class uses the `VTK` library. The class also provides a function to compare the convergence of FD to analytical solution for the special case of a Scherk surface where the convergence rate is measured using both the *Max Norm* as well as the *l2-Norm*.

3.2. Computing the Jacobian

@Chenfei, briefly explain like in the presentation the three methods, and also name that one could use Finite Differences, but this is expected to perform bad (because...), and thus we do not use it (the next lines are already a few months old, use them or get rid of them)

Within the Newton iterations, it is necessary to compute the inverse of the Jacobian of the discrete MSO. We implemented this procedure following two different strategies:

- Based on generating the Jacobian matrix $\nabla \mathbf{F}^h \left[z_k^h\right]$ and computing its inverse
  - Hard-code a manually calculated Jacobian (to verify results)
  - Build a Jacobian matrix from Automatic Differention (AD by hand)

- Based on a linear iterative scheme, where we do not explicitly build the Jacobian, but extract its action on certain vectors from AD and feed this to a linear iterative solver

Argue that, since $\nabla \mathbf{F}$ is not symmetric in general, need stabilized CG (better performance than GMRES according to Eigen library)

Algorithm 3 Newton's method

$y \leftarrow F(z)$
while $\|y\| > \text{TOL}$ **do**
  $A = \nabla F(z)$
  $dz = A^{-1}y$ ▷ Instead of assembling the whole ∇F above, do this matrix-free
  $z \leftarrow z + dz$
  $\texttt{res} \leftarrow F(z)$
end while

Algorithm 4 Matrix-free BiCGSTAB to get dz (adapted from [2])

$z^{(1)} \leftarrow dz$
$(y, y^{(1)}) \leftarrow F^{(1)}(z, z^{(1)})$ ▷ DCO
$p \leftarrow -y - y^{(1)}$
$r \leftarrow p, r_0 \leftarrow r, \rho \leftarrow 1, \alpha \leftarrow 1, \omega \leftarrow 1$
while $\|r\| > \text{TOL}$ **do**
  $\rho_{new} = (r_0, r)$
  $z^{(1)} \leftarrow p$
  $\beta \leftarrow \rho_{new}/\rho \cdot \alpha/\omega$
  $\rho \leftarrow \rho_{new}$
  $p \leftarrow r + \beta(p - \omega v)$
  $z^{(1)} \leftarrow p$
  $(y, y^{(1)}) \leftarrow F^{(1)}(z, z^{(1)})$ ▷ DCO
  $\alpha \leftarrow \rho/(r_0, y^{(1)})$
  $dz \leftarrow dz + \alpha p$
  $s \leftarrow r - \alpha y^{(1)}$
  $z_1 \leftarrow z + dz$
  $(y_1, y_1^{(1)}) \leftarrow F^{(1)}(z_1, z_1^{(1)})$ ▷ DCO
  if $\|y_1\| < \text{TOL}$ **then**
    abort ▷ Converged at intermediate level
  end if
  $z^{(1)} \leftarrow s$
  $(y, y^{(1)}) \leftarrow F^{(1)}(z, z^{(1)})$ ▷ DCO
  $\omega \leftarrow (y^{(1)}, s)/(y^{(1)}, y^{(1)})$
  $dz \leftarrow dz + \omega s$
  $r \leftarrow s - \omega y^{(1)}$
  $z \leftarrow z + dz$
end while

3.3. Solving linear systems

I tested a bit now, and will push also to the code, timings ideally after that: seems like sparseLU is faster for getting the initial guess, so I will implement that.
for the loops, bicgstab is still advantageous as we can greatly reduce TOL_linsolver.

3.4. Testing

@Praveen here the figure as in the presentation, short explanation (basically what you said)

maybe 1-2 results of tests, short explanation

checking of validity by means of scherk, present a result here

4. Results

@Praveen you can refer to Scherk from General background, results for the 2 testcases, some timings (for all solvers for a choice of #gridpoints, not too many), scaling of the three (fix #gridpoints to sth > 500 for jacOption 0,1 and maybe max. 200-300 for 2, and run for 1,2,4,8,16 threads) once timings are implemented, you can also ask us to help determine times (consistent TOL's etc...)

5. Conclusions and outlook

pretty much what we had in the presentation

@all, feel free to add ideas here, I would merge it together in the end

References

[1] Makoto Sakai. *Lecture Notes in Mathematics – Minimal Surfaces in R3*. 1976.

[2] Uwe Naumann. *The art of differentiating computer programs: an introduction to algorithmic differentiation*, volume 24. Siam, 2012.

A. User manual

This section provides a short description on how to run the code. The software accompanying this report is self-contained and guaranteed to run on the RWTH cluster, using either the current versions of the Intel (19) or GCC (9) compiler.

A.1. Compilation

To compile the code, open a terminal inside `source/`.

```
cd build
cmake ..
make
```

The standard setup is the CMAKE compile option `Release` admitting some compiler optimization. If some additional debug information is desired, change the option to `debug` inside `CMakeLists.txt`.

A.2. Running a simulation

To run a simulation, go to the folder testcases or create a new folder with a valid `params.in`-file.

Inside this `params.in`-file, one can find the options to set with descriptions.
To run the a simulation, execute the following, once the input file is set up:

```
cd <folder with params.in>
export NAG_KUSARI_FILE=<path to nag_key.txt>
   # needed if jacobianOpt=2
ln -s <path to executable minSurf in build/> .
   # symbolic link for convenient execution
./minSurf
```

Now, the resulting output can be inspected by opening the `.vts`-files inside `surfaces/` using Paraview[1]. If one is interesting in the convergence, one can find the residual data over iteration inside `residual/`, which can be also plotted using Paraview.

[1] to use this on the cluster, execute `module load GRAPHICS paraview` beforehand.