

1 Simulation of the PDEs

1.1 Model Equations

Let $u = (u_1, u_2)$ be the velocity, where $u_1, u_2 : \Omega \times [0, \infty) \rightarrow \mathbb{R}$ and $p : \Omega \times [0, \infty) \rightarrow \mathbb{R}$ the pressure and $T : \Omega \times [0, \infty) \rightarrow \mathbb{R}$ the temperature variable. We then get the scalar equations:

$$\frac{\partial u_1}{\partial t} + \langle u, \nabla u_1 \rangle = -\frac{1}{\rho} \frac{\partial p}{\partial x} + \nu \nabla^2 u_1 - g_1 \alpha (T - T_0) \quad (1)$$

$$\frac{\partial u_2}{\partial t} + \langle u, \nabla u_2 \rangle = -\frac{1}{\rho} \frac{\partial p}{\partial y} + \nu \nabla^2 u_2 - g_2 \alpha (T - T_0) \quad (2)$$

$$\frac{\partial u_1}{\partial x_1} + \frac{\partial u_2}{\partial x_2} = \varepsilon p \quad (3)$$

$$\frac{\partial T}{\partial t} + \langle u, \nabla T \rangle = \kappa \nabla^2 T \quad (4)$$

where

$g = (g_1, g_2)^T$: gravitational acceleration

ρ : density of the fluid

ν : kinematic viscosity

α : coefficient of expansion

κ : thermal diffusivity

ε : regularisation parameter

T_0 : a reference temperature

with boundary conditions

$$u_1 = u_2 = 0 \quad \text{on } \Gamma \quad (5)$$

$$T = T_{\text{dir}} \quad \text{on } \Gamma_1 \quad (6)$$

$$\partial_\eta T = \langle \nabla T, \eta \rangle = \gamma (T - T_{\text{out}}) \quad \text{on } \Gamma \setminus \Gamma_1 \quad (7)$$

where

η : outer normal of the boundary

T_{dir} : heating

T_{out} : outside temperature

γ : thermal conductivity of the boundary

1.2 Implicit Euler discretisation in time

If we have a differential equation, e.g for u_1

$$\frac{\partial u_1}{\partial t} = F(u_1, u_2, p, T)$$

we can apply implicit Euler with a timestep δt to get

$$\frac{u_1^{\text{new}} - u_1^{\text{old}}}{\delta t} = F(u_1^{\text{new}}, u_2, p, T) \quad (8)$$

where we now have find the root u_1 of the Function

$$u_1 - u_1^{\text{old}} - \delta t F(u_1, u_2, p, T)$$

1.3 Weak formulation

Testing each line (1) – (4) with a test function $v_i, i \in \{1, \dots, 4\}$ and integrating over the domain Ω we can now define

$$F_1(u_1, u_2, p, T)v_1 := \int_{\Omega} \left(-\langle u, \nabla u_1 \rangle - \frac{1}{\rho} \frac{\partial p}{\partial x} + \nu \nabla^2 u_1 - g_1 \alpha (T - T_0) \right) v_1 d\omega \quad (9)$$

$$F_2(u_1, u_2, p, T)v_2 := \int_{\Omega} \left(-\langle u, \nabla u_2 \rangle - \frac{1}{\rho} \frac{\partial p}{\partial y} + \nu \nabla^2 u_2 - g_2 \alpha (T - T_0) \right) v_2 d\omega \quad (10)$$

$$F_3(u_1, u_2, p, T)v_3 := \int_{\Omega} \left(\varepsilon p - \frac{\partial u_1}{\partial x_1} - \frac{\partial u_2}{\partial x_2} \right) v_3 d\omega \quad (11)$$

$$F_4(u_1, u_2, p, T)v_4 := \int_{\Omega} \left(-\langle u, \nabla T \rangle + \kappa \nabla^2 T \right) v_4 d\omega \quad (12)$$

partial integration and using the boundary conditions yields:

(remember, $\nabla^2 u_1 = \Delta u_1 = \sum_i \frac{\partial^2 u_1}{\partial^2 x_i}$)

$$\begin{aligned}
F_1(u_1, u_2, p, T)v_1 &= \int_{\Omega} \left(-\langle u, \nabla u_1 \rangle - \frac{1}{\rho} \frac{\partial p}{\partial x} - g_1 \alpha (T - T_0) \right) v_1 + \nu \nabla^2 u_1 v_1 d\omega \\
&= \int_{\Omega} \left(-\langle u, \nabla u_1 \rangle - \frac{1}{\rho} \frac{\partial p}{\partial x} - g_1 \alpha (T - T_0) \right) v_1 - \nu \langle \nabla u_1, \nabla v_1 \rangle d\omega + \int_{\Gamma} \nu \langle \nabla u_1, \eta \rangle v_1 ds \\
&= \int_{\Omega} \left(-\langle u, \nabla u_1 \rangle - \frac{1}{\rho} \frac{\partial p}{\partial x} - g_1 \alpha (T - T_0) \right) v_1 - \nu \langle \nabla u_1, \nabla v_1 \rangle d\omega, \quad \text{as } v_1 = 0 \text{ on } \Gamma \\
F_2(u_1, u_2, p, T)v_2 &= \int_{\Omega} \left(-\langle u, \nabla u_2 \rangle - \frac{1}{\rho} \frac{\partial p}{\partial y} - g_2 \alpha (T - T_0) \right) v_2 - \nu \langle \nabla u_2, \nabla v_2 \rangle d\omega + \int_{\Gamma} \nu \langle \nabla u_2, \eta \rangle v_2 ds \\
&= \int_{\Omega} \left(-\langle u, \nabla u_2 \rangle - \frac{1}{\rho} \frac{\partial p}{\partial y} - g_2 \alpha (T - T_0) \right) v_2 - \nu \langle \nabla u_2, \nabla v_2 \rangle d\omega \quad \text{as } v_2 = 0 \text{ on } \Gamma
\end{aligned}$$

$$\begin{aligned}
F_4(u_1, u_2, p, T)v_4 &= \int_{\Omega} (-\langle u, \nabla T \rangle + \kappa \nabla^2 T) v_4 d\omega \\
&= \int_{\Omega} -\langle u, \nabla T \rangle v_4 - \kappa \langle \nabla T, \nabla v_4 \rangle d\omega + \int_{\Gamma} \kappa \langle \nabla T, \eta \rangle v_4 ds \\
&= \int_{\Omega} -\langle u, \nabla T \rangle v_4 - \kappa \langle \nabla T, \nabla v_4 \rangle d\omega + \int_{\Gamma_1} \kappa \langle \nabla T, \eta \rangle v_4 ds + \int_{\Gamma \setminus \Gamma_1} \kappa \langle \nabla T, \eta \rangle v_4 ds \\
&= \int_{\Omega} -\langle u, \nabla T \rangle v_4 - \kappa \langle \nabla T, \nabla v_4 \rangle d\omega + \int_{\Gamma_1} \kappa \langle \nabla T, \eta \rangle v_4 ds + \int_{\Gamma \setminus \Gamma_1} \kappa \gamma (T - T_{\text{out}}) v_4 ds
\end{aligned}$$

1.4 Newton's method on the implicit Euler equation

Using the considerations of the last two subsections, we define

$$G(u_1, u_2, p, T) = \begin{pmatrix} \int_{\Omega} (u_1 - u_1^{\text{old}}) v_1 d\omega - \delta t F_1(u_1, u_2, p, T) v_1 \\ \int_{\Omega} (u_2 - u_2^{\text{old}}) v_2 d\omega - \delta t F_2(u_1, u_2, p, T) v_2 \\ F_3(u_1, u_2, p, T) v_3 \\ \int_{\Omega} (T - T^{\text{old}}) v_4 d\omega - \delta t F_4(u_1, u_2, p, T) v_4 \end{pmatrix}$$

We now want to find $(u_1, u_2, p, T)^T$ such that $G(u_1, u_2, p, T) = 0$. Applying Newton's method on the function G , we get the iteration

$$\begin{pmatrix} u_1^{i+1} \\ u_2^{i+1} \\ p^{i+1} \\ T^{i+1} \end{pmatrix} = \begin{pmatrix} u_1^i \\ u_2^i \\ p^i \\ T^i \end{pmatrix} + \begin{pmatrix} \delta u_1^i \\ \delta u_2^i \\ \delta p^i \\ \delta T^i \end{pmatrix}$$

where

$$G'(u_1^i, u_2^i, p^i, T^i) \begin{pmatrix} \delta u_1^i \\ \delta u_2^i \\ \delta p^i \\ \delta T^i \end{pmatrix} = -G(u_1^i, u_2^i, p^i, T^i)$$

and

$$G'(u_1^i, u_2^i, p^i, T^i) = \begin{pmatrix} \frac{\partial G_1}{\partial u_1} & \frac{\partial G_1}{\partial u_2} & \frac{\partial G_1}{\partial p} & \frac{\partial G_1}{\partial T} \\ \frac{\partial G_2}{\partial u_1} & \frac{\partial G_2}{\partial u_2} & \frac{\partial G_2}{\partial p} & \frac{\partial G_2}{\partial T} \\ \frac{\partial G_3}{\partial u_1} & \frac{\partial G_3}{\partial u_2} & \frac{\partial G_3}{\partial p} & \frac{\partial G_3}{\partial T} \\ \frac{\partial G_4}{\partial u_1} & \frac{\partial G_4}{\partial u_2} & \frac{\partial G_4}{\partial p} & \frac{\partial G_4}{\partial T} \end{pmatrix}$$

1.5 Simplifications of the system

Consider a Function $G(z) = C + Az + N(z)$, where C is a constant, Az is the linear and $N(z)$ is the nonlinear part of the function. If we apply Newton's method to find a root of $G(z)$, using $\delta z^i = z^{i+1} - z^i$, we have to solve

$$G'(z^i)\delta z = -G(z^i) \quad (13)$$

$$\Leftrightarrow (A + N'(z^i))(z^{i+1} - z^i) = -(C + Az^i + N(z^i)) \quad (14)$$

and solve this for z^{i+1} we obtain

$$(A + N'(z^i))(z^{i+1}) = -C - Az^i - N(z^i) + (A + N'(z^i))z^i = -C - N(z^i) + N'(z^i)z^i$$

In our context, we split up $G_i(u_1, u_2, p, T)$, $i \in \{1, \dots, 4\}$ and get

$$\begin{aligned} C_{G_1} &= - \int_{\Omega} u_1^{\text{old}} v_1 d\omega - \delta t C_{F_1} = - \int_{\Omega} u_1^{\text{old}} v_1 d\omega - \delta t \int_{\Omega} g_1 \alpha T_0 v_1 d\omega \\ C_{G_2} &= - \int_{\Omega} u_2^{\text{old}} v_2 d\omega - \delta t C_{F_2} = - \int_{\Omega} u_2^{\text{old}} v_2 d\omega - \delta t \int_{\Omega} g_2 \alpha T_0 v_2 d\omega \\ C_{G_3} &= C_{F_3} = 0 \\ C_{G_4} &= - \int_{\Omega} T^{\text{old}} v_4 d\omega - \delta t C_{F_4} = - \int_{\Omega} T^{\text{old}} v_4 d\omega + \delta t \int_{\Gamma \setminus \Gamma_1} \kappa \gamma T_{\text{out}} v_3 d\omega \end{aligned}$$

for the constant part and for the left hand side linear part

$$\begin{aligned}
A_{G_1} z^{i+1} &= \int_{\Omega} u_1^{i+1} v_1 d\omega - \delta t A_{F_1} z^{i+1} \\
&= \int_{\Omega} u_1^{i+1} v_1 d\omega - \delta t \left[\int_{\Omega} \left(-\frac{1}{\rho} \frac{\partial p^{i+1}}{\partial x} - g_1 \alpha T^{i+1} \right) v_1 - \nu \langle \nabla u_1^{i+1}, \nabla v_1 \rangle d\omega \right] \\
&= \int_{\Omega} u_1^{i+1} v_1 d\omega + \delta t \int_{\Omega} \left(\frac{1}{\rho} \frac{\partial p^{i+1}}{\partial x} + g_1 \alpha T^{i+1} \right) v_1 + \nu \langle \nabla u_1^{i+1}, \nabla v_1 \rangle d\omega \\
A_{G_2} z^{i+1} &= \int_{\Omega} u_2^{i+1} v_2 d\omega - \delta t A_{F_2} z^{i+1} \\
&= \int_{\Omega} u_2^{i+1} v_2 d\omega - \delta t \left[\int_{\Omega} \left(-\frac{1}{\rho} \frac{\partial p^{i+1}}{\partial y} - g_2 \alpha T^{i+1} \right) v_2 - \nu \langle \nabla u_2^{i+1}, \nabla v_2 \rangle d\omega \right] \\
&= \int_{\Omega} u_2^{i+1} v_2 d\omega + \delta t \int_{\Omega} \left(\frac{1}{\rho} \frac{\partial p^{i+1}}{\partial y} + g_2 \alpha T^{i+1} \right) v_2 + \nu \langle \nabla u_2^{i+1}, \nabla v_2 \rangle d\omega \\
A_{G_3} z^{i+1} &= \delta t A_{F_3} z^{i+1} \\
&= \int_{\Omega} (\varepsilon p^{i+1} - \frac{\partial u_1^{i+1}}{\partial x} - \frac{\partial u_2^{i+1}}{\partial y}) v_3 \\
A_{G_4} z^{i+1} &= \int_{\Omega} T^{i+1} v_4 d\omega - \delta t A_{F_4} z^{i+1} \\
&= \int_{\Omega} T^{i+1} v_4 d\omega - \delta t \left(\int_{\Omega} -\kappa \langle \nabla T^{i+1}, \nabla v_4 \rangle d\omega + \int_{\Gamma_1} \kappa \langle \nabla T^{i+1}, \eta \rangle v_4 ds + \int_{\Gamma \setminus \Gamma_1} \kappa \gamma T^{i+1} v_4 ds \right) \\
&= \int_{\Omega} T^{i+1} v_4 d\omega + \delta t \left(\int_{\Omega} \kappa \langle \nabla T^{i+1}, \nabla v_4 \rangle d\omega - \int_{\Gamma_1} \kappa \langle \nabla T^{i+1}, \eta \rangle v_4 ds - \int_{\Gamma \setminus \Gamma_1} \kappa \gamma T^{i+1} v_4 ds \right)
\end{aligned}$$

To get the nonlinear part $N(z^i)$ and its linearization $N'(z^i)z^i$ and $N'(z^i)z^{i+1}$ respectively, we first compute with w being a test function

$$\begin{aligned}
&\frac{\partial}{\partial u_1} (\langle u, \nabla u_1 \rangle) w \\
&= \frac{\partial}{\partial u_1} (u_1 \frac{\partial u_1}{\partial x} + u_2 \frac{\partial u_1}{\partial y}) w \\
&= w \frac{\partial u_1}{\partial x} + u_1 \frac{\partial w}{\partial x} + u_2 \frac{\partial w}{\partial y} \quad \text{product rule}
\end{aligned}$$

and

$$\begin{aligned}
& \frac{\partial}{\partial u_2} (\langle u, \nabla u_2 \rangle) w \\
&= \frac{\partial}{\partial u_2} (u_1 \frac{\partial u_2}{\partial x} + u_2 \frac{\partial u_2}{\partial y}) w \\
&= u_1 \frac{\partial w}{\partial x} + w \frac{\partial u_2}{\partial y} + u_2 \frac{\partial w}{\partial y} \quad \text{product rule}
\end{aligned}$$

We then obtain

$$\begin{aligned}
N_{G_1}(z^i) &= -\delta t N_{F_1}(z^i) \\
&= \int_{\Omega} \langle u^i, \nabla u_1^i \rangle v_1 d\omega \\
N'_{G_1}(z^i) z^{i+1} &= -\delta t N'_{F_1}(z^i) z^{i+1} \\
&= \delta t \int_{\Omega} \underbrace{(u_1^{i+1} \frac{\partial u_1^i}{\partial x} + u_1^i \frac{\partial u_1^{i+1}}{\partial x} + u_2^i \frac{\partial u_1^{i+1}}{\partial y} + u_2^{i+1} \frac{\partial u_1^i}{\partial y})}_{-(\frac{\partial N_{F_1}(z^i)}{\partial u_1}) u_1^{i+1}} v_1 d\omega \\
&\quad - (\frac{\partial N_{F_1}(z^i)}{\partial u_2}) u_2^{i+1} \\
N_{G_2}(z^i) &= -\delta t N_{F_2}(z^i) \\
&= \int_{\Omega} \langle u^i, \nabla u_2^i \rangle v_2 d\omega \\
N'_{G_2}(z^i) z^{i+1} &= -\delta t N'_{F_2}(z^i) z^{i+1} \\
&= \delta t \int_{\Omega} \underbrace{(u_1^i \frac{\partial u_2^{i+1}}{\partial x} + u_2^{i+1} \frac{\partial u_2^i}{\partial y} + u_2^i \frac{\partial u_2^{i+1}}{\partial y} + u_1^{i+1} \frac{\partial u_2^i}{\partial x})}_{-(\frac{\partial N_{F_2}(z^i)}{\partial u_2}) u_2^{i+1}} v_2 d\omega \\
&\quad - (\frac{\partial N_{F_2}(z^i)}{\partial u_1}) u_1^{i+1} \\
N_{G_3}(z^i) &= 0 \\
N_{G_4}(z^i) &= -\delta t N_{F_4}(z^i) \\
&= \delta t \int_{\Omega} \langle u, \nabla T \rangle v_4 d\omega \\
N'_{G_4}(z^i) z^{i+1} &= -\delta t N'_{F_4}(z^i) z^{i+1} \\
&= \delta t \int_{\Omega} \underbrace{(u_1^{i+1} \frac{\partial T^i}{\partial x} + u_2^{i+1} \frac{\partial T^i}{\partial y} + \langle u^i, \nabla T^{i+1} \rangle)}_{-(\frac{\partial N_{F_4}(z^i)}{\partial u_1}) u_1^{i+1} - (\frac{\partial N_{F_4}(z^i)}{\partial u_2}) u_2^{i+1} - (\frac{\partial N_{F_4}(z^i)}{\partial T}) T^{i+1}} v_4 d\omega
\end{aligned}$$

1.6 Formulation as linear equation system

Using a Finite Element discretisation, we obtain finite dimensional spaces $V_i, i \in \{1, \dots, 4\}$, where we can just use the Basis functions $\Phi_j, j \in \{1, \dots, N\}$ for each

space as test functions $v_i, \in \{1, \dots, 4\}$. This gives the lines of the equation system. Furthermore, the variables u_1, u_2, p and T are linear combinations of these basis functions. Hence we have, e.g for the temperature T^{i+1} in the next Newton step

$$T^{i+1} = \sum_{j=1}^N \bar{T}_j^{i+1} \Phi_j^{i+1}$$

with coefficients $\bar{T}_j^{i+1} \in \mathbb{R}$.

1.7 Solutions of the linear equation system

1.7.1 No Temperature

If we consider the case without the temperature, we obtain a linear system with a saddle point matrix

$$\begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \begin{pmatrix} u^{i+1} \\ p^{i+1} \end{pmatrix} = \begin{pmatrix} b \\ 0 \end{pmatrix},$$

where $u = (u_1, u_2)$.

Note, that $M_{22} = 0$, if $\varepsilon = 0$ in the continuity equation. In this case, we obtain a unsymmetric, indefinite saddle point matrix. where M_{12} is the gradient and M_{21} the diffusion operator (with boundary conditions), where M_{11} stems from the (nonlinear) advection diffusion part.

An indeph overview of numerical methods can be found in [1], choices for preconditioners in [3, 2]. In [2] the SIMPLE and SIMPLER method for preconditioning are presented.

A possible solution of these systems is by the GMRES method, augmented with an inexact Schur preconditioner $P : X^* \rightarrow X$, namely performs the operation

1. solve $M_{21} \tilde{M}_{11}^{-1} M_{12} p = D \tilde{M}_{11}^{-1} r_1$
2. solve $\tilde{M}_{11} u = r_1 - Gp$

where \tilde{M}_{11} could be the diagonal of M_{11} (SIMPLE method). Note that, if we used $\tilde{M}_{11} = M_{11}$, we converge in one step, as the precondition operation yields the solution. Using the library libmesh, with PETsc as backend, this can be achieved by passing

- -pc.type fieldsplit \rightarrow use fieldsplit preconditioner
- -pc.fieldsplit_type schur \rightarrow use Schur-comp as preconditioner
- -pc.fieldsplit_detect_saddle_point \rightarrow automatic detection of blocks
- -pc.fieldsplit_schur_fact_type <full,diag,upper...> \rightarrow how does \tilde{M}_{11} evolve from M_{11} .

as command line arguments for setting the preconditioner, and

- -ksp_type <richardson,chebyshev,cg,bicg,gmres..>

as Krylov solver. GMRES is the default here.

2 Affine covariant Newton algorithms

Defined by 13, we will compute the Newton step δz at iteration point z . Afterwards, we will compute another (simplified) Newton step, via the solution of

$$G'(z)\bar{\delta z} = -(G(z + \delta z) - G(z) - G'(z)\delta z)$$

In the absence of damping, i.e $-G(z) - G'(z)\delta z = 0$, this yields a second Newton step after δz , with derivative information at z . The idea is now, to estimate the Newton contraction

$$\Theta_{z_*}(x_k) := \frac{\|z_{k+1} - z_*\|}{\|z_k - z_*\|} = \frac{\|G'(z_k)^{-1} (G'(z_k)(z_* - z_k) - (G(z_*) - G(z_k)))\|}{\|z_k - z_*\|}$$

by $z_+ = z - G'(z)^{-1}G(z) = z + \delta z$:

$$\Theta_{z_+}(x) := \frac{\|G'(z)^{-1} (G'(z)(z_+ - z) - (G(z_+) - G(z_k)))\|}{\|z_k - z_*\|}$$

and to extend this to a model around z with

$$[\Theta]_{z_+}(\xi) = \frac{[\omega]}{2} \|\xi - z_+\|$$

and to choose $[\omega]$ such that

$$[\Theta]_{z_+}(z) = \Theta_{x_+}(x) = \frac{\|\bar{\delta z}\|}{\|\delta z\|} \quad \Rightarrow \quad [\omega] = \frac{2\|\bar{\delta z}\|}{\|\delta z\|^2}$$

2.1 Globalization by damping

The problem $G(z) = 0$ might be too difficult, and our starting guess (even the one computed with the explicit Euler) might be too far away from the solution.

Algorithm 1 Damped Newton's method

Require: iterate $z, [\omega]$

repeat // step computation loop

 solve $G'(z)\delta z + G(z) = 0$.

do

 compute $\lambda = \min\{1, \frac{1}{\|\delta z\|[\omega]}\}$

 solve $G'(z)\bar{\delta}z + G(z + \lambda\delta z) = 0$.

 compute $[\omega] = \frac{\|\bar{\delta}z - (1-\lambda)\delta z\|}{\|\lambda\delta z\|^2}$

$\Theta_{z+\lambda\delta z}(z) = \frac{[\omega]}{2}\|\lambda\delta z\|$

while $\Theta_{z+\lambda\delta z}(z) \geq 1$ (divergence)

$z_+ \leftarrow z + \lambda\delta z$

if $\lambda = 1$ and $\Theta_{z_+}(z) \leq 0.5$ and $\|\delta z\| \leq \text{TOL}$ **then**

$z_+ + \bar{\delta}z \leftarrow$ terminate "desired accuracy needed"

end if

$z \leftarrow z_+$

until

References

- [1] M. Benzi, G. H. Golub, and J. Liesen. Numerical solution of saddle point problems. *Acta Numerica*, (14):1–137, 2005.
- [2] A. de Niet and F. Wubs. Two preconditioners for saddle point problems in fluid flows. *INTERNATIONAL JOURNAL FOR NUMERICAL METHODS IN FLUIDS*, 2007.
- [3] J. Schöberl and W. Zulehner. Symmetric indefinite preconditioners for saddle point problems with applications to pde-constrained optimization problems. *SIAM Journal on Matrix Analysis and Applications*, 29(3):752–773, 2007.