“Notes on the simulation of the convection diffusion equation in FEniCS” October 10, 2017; rev. March 14, 2018

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1 Setting

Consider the following equation

$$y_t - \alpha \Delta y + w \nabla y = 0 \text{ on } Q := \Omega \times [0, T] \tag{1}$$

where $y : Q \to \mathbb{R}$ is the temperature, $\alpha \in \mathbb{R}$ is the diffusion coefficient and $w : [0, T] \to \Omega$ is the velocity field. We use the shorthand $y_t = \frac{\partial y}{\partial t}$ to denote the time derivative.

Let Ω be the domain. The boundary is partitioned in an boundary Γ_{out} where some outside temperature is prescribed and a control boundary Γ_c. On one part of the boundary a controllable t is applied which is described by a Dirichlet condition

$$y = u \text{ on } \Gamma_c. \tag{2}$$

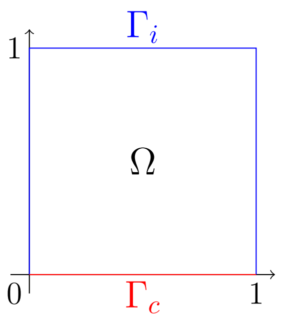
On the other part we have

$$y = y_{out} \text{ on } \Gamma_{out} \tag{3}$$

where $\frac{\partial y}{\partial n}$ is the derivative of y in normal direction. We approximate the Dirichlet boundary conditions by using the following Robin type boundary condition instead

$$\frac{\partial y}{\partial n} + \gamma y = \gamma z \text{ on } \Gamma. \tag{4}$$

By choosing $\gamma := 10^3$ and $z := \begin{cases} y_{out} & \text{on } \Gamma_{out} \\ u & \text{on } \Gamma_c \end{cases}$ we can approximate the Dirichlet boundary conditions. This will also allow us to extend the setting more easily in the future.



2 Numerical simulation of the convection diffusion equation

We simulate the equation using the finite element method.

2.1 Weak form

Multiplying with a test function and integrating over the domain Ω yields

$$\int_\Omega \frac{d}{dt} y v \, dx - \alpha \int_\Omega \Delta y v \, dx + \int_\Omega (w \cdot \nabla y) v \, dx = 0 \tag{5}$$

Using partial integration and substituting the boundary conditions we obtain

$$\int_\Omega \frac{d}{dt} y v \, dx + \alpha \int_\Omega \nabla y \nabla v \, dx + \int_\Omega (w \cdot \nabla y) v \, dx + \alpha \gamma_c \int_{\Gamma_c} (y - u) v \, ds + \alpha \gamma_{out} \int_{\Gamma_{out}} (y - y_{out}) v \, ds = 0 \tag{6}$$

We reorder by terms depending on y:

$$\begin{aligned} \int_\Omega \frac{d}{dt} y v \, dx + \alpha \int_\Omega \nabla y \nabla v \, dx + \int_\Omega (w \cdot \nabla y) v \, dx + \alpha \gamma_c \int_{\Gamma_c} y v \, ds + \alpha \gamma_{out} \int_{\Gamma_{out}} y v \, ds \\ = \alpha \gamma_c \int_{\Gamma_c} u v \, ds + \alpha \gamma_{out} \int_{\Gamma_{out}} y_{out} v \, ds \end{aligned}$$

This can be written more compactly be using the definitions

$$\begin{aligned} \langle \varphi, \psi \rangle_{L^2(\Omega)} &= \int_\Omega \varphi \psi \, dx \\ \langle F(t), \varphi \rangle &= \alpha \gamma_{out} y_{out}(t) \int_{\Gamma_{out}} \varphi \, ds \\ \langle Bu, \varphi \rangle &= \alpha \gamma_c u \int_{\Gamma_c} \varphi \, ds \end{aligned}$$

and the bilinear form

$$a(t; \varphi, \psi) = \alpha \int_\Omega \nabla \varphi \nabla \psi \, dx + \int_\Omega (w \cdot \nabla \varphi) \psi \, dx + \alpha \gamma_c \int_{\Gamma_c} \varphi \psi \, ds + \alpha \gamma_{out} \int_{\Gamma_{out}} \varphi \psi \, ds \tag{7}$$

We get

$$\langle \frac{d}{dt} y, v \rangle_{L^2(\Omega)} + a(t; y, v) = \langle Bu, v \rangle + \langle F(t), v \rangle \tag{8}$$

2.2 Time discretization

We discretize in time using the implicit Euler method. We pick a sampling rate $h > 0$ and define $y_k := y(\cdot, t_0 + hk)$, $y_{out,k} := y_{out}(\cdot, t_0 + hk)$, $u_k := u(t_0 + hk)$, $z_k := z(t_0 + hk)$ for $k \in \{0, 1, \dots, N\}$.
The time derivative of the state is approximated by

$$\frac{d}{dt} y \approx \frac{y_{k+1} - y_k}{h} \tag{9}$$

The initial value y_0 is given. To compute the next state y_{k+1} for each $k \in \{0, 1, \dots, N-1\}$ we replace $\frac{d}{dt} y$ in equation (8) by $\frac{y_{k+1} - y_k}{h}$ and y by y_{k+1}, as well as $y_{out}(t)$ by $y_{out,k+1}$ and $u(t)$ by u_k. Note that we use u_k instead of u_{k+1} since we assume u to be piecewise constant on each time interval. This leads to

$$\langle \frac{y_{k+1} - y_k}{h}, v \rangle_{L^2(\Omega)} + a(t; y_{k+1}, v) = \langle Bu_k, v \rangle + \langle F_k, v \rangle \tag{10}$$

or explicitely

$$\int_\Omega \frac{y_{k+1} - y_k}{h} v \, dx + \alpha \int_\Omega \nabla y_{k+1} \nabla v \, dx + \int_\Omega (w \cdot \nabla y_{k+1}) v \, dx + \alpha \gamma_c \int_{\Gamma_c} y_{k+1} v \, ds + \alpha \gamma_{out} \int_{\Gamma_{out}} y_{k+1} v \, ds$$
$$= \alpha \gamma_c u_k \int_{\Gamma_c} v \, ds + \alpha \gamma_{out} y_{out,k+1} \int_{\Gamma_{out}} v \, ds$$

Again, reordering by the known and unknown terms yields

$$\int_\Omega \frac{y_{k+1}}{h} v \, dx + \alpha \int_\Omega \nabla y_{k+1} \nabla v \, dx + \int_\Omega (w \cdot \nabla y_{k+1}) v \, dx + \alpha \gamma_c \int_{\Gamma_c} y_{k+1} v \, ds + \alpha \gamma_{out} \int_{\Gamma_{out}} y_{k+1} v \, ds$$
$$= \int_\Omega \frac{y_k}{h} v \, dx + \alpha \gamma_c u_k \int_{\Gamma_c} v \, ds + \alpha \gamma_{out} y_{out,k+1} \int_{\Gamma_{out}} v \, ds$$

2.3 Implementation in Firedrake

The above variational equation is solved in FEniCs for each $k \in \{0, 1, \ldots, N-1\}$:

```
# define a mesh
mesh = UnitIntervalMesh(50)

# Compile sub domains for boundaries
left = CompiledSubDomain("near(x[0], 0.)")
right = CompiledSubDomain("near(x[0], 1.)")

# Label boundaries, required for the objective
boundary_parts = MeshFunction("size_t", mesh, mesh.topology().dim() - 1
                               )
left.mark(boundary_parts, 0)  # boundary part for outside temperature
right.mark(boundary_parts, 1)  # boundary part where control is applied
ds = Measure("ds", subdomain_data=boundary_parts)

# Choose a time step size
delta_t = 5.0e-3

# define constants of the PDE
alpha = Constant(1.0)
gamma = Constant(1.0e6)

U = FunctionSpace(mesh, "Lagrange", 1)
```

```
# variational formulation
lhs = (y_k1 / Constant(delta_t) * phi) * dx + alpha * inner(grad(phi),
                               grad(y_k1)) * dx + alpha * gamma *
                               phi * y_k1 * ds
rhs = (y_k0 / Constant(delta_t) * phi) * dx + alpha * gamma * u * phi *
                                ds(1) + alpha * gamma * y_out *
                               phi * ds(0)
```

```
F = inner(y0, v) * dx
for i in range(1, 5):
    F += h * ac * Constant(gamma[i-1]) * Constant(u[i-1]) * v * ds(i)
```

3 Optimal Control Problem

Now that the simulation is running we want to implement an optimal control problem on top of it. Our goal is to solve the following problem:

$$\begin{aligned}\min_{y,u} J(y,u) =& \frac{1}{2}\int_\Omega (y(x,T) - y_\Omega(T,x))^2 \, dx + \frac{1}{2}\int_0^T \int_\Omega (y(x,t) - y_\Omega(t,x))^2 \, dx \, dt \\ &+ \frac{\lambda}{2}\int_0^T \int_\Gamma (u(x,t))^2 \, ds \, dt \\ &\text{s.t.}(1),(4) \\ &\quad \underline{u}(x,t) \le u(x,t) \le \overline{u}(x,t) \\ &\quad \underline{y}(x,t) \le y(x,t) \le \overline{y}(x,t)\end{aligned}$$

While the constraints on the control can be dealt with rather straightforwardly, the state constraints present some challenges. We will use Lavrentiev regularisation to handle the state constraints. The Lavrentiev regularisation replaces the state constraint by a mixed state-control constraint. For this we introduce an additional control variable $v : \Omega \times [0,\infty) \to \mathbb{R}$ defined on the whole domain. This control variable will also be penalized in the cost functional, and so the cost functional is modified to

$$\begin{aligned}\min_{u,v} J(y,u,v) =& \frac{1}{2}\int_\Omega (y(x,T) - y_\Omega(T,x))^2 \, dx + \frac{1}{2}\int_0^T \int_\Omega (y(x,t) - y_\Omega(t,x))^2 \, dx \, dt \\ & \frac{\sigma}{2}\int_0^T \int_\Omega (v(x,t))^2 \, dx \, dt + \frac{\lambda}{2}\int_0^T \int_\Gamma (u(x,t))^2 \, ds \, dt\end{aligned}$$

The state constraint is replaced by the auxiliary control constraint

$$\begin{aligned} & \underline{y}(x,t) \le y(x,t) + \varepsilon v(x,t) \le \overline{y}(x,t) \\ \Leftrightarrow & \underbrace{\frac{1}{\varepsilon}(\underline{y}(x,t) - y(x,t))}_{\underline{v}(x,t)} \le v(x,t) \qquad \le \underbrace{\frac{1}{\varepsilon}(\overline{y}(x,t) - y(x,t))}_{\overline{v}(x,t)}\end{aligned}$$

This kind of optimal control problem (with both a control on the boundary and a control in the domain) is considered in [Tröltzsch, p.221ff]. We look at the general cost functional

$$\begin{aligned}\min_{y,u,v} J(y,u,v) = \int_\Omega \phi(x, y(T)) \, dx + \int\int_Q \varphi(x,t,y,v) \, dx \, dt \\ + \int\int_\Sigma \psi(x,t,y,u) \, ds \, dt\end{aligned}$$

subject to

$$\begin{aligned} y_t - \alpha\Delta y + d(x,t,y,v) = 0 \quad & \text{in } Q \\ \partial_n y + b(x,t,y,u) = 0 \quad & \text{in } \Sigma \\ y(\cdot,0) = y_0 \quad & \text{on } \Omega \\ v_a(x,t) \le v(x,t) \le v_b(x,t) \quad & \text{in } Q \\ u_a(x,t) \le u(x,t) \le u_b(x,t) \quad & \text{in } \Sigma\end{aligned}$$

In our case we have the following identities:

$$
\begin{aligned}
\phi(x, y(x,T)) &= \frac{1}{2}(y(x,T) - y_\Omega(x,T))^2 \\
\phi_y(x, y(x,T)) &= y(x,T) - y_\Omega(x,T)
\end{aligned}
$$

$$
\begin{aligned}
\varphi(x,t,y(x,t),v(x,t)) &= \frac{1}{2}(y(x,t) - y_\Omega(x,t))^2 + \frac{\sigma}{2}(v(x,t))^2 \\
\varphi_y(x,t,y(x,t),v(x,t)) &= y(x,t) - y_\Omega(x,t) \\
\varphi_v(x,t,y(x,t),v(x,t)) &= \sigma v(x,t)
\end{aligned}
$$

$$
\begin{aligned}
\psi(x,t,y(x,t),u(x,t)) &= \frac{\lambda}{2}(u(x,t))^2 \\
\psi_y(x,t,y(x,t),u(x,t)) &= 0 \\
\psi_u(x,t,y(x,t),u(x,t)) &= \lambda u(x,t)
\end{aligned}
$$

$$
\begin{aligned}
d(x,t,y(x,t),v(x,t)) &= 0 \\
d_y(x,t,y(x,t),v(x,t)) &= 0 \\
d_v(x,t,y(x,t),v(x,t)) &= 0
\end{aligned}
$$

$$
\begin{aligned}
b(x,t,y(x,t),u(x,t)) &= \frac{\gamma(x,t)}{\beta(x,t)}(y(x,t) - z(x,t)) \\
b_y(x,t,y(x,t),u(x,t)) &= \frac{\gamma(x,t)}{\beta(x,t)} \\
b_u(x,t,y(x,t),u(x,t)) &= -\frac{\gamma(x,t)}{\beta(x,t)}
\end{aligned}
$$

4 Derivation of the adjoint system

We introduce the adjoint states p_1 and p_2 to remove the PDE equality constraints. The Lagrangian for the problem is given by

$$
\begin{aligned}
\mathcal{L}(y,u,v,p_1,p_2) = &J(y,u,v) - \int_0^T \int_\Omega (\frac{\partial y}{\partial t} - \alpha \Delta y + d(x,t,y,v)) p_1 \, dx \, dt \\
&- \int_0^T \int_\Gamma (\partial_n y + b(x,t,y,u)) p_2 \, dx \, dt
\end{aligned}
$$

For optimality we need

$$
\begin{aligned}
D_y \mathcal{L}(\bar{y},\bar{u},\bar{v},p_1,p_2) y = 0, &\text{ for all } y \text{ with } y(\cdot,0) = 0 \\
D_u \mathcal{L}(\bar{y},\bar{u},\bar{v},p_1,p_2)(u - \bar{u}) \geq 0, &\qquad \text{for all } u \in U_{ad} \\
D_v \mathcal{L}(\bar{y},\bar{u},\bar{v},p_1,p_2)(v - \bar{v}) \geq 0, &\qquad \text{for all } v \in V_{ad}
\end{aligned}
$$

In the following we compute $D_y\mathcal{L}$, $D_u\mathcal{L}$ and $D_v\mathcal{L}$. We start with $D_y\mathcal{L}$:

$$\begin{aligned} D_y\mathcal{L}(y,u,v,p_1,p_2)h =& D_yJ(y,u,v)h - \int_0^T \int_\Omega (\frac{\partial h}{\partial t} - \alpha\Delta h + d_y(x,t,y,v)h)p_1 \, dx \, dt \\ & - \int_0^T \int_\Gamma (\partial_n h + b_y(x,t,y,u)h)p_2 \, dx \, dt, \end{aligned}$$

where for $D_yJ(y,u,v)$ it holds that

$$D_yJ(y,u,v)h = \int_\Omega \phi_y(x,y)h(T)\, dx + \int_0^T \int_\Omega \varphi_y(x,t,y,v)h \, dx \, dt + \int_0^T \int_\Gamma \psi_y(x,t,y,u)h \, ds \, dt. \tag{11}$$

First we consider the term

$$\begin{aligned} & - \int_0^T \int_\Omega (\frac{\partial h}{\partial t} - \alpha\Delta h + d_y(x,t,y,v)h)p_1 \, dx \, dt \\ & = - \int_\Omega \int_0^T \frac{\partial h}{\partial t} p_1 \, dx \, dt + \int_0^T \int_\Omega \alpha \Delta h p_1 \, dx \, dt - \int_0^T \int_\Omega d_y(x,t,y,v)hp_1 \, dx \, dt. \end{aligned}$$

Using partial integration (in time) for the first term and Green's second formula (in space) for the second term we obtain

$$\begin{aligned} & - \int_\Omega \int_0^T \frac{\partial h}{\partial t} p_1 \, dx \, dt + \alpha \int_0^T \int_\Omega \Delta h p_1 \, dx \, dt - \int_0^T \int_\Omega d_y(x,t,y,v)hp_1 \, dx \, dt \\ =& - \int_\Omega [hp_1]_0^T \, dx + \int_\Omega \int_0^T \frac{\partial p_1}{\partial t} h \, dx \, dt + \alpha \int_0^T \int_\Omega \Delta p_1 h \, dx \, dt \\ & + \alpha \int_0^T \int_\Gamma p_1 \frac{\partial h}{\partial n} \, ds \, dt - \alpha \int_0^T \int_\Gamma \frac{\partial p_1}{\partial n} h \, ds \, dt - \int_0^T \int_\Omega d_y(x,t,y,v)p_1 h \, dx \, dt \\ =& \int_\Omega p_1(0)h(0) \, dx - \int_\Omega p_1(T)h(T) \, dx + \int_0^T \int_\Omega \frac{\partial p_1}{\partial t} h \, dx \, dt + \alpha \int_0^T \int_\Omega \Delta p_1 h \, dx \, dt \\ & + \alpha \int_0^T \int_\Gamma p_1 \frac{\partial h}{\partial n} \, ds \, dt - \alpha \int_0^T \int_\Gamma \frac{\partial p_1}{\partial n} h \, ds \, dt - \int_0^T \int_\Omega d_y(x,t,y,v)p_1 h \, dx \, dt \\ \overset{h(0)=0}{=}& - \int_\Omega p_1(T)h(T) \, dx + \int_\Omega \int_0^T \frac{\partial p_1}{\partial t} h \, dx \, dt + \alpha \int_0^T \int_\Omega \Delta p_1 h \, dx \, dt \\ & + \alpha \int_0^T \int_\Gamma p_1 \frac{\partial h}{\partial n} \, ds \, dt - \alpha \int_0^T \int_\Gamma \frac{\partial p_1}{\partial n} h \, ds \, dt - \int_0^T \int_\Omega d_y(x,t,y,v)p_1 h \, dx \, dt \end{aligned}$$

In the last step we used that $h(0) = 0$. This is explained in [Tröltzsch, p.96] and follows from a substitution $y := y - \bar{y}$ for the state.
By substituting the above equation in the original equation and ordering by integration

domains we obtain

$$
\begin{aligned}
D_y J(y,u,v)h &= \int_\Omega (\phi_y(x,y) - p_1(T))h(T)\,dx \\
&+ \int_0^T \int_\Omega (\frac{\partial p_1}{\partial t} + \alpha\Delta p_1 - d_y(x,t,y,v)p_1 + \varphi_y(x,t,y,v))h\,dx\,dt \\
&+ \int_0^T \int_\Gamma (\alpha p_1 - p_2)\frac{\partial h}{\partial n}\,ds\,dt \\
&+ \int_0^T \int_\Gamma (-\alpha\frac{\partial p_1}{\partial n} - b_y(x,t,y,u)p_2 + \psi_y(x,t,y,u))h\,ds\,dt
\end{aligned}
$$

Now we make special choices of h, first $h \in C_0^\infty(Q)$, then with arbitrary $h(T)$, arbitrary $h|_\Sigma$ and finally with arbitrary $\frac{\partial h}{\partial n}$. From this we obtain the following adjoint equation:

$$
\begin{aligned}
-p_{1,t} - \alpha\Delta p_1 + d_y(x,t,\bar{y},\bar{v})p_1 &= \varphi_y(x,t,\bar{y},\bar{v}) \quad \text{in } Q \\
\alpha\partial_n p_1 + b_y(x,t,\bar{y},\bar{u})p_2 &= \psi_y(x,t,\bar{y},\bar{u}) \quad \text{in } \Sigma \\
\alpha p_1 &= p_2 \quad \text{in } \Sigma \\
p_1(x,T) &= \phi_y(x,\bar{y}(x,T)) \text{ in } \Omega
\end{aligned}
\tag{12}
$$

By setting $p := p_1$, $p_2 = \alpha p$ we obtain:

$$
\begin{aligned}
-p_t - \alpha\Delta p + d_y(x,t,\bar{y},\bar{v})p &= \varphi_y(x,t,\bar{y},\bar{v}) \quad \text{in } Q \\
\partial_n p + b_y(x,t,\bar{y},\bar{u})p &= \frac{1}{\alpha}\psi_y(x,t,\bar{y},\bar{u}) \text{ in } \Sigma \\
p(x,T) &= \phi_y(x,\bar{y}(x,T)) \text{ in } \Omega
\end{aligned}
\tag{13}
$$

A similar result (but without the diffusion coefficient α) can be found in [Tröltzsch, p.225f].
Finally we also compute $D_u\mathcal{L}$ and $D_v\mathcal{L}$:

$$
\begin{aligned}
D_u\mathcal{L}(y,u,v,p)h &= D_u J(y,u,v)h - \int_0^T \int_\Gamma b_u(x,t,y,u)ph\,ds\,dt \\
&= \int_0^T \int_\Gamma (\psi_u(x,t,y,u) - b_u(x,t,y,u)p)h\,ds\,dt
\end{aligned}
$$

$$
\begin{aligned}
D_v\mathcal{L}(y,u,v,p)h &= D_v J(y,u,v)h - \int_0^T \int_\Omega d_v(x,t,y,v)ph\,dx\,dt \\
&= \int_0^T \int_\Omega (\varphi_v(x,t,y,v) - d_v(x,t,y,v)p)h\,dx\,dt
\end{aligned}
$$

5 Weak form of the adjoint system

To derive the weak form of the adjoint system (13) we first note that the equation evolves backward in time. To get a forward equation we use the substitution $\tau := T - t$. Define

$$
\begin{aligned}
\tilde{p}(x,\tau) &:= p(x,T-\tau) = p(x,t) \\
\tilde{y}(x,\tau) &:= y(x,T-\tau) \\
\tilde{u}(x,\tau) &:= u(x,T-\tau) \\
\tilde{v}(x,\tau) &:= v(x,T-\tau)
\end{aligned}
$$

Noting that $D_\tau \tilde{p}(x,\tau) = -D_t p(x,t)$, the adjoint system changes to

$$\begin{aligned} \tilde{p}_\tau - \alpha\Delta\tilde{p} + d_y(x, T-\tau, \tilde{y}, \tilde{v})\tilde{p} &= \varphi_y(x, T-\tau, \tilde{y}, \tilde{v}) \quad \text{in } Q \\ \partial_n \tilde{p} + b_y(x, T-\tau, \tilde{y}, \tilde{u})\tilde{p} &= \frac{1}{\alpha}\psi_y(x, T-\tau, \tilde{y}, \tilde{u}) \text{ in } \Sigma \\ \tilde{p}(x,0) &= \phi_y(x, \tilde{y}(x,0)) \qquad \text{in } \Omega \end{aligned} \tag{14}$$

Now the system can be solved again using backward Euler. Replace $\tilde{p}_\tau$ by $\frac{\tilde{p}_{k+1}-\tilde{p}_k}{h}$ and $\tilde{p}$, $\tilde{y}$, $\tilde{u}$ and $\tilde{v}$ by their discrete counterparts. We multiply with the test function v and integrate:

$$\int_\Omega \frac{\tilde{p}_{k+1}-\tilde{p}_k}{h} v\ dx - \int_\Omega \alpha\Delta\tilde{p}_{k+1} v\ dx + \int_\Omega d_y(x, T-\tau_k, \tilde{y}_k, \tilde{v}_k)\tilde{p}_{k+1} v\ dx = \int_\Omega \varphi_y(x, T-\tau_k, \tilde{y}_k, \tilde{v}_k) v\ dx$$

Using partial integration on the second integral and inserting the boundary condition yields

$$\begin{aligned} \int_\Omega \alpha\Delta\tilde{p}_{k+1} v\ dx &= -\int_\Gamma \alpha\frac{\partial\tilde{p}_{k+1}}{\partial n} v ds + \alpha\int_\Omega \nabla\tilde{p}_{k+1}\nabla v\ dx \\ &= \int_\Gamma \alpha b_y(x, T-\tau_k, \tilde{y}_k, \tilde{u}_k)\tilde{p}_{k+1} v\ ds - \int_\Gamma \psi_y(x, T-\tau_k, \tilde{y}_k, \tilde{u}_k) v\ ds \\ &+ \alpha\int_\Omega \nabla\tilde{p}_{k+1}\nabla v\ dx \end{aligned}$$

We insert this in the first equation again and order by integration domain

$$\begin{aligned} \int_\Omega \Big(\frac{\tilde{p}_{k+1}-\tilde{p}_k}{h} &+ d_y(x, T-\tau_k, \tilde{y}_k, \tilde{v}_k)\tilde{p}_{k+1} - \varphi_y(x, T-\tau_k, \tilde{y}_k, \tilde{v}_k)\Big) v + \alpha\nabla\tilde{p}_{k+1}\nabla v dx \\ &+ \int_\Gamma \big(\alpha b_y(x, T-\tau_k, \tilde{y}_k, \tilde{u})\tilde{p}_{k+1} - \psi_y(x, T-\tau_k, \tilde{y}_k, \tilde{u}_k)\big) v\ ds = 0 \end{aligned}$$

After the modified adjoint system was solved we get the original adjoint by substituting back $p(x,t_k) = \tilde{p}(x,\tau_k)$.

5.1 Adjoint equation for our case

In our case the equation simplifies to:

$$\int_\Omega \Big(\frac{\tilde{p}_{k+1}-\tilde{p}_k}{h} - (\tilde{y}_k - \tilde{y}_{\Omega,k})\Big) v + \alpha\nabla\tilde{p}_{k+1}\nabla v\ dx + \int_\Gamma \frac{\alpha\gamma}{\beta}\tilde{p}_{k+1} v\ ds = 0$$

Additionally, we have the initial condition:

$$\tilde{p}_0 = \phi_y(x, \tilde{y}(x,0)) = y_N - y_{\Omega,N}$$

Rewriting (without the time substitution for y) and inserting the different boundaries Γ_{out} and Γ_c:

$$\begin{aligned} \int_\Omega \Big(\frac{\tilde{p}_{k+1}-\tilde{p}_k}{h} &- (y_{N-k} - y_{\Omega,N-k})\Big) v + \alpha\nabla\tilde{p}_{k+1}\nabla v\ dx \\ +\alpha\int_{\Gamma_{out}} \frac{\gamma_{out}}{\beta}\tilde{p}_{k+1} v\ ds &+ \alpha\int_{\Gamma_c} \frac{\gamma_c}{\beta}\tilde{p}_{k+1} v\ ds = 0, \\ &\qquad \text{for } k \in \{0, \ldots, N-1\}. \end{aligned}$$

6 Solution by Projected Gradient Method

Let $N \in \mathbb{N}$ be the MPC horizon and let $u^n := (u_0^n, u_1^n, \dots, u_{N-1}^n)$, $v^n := (v_0^n, v_1^n, \dots, v_{N-1}^n)$ be the iterates of the optimization algorithm.
The gradient of the reduced cost functional $f(v,u) = J(y(v,u), v, u)$ is given by

$$\begin{aligned} f'(v^n, u^n)(v,u) = & \int\int_Q (\varphi_v(x,t,y^n,v^n) - d_v(x,t,y^n,v^n)p^n)\ v\ dx\ dt \\ & + \int\int_\Sigma (\psi_u(x,t,y^n,u^n) - b_u(x,t,y^n,u^n)p^n)\ u\ ds\ dt \end{aligned}$$

This can also be found in [Tröltzsch, p. 243f], for the special case of $d(x,t,y,v) = v$, $b(x,t,y,u) = u$.

Solution algorithm:

1. Solve forward system for given $(u^n, v^n) \rightsquigarrow y_n$

2. Solve adjoint system $\rightsquigarrow p^n$

3. Descent directions

$$\begin{aligned} h^n &:= -(\varphi_v(\cdot, y^n, v^n) - d_v(\cdot, y^n, v^n)p^n) \\ r^n &:= -(\psi_u(\cdot, y^n|_\Sigma, u^n) - b_u(\cdot, y^n, u^n)p^n|_\Sigma) \end{aligned}$$

4. Compute step size $\rightsquigarrow s^n$ (e.g. use $\min_{s>0} f(\mathbb{P}_V(v^n + sh^n), \mathbb{P}_U(u^n + sr^n))$.

5. New iterates:

$$(v^{n+1}, u^{n+1}) := (\mathbb{P}_V(v^n + s^n h^n), \mathbb{P}_U(u^n + s^n r^n)) \tag{15}$$

6.1 Gradient in our case

$$\begin{aligned} f'(v^n, u^n)(v,u) = & \int\int_Q (\sigma v^n)\ v\ dx\ dt \\ & + \int\int_\Sigma (\lambda u^n) + \frac{\gamma}{\beta} p^n)\ u\ ds\ dt \end{aligned}$$

7 Solver Options/Preconditioning

Reference