Implicit Taylor Methods with Truncated PCG Cycles for Solving Semi-Discrete Parabolic Problems

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1. Linear Initial Value Problems with Jumps in Data

Considered are specific linear initial value problems of the type

\[ w'(t) = Aw(t) + f(t), \quad t \in (0, T], \quad w(0) = g \]

with:

\( A \) - symmetric, negative definite, \( f : (0, T] \to \mathbb{R}^N \), \( g \in \mathbb{R}^N \).

In particular, we study the case of \( f \) being sufficiently smooth in each interval of some given time grid

\[ 0 = t^0 < t^1 < \cdots < t^{M_c-1} < t^{M_c} = T, \]

but may have jumps at grid points. An important class with this property form semi-discrete parabolic control problems with piecewise constant controls.
Consider the parabolic initial boundary value problem

\[
\frac{\partial w}{\partial t} - \Delta w = f \quad \text{in} \quad Q := \Omega \times (0, T],
\]
\[
\gamma_D w + \frac{\partial w}{\partial n} = u \quad \text{on} \quad \Gamma_T := \Gamma \times (0, T],
\]
\[
w(\cdot, 0) = 0 \quad \text{on} \quad \overline{\Omega},
\]

\[\Omega \subset \mathbb{R}^2 - \text{bounded domain with piecewise Lipschitz boundary } \Gamma,\]

\[T > 0 - \text{fixed; } \gamma_D \geq 0 - \text{given coefficient, } f \in L^\infty(Q), u \in L^\infty(\Gamma_T).\]

Boundary conditions in (2) are natural ones.
There exists a unique weak solution
\[ w(\cdot, \cdot) \in W(0, T) \cap C(Q) \]
of (2) satisfying the variational equation
\[
\int_Q \frac{\partial w}{\partial t} \varphi dQ + \int_Q \nabla w \circ \nabla \varphi dQ + \gamma_D \int_{\Gamma_T} w \varphi d\Gamma_T
= \int_Q f \varphi dQ + \int_{\Gamma_T} u \varphi d\Gamma_T \quad \forall \varphi \in V := L_2(0, T; H^1(\Omega))
\]
and \( w(\cdot, 0) = 0 \), where \( W(0, T) := \{ v \in V : \frac{\partial v}{\partial t} \in V^* \} \), for a given \( u \in U := L^\infty(\Gamma_T) \) see e.g. Casas[97], Raymond/Zidani[99].

We apply semi-discretization in space (MOL) with piecewise linear triangular finite elements and mass-lumping to (3).

To avoid additional errors assume \( \Omega \) to be a polyhedron and discretizations take into account the sub-structuring of its boundary \( \Gamma \). Furthermore, spatial discretization \( u \in U \) relates to macro-elements of the triangulation.
Let $\Omega$ be covered by triangles (under standard assumptions of FEM) with related grid points and Lagrange piecewise linear basis functions denoted by

$$x_j \quad \text{and} \quad \varphi_j \in C(\bar{\Omega}), \ j = 1, \ldots, N$$

respectively. Let $V_h := \text{span} \{ \varphi_i \}_{i=1}^N \subset H^1(\Omega)$ and corresponding $W_h(0, T)$ with

$$w_h \in W_h \iff w_h(\cdot, t) = \sum_{j=1}^{N} w_j(t) \varphi_j, \ t \in [0, T].$$

FEM semi-discretization with trapezoidal rule mass lumping, i.e.

$$(4) \quad \int_{\Omega} \varphi_j \varphi_j \, d\Omega \approx (\varphi_j, \varphi_i)_{\mu} := \mu_i \delta_{ij}, \ i, j = 1, \ldots, N$$

with $\mu_i := \sum_{j=1}^{N} \int_{\Omega} \varphi_j \varphi_i \, d\Omega$ applied to (3) yields the IVP
\[(5) \quad \mathbf{D} \mathbf{w}'(t) = \mathbf{A}\mathbf{w}(t) + \mathbf{f}(t; \mathbf{u}), \quad t \in (0, T], \quad \mathbf{w}(0) = \mathbf{0}. \]

\[\mathbf{w} = (w_1, \ldots, w_N) : [0, T] \rightarrow \mathbb{R}^N \text{ - coordinate functions of } w_h,\]

\[\mathbf{A} := (a_{ij})_{i,j=1}^N \text{ - stiffness matrix, i.e.}\]

\[a_{ij} := - \int_{\Omega} \nabla \varphi_j \circ \nabla \varphi_i \, d\Omega - \int_{\Gamma} \gamma_D \varphi_j \varphi_i \, d\Gamma, \quad i, j = 1, \ldots, N,\]

\[\mathbf{D} := \text{diag}(\mu_i) \text{ - lumped mass matrix, } \quad \mathbf{f} := (f_i)_{i=1}^N \text{ defined by}\]

\[f_i(t; \mathbf{u}) := \int_{\Omega} f(x, t) \varphi_i(x) \, d\Omega + \int_{\Gamma} u(x, t) \varphi_i(x) \, d\Gamma, \quad i = 1, \ldots, N.\]
Existence and uniqueness for (5) is covered by standard theory and piecewise defined solutions.

Transformation $D^{1/2}w$ and renaming all modified matrices and functions by their former names, (5) is equivalent to the IVP

$$w'(t) = Aw(t) + f(t), \quad t \in (0, T], \quad w(0) = 0$$

with a symmetric, negative definite $A$.

Discretization of control space $U$ over a given time grid

$$0 = t^0 < t^1 < \cdots < t^{M^c-1} < t^{M^c} = T$$

by $P_{0, \rho} \subset U$ with

$$u^\rho \in P_{0, \rho} \iff u^\rho(\cdot, t) = u^k(\cdot), \forall t \in (t^{k-1}, t^k]$$

with $u^k \in L^\infty(\Gamma), k = 1, \ldots, M^c$. 
Piecewise solving of the IVP over subintervals yields

\[ w'(t) = Aw(t) + f(t; u^k), \quad t \in (t^{k-1}, t^k], \]
\[ w(t^{k-1} + 0) = w(t^{k-1}), \quad k = 1, \ldots, M^C. \]

(8)

For time integration we study implicit Taylor methods (cf. CGHKPS[96], Scholz[98]) applied to each interval of (8).

Consider the first step \((t^0, t^1]\), i.e. from \(t = 0\) to \(t = \tau \leq t^1\).

The solution \(w\) of (1) (equivalent to (8)) in \([0, \tau]\) is approximated in ITM-\(q\) by \(w_\tau(\cdot)\) which is of the form

\[ w_\tau(t) = \sum_{j=0}^{q} \frac{\alpha_j}{j!} (\tau - t)^j, \quad t \in [0, \tau]. \]

(9)

\(q \in \mathbb{N}\) is fixed parameter of ITM.
The Coefficients $\alpha_j \in \mathbb{R}^N$, $j = 0, 1, \ldots, q$, are uniquely determined by

\begin{align*}
    w_\tau(0) &= w_0 \\
    w_\tau(\tau) &= w_0 + \int_0^\tau \left( [A w_\tau](t) + f(t) \right) dt
\end{align*}

(10)

and the conditions for the derivatives

\begin{align*}
    w^{(j)}_\tau(\tau) &= A^j w_\tau(\tau) + \sum_{l=0}^{j-1} A^{j-1-l} f^{(l)}(\tau), \quad j = 1, \ldots, q - 1,
\end{align*}

(11)

where due to (1) the initial vector $w_0 \in \mathbb{R}^N$ with $w_0 = g$ is chosen.

Implicit Taylor method (9) - (11) is denoted by ITM-$q$. 
After eliminating the $\alpha_j$ this yields (cf. G/H[00]) for $w_1$ the linear system

\[
\begin{align*}
(12) \quad & \left( I + \sum_{j=0}^{q-1} \frac{(-1)^j}{j!} \left( \frac{1}{q+1} - \frac{1}{j+1} \right) \tau^{j+1} A^{j+1} \right) w_1 = \left( I + \frac{\tau}{q+1} A \right) w_0 \\
& + \sum_{j=1}^{q-1} \frac{(-1)^j \tau^{j+1}}{j!} \left( \frac{1}{j+1} - \frac{1}{q+1} \right) \sum_{i=0}^{j-1} A^{j-1} f(t) (\tau) + \int_0^\tau f(t) \, dt.
\end{align*}
\]

By application to each of the following intervals the $w_j \approx w(t_j)$, $j = 1, \ldots, N$, are recursively generated.
By means of

\[
B := I + \sum_{j=0}^{q-1} \frac{(-1)^j}{j!} \left( \frac{1}{q+1} - \frac{1}{j+1} \right) \tau^{j+1} A^{j+1},
\]

\[
S := I + \frac{\tau}{q+1} A
\]

\[
Rf := \sum_{j=1}^{q-1} \frac{(-1)^j \tau^{j+1}}{j!} \left( \frac{1}{j+1} - \frac{1}{q+1} \right) \sum_{l=0}^{j-1} A^{j-l} f^{(l)},
\]

IPM-\(q\) over a discretization grid \(\{t_k\} \subset \{t^j\}\) can be described by the recursive equations

\[
Bw_k = Sw_{k-1} + [Rf](t_k) + \int_{t_{k-1}}^{t_k} f(t) \, dt, \quad k = 1, \ldots, M
\]

(13)

\[
w_0 = g.
\]
Remark 1 In general, to limit the reduction of sparsity in (12) we focus on the cases \( q = 1, 2, 3 \). Observe that \( q = 1 \) corresponds to a Crank-Nicolson-like method, and \( q = 2 \) is ETF as proposed by Chawla/Al-Zanaidi[99].

ITM-\( q \) is A-stable for \( q = 1, 2, 3 \) and L-stable for \( q = 2, 3 \).

Theorem 1 Let be given a function \( f \) which is sufficiently smooth on each of the subintervals \((t^{j-1}, t^j], \ j = 1, \ldots, M^c\). Then ITM-\( q \) applied to (1) is convergent with order \( q + 1 \).

Sketch of the proof:

Notice that (12) is equivalent to

\[
\begin{align*}
\left( I + \sum_{j=0}^{q} \frac{(-1)^j}{j!} \left( \frac{1}{q+1} - \frac{1}{j+1} \right) \tau^{j+1} A^{j+1} \right) w_1 &= \left( I + \frac{\tau}{q+1} A \right) w_0 \\
+ \sum_{j=1}^{q} \frac{(-1)^j \tau^{j+1}}{j!} \left( \frac{1}{j+1} - \frac{1}{q+1} \right) \sum_{l=0}^{j-1} A^{j-l} f^{(l)}(\tau) + \int_{0}^{\tau} f(t) \, dt.
\end{align*}
\]
Now, replacing $w_\tau$ by the exact solution $w$ of (8), using Taylor expansion and $w(\tau) = e^{A\tau}w_0 + \int_0^\tau e^{A(\tau-s)}f(s)\,ds$ we obtain for the left-hand side

\[
\left(I + \sum_{j=0}^q \frac{(-1)^j}{j!} \left( \frac{1}{q+1} - \frac{1}{j+1} \right)^{\tau} A^{j+1} \right)w(\tau)
\]

\[
= \left( I + \frac{\tau}{q+1} A \right) w_0 + r_q + \left( I + \frac{\tau}{q+1} A \right) \int_0^\tau e^{-As} f(s)\,ds
\]

with

\[
r_q = \frac{(-1)^q \tau^{q+2}}{(q+2)!} \frac{A^{q+2} w(\tau) + O(\tau^{q+3})}{q+1}
\]
By easy calculations it follows

\[
\left( I + \frac{\tau}{q+1} A \right) \int_0^\tau e^{-As} f(s) \, ds
\]

\[
= \int_0^\tau f(s) \, ds + \sum_{j=1}^{q} \tau^{j+1} \frac{(-1)^j}{j!} \left( \frac{1}{j+1} - \frac{1}{q+1} \right) \sum_{l=0}^{j-1} A^j \frac{(-1)^l}{l!} f(l)(\tau) + s_q,
\]

with

\[
s_q = \frac{(-1)^{q+1}}{(q+2)!} \left( A^{q+1} f(\tau) - f^{(q+1)}(\tau) \right) \tau^{q+2}.
\]

Thus for the defect (local consistency) in ITM-\( q \) it holds

\[
d_1 = r_q + s_q
\]

\[
= \frac{(-1)^q}{(q+2)!} \left( \frac{1}{q+1} A^{q+2} w(\tau) - A^{q+1} f(\tau) + f^{(q+1)}(\tau) \right) \tau^{q+2} + O(\tau^{q+3})
\]

With the known stability of one-step methods this proves the assertion. ■
**Remark 2** One should be aware that $\tau^{q+2} A^{q+2}$ and consequently $\left( \frac{\tau}{h^2} \right)^{q+2}$ occurs in the error term. In case of smooth data this effect will be compensated by the smoothness of the solution - not so for nonsmooth data.
2. Efficient Numerical Realization of ITM

In each step of ITM-$q$ (13) linear systems have to be solved. The related coefficient matrix $B$ for $q = 2$ and $q = 3$ has the form

$$B_2 := B = I - \frac{2}{3} \tau A + \frac{1}{6} \tau^2 A^2$$

and

$$B_3 := B = I - \frac{3}{4} \tau A + \frac{1}{4} \tau^2 A^2 - \frac{1}{24} \tau^3 A^3,$$

respectively. Hence, appropriate methods that avoid reduction of sparsity should be applied to (13). The method of choice is PCG with preconditioners of the type

$$P_q := \prod_{j=1}^{q} (I - \sigma_j \tau A), \quad q = 2, 3$$

with appropriately chosen constants $\sigma_j > 0, j = 1, \ldots, q$. 
These matrices provide excellent spectral bounds independent of the discretization parameters $h, \tau > 0$ provided they satisfy the condition

\begin{equation}
\prod_{j=1}^{q} \sigma_j = \frac{1}{q(q+1)},
\end{equation}

that will be supposed.

**Theorem 2** Independently of the discretization parameters $h > 0$ and $\tau > 0$ for

\begin{equation}
c_2 := c_2(\sigma_1, \sigma_2) = \frac{6 + 2\sqrt{6}}{6 + 3\sqrt{6}(\sigma_1 + \sigma_2)}
\end{equation}

we have

\begin{equation}
c_2 \mathbf{v}^T \mathbf{P}_2 \mathbf{v} \leq \mathbf{v}^T \mathbf{B}_2 \mathbf{v} \leq \mathbf{v}^T \mathbf{P}_2 \mathbf{v}, \quad \forall \mathbf{v} \in \mathbb{R}^N.
\end{equation}

Moreover, the constant is optimal, i.e. maximal, in case of $\sigma_1 = \sigma_2 = \frac{1}{\sqrt{6}}$. 
The proof bases on the generalized symmetric eigenvalue problem

\[ B_2 v = \nu P_2 v, \quad v \neq 0. \] (20)

Its eigenvalues can be expressed by

\[ \nu = \frac{1 - \frac{2}{3} \tau \lambda + \frac{1}{6} (\tau \lambda)^2}{(1 - \sigma_1 \tau \lambda)(1 - \sigma_2 \tau \lambda)}, \]

where \( \lambda \) denotes any eigenvalue of \( A \). By straightforward calculations this yields the stated bounds.

The optimal preconditioning for \( q = 2 \) is obtained for \( \sigma_1 = \sigma_2 = 1/\sqrt{6} \), i.e.

\[ P_2 = (I - \frac{1}{\sqrt{6}} \tau A)^2. \] (21)

In the case \( q = 3 \) we concentrate upon the preconditioner

\[ P_3 = (I - \frac{1}{\sqrt{24}} \tau A)^3. \] (22)
Similar to $q = 2$, by elementary calculus we obtain

\begin{equation}
(23) \quad c_3 \, v^T P_3 \, v \leq v^T B_3 \, v \leq v^T P_3 \, v, \quad \forall \, v \in \mathbb{R}^N
\end{equation}

with $c_3 \approx 0.7803$.

In both cases $q = 2, 3$, the estimates (19) and (23), respectively, guarantee that the PCG-method applied to the linear system

\begin{equation}
(24) \quad B \, v = b
\end{equation}

with $B = B_q$ and $b$ the right-hand side of ITM-$q$ with the preconditioner $P = P_q$ generate approximations $v^l \in \mathbb{R}^N$, $l = 1, 2, \ldots$ of the solution $v$. There holds the estimate

\begin{equation}
(25) \quad \|v^l - v\|_{P^{-1}B} \leq 2 \left(\frac{1 - \sqrt{c_q}}{1 + \sqrt{c_q}}\right)^l \|v^0 - v\|_{P^{-1}B}, \quad l = 1, 2, \ldots,
\end{equation}

where $\| \cdot \|_{P^{-1}B}$ is the related discrete energy norm.
This provides at least the estimate

\[(26) \quad \|v^l - v\|_{P^{-1}B} \leq 2\gamma^l \|v^0 - v\|_{P^{-1}B}, \quad l = 1, 2, \ldots\]

with \(\gamma \approx 0.024\) and \(\gamma \approx 0.062\) in the case \(q = 2\) and \(q = 3\), respectively.

If, as a rule, \(\tau/h^2 \gg 1\) then the convergence is even better because of

\[\lim_{s \to +\infty} \nu_q(s) = 1\]

and since this limit is reached rather rapidly.

This effect on PCG-method is illustrated by the graphs of the functions

\[\gamma_q := \frac{1 - \sqrt{c_q}}{1 + \sqrt{c_q}}, \quad q = 2, 3.\]
Due to the rapid reduction of the error only a few iteration steps to solve problem (24) by PCG even up to high accuracy are needed.

Moreover, for systems generated by time discretization good starting iterates are available provided the solution does not change too rapidly. In addition, rapid changes correspond to a dominant influence of higher eigenvalues, but these are damped quite efficiently.
In computational experiments we further studied numerically the convergence behavior of ITM-2 with only one PCG step at each time level.

With a given initial guess \( v^0 \in \mathbb{R}^N \) this truncated version of PCG yields

\[
\tilde{v} = v^0 + \alpha p,
\]

where the search direction \( p \in \mathbb{R}^N \) and the step size \( \alpha > 0 \) are defined by

\[
p := P^{-1}d, \quad \alpha := \frac{p^T d}{p^T B p} \quad \text{with} \quad d := b - Bv^0.
\]

Taking into account that the preconditioning in ITM-2 satisfies \( P^{-1}B \approx I \) from (28) we obtain \( \alpha \approx 1 \). This suggests the following further simplification

\[
\tilde{v} = v^0 + P^{-1}(b - Bv^0).
\]
With the structure of $B = B_2$ and $P = P_2$ the new approximate solution $\tilde{v}$ of (24) is given as solution of the linear system

\begin{equation}
P \tilde{v} = b + \tau \left( \frac{2}{3} - \frac{2}{\sqrt{6}} \right) A v^0.
\end{equation}

Independently of the discretization parameters $h > 0$ and $\tau > 0$ for the spectral radius of the related iteration matrix we obtain the estimate

\begin{equation}
\rho(P^{-1}(P - B)) \leq \frac{1}{2} \left( 1 - \frac{\sqrt{6}}{3} \right) \approx 0.092.
\end{equation}

Hence, a remarkable improvement of an approximate solution of (24) is achieved. However, applying (30) to ITM-2 the order of convergence is reduced compared to the original ITM-2 method.

We apply the described realizations of ITM-2 and ITM-3 combined with different iterative solvers of the occurring linear systems to parabolic boundary control problems.
Quality of approximation of \( f(s) = \exp(-s) \) (black) by the considered schemes on medium ranges.

Fig. 3a: Euler, Crank-Nicolson, ITM-2, ITM-3, ITM-2, ITM-2s
Quality of approximation of $f(s) = \exp(-s)$ (black) by the considered schemes on long ranges.

Fig. 3b: Euler, Crank-Nicolson, ITM-2, ITM-3, ITM-2, ITM-2s
3. ITM Applied to Boundary Control in Heat Conduction

Consider the boundary heat control problem

\( J(u) := \frac{1}{2} \int_{\Omega} [w(x, T; u) - z(x)]^2 \, d\Omega + \frac{\alpha}{2} \int_{\Gamma_T} u(x, t)^2 \, d\Gamma_T \rightarrow \min \)

s.t. \( u \in U \) and \( w(\cdot, \cdot; u) \) defined by the state equations

\[
\frac{\partial w}{\partial t} - \Delta w = f \quad \text{in} \quad Q,
\]

\[
\gamma_D w + \frac{\partial w}{\partial n} = u \quad \text{on} \quad \Gamma_T,
\]

\[
w(\cdot, 0) = 0 \quad \text{on} \quad \overline{\Omega}.
\]

Assumptions on the data in (33) as before. \( \alpha > 0 \) - fixed regularization parameter; \( z \in L^2(\Omega) \) - target temperature at time \( T \).

References e.g. Ito/Kunisch[96], Sammon[83], Troeltzsch[94].
At first we consider FEM semi-discretization with mass-lumping as introduced above. This yields the approximate control problem
\begin{equation}
J_h(u) := \frac{1}{2}(w_h(\cdot, T) - z_h, w_h(\cdot, T) - z_h)_\mu + \frac{\alpha}{2} \int \int_{\Gamma_T} u(x, t)^2 \, d\Gamma_T \rightarrow \min!
\end{equation}

with \(w_h(\cdot, t) = \sum_{j=1}^{N} w_j(t) \varphi_j\) and \(w = (w_1, \ldots, w_N)\) solving the IVP
\begin{equation}
Dw'(t) = Aw(t) + f(t; u), \quad t \in (0, T], \quad w(0) = 0,
\end{equation}

where \(A\) and \(f\) are defined as before.

Further \(z_h \in V_h\) denotes the mass-lumping projection of \(z\) onto \(V_h\), i.e.
\[
(z_h, v_h)_\mu = (z, v_h)_{L^2(\Omega)} \quad \forall v_h \in V_h.
\]

Next we study the application of ITM-\(q\) to the semi-discrete optimal control problem (34).
Again, transformation $\tilde{w} := D^{1/2}w$ is applied to reduce the IVP to its explicit form.

ITM-$q$ generates the following full discretization scheme for the state equations.

(36)

$$
B \tilde{w}_k = S \tilde{w}_{k-1} + R(\tilde{f} + \tilde{u})(t_k) + \int_{t_{k-1}}^{t_k} (\tilde{f} + \tilde{u})(t) \, dt, \quad k = 1, \ldots, M
$$

$$
\tilde{w}_0 = 0,
$$

with $\tilde{f}, \tilde{u} : [0, T] \rightarrow \mathbb{R}^N$ defined by

$$
[\tilde{f}(t)]_i := \frac{1}{\mu_i} \int_{\Omega} f(x, t) \varphi_i(x) \, d\Omega,
$$

$$
[\tilde{u}(t)]_i := \frac{1}{\mu_i} \int_{\Gamma} u(x, t) \varphi_i(x) \, d\Gamma,
$$

i = 1, \ldots, N.
The obtained discrete optimal control problem is

\[
J_{h,\tau}(u) := \frac{1}{2} (\mathbf{w}_M - \mathbf{q}, \mathbf{w}_M - \mathbf{q})_\mu + \frac{\alpha}{2} \int_{\Gamma_T} u^2 d\Gamma_T \to \min
\]

subject to \ \tilde{\mathbf{w}}(\cdot; u) = D^{1/2}\mathbf{w}(\cdot; u) \text{ solution of (36)}.

**Remark 3** Choosing discrete controls that are piecewise constant on the considered grid \(\{t^j\}_{j=0}^{M_c}\) Problem (37) can be interpreted as a fully discrete problem that allows ITM-\(q\) to be applied. If, in addition, we restrict ourselves to the case that both \(f\) and \(u\) are constant in time w.r.t. each of the subintervals \((t_k-1, t_k], \ k = 1, \ldots, M\), then the operator \(R\) reduces to

\[
R := \sum_{j=1}^{q-1} \frac{(-1)^j \tau^{j+1}}{j!} \left( \frac{1}{j+1} - \frac{1}{q+1} \right) \tilde{A}^j,
\]

where according to the transformation we put \(\tilde{A} := D^{-1/2}AD^{-1/2}\).
Important for efficiency of gradient-based optimal control codes is that gradients can be evaluated without excessive numerical costs. For piecewise constant controls since the discrete state equations (36) are linear, it holds

\[
J'_{h,\tau}(u) s = (w_M - q, y_M)_{\mu} + \alpha \sum_{k=1}^{M_c} \tau^k \int_{\Gamma} u_k(x) s_k(x) \, d\Gamma
\]

where \( \tau^k := t^k - t^{k-1} \), \( \tilde{q} = D^{1/2}q \).
The corresponding to \( y_k, \quad k = 0, 1, \ldots, M \), transform \( \tilde{y} = D^{1/2} y \) satisfies

\[
B \tilde{y}_k = S \tilde{y}_{k-1} + R \tilde{s}(t_k) + \tau \tilde{s}(t_k) \, dt, \quad k = 1, \ldots, M \\
\tilde{y}_0 = 0.
\]

(39)

with \( \tilde{s} \) defined by

\[
[\tilde{s}(t)]_i := \frac{1}{\mu_i} \int_{\Gamma} \frac{1}{\gamma N} s(x,t) \varphi_i(x) \, d\Gamma, \quad i = 1, \ldots, N.
\]

The discrete adjoint system

\[
B^T \tilde{v}_{k-1} = S^T \tilde{v}_k, \quad k = M, M - 1, \ldots, 1, \\
S^T \tilde{v}_M = \tilde{w}_M - \tilde{z}
\]

(40)

and \( y_0 = 0 \) lead to

\[
\left( \tilde{w}_M - \tilde{z}, \tilde{y}_M \right) = \sum_{k=1}^{M} \left( \tilde{v}_{k-1}, R \tilde{s}(t_k) \right) + \tau \sum_{k=1}^{M} \left( \tilde{v}_{k-1}, \tilde{s}(t_k) \right).
\]
Hence,

\[
J'_{h,\tau}(u)s = \tau \sum_{k=1}^{M} \left( \tilde{v}_{k-1}, \tilde{s}(t_k) \right) + \sum_{k=1}^{M} \left( \tilde{v}_{k-1}, \mathbf{R}\tilde{s}(t_k) \right) + \alpha \sum_{k=1}^{M^c} \tau^k \int_{\Gamma} u_k(x) s_k(x) \, d\Gamma
\]

**Remark 4** Notice that ITM-\(q\) applied to the semi-discrete adjoint problem yields a system of the form

\[
B \tilde{p}_{i-1} = \mathbf{S} \tilde{p}_i, \quad i = M, M - 1, \ldots, 1 \quad \text{with} \quad \tilde{p}_M = \tilde{w}_M - \tilde{z}.
\]

Simple time integration for the derivative of \(J_h\) in the semi-discrete case leads to

\[
\hat{J}'_{h,\tau}(u)s = \tau \sum_{k=1}^{M} \left( \tilde{p}_k, \tilde{s}(t_k) \right) + \alpha \sum_{k=1}^{M^c} \tau^k \int_{\Gamma} u_k(x) s_k(x) \, d\Gamma,
\]

which differs from the discrete gradient. The additional term \(\sum_{k=1}^{M} (\tilde{v}_{k-1}, \mathbf{R}\tilde{s}(t_k))\) is of higher order and can be widely ignored for small step sizes.
4. Numerical Examples

Example 1

\( \Omega = (-1, 1) \times (-1, 1) \subset \mathbb{R}^2, \quad f \equiv 0, \quad \gamma_D = 1, \quad T = 1. \)

\( u \) along the boundary piecewise constant, either \( u = 1 \) or \( u = -1 \),
alternating w.r.t. subintervals of length 0.5 in space as well as in time.

Spatial uniform triangulation with totally 4225 grid points.

Time integration by Euler implicit, Crank-Nicolson and ITM-2. In all cases equidistant time steps \( \tau = 0.05 \).
Fig. 4: Heat distribution at $t=0.2$

Fig. 5: Behavior at $(-1, 0.0938)$
Example 2

Consider an anchor shaped domain $\Omega$ and $T = 1$. Further, no source term, i.e. $f \equiv 0$.

For the boundary conditions $\gamma_D = 5$ and the control

$$u(x, y) = \begin{cases} 0, & \text{if } y \geq 0.3, \\ -30, & \text{if } y < 0.3 \end{cases}$$

have been chosen.

The grid as given has been generated by the pde-toolbox from MATLAB.

Fig. 6: Anchor with grid
Fig. 7: Euler implicit, $t=0.2$
Fig. 8: Euler implicit, $t=0.4$
Fig. 9: Crank-Nicolson, t=0.2
Fig. 10: Crank-Nicolson, $t=0.4$
Fig. 11: ITM-2, $t=0.2$
Fig. 12: ITM-2, t=0.4
The following figure shows the behavior of Euler implicit, Crank-Nicolson and ITM for the large step size $\tau = 0.2$.

![Graph showing temperature at $(x, y) = (-0.2, 0.3)$](image)

**Fig. 13:** Temperature at $(x, y) = (-0.2, 0.3)$

All computations have been implemented in MATLAB, Version 6.5.
Summary and Outlook

- ITM-$_q$ are practically stable (damping of oscillations) for IVPs with nonsmooth data.
- Preconditioning is possible by matrices that keep sparsity in the LU-factorizations.
- Additional reduction of computational effort by using incomplete Cholesky factorization for the proposed preconditioners.
- Further studies for truncated PCG including its simplified version.
- Discrete adjoints are used to evaluate gradients. They differ from the application of ITM to the adjoint semi-discrete system.
- Optimal adjustment of control discretization and the spatial-time discretization of the state equations has to be studied.
- Bounds on controls and even on states should be incorporated.
Selected References