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Discrete Transparent Boundary Conditions for Parabolic Equations

Transparent boundary conditions for linear parabolic equations for a bounded domain can be derived under the assumption that the coefficients are constant on the exterior of that domain. In 1D these boundary conditions are non–local in time (of memory type). For the Crank–Nicolson finite difference scheme, discrete transparent boundary conditions are derived, and the resulting scheme is proved to be stable. The approach is closely related to [1].

1. Transparent Boundary Conditions for 1D Parabolic Equations

For simplicity of the presentation we restrict ourselves here to a constant coefficient parabolic equation in 1D:

$$u_t = a\,u_{xx} - b\,u_x - c\,u, \quad 0 < x < L, \quad t > 0, \tag{1}$$

with initial data $u^I(x)$ which is assumed to be compactly supported in $(0, L)$. Our goal is to design boundary conditions at $x = 0$, $x = L$, such that the resulting IBVP is well–posed and its solution coincides with the solution of the whole–space problem restricted to $(0, L)$. Such BC's are called *transparent boundary conditions (TBC)*.

The TBC at $x = 0$ is of the form $u_x(0, t) = (Tu)(0, t)$. For its derivation we consider the left exterior problem

$$v_t = a\,v_{xx} - b\,v_x - c\,v, \quad v(x, 0) = 0, \quad v(0, t) = u(0, t), \quad v(-\infty, t) = 0, \quad (Tu)(t) := v_x(0, t), \tag{2}$$

for $x < 0$ and couple it with (1) by the assumption that u, u_x are continuous across the artificial boundary at $x = 0$. Since the initial data vanishes for $x < 0$, we can solve (2) explicitly by the Laplace–method and obtain

$$\hat{u}_x(0, s) = \left(\frac{b}{2a} + \frac{1}{\sqrt{a}}\sqrt[+]{\eta + s}\right)\hat{u}(0, s), \quad \eta := \frac{b^2}{4a} + c \geq 0, \quad \text{Re}\sqrt[+]{\eta + s} > 0.$$

After the inverse Laplace transform the left TBC reads:

$$u_x(0, t) = \frac{b}{2a}\,u(0, t) + \frac{1}{\sqrt{a\pi}}\,e^{-\eta t}\frac{d}{dt}\int_0^t \frac{u(0, \tau)\,e^{\eta\tau}}{\sqrt{t - \tau}}\,d\tau, \tag{3}$$

and it is non–local in t (of memory type). The right TBC is derived similarly. Using the energy method one can easily show $\|u(., t)\|_{L^2(0,L)} \leq \|u^I\|_{L^2(0,L)}$, $t > 0$, and this implies uniqueness of the solution to the parabolic IBVP.

2. The Discrete Transparent Boundary Conditions

Next we shall address the question how to adequately discretize the analytic TBC (3) for a chosen full discretization of (1), which in this example will be the Crank–Nicolson finite difference scheme with the uniform grid points $x_j = j\Delta x$, $t_n = n\Delta t$, and the approximation $u_j^n \approx u(x_j, t_n)$:

$$\Delta_t^+ u_j^n = r\,\Delta_x^2 u_j^{n+\frac{1}{2}} - r\mathit{Pe}\,\Delta_x^0 u_j^{n+\frac{1}{2}} - 2\kappa\,u_j^{n+\frac{1}{2}}, \quad u_j^{n+\frac{1}{2}} := \frac{1}{2}(u_j^{n+1} + u_j^n), \quad \mathit{Pe} := \frac{b\Delta x}{2a}, \quad \kappa := \frac{c}{2}\Delta t, \tag{4}$$

where $r := a\,\Delta t/(\Delta x)^2$ denotes the (parabolic) mesh ratio. In order to avoid any numerical reflections at the boundary and to ensure unconditional stability of the resulting scheme we will construct discrete TBC's instead of choosing a heuristic discretization of (3).

We mimic the derivation from §1 on a discrete level, i.e. we assume $u_j^0 = 0$, $j \leq 1$ and solve the discrete left exterior problem, i.e. (4) for $j \leq 0$, by using the Z–transform: $\mathcal{Z}\{u_j^n\} = \hat{u}_j(z) := \sum_{n=0}^{\infty} u_j^n\,z^{-n}$, j fixed:

$$\hat{u}_j(z) = \alpha_1^{j+1}(z),\ j \leq 0, \quad \text{where} \quad \alpha_1(z) \quad \text{solves} \quad \alpha^2 - \frac{2}{1 - \mathit{Pe}}\left[1 + \frac{1}{r}\left(\frac{z-1}{z+1} + \kappa\right)\right]\alpha + \frac{1 + \mathit{Pe}}{1 - \mathit{Pe}} = 0,$$

and $|\alpha_1(z)| > 1$ since we need decreasing modes as $j \to -\infty$. We obtain the Z–transformed left discrete TBC as $\hat{u}_1(z) = \alpha_1(z)\,\hat{u}_0(z)$, and in a tedious calculation this can be inverse transformed explicitly. The discrete TBC's read:

$$(1-P_e)\,u_1^n = u_0^n * \ell_n = \sum_{k=1}^{n} u_0^k\,\ell_{n-k}, \quad (1+P_e)\,u_{J-1}^n = u_J^n * \ell_n = \sum_{k=1}^{n} u_J^k\,\ell_{n-k}, \quad n \ge 1, \tag{5}$$

$$\ell_n = \left(1 - \frac{1-\kappa}{r}\right)\delta_n^0 + \frac{2}{r}(-1)^n + \frac{1}{r}\,\frac{1}{\sqrt{(1+\kappa)^2 + 2r(1+\kappa) + r^2P_e^2}}\cdot$$

$$\cdot\left[-\left((1-\kappa)^2 - 2r(1-\kappa) + r^2P_e^2\right) f_n + 2(-1)^n \sum_{k=0}^{n} (-1)^k f_k + 2\left(\kappa^2 + 2r\kappa + r^2P_e^2\right)\sum_{k=0}^{n} f_k\right], \tag{6}$$

$$f_n := \lambda^{-n}\left[P_n(\mu) - \lambda\,P_{n-1}(\mu)\right] = Q_n(\mu) - Q_{n-1}(\mu), \quad \lambda := \frac{\sqrt{(1+\kappa)^2 + 2r(1+\kappa) + r^2P_e^2}}{\sqrt{(1-\kappa)^2 - 2r(1-\kappa) + r^2P_e^2}},$$

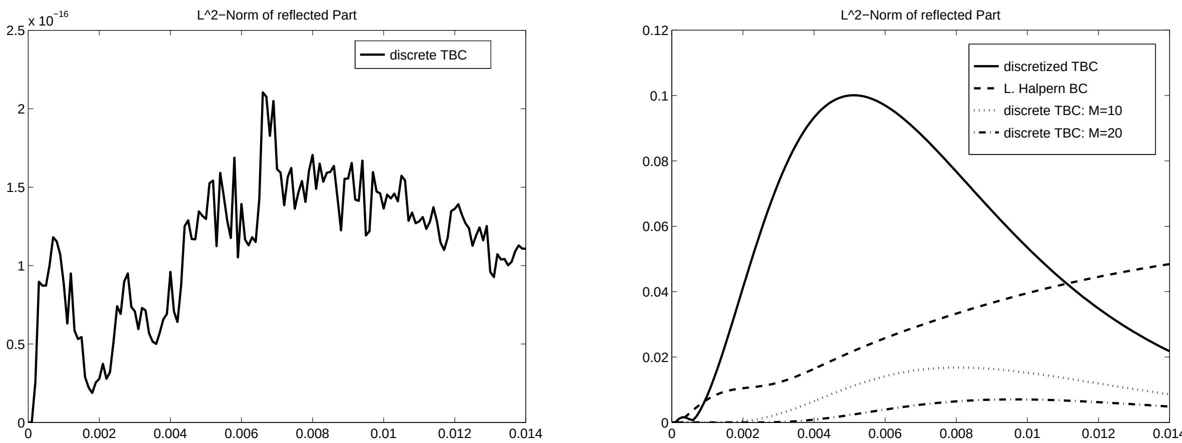
$$\mu := \frac{1 - \kappa^2 - 2r\kappa - r^2P_e^2}{\sqrt{(1+\kappa)^2 + 2r(1+\kappa) + r^2P_e^2}\,\sqrt{(1-\kappa)^2 - 2r(1-\kappa) + r^2P_e^2}}, \quad n \ge 0,$$

where $Q_n(\mu) := \lambda^{-n}P_n(\mu)$ denotes the "damped" Legendre polynomials ($Q_0 \equiv 1$, $Q_{-1} \equiv 0$) and δ_n^0 is the Kronecker symbol. Since the asymptotic behaviour $\ell_n \cong 4(-1)^n/r$ of the convolution coefficients (6) leads to subtractive cancellation in (5) we use $s_n := \ell_n + \ell_{n-1} = \mathrm{O}(n^{-\frac{3}{2}})$, $n \ge 1$ in the implementation. This decay of the s_n allows to restrict (5) to a convolution over the "recent past" (last M time levels — see §3).

To prove stability of the numerical scheme with the discrete TBC's (5) we use the discrete energy method and get $\|u^N\|_h^2 := h\sum_{j=1}^{J-1}\left(u_j^N\right)^2 \le \|u^0\|_h^2$, $N \ge 1$ for $\mu \in \mathbb{R}$.

3. Numerical Results

The numerical example illustrates the superiority of our *discrete TBC's* (5) over both a heuristic discretization of (3) ("discretized TBC") and an approximative absorbing BC [2] (observe the different scales).



Results for : $\Delta x = L/20,\ \Delta t = 10^{-4},\ a = 9,\ b = -100,\ c = 0.$

It is possible to consider (1) with variable coefficients and an inhomogeneity $f(x,t)$ provided that the coefficients are constant outside of $(0,L)$. Most of the results can be generalized to the θ–scheme for $0 < \theta \le 1$.

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4. References

1 Arnold, A.: Numerically Absorbing Boundary Conditions for Quantum Evolution Equations. To appear in: Proceedings of the "International Workshop on Computational Electronics", Tempe, AZ, USA, 1996.

2 Halpern, L.: Artificial BC's for the Linear Advection Diffusion Equation. Math. Comp. **46** (1986), 425–438.

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