Technische Universität Graz

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Bericht 2024/6

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Efficient Solution of State-Constrained Distributed Parabolic Optimal Control Problems

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Abstract

We consider a space-time finite element method for the numerical solution of a distributed tracking-type optimal control problem subject to the heat equation with state constraints. The cost or regularization term is formulated in an anisotropic Sobolev norm for the state, and the optimal state is then characterized as the unique solution of a first kind variational inequality. We discuss an efficient realization of the anisotropic Sobolev norm in the case of a space-time tensor-product finite element mesh, and the iterative solution of the resulting discrete variational inequality by means of a semi-smooth Newton method, i.e., using an active set strategy.

1 Introduction

Optimal control problems arise naturally in a wide range of applications, e.g., [2]. In this work, we consider tracking type optimal control problems to minimze

$$\mathcal{J}(u_\varrho, z_\varrho) = \frac{1}{2}\int_0^T \int_\Omega [u_\varrho(x,t) - \overline{u}(x,t)]^2 \, dx \, dt + \frac{1}{2}\, \varrho \, \|z_\varrho\|_Z^2 \tag{1.1}$$

subject to the Dirichlet boundary value problem for the heat equation,

$$\begin{array}{rcll} \partial_t u_\varrho(x,t) - \Delta_x u_\varrho(x,t) & = & z_\varrho(x,t) & \text{for } (x,t) \in Q := \Omega \times (0,T), \\ u_\varrho(x,t) & = & 0 & \text{for } (x,t) \in \Sigma := \partial\Omega \times (0,T), \\ u_\varrho(x,0) & = & 0 & \text{for } x \in \Omega, \end{array} \tag{1.2}$$

where $\Omega \subset \mathbb{R}^n, n = 2,3$ is a bounded Lipschitz domain, and $T > 0$ is a finite time horizon. In (1.1), we aim to approximate a given, probably discontinuous, target $\overline{u} \in L^2(Q)$ by a more regular function $u_\varrho \in X$ satisfying the heat equation (1.2) with the control z_ϱ as right hand side. For $z_\varrho \in Z$ we write (1.2) as operator equation to find $u_\varrho \in X$ such that

$Bu_\varrho = z_\varrho$ is satisfied, and we assume that $B : X \to Z$ defines an isomorphism. Instead of (1.1) we then consider the reduced functional for $u_\varrho \in X$,

$$\widetilde{\mathcal{J}}(u_\varrho) = \frac{1}{2} \int_0^T \int_\Omega [u_\varrho(x,t) - \overline{u}(x,t)]^2 \, dx \, dt + \frac{1}{2} \, \varrho \, \|Bu_\varrho\|_Z^2 \, . \tag{1.3}$$

The most standard choice is $Z = L^2(Q)$, and hence, using $Y = L^2(0,T; H_0^1(\Omega))$,

$$X := \{ u \in Y : \partial_t u \in Y^*, u(x,0) = 0, \; x \in \Omega, \partial_t u - \Delta_x u \in L^2(Q) \}.$$

For a non-conforming discretization of the resulting reduced optimality system, using piecewise linear continuous space-time finite element functions defined with respect to a simplicial decomposition of the space-time domain Q, see [6]. This finite element discretization becomes conforming if we consider $Z = Y^* = L^2(0,T; H^{-1}(\Omega))$ and $X := \{ u \in Y : \; \partial_t u \in Y^*, u(x,0) = 0, \; x \in \Omega \}$, see [5]. Moreover, following [8], we can consider the Dirichlet boundary value problem (1.2) in anisotropic Sobolev spaces, i.e., $X = H^{1,1/2}_{0;0,}(Q)$, and $Z = [H^{1,1/2}_{0;,0}(Q)]^*$, see also [7]. In all of these cases, the space-time finite element discretization of the reduced optimality system results, after eliminating the discrete adjoint state, in algebraic systems of linear equations of the form $[M_h + \varrho B_h^\top A_h^{-1} B_h]\underline{u} = \underline{f}$. Here, B_h is the space-time finite element matrix which is related to the Dirichlet boundary value problem (1.2), M_h is the mass matrix coming from the first part in (1.3), and A_h is a space-time finite element matrix in order to realize a norm in Z^*. In any case, the structure of the Schur complement matrix $S_h := B_h^\top A_h^{-1} B_h$ may complicate an efficient iterative solution of the discrete reduced optimality system, due to the involved inversion of A_h. Instead of the Schur complement system we may also solve an equivalent block skew-symmetric but positive definite system, see, e.g. [4] in the case of the Poisson equation with L^2 regularization.

To avoid the application of the Schur complement S_h we may replace S_h by any spectrally equivalent space-time finite element stiffness matrix D_h which realizes a norm in $X = H^{1,1/2}_{0;0,}(Q)$. Instead of (1.3) we therefore consider the minimization of

$$\widehat{\mathcal{J}}(u_\varrho) = \frac{1}{2} \, \|u_\varrho - \overline{u}\|^2_{L^2(Q)} + \frac{1}{2} \, \varrho \, \|u_\varrho\|^2_{H^{1,1/2}_{0;0,}(Q)} \tag{1.4}$$

which results in the determination of the optimal state u_ϱ from which we can compute the optimal control $z_\varrho = Bu_\varrho$ by some post processing. While in [7] we have considered the minimization of (1.4) without additional state or control constraints, here we include state constraints, see also [1], i.e.,

$$u_\varrho \in \mathcal{K} = \{ u \in X \mid u_- \leq u \leq u_+ \text{ a.e. in } Q \} \, , \tag{1.5}$$

where $u_\pm \in X \cap C(\overline{Q})$ are given continuous barrier functions, and we assume $0 \in \mathcal{K}$.

The norm in $X = H^{1,1/2}_{0;0,}(Q)$ is realized via

$$\|u\|^2_{H^{1,1/2}_{0;0,}(Q)} := \langle \partial_t u, \mathcal{H}_T u \rangle_Q + \|\nabla_x u\|^2_{L^2(Q)} =: \langle Du, u \rangle_Q \, , \tag{1.6}$$

where $\mathcal{H}_T$ is the modified Hilbert transform [8], that only acts in the temporal direction,

$$\mathcal{H}_T u(x,t) = \sum_{k=0}^{\infty} u_k(x) \cos\left(\left(\frac{\pi}{2}+k\pi\right)\frac{t}{T}\right),$$

and the Fourier coefficients are given as

$$u_k(x) = \frac{2}{T}\int_0^T u(x,t) \sin\left(\left(\frac{\pi}{2}+k\pi\right)\frac{t}{T}\right)\, dt.$$

Note that we can write, using $Bu_\varrho = z_\varrho$,

$$\|u_\varrho\|^2_{H^{1,1/2}_{0;0,}(Q)} = \langle Du_\varrho, u_\varrho\rangle_Q = \|u_\varrho\|^2_D = \|B^{-1}z_\varrho\|^2_D,$$

which defines an equivalent norm for the control z_ϱ in $[H^{1,1/2}_{0;,0}(Q)]^*$.

While in the unconstrained case the minimization of (1.4) results in the gradient equation $u_\varrho + \varrho Du_\varrho = \overline{u}$, in the case of state constraints we find the optimal state $u_\varrho \in \mathcal{K}$ as unique solution of the first kind variational inequality

$$\langle u_\varrho, v - u_\varrho\rangle_{L^2(Q)} + \varrho\,\langle Du_\varrho, v-u_\varrho\rangle_Q \geq \langle \overline{u}, v-u_\varrho\rangle_{L^2(Q)} \quad \text{for all } v \in \mathcal{K}. \tag{1.7}$$

For the numerical solution of (1.7) we define a space-time tensor product finite element space $X_h := W_{h_x} \otimes V_{h_t} \subset X$, where $W_{h_x} = \text{span}\{\psi_i\}_{i=1}^{M_x} \subset H^1_0(\Omega)$ is the spatial finite element space of piecewise linear basis functions ψ_i which are defined with respect to some admissible and globally quasi-uniform finite element mesh with spatial mesh size h_x. Further, $V_{h_t} := S^1_{h_t}(0,T) \cap H^{1/2}_{0,}(0,T) = \text{span}\{\varphi_k\}_{k=1}^{N_t}$ is the space of piecewise linear functions, which are defined with respect to a uniform finite element mesh with temporal mesh size h_t. With this we define

$$\mathcal{K}_h := \{u_h \in X_h : I_h u_- \leq u_h \leq I_h u_+ \text{ in } Q\},$$

and we consider the Galerkin discretization of the variational inequality (1.7) to find $u_{\varrho h} \in \mathcal{K}_h$ such that

$$\langle u_{\varrho h}, v_h - u_{\varrho h}\rangle_{L^2(Q)} + \varrho\,\langle Du_{\varrho h}, v_h - u_{\varrho h}\rangle_Q \geq \langle \overline{u}, v_h - u_{\varrho h}\rangle_{L^2(Q)},\ \forall v_h \in \mathcal{K}_h. \tag{1.8}$$

When assuming $\overline{u} \in \mathcal{K} \cap H^{2,1}(Q)$ and $u_\pm \in H^{2,1}(Q)$ we can prove the following error estimate, see [1, 7],

$$\begin{aligned}
&\|u_{\varrho h} - \overline{u}\|^2_{L^2(Q)} \\
&\leq c\left[h_t^2 + h_x^4 + \varrho(h_t + h_x^2) + \varrho^2\right]\left[\|\overline{u}\|^2_{H^{2,1}(Q)} + \|u_+\|^2_{H^{2,1}(Q)} + \|u_-\|^2_{H^{2,1}(Q)}\right].
\end{aligned}$$

This error estimate motivates the particular choices $\varrho = h_x^2$ and $h_t = h_x^2$ in order to conclude

$$\|u_{\varrho h} - \overline{u}\|^2_{L^2(Q)} \leq c\, h_x^4\left[\|\overline{u}\|^2_{H^{2,1}(Q)} + \|u_+\|^2_{H^{2,1}(Q)} + \|u_-\|^2_{H^{2,1}(Q)}\right].$$

Note that for a more regular target, e.g., for $\overline{u} \in \mathcal{K} \cap H^2(Q)$, we can also use $h_t = h_x$ to obtain the same estimate.

In this note we aim for an efficient iterative solution of the discrete variational inequality (1.8). Albeit D as defined in (1.6) is a non-local operator, since we are using a space-time tensor product ansatz space, we will demonstrate in Section 2 an efficient matrix free discretization of (1.8). These results are then used for an iterative solution of the discretized optimality system. This has the advantage, that we can augment this operator to yield an efficient algorithm for the active set strategy later on. The description of the active set strategy with the augmented operator is presented in Section 3. Numerical results are presented in Section 4.

2 Discretization

The discrete variational inequality (1.8) can be written in the following form to find $\underline{u} \in \mathbb{R}^{N_t \cdot M_x} \leftrightarrow u_h \in \mathcal{K}_h$ such that

$$(K_h \underline{u}, \underline{v} - \underline{u}) \geq (\underline{f}, \underline{v} - \underline{u}) \quad \text{for all } \underline{v} \in \mathbb{R}^{N_t \cdot M_x} \leftrightarrow v_h \in \mathcal{K}_h, \tag{2.1}$$

where K_h is the space-time finite element approximation of $I + \varrho D$, and $\underline{f}$ is the load vector which is related to the given target $\overline{u}$. Since we are using a space-time tensor product ansatz space X_h, we can write the space-time finite element matrix as

$$K_h = M_{h_t} \otimes M_{h_x} + \varrho \left[A_{h_t} \otimes M_{h_x} + M_{h_t} \otimes A_{h_x} \right] \in \mathbb{R}^{N_t \cdot M_x \times N_t \cdot M_x}, \tag{2.2}$$

where

$$A_{h_t}[j,i] = \langle \partial_t \varphi_i, \mathcal{H}_T \varphi_j \rangle_{L^2(0,T)}, \; M_{h_t}[j,i] = \langle \varphi_i, \varphi_j \rangle_{L^2(0,T)}, \; i,j = 1,\ldots,N_t,$$

$$A_{h_x}[\ell,k] = \langle \nabla_x \psi_k, \nabla_x \psi_\ell \rangle_{L^2(\Omega)}, \; M_{h_x}[\ell,k] = \langle \psi_k, \psi_\ell \rangle_{L^2(\Omega)}, \; k,\ell = 1,\ldots,M_x.$$

For the optimal choice $\varrho = h_x^2$, the matrix K_h is spectrally equivalent to the space-time mass matrix $M_{h_t} \otimes M_{h_x}$, allowing for a simple diagonal preconditioning when inverting K_h by applying a preconditioned conjugate gradient scheme. In order to realize the matrix-vector product $\underline{w} = K_h \underline{v}$ efficiently, in [7] we have considered the generalized eigenvalue problem

$$A_{h_t} \underline{v} = \lambda \, M_{h_t} \underline{v}. \tag{2.3}$$

With this we are able to transform any vector $\underline{v} \in \mathbb{R}^{N_t}$ into the eigenvector basis of (A_{h_t}, M_{h_t}) with $\mathcal{O}(N_t \log N_t)$ effort, which translates to $\mathcal{O}(N_t M_x \log N_t)$ for any vector in $\mathbb{R}^{N_t \cdot M_x}$. The temporal transformation matrix into the eigenvector basis is denoted by $C_{h_t}^{-1}$. The respective transformation on $\mathbb{R}^{N_t \cdot M_X}$ is then given by $C_{h_t}^{-1} \otimes I_{h_x}$. For the application $\underline{w} = K_h \underline{v}$ we then conclude $\underline{w} = (M_{h_t} C_{h_t} \otimes I_x) \hat{K}_h (C_{h_t}^{-1} \otimes I_x) \underline{v}$, where $\hat{K}_h$ is the representation of K_h in the temporal eigenbasis, i.e.,

$$\hat{K}_h = (C_{h_t}^{-1} M_{h_t}^{-1} \otimes I_{h_x}) K_h (C_{h_t} \otimes I_{h_x}) = I_{h_t} \otimes M_{h_x} + \varrho (\Lambda_{h_t} \otimes I_{h_x} + I_{h_t} \otimes A_{h_x}),$$

and Λ_{h_t} is the diagonal matrix of the generalized eigenvalues λ_i of (2.3). The application of $\hat{K}_h$ has effort $\mathcal{O}(N_t M_x)$, so we end up with the overall effort of $\mathcal{O}(N_t M_x \log N_t)$ for the matrix free application of K_h. This is a significant improvement over the $\mathcal{O}(N_t^2 M_x)$ effort for the direct application of K_h. Together with the feasibility of the conjugate gradient method with diagonal preconditioning, this yields a quasi optimal solver. Additionally, shared memory parallelization can be easily implemented, due to the Kronecker product structure of the arising matrices.

3 Semi-smooth Newton method

For the solution $\underline{u}$ of the discrete variational inequality (2.1) we define $\underline{\lambda} := K_h \underline{u} - \underline{f}$. By $\mathcal{I}_{A,\pm}$ we denote the index set of all active nodes where $u_j = u_{\pm,j} := u_\pm(x_j, t_j)$, while the complementary set is called the inactive set $\mathcal{I}_I$. Then there hold the discrete complementarity conditions

$$\lambda_j = 0,\ u_{-,j} < u_j < u_{+,j} \text{ for } j \in \mathcal{I}_I,\ \lambda_j \le 0 \text{ for } j \in \mathcal{I}_{A,+},\ \lambda_j \ge 0 \text{ for } j \in \mathcal{I}_{A,-},$$

which are equivalent to

$$\lambda_j = \min\{0, \lambda_j + c(u_{+,j} - u_j)\} + \max\{0, \lambda_j + c(u_{-,j} - u_j)\}, \quad c > 0.$$

Hence we have to solve a system $\underline{F}(\underline{u}, \underline{\lambda}) = \underline{0}$ of (non)linear equations

$$\begin{aligned}
\underline{F}_1(\underline{u}, \underline{\lambda}) &= K_h \underline{u} - \underline{\lambda} - \underline{f} = \underline{0}, \\
\underline{F}_2(\underline{u}, \underline{\lambda}) &= \underline{\lambda} - \min\{0, \underline{\lambda} + c(\underline{u}_+ - \underline{u})\} - \max\{0, \underline{\lambda} + c(\underline{u}_- - \underline{u})\} = \underline{0}.
\end{aligned}$$

One step of the semi-smooth Newton method [3] for the iterative solution of this system reads

$$\begin{pmatrix} \underline{u}^{k+1} \\ \underline{\lambda}^{k+1} \end{pmatrix} = \begin{pmatrix} \underline{u}^{k} \\ \underline{\lambda}^{k} \end{pmatrix} - \left[D\underline{F}(\underline{u}^k, \underline{\lambda}^k) \right]^{-1} \underline{F}(\underline{u}^k, \underline{\lambda}^k), \tag{3.1}$$

where $D\underline{F}$ is the Jacobian of $\underline{F}$ in the sense of slant derivatives. For any iterate $(\underline{u}^k, \underline{\lambda}^k)$ we define the active set $\mathcal{I}_A^k$ as well as the inactive set $\mathcal{I}_I^k$. From the second line in (3.1) we first conclude

$$\begin{cases} \lambda_j^k + c(u_{-,j} - u_j^k) > 0, \\ \lambda_j^k + c(u_{+,j} - u_j^k) < 0, \\ \text{else}, \end{cases} \implies \begin{cases} u_j^{k+1} := u_{-,j}, \\ u_j^{k+1} := u_{+,j}, \\ \lambda_j^{k+1} := 0. \end{cases} \tag{3.2}$$

For the remainder, we first introduce a split into active and inactive parts of all quantities,

$$\underline{u}^{k+1} = \underline{u}_A^{k+1} \oplus \underline{u}_I^{k+1}, \quad \underline{\lambda}^{k+1} = -\underline{\lambda}_A^{k+1} \oplus \underline{\lambda}_I^{k+1}, \tag{3.3}$$

where $\lambda_{I,j}^{k+1} = 0$ for $j \in \mathcal{I}_I^{k+1}$ and $u_{A,j}^{k+1}$ is set according to (3.2) for $j \in \mathcal{I}_A^{k+1}$. Substituting this into the remaining first equation of (3.1) yields

$$\widetilde{K}_h^{k+1} \begin{pmatrix} \underline{u}_I^{k+1} \\ \underline{\lambda}_A^{k+1} \end{pmatrix} := K_h \underline{u}_I^{k+1} + \underline{\lambda}_A^{k+1} = \overline{\underline{u}} - K_h \underline{u}_A^{k+1} =: \underline{f}^{k+1}. \tag{3.4}$$

The left-hand side is a linear map $\widetilde{K}_h^{k+1} : \mathbb{R}^{N_t M_x} \to \mathbb{R}^{N_t M_x}$ for any choice of an active set. Due to the orthogonality of the splitting, $K_h \underline{u}_I^{k+1} + \underline{\lambda}_A^{k+1}$ is also an orthogonal sum and hence $\widetilde{K}_h^{k+1}$ inherits positive definiteness from K_h and the identity. After a correct reordering of the indices, the matrix is even block diagonal,

$$\widetilde{K}_h^{k+1} = \begin{pmatrix} R_I^{k+1} K_h^{k+1} P_I^{k+1} & 0 \\ 0 & R_A^{k+1} I_h P_A^{k+1} \end{pmatrix}, \tag{3.5}$$

where $P_{I/A}^{k+1}$ and $R_{I/A}^{k+1}$ are the canonical prolongation (by zero) and restriction with respect to their subscript index set. Now feasibility of diagonal preconditioning is evident from its feasibility for K_h. In practice the splitting is performed by setting vanishing components to zero. Then all matrices can be applied as in the unconstrained case. As $\widetilde{K}_h$ is not available as a matrix, we take the diagonal of the spectrally equivalent space-time mass matrix for preconditioning, where we set entries corresponding to the active set to one. The semi-smooth Newton method terminates, when the index sets are no longer changing. The algorithm for the overall procedure is summarized in Algorithm 1. Note, that the simple stopping criterion is no longer applicable, when, e.g., underrelaxation or line-search is used. Then one needs to add additional stopping criteria. Underrelaxation is discussed in the next chapter.

Algorithm 1 Active set strategy in the case of state constraints

choose initial guesses for $\underline{u}^0$ and $\underline{\lambda}^0$
for $k = 0, 1, 2, \ldots$ **do**
  compute $\mathcal{I}_A^{k+1}$ and $\mathcal{I}_I^{k+1}$ according to (3.2)
  if $k > 0$ and $\mathcal{I}_A^{k+1} = \mathcal{I}_A^k$ **then**
return $\left(\underline{u}^k, \underline{\lambda}^k\right)$
  end if
  solve (3.4) for $\underline{u}_I^{k+1}$ and $\underline{\lambda}_A^{k+1}$ using matrix free CG with diagonal preconditioning
end for

4 Numerical Results

As an illustrative example, we consider $\Omega = (0,1)^3$ and $T = 1$, i.e., the space-time cylinder $Q = \Omega \times (0,T) = (0,1)^4$. We decompose Ω into a shape regular and simplicial globally quasi-uniform mesh Ω_h with n_x elements of mesh size h_x, and $(0,T)$ into a regular mesh

$\mathcal{T}_h$ consisting of n_t equidistant intervals of length $h_t = 1/n_t$. Then we define the discrete space $X_h = W_{h_x} \otimes V_{h_t}$ with $W_{h_x} = S^1_{h_x}(\Omega_h) \cap H^1_0(\Omega)$ and $V_{h_t} = S^1_{h_t}(\mathcal{T}_h) \cap H^{1/2}_{0,}(0,T)$, where S^1_h denotes the space of piecewise linear continuous functions on the respective mesh. As target function we consider

$$\overline{u}(x,t) = \sin(\pi x_1)\sin(\pi x_2)\sin(\pi x_3)\sin(\pi t) \in C^\infty(Q) \cap X. \tag{4.1}$$

As we have extensively validated the optimality of the strongly related solver for the unconstrained case in [7], here we will only present the more interesting case with state constraints, choosing $u_- \equiv 0$ and $u_+ \equiv 0.8$. This implies that $\overline{u} \notin \mathcal{K}$. But all the given error estimates remain valid when replacing $\overline{u}$ by its projection $P_\mathcal{K}\overline{u} \in \mathcal{K}$. As initial guess in the semi-smooth Newton method we consider $\underline{u}^0 = \frac{1}{2}(\underline{u}_- + \underline{u}_+)$ and $\underline{\lambda}^0 = K_h\underline{u}^0 - \underline{f}$. Further we apply underrelaxation with $\omega_N = 0.1$ in the semi-smooth Newton method with the parameter $c = 1$. We stop the non-linear solver if the active sets do not change anymore and subsequent iterates satisfy

$$\|\underline{u}^{k+1} - \underline{u}^k\|_\infty + \|\underline{\lambda}^{k+1} - \underline{\lambda}^k\|_\infty < 10^{-3}.$$

This condition is needed, due to underrelaxation, which could lead to a non-changing active set, even though the solution is still changing. For this illustrative example, simple underrelaxation is sufficient, but in general, more sophisticated strategies are advised. To gain insight on the condition number of $\widetilde{K}_h$ each nested conjugate gradient iteration starts with a zero initial guess and stops at a relative residual of 10^{-10}. The experiment is conducted for varying mesh sizes $h_t \simeq h_x$. The number of needed Newton as well as CG iterations are given in Table 1. Furthermore the table contains the ratio of conjugate gradient iterations per Newton iterations, which stay at reasonable values. In Figure 1 we plot the solution for different discretization parameters n_x along the line $x_1 = x_2 = x_3 = 0.51$ and compare it to the target function. A point slightly off the center is chosen to exclude benevolent symmetry effects. It is clearly visible, that the solution approaches the target function until it reaches the upper bound. This is exactly the desired behavior.

Table 1: Numerical results for the constrained optimal control problem, with $n = n_t$.

n	**DoF**	**Newton iter.**	**CG iter.**	**CG/Newton**
2	16	36	36	1
4	256	36	612	17
8	4,096	36	1,296	36
16	65,536	38	2,173	57
32	1,048,580	64	3,814	60

Acknowledgements Part of this work has been supported by the Austrian Science Fund (FWF) under the Grant Collaborative Research Center TRR361/F90: CREATOR Computational Electric Machine Laboratory.

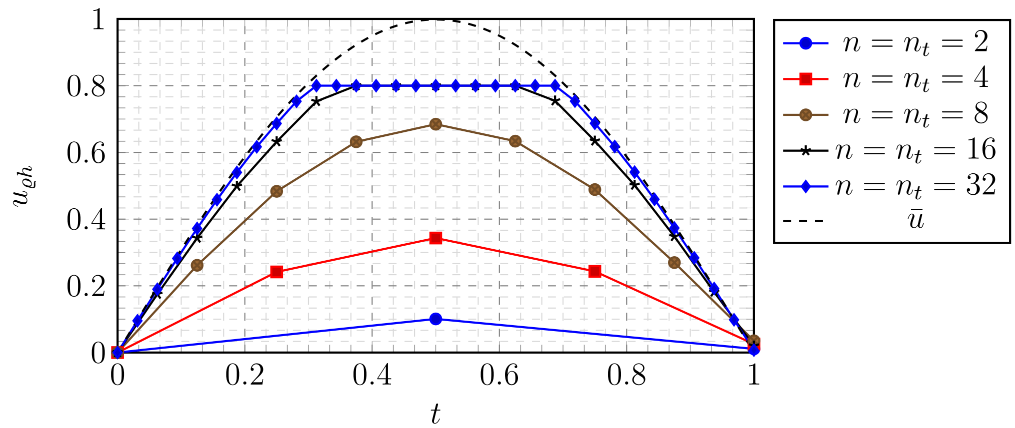

Figure 1: Plot of the constrained solution $u_{\varrho h}$ along the line $x_1 = x_2 = x_3 = 0.51$.

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