Grzegorz Gurgul
Marcin Łoś
Maciej Paszyński
Victor Calo

LINEAR COMPUTATIONAL COST IMPLICIT SOLVER FOR PARABOLIC PROBLEMS

Abstract *In this paper, we use the alternating direction method for isogeometric finite elements to simulate transient problems. Namely, we focus on a parabolic problem and use B-spline basis functions in space and an implicit time-marching method to fully discretize the problem. We introduce intermediate time-steps and separate our differential operator into a summation of the blocks that act along a particular coordinate axis in the intermediate time-steps. We show that the resulting stiffness matrix can be represented as a multiplication of two (in 2D) or three (in 3D) multi-diagonal matrices, each one with B-spline basis functions along the particular axis of the spatial system of coordinates. As a result of these algebraic transformations, we get a system of linear equations that can be factorized in a linear $O(N)$ computational cost at every time-step of the implicit method. We use our method to simulate the heat transfer problem. We demonstrate theoretically and verify numerically that our implicit method is unconditionally stable for heat transfer problems (i.e., parabolic). We conclude our presentation with a discussion on the limitations of the method.*

Keywords isogeometric analysis, implicit dynamics, linear computational cost, direct solvers

Citation Computer Science 21(3) 2020: 335–352

1. Introduction

The alternating directions implicit method (ADI) was first introduced in [4,11,31,33] to deal with finite-difference simulations for time-dependent problems. The method is currently used as a solution for a wide class of problems [18, 19]. In the ADI method for finite-difference simulations, the partial differential equations (PDE) are first discretized in space using spatial stencil and then in time using intermediate time-steps. For example, let us consider the heat equation in two dimensions:

$$\frac{du}{dt} - \Delta u = f \tag{1}$$

with either Dirichlet or Neumann boundary conditions. We now discretize it using central differences with respect to the x and y directions:

$$\frac{du}{dt} - \frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u}{\partial y^2} = f \tag{2}$$

$$\frac{du}{dt} - \frac{u_{i-1,j} - 2u_{i,j} + u_{i+1,j}}{h^2} - \frac{u_{i,j-1} - 2u_{i,j} + u_{i,j+1}}{h^2} = f \tag{3}$$

and the ADS method introduces an intermediate time step:

$$\begin{aligned} \frac{u^{t+0.5}_{i,j} - u^t_{i,j}}{\tau/2} - \frac{u^{t+0.5}_{i-1,j} - 2u^{t+0.5}_{i,j} + u^{t+0.5}_{i+1,j}}{h^2} &= \frac{u^t_{i,j-1} - 2u^t_{i,j} + u^t_{i,j+1}}{h^2} + f^t \\ \frac{u^{t+1}_{i,j} - u^{t+0.5}_{i,j}}{\tau/2} - \frac{u^{t+1}_{i,j-1} - 2u^{t+1}_{i,j} + u^{t+1}_{i,j+1}}{h^2} &= \frac{u^{t+0.5}_{i-1,j} - 2u^{t+0.5}_{i,j} + u^{t+0.5}_{i+1,j}}{h^2} + f^{t+0.5} \end{aligned} \tag{4}$$

where τ is the time-step size, and f^t, $f^{t+0.5}$ denote the forcing term in time-step t and in the middle between steps t and $t+1$, respectively. The resulting two systems of linear equations are tridiagonal and can be solved with a linear computational cost.

In this paper, we apply the above approach to simulations using isogeometric analysis (IGA) [1,8]. The main idea of IGA is to apply B-splines or NURBS [32] basis functions in finite element simulations. It has multiple applications in time-dependent simulations, including phase-field models [9, 10], phase-separation simulations with an application to cancer growth simulations [13, 14], wind turbine aerodynamics [24], incompressible hyper-elasticity [12], turbulent flow simulations [6], the transport of drugs in cardiovascular applications [23], or blood flow simulations and drug transport in artery simulations [3, 5].

An alternating direction solver (ADS) is a fast linear solver that exploits the Kronecker product structure of the matrix that arises in some finite element simulations. It was recently applied [15–17] for a fast solution for the isogeometric L^2 orthogonal projection onto the finite element space of B-splines. There, the authors solved a projection problem discretized with a tensor product basis comprised of basis functions of the following form:

$$B_{i_1,\ldots,i_d}(x_1,\ldots,x_d) = B^{x_1}_{i_1}(x_1)\cdots B^{x_d}_{i_d}(x_d) \tag{5}$$

where $B^{x_1}_{i_1}(x),\ldots,B^{x_d}_{i_d}(x)$ denote one-dimensional B-spline basis functions.

The direction-splitting schemes deliver a fast inversion method for the spatial discretization that is obtained by grouping the one-dimensional B-splines together along particular spatial axes, assuming that the basis functions have a tensor product structure (as Figure 1 sketches). In this case, we can index tensor product basis functions using pairs (in 2D) of indices of one-dimensional basis functions; e.g.,

$$B_{i,j}(x,y) = B_i^x(x)B_j^y(y) \tag{6}$$

For the purpose of visualizing the matrices and vectors in space that are spanned by this basis, such double indices can be linearized by ordering them lexicographically. The Gram (mass) matrix of B-spline basis on 2D domain $\Omega = \Omega_x \times \Omega_y$ can be expressed as follows:

$$\mathcal{M}_{(i,j)(k,l)} = (B_{i,j}, B_{k,l}) = \int_\Omega B_{i,j}B_{k,l}\,\mathrm{d}\Omega = \int_\Omega B_i^x(x)B_j^y(y)B_k^x(x)B_l^y(y)\,\mathrm{d}\Omega$$

$$= \int_\Omega (B_iB_k)(x)\,(B_jB_l)(y)\,\mathrm{d}\Omega = \left(\int_{\Omega_x} B_iB_k\,\mathrm{d}x\right)\left(\int_{\Omega_y} B_jB_l\,\mathrm{d}y\right) = \mathcal{M}^x_{ik}\mathcal{M}^y_{jl} \tag{7}$$

where $(\cdot,\cdot) = (\cdot,\cdot)_{L^2(\Omega)}$. In other words, Gram matrix $\mathcal{M} = \mathcal{M}^x \otimes \mathcal{M}^y$ is the Kronecker product of two multi-diagonal matrices with the corresponding structure of a mass matrix build from one-dimensional B-spline basis functions. Such a matrix can be factorized in a linear computational cost (see Appendix B).

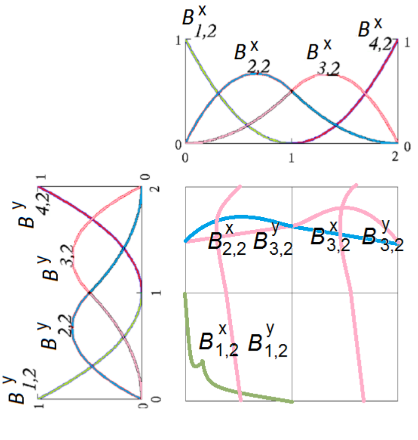

Figure 1. Tensor product structure of quadratic B-spline basis functions, with two exemplary basis functions presented

This idea can be directly applied to speed up simulations using explicit time discretizations, since the simulation of dynamics using the explicit time-stepping scheme can be expressed as a sequence of isogeometric L^2 projections in the following manner.

Given a time-dependent problem with spatial operator L and Dirichlet or Neumann boundary conditions

$$\frac{du}{dt} - Lu = f \tag{8}$$

we discretize time using the explicit Euler scheme and obtain

$$u_{t+1} = u_t + \tau\, Lu_t + \tau\, f \tag{9}$$

where τ is the time-step size. Then, we pass to the weak formulation by multiplying the above equation by test function v, which leads to

$$(u_{t+1}, v) = (u_t + \tau\, Lu_t + \tau\, f, v) \tag{10}$$

where $u_{t+1} = \sum_{i,j} a^{t+1}_{i,j} B^x_{i;p}(x) B^y_{j;q}(y)$ and $u_t = \sum_{i,j} a^t_{i,j} B^x_{i;p}(x) B^y_{j;q}(y)$. Thus, each time-step is equivalent to computing an orthogonal L^2 projection of the right-hand side of Equation (9), which can be done in linear computational cost with respect to the number of degrees of freedom in the system.

The method was used for performing fast simulations of dynamics with explicit time discretization [20, 25–27, 29, 34], since the explicit time integration scheme with isogeometric discretization is equivalent to the sequence of isogeometric L^2 orthogonal projections, which can be solved using the direction splitting of the later kind.

In this paper, we extend this methodology to dynamics simulations with implicit time discretization by collecting different terms as a sequence of multi-diagonal inversions.

The structure of the paper is as follows. In Section 2, we start from a description of the direction splitting for the Laplace operator. Next, in Section 3, we present the numerical results for the two-dimensional model heat transfer problem. Section 4 derives the proof of unconditional stability for our direction-splitting method. We conclude the paper in Section 5. We provide two appendices with some Lemmas used for proving the unconditional stability of the scheme and with the general description of the alternating directions solver.

2. Direction splitting for Laplace operator

We express this parabolic system as a sequence of implicit time-steps, which is

$$\frac{du}{dt} - Lu = f \tag{11}$$

where, for the sake of simplifying the discussion, we assume that the coefficients are constant, the domain is the unit is square, and the differential operator is separable; that is, $L = L_x + L_y$ where L_α contains spatial derivatives only with respect to α (e.g., Laplacian, where $L = L_x + L_y = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}$). Furthermore, we impose either uniform

Dirichlet or zero Neumann boundary conditions. Thus, to apply the alternating direction implicit scheme, we introduce a sequence of intermediate time-steps, which is

$$\frac{u_{t+0.5} - u_t}{\tau/2} - L_x u_{t+0.5} - L_y u_t = f_t \tag{12}$$

$$\frac{u_{t+1} - u_{t+0.5}}{\tau/2} - L_x u_{t+0.5} - L_y u_{t+1} = f_{t+0.5} \tag{13}$$

We rewrite these equations by collecting the known variables on the right-hand side as follows:

$$\begin{aligned} u_{t+0.5} - \frac{\tau}{2} L_x u_{t+0.5} &= u_t + \frac{\tau}{2} L_y u_t + \frac{\tau}{2} f_t, \\ u_{t+1} - \frac{\tau}{2} L_y u_{t+1} &= u_{t+0.5} + \frac{\tau}{2} L_x u_{t+0.5} + \frac{\tau}{2} f_{t+0.5} \end{aligned} \tag{14}$$

Now, we transform the problem into a weak form multiplying by test functions and applying integration by parts to get the following weak forms:

$$(v, u_{t+0.5}) + \frac{\tau}{2}\left(\frac{\partial v}{\partial x}, \frac{\partial u_{t+0.5}}{\partial x}\right) = (v, u_t) - \frac{\tau}{2}\left(\frac{\partial v}{\partial y}, \frac{\partial u_t}{\partial y}\right) + \frac{\tau}{2}(v, f_t) \tag{15}$$

$$(v, u_{t+1}) + \frac{\tau}{2}\left(\frac{\partial v}{\partial y}, \frac{\partial u_{t+1}}{\partial y}\right) = (v, u_{t+0.5}) - \frac{\tau}{2}\left(\frac{\partial v}{\partial x}, \frac{\partial u_{t+0.5}}{\partial x}\right) + \frac{\tau}{2}(v, f_{t+0.5}) \tag{16}$$

where the resulting boundary terms vanish due to the boundary conditions.

In the sequel, we limit the discussion to the first of the above equations; the other can be treated in a similar fashion.

Definition 1. *Let V_x^N be the space of functions $f \in L^2(\Omega)$ such that distributional derivative $\partial f/\partial x$ is a regular distribution and $\partial f/\partial x \in L^2(\Omega)$, which is*

$$V_x^N = \left\{ v \in L^2(\Omega) \colon \frac{\partial v}{\partial x} \in L^2(\Omega) \right\} \tag{17}$$

and let V_x^D be its subspace of functions vanishing on the boundary:

$$V_x^D = V_x^N \cap H_0^1(\Omega) \tag{18}$$

If we consider a problem with Neumann boundary conditions, let $V_x = V_x^N$; otherwise, $V_x = V_x^D$. Space V_y can be defined analogously.

We end up with the following variational problem: Given $w \in H^2(\Omega)$, find $u \in V_x$ such as

$$\begin{aligned} b(v, u) &= l(v) \quad \forall v \in V_x \\ b(v, u) &= (v, u) + \frac{\tau}{2}\left(\frac{\partial v}{\partial x}, \frac{\partial u}{\partial x}\right) \\ l(v) &= (v, w) + \frac{\tau}{2}\left(v, \frac{\partial^2 w}{\partial y^2}\right) + \frac{\tau}{2}(v, f) \end{aligned} \tag{19}$$

We have integrated the right-hand-side term back by parts to keep the continuity of the linear form. This is necessary since, due to the definition of V_x, test function v is not required to possess a weak derivative in the y direction. The assumption that $w \in H^2(\Omega)$ requires that the initial condition satisfies $u(x,0) \in H^2(\Omega)$ as well.

Definition 2. *Let $\tau > 0$. For $u, v \in V_x$, let*

$$(v,u)_{V_x} = (v,u) + \frac{\tau}{2}\left(\frac{\partial v}{\partial x}, \frac{\partial u}{\partial x}\right) \tag{20}$$

It is a scalar product that induces the following norm:

$$\|u\|^2_{V_x} = \|u\|^2_{L^2} + \frac{\tau}{2}\left\|\frac{\partial u}{\partial x}\right\|^2_{L^2} \tag{21}$$

Lemma 1. *Space V_x with norm $\|\cdot\|_{V_x}$ is a Hilbert space.*

Proof. Let $\{u_n\}$ be a Cauchy sequence in V_x. By the definition of the norm of V_x, $\{u_n\}$ and $\{\partial u_n/\partial x\}$ are Cauchy sequences in $L^2(\Omega)$; so, by its completeness, there exist L^2 functions u, u_x such that $u_n \to u$ and $\partial u_n/\partial x \to u_x$ in the sense of the L^2 norm. Let $\phi \in D(\Omega)$ be a test function in the sense of the theory of distributions. We have

$$\left(u, \frac{\partial \phi}{\partial x}\right) = \lim_{n\to\infty}\left(u_n, \frac{\partial \phi}{\partial x}\right) = -\lim_{n\to\infty}\left(\frac{\partial u_n}{\partial x}, \phi\right) = -(u_x, \phi)$$

since $\phi \in L^2(\Omega)$, so u_x is a distributional derivative of u and, thus, $u \in V_x$. Therefore, V_x is complete. □

Theorem 1. *Bilinear form*

$$b(v,u) = (v,u) + \frac{\tau}{2}\left(\frac{\partial v}{\partial x}, \frac{\partial u}{\partial x}\right) \tag{22}$$

defined on V_x is coercive.

Proof. We have

$$\begin{aligned} b(u,u) &= \|u\|^2_{L^2} + \frac{\tau}{2}\left\|\frac{\partial u}{\partial x}\right\|^2_{L^2} \\ &= \|u\|^2_{V_x} \end{aligned} \tag{23}$$

□

Theorem 2. *Abstract variational problem: for a given continuous linear functional $l \in V_x'$, find $u \in V_x$ such that*

$$b(u,v) = l(v) \qquad \forall v \in V_x \tag{24}$$

is well-posed.

Proof. Bilinear form b is obviously continuous and is coercive due to Theorem 1. By the Lax-Milgram theorem, the variational problem is well-posed. □

We discretize the above abstract variational problem using a finite element space $V_h \subset V_x$ comprised of linear combinations of the tensor product of B-spline basis functions of order p, which is

$$V_h = \operatorname{span}\{N_{i,j}\}_{i,j} \qquad N_{i,j}(x,y) = B_i^x(x)B_j^y(y) \tag{25}$$

where B_i^x and B_j^y are basis B-spline functions in the x and y directions, respectively.

Let us first focus on System (15). We approximate $u_{t+0.5} = \sum_{k,l} a_{k,l}^{t+0.5} B_k^x(x)B_l^y(y)$ and test with $v = B_i^x(x)B_j^y(y)$. Our previous sub-step solution is also given as linear combination $u_t = \sum_{k,l} a_{k,l}^t B_k^x(x)B_l^y(y)$.

$$\sum_{k,l} a_{k,l}^{t+0.5}\left[\left(B_k^x(x)B_l^y(y), B_i^x(x)B_j^y(y)\right) + \frac{\tau}{2}\left(\frac{\partial(B_k^x(x)B_l^y(y))}{\partial x}, \frac{\partial(B_i^x(x)B_j^y(y))}{\partial x}\right)\right] =$$
$$\sum_{k,l} a_{k,l}^{t}\left[\left(B_k^x(x)B_l^y(y), B_i^x(x)B_j^y(y)\right) - \frac{\tau}{2}\left(\frac{\partial(B_k^x(x)B_l^y(y))}{\partial y}, \frac{\partial(B_i^x(x)B_j^y(y))}{\partial y}\right)\right] +$$
$$\frac{\tau}{2}(f_t, B_i^x(x)B_j^y(y))$$

Using the fact that $\frac{\partial B_k^x(x)}{\partial y} = \frac{\partial B_k^y(y)}{\partial x} = 0$, we obtain

$$\sum_{k,l} a_{k,l}^{t+0.5}\left[\left(B_k^x(x)B_l^y(y), B_i^x(x)B_j^y(y)\right) + \frac{\tau}{2}\left(\frac{\partial B_k^x(x)}{\partial x}B_l^y(y), \frac{\partial B_i^x(x)}{\partial x}B_j^y(y)\right)\right] =$$
$$\sum_{k,l} a_{k,l}^{t}\left[\left(B_k^x(x)B_l^y(y), B_i^x(x)B_j^y(y)\right) - \frac{\tau}{2}\left(B_k^x(x)\frac{\partial B_l^y(y)}{\partial y}, B_i^x(x)\frac{\partial B_j^y(y)}{\partial y}\right)\right] +$$
$$\frac{\tau}{2}(f_t, B_i^x(x)B_j^y(y))$$

We can separate the directions and use the fact that the y terms are identical, which can be expressed as a Kronecker product:

$$\sum_{k,l} a_{k,l}^{t+0.5}\left[(B_k^x(x),B_i^x(x))+\frac{\tau}{2}\left(\frac{\partial B_k^x(x)}{\partial x},\frac{\partial B_i^x(x)}{\partial x}\right)\right]\left(B_l^y(y),B_j^y(y)\right)=$$
$$\sum_{k,l} a_{k,l}^{t}\left[\left(B_k^x(x)B_l^y(y),B_i^x(x)B_j^y(y)\right)-\frac{\tau}{2}\left(B_k^x(x)\frac{\partial B_l^y(y)}{\partial y},B_i^x(x)\frac{\partial B_j^y(y)}{\partial y}\right)\right]+$$
$$\frac{\tau}{2}(f_t,B_i^x(x)B_j^y(y))$$

These matrices are multi-diagonal and can be factorized in a linear $\mathcal{O}(N)$ cost. An identical procedure yields the following:

$$\sum_{k,l} a_{k,l}^{t+1}\left(B_k^x(x),B_i^x(x)\right)\left[\left(B_l^y(y),B_j^y(y)\right)+\frac{\tau}{2}\left(\frac{\partial B_k^y(y)}{\partial y},\frac{\partial B_j^y(y)}{\partial y}\right)\right]=$$
$$\sum_{k,l} a_{k,l}^{t+0.5}\left[\left(B_k^x(x)B_l^y(y),B_i^x(x)B_j^y(y)\right)-\frac{\tau}{2}\left(B_k^x(x)\frac{\partial B_l^y(y)}{\partial x},B_i^x(x)\frac{\partial B_j^y(y)}{\partial x}\right)\right]+$$
$$\frac{\tau}{2}(f_{t+0.5},B_i^x(x)B_j^y(y))$$

Thus, we obtain an alternating direction implicit IGA discretization with a solution cost of $\mathcal{O}(N)$.

3. Numerical results for Laplace operator

We test the alternating direction implicit solver that we propose for the heat transfer problem with zero forcing over a two-dimensional mesh of 64×64 elements using quadratic B-spline basis functions. The initial state is a ball of heat concentrated in the center of the domain given by

$$u(x,0)=\phi(\min\{1,12\left\|x-(0.5,0.5)\right\|^2\}) \tag{26}$$
$$\phi(s)=(1-s)^2(1+s)^2 \tag{27}$$

and we employ zero Neumann boundary conditions. Due to the boundary conditions and zero forcing, the steady state solution is a constant function with a value equal to the average of the initial state; i.e.,

$$\lim_{t\to\infty} u(\cdot,t)=\frac{1}{|\Omega|}\int_\Omega u(x,0)\,dx=\frac{1}{45}\approx 0.02 \tag{28}$$

We use time-step sizes of 10^{-1}, 10^{-2}, 10^{-3}, and 10^{-4}. We plot the L^2 norm of the solution in Figure 2. From the plots, we can conclude that the solutions always converge to the same final solution even if it is oscillating at the beginning for large time-step sizes (like for 10^{-1}).

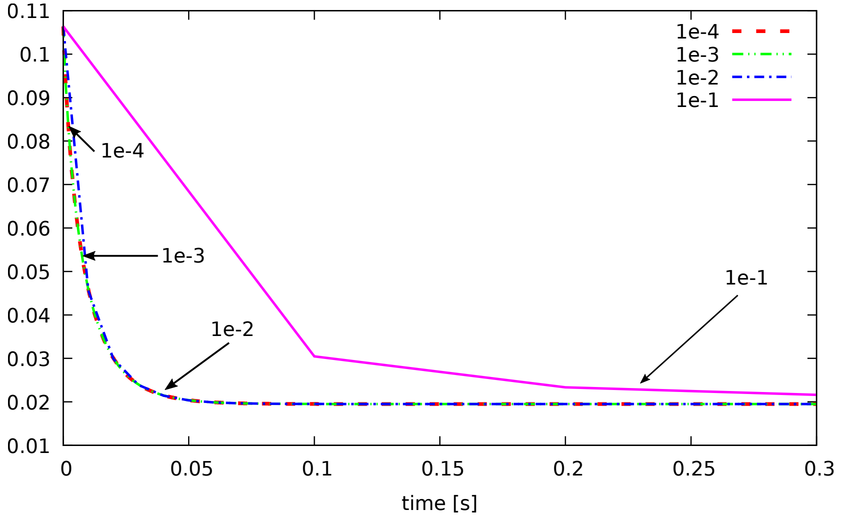

Figure 2. L^2 norm of solution for heat transfer simulations with $\tau = 0.1, 0.01, 0.001$, and 0.0001 for mesh dimensions of 64^2 elements

This is illustrated in Figure 3, where we employ the largest time-step (10^{-1}). Although the quality of the intermediate solutions is very poor for such a large time-step (as expected), the equilibrium solution is ultimately approximated fairly well. We will prove the asymptotic stability of the scheme; thus, the transient local growth of the solution is not discarded. However, these local phenomena disappear as time progresses.

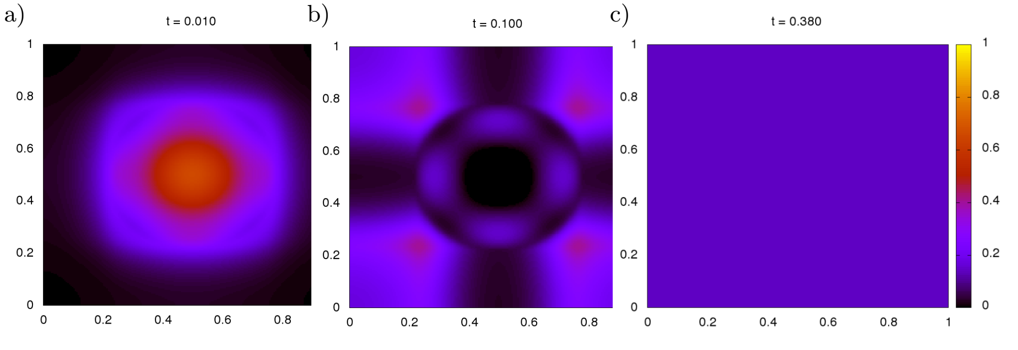

Figure 3. Implicit ADS scheme with time-step 10^{-1}: a) start of oscillations; b) oscillations; c) final state

Snapshots from the simulation with a time-step size of 10^{-4} without any oscillations are presented in Figure 4. These numerical results are obtained for a time-step size of 10^{-3}.

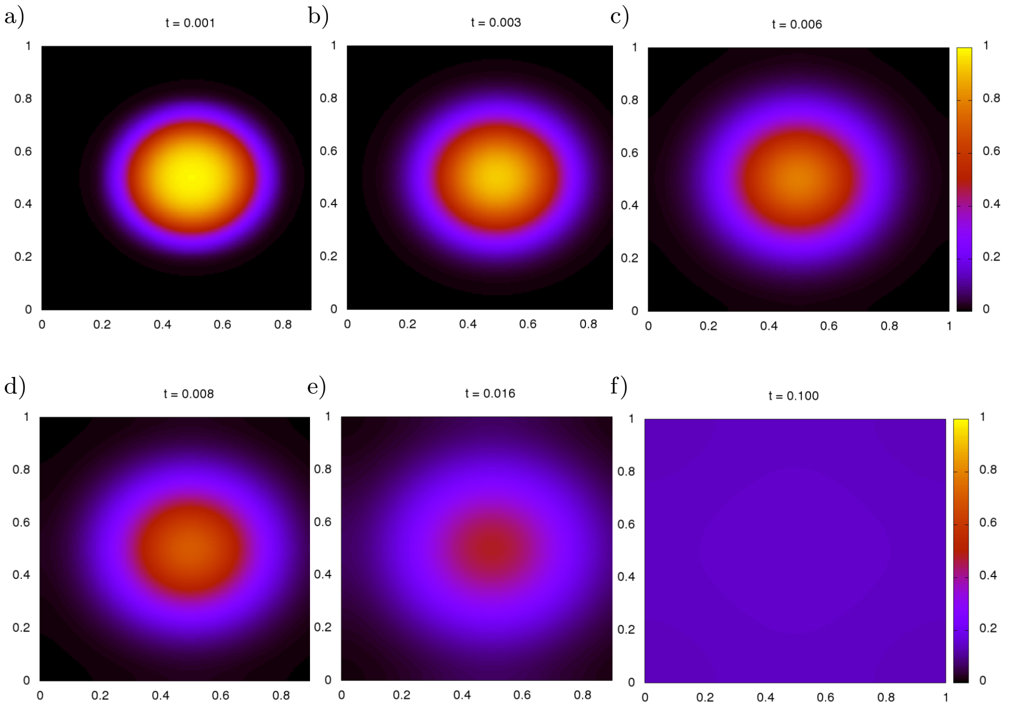

Figure 4. Implicit ADS scheme with time-step 10^{-3}: a) start of simulation; b) time $t = 0.003$; c) time $t = 0.006$; d) time $t = 0.008$; e) time $t = 0.016$; f) final state

Alternative approach for direction splitting is discussed in paper [28], where we focus on hyperbolic wave propagation problems; however, the problem matrix is approximated as a Kronecker product of $(M_x + \alpha S_x) \otimes (M_y + \alpha S_Y)$ (with mass and stiffness matrices) where the higher-order terms with respect to α are neglected. This method also results in an unconditionally stable scheme and a linear computational cost solver. However, the method presented in this paper does not approximate the matrix – it proposes the splitting of the whole system.

4. Stability analysis for heat transfer problem

Let us consider the heat equation on 2D domain $\Omega = \Omega_x \times \Omega_y$

$$\frac{\partial u}{\partial t} - \Delta u = f \tag{29}$$

Assuming zero Dirichlet boundary conditions, the weak formulation is given by

$$\left(\frac{\partial u}{\partial t}, v\right) = -(\nabla u, \nabla v) + (v, f) \tag{30}$$

Let $\mathcal{B}_{ij}(x, y) = \mathcal{B}^x_i(x)\mathcal{B}^y_j(y)$ be the standard tensor product basis. We seek a solution of form

$$u(\mathbf{x}, t) = \sum u^{ij}(t)\, \mathcal{B}_{ij}(\mathbf{x})$$

We will analyze the spectral radius of the step operator for both the explicit Euler method and our implicit method. The method is stable when the spectral radius is less than 1 [21].

Let us denote

$$\mathbf{M} = \left[(\mathcal{B}_{ij}, \mathcal{B}_{kl})_{L^2(\Omega)}\right] \qquad \mathbf{K} = \left[(\nabla\mathcal{B}_{ij}, \nabla\mathcal{B}_{kl})_{L^2(\Omega)}\right] \qquad \mathbf{F} = \left[(f, \mathcal{B}_{ij})_{L^2(\Omega)}\right] \tag{31}$$

and

$$\mathbf{M}_x = \left[(\mathcal{B}^x_i, \mathcal{B}^x_k)_{L^2(\Omega_x)}\right] \qquad \mathbf{K}_x = \left[(\partial_x\mathcal{B}^x_i, \partial_x\mathcal{B}^x_k)_{L^2(\Omega_x)}\right] \tag{32}$$

and similarly for $\mathbf{M}_y$, $\mathbf{K}_y$. These matrices are symmetric and positive definite as Gram matrices of certain sets of linearly independent functions. Under the simple geometrical mapping, we assume that we can express the first two equations of (31) in terms of (32) as

$$\mathbf{M} = \mathbf{M}_x \otimes \mathbf{M}_y \qquad \mathbf{K} = \mathbf{K}_x \otimes \mathbf{M}_y + \mathbf{M}_x \otimes \mathbf{K}_y \tag{33}$$

For simplicity, let us consider the case where forcing term f is time-independent, and we can assume $f = 0$. In the implicit scheme, we have

$$\begin{aligned}
\left(u_{n+\frac{1}{2}}, v\right) + \frac{\tau}{2}\left(\frac{\partial u_{n+\frac{1}{2}}}{\partial x}, \frac{\partial v}{\partial x}\right) &= (u_n, v) - \frac{\tau}{2}\left(\frac{\partial u_n}{\partial y}, \frac{\partial v}{\partial y}\right) \\
(u_{n+1}, v) + \frac{\tau}{2}\left(\frac{\partial u_{n+1}}{\partial y}, \frac{\partial v}{\partial y}\right) &= \left(u_{n+\frac{1}{2}}, v\right) - \frac{\tau}{2}\left(\frac{\partial u_{n+\frac{1}{2}}}{\partial x}, \frac{\partial v}{\partial x}\right)
\end{aligned} \tag{34}$$

which results in the following algebraic relationships:

$$\begin{aligned}
\left(\mathbf{M} + \frac{\tau}{2}\mathbf{K}_x \otimes \mathbf{M}_y\right)\, \mathbf{u}_{n+\frac{1}{2}} &= \left(\mathbf{M} - \frac{\tau}{2}\mathbf{M}_x \otimes \mathbf{K}_y\right)\, \mathbf{u}_n \\
\left(\mathbf{M} + \frac{\tau}{2}\mathbf{M}_x \otimes \mathbf{K}_y\right)\, \mathbf{u}_{n+1} &= \left(\mathbf{M} - \frac{\tau}{2}\mathbf{K}_x \otimes \mathbf{M}_y\right)\, \mathbf{u}_{n+\frac{1}{2}}
\end{aligned} \tag{35}$$

Since $\mathbf{M} = \mathbf{M}_x \otimes \mathbf{M}_y$,

$$\begin{aligned}
\left[\left(\mathbf{M}_x + \frac{\tau}{2}\mathbf{K}_x\right) \otimes \mathbf{M}_y\right]\, \mathbf{u}_{n+\frac{1}{2}} &= \left[\mathbf{M}_x \otimes \left(\mathbf{M}_y - \frac{\tau}{2}\mathbf{K}_y\right)\right]\, \mathbf{u}_n \\
\left[\mathbf{M}_x \otimes \left(\mathbf{M}_y + \frac{\tau}{2}\mathbf{K}_y\right)\right]\, \mathbf{u}_{n+1} &= \left[\left(\mathbf{M}_x - \frac{\tau}{2}\mathbf{K}_x\right) \otimes \mathbf{M}_y\right]\, \mathbf{u}_{n+\frac{1}{2}}
\end{aligned} \tag{36}$$

Let us denote

$$\begin{aligned} \mathbf{S}_x^+ &= \mathbf{M}_x + \frac{\tau}{2}\mathbf{K}_x \qquad & \mathbf{S}_x^- &= \mathbf{M}_x - \frac{\tau}{2}\mathbf{K}_x \\ \mathbf{S}_y^+ &= \mathbf{M}_y + \frac{\tau}{2}\mathbf{K}_y \qquad & \mathbf{S}_y^- &= \mathbf{M}_y - \frac{\tau}{2}\mathbf{K}_y \end{aligned} \tag{37}$$

Then, we can write

$$\begin{aligned} \left[\mathbf{S}_x^+ \otimes \mathbf{M}_y\right] \mathbf{u}_{n+\frac{1}{2}} &= \left[\mathbf{M}_x \otimes \mathbf{S}_y^-\right] \mathbf{u}_n \\ \left[\mathbf{M}_x \otimes \mathbf{S}_y^+\right] \mathbf{u}_{n+1} &= \left[\mathbf{S}_x^- \otimes \mathbf{M}_y\right] \mathbf{u}_{n+\frac{1}{2}} \end{aligned} \tag{38}$$

We can finally combine the two steps:

$$\mathbf{u}_{n+1} = \left[\mathbf{M}_x \otimes \mathbf{S}_y^+\right]^{-1} \left[\mathbf{S}_x^- \otimes \mathbf{M}_y\right] \left[\mathbf{S}_x^+ \otimes \mathbf{M}_y\right]^{-1} \left[\mathbf{M}_x \otimes \mathbf{S}_y^-\right] \mathbf{u}_n \tag{39}$$

which can be simplified by using the properties of the Kronecker product:

- $(\mathbf{A} \otimes \mathbf{B})^{-1} = \mathbf{A}^{-1} \otimes \mathbf{B}^{-1}$
- $(\mathbf{A} \otimes \mathbf{B})(\mathbf{C} \otimes \mathbf{D}) = (\mathbf{AC}) \otimes (\mathbf{BD})$ whenever the products make sense.

Using these, we conclude that

$$\begin{aligned} &\left[\mathbf{M}_x \otimes \mathbf{S}_y^+\right]^{-1} \left[\mathbf{S}_x^- \otimes \mathbf{M}_y\right] \left[\mathbf{S}_x^+ \otimes \mathbf{M}_y\right]^{-1} \left[\mathbf{M}_x \otimes \mathbf{S}_y^-\right] = \\ &\left[\mathbf{M}_x^{-1} \otimes \left(\mathbf{S}_y^+\right)^{-1}\right] \left[\mathbf{S}_x^- \otimes \mathbf{M}_y\right] \left[\left(\mathbf{S}_x^+\right)^{-1} \otimes \mathbf{M}_y^{-1}\right] \left[\mathbf{M}_x \otimes \mathbf{S}_y^-\right] = \\ &\left[\mathbf{M}_x^{-1} \otimes \left(\mathbf{S}_y^+\right)^{-1}\right] \left[\mathbf{S}_x^- \left(\mathbf{S}_x^+\right)^{-1} \otimes \mathbf{I}\right] \left[\mathbf{M}_x \otimes \mathbf{S}_y^-\right] = \\ &\left[\mathbf{M}_x^{-1} \otimes \left(\mathbf{S}_y^+\right)^{-1}\right] \left[\mathbf{S}_x^- \left(\mathbf{S}_x^+\right)^{-1} \mathbf{M}_x \otimes \mathbf{S}_y^-\right] = \\ &\left[\mathbf{M}_x^{-1}\mathbf{S}_x^- \left(\mathbf{S}_x^+\right)^{-1} \mathbf{M}_x\right] \otimes \left[\left(\mathbf{S}_y^+\right)^{-1} \mathbf{S}_y^-\right] \end{aligned} \tag{40}$$

Since the eigenvalues of $\mathbf{A} \otimes \mathbf{B}$ are products of eigenvalues of $\mathbf{A}$ and $\mathbf{B}$, we only seek to determine the eigenvalues of the above two matrices. The first matrix is similar to $\mathbf{S}_x^- \left(\mathbf{S}_x^+\right)^{-1}$ and, thus, has the same eigenvalues. Furthermore, $\mathbf{AB}$ and $\mathbf{BA}$ always have the same spectrum, so $\mathbf{S}_x^- \left(\mathbf{S}_x^+\right)^{-1}$ has the same eigenvalues as $\left(\mathbf{S}_x^+\right)^{-1} \mathbf{S}_x^-$. By Lemma 3 (see Appendix A), the eigenvalues λ of $\left(\mathbf{S}_x^+\right)^{-1} \mathbf{S}_x^-$ and $\left(\mathbf{S}_y^+\right)^{-1} \mathbf{S}_y^-$ satisfy $|\lambda| < 1$, so the full matrix of the single step has a spectral radius of less than 1. Thus, the implicit ADS scheme is unconditionally stable.

5. Conclusion

In this paper, we introduce mixed space-time discretizations based on the alternating direction method for isogeometric discretizations. We introduce intermediate time-steps to use the Kronecker product structure to invert in linear cost of a sequence of semi-implicit discretizations over time. The resulting isogeometric implicit alternating direction method is unconditionally stable for the heat transfer problem in 2D with an arbitrary time-step size. This was verified theoretically and numerically.

Extending the presented method to a more general context poses some challenges. The Kronecker product structure of the matrix required by the alternating directions solver imposes some rather considerable restrictions on the geometry of the domain as well as the problems themselves. Although it is possible to extend our approach to domains that can be parameterized in such a way that the Jacobian of the map is a product of univariate functions, applying it on arbitrarily complicated domains remains an open problem. For similar reasons, the arbitrary variable diffusivity coefficient in the heat equation can break the Kronecker product structure. Nevertheless, the proposed method (when applicable) can greatly decrease computational costs while retaining good stability properties.

Acknowledgments

This work is supported by National Science Center, Poland – Grant No. 2017/26/M/ST1/ 00281.

A. Lemmas

Lemma 2. *Let* $\mathbf{A}$, $\mathbf{B}$ *be symmetric and positive-semidefinite. Then,* $\mathbf{AB}$ *has nonnegative eigenvalues.*

Proof. Exercise 7.2.P21 in [22]. □

Lemma 3. *Let* $\mathbf{A}$, $\mathbf{B}$ *be symmetric and positive-definite. For each eigenvalue* λ *of* $(\mathbf{A}+\mathbf{B})^{-1}(\mathbf{A}-\mathbf{B})$, *we have* $|\lambda| < 1$.

Proof. Let $\lambda \neq 0$ be such an eigenvalue, and let $\mathbf{x}$ be the corresponding eigenvector. Then,

$$(\mathbf{A}+\mathbf{B})^{-1}(\mathbf{A}-\mathbf{B})\,\mathbf{x} = \lambda\mathbf{x} \tag{41}$$

and so

$$\begin{aligned}(\mathbf{A}-\mathbf{B})\,\mathbf{x} &= \lambda\,(\mathbf{A}+\mathbf{B})\,\mathbf{x}\\ (1-\lambda)\mathbf{Ax} &= (1+\lambda)\mathbf{Bx}\end{aligned} \tag{42}$$

Since $\mathbf{B}$ is positive-definite, then it is nonsingular; thus, $\mathbf{Bx} \neq \mathbf{0}$. Thus, $\lambda \neq 1$. Multiplying by $\mathbf{x}^{\mathrm{T}}$ on the left gives

$$\mathbf{x}^{\mathrm{T}}\mathbf{Ax} = \frac{1+\lambda}{1-\lambda}\,\mathbf{x}^{\mathrm{T}}\mathbf{Bx} \tag{43}$$

Since $\mathbf{A}$ and $\mathbf{B}$ are positive definite, both products are positive; thus, $\lambda \in \mathbb{R}$ and

$$\frac{1+\lambda}{1-\lambda} > 0 \Longrightarrow \lambda^2 < 1 \iff |\lambda| < 1 \tag{44}$$

□

B. Linear computational cost solver

Gram matrix $\mathcal{M} = \mathcal{M}^x \otimes \mathcal{M}^y$ (7) is the Kronecker product of two Gram matrices of the one-dimensional B-spline basis functions.

These one-dimensional mass matrices have entries that correspond to the integrals of the multiplication of the one-dimensional B-spline basis functions. These B-spline basis functions of an order of p have local support over $p+1$ elements, so one-dimensional mass matrices $\mathcal{M}^x$, $\mathcal{M}^y$ have a banded structure.

$$\mathcal{M}^x_{ij} = 0 \iff |i-j| > p \tag{45}$$

$$\begin{bmatrix} \mathcal{M}^x_{11} & \mathcal{M}^x_{12} & \mathcal{M}^x_{13} & \mathcal{M}^x_{14} & 0 & 0 & \cdots & 0 \\ \mathcal{M}^x_{21} & \mathcal{M}^x_{22} & \mathcal{M}^x_{23} & \mathcal{M}^x_{24} & \mathcal{M}^x_{25} & 0 & \cdots & 0 \\ \mathcal{M}^x_{31} & \mathcal{M}^x_{32} & \mathcal{M}^x_{33} & \mathcal{M}^x_{34} & \mathcal{M}^x_{35} & \mathcal{M}^x_{36} & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & \dots & \dots & \mathcal{M}^x_{n(n-3)} & \mathcal{M}^x_{n(n-2)} & \mathcal{M}^x_{n(n-1)} & \mathcal{M}^x_{nn} \end{bmatrix}$$

where $\mathcal{M}^x_{ij} = \left(B^x_i, B^x_j\right)$. The same applies for $\mathcal{M}^y_{ij}$.

The Kronecker product structure of the matrix allows us to perform the following trick. Rather than solving a 2D problem, we can solve two one-dimensional problems with multiple right-hand sides.

$$\begin{bmatrix} \mathcal{M}^x_{11} & \mathcal{M}^x_{12} & \mathcal{M}^x_{13} & \mathcal{M}^x_{14} & 0 & \cdots & 0 \\ \mathcal{M}^x_{21} & \mathcal{M}^x_{22} & \mathcal{M}^x_{23} & \mathcal{M}^x_{24} & \mathcal{M}^x_{25} & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & & \vdots \\ 0 & \dots & 0 & \mathcal{M}^x_{n(n-3)} & \mathcal{M}^x_{n(n-2)} & \mathcal{M}^x_{n(n-1)} & \mathcal{M}^x_{nn} \end{bmatrix} \begin{bmatrix} y_{11} & y_{21} & \cdots & y_{m1} \\ y_{12} & y_{22} & \cdots & y_{m1} \\ \vdots & \vdots & \ddots & \vdots \\ y_{1n} & y_{2n} & \cdots & y_{mn} \end{bmatrix} = \begin{bmatrix} b_{11} & b_{21} & \cdots & b_{m1} \\ b_{12} & b_{22} & \cdots & b_{m2} \\ \vdots & \vdots & \ddots & \vdots \\ b_{1n} & b_{2n} & \cdots & b_{mn} \end{bmatrix}$$

$$\begin{bmatrix} \mathcal{M}^y_{11} & \mathcal{M}^y_{12} & \mathcal{M}^y_{13} & \mathcal{M}^y_{14} & 0 & \cdots & 0 \\ \mathcal{M}^y_{21} & \mathcal{M}^y_{22} & \mathcal{M}^y_{23} & \mathcal{M}^y_{24} & \mathcal{M}^y_{25} & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & & \vdots \\ 0 & \dots & 0 & \mathcal{M}^y_{n(n-3)} & \mathcal{M}^y_{n(n-2)} & \mathcal{M}^y_{n(n-1)} & \mathcal{M}^y_{nn} \end{bmatrix} \begin{bmatrix} x_{11} & \cdots & x_{1n} \\ x_{21} & \cdots & x_{2n} \\ \vdots & \ddots & \vdots \\ x_{m1} & \cdots & x_{mn} \end{bmatrix} = \begin{bmatrix} y_{11} & y_{12} & \cdots & y_{1n} \\ y_{21} & y_{22} & \cdots & y_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ y_{m1} & y_{m2} & \cdots & y_{mn} \end{bmatrix}$$

where $\mathcal{M}^x_{ij} = \left(B^x_i, B^x_j\right)$ and $\mathcal{M}^y_{ij} = \left(B^y_i, B^y_j\right)$. The dimensions of the first problem are $n \times n$, where n is the number of B-spline basis functions along the x-axis, and we have m right-hand sides, where m is the number of B-spline basis functions along the y-axis. The computational complexity of the factorization of such a system is $O(n \times m) = O(N)$ [30]. We have an analogous situation in the second problem; namely, an $m \times m$ system with n right-hand sides. This results in $O(m \times n) = O(N)$ linear computational complexity.

This strategy delivers a solution to the isogeometric L^2 orthogonal projection problem with linear $O(N)$ computational cost. This solution's method improves on the standard direct solver cost estimates for ($O(N^{1.5})$ in 2D and $O(N^2)$ in 3D; see [7]) for the factorization of the global problem.

References

[1] Bazilevs Y., Beirao da Veiga L., Cottrell J.A., Hughes T.J.R., Sangalli G.: Isogeometric analysis: Approximation, stability and error estimates for h-refined meshes, *Mathematical Methods and Models in Applied Sciences*, vol. 16, pp. 1031–1090, 2011.

[2] Bazilevs Y., Calo V.M., Cottrell J.A., Hughes T.J.R., Reali A., Scovazzi G.: Variational multiscale residual-based turbulence modeling for large eddy simulation of incompressible flows, *Computer Methods in Applied Mechanics and Engineering*, vol. 197, pp. 173–201, 2007.

[3] Bazilevs Y., Calo V.M., Zhang Y., Hughes T.J.R.: Isogeometric Fluid-Structure Interaction Analysis with Applications to Arterial Blood Flow, *Computational Mechanics*, vol. 38, pp. 310–322, 2006.

[4] Birkhoff G., Varga R.S., Young D.: Alternating Direction Implicit Methods, *Advances in Computers*, vol. 3, pp. 189–273, 1962.

[5] Calo V.M., Brasher N., Bazilevs Y., Hughes T.J.R.: Multiphysics model for blood flow and drug transport with application to patient-specific coronary artery flow, *Computational Mechanics*, vol. 43(1), pp. 161–177, 2008.

[6] Chang K., Hughes T.J.R., Calo V.M.: Isogeometric variational multiscale large--eddy simulation of fully-developed turbulent flow over a wavy wall, *Computers & Fluids*, vol. 68, pp. 94–104, 2012.

[7] Collier N., Pardo D., Dalcin L., Paszyński M., Calo V.M.: The cost of continuity: A study of the performance of isogeometric finite elements using direct solvers, *Computer Methods in Applied Mechanics and Engineering*, vol. 213–216, pp. 353–361, 2012.

[8] Cottrell J.A., Hughes T.J.R., Bazilevs Y.: Isogeometric Analysis: Toward Integration of CAD and FEA, John Wiley and Sons, 2009.

[9] Dedè L., Borden M.J., Hughes T.J.R.: *Isogeometric Analysis for Topology Optimization with a Phase Field Model*, ICES REPORT 11–29, The Institute for Computational Engineering and Sciences, The University of Texas at Austin, 2011.

[10] Dedè L., Hughes T.J.R., Lipton S., Calo V.M.: Structural Topology Optimization With Isogeometric Analysis in a Phase Field Approach. In: *16th U.S. National Conference on Theoretical and Applied Mechanics, USNCTAM 2010*, 2010.

[11] Douglas J., Rachford H.: On the Numerical Solution of Heat Conduction Problems in Two and Three Space Variables, *Transactions of American Mathematical Society*, vol. 82, pp. 421–439, 1956.

[12] Duddu R., Lavier L., Hughes T.J.R., Calo V.M.: A finite strain Eulerian formulation for compressible and nearly incompressible hyperelasticity using high-order B-spline finite elements, *International Journal of Numerical Methods in Engineering*, vol. 89(6), pp. 762–785, 2012.

[13] Gómez H., Calo V.M., Bazilevs Y., Hughes T.J.R.: Isogeometric analysis of the Cahn–Hilliard phase-field model, *Computer Methods in Applied Mechanics and Engineering*, vol. 197, pp. 4333–4352, 2008.

[14] Gómez H., Hughes T.J.R., Nogueira X., Calo V.M.: Isogeometric analysis of the isothermal Navier–Stokes–Korteweg equations, *Computer Methods in Applied Mechanics and Engineering*, vol. 199, pp. 1828–1840, 2010.

[15] Gao L., Calo V.M.: Fast Isogeometric Solvers for Explicit Dynamics, Computer Methods, *Applied Mechanics and Engineering*, vol. 274(1), pp. 19–41, 2014.

[16] Gao L., Calo V.M.: Preconditioners based on the Alternating-Direction-Implicit algorithm for the 2D steady-state diffusion equation with orthotropic heterogeneous coefficients, *Journal of Computational and Applied Mathematics*, vol. 273(1), pp. 274–295, 2015.

[17] Gao L.: Kronecker Products on Preconditioning, PhD. Thesis, King Abdullah University of Science and Technology 2013.

[18] Guermond J.L., Minev P., Shen J.: An overview of projection methods for incompressible flows, *Computer Methods in Applied Mechanics and Engineering*, vol. 195, pp. 6011–6054, 2006.

[19] Guermond J.L., Minev P.: A new class of fractional step techniques for the incompressible Navier-Stokes equations using direction splitting, *Comptes Rendus Mathematique*, vol. 348(9–10), pp. 581–585, 2010.

[20] Gurgul G., Woźniak M., Łoś M., Szeliga D., Paszyński M.: Open source JAVA implementation of the parallel multi-thread alternating direction isogeometric L^2 projections solver for material science simulations, *Computer Methods in Material Science*, vol. 17(1) 2017.

[21] Hairer E., Wanner G.: *Solving Ordinary Differential Equations II: Stiff and Differential-Algebraic Problems* (second ed.), Berlin, Springer-Verlag, section IV.3, 1996.

[22] Horn R.A., Johnson C.R.: *Matrix Analysis*, Cambridge University Press 1990.

[23] Hossain S., Hossainy S.F.A., Bazilevs Y., Calo V.M., Hughes T.J.R.: Mathematical modeling of coupled drug and drug-encapsulated nanoparticle transport in patient-specific coronary artery walls, *Computational Mechanics*, vol. 49, pp. 213–242, 2011. https://doi.org/10.1007/s00466-011-0633-2.

[24] Hsu M.-C., Akkerman I., Bazilevs Y.: High-performance computing of wind turbine aerodynamics using isogeometric analysis, *Computers and Fluids*, vol. 49(1), pp. 93–100, 2011.

[25] Łoś M., Paszyński M., Kłusek A., Dzwinel W.: Application of fast isogeometric L^2 projection solver for tumor growth simulations, *Computer Methods in Applied Mechanics and Engineering*, vol. 316, pp. 1257–1269, 2017.

[26] Łoś M., Woźniak M., Paszyński M., Dalcin L., Calo V.M.: Dynamics with Matrices Possessing Kronecker Product Structure, *Procedia Computer Science*, vol. 51, pp. 286–295, 2015.

[27] Łoś M., Woźniak M., Paszyński M., Lenharth A., Pingali K.: IGA-ADS : Isogeometric analysis FEM using ADS solver, *Computer & Physics Communications*, vol. 217, pp. 99–116, 2017.

[28] Łoś M., Behnoudfar P., Paszyński M., Calo V.M.: Fast isogeometric solvers for hyperbolic wave propagation problems, *Computers & Mathematics with Applications*, vol. 80(1), pp. 109–120, 2020.

[29] Łoś M.,Paszyński M., Applications of Alternating Direction Solver for simulations of time-dependent problems, *Computer Science*, vol. 18(2), pp. 117–128, 2017.

[30] Paszyński M.: *Fast Solvers for Mesh-Based Computations*, Taylor & Francis, CRC Press, 2016.

[31] Peaceman D.W., Rachford Jr. H.H.: The Numerical Solution of Parabolic and Elliptic Differential Equations, *Journal of Society for Industrial and Applied Mathematics*, vol. 3(1), pp. 28–41, 1955.

[32] Piegl L., Tiller W.: *The NURBS Book*, Second Edition, Springer-Verlag, New York, 1997.

[33] Wachspress E.L., Habetler G.J.: An alternating-direction-implicit iteration technique, *Journal of Society for Industrial and Applied Mathematics*, vol. 8(2), pp. 403–423, 1960.

[34] Woźniak M., Łoś M., Paszyński M., Dalcin L.D., Calo V.M.: Parallel Fast Isogeometric Solvers for Explicit Dynamics, *Computing and Informatics*, vol. 36, pp. 1001–1022, 2017.

Affiliations

Grzegorz Gurgul
AGH University of Science and Technology, Department of Computer Sciences, Krakow, Poland

Marcin Łoś
AGH University of Science and Technology, Department of Computer Sciences, Krakow, Poland

Maciej Paszyński
AGH University of Science and Technology, Department of Computer Sciences, Krakow, Poland, maciej.paszynski@agh.edu.pl, ORCID ID: http://orcid.org/0000-0001-7766-6052

Victor Calo
Curtin University, Perth, Western Australia, vmcalo@gmail.com

Received: 23.05.2020
Revised: 22.07.2020
Accepted: 24.07.2020