A parallel-in-time isogeometric BEM for the 3D wave equation using B-spline linear multistep methods

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Introduction

Introduction

Topic of this talk

We present a high-order and easily parallelizable numerical scheme for the wave equation in the interior/exterior of a bounded 3D domain.

Possible real-world application: acoustic propagation and scattering.

Numerical tools

Isogeometric analysis + boundary element method (IgA-BEM), novel time discretization inspired by convolution quadrature.

Comparison with state of the art

Simpler scheme and 10-100x greater efficiency in our benchmarks.

Wave equation

Consider the wave equation with homogeneous wave speed $c > 0$

$$\partial_{tt} u(\boldsymbol{x}, t) = c^2 \Delta u(\boldsymbol{x}, t), \quad \boldsymbol{x} \in \mathbb{R}^3 \setminus \Omega, \quad t \in [0, T],$$

for $\Omega \subset \mathbb{R}^3$ bounded domain with piecewise smooth boundary Γ.
An efficient way to handle such exterior problems is to reformulate the PDE (with boundary conditions) as a boundary integral equation:

$$\frac{1}{2} u(\boldsymbol{x}, t) + \int_0^t \int_\Gamma \frac{\partial \Phi}{\partial \boldsymbol{\nu}}(\boldsymbol{x} - \boldsymbol{y}, t - \tau)\, u(\boldsymbol{y}, \tau)\, d\Gamma_{\boldsymbol{y}}\, d\tau = \int_0^t \int_\Gamma \Phi(\boldsymbol{x} - \boldsymbol{y}, t - \tau)\, \frac{\partial u}{\partial \boldsymbol{\nu}}(\boldsymbol{y}, \tau),$$

outward normal $\boldsymbol{\nu}$, $\quad r = \|\boldsymbol{x} - \boldsymbol{y}\|, \quad \Phi(\boldsymbol{x} - \boldsymbol{y}, t - \tau) = \delta(t - \tau - r/c)(4\pi c r)^{-1}$

for all $\boldsymbol{x} \in \Gamma$, assuming homogeneous initial conditions (δ Dirac delta).

Discretization in space

Collocation schemes

Space discretization: we approximate e.g. $u(\boldsymbol{x}; t)$ by

$$u(\boldsymbol{x}; t) \approx \sum_{i=1}^{N} a_i(t) B_i(\boldsymbol{x})$$

for some basis functions $B_1, \ldots, B_N$. Enforcing the boundary integral equation at $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N \in \Gamma$ gives a linear system for the $a_i(t)$.

Isogeometric analysis (IgA)

We use the same kind of functions to parametrize the boundary Γ and for the basis B_i. We use B-splines, i.e. bell-shaped multivariate piecewise polynomials of degree k with regular joints (usually C^{k-1}).

Discretization in space

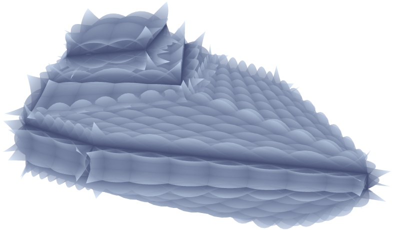


Figure: Quadratic tensor-product B-splines mapped from parametric domains to boundary faces.

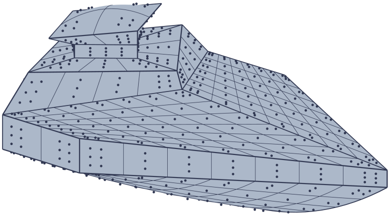
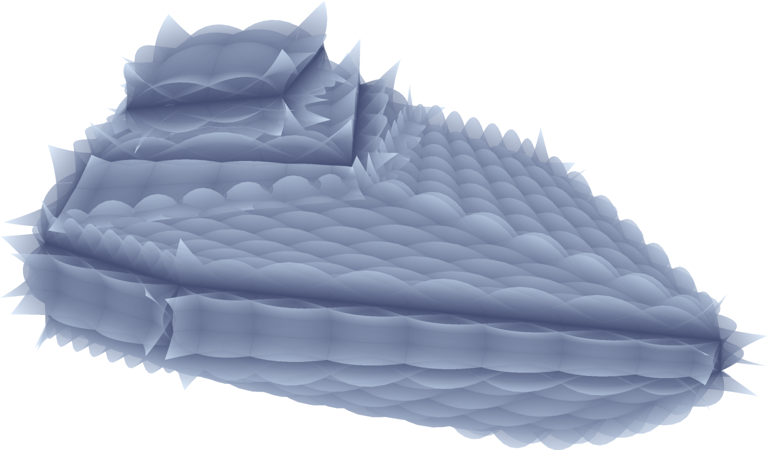


Figure: Collocation points where the boundary integral equation is enforced: modified Greville nodes.

Discretization in space



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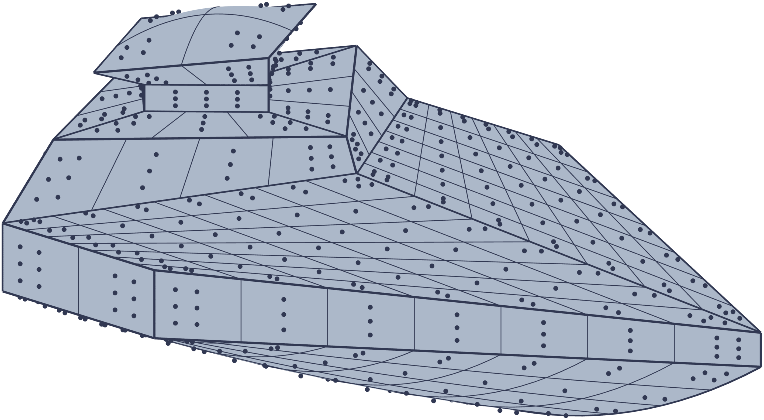

Figure: Collocation points where the boundary integral equation is enforced: modified Greville nodes.

Discretization in time

Space-time collocation is possible, but highly challenging due to the Dirac delta in the integration kernel (assume $c = 1$ from now on):

$$k(r, t-\tau) = \frac{\delta(t-\tau-r)}{4\pi r}, \qquad r = \|\boldsymbol{x} - \boldsymbol{y}\|.$$

Instead, by the inverse Laplace transform,

$$k(r, t-\tau) = \frac{1}{2\pi i} \int_{\mathcal{C}} \frac{e^{s(t-\tau-r)}}{4\pi r}\, ds, \qquad \mathcal{C} = \sigma + i\mathbb{R}.$$

Substituting into the boundary integral equation, we can now collocate in space by integrating (w.r.t. $d\Gamma_{\boldsymbol{y}}$) against the more regular kernel

$$e^{s(t-\tau)} \frac{e^{-sr}}{4\pi r} \qquad \text{linked to the Helmholtz equation.}$$

Convolution quadrature

This is the first step of Convolution Quadrature (CQ), the main Laplace-domain technique for the discretization of time-domain boundary integral equations (TDBIE), introduced by Lubich in 1988.

After a few more steps (to be explained soon), the s-indexed family

$$x_s'(t) = s\, x_s(t) + \varphi(t)$$

of ODEs appears in the TDBIE and has to be solved numerically. This is the key discretization step alternative to naive collocation in time.

Desirable properties of ODE solver:

- A-stability, mandatory in the case of wave equation
- High order of convergence with respect to timestep Δt

Linear multistep formulas

Lubich's original formulation of CQ is for a family of ODE solvers known as linear multistep formulas, such as the A-stable first-order backward Euler method with initial condition $x_{s,0} = 0$:

$$x_{s,n} - x_{s,n-1} = \Delta t(s\, x_{s,n} + \varphi_n)$$

or the A-stable second-order BDF2 with $x_{s,-1} = x_{s,0} = 0$:

$$\frac{3}{2}x_{s,n} - 2x_{s,n-1} + \frac{1}{2}x_{s,n-2} = \Delta t(s\, x_{s,n} + \varphi_n).$$

Dahlquist's second barrier

There are no A-stable linear multistep formulas of order > 2.

Historically, convolution quadrature based on Runge-Kutta schemes was introduced to overcome the barrier. The price to pay is complexity.

Boundary value methods

A subtle point about linear multistep formulas is that Dahlquist's second barrier only applies to discrete initial value problems, where information propagates forward in time, preserving causality.

Linear multistep formulas that combine information from the past and the future into a non-causal global-in-time linear system such as

$$\alpha_{-1}\, x_{s,n-1} + \alpha_0\, x_{s,n} + \alpha_1\, x_{s,n+1} = \Delta t \sum_{j=-1}^{1} \beta_j (s\, x_{s,n+j} + \varphi_{n+j}).$$

subject to both initial conditions and end conditions give boundary value methods (BVM) that break the barrier. For an introduction to BVMs, see the 1998 monograph by Brugnano and Trigiante.

Research question

Can we combine the mature theory of BVMs with CQ?

Convolution quadrature and functions of matrices

Convolution quadrature and functions of matrices

Convolution quadrature is typically derived using formal power series, but this approach does not work for BVMs. We had to find a suitable alternative, and succeeded using the theory of matrix functions.

Recall the Cauchy integral theorem for matrices: for any $A \in \mathbb{C}^{n \times n}$,

$$f(A) = \frac{1}{2\pi i} \int_{\mathcal{C}} f(z)(zI - A)^{-1} \, dz$$

where f is analytic on and inside a closed contour $\mathcal{C}$ that encloses $\Lambda(A)$.

Ignoring the space discretization (for simplicity), convolution quadrature is designed to approximate convolution integrals

$$y(t) = (k * \varphi)(t) = \int_0^t k(t - \tau)\varphi(\tau) \, d\tau, \qquad t \in [0, T].$$

Convolution quadrature and functions of matrices

We introduce a uniform discretization of $[0, T]$ with N timesteps of constant size Δt, and vectors

$$\boldsymbol{y} = \begin{pmatrix} y_0 \\ y_1 \\ \vdots \\ y_N \end{pmatrix} = \begin{pmatrix} y(0) \\ y(\Delta t) \\ \vdots \\ y(T) \end{pmatrix} \qquad \boldsymbol{\varphi} = \begin{pmatrix} \varphi_0 \\ \varphi_1 \\ \vdots \\ \varphi_N \end{pmatrix} = \begin{pmatrix} \varphi(0) \\ \varphi(\Delta t) \\ \vdots \\ \varphi(T) \end{pmatrix}$$

We seek convolution weights $\{\omega_j\}_{j=0,\dots,N}$ such that

$$y_n \approx \sum_{j=0}^{n} \omega_{n-j}\, \varphi_j \qquad \boldsymbol{y} \approx \begin{pmatrix} \omega_0 & 0 & \dots & 0 & 0 \\ \omega_1 & \omega_0 & \dots & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots \\ \omega_{N-1} & \dots & \dots & \omega_0 & 0 \\ \omega_N & \omega_{N-1} & \dots & \omega_1 & \omega_0 \end{pmatrix} \boldsymbol{\varphi}$$

Convolution quadrature and functions of matrices

Let L_j be the matrix with ones on the j-th subdiagonal, and zeros everywhere else. The identity $L_j = (L_1)^j$ implies $\boldsymbol{y} \approx \gamma(L_1)\boldsymbol{\varphi}$, with

$$\gamma(z) = \omega_0 + \omega_1 z + \cdots + \omega_N z^N.$$

Let $K(s)$ be the Laplace transform of $k(t)$. By the inversion formula,

$$y(t) = \int_0^t k(t-\tau)\varphi(\tau)\,d\tau = \int_0^t \frac{1}{2\pi i}\int_{\mathcal{C}} K(s)e^{s(t-\tau)}\,ds\,\varphi(\tau)\,d\tau$$

$$= \frac{1}{2\pi i}\int_{\mathcal{C}} K(s)\left(\int_0^t e^{s(t-\tau)}\phi(\tau)\,d\tau\right)ds =: \frac{1}{2\pi i}\int_{\mathcal{C}} K(s)\,x_s(t)\,ds$$

with $\mathcal{C} = \sigma + i\mathbb{R}$ and $\sigma > 0$.

Convolution quadrature and functions of matrices

By Duhamel's principle, $x_s(t)$ is the solution of

$$x_s'(t) = s\, x_s(t) + \varphi(t), \qquad x_s(0) = 0.$$

Let $\gamma(z)$ be the characteristic quotient of a BDF method with k steps to discretize this s-indexed family of ODEs. For example, $k = 2$ gives

$$\frac{3}{2} x_{s,n} - 2x_{s,n-1} + \frac{1}{2} x_{s,n-2} = \Delta t(s\, x_{s,n} + \varphi_n).$$

with $\gamma(z) = (3/2) - 2z + (1/2)z^2$. In matrix notation,

$$\gamma(L_1)\boldsymbol{x}_s = \Delta t(s\,\boldsymbol{x}_s + \boldsymbol{\varphi}) \qquad (\gamma(L_1)/(\Delta t) - sI)\boldsymbol{x}_s = \boldsymbol{\varphi}$$

$$\boldsymbol{x}_s = (\gamma(L_1)/(\Delta t) - sI)^{-1}\boldsymbol{\varphi}.$$

Convolution quadrature and functions of matrices

Substituting $\boldsymbol{x}_s$ back into the contour integral, we get

$$\boldsymbol{y} \approx \frac{1}{2\pi i} \int_{\mathcal{C}} K(s) \boldsymbol{x}_s \, ds = \frac{1}{2\pi i} \int_{\mathcal{C}} K(s) (\gamma(L_1)/(\Delta t) - sI)^{-1} \, ds \, \boldsymbol{\varphi}.$$

After reversing $\mathcal{C}$ to enclose (at infinity) the spectrum of $\gamma(L_1)/(\Delta t)$, Cauchy's integral theorem for matrices gives

$$\boldsymbol{y} \approx K\big(\gamma(L_1)/(\Delta t)\big) \boldsymbol{\varphi}.$$

A function of a lower triangular Toeplitz matrix is still lower triangular and Toeplitz: we have proved that convolution weights ω_j exist and can be found as the first column of $K\big(\gamma(L_1)/(\Delta t)\big)$.

Diagonalizing B-spline linear multistep methods

Diagonalizable boundary value methods

In the case of a linear multistep boundary value method (BVM), there exist matrices A_L, A_R, with A_L non-triangular, such that

$$A_L \boldsymbol{x}_s = \Delta t \, A_R (s \boldsymbol{x}_s + \varphi), \qquad \boldsymbol{x}_s = (A_R^{-1} A_L / (\Delta t) - sI)^{-1} \varphi.$$

Repeating the same argument as before,

$$\boldsymbol{y} \approx K\big(A/(\Delta t)\big)\varphi \qquad \text{for } A = A_R^{-1} A_L.$$

This time the matrix $K\big(A/(\Delta t)\big)$ is neither triangular nor Toeplitz, so convolution weights ω_j do not exist. Crucially, however, matrices A given by BVMs can be diagonalizable, unlike L_1 which is a Jordan block.

We have traded the causal triangular structure for diagonalizability! It turns out that diagonalizability is extremely useful in the discretization of time-domain boundary integral equations.

Diagonalizable boundary value methods

The matrix $K\big(A/(\Delta t)\big)$ is found by factoring A as

$$A = V \Lambda V^{-1}, \qquad \Lambda = \operatorname{diag}(\lambda_1, \dots, \lambda_N),$$

so that $K\big(A/(\Delta t)\big) = V\, K\big(\Lambda/(\Delta t)\big)\, V^{-1}$.

Our numerical scheme for TDBIEs

Time integrals are discretized by our CQ-like approach based on diagonalizable BVMs. Boundary integrals are discretized by isogeometric collocation. Each λ_i leads to a completely decoupled subproblem that can be solved in parallel.

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Solution: much slower growth with symmetric B-spline BVMs

Symmetric B-spline BVMs

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B-SPLINE LINEAR MULTISTEP METHODS AND THEIR CONTINUOUS EXTENSIONS*

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BVM coefficients are obtained by B-spline collocation in time. Splines of odd degree lead to antisymmetric A_L and symmetric A_R (up to end conditions), improving eigenvalue conditioning of $A = A_R^{-1} A_L$.

For example, with cubic B-splines,

$$A_L = \begin{pmatrix} \ddots & \ddots & \ddots & & \\ & -3 & 0 & 3 & \\ & & \ddots & \ddots & \ddots \end{pmatrix} \quad A_R = \begin{pmatrix} \ddots & \ddots & \ddots & & \\ & 1 & 4 & 1 & \\ & & \ddots & \ddots & \ddots \end{pmatrix}$$

Decoupled Helmholtz subproblems

The decoupled space-only subproblems can be seen as isogeometric collocation schemes for the dissipative Helmholtz equation

$$\Delta \hat{u} + \kappa^2 \hat{u} = 0$$

with wave numbers $\kappa = i\lambda(\Delta t)^{-1}$ for all $\lambda \in \Lambda$. This makes our scheme easy to implement once a Helmholtz solver is available.

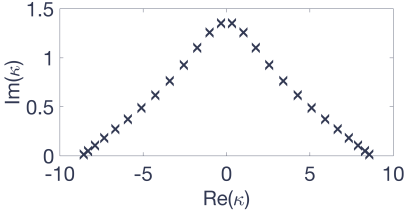


Figure: Helmholtz wave numbers for $\Delta t = 0.2$, $T = 5$, cubic B-spline BVM.

Comparison with Runge-Kutta CQ

We compare the performance of our method with state-of-the-art Runge-Kutta convolution quadrature (RKCQ), in particular parallel-in-time m-stages Radau IIA schemes in the isogeometric setting of Kramer, Marussig, Schanz (2026).

Relative L^2 space-time errors are shown as a function of the number N_H of decoupled Helmholtz subproblems. For RKCQ methods,

$$N_H = N \cdot m.$$

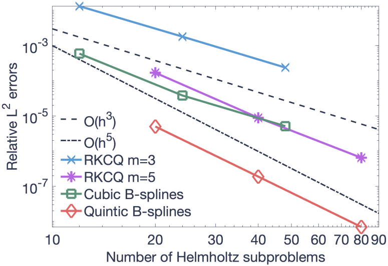
For our B-spline method,

$$N_H = N + 1,$$

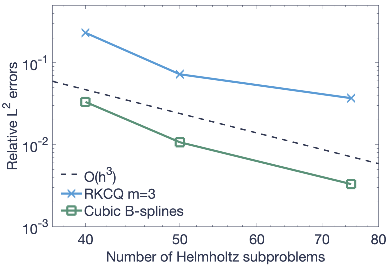
which means that its cost is independent of the BVM order in time.

Comparison with Runge-Kutta CQ

In convergence tests, we subdivide the boundary into elements of size approximately $h \times h$, and choose $\Delta t = 0.5h$.



(a) Wave equation around the unit sphere. Dirichlet BC constant in space, $T = 10$, reference closed-form solution.



(b) Wave equation around the toy boat. Neumann BC from manufactured solution. $T = 5$, cubic splines in space.

Conclusions and outlook

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Our parallel-in-time discretization with B-spline BVMs can be significantly more accurate than state-of-the-art convolution quadrature, such as Runge-Kutta CQ, and is also conceptually simpler. Moreover, it leads to an elegant fully spline-based scheme in both space and time.

Future work

We are now investigating the use of variable timesteps to better resolve localized features of the solution, high-performance computing (HPC) to fully exploit parallelism in time, and hierarchical matrices to speed up the solution of the decoupled Helmholtz subproblems.

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Thank you for your attention!