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## Space-Time Methods for Time-Dependent Partial Differential Equations

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**ABSTRACT.** Modern discretization and solution methods for time-dependent PDEs consider the full problem in space and time simultaneously and aim to overcome limitations of classical approaches by first discretizing in space and then solving the resulting ODE, or first discretizing in time and then solving the PDE in space.

The development of space-time methods for hyperbolic and parabolic differential equation is an emerging and rapidly growing field in numerical analysis and scientific computing. At the first Workshop on this topic in 2017 a large variety of interesting and challenging concepts, methods, and research directions have been presented; now we exchange the new developments.

The focus is on the optimal convergence of discretizations and on efficient error control for space-time methods for hyperbolic and parabolic problems, and on solution methods with optimal complexity. This is complemented by applications in the field of time-dependent stochastic PDEs, non-local material laws in space and time, optimization with time-dependent PDE constraints, and multiscale methods for time-dependent PDEs.

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### Introduction by the Organizers

Space-time finite elements aim for a unified analysis of discretization and solution methods in space and time. The main goal of this research is to develop novel methods with respect to the following paradigms:

- **Discretization:** Develop and analyze discretization methods for parabolic and hyperbolic partial differential equations on the Cartesian product of

the spatial domain and the time interval; methods which can be flexibly adapted to the local space-time behavior of the solution and which may be restricted to cones within the space-time domain.

- **Complexity:** Develop and analyze fast algorithms for solving the arising sparse systems which have less algebraic structure than those which arise in the conventional approaches which often lead to, e.g., block-triangular, block-circulant, or block-Toeplitz matrices.
- **Adaptivity:** Develop and analyze algorithms for full space-time adaptivity on general space-time meshes.
- **Regularity:** Develop a detailed local space-time regularity theory for the solution of parabolic and hyperbolic PDEs which allows to enrich the trial spaces within an adaptive refinement process in an efficient way.
- **Modeling:** Develop and analyze numerical methods for time-dependent stochastic models and a hierarchy of reduced models or multiscale models by intertwining modeling and discretization in space and time. In particular this includes non-local material laws.

Application fields of space-time methods include, in particular, inverse problems and control problems, where iterative solution methods depend on the full space-time information (in particular for the evaluation of the adjoint state equation). The solution of the adjoint problem is also required for efficient and reliable error control. Moreover, a certified model reduction of time-dependent PDEs requires to consider space and time together. These techniques apply, in particular, to time-dependent stochastic PDEs and to multiscale problems, where approximation and solution methods also depend on the full space-time information.

The research on space-time methods is driven by the development of discretizations specially designed for fully coupled approximation schemes together with a strong emphasis on applications for time-dependent PDEs. This includes stochastic PDEs, optimization and hierarchical modeling, where the integrated space-time view is an inherent requirement for analysis and the efficient numerical solution of the problem.

Together, we address the full range of questions arising from space-time discretizations, starting with a rigorous and systematic numerical analysis of the approximation quality and the solution complexity, up to the realization of parallel simulation of challenging applications in engineering and sciences.

## Workshop: Space-Time Methods for Time-Dependent Partial Differential Equations

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## Abstracts

### Fractional Harmonic Maps: Approximation and Convergence

HARBIR ANTIL

(joint work with Sören Bartels, Armin Schikorra)

A fundamental problem in the calculus of variations concerns critical points of energy functionals subject to pointwise constraints. Related applications arise in ferromagnetism to model magnetization fields, liquid crystal theories defining orientations of rod-like molecules, continuum mechanics for describing inextensible rods and unshearable plates, and in quantum mechanics for spin systems.

This talk is based on the article [1] and considers the case of energies related to the fractional Laplace operator. Fractional operators are nonlocal and enable long range interactions. They enforce less smoothness in comparison to their classical counterparts. These features make them attractive for applications leading to certain singularities such as defects in the mathematical description of liquid crystals, which are often modeled by harmonic maps. While some ideas from the treatment of standard, local differential operators can be employed to define stable numerical schemes, new ideas are required to establish the convergence of discrete stationary configurations.

Our point of departure is the fractional Dirichlet energy

$$(1) \quad I[u] = \frac{1}{2} \int_{\Omega} |(-\Delta)^{\frac{s}{2}} u|^2 dx$$

for an appropriate definition of the fractional Laplace operator  $(-\Delta)^{\frac{s}{2}}$  with  $0 < s < 1$ . Here  $\Omega \subset \mathbb{R}^d$  is an open bounded domain with Lipschitz boundary  $\partial\Omega$ . We then consider stationary points for  $I$  subject to a unit-length constraint in the set

$$\mathcal{A} = \{v - \vec{N} \in \tilde{H}^s(\Omega; \mathbb{R}^N) : |v(x)|^2 = 1 \text{ for a.e. } x \in \Omega\},$$

where

$$\tilde{H}^s(\Omega; \mathbb{R}^N) = \{f \in H^s(\mathbb{R}^d; \mathbb{R}^N) : f = 0 \text{ in } \mathbb{R}^d \setminus \Omega\},$$

and  $\vec{N} \in C^\infty(\mathbb{R}^d; \mathbb{R}^N)$  is a fixed vector field that defines a unit-length exterior Dirichlet condition on  $\mathbb{R}^d \setminus \Omega$ . Obviously, a homogeneous boundary condition is incompatible with the unit-length constraint, at least when  $s \in (1/2, 1)$ .

Stationary points for  $I$  in  $\mathcal{A}$  are called *fractional harmonic maps* [5] and are formally characterized by the Euler–Lagrange equations

$$(2) \quad (-\Delta)^s u = \lambda u \text{ in } \Omega, \quad |u|^2 = 1 \text{ in } \Omega, \quad u|_{\mathbb{R}^d \setminus \Omega} = \vec{N},$$

where  $\lambda \in L^1(\Omega)$  is a Lagrange multiplier related to the pointwise unit-length constraint. The function  $\lambda$  depends nonlinearly on the vector field  $u$ , e.g., in the classical case  $s = 1$  we have that  $\lambda = |\nabla u|^2$ . This critical nonlinear dependence requires appropriate arguments to show that accumulation points of bounded sequences of solutions are again solutions of the nonlinear equation. Such stability results are crucial for convergence of numerical approximations.

A useful equivalent characterization of fractional harmonic maps is the weak formulation

$$(3) \quad ((-\Delta)^{\frac{s}{2}} u, (-\Delta)^{\frac{s}{2}} v) = 0$$

for all  $v \in \widetilde{H}^s(\Omega; \mathbb{R}^N)$  satisfying the pointwise orthogonality relation  $u \cdot v = 0$  almost everywhere in  $\Omega$ . If  $N = 3$  then the latter equation is equivalent to

$$(4) \quad ((-\Delta)^{\frac{s}{2}} u, (-\Delta)^{\frac{s}{2}}(u \times \phi)) = 0$$

for all  $\phi \in C_c^\infty(\Omega; \mathbb{R}^3)$ . The latter identity can also be extended to the case  $N \neq 3$ .

Our first result establishes that a limit passage in the nonlinear equation (4) is possible. In particular, if  $\{u_j\}_{j \in \mathbb{N}} \subset \mathcal{A}$ , such that  $u_j \rightharpoonup u$  in an appropriate fractional order Sobolev space, as  $j \rightarrow \infty$ , then

$$(5) \quad ((-\Delta)^{\frac{s}{2}} u_j, (-\Delta)^{\frac{s}{2}}(u_j \times \phi)) \rightarrow ((-\Delta)^{\frac{s}{2}} u, (-\Delta)^{\frac{s}{2}}(u \times \phi))$$

for all  $\phi \in C_c^\infty(\Omega; \mathbb{R}^N)$ . The key challenge here is the fact that due to nonlocality of  $(-\Delta)^s$ , the standard arguments from the case  $s = 1$  cannot be applied.

**Discrete fractional harmonic maps.** The first numerical problem concerns the convergence of discrete fractional harmonic maps as the mesh-sizes of underlying triangulations tend to zero. We consider a sequence  $\{\mathcal{T}_h\}_{h>0}$  of uniformly shape regular triangulations of the polygonal or polyhedral Lipschitz domain  $\Omega \subset \mathbb{R}^d$  with maximal mesh-sizes  $h \rightarrow 0$ . Discrete fractional harmonic maps belong to

$$\mathcal{A}_h = \{v_h - \widetilde{\mathcal{I}}_h \vec{N} \in \mathcal{S}_0^1(\mathcal{T}_h)^N : |v_h(z)|^2 = 1 \text{ for all } z \in \mathcal{N}_h\},$$

where  $\mathcal{S}_0^1(\mathcal{T}_h)$  is the space of piecewise linear, globally continuous functions for a triangulation  $\mathcal{T}_h$  of  $\widetilde{\Omega}$  vanishing in the exterior  $\widetilde{\Omega} \setminus \Omega$ ; the set  $\mathcal{N}_h$  contains the vertices of elements inside  $\Omega$  at which the unit-length constraint is imposed,  $\mathcal{I}_h$  and  $\widetilde{\mathcal{I}}_h$  are the nodal interpolation operators on  $\mathcal{T}_h$  and an extension  $\widetilde{\mathcal{T}}_h$  which provides a triangulation of a domain  $\widetilde{\Omega}$  such that  $\overline{\Omega} \subset \widetilde{\Omega}$  and the support of  $\vec{N}$  is contained in  $\widetilde{\Omega}$ .

The discrete fractional harmonic maps are given by  $u_h \in \mathcal{A}_h$  fulfilling

$$(6) \quad ((-\Delta)^{\frac{s}{2}} u_h, (-\Delta)^{\frac{s}{2}} v_h) = 0$$

for all  $v_h \in \mathcal{F}_h[u_h]$ , where  $\mathcal{F}_h[u_h]$  is defined as

$$\mathcal{F}_h[u_h] = \{v_h \in \mathcal{S}_0^1(\mathcal{T}_h)^N : v_h(z) \cdot u_h(z) = 0 \text{ for all } z \in \mathcal{N}_h\}.$$

We establish that if  $\{u_h\}_{h>0}$  is a bounded sequence of discrete fractional harmonic maps then every weak limit  $u \in \widetilde{H}^s(\Omega; \mathbb{R}^N)$  as  $h \rightarrow 0$  is a fractional harmonic map.

**Fractional harmonic map heat flow.** The second application addresses a parabolic evolution defined by the  $L^2$ -gradient flow for  $I$  given in (1); it was studied analytically in [8, 9]. Its discretization or discretizations of gradient flows for other metrics define fully practical methods to determine discrete fractional harmonic maps. The  $L^2$ -flow of fractional harmonic maps is formally given by the partial differential equation

$$\partial_t u = -(-\Delta)^s u + \lambda u, \quad |u|^2 = 1,$$

where again  $\lambda$  is the Lagrange multiplier subject to the unit-length constraint. Rigorously, we define solutions of the fractional harmonic map heat flow as maps  $u : (0, T) \times \Omega \rightarrow \mathbb{R}^N$  with

$$u - \vec{N} \in H^1(0, T; L^2(\Omega; \mathbb{R}^N)) \cap L^\infty(0, T; \tilde{H}^s(\Omega; \mathbb{R}^N))$$

that satisfy  $u(0) = u_0$  for a given vector field  $u_0 \in \mathcal{A}$ , the constraint  $|u(t, x)|^2 = 1$  almost everywhere in  $(0, T) \times \Omega$ , and with the inner product  $(\cdot, \cdot)$  in  $L^2(\Omega; \mathbb{R}^N)$

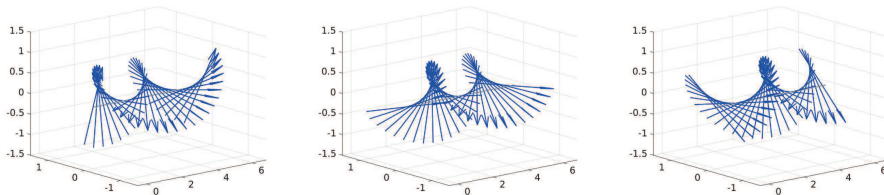
$$(7) \quad (\partial_t u, v) + ((-\Delta)^{\frac{s}{2}} u, (-\Delta)^{\frac{s}{2}} v) = 0$$

for all vector fields  $v \in \tilde{H}^s(\Omega; \mathbb{R}^N)$  and almost every  $t \in (0, T)$  with the orthogonality relation  $u(t, x) \cdot v(x) = 0$  for almost every  $(t, x) \in (0, T) \times \Omega$ , we furthermore require solutions to satisfy an energy-decay property. Our numerical scheme adopts ideas from [2, 3] and imposes the orthogonality condition at the nodes of a triangulation in an explicit way; the evolution equation is discretized implicitly. Convergence of this scheme is shown.

**Hyperbolic system for spin dynamics.** The third numerical problem is a hyperbolic evolution equation determined by the force balance

$$(8) \quad \partial_t u = \delta I[u] \times u = (-\Delta)^s u \times u, \quad |u|^2 = 1,$$

which has been used to model nonlocal effects in spin chains, cf. [10, 7]. This evolution is constraint and energy preserving which follows directly from testing the equation with  $u$  and  $(-\Delta)^s u$ , respectively. To obtain these features for a discretization, we follow [6, 4] and use Crank-Nicolson type midpoint approximations. Convergence of this scheme is established. The figure below shows snapshots of approximations of a solitary wave in a periodic spin chain.



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## Discontinuous Galerkin time-stepping methods: Maximal regularity and a posteriori error estimates

GEORGIOS AKRIVIS

(joint work with Charalambos Makridakis)

Consider an initial value problem for a linear parabolic equation,

$$(1) \quad \begin{cases} u'(t) + Au(t) = f(t), & 0 < t < T, \\ u(0) = 0, \end{cases}$$

in an unconditional martingale differences (UMD) Banach space  $X$ . Our structural assumption is that the operator  $A$  is the generator of an analytic semigroup on  $X$  having *maximal  $L^p$ -regularity*, i.e.,  $u$  satisfies the stability estimate

$$(2) \quad \|u'\|_{L^p((0,T);X)} + \|Au\|_{L^p((0,T);X)} \leq c_{p,X} \|f\|_{L^p((0,T);X)} \quad \forall f \in L^p((0,T);X)$$

for some, or, as it turns out, for all  $p \in (1, \infty)$ , with a constant  $c_{p,X}$  independent of  $T$ , depending only on  $p$  and  $X$ . See [5] for an excellent account of the theory.

*The numerical methods.* We consider the discretization of the initial value problem (1) by discontinuous Galerkin (dG) methods.

Let  $N \in \mathbb{N}$ ,  $k = T/N$  be the constant time step,  $t_n := nk, n = 0, \dots, N$ , be a uniform partition of the time interval  $[0, T]$ , and  $J_n := (t_n, t_{n+1}]$ .

For  $s \in \mathbb{N}_0$ , we denote by  $\mathbb{P}(s)$  and  $\mathbb{P}_{X'}(s)$  the spaces of polynomials of degree at most  $s$  with coefficients in  $\mathcal{D}(A) := \{v \in X : Av \in X\}$  and in the dual  $X'$  of  $X$ , respectively, i.e., the elements  $g$  of  $\mathbb{P}(s)$  and of  $\mathbb{P}_{X'}(s)$  are of the form

$$g(t) = \sum_{j=0}^s t^j w_j, \quad w_j \in \mathcal{D}(A) \quad \text{and} \quad w_j \in X', \quad j = 0, \dots, s.$$

With this notation, let  $\mathcal{V}_k^c(s)$  and  $\mathcal{V}_k^d(s)$  be the spaces of continuous and possibly discontinuous piecewise elements of  $\mathbb{P}(s)$ , respectively,

$$\mathcal{V}_k^c(s) := \{v \in C([0, T]; \mathcal{D}(A)) : v|_{J_n} \in \mathbb{P}(s), \quad n = 0, \dots, N-1\},$$

$$\mathcal{V}_k^d(s) := \{v : [0, T] \rightarrow \mathcal{D}(A), \quad v|_{J_n} \in \mathbb{P}(s), \quad n = 0, \dots, N-1\}.$$

We denote by  $\langle \cdot, \cdot \rangle$  the duality pairing between  $X$  and  $X'$ .



For  $q \in \mathbb{N}$ , with starting value  $U(0) = U_0 = 0$ , we consider the discretization of (1) by the dG( $q - 1$ ) method, i.e., we seek  $U \in \mathcal{V}_k^d(q - 1)$  such that

$$(3) \quad \int_{J_n} (\langle U', v \rangle + \langle AU, v \rangle) dt + \langle U_n^+ - U_n, v_n^+ \rangle = \int_{J_n} \langle f, v \rangle dt \quad \forall v \in \mathbb{P}_{X'}(q - 1)$$

for  $n = 0, \dots, N - 1$ . We use the notation  $v_n := v(t_n)$ ,  $v_n^+ := \lim_{s \searrow 0} v(t_n + s)$ .

With  $0 < c_1 < \dots < c_q = 1$  the Radau nodes, let  $t_{ni} := t_n + c_i k, i = 1, \dots, q$ , be the intermediate nodes, and  $t_{n0} := t_n$ . Using the reconstruction  $\widehat{U} \in \mathcal{V}_k^c(q)$  of the dG approximation  $U \in \mathcal{V}_k^d(q - 1)$ ,

$$\widehat{U}(t_{nj}) = U(t_{nj}), \quad j = 0, \dots, q,$$

we can reformulate the dG method as

$$(4) \quad \int_{J_n} (\langle \widehat{U}', v \rangle + \langle AU, v \rangle) dt = \int_{J_n} \langle f, v \rangle dt \quad \forall v \in \mathbb{P}_{X'}(q - 1).$$

Our basic idea is the interpretation of dG as modified Radau IIA methods. The  $q$ -stage Radau IIA method is specified by the nodes  $c_1, \dots, c_q$  and the coefficients

$$a_{ij} = \int_0^{c_i} \ell_j(\tau) d\tau, \quad b_i = \int_0^1 \ell_i(\tau) d\tau (= a_{qi}), \quad i, j = 1, \dots, q;$$

here,  $\ell_1, \dots, \ell_q \in \mathbb{P}_{q-1}$  are the Lagrange polynomials for  $c_1, \dots, c_q$ . We denote by  $\ell_{ni}$  the corresponding Lagrange polynomials shifted to the interval  $\bar{J}_n$ .

The dG approximations  $U_n := U(t_n), U_{ni} := U(t_{ni}), i = 1, \dots, q$ , satisfy the *modified* Radau IIA method

$$(5) \quad \begin{cases} U_{ni} = U_n - k \sum_{j=1}^q a_{ij} (AU_{nj} - f_{nj}), & i = 1, \dots, q, \\ U_{n+1} = U_n - k \sum_{i=1}^q b_i (AU_{ni} - f_{ni}), \end{cases}$$

$n = 0, \dots, N - 1$ , with the nodal values  $f(t_{ni})$  of  $f$  replaced by the averages

$$(6) \quad f_{ni} := \frac{1}{\int_{J_n} \ell_{ni}(s) ds} \int_{J_n} \ell_{ni}(s) f(s) ds = \frac{1}{b_i k} \int_{J_n} \ell_{ni}(s) f(s) ds, \quad i = 1, \dots, q.$$

Also,  $U_{n+1} = U_{nq}$ . Equivalently, (5) written in terms of  $\widehat{U}$  is a modified collocation method in each interval  $J_n$  with starting value  $\widehat{U}_{n0} = U_n$ , namely,

$$(7) \quad \widehat{U}'(t_{ni}) + A\widehat{U}(t_{ni}) = f_{ni}, \quad i = 1, \dots, q.$$

*Discrete maximal regularity.* Combining the maximal parabolic regularity property for Radau IIA methods, recently established in [3, Corollary 5.2, Theorem 5.1], with the interpretation of dG methods as modified Radau IIA methods, we prove maximal regularity for the dG methods: The dG approximations  $U_0, \dots, U_N \in \mathcal{D}(A)$  are well defined by (3) and satisfy the maximal parabolic regularity stability estimates

$$(8) \quad \|(\partial U_n)_{n=1}^N\|_{\ell^p(X)} + \|(AU_n)_{n=1}^N\|_{\ell^p(X)} \leq C_{p,X} \|f\|_{L^p((0,T);X)}$$

and

$$(9) \quad \sum_{i=1}^q \|(AU_{ni})_{n=0}^{N-1}\|_{\ell^p(X)} \leq C_{p,X} \|f\|_{L^p((0,T);X)}$$

with  $U_{ni} := U(t_{ni})$ . Also, the reconstruction  $\widehat{U}$  satisfies the analogue of (2),

$$(10) \quad \|\widehat{U}'\|_{L^p((0,T);X)} + \|\widehat{A}\widehat{U}\|_{L^p((0,T);X)} \leq C_{p,X} \|f\|_{L^p((0,T);X)},$$

where  $C_{p,X}$  denotes a constant independent of  $N$  and  $T$ .

Here, for a sequence  $(v_n)_{n \in \mathbb{N}} \subset X$ , we used the notation

$$\partial v_n := \frac{v_n - v_{n-1}}{k} \quad \text{and} \quad \|(v_n)_{n=1}^M\|_{\ell^p(X)} := \left(k \sum_{n=1}^M \|v_n\|_X^p\right)^{1/p}.$$

Logarithmically quasi-maximal parabolic regularity results for dG methods were recently established in [6, 7].

*A posteriori error estimates.* Let  $R \in L^p((0,T);X)$  be the *residual* of the reconstruction  $\widehat{U}$  of the dG approximation  $U$ ,

$$(11) \quad R(t) := \widehat{U}'(t) + \widehat{A}\widehat{U}(t) - f(t), \quad t \in (t_n, t_{n+1}], \quad n = 0, \dots, N-1.$$

Then, the error  $e := u - \widehat{U}$  satisfies the *error equation*

$$(12) \quad e'(t) + Ae(t) = -R(t), \quad t \in (t_n, t_{n+1}], \quad n = 0, \dots, N-1.$$

Now, the maximal  $L^p$ -regularity of the operator  $A$  and the triangle inequality, respectively, applied to the error equation (12) yields the upper and lower a posteriori error bounds

$$(13) \quad \|R\|_{L^p((0,t);X)} \leq \|e'\|_{L^p((0,t);X)} + \|Ae\|_{L^p((0,t);X)} \leq c_{p,X} \|R\|_{L^p((0,t);X)}$$

for all  $0 < t \leq T$  for any  $p \in (1, \infty)$  with a constant  $c_{p,X}$  depending only on  $p$  and  $X$ . Since  $R$  is a computable quantity, depending only on the numerical solution  $\widehat{U}$  and the given forcing term  $f$ , (13) is an a posteriori error estimate.

Under suitable regularity assumptions on the solution  $u$ , we first establish a priori error estimates in the discrete  $\ell^p(X)$ -norm. Subsequently, we show that the a posteriori error bound  $\|R\|_{L^p((0,T);X)}$  is of asymptotic optimal order, assuming also regularity of the forcing term  $f$ ; this, in turn, leads to optimal order a priori error estimates in the continuous  $L^p((0,T);X)$ -norm, which complements the corresponding a priori error estimate in the discrete  $\ell^p(X)$ -norm.

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## Space-Time Finite Element and Multigrid Methods for the Navier–Stokes Equations on Evolving and Static Domains

MARKUS BAUSE

(joint work with M. Anselmann)

### 1. INTRODUCTION

The numerical simulation of incompressible viscous flow continues to remain a challenging task, in particular, if three space dimensions are involved. Using space-time finite element methods (cf. [1, 3, 5, 6]) allows the natural construction of higher order methods. They offer the potential to achieve accurate results on computationally feasible grids with a minimum of numerical costs. However, constructing higher order numerical methods maintaining stability and inheriting most of the rich structure of the continuous problem becomes increasingly difficult. In particular, the arising algebraic systems and their solution by iterative methods demand for sophisticated and highly efficient techniques. Geometric multigrid methods are known as the most efficient iterative methods for the solution of large linear systems arising from the discretization of partial differential equations, particularly of elliptic type; cf. [7, 10]. To fully exploit their potential, they need to be adapted to the space-time finite element discretizations; cf. [3]. Time-dependent domains that are also of interest for applications of practical interest (for instance, fluid-structure interaction or free surface flows) put a further facet of complexity on the numerical simulation of the flow problems; cf. [1].

### 2. MATHEMATICAL PROBLEM

In this contribution we study the numerical approximation of solutions to the nonstationary Navier–Stokes equations

$$(1a) \quad \partial_t \mathbf{v} + (\mathbf{v} \cdot \nabla) \mathbf{v} - \nu \Delta \mathbf{v} + \nabla p = \mathbf{f},$$

$$(1b) \quad \nabla \cdot \mathbf{v} = 0,$$

equipped with initial and appropriate boundary conditions, by space-time finite element methods of arbitrary order on static domains  $\Omega \subset \mathbb{R}^d$ , with  $d = 2$  or  $d = 3$ , and on evolving domains  $\Omega \subset \mathbb{R}^2$ . In the latter case, the smooth motion of the domain  $\Omega = \Omega(t)$  for  $t \in [0, T]$  with final time  $T > 0$  is assumed to be given.

### 3. NAVIER–STOKES EQUATIONS ON STATIC DOMAINS

Firstly, we study system (1) on time-independent domains  $\Omega \subset \mathbb{R}^d$ ,  $d \in \{2, 3\}$ . Key ingredients of the proposed space-time finite element approach are (cf. [2, 3]):

- Application of Dirichlet boundary conditions by Nitsche’s method;
- Discontinuous Galerkin time discretization by piecewise polynomials of order  $k \in \mathbb{N}_0$  in time;
- Space discretization by pairs of inf-sup stable finite elements  $(\mathbb{Q}_r)^d \times \mathbb{P}_{r-1}^{\text{disc}}$ , for  $r \geq 2$ , with discontinuous discrete pressure.

A discontinuous temporal test basis, supported on the subintervals of the temporal mesh, is chosen such that a time marching scheme is obtained. A damped version of Newton’s method along with a generalized minimal residual method (GMRES) and a  $V$ -cycle geometric multigrid (GMG) preconditioning technique for the GMRES iterations are applied. For this, hierarchies of successively refined spatial grids built on quadrilateral or hexahedral elements and the canonical grid transfer routines regarding the chosen finite element spaces are used. A cell-based Vanka smoother (cf. [11]) is built. For each of the spatial mesh cells, this operator defines a mapping for the cell’s degrees of freedom. The cell’s unknowns for all of the  $k+1$  time points associated with the temporal degrees of freedom on the subinterval are comprised in the elementwise smoothing step. This Vanka operator, adapted to the Galerkin space-time discretization, is the key component for the solution of the algebraic systems. Finally, the coarse grid problem is solved by a direct solver. For the parallel implementation of the algorithms the deal.II library (cf. [4]) is used.

The proposed approach is carefully validated for the benchmark problem of flow around a cylinder proposed in [9]; cf. Fig 1. The performance properties of the nonlinear and linear solver are evaluated and computed values for the goal quantities of drag and lift coefficient are presented (cf. [3]).

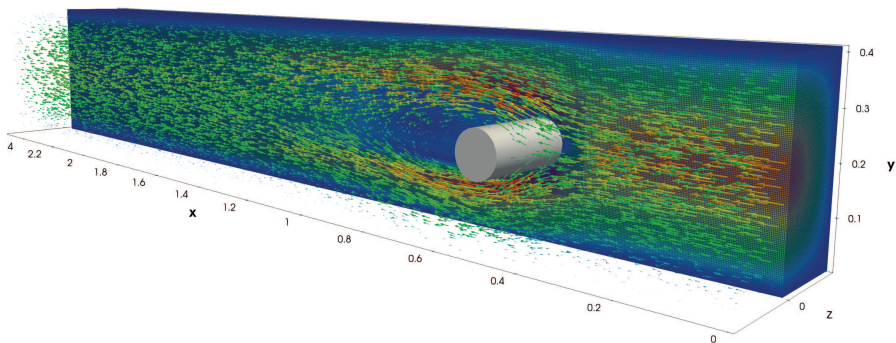


FIGURE 1. Computed flow profile for flow around a cylinder [2, 9].

## 4. NAVIER–STOKES EQUATIONS ON EVOLVING DOMAINS

For flow domains  $\Omega(t)$  evolving in time, a fictitious domain approach is applied; cf. [1, 2]. The physical domain is embedded into a fixed, time-independent computational mesh. Thereby, an expensive remeshing and adaptation of the sparse matrix data structure are avoided and the computations are accelerated. However, an extension of the flow solution to the fictitious or ghost domain is required. Further, mesh cells are intersected in an arbitrary manner by moving boundaries of the domain. This demands for numerical integration over such cut cells.

Key ingredients of the space-time approach for flows on evolving domains are the discretization techniques and algebraic solver of Sec. 3 and:

- Spatial extension of the discrete physical quantities to the entire computational background mesh including fictitious subdomains of fluid flow;
- Iterated integration over cut cells (i.e. intersected quadrilaterals).

Here, an implicitly defined extension, that is free of (computationally expensive) spatial derivatives of the discrete functions, is applied. Simultaneously, the extension stabilizes irregular cuts and prevents spurious oscillations caused by them. The combination of higher order space-time finite element discretizations with the fictitious domain approach, the extension and ghost penalty stabilization and the integration over cut cells has not been studied so far and deserves elucidation.

The stability and convergence properties of this approach are carefully studied for a sequence of numerical experiments of increasing complexity. Further, the performance of the GMG preconditioning technique for the GMRES iterations, proposed in Sec. 3 for time-independent domains, is now investigated for evolving domains. A lack in the smoothing capabilities of the Vanka-type operator that is manifested by a deficit in the reduction of the linear equation’s residuals on the multigrid levels for an increasing number of grid hierarchies is observed and discussed. Possible remedies for future research are outlined.

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## Analysis of a modified Euler scheme for parabolic semilinear stochastic PDEs

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We propose a novel integrator to approximate solutions of parabolic semilinear stochastic evolution equations

$$dX(t) = -\Lambda X(t)dt + F(X(t))dt + dW(t)$$

where  $-\Lambda x(\xi) = \partial_\xi(a(\xi)\partial_\xi x(\xi))$ ,  $\xi \in (0, 1)$  is a second order elliptic operator,  $F$  is a globally Lipschitz nonlinearity, and  $W$  is a cylindrical Wiener process (meaning that the SPDE is driven by space-time white noise). The objective is to overcome some of the limitations of the standard Euler method (see [4, Chapter 10])

$$X_{n+1}^{\tau, \text{st}} = \mathcal{A}_\tau \left( X_n^{\tau, \text{st}} + \tau F(X_n^{\tau, \text{st}}) + \sqrt{\tau} \Gamma_n \right)$$

where  $\tau = T/N$ ,  $\mathcal{A}_\tau = (I + \tau\Lambda)^{-1}$  and  $\sqrt{\tau}\Gamma_n = W(t_{n+1}) - W(t_n)$ . Indeed, for any positive  $\tau$ , the standard Euler method does not preserve the spatial regularity of the solutions of the exact solution  $X(t)$ . As a consequence, approximation of the distribution of  $X(N\tau)$  by the distribution of  $X_N^{\tau, \text{st}}$  can only hold in a weak sense, not in the total variation distance sense for instance.

The proposed modified Euler scheme, introduced in [1], is written as

$$(1) \quad X_{n+1}^\tau = \mathcal{A}_\tau(X_n^\tau + \tau F(X_n^\tau)) + \mathcal{B}_{\tau,1}\sqrt{\tau}\Gamma_{n,1} + \mathcal{B}_{\tau,2}\sqrt{\tau}\Gamma_{n,2},$$

where  $\Gamma_{n,1}, \Gamma_{n,2}$  denote independent Gaussian random variables, distributed like  $\Gamma_n$  from the standard scheme, and the linear operators are assumed to satisfy the conditions  $\mathcal{B}_{\tau,1} = \frac{1}{\sqrt{2}}(I + \tau\Lambda)^{-1}$  and  $\mathcal{B}_{\tau,2}\mathcal{B}_{\tau,2}^* = \frac{1}{2}(I + \tau\Lambda)^{-1}$ . The modified Euler scheme (1) can be combined with a finite difference method for the spatial discretization. It is worth mentioning that the linear operator  $\mathcal{B}_{\tau,2}$  can be computed by a Cholesky decomposition. Another more efficient method than the standard Euler scheme would be the accelerated exponential Euler scheme [3], but it would require knowledge of the eigenvalues and eigenfunctions of the linear operator  $\Lambda$ .

We present the main improvements when the modified Euler scheme (1) is used instead of the standard method, see [1].

- The spatial regularity is preserved at all times, for any value of the time-step size  $\tau$ .
- When  $F = 0$ , the Gaussian invariant distribution  $\nu$  of the Ornstein–Uhlenbeck process  $(X(t))_{t \geq 0}$  is preserved by the numerical scheme, for any value of the time-step size  $\tau$ .
- If  $F = -DV$  and if an appropriate ergodicity condition is satisfied, one can approximate the invariant Gibbs distribution given by

$$d\mu_\star(x) = Z^{-1} \exp(-2V(x))d\nu(x)$$

of the process in the total variation distance: for any  $\tau$ , the scheme admits a unique invariant distribution  $\mu_\infty^\tau$ , and for all  $\kappa \in (0, \frac{1}{2})$ , there exists  $C_\kappa \in (0, \infty)$  such that

$$(2) \quad d_{\text{TV}}(\mu_\infty^\tau, \mu_\star) \leq C_\kappa \tau^{\frac{1}{2}-\kappa}.$$

The error estimate (2) is a major improvement compared with the existing literature: for the standard Euler method, one obtains weak error estimates

$$\left| \int \varphi d\mu_\infty^{\tau, \text{st}} - \int \varphi d\mu_\star \right| \leq C_\kappa \tau^{\frac{1}{2}-\kappa} \|\varphi\|_2$$

only if the test function  $\varphi$  is assumed to be at least of class  $\mathcal{C}^2$ . On the contrary (2) yields weak error estimates

$$\left| \int \varphi d\mu_\infty^\tau - \int \varphi d\mu_\star \right| \leq C_\kappa \tau^{\frac{1}{2}-\kappa} \|\varphi\|_0$$

for measurable and bounded test functions  $\varphi$ .

Finally, an application of the modified Euler scheme to construct asymptotic preserving schemes for a class of slow-fast SPDE systems

$$(3) \quad \begin{cases} dX^\epsilon(t) = -\Lambda X^\epsilon(t)dt + G(X^\epsilon(t), Y^\epsilon(t))dt \\ dY^\epsilon(t) = -\frac{1}{\epsilon} \Lambda Y^\epsilon(t)dt + \frac{1}{\sqrt{\epsilon}} dW(t), \end{cases}$$

is presented. The scheme is defined as

$$(4) \quad \begin{cases} X_{n+1}^{\epsilon, \Delta t} = \mathcal{A}_{\Delta t}(X_n^{\epsilon, \Delta t} + \Delta t G(X_n^{\epsilon, \Delta t}, Y_{n+1}^{\epsilon, \Delta t})) \\ Y_{n+1}^{\epsilon, \Delta t} = \mathcal{A}_{\frac{\Delta t}{\epsilon}} Y_n^{\epsilon, \Delta t} + \sqrt{\frac{\Delta t}{\epsilon}} \mathcal{B}_{\frac{\Delta t}{\epsilon}, 1} \Gamma_{n,1} + \sqrt{\frac{\Delta t}{\epsilon}} \mathcal{B}_{\frac{\Delta t}{\epsilon}, 2} \Gamma_{n,2}, \end{cases}$$

and is such that

$$\lim_{\epsilon \rightarrow 0} \lim_{\Delta t \rightarrow 0} X_N^{\epsilon, \Delta t} = \lim_{\Delta t \rightarrow 0} \lim_{\epsilon \rightarrow 0} X_N^{\epsilon, \Delta t}$$

in the sense of convergence in distribution. We also present the uniform weak error estimates

$$(5) \quad \sup_{\epsilon \in (0, \epsilon_0)} \left| \mathbb{E}[\varphi(X_N^{\epsilon, \Delta t})] - \mathbb{E}[\varphi(X^\epsilon(T))] \right| \leq C_\kappa(T, \varphi, x_0) \Delta t^{\frac{1}{3}-\kappa}$$

obtained in [2]. The asymptotic preserving and uniform accuracy properties are not satisfied if the standard Euler scheme is used, which illustrates the superiority of the proposed modified Euler scheme in this multiscale context.

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***hp*-version space-time discontinuous Galerkin methods on  
general meshes**

ANDREA CANGIANI

(joint work with Zhaonan Dong, Emmanuil H. Georgoulis)

Recent years have witnessed a surge in research into Galerkin procedures on polygonal and polyhedral (polytopic) meshes, aiming at greater resolution flexibility for challenging numerical PDE problems; we refer to our recent monograph [1] for a review.

A technique that naturally lends itself to the exploitation of very general meshes is the discontinuous Galerkin (dG) method. dG is based on employing polynomials of arbitrary degree defined over each mesh element domain without the enforcement of any continuity constraints between neighbouring elements. Instead, elements are coupled via numerical flux functions: in this regard its design is similar to that of Finite Volume Methods. Furthermore, the local space basis may be defined directly in the physical frame, without resorting to local element mappings to a given reference element. In particular, spaces of polynomials of total degree  $p$ , denoted by  $\mathcal{P}_p$ , may be used, *irrespective of the shape of the element*.

One such class of dG methods, known as Interior Penalty (IP-dG) methods, is based on suitable choices of an interior penalty discontinuity penalization parameter used to weakly enforce continuity across the mesh elements boundaries. In a series of works [1, 2, 3], we have shown that IP-dG methods can be defined which provide stable discretisations to a large class of linear PDE problems under extremely general partitions of the computational domain.

Particularly relevant to the topic of the workshop, we have presented the *hp*-version space-time discontinuous Galerkin (dG) finite element method for the numerical approximation of parabolic evolution equations on general spatial meshes consisting of polytopic elements, giving rise to prismatic space-time elements [2]. Here, the  $\mathcal{P}_p$  basis are used in the space-time setting, as opposed to standard dG-time-stepping methods whereby spatial elemental bases are tensorized with temporal basis functions. This approach leads to dG methods which, compared to dG time-stepping schemes employing tensorized space-time basis, use fewer degrees of freedom per time step. It turns out that the reduced number of degrees of



freedom results in an acceptable deterioration of the approximation properties, as proven by extensive comparison with standard approaches, such as the tensorized space-time dG methods, the classical dG-time-stepping, and conforming finite element method in space. Compared to other methods, the new approach has also the advantage that very general spatial meshes consisting of polytopic elements with arbitrary number of faces can be used.

The polytopic dG method has recently been further generalised to the use of meshes made of elements with general Lipschitz boundaries in [3]. Here we show that the IP discontinuity penalization parameter can be defined to be explicitly dependent on the particular element shape, but essentially independent on small shape variations. The resulting IP-dG method is shown to be inf-sup stable for the solution of advection-diffusion-reaction problems in a streamline-diffusion-like norm. A priori error bounds are also presented under very mild structural assumptions restricting the magnitude of the local curvature of the boundary of each element. The stability and a priori error analysis is based on new extensions of classical trace, Markov-type, and  $H^1 - L_2$ -type inverse estimates on essentially arbitrary element shapes which may be of independent interest.

An obvious motivation of polytopic meshes is in their application within adaptive simulations, which are now accepted as the key technology for automatic computational complexity reduction. However, little has been done so far to exploit the endless possibilities offered by polytopic meshes, specifically in the context of mesh adaptive algorithms driven by reliable *a posteriori* error estimators. We finally present ongoing work on the *a posteriori* error analysis of IP-dG methods applied to linear elliptic problems. Here we consider again the case of polytopic meshes with arbitrary number of very small faces, under the mild assumptions already employed in [2]. We remark that simplicial and/or box-type elements are included in the analysis as a special case. As such, the presented analysis generalizes the classical *a posteriori* error analysis of *hp*-dG methods to the case of arbitrary number of irregular hanging nodes per element. The analysis exploits a new recovery strategy in conjunction with a generalized Helmholtz decomposition formula, and results in a new *a posteriori* error bound which involves the usual residual error estimator terms together with a new term depending on the jump of the tangential derivatives along elemental faces. The complexity reduction potential of polytopic meshes within adaptive algorithms is showcased through a series of numerical experiments in which the new *a posteriori* error estimator is used to drive automatic refinement and coarsening of an initial mesh.

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## Sparse grid approximation spaces for space-time boundary integral formulations of the heat equation

ALEXEY CHERNOV

(joint work with Anne Reinarz)

Discretization by piecewise polynomials is a well-established and well-understood approach for the numerical solution of partial differential equations. For time-dependent problems, independent piecewise polynomial approximations can be used in space and time. Given stability of the joint space-time approximation, the accuracy of the method can be expressed in terms of the discretization parameters. It is clear, however, that the space and time discretizations must be balanced for an efficient numerical simulation, since the underrefined discretization space will dictate the accuracy, whereas the overrefined space will determine the overall computational cost.

In this note we address optimal balancing of several piecewise polynomial discretization spaces for the first kind space-time boundary integral formulations for the homogeneous heat equation with Dirichlet boundary conditions. Let  $\Omega \subset \mathbb{R}^d$ ,  $d \geq 2$  be a bounded domain with a smooth boundary  $\Gamma := \partial\Omega$  and  $\mathcal{I} := [0, T]$  be the time interval of interest. After reduction to the mantle of the space-time cylinder  $\Sigma := \Gamma \times \mathcal{I}$ , cf. [6, 3], the problem is rephrased as the boundary integral equation

$$(1) \quad V\psi(x, t) := \int_0^T \int_{\Gamma} G(x - y, t - s) dy ds = f(x, t), \quad x \in \Gamma, t \in \mathcal{I},$$

where  $\psi$  is the unknown flux,  $f$  is the known data (depending on the Dirichlet data) and  $G$  is the fundamental solution of the heat equation

$$(2) \quad G(x, t) = \begin{cases} (4\pi t)^{-d/2} e^{-|x|^2/4t}, & t \geq 0, \\ 0, & t < 0. \end{cases}$$

We write  $H^{r,s}(\Sigma) := L^2(\mathcal{I}, H^r(\Gamma)) \cap H^s(\mathcal{I}, L^2(\Gamma))$  for  $r, s \geq 0$ , equipped with the graph norm, and  $H^{-r,-s}(\Sigma) := H^{r,s}(\Sigma)'$  for its dual. The single layer operator  $V : H^{-1/2,-1/4}(\Sigma) \rightarrow H^{1/2,1/4}(\Sigma)$  is an isomorphism and satisfies the following coercivity estimate [1]

$$(3) \quad \exists c_V > 0 : \quad \langle Vq, q \rangle \geq c_V \|q\|_{H^{-1/2,-1/4}(\Sigma)}^2, \quad \forall q \in H^{-1/2,-1/4}(\Sigma).$$

This remarkable property being typical for *elliptic* operators immediately implies that any conforming discretization  $\mathcal{X}_L \subset H^{-1/2,-1/4}(\Sigma)$  of (1) is stable and that the discrete solution  $\psi_L \in \mathcal{X}_L$  is quasi-optimal, i.e.

$$(4) \quad \|\psi - \psi_L\|_{H^{-1/2,-1/4}(\Sigma)} \leq \frac{\|V\|}{c_V} \inf_{\eta_L \in \mathcal{X}_L} \|\psi - \eta_L\|_{H^{-1/2,-1/4}(\Sigma)}.$$

This allows to construct a number of conforming discretization spaces  $\mathcal{X}_L$  for the numerical solution of (1). In particular, let the polynomial degrees in the space

and time domain  $p_x$  and  $p_t$  be fixed and consider the following nested sequence of discretizations in space and time on meshes defined by bisection

$$\mathcal{X}_0^x \subset \mathcal{X}_1^x \subset \dots \subset \mathcal{X}_i^x \subset \dots \subset H^{-\frac{1}{2}}(\Gamma), \quad \mathcal{X}_0^t \subset \mathcal{X}_1^t \subset \dots \subset \mathcal{X}_j^t \subset \dots \subset H^{-\frac{1}{4}}(\mathcal{I})$$

The individual subspaces admit  $L^2$ -orthogonal representations

$$\mathcal{X}_i^x = W_0^x \oplus W_1^x \oplus \dots \oplus W_i^x, \quad \mathcal{X}_j^t = W_0^t \oplus W_1^t \oplus \dots \oplus W_j^t,$$

so that for any  $\psi \in L^2(\Sigma)$  holds

$$(5) \quad \psi = \sum_{(\ell_x, \ell_t) \in \mathbb{N}_0^2} w_{(\ell_x, \ell_t)}, \quad w_{(\ell_x, \ell_t)} \in W_{\ell_x}^x \otimes W_{\ell_t}^t.$$

Conforming discretizations can now be derived from (5) by restricting the non-negative quadrant to finite, possibly anisotropic index sets  $I_L^\sigma, \hat{J}_L^\sigma \subset \mathbb{N}_0^2$ , where  $\sigma$  indicates the anisotropy and thereby the optimal balance between space and time discretizations.

In view of (4) it is natural to take the  $H^{-1/2, -1/4}(\Sigma)$ -norm as the error measure. As a comparison criterion we take the asymptotic convergence rate  $\gamma$  of the error in this norm with respect to the dimension of the discretization space  $N_L$  for smooth solutions  $\psi$ :

$$(6) \quad \gamma := \sup \left\{ \tilde{\gamma} : \|\psi - \psi_L\|_{H^{-\frac{1}{2}, -\frac{1}{4}}(\Sigma)} \leq cN_L^{-\tilde{\gamma}}, \text{ where } N_L \rightarrow \infty \right\}.$$

In the context of particular discretizations considered below, the smoothness requirement may be replaced by  $\psi \in H^{\mu, \lambda}(\Sigma)$  or  $H_{\text{mix}}^{\mu, \lambda}(\Sigma)$  with  $0 \leq \mu < p_x + 1$  and  $0 \leq \lambda < p_t + 1$ , cf. [2, Remark 1]. This allows the exclusion of the borderline case  $\mu = p_x + 1, \lambda = p_t + 1$ , where the convergence estimates are usually corrupted by logarithmic terms, and thereby simplifying the argument. Here the space  $H_{\text{mix}}^{\mu, \lambda}(\Sigma)$  stands for the hilbertian tensor product  $H^r(\Gamma) \otimes H^s(\mathcal{I})$ .

1. *Anisotropic full-tensor product* discretizations are a natural choice:

$$(7) \quad I_L^\sigma = \{(\ell_x, \ell_t) : \ell_x \leq L/\sigma, \ell_t \leq \sigma L\}$$

Notice that the error measure is given by the anisotropic norm (4), thus nontrivial values  $\sigma \neq 1$  are expected in this case.

2. *Anisotropic sparse-tensor product* discretizations are defined as in [4]

$$(8) \quad \hat{J}_L^\sigma = \{(\ell_x, \ell_t) : \ell_x \sigma + \ell_t / \sigma \leq L\}$$

This choice is potentially more efficient for smooth solutions, since it excludes the largest orthogonal subspace combinations (implying  $\hat{J}_L^\sigma \subset I_L^\sigma$ ) without compromising the accuracy.

The outcomes of the error analysis are summarized in the table below, cf. [2] for the details. The argument is based on appropriate norm equivalences / bounds [2, (17)–(19)] that can be found in [8, Proposition 3], [5, Proposition 1] and derived along the lines of [7, Proposition 3].

The numerical results in [2, 9] validate our theoretical findings. The interested reader will find there also extensions to adaptive sparse grids and numerical solution by combination technique.

We finally remark that for some values  $(p_x, p_t)$  algorithmic accelerations are possible (e.g. when the matrix of the algebraic system is block triangular [9], etc.). Such effects are not considered here.

Full tensor product, $d = 2$			Sparse grids, $d = 2$		
$(p_x, p_t)$	conv. rate $\gamma$	scaling $\sigma^2$	$(p_x, p_t)$	conv. rate $\gamma$	scaling $\sigma^2$
(0, 0)	$\frac{15}{22} \approx 0.68$	$\frac{6}{5}$	(0, 0)	$\frac{7}{6} \approx 1.17$	1
(1, 0)	$\frac{5}{6} \approx 0.83$	2	(1, 0)	$\frac{5}{4} = 1.25$	1
(1, 1)	$\frac{45}{38} \approx 1.18$	$\frac{10}{9}$	(1, 1)	$\frac{13}{6} \approx 2.17$	1
(3, 1)	$\frac{3}{2} = 1.50$	2	(3, 1)	$\frac{9}{4} = 2.25$	1

Full tensor product, $d = 3$			Sparse grids, $d = 3$		
$(p_x, p_t)$	conv. rate $\gamma$	scaling $\sigma^2$	$(p_x, p_t)$	conv. rate $\gamma$	scaling $\sigma^2$
(0, 0)	$\frac{15}{32} \approx 0.47$	$\frac{6}{5}$	(0, 0)	$\frac{3}{4} = 0.75$	2
(1, 0)	$\frac{5}{8} \approx 0.63$	2	(1, 0)	$\frac{9}{8} \approx 1.13$	2
(1, 1)	$\frac{45}{56} \approx 0.80$	$\frac{10}{9}$	(1, 1)	$\frac{5}{4} = 1.25$	2
(3, 1)	$\frac{9}{8} \approx 1.13$	2	(3, 1)	$\frac{17}{8} \approx 2.13$	2

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**Hands on comparison between time-stepping and space-time discretizations of convection-reaction with DPG**

LESZEK DEMKOWICZ

(joint work with Judit Muñoz-Matute, Nathan Roberts)

The Discontinuous Petrov-Galerkin (DPG) method [2] was proposed by Demkowicz and Gopalakrishnan in 2010 where they introduced the idea of optimal test functions for the transport problem [1] considering a weak variational formulation. In the last decade, this method has been extensively studied and applied to many other problems. In general, we can describe the DPG method as a mixed method that delivers a stable solution (the discrete inf-sup condition is guaranteed) and a built-in error representation to perform adaptivity [4, 14]. Recently, in [5], Demkowicz and Roberts revisited the analysis of the DPG method for convection-reaction problem.

In this work, we focus on the transient convection-reaction problem

$$(1) \quad \begin{cases} u_t + b \cdot \nabla u + cu = f, & \text{in } \Omega \times I, \\ u = g, & \text{in } \Gamma_- \times I, \\ u = u_0, & \text{in } \Omega \times \{0\}, \end{cases}$$

where  $\Gamma_- = \{x \in \Gamma : b_n < 0\}$  is the inflow boundary. We compare different approaches to solve (1) using the DPG technology based on previous works of the DPG community on transient problems. In particular, we consider the 1D+time transport case ( $c = 0$ ) over  $\Omega \times I = (0, 1)^2$  with  $b = 1$ ,  $f = g = 0$  and  $u_0$  being a discontinuous function. We know that in this case the solution has a space-time discontinuity so we are interested in a weak variational formulation of (1) both in space and time. We consider three strategies:

1.- Method of discretization in time: We first apply the backward Euler method in time for discretizing in time (1). Then we consider an ultraweak variational formulation of the problem in space. Finally, we discretize the sequence of variational problems employing the DPG method. This strategy has been studied in [7, 8, 15] for parabolic problems.

2.- Space-time slabs: In the spirit of [3, 6, 9], we consider here the time variable as an extra space dimension and we apply the DPG method in the space-time domain. In order to reduce the cost, we solve the problem over a space-time slab  $\Omega \times (t_{k-1}, t_k)$  and then employ the solution of the traces at time  $t_k$  as the initial condition for the next slab.

3.- Method of lines: We first consider an ultraweak variational formulation in space in (1) and then we discretize by a conforming Petrov-Galerkin (PG) method. We select piecewise polynomials of order  $p$  for trial and  $H^1$ -conforming polynomials of order  $p + 1$  vanishing in the outflow boundary for the test space. We know from [1] that this choice corresponds to the optimal testing for the steady-state constant advection problem in 1D. After semidiscretization in space we obtain a system of ODEs and we employ the DPG-based time-marching scheme developed in [11, 12, 13]. This time integrator is based on an ultraweak variational formulation in time

where the optimal test functions are computed analytically. Here, we compute the solution at each time step  $t_k$  (traces in time) and the solution in the interior  $(t_{k-1}, t_k)$ . We know that the DPG time-marching scheme is equivalent to classical exponential time integrators for the trace variables [10] and that it delivers the  $L^2$ -projection of the solution in the time element interior.

In Figure 1 we present the approximated solutions of (1) employing the three different strategies mentioned before at times  $t = 0.25, 0.5, 0.75, 1$ . We selected fine meshes in both space and time where the element size in space and the time step size are of the same order. The top row corresponds to the Backward Euler method in time together with DPG in space, the second row to the ultraweak space-time slabs strategy and the last two rows to the DPG-based time-marching scheme together with the PG method in space. In the third row we show the solution at the traces in time ( $t_k$ ) and in the last row we plot a cross-section of the solution in the element time interior.

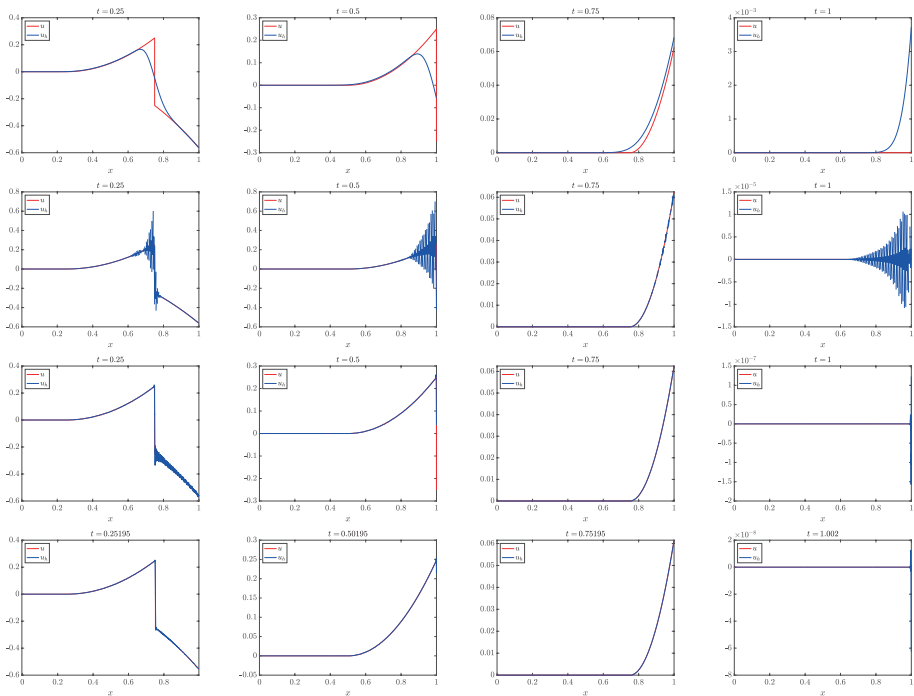


FIGURE 1. Analytical and approximated solutions at times  $t = 0.25, 0.5, 0.75, 1$ .

We conclude that: (a) The Backward Euler method in time with DPG in space has a smoothing effect near the discontinuity. (b) The solution obtained with the ultraweak space-time DPG method is oscillatory for the trace variables. (c) The DPG method in time together with DPG in space it is also oscillatory for the trace

variables. However, it delivers an approximation that captures the discontinuities in the element interior in time.

As future work, we will extend strategy 3 for higher dimensions in space. For that, we need to consider broken test spaces, introduce interface variables in space that will depend upon time and redefine the concept optimal testing. Our final goal is to obtain a time-stepping strategy based on the DPG method capable of capturing space-time discontinuities.

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## Space-time Discontinuous Galerkin Methods for Waves

WILLY DÖRFLER

(joint work with Christian Wieners)

**Elastic and acoustic waves.** *Elastic waves* are described by the displacement field  $\mathbf{u}: (0, T) \times \Omega \rightarrow \mathbb{R}^d$  (with  $\Omega \subset \mathbb{R}^d$  and  $T > 0$ ) satisfying

$$\rho \partial_t^2 \mathbf{u} - \operatorname{div} \boldsymbol{\sigma}(\mathbf{u}) = \mathbf{b},$$

subject to a constitutive law  $\boldsymbol{\sigma} = \boldsymbol{\sigma}(\mathbf{u}) = \mathbf{C}\boldsymbol{\varepsilon}(\mathbf{u})$  ( $\mathbf{C}$  a fourth-order tensor,  $\boldsymbol{\varepsilon}(\mathbf{u})$  the symmetric gradient of  $\mathbf{u}$ ,  $\mathbf{b}$  an external force density) and initial and boundary conditions. For the velocity  $\mathbf{v} = \partial_t \mathbf{u}$  and the stress  $\boldsymbol{\sigma}: (0, T) \times \Omega \rightarrow \mathbb{R}_{\text{Sym}}^{d,d}$  as separate variables this results in the first-order system (1).

*Acoustic waves* are the limit of elastic waves for vanishing shear wave velocity and are modeled by (2) with the pressure function  $p: (0, T) \times \Omega \rightarrow \mathbb{R}$ .

$$(1) \quad \begin{aligned} \rho \partial_t \mathbf{v} - \operatorname{div} \boldsymbol{\sigma} &= \mathbf{b}, \\ \partial_t \boldsymbol{\sigma} - \mathbf{C}\boldsymbol{\varepsilon}(\mathbf{v}) &= \mathbf{0}. \end{aligned} \qquad (2) \quad \begin{aligned} \rho \partial_t \mathbf{v} - \nabla p &= \mathbf{b}, \\ \partial_t p - \kappa \nabla \cdot \mathbf{v} &= 0. \end{aligned}$$

**Linear hyperbolic first-order systems.** Let  $\Omega \subset \mathbb{R}^d$  be bounded with boundary parts  $\Gamma_l \subset \partial\Omega$ ,  $l = 1, \dots, m$ , and denote by  $Q := (0, T) \times \Omega$  the corresponding time-space cylinder.

*Symmetric Friedrichs systems.* The problems above are special instances of the more general equation: Find  $\mathbf{y}: Q \rightarrow \mathbb{R}^m$  solving

$$L\mathbf{y} = M\partial_t \mathbf{y} + A\mathbf{y} = \mathbf{f} \text{ in } Q, \quad \mathbf{y}(0) = \mathbf{y}_0 \text{ in } \Omega, \quad (A_{\mathbf{n}}\mathbf{y})_l = g_l \text{ on } (0, T) \times \Gamma_l$$

with positive definite  $M \in L_\infty(\Omega; \mathbb{R}_{\text{sym}}^{m \times m})$ ,  $A_j \in \mathbb{R}_{\text{sym}}^{m \times m}$ ,  $A_{\mathbf{n}} = \sum_{j=1}^d n_j A_j$  (where  $\mathbf{n}$  is the unit normal vector  $\partial\Omega$ ),  $\mathbf{f} \in L_2(Q; \mathbb{R}^m)$ , and  $g_l \in L_2((0, T) \times \Gamma_l)$ .

*Example:* For the case of acoustic waves we have

$$\begin{aligned} \rho \partial_t \mathbf{v} - \nabla p &= \mathbf{b} && \text{in } (0, T) \times \Omega \\ \kappa^{-1} \partial_t p - \nabla \cdot \mathbf{v} &= 0 && \text{in } (0, T) \times \Omega \\ p(0) = p_0, \mathbf{v}(0) &= \mathbf{v}_0 && \text{in } \Omega \text{ at } t = 0 \\ p(t) &= p_S && \text{on } \Gamma_S \subset \partial\Omega, t \in (0, T) \\ \mathbf{n} \cdot \mathbf{v}(t) &= g_D && \text{on } \Gamma_D = \partial\Omega \setminus \Gamma_S, t \in (0, T). \end{aligned}$$

If we write this as a first-order system we find for  $\mathbf{y} = (\mathbf{v}, p)$  and  $m = d + 1$

$$M\mathbf{y} = \begin{pmatrix} \rho \mathbf{v} \\ \kappa^{-1} p \end{pmatrix}, \quad A\mathbf{y} = \begin{pmatrix} -\nabla p \\ -\nabla \cdot \mathbf{v} \end{pmatrix}, \quad A_{\mathbf{n}}\mathbf{y} = \begin{pmatrix} -p\mathbf{n} \\ -\mathbf{n} \cdot \mathbf{v} \end{pmatrix}, \quad \mathbf{f} = \begin{pmatrix} \mathbf{b} \\ 0 \end{pmatrix}, \quad \mathbf{g} = \begin{pmatrix} -p_S \mathbf{n} \\ -g_D \end{pmatrix}.$$

**Inf-sup stability.** For the case of homogeneous boundary and initial data we introduce spaces  $Y = L_2(\Omega; \mathbb{R}^m)$  and  $W = L_2(Q; \mathbb{R}^m)$  with inner products  $(\cdot, \cdot)_\Omega$ ,  $(\cdot, \cdot)_Q$ , respectively, and norms

$$\|\mathbf{y}\|_Y = \sqrt{(M\mathbf{y}, \mathbf{y})_\Omega}, \quad \|\mathbf{w}\|_W = \sqrt{(M\mathbf{w}, \mathbf{w})_Q}, \quad \|\mathbf{w}\|_{W^*} = \sqrt{(M^{-1}\mathbf{w}, \mathbf{w})_Q},$$



and construct spaces  $V, V^* \subset L_2(Q; \mathbb{R}^m)$  with norms

$$\|\mathbf{w}\|_V = \sqrt{\|\mathbf{w}\|_W^2 + \|L\mathbf{w}\|_{W^*}^2}, \quad \|\mathbf{z}\|_{V^*} = \sqrt{\|\mathbf{z}\|_W^2 + \|L^*\mathbf{z}\|_{W^*}^2}.$$

With the following result one can prove unique existence of  $\mathbf{v} \in V$  for the weak problem  $L\mathbf{v} = \mathbf{f}$  for  $\mathbf{f} \in L_2(\Omega; \mathbb{R}^m)$ .

**Theorem 1** (Inf-sup stability). *The bilinear form  $b: V \times W \rightarrow \mathbb{R}$  defined by  $b(\mathbf{v}, \mathbf{w}) = (L\mathbf{v}, \mathbf{w})_Q$  is inf-sup stable with  $\beta = (4T^2 + 1)^{-1/2}$ :*

$$\inf_{\mathbf{v} \in V \setminus \{0\}} \sup_{\mathbf{w} \in W \setminus \{0\}} \frac{b(\mathbf{v}, \mathbf{w})}{\|\mathbf{v}\|_V \|\mathbf{w}\|_W} = \inf_{\mathbf{w} \in W \setminus \{0\}} \sup_{\mathbf{v} \in V \setminus \{0\}} \frac{b(\mathbf{v}, \mathbf{w})}{\|\mathbf{v}\|_V \|\mathbf{w}\|_W} \geq \beta.$$

**The Petrov–Galerkin setting.** We discretize  $\Omega$  into cells  $K \in \mathcal{K}$  and  $(0, T)$  into time intervals  $I \in \mathcal{I}$ . This induces a decomposition of  $Q$  into space-time cells  $R = I \times K \in \mathcal{R}$ .

For a time-slab  $I$  we let  $Y_{I,h} \subset L_2(\Omega; \mathbb{R}^m)$  be the space of piecewise polynomials of degree  $p_{I,K}$  for  $K \in \mathcal{K}$  over  $\Omega$  and  $Y_h = \oplus_{I \in \mathcal{I}} Y_{I,h}$ . The space-time ansatz space  $V_h \in L_2(Q; \mathbb{R}^m)$  is built of piecewise polynomials on  $R$  with degrees  $p_R = p_{I,K}$  in time and  $q_R = q_{I,K}$  in space, respecting the homogeneous initial conditions, and is required to be *continuous in time*. Accordingly, the test space  $W_h \in L_2(Q; \mathbb{R}^m)$  equals  $V_h$  in space but is discontinuous in time with degree  $p_R = p_{I,K} - 1$ . Note that this gives  $W_h \subset \partial_t V_h$  and is thus named a Petrov–Galerkin method.

We define an approximation  $L_h$  to  $L$  with:

- a)  $M_h \in L_\infty(\Omega; \mathbb{R}_{\text{sym}}^{m \times m})$  is uniformly positive definite, i.e.,  $c_M > 0$  exists with

$$(M_h \mathbf{y}_h, \mathbf{y}_h)_\Omega \geq c_M \|\mathbf{y}_h\|_W^2, \quad \mathbf{y}_h \in Y_h;$$

- b)  $A_h \in \mathcal{L}(Y_h, Y_h)$  is monotone and consistent, i.e.,

$$\begin{aligned} (A_h \mathbf{y}_h, \mathbf{y}_h)_Q &\geq 0, & \mathbf{y}_h &\in Y_h, \\ (A_h \mathbf{z}_h, \mathbf{y}_h)_Q &= (A\mathbf{z}_h, \mathbf{y}_h)_Q, & \mathbf{z}_h &\in Y_h \cap \mathcal{D}(A); \end{aligned}$$

Let  $\Pi_h: L_2(Q; \mathbb{R}^m) \rightarrow W_h$  be the projection with  $(M_h \Pi_h \mathbf{v}, \mathbf{w}_h)_Q = (M_h \mathbf{v}, \mathbf{w}_h)_Q$  and define discrete norms  $\|\mathbf{v}\|_{W_h}^2 = (M_h \mathbf{v}, \mathbf{v})_Q$  and  $\|\mathbf{v}\|_{V_h}^2 = \|\mathbf{v}\|_{W_h}^2 + \|\Pi_h M_h^{-1} L_h \mathbf{v}\|_{W_h}^2$  for  $\mathbf{v} \in V_h$ .

**Theorem 2** (Discrete inf-sup stability). *The bilinear form  $b_h: V_h \times W_h \rightarrow \mathbb{R}$ ,  $b_h(\mathbf{v}_h, \mathbf{w}_h) = (L_h \mathbf{v}_h, \mathbf{w}_h)_Q$ , is inf-sup stable with  $\beta > 0$  defined in Thm. 1:*

$$\inf_{\mathbf{v}_h \in V_h \setminus \{0\}} \sup_{\mathbf{w}_h \in W_h \setminus \{0\}} \frac{b_h(\mathbf{v}_h, \mathbf{w}_h)}{\|\mathbf{v}_h\|_{V_h} \|\mathbf{w}_h\|_{W_h}} \geq \beta.$$

Discretizations that lead to approximations  $A_h$  as required can be obtained by taking upwind schemes. A construction of such schemes uses the flux computed from local Riemann problems [2, Sect. 3].

For this scheme one can derive error estimates in the  $V_h$ -norm for smooth solutions of order  $\tau^p + h^q$  (in time and spatial step size), where  $1 \leq p \leq \min_{R \in \mathcal{R}} p_R$ ,  $1 \leq q \leq \min_{R \in \mathcal{R}} q_R$  [1, Thm. 4.3] [2, Thm. 4.1].

The case of non-homogeneous initial and boundary conditions can be treated in this fashion if we assume that there is a  $\hat{\mathbf{u}} \in V$  that attains initial and boundary values. The problem is then reformulated to seek the solution  $\mathbf{u} \in V$  of  $L\mathbf{u} = \mathbf{f} - L\hat{\mathbf{u}}$  [3, Rem. 10].

As solutions to hyperbolic problems can be of low regularity, we are interested in weaker notions of solutions. In the following we allow more general non-homogeneous initial conditions  $\mathbf{u}_0$ , but assume that  $M = M_h$ . For convenience, the notion  $h \in \mathcal{H}$  means that there is a sequence of nested problems with accumulation at  $h \rightarrow 0$ .

**Theorem 3** (Convergence of Petrov–Galerkin solutions in  $L_2$ ). *Let  $\mathbf{u}_0 \in L_2(\Omega; \mathbb{R}^m)$  such there exists a sequence  $(\mathbf{u}_{0,h})_{h \in \mathcal{H}} \subset L_2(Q; \mathbb{R}^m)$  with  $\mathbf{u}_{0,h}(0) \rightarrow \mathbf{u}_0$  in  $L_2(\Omega; \mathbb{R}^m)$  and  $\sup_{h \in \mathcal{H}} \|\mathbf{u}_{0,h}\|_{V_h} \leq C$ . Then the discrete solutions  $(\mathbf{u}_h)_{h \in \mathcal{H}}$  are weakly converging in  $L_2(\Omega; \mathbb{R}^m)$  to the weak solution  $\mathbf{u} \in W$  of the equation*

$$(3) \quad (\mathbf{u}, L^* \mathbf{z})_Q = (\mathbf{f}, \mathbf{z})_Q + (M\mathbf{u}_0, \mathbf{z}(0))_\Omega, \quad \mathbf{z} \in V^*.$$

A corresponding result can be proved also for the DG space-time setting where we use discontinuous ansatz functions in time and the same space for the test functions. Here, the condition for the initial value is relaxed.

**Theorem 4** (Convergence of DG space-time solutions in  $L_2$ ). *For  $\mathbf{u}_0 \in L_2(\Omega; \mathbb{R}^m)$  and  $\mathbf{f} \in L_2(Q; \mathbb{R}^m)$  the discrete solutions  $(\mathbf{u}_h)_{h \in \mathcal{H}}$  of the acoustic wave equation are weakly converging in  $L_2(\Omega; \mathbb{R}^m)$  to the weak solution  $\mathbf{u} \in W$  of the equation (3).*

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## Low-rank space-time Galerkin methods for parabolic equations

ALEXANDRE ERN

(joint work with T. Boiveau, V. Ehrlacher, A. Nouy)

We devise a space-time tensor method for the low-rank approximation of linear parabolic evolution equations. The proposed method is a stable Galerkin method, uniformly in the discretization parameters, based on a Minimal Residual formulation of the evolution problem in Hilbert–Bochner spaces. The discrete solution is sought in a linear trial space composed of tensors of discrete functions in space

and in time and is characterized as the unique minimizer of a discrete functional where the dual norm of the residual is evaluated in a space semi-discrete test space. The resulting global space-time linear system is solved iteratively by a greedy algorithm. Numerical results are presented to illustrate the performance of the proposed method on test cases including non-selfadjoint and time-dependent differential operators in space. Further insight can be found in [1].

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**A FEM-BEM method for the numerical solution of 2D exterior linear elastodynamics problems using scalar potentials**

SILVIA FALLETTA

(joint work with G. Monegato, L. Scuderi)

Let  $\Omega^i \subset \mathbb{R}^2$  be an open, bounded and rigid domain, whose boundary  $\Gamma$  is assumed to be closed and smooth. We aim at studying the propagation of elastic waves in the homogeneous isotropic elastic medium  $\Omega^e := \mathbb{R}^2 \setminus \overline{\Omega^i}$ , caused by a body force  $\mathbf{f}$ , a Dirichlet datum  $\mathbf{g}$  and trivial initial conditions. Assuming small variations of the vector field  $\mathbf{u}^e(\mathbf{x}, t) = (u_1^e(\mathbf{x}, t), u_2^e(\mathbf{x}, t))$ ,  $\mathbf{x} = (x_1, x_2)$ , this latter is uniquely defined by the following system:

$$\begin{cases} \rho \frac{\partial^2 \mathbf{u}^e}{\partial t^2}(\mathbf{x}, t) - (\lambda + \mu) \nabla(\operatorname{div} \mathbf{u}^e)(\mathbf{x}, t) - \mu \nabla^2 \mathbf{u}^e(\mathbf{x}, t) &= \mathbf{f}(\mathbf{x}, t) & \mathbf{x} \in \Omega^e, t \in (0, T] \\ \mathbf{u}^e(\mathbf{x}, t) &= \mathbf{g}(\mathbf{x}, t) & \mathbf{x} \in \Gamma, t \in (0, T] \\ \mathbf{u}^e(\mathbf{x}, 0) &= \mathbf{0} & \mathbf{x} \in \Omega^e \\ \mathbf{u}_t^e(\mathbf{x}, 0) &= \mathbf{0} & \mathbf{x} \in \Omega^e, \end{cases}$$

where  $\rho > 0$  is the constant material density,  $\lambda > 0$  and  $\mu > 0$  are the Lamé constants. Using the Helmholtz decomposition of a vector field (see [1]), we decompose the unknown displacement by two unknown scalar potentials  $\mathbf{u}^e = \nabla \varphi_P^e + \mathbf{curl} \varphi_S^e$  where, for a generic scalar function  $w = w(x_1, x_2)$ , its vectorial curl is defined as  $\mathbf{curl} w = (\partial_{x_2} w, -\partial_{x_1} w)$ . The unknowns  $\varphi_P^e$  and  $\varphi_S^e$  are called Primary (or longitudinal) and Secondary (or transverse) waves.

Referring to [2] for details, we recall the main relations that allows us to rewrite the elastodynamic equation in terms of a couple of wave equations. In particular, by using the decomposition of the Dirichlet datum on  $\Gamma$ ,  $\mathbf{g} = \nabla \varphi_P^e + \mathbf{curl} \varphi_S^e$ , and introducing the anti-clockwise oriented unit tangent vector  $\boldsymbol{\tau}_\Gamma = (n_{\Gamma,2}, -n_{\Gamma,1})$ ,  $\mathbf{n}_\Gamma = (n_{\Gamma,1}, n_{\Gamma,2})$  being the ingoing unit normal vector on  $\Gamma$ , the following relations hold:

$$\frac{\partial \varphi_P^e}{\partial \mathbf{n}_\Gamma} - \frac{\partial \varphi_S^e}{\partial \boldsymbol{\tau}_\Gamma} = \mathbf{g} \cdot \mathbf{n}_\Gamma, \quad \frac{\partial \varphi_S^e}{\partial \mathbf{n}_\Gamma} + \frac{\partial \varphi_P^e}{\partial \boldsymbol{\tau}_\Gamma} = \mathbf{g} \cdot \boldsymbol{\tau}_\Gamma.$$

Hence, we obtain that the exterior elastodynamics problem is formally equivalent (see [3]) to the following exterior potentials problem:

$$(1) \quad \begin{cases} \frac{\partial^2 \varphi_P^e}{\partial t^2} - v_P^2 \nabla^2 \varphi_P^e = \frac{1}{\rho} f_P & (\mathbf{x}, t) \in \Omega^e \times (0, T] \\ \frac{\partial^2 \varphi_S^e}{\partial t^2} - v_S^2 \nabla^2 \varphi_S^e = \frac{1}{\rho} f_S & (\mathbf{x}, t) \in \Omega^e \times (0, T] \\ \frac{\partial \varphi_P^e}{\partial \mathbf{n}_\Gamma} = \frac{\partial \varphi_S^e}{\partial \boldsymbol{\tau}_\Gamma} + \mathbf{g} \cdot \mathbf{n}_\Gamma =: \frac{\partial \varphi_S^e}{\partial \boldsymbol{\tau}_\Gamma} + g_{\mathbf{n}_\Gamma} & (\mathbf{x}, t) \in \Gamma \times (0, T] \\ \frac{\partial \varphi_S^e}{\partial \mathbf{n}_\Gamma} = -\frac{\partial \varphi_P^e}{\partial \boldsymbol{\tau}_\Gamma} + \mathbf{g} \cdot \boldsymbol{\tau}_\Gamma =: -\frac{\partial \varphi_P^e}{\partial \boldsymbol{\tau}_\Gamma} + g_{\boldsymbol{\tau}_\Gamma} & (\mathbf{x}, t) \in \Gamma \times (0, T], \end{cases}$$

endowed with null initial conditions.

Aiming at determining the solution of (1) in a bounded subregion of  $\Omega^e$ , surrounding the physical domain  $\Omega^i$ , we truncate the infinite domain  $\Omega^e$  by introducing an artificial smooth boundary  $\mathcal{B}$ , hence obtaining a finite computational domain  $\Omega$ , which is bounded internally by  $\Gamma$  and externally by  $\mathcal{B}$ . Then, assuming  $f_P$  and  $f_S$  locally supported in  $\Omega^i$ , we define on  $\mathcal{B} \times [0, T]$  a couple of scalar TD-NRBCs:

$$\frac{1}{2} \varphi_\star^e(\mathbf{x}, t) + (\mathcal{K}_\star \varphi_\star^e)(\mathbf{x}, t) - (\mathcal{V}_\star(\partial_{\mathbf{n}_D} \varphi_\star^e))(\mathbf{x}, t) = 0, \quad \star := P, S$$

$\mathcal{V}_\star$  and  $\mathcal{K}_\star$ , being the well known single and double layer operators associated with the scalar  $\star = P, S$ -wave equations:

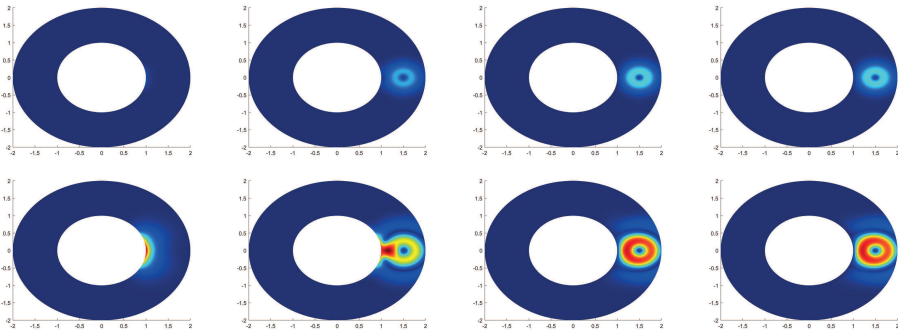
$$\begin{aligned} (\mathcal{V}_\star \psi)(\mathbf{x}, t) &:= \int_0^t \int_{\mathcal{B}} G_\star(\mathbf{x} - \mathbf{y}, t - s) \psi(\mathbf{y}, s) \, d\mathcal{B}_\mathbf{y} \, ds \\ (\mathcal{K}_\star \lambda)(\mathbf{x}, t) &:= \int_0^t \int_{\mathcal{B}} G_{\mathbf{n}_D, \star}(\mathbf{x} - \mathbf{y}, t - s) \lambda(\mathbf{y}, s) \, d\mathcal{B}_\mathbf{y} \, ds. \end{aligned}$$

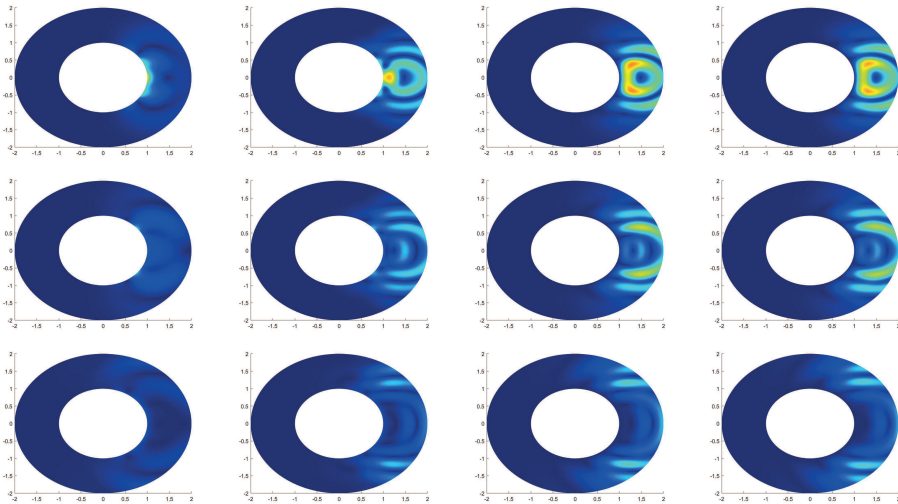
To restrict the original problem in the finite computational domain  $\Omega$ , we impose the continuity transmission conditions of the  $P$  and  $S$ -waves as well as of their normal derivatives on the artificial boundary  $\mathcal{B}$ . Hence, denoting by  $\varphi_P$  and  $\varphi_S$  the restriction of the solutions  $\varphi_P^e$  and  $\varphi_S^e$  to  $\Omega$ , we get:

$$(2) \quad \begin{cases} \frac{\partial^2 \varphi_P}{\partial t^2}(\mathbf{x}, t) - v_P^2 \nabla^2 \varphi_P(\mathbf{x}, t) = \frac{1}{\rho} f_P(\mathbf{x}, t) & (\mathbf{x}, t) \in \Omega \times (0, T] \\ \frac{\partial^2 \varphi_S}{\partial t^2}(\mathbf{x}, t) - v_S^2 \nabla^2 \varphi_S(\mathbf{x}, t) = \frac{1}{\rho} f_S(\mathbf{x}, t) & (\mathbf{x}, t) \in \Omega \times (0, T] \\ \frac{\partial \varphi_P}{\partial \mathbf{n}_\Gamma}(\mathbf{x}, t) = \frac{\partial \varphi_S}{\partial \boldsymbol{\tau}_\Gamma}(\mathbf{x}, t) + g_{\mathbf{n}_\Gamma}(\mathbf{x}, t) & (\mathbf{x}, t) \in \Gamma \times (0, T] \\ \frac{\partial \varphi_S}{\partial \mathbf{n}_\Gamma}(\mathbf{x}, t) = -\frac{\partial \varphi_P}{\partial \boldsymbol{\tau}_\Gamma}(\mathbf{x}, t) + g_{\boldsymbol{\tau}_\Gamma}(\mathbf{x}, t) & (\mathbf{x}, t) \in \Gamma \times (0, T] \\ \frac{1}{2} \varphi_P(\mathbf{x}, t) + (\mathcal{K}_P \varphi_P)(\mathbf{x}, t) + (\mathcal{V}_P(\partial_{\mathbf{n}} \varphi_P))(\mathbf{x}, t) = 0, & (\mathbf{x}, t) \in \mathcal{B} \times (0, T] \\ \frac{1}{2} \varphi_S(\mathbf{x}, t) + (\mathcal{K}_S \varphi_S)(\mathbf{x}, t) + (\mathcal{V}_S(\partial_{\mathbf{n}} \varphi_S))(\mathbf{x}, t) = 0, & (\mathbf{x}, t) \in \mathcal{B} \times (0, T]. \end{cases}$$

We discretize the space-time integral equations in (2) defined on  $\mathcal{B}$  by combining a second order BDF convolution quadrature in time and a collocation method in space. Such a discretization is then coupled with an unconditionally stable ODE integrator in time and a FEM in space.

**Example.** In our experiment, the domain of computation is an annulus, whose interior physical boundary  $\Gamma$  is the unit circle, and the artificial one  $\mathcal{B}$  is the circle of radius 2. We have chosen an S-wave source term, localized in space at  $\mathbf{x} = (1.5, 0)$ , which varies in time as a Ricker pulse. In the plots we present the snapshots of the numerical solution obtained at the fixed time instants  $t_n = 0.75, 1.25, 1.75, 2, 2.5$ . The first three columns represent the solution obtained by the scalar FEM-BEM method ( $|\nabla \varphi_P|$ ,  $|\mathbf{curl} \varphi_S|$  and  $|\mathbf{u}|$ , respectively) while the last one refers to the solution obtained by applying a FEM-BEM approach for the classical vector displacement formulation. As we can see, there is a very good agreement between the new scalar and the standard vector solutions, depicted in the second last and last columns of the figure, respectively.





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## Two Time Parallel Algorithms for PDE Constraint Optimization: Difference with Time Parallel Algorithms for Evolution Problems

MARTIN J. GANDER

Parallel in Time (PinT) algorithms have received a lot of attention over the past two decades, following the invention in 2001 of the Parareal algorithm by Lions, Maday and Turinici [1]; for a detailed convergence analysis, see [2] for linear partial differential equations, and [3] for nonlinear problems. PinT algorithms have gained tremendous importance for the parallelization of evolution problems on the massively parallel computing architectures available today, since the millions of computing cores can often not be used effectively when only parallelizing such problems in space. PinT algorithms have however a long history spanning more than 5 decades; for a review, see [4]. More recently, PinT algorithms have also been developed for optimal control problems and PDE constraint optimization, where the constraints are given by evolution problems [5, 6, 7, 8, 9, 10, 11], for a historical introduction to such problems, see [12]. These algorithms have become known under the name ParaOpt algorithms.

Solving evolution problems with PinT algorithms is however quite different from solving optimal control or PDE constraint optimization problems with evolution

problems as constraints using PinT algorithms. I illustrated this in my presentation with two ParaOpt algorithms, the first one from [13, 14] based on Schwarz domain decomposition in time, motivated by [8], and the second one from [15] based on Parareal techniques.

Consider the PDE constraint optimization problem

$$(1) \quad \min_{y,u} \mathcal{J}(y, u), \quad \text{subject to } \dot{y} + Ay = u, \quad y(0) = y_0,$$

where  $y$  is the state,  $u$  the control,  $A$  a linear operator, and the functional to be minimized is defined by

$$(2) \quad \mathcal{J}(y, u) := \frac{1}{2} \int_0^T \|y - \hat{y}\|^2 + \frac{\gamma}{2} \|y(T) - \hat{y}(T)\|^2 + \frac{\nu}{2} \int_0^T \|u\|^2,$$

$\gamma$  and  $\nu$  being two positive parameters to give weights to the terms to be minimized. Using a Lagrange multiplier  $\lambda(t)$ , see e.g. [12], we have to minimize

$$(3) \quad \min_{y,u,\lambda} \left( \mathcal{J}(y, u) + \int_0^T (\dot{y} + Ay - u)^T \lambda \right).$$

Taking derivatives with respect to  $\lambda$ ,  $y$  and  $u$ , we find the optimality condition

$$(4) \quad \begin{cases} \dot{y} + Ay = u \text{ on } (0, T), \\ y(0) = y_0, \end{cases} \quad \begin{cases} \dot{\lambda} - A^T \lambda = y - \hat{y} \text{ on } (0, T), \\ \lambda(T) = -\gamma(y(T) - \hat{y}(T)), \end{cases} \quad \lambda(t) = \nu u(t).$$

We can eliminate  $u(t) = \frac{1}{\nu} \lambda(t)$  to obtain the PDE first order optimality system

$$(5) \quad \begin{bmatrix} \dot{y} \\ \dot{\lambda} \end{bmatrix} + \begin{bmatrix} A & -\nu^{-1}I \\ -I & -A^T \end{bmatrix} \begin{bmatrix} y \\ \lambda \end{bmatrix} = \begin{bmatrix} 0 \\ -\hat{y} \end{bmatrix},$$

with initial and final conditions  $y(0) = y_0$ ,  $\lambda(T) = -\gamma(y(T) - \hat{y}(T))$ . The fact that we have now initial and final conditions is very important, the problem we have to solve is now a boundary value problem in time, not an initial value problem any more!

To use a Schwarz domain decomposition method in time<sup>1</sup>, we divide the time interval  $(0, T)$  into  $I_1 = (0, \beta)$  and  $I_2 = (\alpha, T)$ ,  $\alpha \leq \beta$  and for  $n = 1, 2, \dots$ , solve

$$\begin{cases} \begin{bmatrix} \dot{y}_1^n \\ \dot{\lambda}_1^n \end{bmatrix} + \begin{bmatrix} A & -\nu^{-1}I \\ -I & -A^T \end{bmatrix} \begin{bmatrix} y_1^n \\ \lambda_1^n \end{bmatrix} = \begin{bmatrix} 0 \\ -\hat{y} \end{bmatrix} & \text{on } I_1 = (0, \beta), \\ y_1^n(0) = y_0, \\ \lambda_1^n(\beta) + p y_1^n(\beta) = \lambda_2^{n-1}(\beta) + p y_2^{n-1}(\beta), \end{cases}$$

---

<sup>1</sup>This would make very little sense, without further mechanisms like a coarse propagation, for the pure evolution problem, since solving the subdomain problem earlier in time followed by the subdomain problem later in time would immediately lead to the solution of the evolution problem, due to causality, and this independently of the overlap.

$$\left\{ \begin{array}{l} \begin{bmatrix} \dot{y}_2^n \\ \dot{\lambda}_2^n \end{bmatrix} + \begin{bmatrix} A & -\nu^{-1}I \\ -I & -A^T \end{bmatrix} \begin{bmatrix} y_2^n \\ \lambda_2^n \end{bmatrix} = \begin{bmatrix} 0 \\ -\hat{y} \end{bmatrix} \\ y_2^n(\alpha) - q\lambda_2^n(\alpha) = y_1^{n-1}(\alpha) - q\lambda_1^{n-1}(\alpha), \\ \lambda_2^n(T) = -\gamma(y_2^n(T) - \hat{y}(T)), \end{array} \right. \quad \text{on } I_2 = (\alpha, T),$$

where  $p$  and  $q$  are two real parameters that can be tuned to get best performance of the algorithm. If the PDE is discretized, and  $A = A^T \in \mathbb{R}^{m \times m}$ ,  $A = QDQ^T$ , with  $Q^T Q = I$  and  $D = \text{diag}(d_1, \dots, d_m)$ , then we can diagonalize the subdomain problems, and obtain for example for the first one

$$\left\{ \begin{array}{l} \begin{bmatrix} \dot{z}_1^n \\ \dot{\mu}_1^n \end{bmatrix} + \begin{bmatrix} D & -\nu^{-1}I \\ -I & -D \end{bmatrix} \begin{bmatrix} z_1^n \\ \mu_1^n \end{bmatrix} = \begin{bmatrix} 0 \\ -\hat{z} \end{bmatrix} \\ z_1^n(0) = z_0, \\ \mu_1^n(\beta) + pz_1^n(\beta) = \mu_2^{n-1}(\beta) + pz_2^{n-1}(\beta), \end{array} \right. \quad \text{on } I_1 = (0, \beta),$$

which are now  $m$  independent  $2 \times 2$  systems of the form

$$\dot{z}_1^{(i),n} + d_i z_1^{(i),n} - \nu^{-1} \mu_1^{(i),n} = 0, \quad \dot{\mu}_1^{(i),n} - d_i \mu_1^{(i),n} - z_1^{(i),n} = \hat{z}^{(i)}.$$

Isolating  $\mu_1$  from the first equation and substituting into the second yields

$$(6) \quad \ddot{z}_1^{(i),n} - (d_i^2 + \nu^{-1})z_1^{(i),n} = -\nu^{-1}\hat{z}^{(i)},$$

with  $z_1^{(i),n}(0) = z_0^{(i)}(0)$  and transmission condition at  $t = \beta$

$$(7) \quad \dot{z}_1^{(i),n} + (d_i + p\nu^{-1})z_1^{(i),n} = \dot{z}_2^{(i),n-1} + (d_i + p\nu^{-1})z_2^{(i),n-1},$$

and similarly on the second subdomain. Equation (6) shows us that in fact we have now a Laplace like equation to solve in time, not a parabolic evolution problem any more, and thus a Schwarz algorithm in time makes sense for the optimality system. Furthermore, the transmission conditions are automatically Robin transmission conditions in (7), even without the parameters  $p$  and  $q$ , so applying Schwarz to the optimality system (5) leads automatically to an algorithm in the class of Optimized Schwarz Methods, see [16] for an introduction to such methods. In [13], we show that this algorithm converges linearly, in contrast to the superlinear convergence PinT algorithms often show for parabolic evolution problems, and we show also how to optimize the parameters  $p$  and  $q$ , see also [14].

Similarly, I showed a second new such ParaOpt algorithm, based on Parareal techniques, introduced and analyzed in [15], and it also converges linearly, in contrast to the Parareal algorithm that converges superlinearly when applied to parabolic evolution problems [2]. There is therefore an important difference for PinT algorithms when they are used to solve evolution problems, in contrast to solving optimal control problems with these evolution problems as constraints, since the optimality condition transforms the evolution problems into boundary value problems.



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**Higher-order boundary elements in the time domain:  
adaptivity, graded meshes and hp-versions**

HEIKO GIMPERLEIN

(joint work with Alessandra Aimi, Giulia Di Credico, Ceyhan Özdemir,  
Ernst P. Stephan)

Solutions to the wave equation in the exterior of a polyhedral domain or a screen in  $\mathbb{R}^3$  exhibit singular behavior from the edges and corners. For time-independent problems,  $p$ - and  $hp$ -versions of boundary element methods, as well as  $h$ -versions on graded meshes, give rise to fast approximations of both smooth solutions and geometric singularities. Optimal convergence rates on quasi-uniform meshes have

been obtained in [2], while exponential convergence is known on geometrically graded meshes for suitable data. On the other hand, adaptive mesh refinements based on a posteriori error estimates are of interest for the approximation of non-smooth solutions [3].

The talk discussed the extension of these classical results for  $h$ -,  $p$ - and  $hp$ -versions of the Galerkin boundary element method in the time domain, with quasi-optimal error estimates. To be specific, for  $n = 2, 3$  in the exterior  $\Omega \subset \mathbb{R}^n$  of a closed polyhedral surface or screen  $\Gamma$  we considered the initial-boundary value problem for the (scalar) wave equation

$$(1) \quad \partial_t^2 u(t, x) - \Delta_x u(t, x) = 0 \quad \text{in } \mathbb{R}_t^+ \times \Omega_x$$

and the (vector-valued) elastodynamic equations

$$(2) \quad (\lambda + \mu)\nabla(\nabla \cdot u) + \mu\Delta u - \rho\ddot{u} = 0 \quad \text{in } \mathbb{R}_t^+ \times \Omega_x$$

for given Dirichlet data  $u|_\Gamma = g$  on  $\Gamma = \partial\Omega$ . For simplicity, homogeneous initial conditions are  $u(0, x) = \partial_t u(0, x) = 0$  are considered.

Flat polygonal screens  $\Gamma$  pose the greatest numerical challenges. To solve the Dirichlet problem for (1) or (2) numerically, we reformulate it as a time dependent integral equation

$$(3) \quad \mathcal{V}\psi = \left(\mathcal{K} + \frac{1}{2}\right)g$$

on  $\Gamma$  for the single layer operator  $\mathcal{V}$ . This integral equation is approximated using Galerkin boundary elements, based on tensor products  $V_{\Delta t, h}^p$  of piecewise polynomial functions of degree  $p$  on a quasi-uniform mesh in space and a uniform mesh in time.

The approximation rate is governed by the singularities of the solution at non-smooth boundary points of the domain. In conical or wedge domains the singular behavior of the solution to inhomogeneous wave and elastodynamic equations with homogeneous boundary conditions has been clarified by Plamenevskii and collaborators since the late 1990's [8]. Their results show that at fixed time  $t$ , the solution admits an explicit singular expansion with exactly the same singular behavior as for elliptic equations. The results were used by Müller and Schwab to prove optimal convergence rates for a finite element method on algebraically graded meshes for the wave and elastodynamic equations in polygonal domains in  $\mathbb{R}^2$  [7].

Corresponding results for the wave equation in  $\mathbb{R}^3$  were obtained in [4, 5] and for the elastodynamic equations in [1]. They imply approximation results for boundary element methods on graded meshes [4],  $hp$  versions [5] and the efficiency of a posteriori error estimates for adaptive refinement procedures [6].

For example, in [5] we obtain:

**Theorem.** Let  $\psi$  be the solution to the single layer integral equation (3) and  $\psi_{h, \Delta t}$  the best approximation in the norm of  $H_\sigma^r(\mathbb{R}^+, \tilde{H}^{-\frac{1}{2}}(\Gamma))$  to  $\psi$  in  $V_{\Delta t, h}^p$  on a quasi-uniform spatial mesh with  $\Delta t \leq Ch$ . Then

$$\|\psi - \psi_{h, \Delta t}\|_{r, -\frac{1}{2}, \Gamma, *} \leq C \left( \left(\frac{h}{p^2}\right)^{\frac{1}{2}-\varepsilon} + \left(\frac{h}{p}\right)^{\frac{1}{2}+\eta} + \left(\frac{\Delta t}{p}\right)^{\mu+1-r} \right),$$

where  $r \in [0, p + 1)$  and the regular part  $\psi_0 \in H_\sigma^{\mu+1}(\mathbb{R}^+, \tilde{H}^\eta(\Gamma))$  of the singular expansion of  $\psi$ , with  $\eta, \mu$  sufficiently large.

In addition to the a priori error analysis, in [6] we obtain a posteriori error estimates and discuss the resulting adaptive mesh refinement procedures in 3d. The results extend those from the time-independent case [3], and the reader should consult [6] for detailed information.

**Theorem.** Let  $\psi \in H_\sigma^1(\mathbb{R}^+, \tilde{H}^{-\frac{1}{2}}(\Gamma))$  be the solution to (3), and let  $\psi_{h,\Delta t} \in H_\sigma^1(\mathbb{R}^+, H^{-\frac{1}{2}}(\Gamma))$  such that  $\mathcal{R} = \partial_t f - \mathcal{V}\partial_t \phi_{h,\Delta t} \in H_\sigma^0(\mathbb{R}^+, H^1(\Gamma))$ . Then

$$\|\psi - \psi_{h,\Delta t}\|_{0,-\frac{1}{2},\Gamma,*}^2 \leq C \sum_{i,\Delta} \max\{(\Delta t)_i, h_\Delta\} \|\mathcal{R}\|_{0,1,[t_i,t_{i+1}) \times \Delta}^2 .$$

A lower bound is obtained on globally quasi-uniform meshes on  $\Gamma$ , showing a (weak) efficiency of the error estimator:

$$\max\{\Delta t, h\} \|\mathcal{R}\|_{0,1-\epsilon,\Gamma}^2 \leq C \|\phi - \phi_{h,\Delta t}\|_{2,-\frac{1}{2},\Gamma}^2 .$$

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**Stabilized Leapfrog Based Local Time-stepping Method  
For the Wave Equation**

MARCUS J. GROTE

(joint work with Simon Michel, Stefan Sauter)

Local time-stepping methods permit to overcome the severe stability constraint on explicit methods caused by local mesh refinement without sacrificing explicitness. In [6], a leapfrog based explicit local time-stepping (LF-LTS) method was proposed for the time integration of second-order wave equations. Recently, optimal convergence rates were proved for a conforming FEM discretization, albeit under

a CFL stability condition where the global time-step,  $\Delta t$ , depends on the smallest elements in the mesh [10]. In general one cannot improve upon that stability constraint, as the LF-LTS method may become unstable at certain discrete values of  $\Delta t$ . To remove those critical values of  $\Delta t$ , we apply a slight modification (as in recent work on LF-Chebyshev methods [2]) to the original LF-LTS method which nonetheless preserves its desirable properties: it is fully explicit, second-order accurate, satisfies a three-term (leapfrog like) recurrence relation, and conserves the energy. The new stabilized LF-LTS method [11] also yields optimal convergence rates for a standard conforming FE discretization, yet under a CFL condition where  $\Delta t$  no longer depends on the mesh size inside the locally refined region.

## 1. INTRODUCTION

As our model problem, we consider the homogeneous wave equation

$$(1) \quad u_{tt} - \nabla \cdot (c^2 \nabla u) = 0 \quad \text{in } \Omega \times (0, T)$$

$$(2) \quad u|_{t=0} = u_0 \quad u_t|_{t=0} = v_0 \quad \text{in } \Omega,$$

where  $\Omega$  denotes a bounded domain in  $\mathbb{R}^d$ , and  $u_0, v_0$  are prescribed initial conditions. The speed of propagation,  $c = c(x)$ , is assumed piecewise smooth and strictly positive. At the boundary, we impose appropriate boundary conditions for well-posedness.

For the spatial discretization of (1), we consider a conforming finite element (FE) method with mass-lumping. For the time discretization, we opt for the leapfrog based local time-stepping (LTS-LF) method to circumvent the bottleneck caused by the overly stringent CFL condition in the presence of local refinement [6, 7, 15]. Hence we split the mesh into a "coarse" and a "fine" sub-region with mesh size  $h$  and  $h_f$ , respectively. During each time-step  $\Delta t$  inside the "coarse" region, we use  $p$  time-steps of smaller size  $\Delta \tau = \Delta t/p$  inside the "fine" region, where  $p \simeq h/h_f$  — see [6] for details.

Despite the many different explicit LTS methods that were proposed and successfully used for wave propagation in recent years (see [9] and references therein), a rigorous general space-time convergence theory (in the PDE sense) is still lacking. Until recently, convergence had been proved only for the method of Collino et al. [4, 13] and for the locally implicit method for Maxwell's equations by Verwer [17, 5, 12], which combines the explicit Verlet scheme with the implicit Crank–Nicolson, neither fully explicit.

In [10], optimal convergence rates for the fully explicit LF-LTS method from [6] were derived for a conforming FEM discretization, albeit under a CFL condition where the global time-step  $\Delta t$  in fact depends on the smallest elements in the mesh [10]. In doing so, the inner loop over the  $p$  local LF steps of size  $\Delta t/p$  was rewritten in terms of a single global time-step  $\Delta t$ , which involves Chebyshev polynomials. In general one cannot improve upon the stability constraint on  $\Delta t$ , as the LF-LTS method may become unstable at certain discrete values of  $\Delta t$ . Although those instabilities only matter in special situations and for long time simulation, they

nonetheless thwart any attempt to guarantee that the numerical solution remains bounded for all time independently of  $p$ , that is under a CFL condition imposed by the coarse mesh only. In fact, similar instabilities can also occur in leapfrog-Chebyshev (LFC, discrete Gautschi-type) methods without added stabilization [8, 2], which are closely related to LTS schemes. As a remedy, Carle, Hochbruck and Sturm [2] introduced a class of stabilized LFC methods based on stabilized Chebyshev polynomials together with a special starting value. Note that the idea of replacing standard Chebyshev polynomials by their stabilized version for added stability is well-known in the parabolic context and was also recently used to stabilize a Lagrange multiplier based LTS approach [3].

The reformulation of the original LF-LTS method [6] using Chebyshev polynomials in [10] is key for its subsequent stabilization. More concretely, by replacing the Chebyshev polynomials by their stabilized analogues, as in [2] for LFC methods, we devise a stabilized version of the original LF-LTS method [6], which completely removes the potentially unstable behavior at discrete time-steps while preserving all the desirable properties of the original method: it is fully explicit, proceeds by a three-term recurrence relation and conserves (a discrete version of) the energy; hence, the (leapfrog-like) structure of the resulting algorithm remains unchanged [11]. The same stabilized LF-LTS algorithm was developed independently and in parallel by the group of M. Hochbruck [1]. Here we develop a convergence analysis for the fully discrete stabilized LF-LTS method under a CFL condition where  $\Delta t$  no longer depends on the mesh size inside the locally refined region.

## 2. CONVERGENCE THEORY

To develop a general convergence theory for explicit LTS methods, we first define finite-dimensional restriction operators to the “fine” grid and formulate the leapfrog (LF) based LTS method from [6] in a Galerkin conforming finite element setting. Next, we prove continuity and coercivity estimates for the LTS operator that are robust with respect to the number of local time-steps  $p$ , provided a genuine CFL condition is satisfied. Here, new estimates on the coefficients that appear when rewriting the LTS-LF scheme in “leap-frog manner” play a key role. Those estimates pave the way for the stability estimate of the time iteration operator, for which we then prove a stability bound independently of  $p$ .

Due to the local restriction, however, a judicious splitting of the iteration operator and its inverse is required to avoid negative powers of  $h$  via inverse inequalities. By combining our analysis of the semi-discrete formulation, which takes into account the effect of local time-stepping, with classical error estimates, we eventually obtain optimal space-time convergence rates.

Let  $u_h$  denote the fully discrete Galerkin solution of the stabilized LF-LTS method with stabilization parameter  $\nu > 0$  using continuous piecewise polynomial finite elements of order  $\ell$ . Under standard smoothness assumptions on the solution  $u$  of (1)–(2), we prove in [11] under a  $p$ -independent CFL stability condition on

the time-step  $\Delta t > 0$  and the mesh size  $h > 0$  in the coarse region that

$$\|u - u_h\|_{L^\infty([0,T];L^2(\Omega))} \leq C(1+T)(h^{\ell+1} + \Delta t^2),$$

where the constant  $C$  depends only on  $u$  and  $\nu$ , but not on  $h$ ,  $\Delta t$ ,  $p$  or  $T$ .

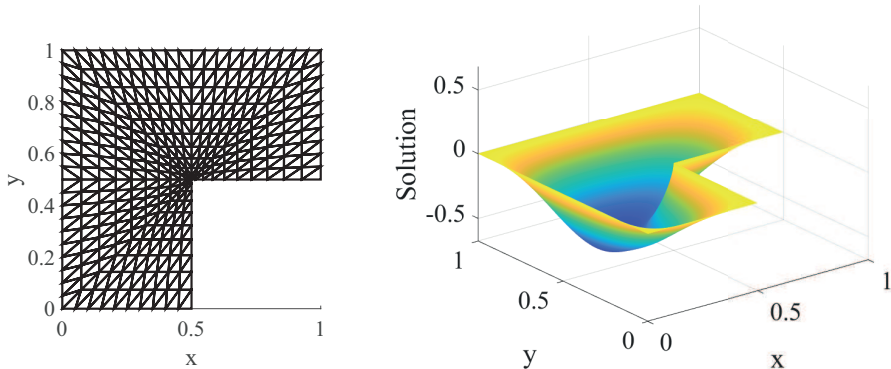


FIGURE 1. Left: Graded mesh with grading parameter  $\beta = 1.5$ . Right: LF-LTS solution of (1) for initial conditions (3) at  $t = 0.3$

### 3. NUMERICAL EXPERIMENT

We consider (1)–(2) in an L-shaped domain  $\Omega$ , with a reentrant corner,  $\Omega = (0, 1)^2 \setminus ([0.5, 1] \times (0.5, 1])$ . Due to characteristic singularities of the solution at reentrant corners, uniform meshes generally do not yield optimal convergence rates [14]. A common remedy to restore the accuracy and achieve optimal convergence rates is to use (a-priori) graded meshes [16, Chapt. 3.3.7] toward the reentrant corner. Hence, we first partition  $\Omega$  into six triangles of equal size with a common vertex at the center  $(0.5, 0.5)$ . Then on every edge  $e$  connected to the center, we allocate  $N + 1$  points at distance

$$|e| \left( \frac{k}{N} \right)^\beta, \quad k = 0, 1, \dots, N,$$

from it, where  $\beta \geq 1$  is a fixed grading parameter; the larger  $\beta$ , the more strongly the triangles will cluster near the reentrant corner, whereas for  $\beta = 1$  the mesh is uniform throughout  $\Omega$ . All other vertices within the same  $k$ -th layer are distributed uniformly, as shown in Fig. 1 for a graded mesh with  $\beta = 1.5$  and  $N = 10$ .

Now, we consider (1)–(2) in  $\Omega$  with homogeneous Dirichlet boundary conditions and the initial conditions

$$(3) \quad \begin{cases} u_0(x) = 0, \\ v_0(x) = -w(x), \end{cases}$$

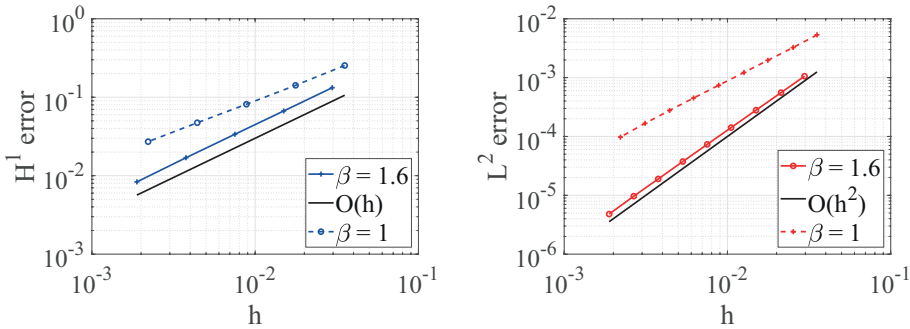


FIGURE 2. L-shaped domain: Absolute errors vs.  $h = \max_{\tau} h_{\tau}$  at  $t = 0.3$  either for graded meshes with  $\beta = 1.6$  and LF-LTS time integration (solid), or for uniform meshes (with  $\beta = 1$ ) and standard LF time integration (dashed). Left:  $H^1$ -error with reference line  $\mathcal{O}(h)$ ; right:  $L^2$ -error with reference line  $\mathcal{O}(h^2)$ .

where  $w$  is the (singular) solution of the elliptic problem  $\Delta w = 100$  in  $\Omega$  with homogeneous Dirichlet boundary conditions, numerically computed on a highly refined mesh.

We solve this problem numerically using  $\mathbb{P}_1$ -FE and the stabilized LF-LTS method with  $\nu = 0.01$  for time integration on a sequence of graded meshes. On every mesh, we let the locally refined region  $\Omega_f$  consist of those elements which lie inside the nearest  $\lfloor \sqrt{N} \rfloor$  layers from the reentrant corner. Hence, the number of local time-steps,  $p$ , depends on  $N$  and thus varies from one mesh to another. The numerical solution for  $\beta = 1.5$  and  $N = 320$  is shown at time  $t = 0.3$  in Fig. 1.

Next, we study the convergence of the stabilized LF-LTS scheme on a sequence of graded meshes with  $\beta = 1.6$  and  $h = \max_{\tau} h_{\tau}$ . As shown in Fig. 2, the error converges optimally as  $\mathcal{O}(h)$  with respect to the  $H^1$ -norm and as  $\mathcal{O}(h^2)$  with respect to the  $L^2$ -norm. The  $L^2$ - and  $H^1$ -errors are both computed at the final time  $t = 0.3$  with respect to a reference solution on a finer mesh.

For the sake of comparison, we also display the errors obtained with a standard LF method on a sequence of uniform meshes. As expected, the LF method with a uniform FE discretization fails to achieve the optimal convergence rates due to the corner singularity. Moreover, for any mesh size  $h$ , the LF-LTS method on the corresponding graded mesh is more accurate than the standard LF method on a uniform mesh.

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## On the use of potentials for finite element computations in elastodynamics

PATRICK JOLY

(joint work with J. Albella, S. Imperiale, J. Rodríguez)

### 1. INTRODUCTION

In nearly incompressible media such as soft tissues, the simulation of elastic wave propagation based on displacement formulations are highly penalized by the fact that shear (S) waves propagate much more slowly than pressure (P) waves. On the other hand, in the case of locally homogeneous media, decomposing of the displacement field as the sum of the gradient and the rotational of two scalar potentials allows the decoupling of the two dynamics giving the hope to build space and time discretizations adapted to each type of wave. For finite element



methods, the challenge is to treat in a stable way boundaries and interfaces, where the two waves are recoupled. In this report, we give the main idea of our approach on a transmission model problem. Due to page limitation, we restrict ourselves to the continuous problem and refer to the bibliography for computational issues.

2. MODEL PROBLEM AND POTENTIAL FORMULATION

We consider a 2D bounded domain of propagation  $\Omega$  that is made of the union of two subsets  $\Omega_1$  and  $\Omega_2$  which are separated by an interface  $\Sigma$  according to figure 1 where the needed notation is also introduced. Each domain  $\Omega_j$  is filled with a homogeneous isotropic medium with density  $\rho_j$  and Lamé's coefficients  $(\lambda_j, \mu_j)$  (all positive). Denoting  $\mathbf{u}_j$  the displacement field in  $\Omega_j$ , the transmission problem to be solved is composed with the following PDE's

$$(1) \quad \rho_j \partial_t^2 \mathbf{u}_j - \mathbf{div} \boldsymbol{\sigma}(\mathbf{u}_j) = 0, \quad \boldsymbol{\sigma}(\mathbf{u}) = \lambda_j \operatorname{div} \mathbf{u} \mathbf{I} + 2\mu_j \boldsymbol{\varepsilon}(\mathbf{u}_j) \quad \text{in } \Omega_j, j = 1, 2$$

with  $\boldsymbol{\varepsilon}(\mathbf{u}_j) := (\nabla \mathbf{u}_j + \nabla \mathbf{u}_j^t)/2$  the strain tensor,  $\mathbf{I}$  the identity matrix and  $\mathbf{div}$  the divergence operator for a matrix field. (1) is completed with the transmission and boundary conditions (the exterior boundary  $\Gamma_D$  is a clamped boundary):

$$(2) \quad \mathbf{u}_1 = \mathbf{u}_2, \quad \boldsymbol{\sigma}(\mathbf{u}_1)\mathbf{n} = \boldsymbol{\sigma}(\mathbf{u}_2)\mathbf{n}, \quad \text{on } \Sigma, \quad \mathbf{u}_1 = 0 \quad \text{on } \Gamma_D.$$

Thanks to the identity  $\mathbf{div} \boldsymbol{\sigma}(\mathbf{u}_j) = (\lambda_j + 2\mu_j)\nabla \operatorname{div} \mathbf{u}_j - \mu_j \mathbf{curl} \operatorname{curl} \mathbf{u}_j$ , where  $\mathbf{curl}$  and  $\operatorname{curl}$  are respectively the 2D vector and scalar curl's, one can show that

$$(3) \quad \partial_t \mathbf{u}_j = \nabla \varphi_{P,j} + \mathbf{curl} \varphi_{S,j}$$

where the two scalar potentials  $\varphi_{P,j}$  (for P waves) and  $\varphi_{S,j}$  (for S waves) satisfy the two decoupled wave equations (that replace(1))

$$(4) \quad \rho_j \partial_t^2 \varphi_{P,j} - (\lambda_j + 2\mu_j)\Delta \varphi_{P,j} = 0, \quad \rho_j \partial_t^2 \varphi_{S,j} - \mu_j \Delta \varphi_{S,j} = 0.$$

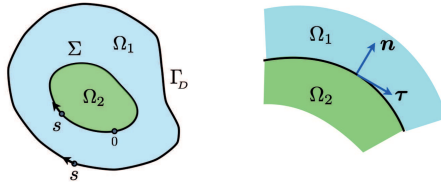


FIGURE 1. Geometry and main notation

The Dirichlet boundary on  $\Gamma_D$  simply becomes ( $\partial_\tau$  denotes the tangential derivative oriented with the curvilinear abscissa  $s$ , cf figure 1)

$$(5) \quad \partial_n \varphi_{P,1} - \partial_\tau \varphi_{S,1} = 0, \quad \partial_n \varphi_{S,1} + \partial_\tau \varphi_{P,1} = 0, \quad \text{on } \Gamma_D.$$

The transmission conditions are more delicate to express in terms of the potentials. To do so, the idea is to introduce an auxiliary unknown  $\mathbf{v}_\Sigma$  which is the

common value of the velocities  $\partial_t \mathbf{u}_1$  and  $\partial_t \mathbf{u}_2$  on  $\Sigma$  (this already encodes the first transmission condition on the continuity of the displacement).

$$\mathbf{v}_\Sigma = (v_1, v_2) := (\partial_t \mathbf{u}_1)_\Sigma \equiv (\partial_t \mathbf{u}_2)_\Sigma$$

which gives, using (3),

$$(6) \quad \partial_n \varphi_{P,j} - \partial_\tau \varphi_{S,j} = \mathbf{v}_\Sigma \cdot \mathbf{n}, \quad \partial_n \varphi_{S,j} + \partial_\tau \varphi_{P,j} = \mathbf{v}_\Sigma \cdot \boldsymbol{\tau}, \quad \text{on } \Gamma_D, \quad j = 1, 2.$$

In what follows, given  $f = (f_1, f_2)$  with  $f_j$  defined in  $\Omega_j$ , we set  $[f] := (f_1 - f_2)|_\Sigma$  (jump across  $\Sigma$ ) and we define the 2D vector potentials

$$\boldsymbol{\varphi}_j := (\varphi_{P,j}, \varphi_{S,j}), \quad \boldsymbol{\varphi} = (\boldsymbol{\varphi}_1, \boldsymbol{\varphi}_2).$$

It can be shown that the second transmission condition (continuity of the normal stress) is equivalent to the existence of two constants  $c_1$  and  $c_2$  such that

$$(7) \quad 2[\mu] v_1 = \mathcal{I}(\partial_t^2 [\rho \boldsymbol{\varphi}] \cdot \boldsymbol{\tau}) + c_1, \quad 2[\mu] v_2 = -\mathcal{I}(\partial_t^2 [\rho \boldsymbol{\varphi}] \cdot \mathbf{n}) + c_2,$$

where  $\mathcal{I}$  is the integration operator along  $\Sigma : \mathcal{I}g(s) := \int_0^s g(s') ds'$ . Note that (7) implies the Gauge conditions

$$(8) \quad \int_\Sigma [\rho \boldsymbol{\varphi}] \cdot \boldsymbol{\tau} = 0, \quad \int_\Sigma [\rho \boldsymbol{\varphi}]_\Sigma \cdot \mathbf{n} = 0.$$

### 3. VARIATIONAL FORMULATIONS

(i) **The case  $\mu_1 = \mu_2$ .** We look for the weak formulation of (4, 6, 7, 8). When there is no jump is  $\mu$ , the easy case, (7) degenerates and implies that the good variational space for  $\boldsymbol{\varphi}$  is, setting  $\mathbf{V}_j := H(\text{div}, \Omega_j) \cap H(\text{curl}, \Omega_j)$ ,

$$(9) \quad \boldsymbol{\varphi} \in \mathbf{V}_\Sigma := \{ \boldsymbol{\psi} \in \mathbf{V}_1 \times \mathbf{V}_2 / [\rho \boldsymbol{\psi}] \cdot \boldsymbol{\tau} = [\rho \boldsymbol{\psi}] \cdot \mathbf{n} = 0 \}$$

After eliminating  $\mathbf{v}_\Sigma$ ,  $c_1$  and  $c_2$  one sees that  $\boldsymbol{\varphi}(t) : \mathbb{R}^+ \rightarrow \mathbf{V}_\Sigma$  satisfies

$$(10) \quad \frac{d^2}{dt^2} m(\boldsymbol{\varphi}(t), \boldsymbol{\psi}) + a(\boldsymbol{\varphi}(t), \boldsymbol{\psi}) = 0, \quad \forall \boldsymbol{\psi} \in \mathbf{V}_\Sigma.$$

with  $m_\Omega(\boldsymbol{\varphi}, \boldsymbol{\psi}) = \sum m_{\Omega,j}(\boldsymbol{\varphi}_j, \boldsymbol{\psi}_j)$ ,  $a(\boldsymbol{\varphi}, \boldsymbol{\psi}) = \sum a_j(\boldsymbol{\varphi}_j, \boldsymbol{\psi}_j)$  (sums on  $j = 1, 2$ ) and

$$(11) \quad \begin{cases} m_{\Omega,j}(\boldsymbol{\varphi}_j, \boldsymbol{\psi}_j) = \frac{\rho_j^2}{\lambda_j + 2\mu_j} \int_{\Omega_j} \varphi_{P,j} \psi_{P,j} + \frac{\rho_j^2}{\mu_j} \int_{\Omega_j} \varphi_{S,j} \psi_{S,j} \\ a_j(\boldsymbol{\varphi}_j, \boldsymbol{\psi}_j) = \rho_j \int_{\Omega_j} (\text{div } \boldsymbol{\varphi}_j \text{ div } \boldsymbol{\psi}_j + \text{curl } \boldsymbol{\varphi}_j \text{ curl } \boldsymbol{\psi}_j) \end{cases}$$

Moreover, it is easy to see that, as soon as  $\boldsymbol{\varphi}$  and  $\boldsymbol{\psi}$  belong to  $H^1(\Omega_1)^2 \times H^1(\Omega_2)^2$ ,

$$a_j(\boldsymbol{\varphi}_j, \boldsymbol{\psi}_j) = \rho_j \int_{\Omega_j} (\nabla \varphi_{P,j} \cdot \nabla \psi_{P,j} + \nabla \varphi_{S,j} \cdot \nabla \psi_{S,j}) + \int_{\partial \Omega_j} (\partial_\tau \varphi_{P,j} \psi_{S,j} + \varphi_{P,j} \partial_\tau \psi_{S,j})$$

which shows that the  $P$  and  $S$  potentials are only coupled on  $\Sigma$  : this allows to discretize independently in space these potentials in each subdomain  $\Omega_j$ .

(ii) **The case  $\mu_1 \neq \mu_2$ .** This time the appropriate variational space is

$$(12) \quad \boldsymbol{\varphi} \in \mathbf{V}_0 := \{ \boldsymbol{\psi} \in \mathbf{V}_1 \times \mathbf{V}_2 / \boldsymbol{\psi} \text{ satisfies (8)} \}$$

Proceeding as in (i), a naive weak formulation is : find  $\varphi(t) : \mathbb{R}^+ \rightarrow \mathbf{V}_0$  such that

$$(13) \quad \frac{d^2}{dt^2} m(\varphi(t), \psi) + a(\varphi(t), \psi) = 0, \quad \forall \psi \in \mathbf{V}_0.$$

where the new mass bilinear form  $m(\cdot, \cdot)$  is given by

$$(14) \quad m(\varphi, \psi) = m_\Omega(\varphi, \psi) + \frac{1}{2[\mu]} \int_\Sigma \left( [\mathcal{I}(\rho\varphi)] [\rho\psi] + [\rho\varphi] [\mathcal{I}(\rho\psi)] \right)$$

The problem comes from the interface term in (14) which has no sign. As a matter of fact, one shows that  $m(\varphi, \psi)$  is not positive in the space  $\mathbf{V}_0$ . More precisely, if  $\mathcal{H}_j$  denotes the subspace functions  $p_j \in H^1(\Omega_j)$  which are harmonic ( $\Delta p_j = 0$ ), one shows that, setting  $p = (p_1, p_2) \in \mathcal{H} := \mathcal{H}_1 \times \mathcal{H}_2$  and  $\nabla p = (\nabla p_1, \nabla p_2)$

$$\forall p \in \mathcal{H}, \nabla p \in \mathbf{V}_0 \quad \text{and} \quad m(\nabla p, \nabla p) = - \sum \frac{\mu_j(\lambda_j + \mu_j)}{\lambda_j + 2\mu_j} \int_{\Omega_j} |\partial_1 p_j|^2 dx < 0.$$

For this reason, the problem (13) is strongly ill posed. The solution consists in reduce the variational space to the following subspace of  $\mathbf{V}_0$ :

$$(15) \quad \nabla \mathcal{H}^\perp := \{ \psi \in \mathbf{V}_0 / m(\psi, \nabla p) = 0, \forall p \in \mathcal{H} \}.$$

Indeed, it can be shown that for the solution,  $\varphi(t) \in \nabla \mathcal{H}^\perp$  for each  $t$  and that

$$(16) \quad \forall \varphi \in \nabla \mathcal{H}^\perp, \quad m(\varphi, \varphi) \geq \alpha \sum \int_{\Omega_j} |\varphi_j|^2, \quad \text{for some } \alpha > 0.$$

so that the variational problem (13) posed in  $\nabla \mathcal{H}^\perp$  instead of  $\mathbf{V}_0$  is a nice variational problem. Treating  $m(\psi, \nabla p) = 0$  as an equality constrain and exploiting the fact that  $\mathcal{H}$  is isomorphic (with an explicit isomorphism involving Poisson problems in each  $\Omega_j$ ) to a space of couples scalar functions defined on  $\partial\Omega_1$  and  $\partial\Omega_2$ , one replaces (13) by a stabilized mixed problem in which appear boundary Lagrange multipliers living on  $\partial\Omega_1$  and  $\partial\Omega_2$ ,

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### On time-domain Foldy-Lax models

MARYNA KACHANOVSKA

**Introduction.** We are interested in constructing accurate asymptotic models for scattering by small particles. Such models have been studied and used extensively in the frequency domain [1, 2, 3, 4, 5], but not much had been done in the time domain, cf. [6, 7]. The goal of this work is to fill in this gap for the case of the 2D sound-soft scattering by circular particles.

More precisely, we study the following model problem. Let the centers of  $N$  circular particles be located at  $\mathbf{c}_j \in \mathbb{R}^2$ ,  $j = 1, \dots, N$ . Given  $R_j > 0$ ,  $j = 1, \dots, N$ , we set a radius of  $j$ 'th particle to  $r_j^\varepsilon = \varepsilon R_j$ , where  $\varepsilon > 0$ . We denote by  $\Omega^\varepsilon := \cup_j B(\mathbf{c}_j, r_j^\varepsilon)$ , by  $\Gamma_j^\varepsilon = \partial B(\mathbf{c}_j, r_j^\varepsilon)$ , and by  $\Gamma^\varepsilon = \partial\Omega^\varepsilon = \cup_j \Gamma_j^\varepsilon$ .

Let the (known) incident field  $u^{inc} : \mathbb{R}_{\geq 0} \times \mathbb{R}^2 \rightarrow \mathbb{R}$  solve

$$\begin{aligned} \partial_t^2 u^{inc}(t, \mathbf{x}) - \Delta u^{inc}(t, \mathbf{x}) &= 0, \text{ for } (t, \mathbf{x}) \in \mathbb{R}_{> 0} \times \mathbb{R}^2, \\ u^{inc}(0, \mathbf{x}), \quad \partial_t u^{inc}(0, \mathbf{x}) &= u_1(\mathbf{x}), \end{aligned}$$

where the initial conditions  $u_0, u_1$  are assumed to be sufficiently regular, compactly supported, with  $\text{supp } u_0, \text{supp } u_1 \subset \mathbb{R}^2 \setminus \Omega^{\varepsilon_0}$ , for some  $\varepsilon_0 > 0$ .

Our goal is to find an accurate approximation to the so-called scattered field  $u^\varepsilon : \mathbb{R}_{\geq 0} \times \mathbb{R}^2 \rightarrow \mathbb{R}$ , which is a solution to

$$\begin{aligned} (1) \quad & \partial_t^2 u^\varepsilon - \Delta u^\varepsilon = 0 \quad \text{in } \mathbb{R}_{> 0} \times (\mathbb{R}^2 \setminus \overline{\Omega^\varepsilon}), \\ & \gamma_0 u^\varepsilon = -\gamma_0 u^{inc} \text{ on } \Gamma^\varepsilon, \\ & u^\varepsilon(0, \mathbf{x}) = \partial_t u^\varepsilon(0, \mathbf{x}) = 0. \end{aligned}$$

There exist  $u^{inc}$ , and  $(t, \mathbf{x}) \in \mathbb{R}_{\geq 0} \times \mathbb{R}^+ \setminus \overline{\Omega^{\varepsilon_0}}$ , s.t., as  $\varepsilon \rightarrow 0$ ,  $|u^\varepsilon(t, \mathbf{x})| > c \log^{-1} \varepsilon$ , for  $c > 0$ . We are interested in higher-order asymptotics of  $u^\varepsilon(t, \mathbf{x})$ , as  $\varepsilon \rightarrow 0$ .

There exist several ways to derive such asymptotics: matched asymptotic expansions, integral equation formulations, and more heuristic Foldy-Lax models. The models obtained by the two latter approaches are typically of the same type: e.g. in the frequency domain the scattered field is expressed as a linear combination of  $N$  free-space Green functions 'centered' in  $\mathbf{c}_j$ , with the coefficients satisfying an  $N \times N$  system of equations. Here we adhere to such an approach as well.

**First idea: recasting frequency-domain Foldy-Lax models into the time domain.** One way to obtain a time-domain Foldy-Lax model is to recast an available frequency-domain model into the time-domain. The goal of this section is to show that this procedure may lead to unstable and thus non-convergent models. For this we will consider the model of [3], which can be rewritten in the time domain as follows: the field  $u^\varepsilon$  is approximated by

$$u^\varepsilon(t, \mathbf{x}) \approx u_{FL}^\varepsilon(t, \mathbf{x}) = \sum_{k=1}^N \mathcal{G}(t, \|\mathbf{x} - \mathbf{c}_k\|) *_t \mu_k^\varepsilon,$$

where  $\mathcal{G}(t, r) = \frac{1}{2\pi} \frac{\mathbb{1}_{t>r}}{\sqrt{t^2-r^2}}$  (the 2D free-space wave equation Green function), and the  $N$  unknown functions  $\mu_k^\varepsilon : \mathbb{R}_{\geq 0} \rightarrow \mathbb{R}$  satisfy the following system:

$$\mathcal{G}(t, r_k^\varepsilon) *_t \mu_k^\varepsilon + \sum_{n \neq k} \mathcal{G}(t, \|\mathbf{c}_k - \mathbf{c}_n\|) *_t \mu_n^\varepsilon = -\mathcal{G}(t, r_k^\varepsilon) *_t u^{inc}(t, \mathbf{c}_k), \quad k = 1, \dots, N.$$

However, for some geometric configurations the above system is unstable. The simplest result of this type is given in the proposition below.

**Proposition.** *Let  $N = 3$ ,  $\varepsilon > 0$  and  $r_i^\varepsilon = \varepsilon$  for all  $i$ . Let  $\|\mathbf{c}_i - \mathbf{c}_j\| = c > 0$  for all  $i \neq j$  (in other words, the centers of the particles are located in the vertices of an equilateral triangle of side length  $c$ ). Assume that  $c/\varepsilon < 4$ .*

*Then there exists  $u^{inc} \in C_0^\infty(\mathbb{R}_{\geq 0} \times \mathbb{R}^2)$ , s.t. the following holds true. There exist  $\alpha, A > 0$  and a sequence  $t_n \rightarrow +\infty$ , s.t.  $\|u_{FL}^\varepsilon(t_n)\|_{L^2(\mathbb{R}^2)} \geq \alpha e^{At_n}$ .*

To deal with such potential instabilities, we propose an alternative Foldy-Lax model, which we will call the Galerkin Foldy-Lax model (name due to P. Joly (POEMS)).

**Second idea: Galerkin Foldy-Lax model.** For sufficiently regular scattered field  $u^{inc}$ , any solution to the scattering problem (1) can be represented as the single layer potential of an unknown density  $\boldsymbol{\lambda}^\varepsilon \in C^0(\mathbb{R}_{\geq 0}; H^{-1/2}(\Gamma^\varepsilon))$  (where we use the notation  $\boldsymbol{\lambda}^\varepsilon|_{\Gamma_k^\varepsilon} = \lambda_k^\varepsilon$ ):

$$(2) \quad u(t, \mathbf{x}) = \sum_{k=1}^N \int_{\Gamma_k^\varepsilon} \mathcal{G}(t, \|\mathbf{x} - \mathbf{y}\|) *_t \lambda_k^\varepsilon(t, \mathbf{y}) d\Gamma_{\mathbf{y}}.$$

Applying  $\gamma_0$  to both sides of the above identity yields a well-posed boundary integral equation for the unknown density  $\boldsymbol{\lambda}^\varepsilon$ :

$$-\gamma_0 u^{inc}(t, \mathbf{x}) = S^\varepsilon \boldsymbol{\lambda}^\varepsilon = \sum_{k=1}^N \int_{\Gamma_k^\varepsilon} \mathcal{G}(t, \|\mathbf{x} - \mathbf{y}\|) *_t \lambda_k^\varepsilon(t, \mathbf{y}) d\Gamma_{\mathbf{y}}.$$

Because of coercivity-like properties of the above operator, the Galerkin semidiscretizations in space of the above equation are a priori stable. We then obtain a Foldy-Lax model as one such Galerkin semidiscretization of the above equation. We define a coarse Galerkin space

$$\mathbb{S}_0(\Gamma_k^\varepsilon) := \{\phi \in H^{-1/2}(\Gamma_k^\varepsilon) : \phi = \text{const}\}, \quad \mathbb{S}_0^\varepsilon := \prod_{k=1}^N \mathbb{S}_0(\Gamma_k^\varepsilon).$$

We then look for the approximation of the density  $\boldsymbol{\lambda}^\varepsilon$

$$\boldsymbol{\lambda}^\varepsilon(t, \mathbf{x}) \approx \boldsymbol{\lambda}_{app}^\varepsilon = \sum_{k=1}^N \lambda_{app,k}^\varepsilon(t) \mathbb{1}_{\mathbf{x} \in \Gamma_k^\varepsilon},$$

which satisfies

$$-\int_{\Gamma_k^\varepsilon} \gamma_0 u^{inc}(t, \mathbf{x}) d\Gamma_{\mathbf{x}} = \langle S^\varepsilon \boldsymbol{\lambda}^\varepsilon, 1 \rangle_{\Gamma_k^\varepsilon} = \sum_{\ell=1}^N \int_{\Gamma_\ell^\varepsilon} \int_{\Gamma_k^\varepsilon} \mathcal{G}(t, \|\mathbf{x} - \mathbf{y}\|) *_t \lambda_{app,\ell}^\varepsilon(t) d\Gamma_{\mathbf{y}} d\Gamma_{\mathbf{x}}.$$

Remark that in order to find the densities  $\lambda_{app,k}^\varepsilon(t)$ , we need to solve the system of  $N$  convolutional equations. Next, knowing the densities  $\lambda_k^\varepsilon$ , the approximated field  $u_{app}^\varepsilon$  can be restored using (2):

$$u^\varepsilon(t, \mathbf{x}) \approx u_{app}^\varepsilon(t, \mathbf{x}) = \sum_{\ell=1}^N \int_{\Gamma_\ell^\varepsilon} \mathcal{G}(t, \|\mathbf{x} - \mathbf{y}\|) *_t \lambda_{app,\ell}^\varepsilon(t) d\Gamma_{\mathbf{y}}.$$

We then have the following convergence result.

**Theorem 1.** *Let  $K$  be compact, and, for some  $\varepsilon_0 > 0$ ,  $\text{dist}(K, \Omega^{\varepsilon_0}) > d > 0$ . As  $\varepsilon \rightarrow 0$ , with  $C$  depending only on the distance between particles,*

$$\|u_\varepsilon - u_\varepsilon^{app}\|_{L^\infty(0,T;L^\infty(K))} \leq \varepsilon^2 \times CN^{5/2} \max(1, T^6 \log T) \|u^{inc}\|_{H^9(0,T;W^{1,\infty}(\mathbb{R}^2))}.$$

**Conclusions and open questions.** We have constructed an unconditionally stable Foldy-Lax model for sound-soft scattering by circular particles and obtained corresponding convergence estimates.

However, there remain several open questions that we would like to address. First of all, it is extension of the analysis for the non-circular obstacles. Second, our convergence estimates fail when the distance between the obstacles reduces proportionally to their size; it would be interesting to see whether adding more functions into the Galerkin approximation space could help obtaining a more accurate model in this case. Finally, we would like to investigate a more difficult case of the electromagnetic scattering by small particles.

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## Connecting random fields on manifolds and stochastic partial differential equations in simulations

ANNIKA LANG

(joint work with David Cohen, Erik Jansson, Mihály Kovács, Mike Pereira)

The simulation of random fields on manifolds can be connected to stochastic partial differential equations (SPDEs) in two ways. These two directions divided the presentation naturally in two parts. In the first part, we looked at approximation methods for random fields when interpreted as solutions to a specific type of SPDEs. The second part used the theory and algorithms for isotropic Gaussian random fields to solve and simulate the stochastic wave equation on the sphere.

Let  $(\Omega, \mathcal{A}, (\mathcal{F}_t), P)$  be a filtered probability space and denote by  $\mathbb{S}^2 \subset \mathbb{R}^3$  the unit sphere. By [6], an isotropic Gaussian random field  $T$  admits a Karhunen–Loève expansion  $T = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} a_{\ell m} Y_{\ell m}$ , where  $(Y_{\ell m}, \ell \in \mathbb{N}_0, m = -\ell, \dots, \ell)$  denotes the sequence of spherical harmonic functions and  $(a_{\ell m}, \ell \in \mathbb{N}_0, m = -\ell, \dots, \ell)$  is a sequence of normally distributed random variables, whose properties are characterized by the angular power spectrum  $(A_{\ell}, \ell \in \mathbb{N}_0)$ . A truncation of the series expansion at level  $L$  leads to the random field  $T^L$  which converges to  $T$  depending on the decay of the angular power spectrum as has been shown in [5].

**Theorem 1.** *Assume that  $A_{\ell} \leq C \cdot \ell^{-\alpha}$  for some  $\alpha > 2$  and  $C > 0$ . Then for all  $1 \leq p < +\infty$  there exists a constant  $\hat{C}_p$  such that*

$$\|T - T^L\|_{L^p(\Omega; L^2(\mathbb{S}^2))} \leq \hat{C}_p \cdot L^{-(\alpha-2)/2}.$$

*Furthermore, for all  $\beta < (\alpha - 2)/2$  it holds asymptotically  $\|T - T^L\|_{L^2(\mathbb{S}^2)} \leq L^{-\beta}$ , P-a. s..*

The first application of this result in the talk was to consider spectral approximations of Whittle–Matérn random fields which are given as solutions to the SPDEs

$$(1) \quad (\kappa^2 - \Delta_{\mathbb{S}^2})^{\beta} u = \mathcal{W},$$

where  $\mathcal{W}$  denotes white noise on  $\mathbb{S}^2$ ,  $\Delta_{\mathbb{S}^2}$  the Laplace–Beltrami operator, and  $\kappa, \beta > 0$  are real-valued parameters. It implies that a spectral approximation with truncation at level  $L$  leads to convergence

$$\|u - u_L\|_{L^2(\Omega; L^2(\mathbb{S}^2))} \leq C_{\kappa, \beta} L^{1-2\beta}.$$

We continued with an alternative approach that paves the way for generalizations to more general operators and manifolds. More specifically, we represent the fractional operator in (1) as a Dunford–Taylor integral that is approximated by a quadrature. The resulting linear equations are solved by the surface finite element method (SFEM) [2]. As shown in [3], we obtain for mesh size  $h$  on the discretized sphere and  $k$  in the quadrature the convergence of the approximate solution  $u_{L,h}^l$ , where  $l$  refers to the lift of the function from the discretized sphere to  $\mathbb{S}^2$ .

**Theorem 2.** *If  $\mathcal{W}_{L,h}^l = P_h \mathcal{W}_L$  is given by the  $L^2$  projection, then for  $s \in [0, 2]$  and some constant  $C$  the error is bounded by*

$$\|u - u_{L,h}^l\|_{L^2(\Omega; L^2(\mathbb{S}^2))} \leq C(L + 1)(L^{-2\beta} + e^{-\pi^2/(4k)} + h^s(L + 1)^s).$$

We continue with extending this approach to a Riemannian manifold  $\mathcal{M}$  and more general functions of the Laplace–Beltrami operator  $\Delta_{\mathcal{M}}$  in the next step. Let  $\gamma \in C^\nu$  with  $|\gamma'(\lambda)| \leq C|\lambda|^{-1+\beta}$  for  $\lambda \in \mathbb{R}$  and consider

$$u = \gamma(-\Delta_{\mathcal{M}})\mathcal{W} \quad \text{and} \quad u_n = \gamma(-\Delta_n)\mathcal{W}_n,$$

where  $u_n$  denotes an approximation of  $u$  on a finite-dimensional space  $V_n$  with basis functions  $(\psi_k, k = 1, \dots, n)$ . Examples include the truncation of a possibly known eigenbasis of  $\Delta_{\mathcal{M}}$  or a finite element space. A key step in the approximation is the simulation of the correlated random vectors in the expansion with respect to the basis  $(\psi_k, k = 1, \dots, n)$ . Its distribution can be characterized by a Galerkin approximation. In order to be more efficient, we approximate the possibly non-linear function  $\gamma$  by Chebyshev polynomials of order  $K$ . Together we obtain the following convergence result of our Galerkin–Chebyshev approximation of  $u$  [4]:

**Theorem 3.** *Let  $r$  and  $s$  characterize the quality of approximation of eigenvalues and eigenfunctions of  $\Delta_{\mathcal{M}}$  in  $V_n$  and let  $\alpha$  be the asymptotic growth rate of the eigenvalues of  $\Delta_{\mathcal{M}}$ . Then the Galerkin–Chebyshev approximation  $\hat{u}_{n,K}$  converges strongly to  $u$  and the error is bounded by*

$$\|u - \hat{u}_{n,K}\|_{L^2(\Omega; L^2(\mathcal{M}))} \leq C \left( n^{-\min\{s, r, (\alpha\beta-1/2)\}} + \sqrt{n}(K - \nu)^{-\nu} \right)$$

for some constant  $C$ . Furthermore, the weak error satisfies in terms of the covariance

$$|\text{Cov}((u, \theta)_0, (u, \varphi)_0) - \text{Cov}((u_n, \theta)_0, (u_n, \varphi)_0)| \leq C n^{-\min\{s, r, (2\alpha\beta-1)\}},$$

where  $(\cdot, \cdot)_0$  denotes the inner product of  $L^2(\mathcal{M})$ .

In the second part of the talk we went back to  $\mathbb{S}^2$  and spectral representations. Based on Theorem 1, we considered spectral approximations of solutions to the stochastic wave equation driven by additive noise

$$\partial_{tt}u(t) - \Delta_{\mathbb{S}^2}u(t) = \dot{W}(t)$$

with initial condition  $u(0) = v_1$  and  $\partial_t u(0) = v_2$ , where  $W = (W(t), t \in [0, T])$  denotes a  $Q$ -Wiener process on the sphere generated by the Gaussian random fields of the first part of the talk and  $Q$  is the covariance operator characterized by the angular power spectrum. Rewriting the equation as the system

$$u_1(t) = v_1 + \int_0^t u_2(s) \, ds \quad \text{and} \quad u_2(t) = v_2 + \int_0^t \Delta_{\mathbb{S}^2}u_1(s) \, ds + W(t)$$

and expanding each component with respect to the spherical harmonics, we obtain a system of stochastic differential equations given by



$$\begin{cases} u_1^{\ell,m}(t) &= \cos(t\lambda_\ell)v_1^{\ell,m} + \lambda_\ell^{-1} \sin(t\lambda_\ell)v_2^{\ell,m} + \hat{W}_1^{\ell,m}(t), \\ u_2^{\ell,m}(t) &= -\lambda_\ell \sin(t\lambda_\ell)v_1^{\ell,m} + \cos(t\lambda_\ell)v_2^{\ell,m} + \hat{W}_2^{\ell,m}(t), \end{cases}$$

where  $(\hat{W}_1^{\ell,m}, \hat{W}_2^{\ell,m})$  are correlated Brownian motions and  $\lambda_\ell = (\ell(\ell + 1))^{1/2}$ .

Since we are able to compute the solutions to the equations exactly, we only have an error in the truncation of the series expansion. Based on Theorem 1, we show a strong convergence result [1].

**Proposition.** *Assume that  $A_\ell \leq C \cdot \ell^{-\alpha}$  for  $\alpha > 2$ . Then the truncated solution  $u^L$  converges strongly to  $u$  and the error is bounded by*

$$\begin{aligned} \|u_1(t) - u_1^L(t)\|_{L^p(\Omega; L^2(\mathbb{S}^2))} &\leq \hat{C}_p L^{-\alpha/2}, \\ \|u_2(t) - u_2^L(t)\|_{L^p(\Omega; L^2(\mathbb{S}^2))} &\leq \hat{C}_p L^{-(\alpha/2-1)} \end{aligned}$$

for sufficiently smooth initial conditions and some constant  $\hat{C}_p$ . Additionally the approximation converges  $P$ -a.s., and for all  $\delta < \alpha/2$  the error is asymptotically bounded by

$$\|u_1(t) - u_1^L(t)\|_{L^2(\mathbb{S}^2)} \leq L^{-\delta} \quad \text{and} \quad \|u_2(t) - u_2^L(t)\|_{L^2(\mathbb{S}^2)} \leq L^{-(\delta-1)}.$$

Using strong convergence in negative Sobolev spaces, we can extend the convergence analysis and show weak convergence rates [1].

**Proposition.** *Assume that the derivative of the test function  $\varphi$  is of polynomial growth and the initial conditions are sufficiently smooth. Then for all  $s < \alpha/2$  and some constant  $\hat{C}$  the weak error is bounded by*

$$\begin{aligned} |\mathbb{E} [\varphi(u_1(t)) - \varphi(u_1^L(t))]| &\leq \hat{C} L^{-(\alpha/2+s)}, \\ |\mathbb{E} [\varphi(u_2(t)) - \varphi(u_2^L(t))]| &\leq \hat{C} L^{-(\alpha/2+s-1)}. \end{aligned}$$

In conclusion we showed that the weak convergence rate is essentially twice the strong one under sufficient smoothness of the initial condition and the test function  $\varphi$ .

In the talk all approximation schemes and convergence results were accompanied by simulation results. Most figures can be found in the referenced publications.

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## Adaptive Space-Time Finite Element Methods for Parabolic Optimal Control Problems

ULRICH LANGER

(joint work with A. Schafelner, O. Steinbach, F. Tröltzsch, H. Yang)

We consider tracking-type optimal control problems constrained by linear parabolic partial differential equations with distributed source control that read as follows: Minimize the cost functional

$$(1) \quad J(y, u) = \frac{1}{2} \int_{\Omega_T} [y(x, t) - y_d(x, t)]^2 dxdt + \frac{1}{2} \lambda R(u)$$

over  $y$  from a suitable state space  $Y$  and  $u$  from a suitable control space subject to the parabolic initial-boundary value problem (state equation)

$$(2) \quad \partial_t y - \Delta_x y = u \text{ in } \Omega_T, \quad u = 0 \text{ on } \Sigma, \quad u = u_0 := 0 \text{ on } \Sigma_0,$$

where  $\Omega_T = \Omega \times (0, T) \subset \mathbb{R}^{d+1}$  denotes the space-time cylinder,  $\Sigma = \partial\Omega \times (0, T)$  is its lateral surface,  $\Sigma_0 := \Omega \times \{0\}$ ,  $\Omega \subset \mathbb{R}^d$  denotes the spatial domain that is supposed to be Lipschitz and bounded,  $y_d \in L_2(\Omega_T)$  is the given desired state, and  $\lambda$  in front of the regularization term  $R(u)$  is a suitably chosen positive regularization parameter. Besides the standard  $L_2$ -regularization  $R(u) = \|u\|_{U=L_2(\Omega_T)}^2$ , we also consider the energy regularization  $R(u) = \|u\|_{U=L_2(0,T;H^{-1}(\Omega))}^2$ , and compare numerically both regularizations with the sparse control where a sparsity term  $\mu \|u\|_{L_1(\Omega_T)}$  with a non-negative sparsity parameter  $\mu$  is added to the  $L_2$ -regularization. Since the state equation (2) has a unique weak solution  $y \in Y_0 = \{y \in W(0, T) = \{y \in V = L_2(0, T; H_0^1(\Omega)) : \partial_t y \in V^*\} : y = 0 \text{ on } \Sigma_0\}$ , we can conclude unique solvability of the corresponding optimal control problem (1) - (2). The solution of the optimal control problem (1) - (2) is equivalent to the solution of the reduced (by means of the gradient equation) optimality system consisting of the primal and adjoint equations: Find  $(y, p) \in Y \times P$  such that

$$(3) \quad B(y, p; v, q) = (y_d, q) \quad \forall (v, q) \in V \times Q,$$

where the spaces  $Y, P, V, Q$  and the bilinear form  $B(\cdot; \cdot)$  are defined as follows:

- *$L_2$  regularization:*  $Y = Y_0, P = P_T = \{p \in W(0, T) : p = 0 \text{ on } \Sigma_T\}, Q = V$ , and  $B(y, p; v, q) := \lambda[\langle \partial_t y, v \rangle + (\nabla_x y, \nabla_x v)] + (p, v) - (y, q) - \langle \partial_t p, q \rangle + (\nabla_x p, \nabla_x q)$ , where  $\Sigma_T = \Omega \times \{T\}$ , and the optimal control  $u$  can be computed from the gradient equation  $p + \lambda u = 0$ ; see [2],
- *energy regularization:*  $Y = Y_0, P = V, Q = Y_0$ , and  $B(y, p; v, q) := \lambda^{-1}(\nabla_x p, \nabla_x v) + \langle \partial_t y, v \rangle + (\nabla_x y, \nabla_x v) - \langle \partial_t q, p \rangle - (\nabla_x p, \nabla_x q) + (y, q)$ , where the optimal control  $u$  can be computed from the gradient equation  $p + \lambda w_u = 0$ , and  $w_u \in V$  solves  $(\nabla_x w_u, \nabla_x v) = \langle u, v \rangle \forall v \in V$ ; see [3].

Here  $(\cdot, \cdot) : L_2(\Omega_T) \times L_2(\Omega_T) \rightarrow \mathbb{R}$  always denotes the  $L_2(\Omega_T)$ -inner product, and  $\langle \cdot, \cdot \rangle : V^* \times V \rightarrow \mathbb{R}$  is the corresponding duality product. For both the  $L_2$ - and the energy regularizations, well-posedness of (3) was shown in [2] and [3] by means of the Banach-Nečas-Babuška theorem. More precisely, the operator  $B : Y \times P \rightarrow V^* \times Q^*$ , generated by the bilinear form  $B(\cdot; \cdot)$ , is an isomorphism.

Now we look for a full space-time finite element (f.e.) discretization of (3) on unstructured simplicial meshes  $\mathcal{T}_h = \{\Delta\}$  such that  $\overline{Q}_T = \cup \overline{\Delta}$ . As in the elliptic case, we construct suitable conforming f.e. trial and test spaces  $Y_h \subset Y, P_h \subset P, V_h \subset V, Q_h \subset Q$ , and look for the f.e. solution  $(y_h, p_h) \in Y_h \times P_h$  such that

$$(4) \quad B(y_h, p_h; v_h, q_h) = (y_d, q_h) \quad \forall (v_h, q_h) \in V_h \times Q_h.$$

More precisely, we choose  $Y_h = V_h = S_h^k(\Omega_T) \cap Y \subset Y \subset V$  and  $P_h = Q_h = S_h^k(\Omega_T) \cap P \subset P \subset Q$  for the  $L_2$ -regularization, and  $Y_h = Q_h = S_h^k(\Omega_T) \cap Y \subset Y = Q \subset V$  and  $P_h = V_h = S_h^k(\Omega_T) \cap P \subset P = V$  for the energy regularization, where  $S_h^k(\Omega_T)$  denotes the usual continuous f.e. space based on polynomials of degree  $k$ . In both cases, we can establish discrete inf-sup conditions, from which existence and uniqueness of the solution  $(y_h, p_h) \in Y_h \times P_h$  of the f.e. scheme (4) follows. Moreover, we can derive a Céa-like discretization error estimates by the best-approximation error. Finally, these estimates imply convergence rate estimates under additional regularity assumptions. For instance, if the state  $y$  and the co-state (adjoint)  $p$  belong to  $H^{1+s}(\Omega_T)$  for some real positive  $s$ , then we get convergence rate estimates of the form

$$\|(y, p) - (y_h, p_h)\| \leq c(y, p) h^{\min\{s, k\}},$$

where  $h$  denotes the usual mesh-size parameter (maximal length of the edges of the simplices  $\Delta$ ) of the regular mesh  $\mathcal{T}_h$ . The norm is defined by

$$\|(y, p)\| := [\lambda \|y\|_V^2 + \|p\|_P^2]^{0.5} \quad \text{and} \quad \|(y, p)\| := [\|y\|_{Y_h}^2 + \|p\|_P^2]^{0.5}$$

for the  $L_2$  and energy regularizations, respectively, with  $\|y\|_{Y_h}^2 = \|y\|_V^2 + \|w_{\partial_t y, h}\|_V^2$ , where  $w_{\partial_t y, h} \in V_h$  solves the parameter-dependent elliptic boundary value problem

$$(\nabla_x w_{\partial_t y, h}, \nabla_x v_h) = \langle \partial_t y, v_h \rangle \quad \forall v_h \in V_h.$$

We refer to [2] ( $L_2$  regularization) and [3] (energy regularization) for more details, the proofs, and the discussion of the results of extensive numerical experiments including results obtained by adaptive schemes based on residual error indicators. In [2], we extend this adaptive space-time approach to space-time tracking-type,  $L_2$ -regularized optimal control of semilinear parabolic equations (Schlögl model) with box constraints imposed on the control  $u$ . In [3], we compare the energy regularization with the  $L_2$ -regularization and with the sparse optimal control in the full space-time adaptive setting. Adaptive space-time sparse optimal control of semilinear parabolic problems is studied in [4].

In the case of the  $L_2$ -regularization, we easily observe maximal parabolic regularity, i.e., the solution  $(y, p) \in Y \times P$  of (3) belongs to the space  $H^{\Delta, 1}(\Omega_T) \times H^{\Delta, 1}(\Omega_T)$ , where  $H^{\Delta, 1}(\Omega_T) := \{y \in H^1(\Omega_T) : \Delta_x y \in L_2(\Omega_T)\}$ . Thus the reduced

optimality system

$$(5) \quad \lambda(\partial_t y - \Delta_x y) + p = 0 \quad \text{in } L_2(\Omega_T),$$

$$(6) \quad -\partial_t p - \Delta_x p - y = -y_d \quad \text{in } L_2(\Omega_T)$$

holds in  $L_2(\Omega_T)$ , with homogeneous Dirichlet boundary conditions for  $y$  and  $p$  on  $\Sigma$ , homogeneous initial conditions for  $y$  on  $\Sigma_0$ , and homogeneous terminal conditions for  $p$  on  $\Sigma_T$ . This remains even valid for inhomogeneous initial data  $u_0 \in H_0^1(\Omega)$  and more general non-autonomous parabolic problems under certain assumptions. Now we can look at the terms  $\partial_t y$  and  $-\partial_t p$  as forward and backward convection terms in time, and we can treat them by upwind and downwind stabilized test functions. Multiplying (5) by upwind test functions  $v_h + \theta \varrho_h^2 \partial_t v_h$  and (6) by downwind test functions  $q_h - \theta \varrho_h^2 \partial_t q_h$ , integrating over  $\Delta$ , integrating by parts in the elliptic terms where the scaling parameter  $\theta$  does not appear, and summing over all space-time f.e.  $\Delta \in \mathcal{T}_h$ , we arrive at the consistent f.e. scheme: Find  $(y_h, q_h) \in (Y_{0h} = S_h^k(\Omega_T) \cap Y_0) \times (P_{Th} = S_h^k(\Omega_T) \cap P_T)$  such that

$$B_h(y_h, p_h; v_h, q_h) = -(y_d, q_h - \theta \varrho_h^2 \partial_t q_h) \quad \forall (v_h, q_h) \in Y_{0h} \times P_{Th}.$$

The mesh-density function  $\varrho_h$  is simply equal to  $h$  in the case of uniform meshes, and can be chosen as a continuous, piecewise linear function in the case of adaptively generated meshes. The consistency yields Galerkin orthogonality, and Galerkin orthogonality, together with  $(Y_{0h} \times P_{Th})$ -ellipticity and the extended boundedness of the mesh-dependent bilinear form  $B_h(\cdot; \cdot)$ , implies discretization error estimates. Finally, assuming that  $y, p \in H^{1+s}$  with some positive  $s$ , we arrive at the convergence rate estimate

$$\|(y, p) - (y_h, p_h)\|_h \leq (1 + (\mu_b/\mu_e)c(y, p))h^{\min\{s, k\}},$$

where the mesh-dependent norm  $\|\cdot\|_h$  is related to the ellipticity and boundedness of the bilinear form  $B_h(\cdot; \cdot)$ , and  $\mu_e$  and  $\mu_b$  are the constants in the ellipticity and boundedness inequalities; see [1] for details and proofs. Therein adaptive space-time schemes, which are based on new functional a posteriori error estimates, are proposed and numerically tested. These a posteriori estimates have the form

$$\begin{aligned} & \left[ \lambda \|y - \tilde{y}\|_{X_0}^2 + \|p - \tilde{p}\|_{X_T}^2 \right]^{1/2} \\ & \leq \sqrt{2} \left[ (1 + \alpha) \|\nabla_x \tilde{p} - \sigma\|^2 + (1 + \alpha^{-1}) C_F^2 \|-\partial_t \tilde{p} - \operatorname{div}_x \sigma - \tilde{y} + y_d\|^2 \right. \\ & \quad \left. + (1 + \beta) \|\nabla_x \tilde{y} - \tau\|^2 + (1 + \beta^{-1}) C_F^2 \|\partial_t \tilde{y} - \operatorname{div}_x \tau + \lambda^{-1} \tilde{p}\|^2 \right], \end{aligned}$$

where  $\|\cdot\| := \|\cdot\|_{L_2(Q)}$ ,  $C_F = C_F(\Omega)$  denotes the Friedrichs constant for the spatial domain  $\Omega$ ,  $\tilde{y} \in Y_0 \cap H^1(\Omega_T)$  and  $\tilde{p} \in P_T \cap H^1(\Omega_T)$  are any approximations to the solution  $y \in Y_0$  and  $p \in P_T$ ,  $\tau, \sigma \in H(\operatorname{div}_x, \Omega_T)$  are suitably reconstructed fluxes, and  $\alpha$  and  $\beta$  are positive real scaling parameters.

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### Space-Time CutFEMs on Overlapping Meshes

CARL LUNDHOLM

(joint work with Mats G. Larson and Anders Logg)

We present two cut finite element methods (CutFEMs) for the heat equation on overlapping meshes. By overlapping meshes we mean a mesh hierarchy with a stationary background mesh at the bottom and an overlapping mesh that is allowed to move around on top of the background mesh. Overlapping meshes can be used as an alternative to costly remeshing for problems with changing or evolving interior geometry. The two CutFEMs were first presented in [1] which we refer to for details and relevant literature. The pivotal difference between the two methods is how the movement of the overlapping mesh is represented discretely.

In Method I, the overlapping mesh is prescribed a *simple continuous* movement, meaning that its location as a function of time is *continuous* and *piecewise linear*. This results in a space-time discretization with skewed and spatiotemporally cut space-time prisms. See Figure 1. In Method II, the overlapping mesh is prescribed a *simple discontinuous* movement, meaning that its location as a function of time is *discontinuous* and *piecewise constant*. This results in a space-time discretization with a slabwise product structure between space and time. See Figure 1.

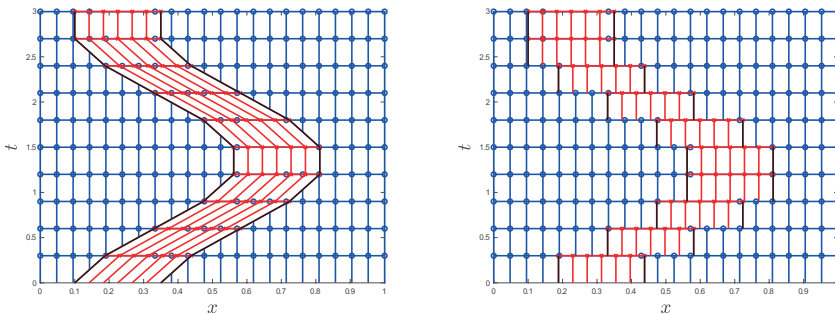


FIGURE 1. Space-time discretization from *continuous* mesh movement used in Method I (left) and *discontinuous* mesh movement used in Method II (right).

In both methods, to define the global discrete space  $V_h$  we use  $dG(q)$  in time and  $cG(p)$  in space with the addition of a discontinuity on the boundary between

the two meshes. Both finite element formulations are based on Nitsche's method and have the form: Find  $u_h \in V_h$  such that

$$(1) \quad B_h(u_h, v) = \int_0^T (f, v)_{\Omega_0} dt + (u_0, v_0^+)_{\Omega_0}, \quad \forall v \in V_h.$$

Here,  $B_h$  is a mesh-dependent space-time bilinear form that for Method I is

$$(2) \quad \begin{aligned} B_h(w, v) := & \sum_{i=1}^2 \sum_{n=1}^N \int_{I_n} (\dot{w}, v)_{\Omega_i(t)} dt + \sum_{n=1}^N \int_{I_n} A_{h,t}(w, v) dt \\ & + \sum_{n=1}^{N-1} ([w]_n, v_n^+)_{\Omega_0} + (w_0^+, v_0^+)_{\Omega_0} - \sum_{n=1}^N \int_{\bar{\Gamma}_n} \bar{n}^t [w] v_\sigma d\bar{s}, \end{aligned}$$

and for Method II is

$$(3) \quad \begin{aligned} B_h(w, v) := & \sum_{n=1}^N \int_{I_n} (\dot{w}, v)_{\Omega_0} dt + \sum_{n=1}^N \int_{I_n} A_{h,t_n}(w, v) dt \\ & + \sum_{n=1}^{N-1} ([w]_n, v_n^+)_{\Omega_0} + (w_0^+, v_0^+)_{\Omega_0}. \end{aligned}$$

The time-dependent spatial bilinear form  $A_{h,t}$  is the same as in the elliptic case but with the addition of an overlap stability term to handle badly cut mesh cells. The last term on the right-hand side of (2) is present to mimic the standard dG time-jump term but over the space-time boundary between the meshes.

The space-time discretization in Method I gives discrete spatial operators, e.g., the discrete Laplacian, an intrinsic time-dependence which makes standard analysis methodologies fail. We therefore propose a new space-time energy analysis framework that is general and robust enough to be applicable to Method I. It seems that the core components of this new analysis framework have been discovered independently by us and [2]. The new energy analysis follows a Céa's lemma type argument just as the standard energy analysis. The defining characteristic of the new energy analysis is how the time derivative is included in an energy norm. In the standard energy analysis, the  $H^{-1}$ -norm is used. In the new energy analysis, we use the  $L^2$ -norm scaled with the time step  $k_n$ . Thus, the main space-time energy norm is

$$(4) \quad \|v\|_X^2 := \sum_{i=1}^2 \sum_{n=1}^N \int_{I_n} k_n \|D_t v\|_{\Omega_i(t)}^2 dt + \|v\|_{B_h}^2,$$

where  $D_t$  is a domain-dependent material derivative and the  $B_h$ -norm is the natural coercivity norm for  $B_h$ . Due to the new energy norm, slightly different inf-sup condition and continuity are needed. By proving some technical inverse estimates for the space-time discretization in Method I, one may obtain the following discrete inf-sup condition

$$(5) \quad \|w\|_X \lesssim \sup_{v \in V_h \setminus \{0\}} \frac{B_h(w, v)}{\|v\|_X} \quad \forall w \in V_h.$$

Integrating by parts with respect to time in  $B_h$  yields the alternative but equivalent form  $B_h^-$  which may be used to obtain the following alternative continuity

$$(6) \quad B_h(w, v) = B_h^-(w, v) \lesssim \|w\|_{Y_-} \|v\|_X,$$

where the  $Y_-$ -norm is the natural auxiliary norm. Using the inf-sup condition (5), followed by Galerkin orthogonality, and finally the continuity (6), gives an a priori energy error estimate for Method I that is of optimal order with respect to both time step  $k$  and mesh size  $h$ , namely

$$(7) \quad \|e\|_X \sim k^{q+1/2} + h^p.$$

The space-time discretization in Method II allows for standard analysis methodologies to be applied with some modifications. We follow standard analysis methodology that gives an estimate for the error at the final time in the  $L^2$ -norm. A cornerstone of this analysis is the strong stability estimate. At one point in its proof, one would like to use the Ritz projection operator  $R_n$  on a function from the *previous* slab, but this is not defined because of the shift in discontinuity between slabs. Instead we use a shift operator  $\mathcal{S}_n : V_{h,n-1} \rightarrow V_{h,n}$  defined by

$$(8) \quad A_n(\mathcal{S}_n v, w) = \mathcal{A}_{n-1,n}(v, w) \quad \forall w \in V_{h,n},$$

where  $\mathcal{A}_{n-1,n}$  is a special non-symmetric bilinear form. The rest of the analysis is essentially the same as in the standard case and thus gives an a priori estimate of the error at the final time in the  $L^2$ -norm for Method II that is of optimal order with respect to both time step  $k$  and mesh size  $h$ , namely

$$(9) \quad \|e(T)\|_{\Omega_0} \sim k^{2q+1} + h^{p+1}.$$

For both methods, numerical results for a problem in one spatial dimension verify the analytic error convergence orders. Numerical solutions computed with both methods are presented in Figure 2.

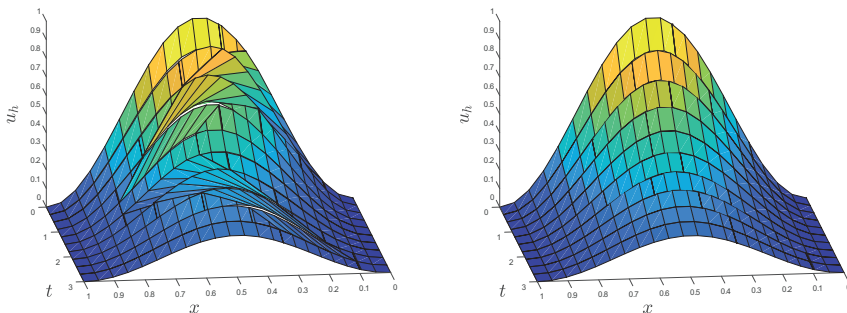


FIGURE 2. dG(1)cG(1)-solution from Method I (left) and Method II (right).

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**Time-dependent electromagnetic scattering from thin layers**

CHRISTIAN LUBICH

(joint work with Balázs Kovács, Jörg Nick)

We study time-dependent electromagnetic scattering. On an exterior domain  $\Omega$ , which is the complement of one or multiple bounded domains, the time-dependent Maxwell's equations for the total electric field  $\mathbf{E}^{\text{tot}}(\mathbf{x}, t)$  and the total magnetic field  $\mathbf{H}^{\text{tot}}(\mathbf{x}, t)$  are

$$(1) \quad \begin{aligned} \varepsilon \partial_t \mathbf{E}^{\text{tot}} - \text{curl} \mathbf{H}^{\text{tot}} &= 0 \\ \mu \partial_t \mathbf{H}^{\text{tot}} + \text{curl} \mathbf{E}^{\text{tot}} &= 0 \end{aligned} \quad \text{in the exterior domain } \Omega,$$

where  $\varepsilon$  and  $\mu$  are positive constants. We assume to be given incident electric and magnetic fields  $(\mathbf{E}^{\text{inc}}, \mathbf{H}^{\text{inc}})$ , which are a solution to Maxwell's equations in  $\mathbb{R}^3$ , and which initially, at time  $t = 0$ , have their support in  $\Omega$  and are thus bounded away from the boundary  $\Gamma = \partial\Omega$ . The objective is to compute the scattered fields  $\mathbf{E}^{\text{scat}} = \mathbf{E}^{\text{tot}} - \mathbf{E}^{\text{inc}}$  and  $\mathbf{H}^{\text{scat}} = \mathbf{H}^{\text{tot}} - \mathbf{H}^{\text{inc}}$  on a time interval  $0 \leq t \leq T$ , possibly only at selected space points  $\mathbf{x} \in \Omega$ , such that the total fields  $(\mathbf{E}^{\text{tot}}, \mathbf{H}^{\text{tot}})$  are a solution to Maxwell's equations (1) that satisfies a prescribed boundary condition.

The scattering of electromagnetic waves from obstacles with wave-material interaction in thin layers on the surface is described by generalized impedance boundary conditions, which provide effective approximate models. They are of the general form

$$(2) \quad (\mathbf{E}^{\text{tot}} \times \boldsymbol{\nu}) \times \boldsymbol{\nu} = \mathbf{Z}(\partial_t) (\mathbf{H}^{\text{tot}} \times \boldsymbol{\nu}) \quad \text{on } \Gamma = \partial\Omega,$$

where  $\boldsymbol{\nu}$  denotes the unit surface normal pointing into the exterior domain  $\Omega$  and the time-dependent impedance operator  $\mathbf{Z}(\partial_t)$  is a combined surface differential operator and temporal convolution operator. This situation includes a thin coating around a perfect conductor and the skin effect of a highly conducting material. The Engquist–Nédélec effective boundary condition for the thin coating has (omitting material-dependent constants)

$$(3) \quad \mathbf{Z}(\partial_t) = \delta (\partial_t - \partial_t^{-1} \nabla_{\Gamma} \text{div}_{\Gamma})$$

with a small positive parameter  $\delta$ , which is proportional to the layer depth. For a highly conductive obstacle, the effective boundary condition derived by Haddar, Joly & Nguyen has

$$(4) \quad \mathbf{Z}(\partial_t) = \delta \partial_t^{1/2},$$



where  $\delta$  is inversely proportional to the high conductivity, and the fractional derivative  $\partial_t^{1/2}$  is the time derivative of convolution with the kernel  $(\pi t)^{-1/2}$ . The general framework works with temporal convolution operators  $\mathbf{Z}(\partial_t)$  on a subspace of the trace space such that the Laplace transform  $\mathbf{Z}(s)$  of the convolution kernel is polynomially bounded in a complex half-space  $\operatorname{Re} s \geq \sigma > 0$  and satisfies a positivity condition.

We derive, analyse and discretize a system of time-dependent boundary integral equations that determines the tangential traces of the scattered electric and magnetic fields. The fields are then evaluated in the exterior domain by a representation formula, which uses the time-dependent potential operators of Maxwell's equations. In our numerical approach, time discretization of the boundary integral equation and the representation formula is done by convolution quadrature. Space discretization is done with appropriate boundary elements.

Via newly derived frequency-explicit bounds for the time-harmonic scattering problem with frequencies in a complex half-plane, we prove both the well-posedness of the time-dependent scattering problem and the stability and convergence of the numerical method, with explicitly given orders of convergence in the case of sufficient regularity. The bounds are robust in the singular perturbation limit  $\delta \searrow 0$  in (3) and (4). Taking the same Radau-type Runge–Kutta convolution quadrature for discretizing both the time-dependent boundary integral equation and the representation formulas, the optimal order of convergence is obtained away from the scattering boundary, whereas an order reduction to half the optimal temporal order occurs close to the boundary.

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### Navier-Stokes equations on evolving surfaces

ARNOLD REUSKEN

(joint work with Philip Brandner, Paul Schwering, Maxim Olshanskii)

In recent years there has been a strongly growing interest in *surface* Navier-Stokes equations, in particular concerning physical principles related to these equations and to tailor-made numerical discretization methods. One reason for this recent growing interest lies in the fact that these equations are used in the modeling of biological interfaces.

In the first part of this presentation we discuss *derivations* of surface Navier-Stokes equations for *evolving* surfaces. In the past few years several derivations have been presented in the literature [1, 2, 3, 4, 5], which differ in the physical principles used in the modeling approach and in the coordinate systems in which the resulting equations are represented. In [1, 3] mass and momentum conservation laws for material *surfaces* are used as basic physical principles, whereas in [4, 5] similar conservation laws for mass and momentum for a material *volume* are

used and combined with a thin film technique. In [2] the derivation is based on energy minimization principles. Besides these differences in physical principles, there is also a difference in the representation of the resulting flow equations. In some papers, e.g. [3, 5], local coordinate systems (curvilinear coordinates) are used, whereas in other literature [1, 2, 4] the standard Euclidean basis of  $\mathbb{R}^3$ , in which the evolving surface is embedded, is used. Such different coordinate systems lead to different representations of surface differential operators such as a covariant derivative or a surface divergence, and one has to be careful when comparing equations formulated in such different coordinate systems. Both the local curvilinear and the global Cartesian coordinate system have attractive properties. The local coordinate system can be very useful for modeling of more complex fluid properties, e.g. in certain classes of fluid membranes [3] or in flows of liquid crystals [5]. The representation in global Cartesian coordinates is very convenient for the development of numerical simulation methods for these flow equations. In the recent work [6] these different derivations of surface Navier-Stokes equations are compared. In the presentation we explain the basic ideas of these derivations and discuss the resulting system of surface Navier-Stokes equations, which is of the form

$$\begin{cases} \rho \dot{\mathbf{u}} = -\nabla_{\Gamma} \pi + 2\mu \operatorname{div}_{\Gamma}(E_s(\mathbf{u})) + \pi \kappa \mathbf{n} \\ \operatorname{div}_{\Gamma} \mathbf{u} = 0 \\ \dot{\rho} = 0 \end{cases} \quad \text{on } \Gamma(t),$$

with  $\mathbf{u}$  the velocity,  $\pi$  the surface fluid pressure,  $\rho$  the surface material density,  $E_s(\mathbf{u}) = \frac{1}{2}(\nabla_{\Gamma} \mathbf{u} + \nabla_{\Gamma} \mathbf{u}^T)$  the surface strain tensor,  $\kappa$  the mean curvature and  $\mu$  the viscosity coefficient. Starting from an initial closed smooth surface  $\Gamma(0)$ , the velocity field defines the evolving surface  $\Gamma(t)$ ,  $t > 0$ . We consider a major simplification by assuming that the *geometric* evolution of  $\Gamma(t)$  is known. More precisely, we assume a smooth velocity field  $\mathbf{w} = \mathbf{w}(t, \mathbf{x})$  in  $[0, T] \times \mathbb{R}^3$  that passively advects the embedded surface  $\Gamma(t)$  given by  $\Gamma(t) = \{ \mathbf{y} \in \mathbb{R}^3 \mid \mathbf{y} = \mathbf{x}(t, \mathbf{z}), \mathbf{z} \in \Gamma(0) \}$ , where the trajectories  $\mathbf{x}(t, \mathbf{z})$  are the unique solutions of the Cauchy problem

$$\begin{cases} \mathbf{x}(0, \mathbf{z}) = \mathbf{z} \\ \frac{d}{dt} \mathbf{x}(t, \mathbf{z}) = \mathbf{w}(t, \mathbf{x}(t, \mathbf{z})), \end{cases}$$

for all  $\mathbf{z}$  on  $\Gamma(0)$ . The velocity is split into a tangential and normal part, denoted by  $\mathbf{u} = \mathbf{u}_T + (\mathbf{u} \cdot \mathbf{n})\mathbf{n} =: \mathbf{u}_T + u_N \mathbf{n}$ . We are then interested in the *tangential* velocity  $\mathbf{u}_T$  on  $\Gamma(t)$  only. For the pair  $(\mathbf{u}_T, \pi)$  a closed system of equations can be derived from the full surface Navier-Stokes system given above. For this we introduce the flow map of the pure geometric *normal* evolution of the surface, denoted by  $\Phi_t^n : \Gamma(0) \rightarrow \Gamma(t)$ . The Lagrangian derivative for the flow map  $\Phi_t^n$  is denoted by  $\partial^\circ$ :

$$\partial^\circ \mathbf{v}(t, \mathbf{x}) = \frac{d}{dt} \mathbf{v}(t, \Phi_t^n(\mathbf{z})), \quad \mathbf{x} = \Phi_t^n(\mathbf{z}).$$

Let  $\mathbf{H}$  be the second fundamental form (Weingarten mapping) and  $\mathbf{P}$  the orthogonal projection on the tangential plane. For the tangential flow one obtains the

following tangential surface Navier-Stokes equations (TSNSE):

$$\begin{cases} \mathbf{P}\partial^\circ \mathbf{u}_T + (\nabla_\Gamma \mathbf{u}_T)\mathbf{u}_T + w_N \mathbf{H}\mathbf{u}_T - 2\mu \mathbf{P} \operatorname{div}_\Gamma E_s(\mathbf{u}_T) + \nabla_\Gamma \pi = \mathbf{f} \\ \operatorname{div}_\Gamma \mathbf{u}_T = g, \end{cases}$$

with right-hand sides known in terms of geometric quantities and  $w_N = \mathbf{w} \cdot \mathbf{n}$ :

$$g = -w_N \kappa, \quad \mathbf{f} = 2\mu \mathbf{P} \operatorname{div}_\Gamma (w_N \mathbf{H}) + \frac{1}{2} \nabla_\Gamma w_N^2.$$

In the second part of the presentation we discuss well-posedness of the TSNSE. Based on results presented in [7] we propose a variational formulation of the TSNSE in appropriate Hilbert spaces and formulate a well-posedness result for this formulation.

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**Time fractional gradient flows: Theory and numerics**

ABNER J. SALGADO

(joint work with Wenbo Li)

1. PROBLEM DESCRIPTION

Let  $\mathcal{H}$  be a separable Hilbert space with inner product  $\langle \cdot, \cdot \rangle$  and norm  $\|\cdot\|$ . Let  $\Phi : \mathcal{H} \rightarrow \mathbb{R} \cup \{+\infty\}$  be a convex and lower semicontinuous (lsc) functional, and  $T > 0$  a final time. Given  $u_0 \in \mathcal{H}$  and  $f : [0, T] \rightarrow \mathcal{H}$  we seek for  $u : [0, T] \rightarrow \mathcal{H}$  that solves, in a sense to be specified, the following evolutionary inclusion

$$(1) \quad \begin{cases} D_c^\alpha u(t) + \partial\Phi(u(t)) \ni f(t), & t \in (0, T], \\ u(0) = u_0. \end{cases}$$

Here, for  $\alpha \in (0, 1)$ , we denote by  $D_c^\alpha w(t)$  the Caputo derivative of order  $\alpha$  which, for sufficiently smooth functions is defined as

$$D_c^\alpha w(t) = I^{1-\alpha}[\dot{w}](t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t (t-r)^{-\alpha} \dot{w}(r) dr,$$

where  $I^{1-\alpha}$  is the (Riemann–Liouville) fractional integral of order  $1 - \alpha$ .

Problem (1) entails an abstraction of several models of interest. For instance, fractional differential equations with nonsmooth slope functions [3], subdiffusion equations [9, 5] and its nonlinear variants [10, 14], time fractional parabolic obstacle problems [4, 13], fractional porous medium equations [1], and the time fractional Allen Cahn and Cahn Hilliard equations [12].

## 2. THE CAPUTO DERIVATIVE AND ITS DISCRETIZATION

**2.1. The Caputo derivative.** The classical definition of the Caputo derivative of order  $\alpha \in (0, 1)$  requires already for a function to be differentiable. There have been several attempts to extend the definition of Caputo derivative to less regular functions [2, 6]. We will follow the one proposed by Li and Liu [6, 7] which, essentially, reads

$$D_c^\alpha w(t) = \frac{d}{dt} I^{1-\alpha}[w - w(0)\theta](t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t (t-s)^{-\alpha} (w(s) - w(0)\theta(s)) ds,$$

where  $\theta$  is the Heaviside function. This extended definition of the Caputo derivative satisfies, whenever the identity makes sense, the following *fundamental theorem of fractional calculus*

$$(2) \quad w(t) = w(0) + I^\alpha[D_c^\alpha w](t) = w(0) + \frac{1}{\Gamma(\alpha)} \int_0^t (t-s)^{\alpha-1} D_c^\alpha w(s) ds.$$

In addition, for every  $\Psi : \mathcal{H} \rightarrow \mathbb{R}$  that is convex and lsc we have the following *key inequality*

$$(3) \quad D_c^\alpha \Psi(w(t)) \leq \langle \partial \Psi(w(t)), D_c^\alpha w(t) \rangle.$$

**2.2. Discretization.** Let  $\mathcal{P} = \{t_n\}_{n=0}^N$  be an arbitrary partition of  $[0, T]$ , i.e.,  $0 < t_0 < \dots < t_N = T$ . Set  $\tau_n = t_n - t_{n-1}$  and  $\boldsymbol{\tau} = \max\{\tau_n\}_{n=1}^N$ .

Recall (2). Assume now that the Caputo derivative  $D_c^\alpha w$  is piecewise constant over the partition  $\mathcal{P}$  to obtain

$$\mathbf{W} = w_0 \mathbf{1} + \mathbf{K}_{\mathcal{P}} \mathbf{V}_\alpha,$$

where  $\mathbf{1}$  is a vector having one in all coordinates,  $\mathbf{W} = \{w(t_n)\}_{n=1}^N \subset \mathcal{H}^N$ ,  $\mathbf{V}_\alpha = \{D_c^\alpha w(t_n)\}_{n=1}^N$ , and

$$[\mathbf{K}_{\mathcal{P}}]_{ni} = \frac{1}{\Gamma(1-\alpha)} \int_{t_{i-1}}^{t_i} (t_n - r)^{-\alpha} dr, \quad i \leq n.$$

Clearly the matrix  $\mathbf{K}_{\mathcal{P}}$  is lower triangular and nonsingular. This allows us to define the following discretization of the Caputo derivative

$$D_{\mathcal{P}}^\alpha \mathbf{W} = \mathbf{V}_\alpha = \mathbf{K}_{\mathcal{P}}^{-1} [\mathbf{W} - w_0 \mathbf{1}],$$

which is a generalization of the deconvolutional schemes studied in [7]. Many properties of this discretization follow from the structure of  $\mathbf{K}_{\mathcal{P}}^{-1}$ .

**Proposition 1** (properties of  $\mathbf{K}_{\mathcal{P}}$ ). *For any partition  $\mathcal{P}$ , all  $n \in \{1, \dots, N\}$ , and all  $i \in \{0, \dots, n - 1\}$  we have*

$$[\mathbf{K}_{\mathcal{P}}^{-1}]_{nn} > 0, \quad [\mathbf{K}_{\mathcal{P}}^{-1}]_{ni} < [\mathbf{K}_{\mathcal{P}}^{-1}]_{(n+1)i},$$

where  $[\mathbf{K}_{\mathcal{P}}]_{n0} = -\sum_{j=1}^n [\mathbf{K}_{\mathcal{P}}]_{nj}$ .

**Corollary 2** (discrete key inequality). *For any convex and lsc  $\Psi : \mathcal{H} \rightarrow \mathbb{R}$ , and all  $\mathbf{W} \in \mathcal{H}^N$  we  $\Psi(\mathbf{W}) = \{\Psi(W_n)\}_{n=1}^N$ . Then,*

$$D_{\mathcal{P}}^\alpha \Psi(\mathbf{W}) \leq \langle \partial \Psi(\mathbf{W})_n, (D_{\mathcal{P}}^\alpha \mathbf{W})_n \rangle.$$

### 3. THEORY

We introduce the following notion of solutions for (1).

**Definition 3** (energy solution). A function  $u \in L^2(0, T; \mathcal{H})$  such that  $D_c^\alpha u \in L^2(0, T; \mathcal{H})$  is called an *energy solution* of (1) if

$$\frac{1}{t} \int_0^t \|u(r) - u_0\|^2 dr \rightarrow 0, \quad t \downarrow 0,$$

and, for every  $w \in \mathcal{H}$ , we have

$$\langle D_c^\alpha u(t), u(t) - w \rangle + \Phi(u(t)) - \Phi(w) \leq \langle f(t), u(t) - w \rangle, \quad \text{a.e. } t \in (0, T).$$

This notion of solution seems natural in light of the following result.

**Theorem 4** (uniqueness). *Energy solutions are unique.*

To show existence we develop a *fractional minimizing movements* scheme. Starting from  $U_0 \approx u_0$  we compute, for  $n \geq 0$ , and  $F_n = \frac{1}{\tau_n} \int_{t_{n-1}}^{t_n} f(t) dt$

$$(4) \quad U_n = \operatorname{argmin}_{w \in \mathcal{H}} \left[ \Phi(w) - \frac{1}{2} \sum_{i=0}^{n-1} [\mathbf{K}_{\mathcal{P}}^{-1}]_{ni} \|w - U_i\|^2 - \langle F_n, w \rangle \right].$$

Owing to the strict convexity of the norm, we have existence and uniqueness of  $U_n$ . In addition, the optimality conditions of (4) read

$$(5) \quad (D_{\mathcal{P}}^\alpha \mathbf{U})_n + \partial \Phi(\mathbf{U})_n \ni F_n.$$

On the basis of the sequence  $\{U_n\}_{n=0}^N$  we construct two functions. The function  $\overline{U}_{\mathcal{P}} \in L^\infty(0, T; \mathcal{H})$  is piecewise constant subject to the triangulation, i.e., for  $t \in (t_{n-1}, t_n]$ , we have  $\overline{U}_{\mathcal{P}}(t) = U_n$ . The other function  $\widehat{U}_{\mathcal{P}} \in C([0, T]; \mathcal{H})$  is such that its Caputo derivative is piecewise constant: if  $t \in (t_{n-1}, t_n]$  we have  $D_c^\alpha \widehat{U}_{\mathcal{P}}(t) = (D_{\mathcal{P}}^\alpha \mathbf{U})_n$ . It is important to note, using the fundamental theorem of fractional calculus (2), we can define functions  $\{\varphi_i\}_{i=0}^N \in C([0, T]; \mathcal{H})$  that are such that

$$(6) \quad (D_{\mathcal{P}}^\alpha \varphi_i)_j = \delta_{i,j}.$$

With these functions at hand we can write

$$(7) \quad \widehat{U}_{\mathcal{P}}(t) = \sum_{i=0}^n U_i \varphi_i(t).$$

The properties of these functions allow us to rewrite (4) or (5) as

$$(8) \quad \left\langle D_c^\alpha \widehat{U}_{\mathcal{P}}(t), \overline{U}_{\mathcal{P}}(t) - w \right\rangle + \Phi(\overline{U}_{\mathcal{P}}(t)) - \Phi(w) \leq \left\langle \overline{F}_{\mathcal{P}}(t), \overline{U}_{\mathcal{P}}(t) - w \right\rangle, \quad \forall w \in \mathcal{H}.$$

This variational inequality allows us to obtain suitable a priori estimates on these discrete solutions and, as a consequence, pass to the limit via compactness.

**Theorem 5** (existence). *Assume  $\Phi(u_0) < \infty$  and that*

$$\sup_{t \in [0, T]} \int_0^t (t-s)^{\alpha-1} \|f(s)\|^2 ds < \infty.$$

*Then, for any  $\mathcal{P}$  we have*

$$\sup_{t \in [0, T]} \int_0^t (t-s)^{\alpha-1} \|D_c^\alpha \widehat{U}_{\mathcal{P}}(s)\|^2 ds < \infty.$$

*Consequently, the time fractional gradient flow (1) has an energy solution which, moreover, verifies  $u \in C^{0, \alpha/2}([0, T]; \mathcal{H})$ .*

We remark that, in the integer order case [11], energy solutions to gradient flows belong to  $C^{0, 1/2}([0, T]; \mathcal{H})$ , so there is a sort of continuity with respect to  $\alpha$  in the previous result.

#### 4. NUMERICS

We notice, first of all, that (5) is a viable numerical scheme. We now intend to analyze it.

**4.1. A posteriori error analysis.** Setting  $w = U_{n-1}$  in (5) we obtain

$$\mathcal{E}_\alpha(t) = \left\langle D_c^\alpha \widehat{U}_{\mathcal{P}}(t) - \overline{F}_{\mathcal{P}}(t), \widehat{U}_{\mathcal{P}}(t) - \overline{U}_{\mathcal{P}}(t) \right\rangle + \Phi(\widehat{U}_{\mathcal{P}}(t)) - \Phi(\overline{U}_{\mathcal{P}}(t)) \geq 0,$$

which only depends on data and the discrete solution, and so it is a *computable* quantity. This will be our a posteriori error estimator.

Using the convexity of  $\Phi$ , we can rewrite (8) as, for all  $w \in \mathcal{H}$ ,

$$(9) \quad \left\langle D_c^\alpha \widehat{U}_{\mathcal{P}}(t), \widehat{U}_{\mathcal{P}}(t) - w \right\rangle + \Phi(\widehat{U}_{\mathcal{P}}(t)) - \Phi(w) \leq \left\langle \overline{F}_{\mathcal{P}}(t), \widehat{U}_{\mathcal{P}}(t) - w \right\rangle + \mathcal{E}_\alpha(t).$$

This allows us to prove the following result.

**Theorem 6** (a posteriori error estimate). *Assume that  $\Phi(u_0) < \infty$ . For every  $\mathcal{P}$  we have*

$$\begin{aligned} \|u - \widehat{U}_{\mathcal{P}}\|_{L^\infty(0, T; \mathcal{H})} &\lesssim \left( \sup_{t \in [0, T]} \int_0^t (t-s)^{\alpha-1} \mathcal{E}_\alpha(s) ds \right)^{1/2} \\ &+ \sup_{t \in [0, T]} \int_0^t (t-s)^{\alpha-1} \|f(s) - \overline{F}_{\mathcal{P}}(s)\| ds. \end{aligned}$$

**4.2. A priori error analysis.** It turns out that, the functions  $\{\varphi_i\}_{i=0}^N$ , defined in (6) form a partition of unity. Consequently, (7) is a convex combination of the nodal values  $\{U_i\}_{i=0}^n$ . This, together with a few manipulations of the error estimator  $\mathcal{E}_\alpha$ , allow us to obtain the following estimate.

**Theorem 7** (a priori error estimate). *In the same setting as Theorem 5 we have*

$$\left\| u - \widehat{U}_{\mathcal{P}} \right\|_{L^\infty(0,T;\mathcal{H})} \lesssim \tau^{\alpha/2}.$$

We recall that energy solutions are, in general, no better than  $C^{0,\alpha/2}([0, T]; \mathcal{H})$  so the previous result is optimal.

## 5. CONCLUSIONS AND OPEN PROBLEMS

Let us summarize the results of this work, for more details we refer the reader to [8].

- We provided a discretization of the Caputo derivative which is unconditionally stable on any time partition  $\mathcal{P}$ .
- With the help of this discretization we developed a fractional minimizing movements scheme which allowed us to show existence and uniqueness of energy solutions to time fractional gradient flows.
- We developed an a posteriori error estimate which is reliable.
- We provided an a priori error analysis which, given the regularity of the solutions, is optimal.

Some other results, that we have not discussed, include:

- Extensions of the theory and numerics to the cases when  $\Phi$  is merely  $\lambda$ -convex, and/or the case of a Lipschitz perturbation of the subdifferential.
- For some particular cases of energy  $\Phi$  and initial condition  $u_0$ , we have improved convergence rates.
- When  $f = 0$  we have studied the asymptotic behavior of the solution.

Finally, some open questions are

- Development of the theory and numerics in the case that  $\partial\Phi$  is replaced by a maximal monotone operator.
- Development of the theory and numerics in Banach spaces.
- Space discretization.

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## FOSLS for parabolic and instationary Stokes equations

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(joint work with Gregor Gantner)

**Space-time variational formulation.** We consider parabolic evolution equations in a simultaneous space-time variational formulation: For a Gelfand triple  $V \hookrightarrow H \simeq H' \hookrightarrow V'$  of function spaces on a spatial domain  $\Omega \subset \mathbb{R}^d$ , and a.e.  $t \in I := (0, T)$ , let  $a(t; \cdot, \cdot)$  be a bilinear form on  $V \times V$  that is bounded and satisfies a Gårding inequality, both uniform in  $t$ . Then with  $A(t) \in \mathcal{L}(V, V')$  defined by  $(A(t)\eta)(\zeta) := a(t; \eta, \zeta)$ , given  $f$  and  $u_0$  we search  $u(t): \Omega \rightarrow \mathbb{R}$  that satisfies

$$(1) \quad \begin{cases} \frac{du}{dt}(t) + A(t)u(t) = f(t) & (t \in I), \\ \gamma_0 u = u_0. \end{cases}$$

With

$$(Bu)(v) := \int_I \left\langle \frac{du}{dt}(t), v(t) \right\rangle_H dt + \int_I (A(t)u(t))(v(t)) dt = \int_I \langle f(t), v(t) \rangle_H dt =: f(v),$$

$Y := L_2(I; V)$  and  $X := Y \cap H^1(I; V')$ , it is known that the pair  $(B, \gamma_0) \in \mathcal{L}\text{is}(X, Y' \times H)$ , where  $\mathcal{L}\text{is}(E, F)$  denotes the set of boundedly invertible operators  $E \rightarrow F$ .



**Minimal residual methods.** An approach to construct a numerical approximation to the solution  $u$  from a finite dimensional subspace  $X^\delta \subset X$  is to compute  $u^\delta \in X^\delta$  that minimizes the residual over  $X^\delta$ . In [1] this minimal residual method is made practical by replacing the dual norm  $\|\cdot\|_{Y'}$  by a discretized dual norm  $\|\cdot\|_{Y^{\delta'}}$  for some finite dimensional subspace  $Y^\delta \subset Y$ . W.l.o.g. assuming that  $a(t; \cdot, \cdot)$  is coercive (unif. in  $t$ ), with  $(Au)(v) := \int_I (A(t)u(t))(v(t))dt$ ,  $A_s := \frac{1}{2}(A+A')$ ,  $A_a := \frac{1}{2}(A-A')$ , and by equipping  $Y$  and  $X$  with ‘energy-norms’  $\|\cdot\|_Y := \sqrt{(A_s \cdot)(\cdot)}$  and  $\|\cdot\|_X := \sqrt{\|\cdot\|_Y^2 + \|\partial_t \cdot\|_{Y'}^2 + \|\gamma_T \cdot\|^2}$ , the following result is valid:

**Theorem 1** ([7]). *Let  $\alpha := \|A_a\|_{\mathcal{L}(Y, Y')} = \rho(A_s^{-1}A_aA_s^{-1}A_a)^{\frac{1}{2}}$ ,  $X^\delta \subseteq Y^\delta$  and  $\gamma_\delta := \inf_{w \in X^\delta} \frac{\|\partial_t w\|_{Y^{\delta'}}}{\|\partial_t w\|_{Y'}} > 0$ . Then  $u^\delta := \operatorname{argmin}_{w \in X^\delta} \|Bw - f\|_{Y^{\delta'}}^2 + \|\gamma_0 w - u_0\|_H^2$  satisfies*

$$\|u - u^\delta\|_X \leq \sqrt{\frac{2 + \alpha^2 + \alpha\sqrt{\alpha^2 + 4}}{\gamma_\delta^2 + \alpha^2 + 1 - \sqrt{(\gamma_\delta^2 + \alpha^2 + 1)^2 - 4\gamma_\delta^2}}} \inf_{w \in X^\delta} \|u - w\|_X.$$

Uniform stability  $\inf_{\delta \in \Delta} \gamma_\delta > 0$ , which yields quasi-best approximations, has so far been verified for families  $(X^\delta)_{\delta \in \Delta}$ ,  $(Y^\delta)_{\delta \in \Delta}$  that consist of finite element spaces w.r.t. partitions of type  $\cup_i [t_i, t_{i+1}] \times \Omega_{h_i}$  (‘time-slab setting’).

**FOSLS.** To describe the First Order System Least Squares Formulation, which applies to parabolic equations of second order, for ease of presentation we restrict ourselves to the model problem of the heat equation

$$\begin{cases} (\partial_t - \Delta_{\mathbf{x}})u = f & \text{on } I \times \Omega, \\ u = 0 & \text{on } I \times \partial\Omega, \\ \gamma_0 u = u_0 & \text{on } \Omega. \end{cases}$$

Introducing  $-\nabla_{\mathbf{x}}u$  as an additional variable, this equation can be recast as a first order system

$$G(u, w) := (\partial_t u + \operatorname{div}_{\mathbf{x}} w, -w - \nabla_{\mathbf{x}}u, \gamma_0 u) = (f, 0, u_0).$$

(with  $u = 0$  on  $I \times \partial\Omega$ ). From  $(B, \gamma_0) \in \mathcal{L}\text{is}(X, Y' \times H)$ ,  $\nabla_{\mathbf{x}} \in \mathcal{L}(X, L_2(I \times \Omega)^d)$ ,  $\operatorname{div}_{\mathbf{x}} \in \mathcal{L}(L_2(I \times \Omega)^d, Y')$  one infers that  $G \in \mathcal{L}\text{is}(X \times L_2(I \times \Omega)^d, Y' \times L_2(I \times \Omega)^d \times L_2(\Omega))$ . To get rid of the dual norm at the right hand side, which is inconvenient for minimal residual discretisations, in [2] it was proposed to incorporate the condition  $\operatorname{div}(u, w) := \partial_t u + \operatorname{div}_{\mathbf{x}} w \in L_2(I \times \Omega)$  into the definition of the ‘trial space’. In [3] it was proven that the resulting least squares formulation, with  $Y'$  replaced by  $L_2(I \times \Omega)$ , is well-posed. A somewhat stronger statement, where also the dual space is removed from the definition of the trial space, reads as follows:

**Theorem 2** ([3]). *With  $U := \{\vec{u} := (u, w) \in L_2(I; H_0^1(\Omega)) \times L_2(I \times \Omega)^d : \operatorname{div} \vec{u} \in L_2(I \times \Omega)\}$  and  $L := L_2(I \times \Omega) \times L_2(I \times \Omega)^d \times L_2(\Omega)$ ,*

$$G \in \mathcal{L}\text{is}(U, L),$$

*and by decomposing  $f \in Y'$  as  $f = f_1 + \operatorname{div}_{\mathbf{x}} f_2$ ,*

$$(B, \gamma_0)u = (f, u_0) \iff G\vec{u} = \vec{f} := (f_1, f_2, u_0).$$

The advantages of this first order system formulation are that for *any* closed subspace  $U^\delta \subset U$ ,  $\vec{u}^\delta := \operatorname{argmin}_{\vec{v} \in U^\delta} \|G\vec{v} - \vec{f}\|_L$  is quasi-best approximation from  $U^\delta$

to  $\vec{u}$  w.r.t.  $\|\cdot\|_U$ ; the bilinear form  $\langle G\cdot, G\cdot \rangle_L$  is bounded, symmetric and coercive on  $U \times U$ ; the a posteriori error estimator  $\|\vec{f} - G\vec{u}^\delta\|_L$  is equivalent to  $\|\vec{u} - \vec{u}^\delta\|_L$ .

The formulation of a parabolic PDE as a variational problem with a bounded and coercive bilinear form has several interesting applications. In [5] we discuss the application of this formulation within a reduced basis method for solving a parameter-dependent parabolic PDE, and for solving a parabolic PDE constraint optimal control problem.

The inclusion of the constraint  $\operatorname{div}(u, w) \in L_2(I \times \Omega)$  in the definition of the trial space also has its price. The term  $\|\operatorname{div}(u, w)\|_{L_2(I \times \Omega)}$  is part of the graph norm  $\sqrt{\|u\|_{L_2(I; H_0^1(\Omega))}^2 + \|w\|_{L_2(I \times \Omega)^d}^2 + \|\operatorname{div}(u, w)\|_{L_2(I \times \Omega)}^2}$  in which the error is minimized. With for example linear trial spaces for  $u$  and  $w$ , the local approximation error in  $\operatorname{div}(u, w)$  in  $L_2$ -norm is of the order of the local mesh-size times the maximum of the local  $H^2$  semi-norms of  $u$  and  $w$ . Realizing that, for  $f_2 = 0$ ,  $w = -\nabla_{\mathbf{x}} u$ , we conclude that this local approximation error is of the order of the local mesh-size times the maximum of the second and *third* order derivatives of  $u$ . On the other hand similar bounds on the local approximation errors in  $u$  and  $w$  in  $L_2(I; H_0^1(\Omega))$  or  $L_2(I \times \Omega)^d$ -norms involve at most second order derivatives of  $u$ . Numerical experiments reported on in [3] show for non-smooth  $u$  convergence rates in terms of the number of DoFs for both uniform and adaptively refined meshes that are much smaller than the optimal rate  $\frac{1}{d+1}$ .

To cure the problem of the disappointingly low rates for non-smooth solutions, in [6] we consider finite element spaces w.r.t. prismatic elements. By constructing them so that a commuting diagram is valid, the error in  $\operatorname{div}(u, w)$  in  $L_2$ -norm depends only on higher order norms of  $\operatorname{div}(u, w)$ , i.e., of  $f_1$ , which in many cases is much smoother than the terms  $\partial_t u$  and  $\operatorname{div}_{\mathbf{x}} w$ .

**Instationary Stokes equations.** In [4] we followed an analogous FOSLS program for the instationary Stokes equations with slip boundary conditions. By introducing the deformation tensor as an additional variable, we write these Stokes equations as a first order system for the triple of the velocities, deformation tensor, and pressure. For a spatial domain  $\Omega$  that is convex or has a  $C^2$  boundary, this system is shown to be well-posed in a least-squares sense. All norms that arise in the residual minimization can be exactly evaluated.

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**Space-time finite element methods**

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 (joint work with Marco Zank)

The space-time variational formulation for the Dirichlet boundary value problem for the heat equation,

(1)  $\partial_t u - \Delta_x u = f$  in  $Q := \Omega \times (0, T)$ ,  $u = 0$  on  $\Sigma := \partial\Omega \times (0, T)$ ,  $u(0) = 0$  in  $\Omega$ , is to find  $u \in L^2(0, T; H_0^1(\Omega)) \cap H_0^1(0, T; H^{-1}(\Omega))$  such that

$$(2) \quad \int_0^T \int_{\Omega} [\partial_t u v + \nabla_x u \cdot \nabla_x v] dx dt = \int_0^T \int_{\Omega} f v dx dt$$

is satisfied for all  $v \in L^2(0, T; H_0^1(\Omega))$ . Unique solvability of (2) follows from the Babuška–Nečas theory. A stability and error analysis of unstructured space-time finite element methods for (2) is given in [4], for an overview see [6]. This approach was used for the solution of distributed optimal control problems subject to the heat equation (1) with  $L^2(Q)$  regularization [1], and alternatively with a regularization in the energy space  $L^2(0, T; H^{-1}(\Omega))$ , see [2]. When doing integration by parts also in time, instead of the primal variational formulation (2) we have to solve an adjoint variational formulation to find  $u \in L^2(0, T; H_0^1(\Omega))$  such that

$$(3) \quad \int_0^T \int_{\Omega} [-u \partial_t v + \nabla_x u \cdot \nabla_x v] dx dt = \int_0^T \int_{\Omega} f v dx dt$$

is satisfied for all  $v \in L^2(0, T; H_0^1(\Omega)) \cap H_0^1(0, T; H^{-1}(\Omega))$ . Note that the test space covers a zero terminal condition  $v(x, T) = 0$  for  $x \in \Omega$ . While unique solvability of the adjoint formulation (3) follows as for the primal formulation (2), the consideration of the variational formulations (2) and (3) motivates, by using an interpolation argument, a variational formulation of (1) in anisotropic Sobolev spaces to find  $u \in H_{0;0}^{1;1/2}(Q)$  such that

$$(4) \quad \int_0^T \int_{\Omega} [\partial_t u v + \nabla_x u \cdot \nabla_x v] dx dt = \int_0^T \int_{\Omega} f v dx dt$$

is satisfied for all  $v \in H_{0;0}^{1;1/2}(Q)$ . An important tool in proving unique solvability of (4) is a modified Hilbert transformation  $\mathcal{H}_T : H_{0;0}^{1;1/2}(Q) \rightarrow H_{0;0}^{1;1/2}(Q)$ , see [7]. For  $u \in L^2(0, T)$ , the modified Hilbert transformation is defined as the adjoint

$$(5) \quad \mathcal{H}_T u(t) = \sum_{k=0}^{\infty} u_k \cos\left(\left(\frac{\pi}{2} + k\pi\right) \frac{t}{T}\right)$$

of the Fourier series

$$u(t) = \sum_{k=0}^{\infty} u_k \sin\left(\left(\frac{\pi}{2} + k\pi\right) \frac{t}{T}\right) dt, \quad u_k = \frac{2}{T} \int_0^T u(t) \sin\left(\left(\frac{\pi}{2} + k\pi\right) \frac{t}{T}\right) dt.$$

It turns out that the bilinear form  $\langle \partial_t u, \mathcal{H}_T v \rangle_{(0,T)}$  is symmetric, bounded, and elliptic for all  $u, v \in H_{0,0}^{1/2}(0, T)$ , and  $\langle v, \mathcal{H}_T v \rangle_{L^2(0,T)} \geq 0$  is non-negative.

The modified Hilbert transformation  $\mathcal{H}_T$  as defined in (5) allows for a closed representation [7],

$$(6) \quad \mathcal{H}_T u(t) = \frac{1}{2T} \text{p.v.} \int_0^T \left[ \frac{1}{\sin\left(\frac{\pi}{2} \frac{s-t}{T}\right)} + \frac{1}{\sin\left(\frac{\pi}{2} \frac{s+t}{T}\right)} \right] u(s) ds \quad \text{for } t \in (0, T).$$

The representation (6) can be used for an efficient discretization of the resulting Galerkin–Bubnov variational formulation to find  $u \in H_{0,0}^{1,1/2}(Q)$  such that

$$(7) \quad \langle \partial_t u, \mathcal{H}_T v \rangle_Q + \langle \nabla_x u, \nabla_x \mathcal{H}_T v \rangle_{L^2(Q)} = \langle f, \mathcal{H}_T v \rangle_{L^2(Q)}$$

is satisfied for all  $v \in H_{0,0}^{1,1/2}(Q)$ .

It turns out that the modified Hilbert transformation  $\mathcal{H}_T$  is a generalization of the Hilbert transformation

$$\mathcal{H}\bar{u}(t) := \frac{1}{\pi} \text{p.v.} \int_{\mathbb{R}} \frac{\bar{u}(s)}{t-s} ds \quad \text{for } t \in \mathbb{R},$$

i.e., we have [5]

$$(8) \quad \mathcal{H}_T u = -\mathcal{H}\bar{u} + Bu \quad \text{on } (0, T),$$

where  $\bar{u}$  is an extension of  $u$  from  $(0, T)$  onto  $\mathbb{R}$  by reflection,

$$(9) \quad \bar{u}(s) := \begin{cases} u(s) & \text{for } s \in (0, T), \\ u(2T-s) & \text{for } s \in (T, 2T), \\ -u(-s) & \text{for } s \in (-T, 0), \\ -u(2T+s) & \text{for } s \in (-2T, -T), \\ 0 & \text{else,} \end{cases}$$

and  $B : L^2(0, T) \rightarrow H^1(0, T) \subset L^2(0, T)$  is compact. Hence, and up to a compact perturbation, we can replace in (7) the modified Hilbert transformation  $\mathcal{H}_T$  by the classical Hilbert transformation  $\mathcal{H}$  which simplifies the implementation. Moreover, the representation (8) provides a relation of the above considerations in a finite time interval  $(0, T)$  with some recent results in the mathematical analysis for more general parabolic evolution equations, and for the ellipticity of boundary integral operators for the wave equation on flat objects, considering both in the infinite time interval  $\mathbb{R}_+$ , see also the discussion in [5].

As a second model problem, we consider the Dirichlet boundary value problem for the wave equation,

$$(10) \quad \partial_{tt} u - \Delta_x u = f \text{ in } Q, \quad u = 0 \text{ on } \Sigma, \quad u(0) = \partial_t u(t)|_{t=0} = 0 \text{ in } \Omega.$$

The variational formulation of (10) is to find  $u \in H_{0;0}^{1,1}(Q)$  such that

$$(11) \quad -\langle \partial_t u, \partial_t v \rangle_{L^2(Q)} + \langle \nabla_x u, \nabla_x v \rangle_{L^2(Q)} = \langle f, v \rangle_{L^2(Q)}$$

is satisfied for all  $v \in H_{0;0}^{1,1}(Q)$ . Note that the ansatz space covers a zero initial condition  $u(0) = 0$ , while the test space has a zero terminal condition  $v(T) = 0$ . For  $f \in L^2(Q)$ , there exists a unique solution  $u$  of (11), satisfying, e.g., [7],

$$\|u\|_{H_{0;0}^{1,1}(Q)}^2 = \|\partial_t u\|_{L^2(Q)}^2 + \|\nabla_x u\|_{L^2(Q)}^2 \leq \frac{1}{2} T^2 \|f\|_{L^2(Q)}^2.$$

For the Galerkin space-time finite element discretization of (11) using the same test and ansatz functions we introduce some bijective operator  $A : H_{0;0}^{1,1}(Q) \rightarrow H_{0;0}^{1,1}(Q)$ , e.g., the time reversal map  $\kappa_T w(x, t) = w(x, T - t)$ , or, in the case of tensor-product space-time finite element spaces, the transformation  $Aw_h(x, t) := w_h(x, T) - w_h(x, t)$ , see [7]. However, the resulting numerical scheme is only stable when a CFL condition is satisfied, e.g.,  $h_t < h_x \sqrt{n}$  when using piecewise linear basis functions and a tensor-product structure also in the spatial domain  $\Omega \subset \mathbb{R}^n$ . However, using the modified Hilbert transformation  $\mathcal{H}_T$  as defined in (5) and its properties, we end up with a variational formulation [3] to find  $u \in H_{0;0}^{1,1}(Q)$  such that

$$(12) \quad \langle \mathcal{H}_T \partial_t u, \partial_t w \rangle_{L^2(Q)} + \langle \partial_x u, \mathcal{H}_T \nabla_x w \rangle_{L^2(Q)} = \langle f, \mathcal{H}_T w \rangle_{L^2(Q)}$$

is satisfied for all  $w \in H_{0;0}^{1,1}(Q)$ . The Galerkin finite element discretization of (12) results in a linear system  $K_h \underline{u} = \underline{f}$  with a stiffness matrix  $K_h$ , which is positive definite. Hence, unique solvability of the Galerkin system follows for any conforming space-time finite element space. First numerical results are given in [3] which illustrate unconditional stability and optimal convergence rates.

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## Interpolation Operators on negative Sobolev Spaces

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(joint work with Lars Diening, Tabea Tscherpel)

Local interpolation operators are of uttermost importance in a priori error analysis, the design and analysis of a posteriori error estimators, and further applications like preconditioning. These aspects led to huge scientific activity resulting in several interpolation operators that are well suited for elliptic problems. However, suitable interpolation operators for parabolic space-time finite element methods are missing. Indeed, interpolation operators that have been used in the literature require additional smoothness of the solution.

A downside of this requirement is that it hides the need of parabolic scaling for irregular solutions. In particular, a special case of the parabolic Poincaré inequality in [2] states that a function  $v: K \rightarrow \mathbb{R}$  on a time-space cell  $K = I \times T$  with time interval  $I$  of length  $h_t$  and simplex  $T$  with diameter  $h_x$  satisfies

$$(1) \quad \left\| \nabla_x v - |K|^{-1} \int_K \nabla_x v \, dx \right\|_{L^2(K)} \lesssim h_x \|\nabla_x^2 v\|_{L^2(K)} + h_t h_x^{-1} \|\partial_t v\|_{L^2(K)}.$$

This estimate indicates that for solutions to parabolic problems with time derivatives merely in  $L^2$  the underlying mesh of the space-time FEM needs to be refined parabolically in the sense that  $h_t \approx h_x^2$ . Indeed, numerical experiments in [3] for a space-time DPG method indicate a significant improvement for parabolically scaled meshes, cf. Figure 1.

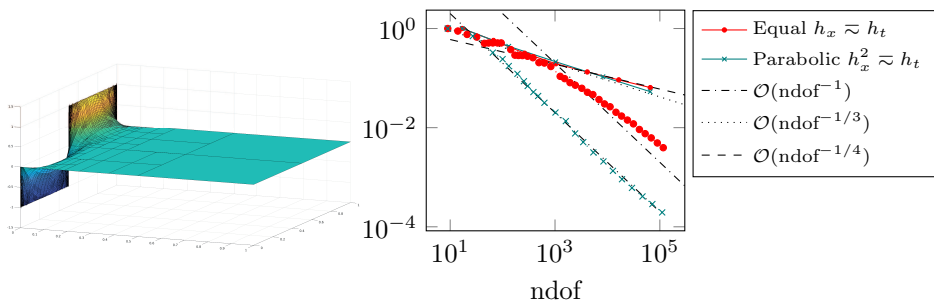


FIGURE 1. Solution to the heat equation in 1D with rough initial data and source term zero and the corresponding convergence history plot of the squared error. The solid lines result from uniform and the dotted lines result from adaptive mesh refinements.

Another difficulty of interpolation operators for parabolic problems is the treatment of the  $L^2(\mathcal{I}; H^{-1}(\Omega))$  norm of the time derivative. Even in the stationary case classical interpolation operators like the Scott–Zhang projector [6] are not well defined for functions in  $H^{-1}(\Omega) := (H_0^1(\Omega))^*$ . This can be seen immediately from its definition: Let  $\varphi_j \in \mathcal{L}_{k,0}^1(\mathcal{T}) \subset H_0^1(\Omega)$  denote the Lagrange basis function of polynomial degree  $k$  related to an interior Lagrange node  $j \in \mathcal{N}^\circ$  and let  $\varphi_\ell^*$  be a piece-wise polynomial of degree  $k$  supported on a single simplex  $T_\ell \in \mathcal{T}$  such that  $\langle \varphi_j, \varphi_\ell^* \rangle_\Omega = \delta_{j,\ell}$ , then the Scott–Zhang projection reads

$$(2) \quad \Pi v := \sum_{j \in \mathcal{N}^\circ} \langle v, \varphi_j^* \rangle_\Omega \varphi_j \quad \text{for all } v \in L^2(\Omega).$$

The functions  $\varphi_j^*$  are not in  $H_0^1(\Omega)$  and hence the  $L^2$  inner products do not extend to functions in  $H^{-1}(\Omega)$ . A simple remedy is the replacement of the discontinuous weight functions by continuous ones. However, the following result from [5, Lem. 15] shows that we have to increase their polynomial degrees.

**Lemma 1.** *Any projection defined as in (2) with weight functions  $\varphi_j^* \in \mathcal{L}_{k,0}^1(\mathcal{T})$  is the  $L^2$  projection.*

It is possible to design an operator with weight functions  $\varphi_j^* \in \mathcal{L}_{k,0}^1(\mathcal{T})$  that is not a projection but self-adjoint. The design for the lowest-order case goes back to Carstensen [1]. We generalized the operator in [4] to all polynomial degrees. Due to its self-adjointness the operator is well suited for approximations in  $H^{-1}(\Omega)$ . However, since it is not a projection, the maximal order of convergence is reduced by one; cf. [5, Thm. 17].

Tantardini designed a  $H^{-1}$  stable projection with higher order weights for the lowest-order case  $k = 1$  in her PhD thesis [7]. We extended this operator to all polynomial degrees  $k \in \mathbb{N}$ . Our main result [5, Thm. 1] shows localized (with respect to nodal patches  $\omega_j := \bigcup\{T \in \mathcal{T} : j \in T\}$  and  $\omega_j^2 := \bigcup\{T \in \mathcal{T} : T \cap \omega_j \neq \emptyset\}$  for vertices  $j \in \mathcal{V}$ ) approximation and stability results.

**Theorem 2 (Main Result).** *There exists a linear projection  $\Pi$  onto  $\mathcal{L}_{k,0}^1(\mathcal{T})$  such that for  $0 \leq m \leq s \leq k + 1$ , all  $\xi \in H^{-1}(\Omega)$ , and all  $w \in H_0^1(\Omega)$*

**Localization**  $\quad \|\xi - \Pi\xi\|_{H^{-1}(\Omega)} \approx \left( \sum_{j \in \mathcal{V}} \|\xi - \Pi\xi\|_{H^{-1}(\omega_j)}^2 \right)^{1/2},$

**Approximability**  $\quad \|\xi - \Pi\xi\|_{H^{-1}(\omega_j)} \lesssim h_j \|\xi\|_{L^2(\omega_j^2)},$   
 $\quad \|w - \Pi w\|_{H^{-1}(\omega_j)} \lesssim h_j^{s+1} \|\nabla^s w\|_{L^2(\omega_j^2)},$   
 $\quad \|\nabla^m(w - \Pi w)\|_{L^2(T)} \lesssim h_T^{s-m} \|\nabla^s w\|_{L^2(\omega_T)},$

**Local Stability**  $\quad \|\Pi\xi\|_{H^{-1}(\omega_j)} \lesssim \|\xi\|_{H^{-1}(\omega_j^2)},$   
 $\quad \|\nabla^s \Pi w\|_{L^2(T)} \lesssim \|\nabla^s w\|_{L^2(\omega_T)}.$

The structure of the operator  $\Pi$  in Theorem 2 is as in (2) with weights  $\varphi_j^* \in \mathcal{L}_{3k,0}^1(\mathcal{T})$ . A key in the design of  $\Pi$  is the property  $\Pi^*1 = 1$  of the adjoint operator

on simplices  $T \in \mathcal{T}$  that do not touch the boundary of  $\Omega$ . The importance of this property for  $H^{-1}$  stability is illustrated by the upper bound

$$(3) \quad \|\Pi v\|_{H^{-1}(\Omega)} = \sup_{w \in H_0^1(\Omega)} \frac{\langle v, \Pi^* w \rangle_\Omega}{\|\nabla w\|_{L^2(\Omega)}} \leq \|v\|_{H^{-1}(\Omega)} \sup_{w \in H_0^1(\Omega)} \frac{\|\nabla \Pi^* w\|_{L^2(\Omega)}}{\|\nabla w\|_{L^2(\Omega)}}.$$

The property  $\Pi^* 1 = 1$  additionally yields a first-order approximation property of the adjoint  $\Pi^* w = \sum_{j \in \mathcal{N}^\circ} \langle w, \varphi_j \rangle_\Omega \varphi_j^*$  resulting in the localization of the  $H^{-1}$  norm and the improved order of convergence in Theorem 2; cf. [5, Lem. 11–12].

The weight functions are constructed by local weight functions designed on a reference simplex  $T_{\text{ref}}$ . Let  $b_\alpha := |\alpha|!/\alpha! \lambda^\alpha$  with multi-indices  $\alpha \in \mathbb{N}_0^{d+1}$  and barycentric coordinates  $\lambda$  denote the Bernstein basis function on  $T_{\text{ref}}$ . Then we define, with polynomials  $q_\gamma$  of maximal degree  $k$  to be determined, the local weight function

$$(4) \quad p_\alpha := b_\alpha \left( c_k^{-1} + \left( q_\alpha - \sum_{|\gamma|=k} b_\gamma q_\gamma \right) \right).$$

The well-posedness of a related linear system of equations ensures the existence of suitable polynomials  $q_\gamma$  such that the weights form an orthonormal system. By the ansatz in (4) the resulting global basis functions have a local support  $\text{supp}(\varphi_j^*) \subset \text{supp}(\varphi_j)$ . Moreover, since the Bernstein basis functions form a partition of unity, the summation over all weights leads to a constant function. This leads to the property  $\Pi^* 1 = 1$ .

The novel operator  $\Pi$  allows us to design a local interpolation operator for semi-discretizations and tensor-product spaces for parabolic problems with optimal rates of convergence; c.f. [5, Sec. 4.1–4.2]. Moreover, it allows us to smoothen rough right-hand sides in least-squares finite element methods which allows us to conclude quasi-optimality with respect to the energy norm plus some higher-order data-approximation error; c.f. [5, Sec. 4.3].

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### A space-time multiscale mortar mixed finite element method for parabolic equations

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(joint work with Manu Jayadharan, Michel Kern, and Ivan Yotov)

We develop a space-time mortar mixed finite element method for the model parabolic problem: find a fluid pressure  $p$  and a Darcy velocity  $\mathbf{u}$  such that

$$(1) \quad \mathbf{u} = -K\nabla p \quad \text{and} \quad \frac{\partial p}{\partial t} + \nabla \cdot \mathbf{u} = q \quad \text{in } \Omega \times (0, T],$$

subject to appropriate initial and boundary conditions (here  $q$  is a source term and  $K$  is a diffusion tensor). The spatial computational domain  $\Omega$  is decomposed into a union of subdomains  $\Omega_i$  discretized with non-matching spatial grids with typical mesh-sizes  $h_i$ , whereas asynchronous (individual for each subdomain  $\Omega_i$ ) time steps of size  $\Delta t_i$  are considered for the time interval  $(0, T]$ .

Our method is based on a space-time variational formulation that couples mixed finite elements employing polynomial degrees  $k, l$  in space with the discontinuous Galerkin method of degree  $q$  in time. Continuity of flux (mass conservation) across the space-time interfaces  $\Gamma_{ij} \times (0, T]$  is imposed via a space-time mortar variable that lives on the interfaces  $\Gamma_{ij} \times (0, T]$ . Following [1], we typically use coarser meshes (of typical mesh-sizes  $H_{ij}$  and time steps  $\Delta T_{ij}$ ) and higher-degree polynomial approximations ( $m$  in space and  $s$  time) in comparison with respect to the subdomains. This setting is illustrated in Figure 1.

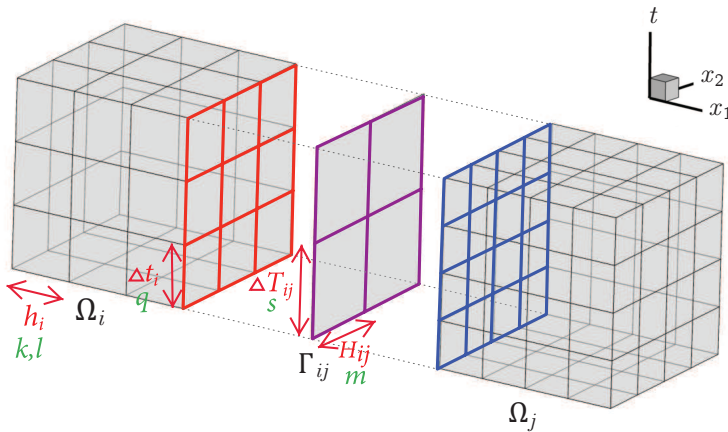


FIGURE 1. Space-time meshes and discretizations

We establish existence, uniqueness, and stability of our method. We also prove a priori error estimates for the spatial and temporal errors, optimal under some technical conditions. We finally develop a space-time non-overlapping domain

decomposition method that reduces the global problem to a space-time coarse-scale mortar interface problem. Every iteration here involves solving a space-time problem on each individual space-time subdomain  $\Omega_i \times (0, T]$ , which can be done in parallel. The spectral properties of the interface operator and the convergence of the interface iteration of our domain decomposition method are analyzed.

Numerical experiments are provided that illustrate the theoretical results and the flexibility of the method for modeling problems with features that are localized in space and in time. The details can be found in [2].

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