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Low-rank techniques for integrating large Sylvester-like equations with Parareal

Author and Presenter: Benjamin Carrel (University of Geneva)

Co-authors: Martin J. Gander (University of Geneva) Bart Vandereycken (University of Geneva)

Abstract: In this poster, we apply Parareal to evolution problems that admit good low-rank approximations that can be obtained from the dynamical low-rank approximation (DLRA) algorithm. In this context, the cost and accuracy of each time step are dominated by the rank chosen for the approximation. We use these properties in a new method, which we call low-rank Parareal, to obtain a time-parallel DLRA solver for evolution problems. Low-rank Parareal is shown, both experimentally and theoretically, to work well on parabolic problems. Furthermore, we present a new method to efficiently integrate the time steps in the fine and coarse levels of low-rank Parareal. The idea is to apply a projected exponential Runge–Kutta integrator, specific to Sylvester-like equations, in an extended Krylov subspace. The method is robust to stiffness and keeps all computations in a low-rank format. Numerical experiments show that it is superior compared to other low-rank methods for stiff problems.

Generic bounds on the approximation error for physics-informed (and) operator learning

Author and Presenter: Tim De Ryck (ETH Zürich, Switzerland)

Co-author: Siddhartha Mishra (ETH Zürich, Switzerland)

Abstract: We propose a very general framework for deriving rigorous bounds on the approximation error for physics-informed neural networks (PINNs) and operator learning architectures such as DeepONets and FNOs as well as for physics-informed operator learning. These bounds guarantee that PINNs and (physics-informed) DeepONets or FNOs will efficiently approximate the underlying solution or solution operator of generic partial differential equations (PDEs). Our framework utilizes existing neural network approximation results to obtain bounds on more involved learning architectures for PDEs. We illustrate the general framework by deriving the first rigorous bounds on the approximation error of physics-informed operator learning and by showing that PINNs (and physics-informed DeepONets and FNOs) mitigate the curse of dimensionality in approximating nonlinear parabolic PDEs.

References

 T. De Ryck and S. Mishra, Generic bounds on the approximation error for physics-informed (and) operator learning. Report 2022-20, Seminar for Applied Mathematics, ETH Zürich, Switzerland (in review).

Approximation of polynomials with Neural Networks and Machine Learning

Author and Presenter: Bruno Després (Sorbonne LJLL Université France)

Abstract: Neural Networks representations of real monovariate polynomials defined on the closed segment $x \in I = [0, 1]$ play a central role in the numerical analysis of Neural Networks [4, 3, 1, 2]. A central result is the Yarostky Theorem [5] which provides an approximation result of general functions, by means of a specific Neural Network approximation of the polynomial $x \mapsto x^2$ where the activation function is ReLU $R(x) = \max(0, x)$. This specific Neural Network can have an arbitrary large number of hidden layers, so it provides a simple example of a Deep Neural Network with perfectly known coefficients.

However, as pointed out by Ronald DeVore in 2019, the stability of the approximation of polynomial functions by Deep Neural Networks (i.e. with many hidden layers) is not addressed in the current theory. In particular it is already not the case for the Deep Neural Network which approximates the polynomial $x \mapsto x^2$. Most of the recent developments are devoted to abstract approximation theory and are scarcely related to constructive algorithms.

Recent progress https://hal.sorbonne-universite.fr/hal-03762185 on the approximation of polynomials will be explained. I will detail an original algorithm for the numerical approximation of polynomials with Machine Learning tools. The algorithm is proved to be convergent in L^{∞} norm.

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The skeleton equation method for acoustic transmission problems with varying coefficients

Author and Presenter: Francesco Florian (Universitt Zrich, Switzerland)

Co-authors: Stefan Sater (Universitt Zrich, Switzerland) Ralf Hiptmair (ETH Zrich, Switzerland)

Abstract: We consider transmission problems in either the \mathbb{R}^3 or a subset and solve the heterogeneous Helmholtz equation. We construct abstract layer potentials as solution of a transmission problem, avoiding Green's functions. We derive a well posed formulation as boundary equations.

Keywords: Boundary element methods, layer potentials, frequency-domain wave equation

Introduction We consider the domain $\Omega \subseteq \mathbb{R}^3$, partitioned in Ω_j , $1 \leq j \leq n_\Omega$. The *skeleton* is $\bigcup_{1 \leq j \leq n_\Omega} \partial \Omega_j$. We analyze the *Helmholtz transmission problem*: for Re s > 0 and general positive coefficients $\mathbf{A} \in L^{\infty}(\Omega, \mathbb{R}^{3 \times 3}_{\text{sym}}), p \in L^{\infty}(\Omega, \mathbb{R})$

$\int p^2 s^2 u - \operatorname{div}(\mathbf{A}\nabla u) = 0$	in $\Omega_j, 1 \le j \le n_\Omega$,
(Inhomogeneous) transmission conditions	on $\partial \Omega_j \cap \partial \Omega_k, 1 \leq j, k \leq n_{\Omega}$,
(Inhomogeneous) boundary conditions	$\text{if }\partial\Omega\neq\emptyset,$
Radiation conditions	if Ω is unbounded.

Layer Potentials The layer potentials are defined in each subdomain Ω_j separately, using PDE techniques, without the Green's function [2].

For this goal we extend $p|_{\Omega_j}$, $\mathbf{A}|_{\Omega_j}$ to positive L^{∞} coefficients p_j , \mathbf{A}_j defined on \mathbb{R}^3 . We introduce the sesquilinear form

$$\ell_j(s)(u,v) := \left\langle p_j^2 s^2 u, \overline{v} \right\rangle_{\mathbb{R}^3} + \left\langle \mathbf{A}_j \nabla u, \overline{\nabla v} \right\rangle_{\mathbb{R}^3} : H^1(\mathbb{R}^3) \times H^1(\mathbb{R}^3) \to \mathbb{C}$$

with $L_j(s): H^1(\mathbb{R}^3) \to H^{-1}(\mathbb{R}^3)$ being the associated operator.

The solution operator $N_j(s)$ and the single layer potential $S_j(s)$ are defined as solutions of full space problems [2, 4]:

$$\begin{split} \ell_j(s)(\mathsf{N}_j(s)f,w) &= \langle f,\overline{w}\rangle_{\mathbb{R}^3} \quad \forall w \in H^1(\mathbb{R}^3);\\ \ell_j(s)\left(\mathsf{S}_j(s)\phi,w\right) &= \left\langle \phi,\overline{s^{-1/2}\gamma_{\mathrm{D};j}w}\right\rangle_{\partial\Omega_j} \quad \forall w \in H^1(\mathbb{R}^3). \end{split}$$

The double layer potential is defined piecewise: given any $\phi \in H^{1/2}(\partial \Omega_j)$ consider a function $f \in H^1(\mathbb{R}^3)$ such that $\gamma_{\mathrm{D};j}f = s^{-1/2}\phi$; then

$$\mathsf{D}_{j}(s)\phi|_{\Omega_{j}^{\pm}} := \mp f|_{\Omega_{j}^{\pm}} + \left(\mathsf{N}_{j}(s)\mathsf{L}_{j}(s) f|_{\Omega_{j}^{\pm}}\right)\Big|_{\Omega_{j}^{\pm}}.$$

The definition does not depend on f, only on its trace [2, 4].

Skeleton Operators The skeleton operators are obtained in the usual way as mean values of the layer potentials. The Caldern operators are first constructed for a single domain:

$$\mathbf{C}_{j}(s) := \begin{bmatrix} -\mathsf{K}_{j}(s) & \mathsf{V}_{j}(s) \\ \mathsf{W}_{j}(s) & \mathsf{K}_{j}(s)' \end{bmatrix} - \frac{Id}{2};$$

they are then collected in the block-diagonal operator $\mathbf{C}(s) := \operatorname{diag}_{1 \leq j \leq n_{\Omega}} \mathbf{C}_{j}(s)$.

We incorporate homogeneous transmission and boundary conditions into the function space where the solution is sought by using the *single trace* space. Inhomogeneities are treated with suitable offset functions[3, 5].

Theorem. The operator $\mathbf{C}(s)$ is continuous. Let $\langle \cdot, \overline{\cdot} \rangle_{\mathbf{X}}$ the natural scalar product in the skeleton and $\sigma := \frac{s}{|s|}$; then for all Φ with homogeneous boundary conditions in the single trace space, for some C > 0 independent of s:

$$\operatorname{Re}\left\langle \mathbf{C} \mathbf{\Phi}, \overline{\sigma \mathbf{\Phi}} \right\rangle_{\mathbf{X}} \geq C \min\{1, |s|^2\} \frac{\operatorname{Re} s}{|s|^2} \left\| \mathbf{\Phi} \right\|_{\mathbf{X}}^2,$$

It follows that the resulting problem in weak form is well-posed [1, 3, 4].

Conclusions

- We present a general method to transform acoustic transmission problems with mixed boundary conditions to a system of non-local Caldern operators on the skeleton, without relying on the Green's function. The resulting operators are coercive, self-dual and continuous.
- If the Green's function is explicitly known, the Caldern operators admit a representation as skeleton integrals, which allow for a standard discretization by conforming Galerkin BEM.

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Adaptive Spectral Decomposition for Inverse Problems

Author and Presenter: Yannik G. Gleichmann (University of Basel, Switzerland)

Co-authors: Daniel H. Baffet (University of Basel, Switzerland) Marcus J. Grote (University of Basel, Switzerland)

Abstract: Inverse medium problems involve the reconstruction of a spatially varying medium, u(x), from available observations. Typically, they are formulated as PDE-constrained optimization problems and solved by an inexact Newton-like iteration. Clearly, standard grid-based representations of u are very general but often too expensive due to the resulting high-dimensional search space. Adaptive spectral inversion (ASI) instead expands the unknown medium in a basis of eigenfunctions of a judicious elliptic operator, which depends itself on the current iterate. Rigorous L^2 -error estimates of the adaptive spectral (AS) approximation are proved for an arbitrary piecewise constant medium.

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Numerical approximation of the deformation of thin plates

Author and Presenter: Diane Guignard (University of Ottawa, Canada)

Abstract: We study the elastic behavior of prestrained and bilayer thin plates which can undergo large deformations and achieve non-trivial equilibrium shapes even without external forces or prescribed boundary conditions. These phenomena can be observed in nature (e.g., the growth of soft tissues or the snap of the venus flytrap) or be manufactured (e.g., engineered polymer gels). Being able to simulate the deformation of such plates can be benificial for many engineering and medical applications, for instance to develop micro-mechanical devices or to design climate-responsive architecture. We are mainly interested in the bending regime, namely when the three-dimensional hyper-elastic energy scales like the third power of the thickness of the plate. From a mathematical point of view, the dimensionally reduced problem consists of the minimization of a bending energy involving the second fundamental form of the deformed midplane subject to a nonlinear and nonconvex metric constraint.

In this talk, we introduce the mathematical model and derive the dimensionally reduced problem. We then present the proposed numerical method, which is based on a local discontinuous Galerkin approach for the discretization and a gradient flow for the energy minimization, discuss its properties and illustrate its performances throught several numerical experiments.

This is joint work with Andrea Bonito and Angelique Morvant (Texas A&M University), Ricardo H. Nochetto (University of Maryland), and Shuo Yang (Tsinghua University).

Randomized Joint Orthogonal Diagonalization of Real Symmetric Matrices

Author and Presenter: Haoze He (EPFL, Switzerland)

Co-author: Daniel Kressner (EPFL, Switzerland)

Abstract: The classical problem of joint diagonalization of an almost commuting family of real symmetric matrices is to find an orthogonal matrix that almost diagonalizes every matrix in the family. Most current methods solve this problem using optimization techniques. We propose a novel randomized method that reduces the problem to a standard eigenvalue problem through random linear combinations. Unlike existing optimization-based methods, our algorithm is easy to implement and leverages existing high-quality linear algebra software packages. We prove its robustness by proving that the backward error of the output orthogonal joint diagonalizer will be small with high probability through a perturbation analysis. The algorithm can be further improved by deflation techniques. Through numerical experiments on synthetic and real-world data, we show that our algorithm reaches state-of-the-art performance.

References

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Analytic regularity for the Navier-Stokes equations in polygons with mixed boundary conditions

Author and Presenter: Yanchen He (ETH Zurich, Switzerland)

Co-authors: Carlo Marcati (University of Pavia, Italy; ETH Zurich, Switzerland) Christoph Schwab (ETH Zurich, Switzerland).

Abstract: We prove weighted analytic regularity of Leray-Hopf variational solutions for the stationary, incompressible Navier-Stokes Equations (NSE) in plane polygonal domains, subject to analytic body forces. We admit mixed boundary conditions which may change type at each vertex. The weighted analytic regularity results are established in Hilbertian Kondrat'ev spaces. The proofs rely on a priori estimates for the corresponding linearized boundary value problem in sectors in corner-weighted Sobolev spaces and on an induction argument for the weighted norm estimates on the quadratic nonlinear term in the NSE, in a polar frame.

References

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Mathematical foundation of sparsity-based multi-illumination super-resolution

Author and Presenter: Ping Liu (ETH Zürich, Switzerland)

Co-authors: Habib Ammari (ETH Zürich, Switzerland) Sanghyeon Yu (Korea University, Korea) Ola Sabet (University of Zrich, Switzerland) Lucas Pelkmans (University of Zrich, Switzerland)

Abstract: It is well-known that the resolution of traditional optical imaging system is limited by the so-called Rayleigh resolution or diffraction limit, which is of several hundreds of nanometers. By employing fluorescence techniques, modern microscopic methods can resolve point scatterers separated by a distance much lower than the Rayleigh resolution limit. Localization-based fluorescence subwavelength imaging techniques such as PALM and STORM can achieve spatial resolution of several tens of nanometers. However, these techniques have limited temporal resolution as they require tens of thousands of exposures. Employing sparsity-based models and recovery algorithms is a natural way to reduce the number of exposures, and hence obtain high temporal resolution. Nevertheless, to date fluorescence techniques suffer from the tradeoff between spatial and temporal resolutions.

Recently, a new multi-illumination imaging technique called Brownian Excitation Amplitude Modulation microscopy (BEAM) is introduced. BEAM achieves a threefold resolution improvement by applying a compressive sensing recovery algorithm over only few frames. Motivated by BEAM, our aim in this paper is to pioneer the mathematical foundation for sparsity-based multiillumination super-resolution. More precisely, we consider several diffractionlimited images from sample exposed to different illumination patterns and recover the source by considering the sparsest solution. We estimate the minimum separation distance between point scatterers so that they could be stably recovered. By this estimation of the resolution of the sparsity recovery, we reveal the dependence of the resolution on the cut-off frequency of the imaging system, the signal-to-noise ratio, the sparsity of point scatterers, and the incoherence of illumination patterns. Our theory particularly highlights the importance of the high incoherence of illumination patterns in enhancing the resolution. It also demonstrates that super-resolution can be achieved using sparsity-based multi-illumination imaging with very few frames, whereby the spatio-temporal super-resolution becomes possible. BEAM can be viewed as the first experimental realization of our theory, which is demonstrated to hold in both the oneand two-dimensional cases.

References

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Flux Globalization Based Well-Balanced Path-Conservative Central-Upwind Schemes for Shallow Water Models

Yongle Liu (University of Zurich)

Co-authors:

Alexander Kurganov (Southern University of Science and Technology, China) Yangyang Cao (Southern University of Science and Technology, China) Ruixiao Xin (Southern University of Science and Technology, China).

Abstract: I will introduce a new approach for constructing robust wellbalanced (WB) finite-volume methods for nonconservative one-dimensional hyperbolic systems of nonlinear PDEs. The WB property, namely, the ability of the scheme to exactly preserve physically relevant steady-state solutions is enforced using a flux globalization approach according to which a studied system is rewritten in an equivalent quasi-conservative form with global fluxes. To this end, one needs to incorporate nonconservative product terms into the global fluxes. The resulting system can then be solved using a Riemann-problemsolver-free central-upwind (CU) scheme. However, a straightforward integration of the nonconservative terms would result in a scheme capable of exactly preserving very simple smooth steady states only and failing to preserve discontinuous steady states naturally arising in the nonconservative models.

In order to ameliorate the flux globalization based CU scheme [1], we evaluate the integrals of the nonconservative product terms using a path-conservative technique [2]. This results in a new WB flux globalization based path-conservative central-upwind scheme (PCCU) scheme [3, 4], which is much more accurate and robust than its predecessors. We illustrate the property of the proposed WB PCCU scheme on a variety of shallow water models including shallow water equations with/without Manning friction term [4], the shallow water equations with Coriolis force [4], the two-layer shallow water equations [3], and the thermal rotating shallow water equations [5].

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A mixed precision Jacobi SVD algorithm

Author and Presenter: Yuxin Ma (EPFL, Switzerland and Fudan University, China)

> Co-authors: Weiguo Gao (Fudan University, China) Meiyue Shao (Fudan University, China)

Abstract: We propose a mixed precision Jacobi algorithm for computing the singular value decomposition (SVD) of a dense matrix. After appropriate preconditioning, the proposed algorithm computes the SVD in a lower precision as an initial guess, and then performs one-sided Jacobi rotations in the working precision as iterative refinement. By carefully transforming a lower precision solution to a higher precision one, our algorithm achieves about $2\times$ speedup on the x86-64 architecture compared to the usual one-sided Jacobi SVD algorithm in LAPACK, without sacrificing the accuracy.

Extrapolation methods as nonlinear Krylov methods

Author and Presenter: Conor McCoid (Université de Genève, Switzerland)

Co-author: Martin J. Gander (Université de Genève, Switzerland)

Abstract: Krylov methods are commonplace for solving of linear problems. Their use for nonlinear problems requires generalizing them. In linear examples some extrapolation methods have been shown to be equivalent to Krylov subspace methods. Since extrapolation methods can be applied to nonlinear problems, we can view these methods as nonlinear Krylov methods. To show the broad class of equivalences between these methods and others, we build each from their ancestral root-finding method, the multisecant equations, which are an extension of the secant equations to higher dimensions.

A novel well-balanced global flux formulation for continuous $$\rm FEM/RD$$

Author and Presenter: Lorenzo Micalizzi (Universität Zürich, Switzerland)

Co-authors: Rémi Abgrall (Universität Zürich, Switzerland) Mario Ricchiuto (Inria Bordeaux sud-ouest, France)

Abstract: In the context of the numerical solution of hyperbolic problems, one has to deal with several challenges among which: the presence of instabilities and the exact preservation of some analytical solutions at the discrete level (well-balancing). The instability issues are usually solved through an upwinding in the finite volume/discontinuous Galerkin finite element method setting, through stabilization techniques in the Residual Distribution/continuous finite element method setting. In particular, in this last context, the existing literature offers many possible options: Lax-Friedrichs, Streamline-Upwind Petrov-Galerkin (SUPG), orthogonal subscale stabilization (OSS), continuous interior penalty (CIP, introduced in [1]), etc... Several strategies have been introduced to achieve well-balancing. In particular, a successful approach is based on the definition of a global flux [2], i.e., a new flux which keeps into account the source term allowing to recast the initial problem into an equivalent one which is homogeneous.

In this work, in a one dimensional setting, the accuracy and the well-balanced properties of a global flux formulation of the RD/continuous FEM method for the Shallow Water equations coupled with some novel CIP stabilizations are investigated. The time-stepping technique is given by the Deferred Correction [3] to have a fully-explicit scheme avoiding the inversion of the mass matrix. The numerical results confirm the ability of the approach to exactly preserve a particular steady state (lake at rest) and the high order accuracy. In particular, one of the novel CIP stabilizations based on the jump of the derivative of the global flux has shown very good performances and superconvergences towards general steady solutions. Despite the simulations addressing the monodimensional Shallow Water equations only, most of the elements can be generalized to other systems of equations (such as the Euler equations) and, in particular, some of the novel CIP stabilizations can be extended to the multidimensional case. For these reasons generalizations will be investigated in the future.

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Anisotropic Adaptive Finite Elements for Aluminium Electrolysis

Author and Presenter: Paride Passelli (EPFL, Switzerland)

Co-authors: Marco Picasso (EPFL, Switzerland)

Abstract: A linear and a nonlinear elliptic problem will be considered, the first having strongly varying diffusion coefficient as in [1] and the second one being a p-laplacian like problem.

Anisotropic a posteriori error estimates will be discussed. For the linear case an error estimator, being equivalent to the true error (up to some higher orders terms) will be presented. For the nonlinear case an upper bound will be discussed.

Finally an adaptive strategy, a numerical study of the effectivity index for both problems and an industrial application to aluminium electrolysis will be presented.

References

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Randomized low-rank approximation of monotone matrix functions

Author and Presenter: David Persson (EPFL, Switzerland)

Co-author: Daniel Kressner (EPFL, Switzerland)

Abstract: This work is concerned with computing low-rank approximations of a matrix function f(A) for a large symmetric positive semi-definite matrix A, a task that arises in, e.g., statistical learning and inverse problems. The application of popular randomized methods, such as the randomized singular value decomposition or the Nystrm approximation, to f(A) requires multiplying f(A) with a few random vectors. A significant disadvantage of such an approach, matrix-vector products with f(A) are considerably more expensive than matrix-vector products with A, even when carried out only approximately via, e.g., the Lanczos method. In this work, we present and analyze funNyström, a simple and inexpensive method that constructs a low-rank approximation of f(A) directly from a Nyström approximation of A, completely by passing the need for matrix-vector products with f(A). It is sensible to use funNyström whenever f is monotone and satisfies f(0) = 0. Under the stronger assumption that f is operator monotone, which includes the matrix square root $A^{1/2}$ and the matrix logarithm $\log(I + A)$, we derive probabilistic bounds for the error in the Frobenius, nuclear, and operator norms. These bounds confirm the numerical observation that funNyström tends to return an approximation that compares well with the best low-rank approximation of f(A). Our method is also of interest when estimating quantities associated with f(A), such as the trace or the diagonal entries of f(A). In particular, we propose and analyze funNyström++, a combination of funNyström with the recently developed Hutch++ method for trace estimation.

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Convergence Bound for Parareal with Spatial Coarsening

Author and Presenter: Aušra Pogoželskytė (Université de Genève, Switzerland)

Co-authors: Martin J. Gander (Université de Genève, Switzerland)

Abstract:

Over the last two decades, the number of processors per computer has greatly increased, which enabled the full exploitation of parallelism when solving partial differential equations. However, nowadays, communication between those processors has become a bottleneck.

Parallel-in-time algorithms enable us to parallelize our problem along the time dimension allowing us to relieve that bottleneck. One such method is Parareal [3]. For performance and stability reasons, we consider the sequential operator on a coarser grid in space (additionally to time) [2].

Following the method of Dobrev, Kolev, Petersson and Schroder [1], we will prove a linear convergence bound for Parareal with coarsening in space of factor two. The bound will be valid for most classical spatial restriction and prolongation operators.

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Hermite interpolation with retractions on manifolds

Author and Presenter: Axel Séguin (EPFL, Switzerland)

Co-authors: Daniel Kressner (EPFL, Switzerland)

Abstract: Interpolation of data belonging to non-Euclidean spaces is an active research area fostered by its numerous applications. In this work we focus on the Hermite interpolation problem: finding a smooth manifold curve that interpolates a collection of data points belonging to a Riemannian manifold while matching prescribed velocities at each point. We propose a novel procedure relying only on retractions to solve this problem on a large class of manifolds, including those for which tractable computations of the Riemannian exponential and logarithmic maps are not available, like for instance the manifold of fixed-rank matrices. We analyze the well-posedness of the method by introducing and showing the existence of retraction-convex sets, generalization of geodesically convex sets. We extend to the manifold setting the classical result characterizing the asymptotic interpolation error of Hermite interpolation for the case where data points are equispaced samples from an underlying smooth manifold curve. We finally illustrate these results and the effectiveness of the method with numerical experiments on the manifold of fixed-rank matrices and the Stiefel manifold of matrices with orthonormal columns.

Multilevel Monte Carlo FEM for Elliptic PDEs with Besov Random Tree Priors

Author and Presenter: Andreas Stein (ETH Zrich)

Co-author: Christoph Schwab (ETH Zrich)

Abstract: We develop a Multilevel Monte Carlo (MLMC) FEM algorithm for linear, elliptic diffusion problems in polytopal domain $\mathcal{D} \subset \mathbb{R}^d$, with Besovtree random coefficients. This is to say that the logarithms of the diffusion coefficients are sampled from so-called Besov random tree priors, which add a random tree structure to the wavelet expansion of the well-known Besov prior.

Numerical analysis of the fully discrete FEM includes quadrature approximation and accounts for a) nonuniform pathwise upper and lower coefficient bounds, and for b) low path-regularity of the Besov random tree coefficients. Admissible non-parametric random coefficients correspond to random functions exhibiting singularities on random fractals with tunable fractal dimension, but involve no a-priori specification of the fractal geometry of singular supports of sample paths. Optimal complexity and convergence rate estimates for quantities of interest are proved. A convergence analysis for MLMC-FEM is performed which yields choices of the algorithmic steering parameters for efficient implementation. A complexity ("error vs work") analysis of the MLMC-FEM approximations is provided.

References

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Low-rank multi-marginal optimal transport

Author and Presenter: Christoph Strössner (EPFL, Switzerland)

Co-author: Daniel Kressner (EPFL, Switzerland)

Abstract: By adding entropic regularization, multi-marginal optimal transport problems can be transformed into tensor scaling problems, which can be solved numerically using the multi-marginal Sinkhorn algorithm. The main computational bottleneck of this algorithm is the repeated evaluation of marginals. Recently, it has been suggested that this evaluation can be accelerated when the application features an underlying graphical model. In this work, we accelerate the computation further by combining the tensor network dual of the graphical model with additional low-rank approximations. We provide an example for the color transfer between several images, in which these additional low-rank approximations save more than 96% of the computation time.

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On the Combination between Space–Time Model Order Reduction Methods and Deep Learning for Hæmodynamic Problems

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Abstract: Over the last decade, several works aimed at exploiting deep learning (DL) techniques for the numerical approximation of PDEs appeared and the topic of physics-informed neural networks emerged. In particular, Dal Santo et al. [1] combined the Reduced Basis (RB) method with DL algorithms, coming up with a model — called RB-DNN — able to encode scattered values of solutions to steady parametrized PDEs to the underlying parameters. The model features an asymmetric autoencoder structure: a data-driven encoder learns the parameter values from the input and a deterministic PDE-based decoder uses such latent values to reconstruct the desired output. The goal of this talk is to investigate how the paradigm of the RB–DNN model could be extended to unsteady parametrized PDEs. To this end, two elements are crucial. Firstly, efficient ad hoc model order reduction (MOR) techniques are needed to embed unsteady PDE solvers into the RB-DNN model structure. Indeed, the numerical approximation of the PDE should undermine neither the training procedure nor the evaluation phase. Spatio-temporal MOR techniques, allowing for a dramatic dimensionality reduction of the problem at hand along both the spatial and the temporal dimensions, are exploited to this aim. Such methods have been recently introduced for some classes of linear problems, while their extension to non-linear ones remains an open issue. We thoroughly analyzed their application to saddle point problems, with a specific focus on the Stokes equations. Secondly, the structure of RB–DNN models has to be tailored to unsteady PDEs. On the one side, this involves the design a trainable encoder able to estimate the parameters from scattered values of the PDE solution in the spatio-temporal domain. On the other side, the development of a fast tensorial solver for the problem at hand is necessary, in order to be compliant with the backpropagation training algorithm. Numerical tests have been conducted considering two different problems: the thermal-block problem in 2 dimensions and the Stokes equations in a fixed 3D geometry. In both cases, (1) space-time MOR techniques allowed for accurate approximations of the solution, attaining significant speedups with respect to the high-fidelity model; (2) the RB-DNN model managed to provide good estimates of the underlying parameter values. being given scattered values of the solution in input. Further extensions of the proposed model to the Navier-Stokes equations, suitably handling the convective non-linear term, are being planned.

Keywords: Partial Differential Equations, Space–Time Model Order Reduction, Stokes Equations, Hæmodynamic Problems, Physics–aware Deep Learning

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Asymptotic-Preserving Scheme for Plasma Simulation in 3D

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Abstract: A key coefficient characterizing plasmas is the so-called Debye length λ_D , whose size indicates to what extent electric charges can deviate from the neutral case: If $\lambda_D = \mathcal{O}(1)$ we face the non-neutral regime, while for $\lambda_D \to 0$ the plasma becomes quasi-neutral. Plasma models have rather different properties in these two regimes due to the singular perturbation arising from the $\lambda_D \to 0$ limit. Since both regimes may coexist in some plasma phenomena, it is desired to design numerical schemes that are *robust* for arbitrary λ_D . More precisely, they should be *asymptotic-preserving* (AP), in the sense that the limit $\lambda_D \to 0$ of the scheme yields a viable discretization for the continuous limit model.

An asymptotic-preserving scheme for single- and multi-fluid Euler-Maxwell systems was proposed in [1] for one spatial dimension. We start from their dimensionless model and extend the scheme to three dimensions. The key ingredients are (i) a discretization of Maxwell's equations based on primal and dual meshes in the spirit of discrete exterior calculus (DEC)/the finite integration technique (FIT), (ii) finite volume method (FVM) for the fluid equations on the dual mesh, and (iii) mixed implicit-explicit timestepping. This scheme turns out to be AP for $\lambda_D \rightarrow 0$ both in terms of structure and empirically in the numerical test. Special care is necessary for the boundary conditions which must be valid in both regimes. Additionally, if the electromagnetic fields have to be modeled in an insulating region beyond the plasma domain, additional stabilization is necessary to accommodate Gauss's law.

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Inference for interacting particle systems based on eigenfunction estimators

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Abstract: We study the problem of inference of unknown parameters for large systems of interacting particles. In particular, we aim to fit their mean field limit, i.e., a reduced model which is valid at macroscopic scales, given a set of discrete observations of one single particle. Our approach consists in constructing martingale estimating functions based on eigenvalues and eigenfunctions of the generator of the mean field limit, where the law of the process is replaced by the invariant measure of the simplified dynamics [1]. Then, the estimator we propose is the zero of these estimating functions. We analyze theoretically the asymptotic properties of our estimator in the limit of infinite data and particles, showing that it is unbiased and normal and providing a rate of convergence. Finally, we present several numerical experiments which highlight the potentiality of our methodology.

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