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Invited Lectures
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Machine learning in numerical simulations: results, challenges, and open problems

Author and Presenter:
Ivan Oseledets (INM, RAS, Moscow, Russia)

Abstract: Machine learning (especially deep learning) has achieved tremendous success in many cognitive tasks, like image classification and text mining.

Modern machine learning can be considered as a collection of algorithms and software packages that are able to solve complex function interpolation tasks. For "numerical people" an obvious question is if these technologies can be efficiently used to solve computational modeling tasks and create faster solvers. This has been already tried, and neural networks have gained a bad reputation in numerical simulations due to the fact that they produce non-robust approximations, and the accuracy is difficult to control. One of the promising ways is to use tensor methods for multivariate function approximations: it has been recently shown that tensor decomposition can be viewed as a special type of neural networks, but can be computed using fast and stable algorithms. I will highlight recent results in this area.

Finally, I will talk about open problems in the attempts that try to bridge the gap between data science and computational science.

Domain-decomposition preconditioning for frequency-domain wave problems

Author and Presenter:
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Abstract: There is currently large research interest in finding optimal-in-time solvers for finite-element discretisations of frequency-domain wave problems, such as the Helmholtz and time-harmonic Maxwell equations, when the frequency is large. Ideally such solvers should also have good parallel scaling properties, be robust to heterogeneities in the material coefficients and come with theorems rigorously justifying their behaviour.

A common approach to this problem is trying to find good preconditioners to use when solving the linear systems with (F)GMRES. This talk will be about preconditioners built using

(i) variants of classical additive-Schwarz domain-decomposition methods, and

(ii) artificial absorption (similar to in the "shifted Laplacian" preconditioner involving multigrid).

The overall philosophy is to use PDE theory of the underlying boundary-value problems to tackle this linear-algebra problem of developing fast solvers.

The work on Helmholtz is joint with Ivan Graham (Bath), Eero Vainikko (Tartu), and Jun Zou (Chinese University of Hong Kong). The work on Maxwell is joint with Marcella Bonazzoli (Paris 6), Victorita Dolean (Strathclyde/Côte d'Azur), Ivan Graham (Bath), and Pierre-Henri Tournier (Paris 6).

Optimal explicit stabilized integrator of weak order one for stiff and ergodic stochastic differential equations

Author and Presenter:
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Co-authors:
Assyr Abdulle (EPFL, Switzerland)
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Abstract: Explicit stabilized Runge-Kutta methods are efficient for solving stiff (deterministic or stochastic) differential equations in large dimensions. In this talk, we present a new explicit stabilized scheme of weak order one for stiff and ergodic stochastic differential equations (SDEs). In the absence of noise, the new method coincides with the classical deterministic stabilized scheme (or Chebyshev method) for diffusion dominated advection-diffusion problems and it inherits its optimal stability domain size, in contrast to known existing methods for mean-square stable stiff SDEs. In addition, the new method can be used to sample the invariant measure of a class of ergodic SDEs, and combined with postprocessing techniques of geometric numerical integration originally from the deterministic literature, it achieves a convergence rate of order two at a negligible overcost.

References

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A fully parallel space-time multigrid solver for computational electrophysiology

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Abstract: We present a parallel and efficient multilevel solution strategy for solving non-linear time-dependent problems. We consider in particular the monodomain model, a non-linear reaction-diffusion equation arising from a problem in electrophysiology: the electrical activation in the human heart. Different strategies for the space-time discretization and solution of the mono-domain equation are discussed, which are based on domain decomposition and multilevel approach. For the latter, we propose a semi-geometric multigrid method, for which the coarse level approximation spaces are created using arbitrary hierarchies of non-nested meshes. Interpolation and restriction in the multilevel context is then realized by means of a discrete L^2-projection between the non-matching meshes. This approach allows for creating the coarser levels of a multigrid hierarchy, even if only a single "fine" mesh is available. Hence, multigrid hierarchies can be created for arbitrary geometries in any dimension. We discuss how this approach can be applied to the monodomain equation discretised with space-time finite elements. While we use continuous finite elements in space, for stability reasons we adopt discontinuous elements in time. We discuss shortly the properties of this time discretization scheme. We investigate how different block smoothers, coarsening strategies and ordering of the space-time variables effect the overall convergence and robustness of the solver. Furthermore, we comment on local time-stepping for space-time discretizations. Finally, we investigate numerically the scalability and the convergence of our multilevel and domain decomposition solution strategies.

Exploring chemical reaction networks with KiNetX

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Abstract: A tool for automated quantum mechanical exploration of molecular reactivity previously published by our group, Chemoton [1], generates complex chemical reaction networks and associated properties such as activation energies. The size of the networks quickly becomes intractable, in particular if the involved species cause multiple side reactions. Then, the relevant kinetics of a chemical species might be hidden under a myriad of reactive conformers. For a kinetic analysis, the chemical reaction network must be converted to a set of possibly stiff ordinary differential equations (ODE). Ideally, the resulting chemical kinetics analysis is then carried out under full error control. KiNetX [2] is a C++ software aimed at the analysis of complex chemical reaction networks and their efficient exploration. Our software has been developed to possess four features. It is able to convert the graph structure of the network into a set of ODE and to identify and prune kinetically irrelevant species. Moreover, it propagates the first-principle uncertainty in activation energies estimated by Chemoton [3] as uncertainty in concentration trajectories. Most importantly, it collects the knowledge acquired through this analysis and drives the chemical reaction network exploration of Chemoton, for instance, avoiding wasting resources exploring kinetically irrelevant portions of the graph or identifying critical paths where more refined calculation methods should be employed.

References

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Fast maximum likelihood estimation via equilibrium expectation for large network data

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Abstract: Network data may be analyzed by constructing statistical models that accurately reproduce the structural properties that may be of theoretical relevance or empirical interest. Examples of such models are Exponential Random Graph Models for social networks and Markov Random Field for image processing. Typically, Markov chain Monte Carlo (MCMC) methods are used when normalizing constants of statistical models cannot be computed. We improve on a recently developed Auxiliary Parameter Markov Chain Monte Carlo method [1] and propose a new MCMC approach for the Maximum Likelihood Estimation (MLE) of parameters of statistical models from exponential family. The existing MCMC approaches for parameter estimation (Bayesian, MCMCMLE of Geyer and Thompson [2], and stochastic approximation for Method of Moments [3]) require many MCMC simulations until convergence. The approach we propose does not require many converged simulations and, in a result, is much less computationally expensive. It relies on properties of Markov chains at equilibrium and, for this reason, we call it Equilibrium Expectation (EE). Using this approach we design a simple and efficient algorithm to find the MLE when it exists and is unique. The EE algorithm is similar to the Metropolis-Hastings algorithm, but allows MCMC simulation to be performed while constraining the desired networks properties.

We demonstrate the performance of the EE algorithm in the context of Exponential Random Graph Models (ERGMs) - a family of statistical models for network data. The EE algorithm is first tested on simulated networks. We compute bias and variance of the estimates and show that the estimates obtained with the proposed method are not less accurate than those obtained with stochastic approximation. Thus far, the lack of efficient computational methods has limited the empirical scope of ERGMs to relatively small networks with a few thousand nodes. Good scaling properties of the EE algorithm allow a dramatic increase in the size of networks that may be analyzed with ERGMs. This is illustrated in an analysis of several biological and one social network with 104,103 nodes.

References

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Coupling Finite Elements and auxiliary sources

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Abstract: We propose to solve boundary value problems stemming from Maxwell's equations by using two numerical techniques in different domains: the Finite Element Method (FEM) and the Multiple Multipole Program (MMP). MMP is a Trefftz method for computational electromagnetics, successfully employed in the code OpenMaXwell for many years.

FEM and MMP enjoy complementary capabilities. FEM requires a mesh of the computational domain of interest. This is expensive, but can treat nonlinear materials, nonsmooth shapes, or complicated geometries. At the same time, FEM allows a purely local construction of the discrete system of equations.

On the other hand, MMP is a boundary method using global basis functions that solve exactly the PDE: only integrals on a hypersurface have to be computed, and the obtained linear combination is valid in the whole domain where the PDE holds. MMP performs well where the electromagnetic field is smooth, i.e. in the free space far from physical sources and material interfaces.

Thus, a natural way to combine the strengths of these methods arises when one needs to simulate the electromagnetic field of components with nonlinear or nonsmooth properties surrounded by free space: use FEM on a mesh defined on the components and MMP in the unbounded domain outside. The boundary between the FEM and MMP domains can be nonphysical if one surrounds the components by a conforming mesh of an "air box" also modeled by FEM.

The interface conditions on the surface of the FEM domain are key to accurate coupled FEM–MMP solutions. Integrating by parts the variational form of the PDE solved by FEM, surface integrals appear, through which one can impose interface conditions by substituting the ansatz of MMP. However, one interface condition cannot be imposed in this way.

We have explored four ways to include the additional condition. The first approach relies on optimizing a functional for the additional condition, subject to a constraint expressed by the variational form of FEM. The second approach introduces a weak formulation of the additional condition, where MMP basis functions are chosen as test functions. The third and fourth approaches are based on the mortar element method and Discontinuous Galerkin, respectively.

Convergence tests have been performed for scalar and vector configurations of Maxwell's equations with exact solutions, obtaining the expected results. Moreover, non-trivial physical configurations have been simulated. An extension to transient Maxwell's equations will be considered in future research.

References

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A new coarse space correction for a well defined Neumann-Neumann method at the continuous level

Author and Presenter:
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Abstract: The Neumann-Neumann domain decomposition preconditioner is well understood, and polylogarithmic condition number estimates show its effectiveness for many elliptic problems. The method as a stationnary iteration is however divergent, and not well posed at the continuous level when cross points are present in the domain decomposition. While coarse space components are usually added to domain decomposition methods to make them scalable, we propose here new coarse space components which permit to obtain a well posed and convergent stationary two level Neumann-Neumann iteration in H2, also in the presence of cross points in the domain decomposition. We then show that the discretization of this new two level Neumann-Neumann method leads to effective preconditioners without logarithmic growth.

Convolution quadrature for wave equations with transmission boundary condition

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Abstract: This talk presents the application of the *generalised Convolution Quadrature* (gCQ) [1, 2] to a 3D time-space geophysical problem that arises from the problem of evaluating the ice volume of glaciers in the Swiss Alps.

The geophysical problem is described mathematically by 3D wave equations in two disjoint bounded domains of different media, namely the ice domain and the air domain, which are related to each other via the transmission boundary condition. Let Ω_{ice} denote the domain of the ice with the boundary $\partial\Omega_{ice} = \Gamma_0 \cup \Gamma_{01}$, and let Ω_{air} denote the domain of the air with the boundary $\partial\Omega_{air} = \Gamma_{01} \cup \Gamma_1$. The boundary Γ_{01} denotes the interface between the ice and the air, while the boundary Γ_0 denotes the interface between the ice and the rock underneath. The goal is to solve the following 3D time-space problem by using retarded potential ansatzs [3]

$$\begin{aligned}
u_{tt}^{ice} - a_{ice}^2 \Delta u^{ice} &= 0 \quad \text{in } \Omega_{ice} \times [0,T], \\
u_{tt}^{air} - a_{air}^2 \Delta u^{air} &= 0 \quad \text{in } \Omega_{air} \times [0,T], \\
u &= g \quad \text{on } \Gamma_0 \quad \times [0,T], \\
[u]_{\Gamma_{01}} = \left[a^2 \frac{\partial u}{\partial n} \right]_{\Gamma_{01}} &= 0 \quad \text{on } \Gamma_{01} \quad \times [0,T], \\
\frac{\partial u}{\partial n} + \frac{1}{a_{air}} u_t &= 0 \quad \text{on } \Gamma_1 \quad \times [0,T], \\
u(0,x) = u_t(0,x) &= 0 \quad \text{in } \Omega,
\end{aligned}$$

where $\Omega := \Omega_{ice} \cup \Omega_{air}$.

With the single layer retarded potentials $\phi^{ice} : \Gamma_{ice} \times [0,T] \to C$ and $\phi^{air} : \Gamma_{air} \times [0,T] \to C$, the solutions u^{ice} and u^{air} can be expressed respectively by

$$\begin{aligned}
u^{ice}(x,t) &:= \int_{\Gamma_{ice}} \frac{\phi^{ice}\left(y, t - \frac{\|x-y\|}{a_{ice}}\right)}{4\pi\|x-y\|} ds_y \quad \forall (x,t) \in \Omega_{ice} \times [0,T], \\
u^{air}(x,t) &:= \int_{\Gamma_{air}} \frac{\phi^{air}\left(y, t - \frac{\|x-y\|}{a_{air}}\right)}{4\pi\|x-y\|} ds_y \quad \forall (x,t) \in \Omega_{air} \times [0,T].
\end{aligned}$$

The substitution of the solution ansatzs into the boundary conditions results in a 4×4 system of time-domain boundary integral equations. The unknowns ϕ^{ice} and ϕ^{air} in the system are then solved by using the gCQ based on the implicit

Euler method for temporal discretisation and the Galerkin boundary element method (BEM) of constant basis function for spatial discretisation.

The numerical simulation produces stable results, and shows the feasibility of solving real-world complex problems of such a type by using gCQ with BEM.

References

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An adaptive method to verify the lack of collision between solid bodies in a 2D incompressible viscous flow

Author and Presenter:
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Abstract: Our goal is to check numerically a Theorem of Hillairet [1] which says that a solid body falling in a constant-density incompressible viscous fluid cannot reach the bottom of the cavity in finite time. A penalty method is used to formulate the fluid flow problem in the whole cavity, thus avoiding the solid-liquid interface to be tracked. However, an adaptive method in space an time is advocated, the error indicators in space and time being derived on simplified problems. Numerical experiments indeed show that the solid body does not reach the bottom of the cavity in finite time.

References

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Parallelized sparse inverse covariance matrix estimation

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Abstract: We consider the problem of estimating sparse inverse covariance matrices for high-dimensional datasets using the ℓ_1-regularized Gaussian maximum likelihood method. This problem is particularly challenging as the required computational resources increase superlinearly with the number of random variables. We introduce a performant and scalable algorithm, which builds on recent advancements of second-order methods for sparse problems [1, 2]. The routine leverages the intrinsic parallelism in the linear algebra operations and exploits the underlying sparsity of the problem. The computational bottlenecks are identied, and the respective subroutines are parallelized using a hybrid MPI-OpenMP approach. Numerical examples conducted at the Swiss National Supercomputing Center (Cray XC40) show that, in comparison to the state-of-the-art algorithms, the proposed routine provides signicant speed-up with scalability up to 128 nodes. The developed framework is used to approximate the sparse inverse covariance matrix for datasets with up to 10 million random variables.

References

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Random time steps geometric integrators of ordinary differential equations for uncertainty quantification of numerical errors

Author and Presenter:
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Abstract: We introduce a probabilistic integrator for ordinary differential equations (ODEs) based on randomised time steps [1]. The random perturbation that is introduced allows to build a probability measure on the numerical solution and thus to provide an uncertainty quantification of the error. Convergence of this probability measure towards the true solution is studied both in strong and weak sense. Unlike an additive random perturbation, randomising the time steps guarantees the conservation of some geometric properties of deterministic Runge-Kutta methods, hence improving the robustness of the probabilistic solution. Probabilistic methods for differential equations allow for a substantial qualitative improvement of the solution of Bayesian inverse problems. Hence, we show how to incorporate our probabilistic integrator in this framework, providing examples of inverse problems based on Hamiltonian systems.

References

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Numerical approximation of the three-dimensional elliptic Monge-Ampère equation

Author and Presenter:
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Abstract: In this work, a numerical method for solving the three-dimensional elliptic Monge-Ampère equation is presented. The Monge-Ampère equation is a fully nonlinear second-order elliptic equation with many application in various fields. The method that is used to solve the problem is based on least squares/relaxation approach. The relaxation algorithm allows to decouple the problem into a sequence of local nonlinear problems and linear variational problems. The local nonlinear problems are solved using Newton-type methods, while the variational problems are approximated using mixed low order finite elements with regularization techniques. The results of numerical experiments show the convergence of our relaxation method to a convex classical solution if such a solution exists, or to a generalized solution in a least-squares sense otherwise. These results also show the robustness of our methodology and its ability at handling curved boundaries and non-convex domains.

This is joint work with A. Caboussat (Geneva School of Business Administration, University of Applied Sciences Western Switzerland (HES-SO)) and Prof. R. Glowinski (University of Houston).

References

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ε-rank estimations for $\mathcal{H}$-matrix subblocks of the Helmholtz equation

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Abstract: $\mathcal{H}$-matrix techniques are known to be an efficient tool for solving linear systems arising from PDEs with asymptotically smooth kernel (e.g. the Laplace kernel). However, for highly oscillatory kernels (e.g. the Helmholtz kernel for large wave numbers), methods based on these techniques lose their advantage. In this talk, we want to investigate the order of rank growth (w.r.t. the wave number) for different subblock choices. First, we will show some brand new theoretical results obtained by Engquist and Zhao and provide insight in the main ideas of the theory. Then we will see in the numerical tests that there is indeed a signicant influence of the geometrical constellation of the two subblock index sets on the order of rank growth.

Sparse approximation of solutions to parametric diffusion problems

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Abstract: Sparsity of solutions to parametric diffusion problems is analyzed with general non-isotropic, non-affine parametric input. Locally supported representation systems are admitted for the parametric input. Best N-term approximation rates are implied that generalize those in the usual case of affine-parametric inputs. Also non-local operators such as parametric fractional diffusion operators are admissible. This work is supported in part by the Swiss National Science Foundation (SNSF) under grant SNF 159940.

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Security constrained optimization of large scale energy systems on high performance computers[1]

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Abstract: The electrical power grid is a critical infrastructure that should be resilient to failures. Increased penetration of the renewable energy sources is placing greater stress on the grid, shifting operation of the power grid equipment towards their operational limits [1]. Thus, any unexpected contingency could be critical to the overall operation. Consequently, it is essential to operate the grid with a focus on the security measures. Security constrained optimal power flow (SCOPF) imposes additional security constraints to the optimal power flow problem. It aims for minimum adjustments in the pre-contingency operating state, such that in the event of any contingency, the operation will remain secure and within operating limits. For a realistic power network, however, with numerous contingencies considered, the overall problem size becomes intractable for single-core optimization tools in short time frames for real-time industrial operations, such as real-time electricity market responses to electricity prices. We propose a distributed primal-dual interior-point framework exploiting the block-structured KKT linear system arising from the SCOPF problem using a Schur complement technique [2]. In order to utilize node-level parallelism, an incomplete augmented multicore sparse factorization is used, which further exploits sparse structure of the problem. The performance of the implementation is evaluated on the "Piz Daint" supercomputer.

References

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[1] We gratefully acknowledge financial support from the Swiss Commission for Technology and Innovation (CTI - SCCER program). This project is carried out in the frame of the Swiss Centre for Competence in Energy Research on the Future Swiss Electrical Infrastructure (SCCER-FURIES).

Porting physical parameterizations from a climate model to accelerators

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Abstract: ICON [1] (ICOsahedral Non-hydrostatic) is a climate and numerical weather prediction model being developed by the Max Planck Institute for Meteorology (MPI-M) and the German Weather Service (DWD). Together with MPI-M and DWD, MeteoSwiss, the Center for Climate Systems Modeling (C2SM/ETH), and the Swiss National Supercomputing Center (CSCS) are porting ICON to GPUs and many-core architectures. Within the model, physical parameterizations calculate the collective effect of physical phenomena which occur on a sub-grid scale. We suggest multiple directive-based approaches of porting these parameterizations to accelerators, such as using the OpenACC standard or the CLAW source-to-source translator. Allowing the retention of a single Fortran code, directive approach can offer a high degree of performance portability. Using the FortranTestGenerator tool for automatic unit test generation for Fortran subroutines, the turbulence parameterization is isolated in a testbed subset of the model, so that subsequent changes can be easily validated. Tool-based analysis of loop kernels using the Rooine model is used to estimate attainable performance of the tri-diagonal algorithm on various platforms, in particular i86-based multi-core CPUs as well as NVIDIA GPUs. The validated turbulence parameterization, running within a testbed framework, can be integrated into the overall ICON model.

References

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Analysis of overlap in optimized waveform relation methods for RLCG transmission line type circuits

Author and Presenter:
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Abstract: Among many applications of parallel computing, solving large systems of ordinary differential equations (ODEs) which arise from large scale electronic circuits, or discretizations of partial differential equations (PDEs), form an important part. A systematic approach for their parallel solution are Waveform Relaxtion (WR) techniques, which were introduced in 1982 for circuit solver applications. These techniques are based on partitioning large circuits into smaller sub-circuits, which are then solved separately over multiple time steps, and the overall solution is obtained by an iteration between the sub-circuits. However, this technique can lead to non-uniform and potentially slow convergence over large time windows. To overcome this issue, optimized waveform relaxation techniques were introduced, which are based on optimizing a parameter. We show how this method improves the convergence for RLCG transmission line type circuits. We introduce overlap between sub circuits and analyze its effect on the convergence factor. For $R = 0$, we find that these RLCG circuit equations represent discretizations of the well known Maxwell equations. We relate these two models and give some asymptotic results.

Exotic aromatic B-series for the order conditions of the long time numerical integration of ergodic stochastic differential equations

Author and Presenter:
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Abstract: We introduce a new algebraic framework based on aromatic trees and Butcher-series for the systematic study of the accuracy of numerical integrators for sampling the invariant measure of a class of ergodic stochastic differential equations.

References

[1] A. Laurent and G. Vilmart. Exotic aromatic B-series for the study of long time integrators for a class of ergodic SDEs. *Submitted*, arXiv:1707.02877, 2017.

Robust Rayleigh quotient minimization and nonlinear eigenvalue problems

Author and Presenter:
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Abstract: In this talk, we consider the robust Rayleigh quotient optimization problem. Such type of problems commonly arise from Rayleigh quotient optimization with data uncertainty in the coefficient matrices. By exploiting the stationary conditions, we show that the minimizer is a solution of a nonlinear eigenvalue problem with eigenvector nonlinearity. This allows us to explain the potential divergence issue of a commonly applied simple iterative method for the robust solution. Two schemes are proposed to address this issue, including a nonlinear spectral transformation, and a reformulation of the objective nonlinear eigenvalue problems using second order conditions. Numerical examples, with applications in data sciences, are provided to demonstrate the effectiveness of our approaches.

Computing statistical solutions of hyperbolic conservation laws

Author and Presenter:
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Abstract: An open question in the field of hyperbolic conservation laws is the question of well-posedness. Recent theoretical and numerical evidence have indicated that multidimensional systems of hyperbolic conservation laws exhibit random behavior, even with deterministic initial data. We use the framework of statistical solutions to model this inherit randomness. We review the theory of statistical solutions for conservation laws.

Afterwards, we introduce a convergent numerical method for computing the statistical solution of conservation laws, and prove that it converges in the Wasserstein distance through narrow convergence for the case of scalar conservation laws. For the scalar case, we validate our theory by computing the structure functions of the Burgers equation with random initial data. We especially focus on Brownian initial data, and the measurement of the scalings of the structure functions. The results agree well with the theory, and we get the expected convergence rate. We furthermore show that we can get faster computations using Multilevel Monte-Carlo for computing the statistical solutions of scalar conservation laws.

In the case of systems of equations, we test our theory against the compressible Euler equations in two space dimensions. We check our numerical algorithm against two ill-behaved initial data, the Kelvin-Helmholtz instability and the Richtmeyer-Meshkov instability. We observe Wasserstein convergence for the two point correlation marginals.

Symplectic model order reduction

Author and Presenter:
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(Supervised by Jan S. Hesthaven (EPF Lausanne, Switzerland))

Abstract: Over the past decade, reduced basis methods have demonstrated great success in lowering the computational costs of solving elliptic and parabolic differential equations. However, model order reduction of hyperbolic problems remains a challenge. Recently, considerable attention has been paid to preserving structures and invariants in reduced basis methods, in order to enhance the stability and robustness of the reduced systems of hyperbolic systems. In the context of Hamiltonian systems, symplectic model reduction seeks to construct a reduced system that preserves the symplectic symmetry of Hamiltonian systems. Unlike the conventional model reduction routines that construct an orthogonal basis for the reduced space with respect to the Euclidean inner product, the symplectic model reduction constructs an orthogonal basis with respect to the symplectic differential form. This way, the reduced system inherits the physical meanings and properties of the original Hamiltonian system and it helps with robustness and the long-time stability of the reduced system. We propose a greedy approach for a symplectic basis generation that retains the convergence properties of conventional greedy basis generation. Furthermore, we shall discuss how the method can be generalized to reduce the computational costs of more complex problems.

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Bayesian approaches to a seismic source inversion problem

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Abstract: According to the American National Earthquake Information Center (NEIC), there is an occurrence of about 13'000 earthquakes every year, spanning different values on the Richter scale from very mild (2) to giant earthquakes (8 and above). Being able to study these earthquakes provides useful information for a wide range of applications in geophysics. In earthquake source inversion, we try to estimate certain physical parameters characterizing an earthquake rupture process. Examples of these parameters are the source location (epicenter), the spatially variable displacement across the fault surface (slip), the slip direction, duration, among others. In this poster we focus on implementing a sampling strategy using Bayesian inversion, in particular Markov Chain Monte Carlo (MCMC), in order to recover the probability distribution of the spatial location of the epicenter of an earthquake in a bounded domain. To this end, we first postulate a computational elasticity model (usually arising from the discretization of a partial differential equation) that describes the earthquake dynamics. In particular, this so called forward problem is described by the ellas-todynamic wave equitation, and is discretized using a spectral element method and efficiently implemented via the software package SPECFEM2D presented in [1]. Despite having an efficient solver for the forward problem, sampling from the posterior distribution is not a trivial task. In particular, the source term of the wave equation involves a delta functional representing the location of the source, which complicates the exploration of the posterior distribution, given that this delta functional greatly affects the shape of the likelihood. In addition, material properties of the ground are typically uncertain and as such will be treated as random parameters in the source inversion problem. We discuss possible Markov Chain Monte Carlo strategies suited for the problem at hand and eventual extensions to a multilevel framework.

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The domain decomposition method of Bank and Jimack as an optimized Schwarz method

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Abstract: In 2001, Bank and Jimack introduced a new domain decomposition algorithm for the adaptive finite element solution of elliptic partial differential equations. The novel feature of this algorithm is that the subdomain problems are defined over the entire domain, consisting of a fine grid in the area where the subdomain is responsible for an accurate solution, and a coarse grid elsewhere. A convergence analysis of this algorithm was given in 2008 by Bank and Vassilevski. We are interested here in understanding what the precise contribution of the outer coarse mesh is to the convergence behavior of the domain decomposition method proposed by Bank and Jimack. We show for a two subdomain decomposition that the outer coarse mesh can be interpreted as computing an approximation to the optimal transmission condition represented by the Dirichlet to Neumann map, and thus the method of Bank and Jimack can be viewed as an optimized Schwarz method, i.e. a Schwarz method that uses Robin or higher order transmission conditions instead of the classical Dirichlet ones. In particular, we show that when applied to the Laplace equation in one spatial dimension, the algorithm of Bank and Jimack computes an optimal Robin parameter for any choice of the outer coarse mesh, and the method thus converges in two iterations in this case. We then present more general situations, and we illustrate our results with numerical experiments.

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Risk average optimal control problem for elliptic PDEs with uncertain coefficients

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Abstract: We consider a risk averse optimal control problem for an elliptic PDE with uncertain coefficients. The control is a deterministic distributed forcing term and is determined by minimizing the expected L^2-distance between the state (solution of the PDE) and a target deterministic function. An L^2-regularization term is added to the cost functional (see e.g. [1]).

We consider a finite element discretization of the underlying PDE and derive an error estimate on the optimal control.

Concerning the approximation of the expectation in the cost functional and the practical computation of the optimal control, we analyze and compare two strategies.

In the first one, the expectation is approximated by either a Monte Carlo estimator, and a steepest descent algorithm is used to find the discrete optimal control.

The second strategy, named Stochastic Gradient (see e.g. [2, 3]) is again based on a steepest-descent type algorithm. However the expectation in the computation of the steepest descent is approximated with independent Monte Carlo estimators at each iteration using possibly a very small sample size. The sample size and possibly the mesh size in the finite element approximation could vary during the iterations. We present error estimates and complexity analysis for both strategies and compare them on few numerical test cases.

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A discrete duality finite volume method on non-convex domains

Author and Presenter:
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Abstract: We consider a diffusion problem on a polygonal domain presenting a reentrant corner and use a discrete duality finite volume method to solve it. In order to compensate for the loss of regularity of the solution near the nonsmooth part of the boundary, we introduce a refinement of the grid at the reentrant corner. This technique allows to restore the optimal order of convergence. This work is originated from a collaboration with the swiss weather prediction service MeteoSwiss, we thus restrict ourselves to a specific grid and compare two ways to refine it.

A semi-Lagrangian splitting method for the numerical simulation of sediment transport with free surface flows

Author and Presenter:
Arwa Mrad (EPF Lausanne, Switzerland)

Abstract: We present a numerical model for the simulation of 3D polydispersed sediment transport in a Newtonian flow with free surfaces. The physical model is a macroscopic model based on a concentration of sediment in water. This model couples the incompressible Navier-Stokes equations with a volume-of-fluid approach for the tracking of the free surface between water and air, and a non-linear hyperbolic equation for the evolution of the sediment concentration in water. The numerical algorithm relies on operator-splitting to decouple advection and diffusion phenomena and a two-grid method. Unstructured finite elements are used to solve the diffusion problem, while a characteristics method and a Godunov scheme are reepctively used to solve advection and hyperbolic problems on a structured grid. The numerical model is validated through numerical experiments. Simulation results are compared with experimental results in various situations. In particular, we present here the deposition of particles in a still fluid and the bedload erosion by a vertical jet.

Graph partition refinement using the graph p-Laplacian

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Abstract: A continuous formulation of the optimal 2-way graph partitioning based on the p-norm minimization of the graph Laplacian Rayleigh quotient is presented, which provides a sharp approximation to the balanced graph partitioning problem, the optimality of which is known to be NP-hard. The minimization is initialized from a cut provided by a state-of-the-art multilevel recursive bisection algorithm, and then a continuation approach reduces the p-norm from a 2-norm towards a 1-norm, employing for each value of p a feasibility-preserving steepest-descent method that converges on the p-Laplacian eigenvector. A filter favors iterates advancing towards minimum edge-cut and partition load imbalance. The simplicity and the linear complexity in edges of the steepest-descent algorithm allows highly scalable parallel implementations in both distributed multi-core CPU platforms and GPU accelerators, thus enabling the recursive bisection of large-scale graphs with up to 1.9 billion tetrahedra. The suggested approach exhibits significant improvements over both METIS and KaHIP for graphs originating from various application domains of graph partitioning, ranging from triangular Delaunay meshes to power networks. Particular emphasis is placed on the benefits of applying the p-Laplacian method on graphs emerging from social networks.

Coupling non-conforming discretizations of PDEs by spectral approximation of the Lagrange multiplier space

Author and Presenter:
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Abstract: Our work focuses on the development of a non-conforming domain decomposition method for the approximation of PDEs based on weakly imposed transmission conditions: the continuity of the global solution is enforced by a discrete number of Lagrange multipliers defined over the interfaces of adjacent subdomains. The method falls into the class of primal hybrid methods, which also include the well-known mortar method. Differently from the mortar method, we discretize the space of basis functions on the interface by spectral approximation independently of the discretization of the two adjacent domains; one of the possible choices is to approximate the interface variational space by Fourier basis functions. As we show in the numerical simulations presented in [1], our approach is well-suited for the solution of problems with non-conforming meshes or with finite element basis functions with different polynomial degrees in each subdomain. Another application of the method that still needs to be investigated is the coupling of solutions obtained from otherwise incompatible methods, such as the finite element method, the spectral element method or isogeometric analysis.

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Numerical homogenization methods for long time wave propagation in locally periodic media

Author and Presenter:
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Abstract: The approximation of the wave equation in heterogeneous media is challenging. Indeed, to be accurate, standard numerical methods require a grid that resolves the fine scale of the medium, leading to a prohibitive cost. Homogenization theory provides an effective equation that does not depend on the fine scale. Based on this equation, numerical homogenization methods approximate the effective wave at an affordable cost. However, at large timescales, the original wave exhibits a dispersive behaviour at the macroscopic scale, which is not captured by the homogenized equation.

In this talk, we introduce a family of effective equations that describe these long time effects in locally periodic media [3, 4]. Based on these effective models, we design efficient numerical homogenization methods for long time wave propagation. Furthermore, we provide a long time a priori error analysis of the finite element heterogeneous multiscale method, proposed in [1, 2], for locally periodic media.

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An efficient algorithm for Padé-type approximation of the frequency response for the Helmholtz problem

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Abstract: Given an open bounded Lipschitz domain $D \subset \mathbb{R}^d (d = 1, 2, 3)$, whose boundary is partitioned into Γ_D and Γ_N, and $f \in L^2(D)$, we consider the map $\mathcal{S} : \mathbb{C} \to H^1_{\Gamma_D}(D) = \{v \in H^1(D),\ v|_{\Gamma_D} = 0\}$, which associates a complex value z with the weak solution of the (complex) Helmholtz problem

$$\begin{aligned}&\text{find } \mathcal{S}(z) \in H^1_{\Gamma_D}(D):\\ &\langle \nabla \mathcal{S}(z), \nabla v\rangle_{L^2(D)} - z\langle \mathcal{S}(z), v\rangle_{L^2(D)} = \langle f, v\rangle_{L^2(D)} \quad \forall v \in H^1_{\Gamma_D}(D).\end{aligned}$$

Several results (see e.g. [1]) show that $\mathcal{S}$ is well-defined and meromorphic in $\mathbb{C}\backslash\Lambda, \Lambda = \{\lambda_\alpha\}_{\alpha=1}^{\infty}$ being the (countable, unbounded) set of (real, non-negative) eigenvalues of the Laplace operator (restricted to $H^1_{\Gamma_D}(D)$, with homogeneous Neumann boundary conditions on Γ_N). In particular, it holds

$$\mathcal{S}(z) = \sum_{\alpha=1}^{\infty} \frac{s_\alpha}{\lambda_\alpha - z},$$

where the elements of $\{s_\alpha\}_{\alpha=1}^{\infty} \subset H^1_{\Gamma_D}(D)$ are pair-wise orthogonal with respect to the $H^1_{\Gamma_D}(D)$ inner product and the equality in (1) has to be understood with respect to the $H^1_{\Gamma_D}(D)$ norm.

It is possible to define a Padé-type approximant of any map (1) around $z_0 \in \mathbb{C}$: given $M, N \in \mathbb{N}$, the exact map is approximated by a rational map $\mathcal{S}_{[M/N]}$: $\mathbb{C}\backslash\Lambda \to H^1_{\Gamma_D}(D)$ of the form

$$\mathcal{S}_{[M/N]}(z) = \frac{\mathcal{P}_{[M/N]}(z)}{\mathcal{Q}_{[M/N]}(z)} = \frac{\sum_{j=0}^{M} P_j (z - z_0)^j}{\sum_{i=0}^{N} Q_i (z - z_0)^i},$$

with $\{P_j\}_{j=0}^{M} \subset H^1_{\Gamma_D}(D)$ and $\{Q_i\}_{i=0}^{N} \subset \mathbb{C}$.

In [1] the authors define such approximant within a Least-Squares framework, through the minimization of a suitable functional which involves $E' \geq M + N$ derivatives of $\mathcal{S}$ in z_0. This poster introduces a new definition, which relies on a simplified version of the functional, and only requires $E \geq M$ derivatives of the solution map. As such, starting from the same amount of information on $\mathcal{S}$, it is possible to find a higher order - hence more accurate - approximant.

In particular, the denominator $\mathcal{Q}_{[M/N]}$ is the minimizer (under some normalization constraints) of the $H^1_{\Gamma_D}(D)$ norm of the E-th Taylor coefficient of $Q\mathcal{S}$, as Q varies in the space of polynomials with degree $\leq N$. The numerator is then computed by matching as many terms as possible of the Taylor series of $\mathcal{S}$ with those of $\mathcal{S}_{[M/N]}$, analogously to the classical Padé approach.

The resulting approximant is shown to converge, as $M+N$ goes to infinity, to the exact map $\mathcal{S}$ in the $H^1_{\Gamma_D}(D)$ norm within $B_N \backslash \Lambda$, B_N being an open disk centered at z_0 whose boundary includes the $(N+1)$-th element of Λ closer to z_0. Moreover, it is proven that the roots of the denominator $\mathcal{Q}_{[M/N]}$ converge exponentially (as M goes to infinity) to the N elements of Λ closer to z_0.

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Low-rank Riemannian optimization for high-dimensional eigenvalue problems

Author and Presenter:
Maxim Rakhuba (ETH Zurich, Switzerland)

Abstract: In this work we focus on a solution of symmetric eigenvalue problems with eigenvectors that admit a low-rank representation in the Tensor Train format. The straightforward extension of iterative methods, e.g. locally-optimal block preconditioned conjugate gradient method (LOBPCG), leads to the instability and/or to the rank growth. Alternatively one can solve an eigenvalue problem as an optimization procedure, which is time-consuming when a large number of eigenvectors is to be found. We present a new solver which is based on the Riemannian optimization approach and which is capable of computing hundreds of eigenstates in high dimensions. The solver is implemented using TensorFlow software library and hence allows for a natural GPU parallelization. We showcase our method by calculating up to 100 eigenvalues and eigenvectors of a realistic Hamiltonian.

A priori and a posteriori analysis of a local scheme for elliptic equations

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Abstract: We consider a new local finite element scheme for convection-diffusion-reaction problems and present a priori and a posteriori error analysis of the method. The algorithm is based on a coarse solution in the whole domain, it proceeds by refining the mesh where the error is estimated to be large and improves the solution by solving local elliptic problems with artificial boundary conditions. The a priori analysis is performed in the Gradient Discretization framework under minimal regularity assumptions [1]. Convergence for linear and semi linear problems is established. The a posteriori error estimators [2] allow to select the local domains and provide bounds that are robust in singularly perturbed regimes.

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Modelling of a biphasic fluid for a 3D aluminium reduction cell

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Abstract: Metallic aluminium is produced by the Hall Heroult process [1], which involves the electrolysis of dissolved aluminium oxyde Al_2O_3 in an electrolytic bath composed mostly of cryolite. The aluminium liquid generated by various chemical reactions is dragged down by gravity, while important electromagnetic forces are agitating the liquid. At the boundary of the upper part of the cell, the anode, CO_2 is produced and forms millimetric bubbles which escape towards the upper free surface of the bath. Our work focuses in the modelling of this CO_2, and how the presence of this gas impacts the liquid flow. Considering a one-pressure model and an incompressible gas, we establish, following [2, 3], from mass and momentum conservation, a mathematical system, the different unknowns being: the velocity of the bath mixture (in which the gas is diffused), the pressure, the velocity of the gas, and the average density. A particular attention is given to the mass transport of the gas. The discretization is performed using piecewise linear finite elements on tetrahedrons. Preliminar results will be presented.

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Connecting geodesics for the Stiefel manifold

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Abstract: Several applications in optimization, image and signal processing deal with data that belong to the Stiefel manifold $\mathrm{St}(n,p)$, that is, the set of $n \times p$ matrices with orthonormal columns. Some applications, for example, the computation of the Karcher mean, require evaluating the geodesic distance between two arbitrary points on $\mathrm{St}(n,p)$. This can be done by explicitly constructing the geodesic connecting these two points.

An existing method for nding geodesics is the leapfrog algorithm introduced by J.L. Noakes, which enjoys global convergence properties. We reinterpret this algorithm as a nonlinear block Gauss-Seidel process and propose a new convergence proof based on this framework for the case of $\mathrm{St}(n,p)$.

Parallel HPC solution of the Helmholtz equation with controllability methods

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Abstract: The exact controllability approach [1, 2] reformulates the Helmholtz equation in the time domain and seeks the time-harmonic solution of the corresponding wave equation by iteratively minimizing an appropriate penalty functional. Then each conjugate gradient iteration solely relies on standard numerical algorithms, which are inherently parallel and robust against higher frequencies. In [3], new penalty functionals were introduced which extend the controllability approach to general boundary value problem governed by the Helmholtz equation. Here, we study the parallel performance of controllability methods using FreeFem++ [4, 5] on massively parallel HPC architectures for large-scale Helmholtz problems.

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Multilevel optimized Schwarz methods

Author and Presenter:
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Abstract: Optimized Schwarz methods (OSMs) are non overlapping domain-decomposition methods based on enhanced transmission conditions which are optimized in order to accelerate the convergence. We present a multilevel optimized Schwarz method where the transmission conditions are tuned not to improve the convergence behavior but instead the smoothing property of the iterative scheme. Numerical results show the effectiveness of our approach both compared to the one-level OSM and the multigrid scheme.

Dynamical low rank approximation of random time dependent PDEs

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Abstract: Partial differential equations with random coefficients and input data arise in many real world applications. What they often have in common is that the data describing the PDE model are subject to uncertainties either due to a lack of knowledge of the system or to its inherent variability. The numerical approximation of statistics of this random solution poses several challenges, in particular when the number of random parameters is large and/or the parameter-to-solution map is complex. Therefore, effective surrogate or reduced models are of great need.

We consider a class of time dependent PDEs with random parameters and search for an approximate solution in a separable form, i.e. at each time instant expressed as a linear combination of linearly independent spatial functions multiplied by linearly independent random variables (low rank approximation) in the spirit of a truncated Karhunen-Loève expansion. Since the optimal deterministic and stochastic modes can significantly change over time, static versions, such as proper orthogonal decomposition or polynomial chaos expansion, may lose their effectiveness. Instead, here we consider a dynamical approach in which those modes are computed on-the-fly as solutions of suitable auxiliary evolution equations. From a geometric point of view, this approach corresponds to constraining the original dynamics to the manifold of fixed rank functions. The original equations are projected onto the tangent space of this manifold along the approximate trajectory.

In this poster we recall the construction of the method introduced in [2] and give some implementation details. The spatial discretization is carried out by the finite element method and the discretization of the random variables relies on an adaptive choice of sparse grid. We will present some numerical test cases including the heat equation with a random diffusion coefficient and initial condition [1].

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Non-intrusive reduced-order modeling of combustor flow

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Abstract: A non-intrusive reduced basis method is proposed for the quasi-1D continuous variable resonance combustor (CVRC) flow, which is a typical complex non-linear time-dependent problem. The reduced basis from a collection of high-fidelity solutions is extracted via proper orthogonal decomposition (POD). The coefficients of reduced basis are approximated by artificial neural networks (ANNs). The offline stage consists of the generation of reduced basis and the training of ANNs, while the online stage only perform evaluation of the reduced basis coefficients via the ANNs. Therefore, the proposed reduced basis method is efficient. Numerical results demonstrate that, the proposed method can recover unsteady solution of the CVRC flow with physical parametrization accurately and efficiently.

Scalable parallel BEM solvers on many-core clusters

Author and Presenter:
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Abstract: Our aim is to solve large scale problems discretized by the boundary element method. To this end, we propose to use parallel computers equipped with graphics processing units to assemble and solve the linear systems involved in the discretization. Depending on the application case, we either assemble the full dense system matrix (in parallel) or we compress the matrix by hierarchical matrices with adaptive cross approximation. In either case, Krylov subspace solvers are applied to solve the linear system. Our multi-GPU parallel implementation is achieved by porting a sequential CPU BEM code to GPUs and by applying a multi-GPU library for generic Krylov subspace solvers ([1, 3]) and a GPU-based hierarchical matrix library ([2]). In our presentation, we will give details on the parallel implementation and we will show our latest parallel performance benchmarks.

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