Contents

About

Sparse Grids and Applications Seminar 2024

This is the book of abstracts and timetable for the seminar on Sparse Grids and Applications 2024. The seminar is held on September 11th and September 12th of 2024 at the Institute for Numerical Simulation (Friedrich-Hirzebruch-Allee 7, 53115 Bonn) of the University of Bonn, Germany.

Sparse grids have gained increasing interest in recent years for the numerical treatment of high-dimensional problems. Where classical numerical discretization schemes fail in more than three or four dimensions, sparse grids allow to overcome the curse of dimensionality to some extent - extending the number of dimensions that can be dealt with.

Organizing committee

Bastian Bohn	University of Bonn
Jochen Garcke	University of Bonn & Fraunhofer SCAI

List of Speakers

Naya Baslan	Robert Bosch GmbH, Stuttgart
Ivana Jovanovic Buha	Technical University of Munich
Tucker Carrington	Queen’s University, Kingston
Dinh Dũng	Vietnam National University, Hanoi
Ionut Farcas	University of Texas, Austin
Bernd Käßemodel	Chemnitz University of Technology
Rüdiger Kempf	University of Bayreuth
Guanglian Li	The University of Hong Kong
Kateryna Pozharska	Chemnitz University of Technology
Kislaya Ravi	Technical University of Munich
Andrea Scaglioni	Vienna University of Technology
Riccarda Scherner-Grießhammer	University of Erlangen-Nürnberg
Uta Seidler	University of Bonn
Laura Weidensager	Chemnitz University of Technology
Andreas Zeiser	University of Applied Sciences for Engineering and Economics, Berlin

Useful Information

Talks

Talks will be held at the seminar room 2.035 at the Institute for Numerical Simulation (INS) at **Friedrich-Hirzebruch-Allee 7, 53115 Bonn**. It is situated on the second floor.

For each contributed talk (marked by CT in the timetable) we reserved a **30 minutes slot**, which is intended to cover a **25 minutes talk + 5 minutes discussion**.

We are glad to announce that this year's SGA **invited speakers**

- Tucker Carrington
- Ionut Farcas
- Kateryna Pozharska

agreed to give their talk at the seminar instead. For these talks (marked by IS in the timetable) we reserved a **45 minutes slot**, i.e. **40 minutes talk + 5 minutes discussion**.

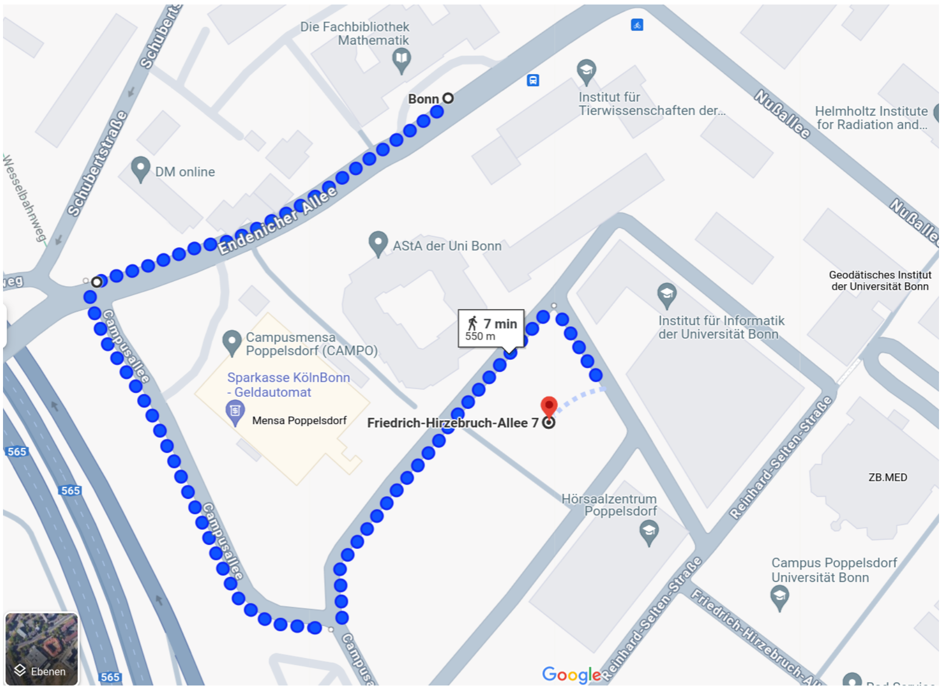
We will offer **coffee** and **tea** during the breaks.

Eduroam Wi-Fi will be available during the seminar (`https://eduroam.org/`).

How to get to the INS?

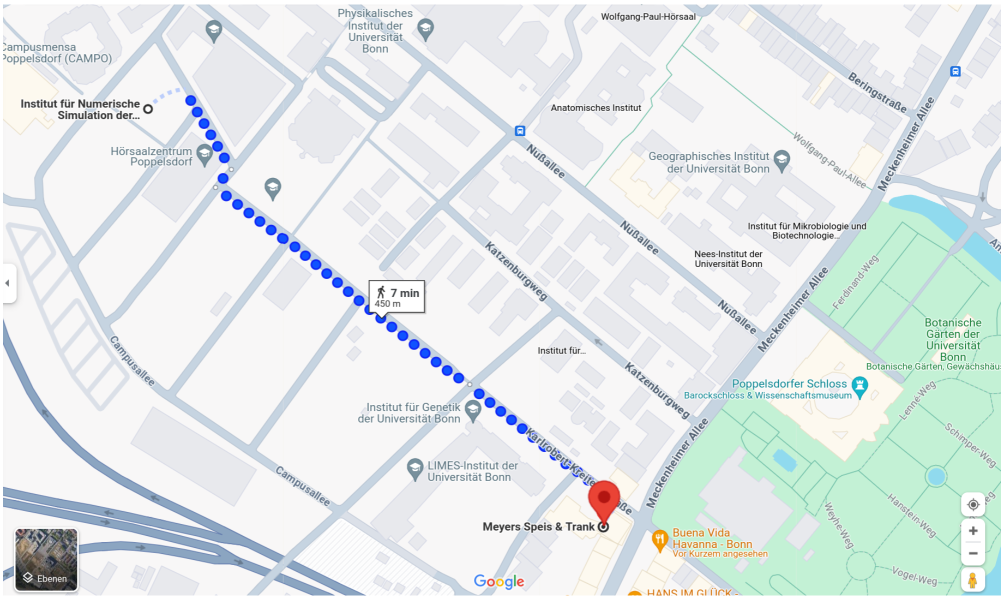
The INS building is located on the university campus in Bonn Poppelsdorf at Friedrich-Hirzebruch-Allee 7 and can be reached by:

- **Plane:** arrival at Flughafen Cologne/Bonn. Then take Bus SB60 to Bonn central station (runs about every 30 minutes, 35-minute ride). From there take one of the bus lines 604, 605, 606, 607 to Kaufmannstraße.
- **Train:** travel to Bonn central station and take one of the bus lines 604, 605, 606, 607 to Kaufmannstraße,
- **Bus:** lines 604, 605, 606, 607 stopping at Kaufmannstraße.
- **Foot:** From bus stop Kaufmannstraße it is a short walk to the INS:



Dinner

We will have an informal **dinner on Wednesday, September 11th**. We reserved tables for **7 p.m.** at ***Meyers Speis & Trank*** (Clemens-August-Straße 2-4), which is located just 450m from the INS building, where the seminar takes place. Please note that everyone is responsible for paying for their own food and drinks.



Timetable

Wednesday, 11th of September, 2024

14:00–14:15	**Welcome**		
14:15–14:45	CT	**Andrea Scaglioni** Vienna, Austria	Sparse grid approximation of nonlinear SPDEs: The Landau–Lifshitz–Gilbert equation
14:45–15:15	CT	**Kislaya Ravi** Munich, Germany	Dimension adaptive Multi-fidelity Polynomial Chaos Expansion using Leja points
15:15–15:45	CT	**Ivana Jovanovic Buha** Munich, Germany	Efficient Uncertainty Quantification and Global Sensitivity Analysis of Time-dependent outputs in Hydrology Modeling
15:45–16:15	**Coffee break**		
16:15–17:00	IS	**Kateryna Pozharska** Chemnitz, Germany	Sampling recovery in the uniform norm and sampling projections
17:00–17:30	CT	**Bernd Käßemodel** Chemnitz, Germany	Quantum information-based complexity
17:30–18:00	CT	**Dinh Dung** Hanoi, Vietnam	Gaussian-weighted numerical integration in Sobolev spaces of mixed smoothness
19:00–21:00	**Informal dinner at *Meyer's Speis & Trank***		

Thursday, 12th of September, 2024

09:15–09:45	CT	**Naya Baslan** Stuttgart, Germany	Adaptive Sparse Grids Kriging: An Active Learning Framework for Reliability Analysis and Rare Event Estimation
09:45–10:15	CT	**Guanglian Li** Hong Kong, Hong Kong	On Sparse Grid Interpolation for American Option Pricing with Multiple Underlying Assets
10:15–10:45	CT	**Andreas Zeiser** Berlin, Germany	Sparse Grid Time-Discontinuous Galerkin Method with Streamline Diffusion for Transport Equations
10:45–11:15	**Coffee break**		
11:15–12:00	IS	**Tucker Carrington** Kingston, Canada	Solving the vibrational Schrödinger equation using a sparse gird collocation method with more points than basis functions: obviating integrals
12:00–12:30	CT	**Uta Seidler** Bonn, Germany	Adaptive Sparse Grid Techniques for Stochastic Elliptic PDEs in Uncertainty Quantification
12:30–13:00	CT	**Riccarda Scherner-Grießhammer** Erlangen, Germany	Hybrid Parallelization of a Solver for PDEs with Variable Coefficients on Locally Adaptive Sparse Grids
13:00–14:30	**Lunch break**		
14:30–15:00	CT	**Laura Weidensager** Chemnitz, Germany	High-Dimensional Approximation Using ANOVA-Boosting
15:00–15:30	CT	**Rüdiger Kempf** Bayreuth, Germany	High-Dimensional Approximation on Sparse Grids by Tensorized Moving Least-Squares
15:30–16:00	IS	**Ionut Farcas** Austin, USA	Structure-exploiting sparse grid approximations for efficient uncertainty quantification and surrogate model construction
16:00-16:10	**Concluding remarks**		

List of Abstracts – Talks

Wednesday 11th

14:15 - 14:45

Sparse grid approximation of nonlinear SPDEs: The Landau–Lifshitz–Gilbert equation

***X. An*[1], *J. Dick*[2], *M. Feischl*[3], *A. Scaglioni*[3], *T. Tran*[2]**

[1] NSW Cancer Council, Sydney, Australia
[2] University of New South Wales, Sydney, Australia
[3] Vienna University of Technology, Austria

We consider the Stochastic Landau–Lifshitz–Gilbert (SLLG) problem as an example of nonlinear, time-dependent stochastic PDE (SPDE) driven by Gaussian noise. Beyond being a popular model for magnetic materials immersed in heat baths, the forward uncertainty quantification (UQ) task poses several interesting challenges that did not appear simultaneously in previous works: The equation is strongly nonlinear, time-dependent, and has a non-convex side constraint. We first use the Doss-Sussmann transform to reduce the SPDE to a random coefficient PDE. We then parametrize the Wiener process using the Lévy-Ciesielski construction to obtain a parametric coefficient PDE. We study the regularity and sparsity properties of the parameter-to-solution map, which features countably many unbounded parameters and low regularity compared to other elliptic and parabolic model problems in UQ. We use a novel technique to establish uniform holomorphic regularity of the parameter-to-solution map based on a Gronwall-type estimate combined with previously known methods that employ the implicit function theorem. This regularity result is used to design a piecewise-polynomial sparse grid approximation through a profit maximization approach. We prove algebraic dimension-independent convergence and validate the result with numerical experiments. If time allows, we discuss the finite element discretization and multi-level approximation. A detailed exposition can be found in [1].

References

[1] An, X. and Dick, J. and Feischl, M. and Scaglioni, A. and Tran, T. - Sparse grid approximation of stochastic parabolic PDEs: The Landau–Lifshitz–Gilbert equation (2024). ArXiv preprint.

14:45 - 15:15

Dimension adaptive Multi-fidelity Polynomial Chaos Expansion using Leja points

K. Ravi[1]***, T. Neckel***[1]***, H.-J. Bungartz***[1]

[1] Technical University of Munich, Germany

The high computational demands of models pose a significant challenge for conducting forward uncertainty quantification (UQ) analyses. We employ multi-fidelity modeling within the forward UQ framework to address this issue. We extract statistical moments from the highest fidelity model using minimal computational resources by integrating information from different fidelity levels. We leverage polynomial chaos expansion (PCE) to compute these statistical moments. We use a low-fidelity and discrepancy function to construct the PCE [1]. The discrepancy function represents the transformation applied to the low-fidelity model to convert it into a high-fidelity model, modeled as a linear combination of an additive and multiplicative term. This transformation is applied recursively at each level to derive the PCE of the highest fidelity model. We employ a sparse combination technique [2] to merge polynomials of different orders and adaptively select model evaluation points based on variance surplus [3, 4]. Additionally, we utilize Leja grid points to reduce the number of model evaluations further. Through various examples, we demonstrate the efficiency of our proposed method in obtaining statistical moments.

References

[1] Eldred, M. and Ng., L. and Barone, M. and Domino, S. - Multifidelity Uncertainty Quantification Using Spectral Stochastic Discrepancy Models (2015). Sandia National Lab.(SNL-NM), Albuquerque, NM (United States).
[2] Griebel, M. and Schneider, M. and Zenger, C. - A combination technique for the solution of sparse grid problems (1990), Citeseer.
[3] Conrad, P. and Marzouk, Y. - Adaptive Smolyak pseudospectral approximations (2013). SIAM Journal on Scientific Computing, 35(6):A2643–A2670.
[4] Farcas, I.-G. and Görler, T. and Bungartz, H.-J. and Jenko, F. and Neckel, T. - Sensitivity-driven adaptive sparse stochastic approximations in plasma microinstability analysis (2020). Journal of Computational Physics, 410:109394.

15:15 - 15:45

Efficient Uncertainty Quantification and Global Sensitivity Analysis of Time-dependent outputs in Hydrology Modeling

I. Jovanovic Buha[1], ***M. Obersteiner***[1]

Chair of Scientific Computing, TUM School of Computation, Information and Technology, Technical University of Munich, Germany

Hydrology models, which conceptualize complex, spatially distributed processes, inevitably result in non-unique input-output relationships and significant predictive uncertainties. The reliable assessment of these uncertainties is crucial for models simulating real-world problems. In this study, we explore computationally efficient methods for Forward Uncertainty Quantification (FUQ) and Global variance-based Sensitivity Analysis (SA) of hydrology models that produce time-dependent quantities of interest (QoI). We utilize a polynomial chaos expansion (PCE) surrogate model, combined with non-intrusive pseudo-spectral projection (PSP) and sparse grid (SG) strategies, to explicitly express uncertainty evolution and conduct SA while keeping the necessary model runs small. To maintain the combination technique's black-box property while focusing on regions of interest adaptively, we rely on a recently proposed spatially adaptive SG combination technique with a dimension-wise refinement algorithm [1]. The particular focus of our work is on how to combine time-dependent QoIs with adaptive SG. Traditional approaches for FUQ and SA treat each model output at individual time steps as separate QoIs. Still, this approach neglects the dynamic nature of the response and can substantially increase computational demands, especially if adaptivity is performed independently for each time step. To address this, we further integrate the Karhunen–Loève (KL) expansion model as an intermediate surrogate to capture the system dynamics, as recently proposed in [2]. Coefficients of the truncated KL-based model are treated as separate QoIs, with a single PCE model computed for each using an adaptive SG strategy. We expect that this approach can efficiently identify key uncertain parameters and their interactions that drive the dynamic behavior of hydrology models. Our work aims to bridge the gap between theoretical advancements in UQ and Adaptive SG and their practical application in real-world scenarios.

References

[1] Obersteiner, M. and Bungartz, H.-J. - A generalized spatially adaptive sparse grid combination technique with dimension-wise refinement (2021). SIAM Journal on Scientific Computing, 43(4):A2381–A2403.

[2] Alexanderian, A. and Gremaud, P. and Smith, C. - Variance-based sensitivity analysis for time-dependent processes (2020). Reliability Engineering and System Safety, 196.

16:15 - 17:00

Sampling recovery in the uniform norm and sampling projections

K. Pozharska[1,2]

IS

[1] Institute of Mathematics of the NAS of Ukraine, Ukraine
[2] Faculty of Mathematics, Chemnitz University of Technology, Germany

In the talk, we will give an overview of the problem of optimal recovery of functions from their samples and conditions under which linear sampling algorithms are optimal among all (possibly non-linear) algorithms.

The main emphasis will be made on the uniform recovery of bounded complex-valued functions. Besides, we will show how to lift L_2-error bounds to error bounds in general semi-normed spaces G using the spectral function.

We will also discuss a new sharp bound for the norms of sampling projections onto arbitrary n-dimensional subspaces of the space of bounded functions. The result is based on a specific type of discretization of the uniform norm, connected to the Marcinkiewicz-Zygmund inequalities.

17:00 - 17:30

Quantum information-based complexity

B. Käßemodel

Chemnitz University of Technology, Germany

We start with a short introduction to the concepts of quantum algorithms. Based on this, we study quantum information-based complexity of numerical problems (in the sense of S. Heinrich and E. Novak) such as integration and approximation of functions from a given function class, in particular functions with mixed smoothness.

17:30 - 18:00

Gaussian-weighted numerical integration in Sobolev spaces of mixed smoothness

D. Dũng

Vietnam National University, Hanoi, Vietnam

We investigated optimal Gaussian-weighted numerical integration for functions on $\mathbb{R}^d$ in the Sobolev space $W_p^r(\mathbb{R}^d;\gamma)$ of mixed smoothness $r \in \mathbb{N}$, defined in the Gaussian-weighted p-integral norm, where $1 \le p < \infty$ and γ is the standard Gaussian measure. In the high-dimensional case $(d > 1)$, we proved the right convergence rate of optimal quadrature for $1 < p < \infty$ and upper bound of optimal quadrature for $p = 1$. In the one-dimensional case $(d = 1)$, we obtained the right convergence rate of optimal quadrature for $1 \le p < \infty$. We constructed completely different algorithms for the cases $1 < p < \infty$ and $p = 1$ based on new sparse grids, which realize the optimal optimal rate in the case $1 < p < \infty$ and the upper bound in the case $p = 1$, respectively.

This talk is based on the papers [1] and [2].

References

[1] Dũng, D. - Numerical weighted integration of functions having mixed smoothness (2023). Journal of Complexity, 78:101757.

[2] Dũng, D. and Nguyen, V. - Optimal numerical integration and approximation of functions on $\mathbb{R}^d$ equipped with Gaussian measure (2024). IMA Journal of Numerical Analysis, 44:1242–1267.

Thursday 22nd

09:15 - 09:45

Adaptive Sparse Grids Kriging: An Active Learning Framework for Reliability Analysis and Rare Event Estimation

N. Baslan[1,2], ***J. Schmidt***[1], ***A. Kerschl***[1], ***D. Pflüger***[2]

[1] Robert Bosch GmbH, Stuttgart, Germany
[2] University of Stuttgart, Germany

In this talk, we present our active-learning-based reliability analysis framework, which we utilise for rare event estimation and testing automated driving systems. A Gaussian Process, enhanced by incorporating an adaptive Sparse Grid discretizaion, is developed and used as a surrogate model in a search-based testing approach [1]. The objective is to enhance the technology employed in the assessment of the safety of automated driving systems. The primary goal is to evaluate the probability of system failure in the system under test. To achieve this, a variety of scenarios are parameterised, and the system's performance is assessed under different conditions. A significant challenge faced by automated driving systems is the infrequent occurrence of critical cases. Despite occurring only rarely, these critical scenarios are potentially very dangerous and can lead to accidents or hazardous situations, particularly when driving in normal conditions over extended periods. Consequently, it is crucial to utilize specialized techniques to effectively estimate rare events and allocate computational resources accordingly. The proposed approach implements a two-stage surrogate modeling technique. In the initial stage, the open-source SG^{++} toolbox [2] is used to generate an initial Sparse Grid with B-spline boundary basis functions. Following that, an iterative refinement algorithm is implemented to identify and refine informative grid points in proximity to the limit state function. In this context, the limit state function is defined as the boundary between the fail and pass cases, incorporating critical events. The refinement process enhances the precision of the B-Spline meta-model in the aforementioned regions of interest. In the second stage, the Sparse Grid meta-model is introduced as a prior mean term in the Gaussian Process. Furthermore, active learning is implemented to direct the algorithm towards enhancing the confidence measure surrounding the limit state function. The results demonstrate that the surrogate model outperforms the commonly used zero-mean Gaussian process. We use benchmark experiments to compare our method to existing methods in the literature, such as the PC-Kriging surrogate model used in reliability analysis [3]. Furthermore, we present the application of our framework to the safety assessment of an automated driving system. We utilise the OpenScenario industrial standard to define driving scenarios and use our algorithm for testing and parameter variation in order to identify critical cases. In conclusion, our framework contributes to the safety assessment of highly automated and autonomous driving vehicles in accordance with safety standards.

References

[1] Baslan, N. and Schmidt, J. and Kerschl, A. and Pflüger, D. - Towards reliable automated driving systems: Surrogate modeling using sparse grids and Gaussian processes (2023). In: P. Langley - 5th International Conference on UQ in Computational Sciences and Engineering, Athens, Greece. Institute of Structural Analysis and Antiseismic Research National Technical University of Athens.
[2] Pflüger, D. and others - SG++ – Software for Spatially Adaptive Sparse Grids. `http://sgpp.sparsegrids.org`.
[3] Schöbi, R. - Surrogate models for uncertainty quantification in the context of imprecise probability modelling (2017). PhD Thesis. ETH Zürich, Switzerland. `https://api.semanticscholar.org/CorpusID:54959341`.

09:45 - 10:15

On Sparse Grid Interpolation for American Option Pricing with Multiple Underlying Assets

Li, G.

The University of Hong Kong, Hong Kong

In this work, we develop a novel efficient quadrature and sparse grid based polynomial interpolation method to price American options with multiple underlying assets. The approach is based on first formulating the pricing of American options using dynamic programming, and then employing static sparse grids to interpolate the continuation value function at each time step. To achieve high efficiency, we first transform the domain from $\mathbb{R}^d$ to $(-1,1)^d$ via a scaled tanh map, and then remove the boundary singularity of the resulting multivariate function over $(-1,1)^d$ by a bubble function and simultaneously, to significantly reduce the number of interpolation points. We rigorously establish that with a proper choice of the bubble function, the resulting function has bounded mixed derivatives up to a certain order, which provides theoretical underpinnings for the use of sparse grids. Numerical experiments for American arithmetic and geometric basket put options with the number of underlying assets up to 16 are presented to validate the effectiveness of our approach. This is a joint work with my PhD student Miss Jiefei Yang.

10:15 - 10:45

Sparse Grid Time-Discontinuous Galerkin Method with Streamline Diffusion for Transport Equations

A. Zeiser

Faculty 1: School of Engineering – Energy and Information, HTW Berlin – University of Applied Sciences, Berlin, Germany

High-dimensional transport equations frequently occur in science and engineering. Computing their numerical solution, however, is challenging due to its high dimensionality. In [1] we develop an algorithm to efficiently solve the transport equation in moderately complex geometrical domains using a Galerkin method stabilized by streamline diffusion. The ansatz spaces are a tensor product of a sparse grid in space and discontinuous piecewise polynomials in time. Here, the sparse grid is constructed upon nested multilevel finite element spaces to provide geometric flexibility. This results in an implicit time-stepping scheme which we prove to be stable and convergent. If the solution has additional mixed regularity, the convergence of a 2d-dimensional problem equals that of a d-dimensional one up to logarithmic factors. For the implementation, we rely on the representation of sparse grids as a sum of anisotropic full grid spaces. This enables us to store the functions and to carry out the computations on a sequence regular full grids exploiting the tensor product structure of the ansatz spaces. In this way existing finite element libraries and GPU acceleration can be used. The combination technique is used as a preconditioner for an iterative scheme to solve the transport equation on the sequence of time strips. Numerical tests show that the method works well for problems in up to six dimensions. Finally, the method is also used as a building block to solve nonlinear Vlasov-Poisson equations.

References

[1] Zeiser, A. - Sparse Grid Time-Discontinuous Galerkin Method with Streamline Diffusion for Transport Equations (2023). Partial Differential Equations and Applications, 4(4):2662–2971.

11:15 - 12:00

Solving the vibrational Schrödinger equation using a sparse gird collocation method with more points than basis functions: obviating integrals

R. Wodraszka[1]***, J. Simmons***[1]***, T. Carrington***[1]

IS

Queen's University, Kingston, Canada

To use quantum mechanics to study the motion of nuclei in a molecule or a reacting system one must solve a Schrödinger equation. It is a high-dimensional equation because each nucleus moves in 3-D space. If there are N nuclei, the dimensionality of the equation is $3N$. Problems of molecular quantum dynamics are therefore well-suited to sparse grid methods. To discretize the Schrödinger equation, one represents its solutions, called wavefunctions, as a linear combination of basis functions. The best univariate basis functions are not the commonly used piece-wise linear "hat" functions, but polynomials. The appropriate polynomials depend on the choice of the coordinates used to specify the positions of the nuclei. The choice of the basis functions is motivated by the physics of the problem. The polynomial univariate functions are combined using the sparse grid recipe to make a "sparse basis". The underlying structure of the sparse basis is critical for efficiently evaluating the matrix-vector products required to use a Krylov method to solve the linear algebra problem obtained by discretizing the Schrödinger equation. The sparse basis used in most of our calculations is a pruned tensor product basis. For a 12-D problem, it is orders of magnitude smaller than the tensor product basis from which it is extracted. If one uses a Galerkin approach, it is not enough to have a sparse basis because matrix elements required to build the discretized problem are themselves high-dimensional integrals. A sparse grid is also required. One option is to compute the matrix elements with a sparse grid (Smolyak) quadrature. In this talk, I concentrate instead on collocation methods. They require computing matrix-vector products with, $\mathbf{B}$, the matrix whose elements are (multi-dimensional) basis functions evaluated at points (in a high-dimensional space) and with $\mathbf{B}^{-1}$. It is well known that, if the univariate basis functions are "hat" functions, these matrix-vector products can be evaluated efficiently by using what is known as the unidirectional principle. The matrix-vector products can *also* be efficiently evaluated with *any* (e.g. non-"hat") univariate basis functions. Collocation methods obviate all the integrals required when using a Galerkin approach. In this talk, I present a collocation method with more points than basis functions, that systematically approaches Galerkin accuracy. This means using rectangular matrices. Excellent results are obtained for molecules with as many as six atoms without any need to optimize points.

12:00 - 12:30

Adaptive Sparse Grid Techniques for Stochastic Elliptic PDEs in Uncertainty Quantification

U. Seidler[1], ***M. Griebel***[1,2]

[1] Institute for Numerical Simulation, University of Bonn, Germany,
[2] Fraunhofer Institute for Algorithms and Scientific Computing SCAI

In this talk, we present an adaptive sparse grid approach for forward problems in uncertainty quantification, particularly focusing on the computation of quantities of interests for stochastic elliptic PDEs. The approximation of the equivalent parametric problem requires a restriction of the countably infinite dimensional parameter space to a finite-dimensional parameter set, a spatial discretization and an approximation in the parametric variables.

Our approach uses a sparse grid method between these three approximation directions, employing a dimension-adaptive combination technique that balances computational effort with accuracy based on the benefit-cost ratio. For the high-dimensional parametric approximation on its own, we also make use of a sparse grid structure which is simultaneously detected. By this approach the anisotropy in the parametric variables can be detected and exploited as the algorithm adjusts to it.

We further extend our method to incorporate adaptive spatial discretizations. Instead of relying on predefined uniform finite element meshes, our sparse grid approach uses spatial approximation spaces that are constructed based on an error estimator. This enables the algorithm to adjust to geometric singularities within the spatial domain. Numerical examples demonstrate the algorithm's performances for both uniform and adaptive spatial approximations.

12:30 - 13:00

Hybrid Parallelization of a Solver for PDEs with Variable Coefficients on Locally Adaptive Sparse Grids

R. Scherner-Grießhammer[1], ***C. Pflaum***[1]

[1] Department of Computer Science, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany

Elliptic partial differential equations with variable coefficients can be discretized using prewavelets on locally adaptive sparse grids. With prewavelets being L^2-orthogonal, one can apply the Ritz-Galerkin discretization, resulting in a linear equation system with $O(N(\log N)^{d-1})$ or fewer unknowns in the case of adaptivity.

An algorithm for the corresponding matrix-vector multiplication based on [1] is applied to locally adaptive sparse grids, see [2]. These grids are constructed by local tensor product grids to generate adaptivity while maintaining a local unidirectional approach. The numerical computation of the underlying bilinear form requires the use of so-called hanging nodes.

In order to optimize the performance of the underlying C++ Finite-Element Library ExPDESG (Expression Templates for Partial Differential Equations on Sparse Grids), a hybrid parallelization strategy is employed, which utilizes both shared memory (OpenMP) and distributed memory (MPI) parallelization. This hybrid approach makes use of 2^d independent cases of prolongations and restrictions, allowing parallelization via MPI. Additionally, it utilizes a cell-based computation of local stiffness matrices, which enables the distribution of local stiffness matrices via OpenMP. Numerical quadrature must be applied to compute the entries of the local stiffness matrices.

The system is solved by the conjugate-gradient method with a simple diagonal Jacobi preconditioner being applied. As the entries of the preconditioner are also dependent on variable coefficients, they must be computed by numerical quadrature. This leads to a further need for parallelization.

The parallelizations described above were carried out on the parallel CPU cluster Fritz provided by the Erlangen National High Performance Computing Center [3]. We present numerical results, demonstrating the convergence of the underlying discretization and the boundedness of the condition number of the stiffness matrix.

References

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[2] Scherner-Grießhammer, R. and Pflaum, C. - Discretization of PDEs with variable coefficients using locally adaptive sparse grids (2017). PAMM, 23(4):e202300076.
[3] NHR@FAU - Fritz Cluster. `https://doc.nhr.fau.de/clusters/fritz/`.

14:30 - 15:00

High-Dimensional Approximation Using ANOVA-Boosting

L. Weidensager

Chemnitz University of Technology, Germany

We study the problem of scattered-data approximation, where we have given sample points and the corresponding function evaluations. We use the classical analysis of variance (ANOVA) decomposition for approximating high-dimensional functions having only low dimensional variable interactions. In the case for dependent input variables, the ANOVA decomposition is generalized, such that the orthogonality conditions between the terms are softened to hierarchical orthogonality conditions. We propose interpretable algorithms with the aim to detect the structure of the function, i.e. to find which input variables and variable interactions are important to boost already existing algorithms by adapting the basis function choice to the ANOVA decomposition of the function.

We consider two cases:

- For periodic functions on $\mathbb{T}^d$ we give a relation between the ANOVA terms and wavelet coefficients. We then use hyperbolic wavelet regression with compactly supported Chui-Wang wavelets for the fast function reconstruction.

- On $\mathbb{R}^d$, we give a relation between the Fourier transform of the function and the ANOVA terms. In the random Fourier feature approach, we draw frequencies at random and learn coefficients from the given data to construct the approximant. We generalize already existing random Fourier feature models to an ANOVA setting, where terms of different order can be used.

Our algorithms have the advantage of interpretability, meaning that the influence of every input variable is known, even for dependent input variables. We give theoretical as well as numerical results that our algorithms perform well for sensitivity analysis. The ANOVA-boosting step reduces the approximation error of existing methods significantly. This talk is based on joint work with Daniel Potts and Tino Ullrich.

15:00 - 15:30

High-Dimensional Approximation on Sparse Grids by Tensorized Moving Least-Squares

R. Kempf[1,2]

[1] University of Bayreuth, Germany
[2] University of Basel, Switzerland

The easiest representation of an approximation to a function f using only point-wise data has the form $Q(f) = \sum_j f(\boldsymbol{x}_j)\varphi_j$ with suitable *shape-functions* φ_j. Usually, one demands for such *quasi-interpolation processes* Q that they reproduce a certain class of functions, e.g., polynomials of a given degree. One way to construct shape functions that provide polynomial reproduction is by solving weighted least-squares problems, leading to a method commonly referred to as *moving least-squares*. Using compactly supported weight functions yields a fast, high-order reconstruction method using scattered data in arbitrary domains.

Furthermore, the specific form of the quasi-interpolation operators allow an easy application of the combination technique to obtain a high-order approximation method of high-dimensional functions on sparse grids that are constructed with nearly arbitrary low-dimensional point sets.

In this talk, I will repeat the basics of the low dimensional approximation process, the moving least-squares method. Then I introduce the new Smolyak moving least-squares method and discuss its properties. Additionally, I will confirm the theoretical results with numerical examples.

15:30 - 16:00

Structure-exploiting sparse grid approximations for efficient uncertainty quantification and surrogate model construction

I. Farcas

IS

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Gyrokinetic simulations on parallel supercomputers provide the gold standard for theoretically determining turbulent transport in magnetized fusion plasmas. Applications to large and costly future machines, in particular burning plasma devices like ITER, call for a proper Uncertainty Quantification (UQ) in order to assess the reliability of certain predictions. However, the high computational cost of gyrokinetic simulations prevents straightforward applications of conventional UQ approaches. Here, we discuss a sensitivity-driven dimension-adaptive sparse grid interpolation approach that can enable UQ in such expensive simulations. This approach explores and exploits, via dimension-adaptive refinement driven by sensitivity information, the fact that in most problems (i) only a subset of the uncertain parameters is important and (ii) these parameters interact anisotropically. This approach will be used in a realistic description of turbulent transport in the edge of fusion experiments. In a non-linear scenario with more than 264 million degrees of freedom and eight uncertain inputs, it requires a mere total of 57 high-fidelity simulations. In addition, we will show that a byproduct of our approach is that it also enables the construction of surrogate transport models, which is crucial for tasks such as profile predictions or the design of optimized devices.

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