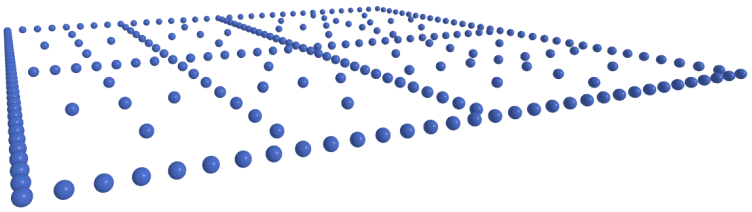
3rd Workshop on

Sparse Grids and Applications

2014

PROGRAM and ABSTRACTS



University of Stuttgart
Germany

SimTech
Cluster of Excellence

infos e. V.
Informatik-Forum Stuttgart

September 1–5, 2014

Stuttgart, Germany

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Sparse Grids and Applications

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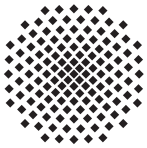
Organized by

Institute of Parallel and Distributed Systems, Simulation of Large Systems,
University of Stuttgart

Sponsored by

Informatik Forum Stuttgart e. V.
Cluster of Excellence "Simulation Technology", University of Stuttgart



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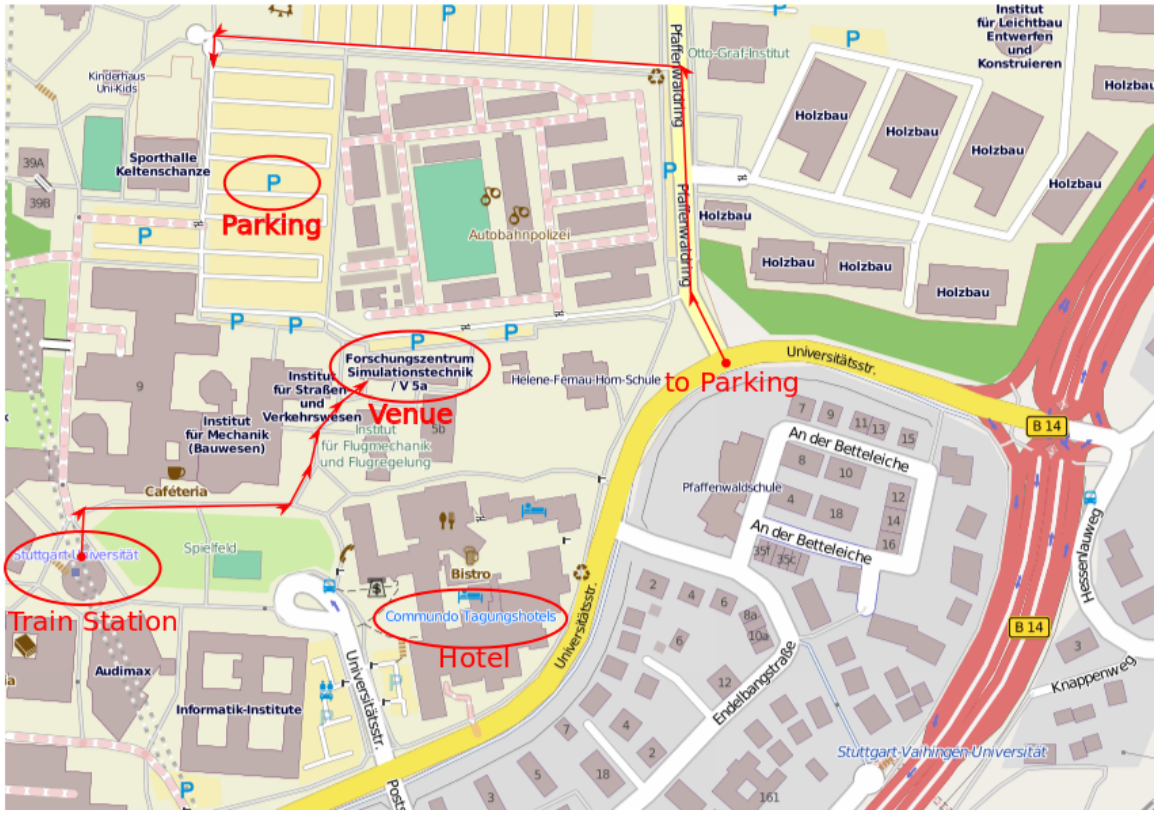
Local organization

Fabian Franzelin
Mario Heene
David Pfander
Dirk Pflüger

Program Overview

	Monday	Tuesday	Wednesday	Thursday	Friday
8:30-9:00	Registration (8:30-9:15)	Registration	Registration	Registration	Registration
09:00-10:10	1 (9:15 – 10:10) Welcome and Overview Hamaekers	5 Oettershagen Volkmer	9 Chen Hellebrand	11 Pflüger Peherstorfer	15 Fuchs Haji Ali
10:10-10:45	Coffee Break	Coffee Break	Coffee Break	Coffee Break	Coffee Break
10:45-12:30	2 Kormann Kröner De Dios	6 Carrington Anderson Wang	10 Garcke Kowitz Hullmann	12 Heene Hinojosa Hupp	16 Bohn Röhner Khakhutsky
12:30-13:45	Lunch Break	Lunch Break	Lunch Break	Lunch Break	Lunch Break
13:45-15:20	3 Invited Talk: Hiptmair Buse	7 Invited Talk: Gunzburger Nance		13 Invited Talk: Rahman Peters	17 Invited Talk: Nobile Litvinenko
15:20-15:50	Coffee Break	Coffee Break	15:15 – 18:00 Social Excursion to the Mercedes-Benz Museum with guided tour (English language)	Coffee Break	Coffee Break
15:50-17:00	4 Zhang Siebenmorgen	8 Franzelin Jantsch		14 Scheidegger Pfander	
			19:00 Conference Dinner Stuttgarter Stäffele Buschlestraße 2 70178 Stuttgart		

Directions and Orientation



Address of the venue

Stuttgart Research Centre for Simulation Technology (SRC SimTech)
Pfaffenwaldring 5a, 70569 Stuttgart

By train from the main railway station *(Hauptbahnhof)*

From Stuttgart main station (*Hauptbahnhof*), take the commuter train (S-Bahn) **S1**, **S2** or **S3** towards *Herrenberg*, *Filderstadt* or *Flughafen/Messe*. Exit the train at *Universität*. Leave the train station towards *Universitätszentrum*.
Travel time approx.: 10 min.

By train from the airport

From the airport, take the commuter train (S-Bahn) **S2** or **S3** towards *Hauptbahnhof*, *Schorndorf* or *Backnang*. Exit the train at *Universität*. Leave the train station towards *Universitätszentrum*.
Travel time approx.: 16 min.

By car

There is free parking available close to the venue. We recommend you to use the parking area marked on the map.

If you are a guest at the *Commundo Hotel*, there might be parking spaces available in the hotel's own underground parking.

Social Event, Wednesday, September 3

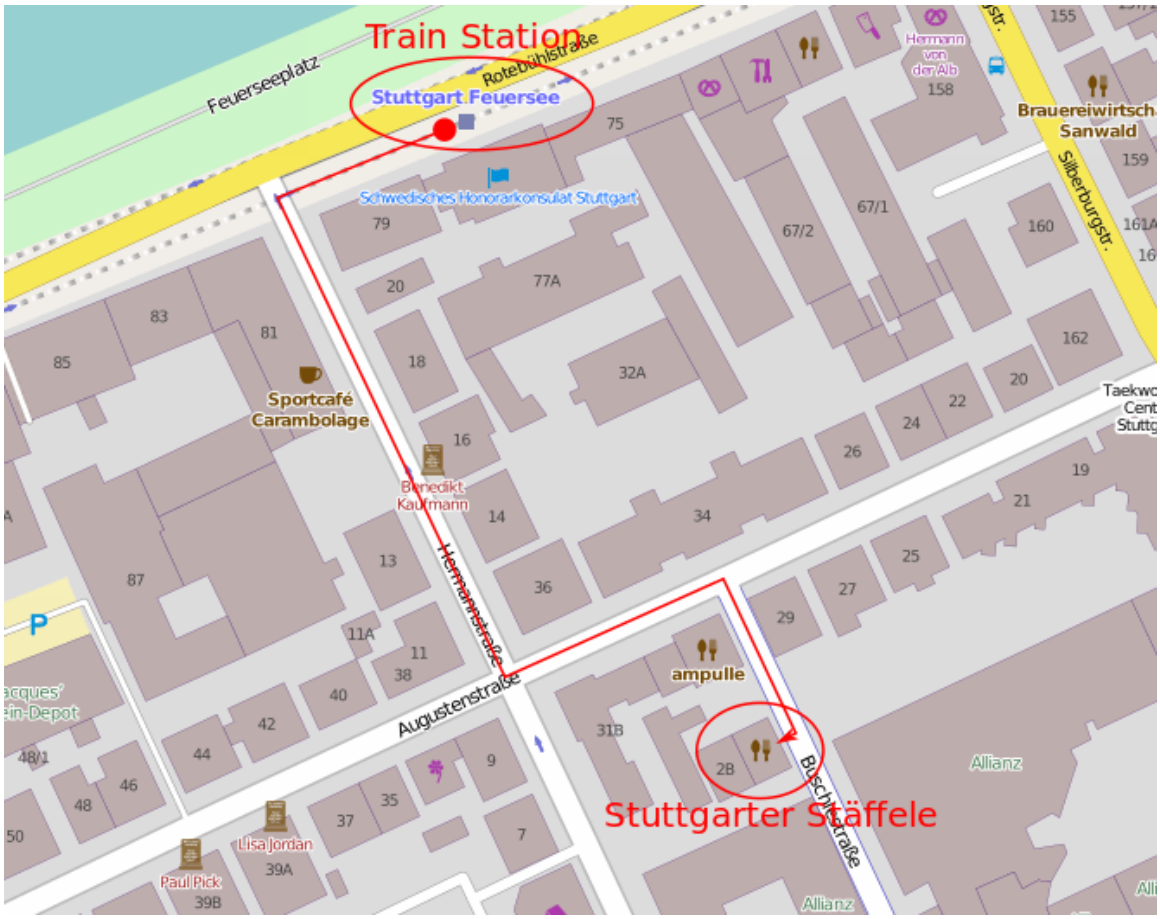
15:15 Excursion to the Mercedes-Benz Museum with guided tour

There will be a guided tour for us at the Mercedes-Benz Museum in English. We will meet in front of the conference venue and go together by train. The train ticket and entrance are included in the conference fee.

The tour will start at 16:00 and will take two hours. After the tour we will directly proceed to the conference dinner.

19:00 Conference dinner at Stuttgarter Stäffele

Address:
Stuttgarter Stäffele
Buschlestrasse 2a/b, 70178 Stuttgart



For those who do not join the excursion: From the train station *Universität* close to the venue take commuter train **S1**, **S2** or **S3** towards *Hauptbahnhof*, *Schorndorf*, *Backnang* or *Kirchheim (T)*. Exit the train at *Feuersee* and walk to the *Stuttgarter Stäffele* as indicated on the map.

In case you get lost or if there are any problems/questions etc. please contact:

Mario Heene: +49 151 28432862

8.30–9.15 **Registration**

9.15–9.35 **Welcome and Overview**

9.35–10.10 **Session**

1. **HCFFT: A fast Fourier transformation software library for general hyperbolic cross/sparse grid spaces** – *Jan Hamaekers*

10.10–10.45 **Coffee Break**

10.45–12.30 **Session**

1. **Sparse grids for the Vlasov equation** – *Katharina Kormann and Eric Sonnendrücker*
2. **Solving optimal feedback control problems for partial differential equations using adaptive sparse grids** – *Axel Kröner and Jochen Garcke*
3. **A sparse discontinuous Galerkin method for the Vlasov-Poisson system** – *Blanca Ayuso de Dios and Saverio Castelanelli*

12.30–13.45 **Lunch**

13.45–14.45 **Invited Talk**

1. **Multiple point evaluation on combined tensor product supports** – *Ralf Hiptmair*

14.45–15.20 **Session**

1. **A slim dynamic data layout for more localized operations on spatially adaptive sparse grids** – *Gerrit Buse and Riko Jacob*

15.20–15.50 **Coffee Break**

15.50–17.00 **Session**

1. **Adaptive sparse-grid methods for backward stochastic differential equations and applications in solving partial differential equations** – *Guannan Zhang, Max Gunzburger and Weidong Zhao*
2. **Multilevel quadrature methods for stochastic PDEs with lognormal diffusion coefficients** – *Markus Siebenmorgen, Helmut Harbrecht and Michael Peters*

9.00–10.10 **Session**

1. **Multivariate integration in reproducing kernel Hilbert spaces** – *Jens Oettershagen and Michael Griebel*
2. **Approximation of multivariate periodic functions by trigonometric polynomials based on rank-1 lattice sampling** – *Toni Volkmer*

10.10–10.45 **Coffee Break**

10.45–12.30 **Session**

1. **A new sparse collocation method for solving the vibrational Schrödinger equation** – *Tucker Carrington and Gustavo Avila*
2. **LSE approach to solving the electronic Schrödinger equation** – *James Anderson, Hiroyuki Nakashima and Hiroshi Nakatsuji*
3. **Efficient spectral Galerkin methods for electronic structure calculations** – *Yingwei Wang and Jie Shen*

12.30–13.45 **Lunch**

13.45–14.45 **Invited Talk**

1. **Multilevel stochastic collocation methods for SPDEs and optimal points for Lagrange interpolation on hypercubes** – *Max Gunzburger*

14.45–15.20 **Session**

1. **A sparse interpolation algorithm for dynamical simulations in computational chemistry** – *James Nance, C. T. Kelley and Elena Jakubikova*

15.20–15.50 **Coffee Break**

15.50–17.00 **Session**

1. **Datadriven uncertainty quantification with adaptive sparse grids in underground flow simulations** – *Fabian Franzelin and Dirk Pflüger*
2. **Multilevel sparse grid stochastic collocation methods** – *Peter Jantsch, Max Gunzburger and Aretha Teckentrup*

9.00–10.10 **Session**

1. **Sparse-grid, reduced basis approximation of Bayesian inverse problems** – *Peng Chen and Christoph Schwab*
2. **Sparse grid interpolants as surrogate models in statistical inverse problems** – *Emily Mo-Hellenbrand and Benjamin Peherstorfer*

10.10–10.45 **Coffee Break**

10.45–12.30 **Session**

1. **On the optimised combination technique for eigenvalue problems** – *Jochen Garcke*
2. **The combination technique for large scale gyrokinetic eigenvalue problems** – *Christoph Kowitz and Markus Hegland*
3. **Optimal scaling parameters for sparse grid discretizations** – *Alexander Hullmann*

12.30–13.45 **Lunch**

15.15–18.00 **Excursion to the Mercedes Benz Museum with guided tour**

19.00–22.00 **Conference Dinner**

9.00–10.10 **Session**

1. **Sparse grids and battleships in higher dimensions** – *Dirk Pflüger*
2. **Sparse grid density estimation with data independent quantities** – *Benjamin Peherstorfer, Dirk Pflüger and Hans-Joachim Bungartz*

10.10–10.45 **Coffee Break**

10.45–12.30 **Session**

1. **Massively parallel simulation of time-dependent initial value problems with the sparse grid combination technique** – *Mario Heene and Dirk Pflüger*
2. **Overcoming the fault tolerance (exa)challenge using sparse grids in plasma physics simulations** – *Alfredo Parra Hinojosa*
3. **Cache-optimal component grid hierarchization outperforming the unidirectional algorithm** – *Philipp Hupp and Riko Jacob*

12.30–13.45 **Lunch**

13.45–14.45 **Invited Talk**

1. **High-dimensional stochastic computing by adaptive-sparse polynomial dimensional decomposition** – *Sharif Rahman*

14.45–15.20 **Session**

1. **Combination technique based k-th moment analysis of elliptic problems with random diffusion** – *Michael Peters, Helmut Harbrecht and Markus Siebenmorgen*

15.20–15.50 **Coffee Break**

15.50–17.00 **Session**

1. **Using adaptive sparse grids to solve high-dimensional dynamic economic models** – *Simon Scheidegger and Johannes Brumm*
2. **Improving the efficiency of data mining on spatially adaptive sparse grids** – *David Pfander, Dirk Pflüger and Alexander Heinecke*

9.00–10.10 **Session**

1. **Stochastic collocation for differential algebraic qquations arising from gas network simulation** – *Barbara Fuchs and Jochen Garcke*
2. **Multi Index Monte Carlo: when sparsity meets sampling** – *Abdul Lateef Haji Ali, Fabio Nobile and Raul Tempone*

10.10–10.45 **Coffee Break**

10.45–12.30 **Session**

1. **Convergence results for discretized regression applied to sparse grids** – *Bastian Bohn and Michael Griebel*
2. **Online data mining with sparse grids** – *Kilian Röhner and Benjamin Peherstorfer*
3. **Greedy sparse grids adaptivity in the context of online learning** – *Valeriy Khakhutskyy*

12.30–13.45 **Lunch**

13.45–14.45 **Invited Talk**

1. **Quasi-optimal sparse grids for PDEs with random coefficients** – *Fabio Nobile*

14.45–15.20 **Session**

1. **Computation of the response surface and post-processing in the tensor train data format** – *Alexander Litvinenko, Sergey Dolgov and Hermann Matthies*

ABSTRACTS

Session

HCFFT: A fast Fourier transformation software library for general hyperbolic cross/sparse grid spaces

Jan Hamaekers

Fraunhofer Institute for Algorithms and Scientific Computing SCAI, Germany; jan.hamaekers@scai.fraunhofer.de

In this talk, we will present our software library HCFFT for fast Fourier transformations on general sparse grid approximation spaces. The curse of dimension limits the application of standard full grid spaces to low dimensional approximation problems and thus limits also the application of the conventional multi-dimensional fast Fourier transformation method. For functions which fulfill certain additional regularity assumptions, sparse grid spaces allows us to circumvent the curse of dimension at least to some extend. Our library HCFFT enables us to perform a fast Fourier transformation on these spaces. In particular, this includes optimized sparse grid approximation spaces, e.g. energy-norm sparse grid like spaces, and also dimension-adaptive sparse grid approximation spaces. We will discuss costs, accuracy, convergence rates, and some implementational details and applications.

Session

Sparse grids for the Vlasov equation

Katharina Kormann[1] *and Eric Sonnendrücker*[2]

[1]Technische Universität München, Germany; katharina.kormann@tum.de
[2]Max-Planck-Institut für Plasmaphysik, Germany; eric.sonnendruecker@ipp.mpg.de

The Vlasov equation models the evolution of a plasma in an external or self-consistent field. In its full generality, the model consists of an advection equation in six dimensional phase space coupled to Maxwell's or Poisson's equation. Due to the high dimensionality and the development of small structures the numerical solution is quite challenging. For two or four dimensional Vlasov problems, semi-Lagrangian solvers have been successfully applied. Introducing a sparse grid, the number of grid points can be reduced in higher dimensions. In this talk, we present a semi-Lagrangian Vlasov-Poisson solver on a tensor product of two sparse grids. In order to defeat the problem of poor representation of Gaussians on the sparse grid, we use a delta-f method and separate a Gaussian part that is then handled analytically. In the semi-Lagrangian setting, we have to evaluate the hierarchical surplus on each mesh point. This interpolation step is quite expensive on a sparse grid due to the global nature of the basis function. In our method, we use an operator splitting so that the advection steps boil down to a number of one dimensional interpolation problems. With this structure in mind we devise an evaluation step with constant instead of logarithmic complexity per grid point. Results are shown for standard test cases like the Landau damping problem and in four dimensional phase space the results are compared to a full-grid solution and a solution on the four dimensional sparse grid.

Solving optimal feedback control problems for partial differential equations using adaptive sparse grids

Axel Kröner[1] *and Jochen Garcke*[2]

[1]RICAM, Austria; axel.kroener@ricam.oeaw.ac.at
[2]Universität Bonn, Germany; garcke@ins.uni-bonn.de

An approach to solve finite time horizon optimal feedback control problems for partial differential equations using adaptive sparse grids is proposed. A semi-discrete optimal control problem is introduced and the feedback control is derived from the corresponding value function. The value function can be characterized as the solution of an evolutionary Hamilton-Jacobi Bellman (HJB) equation which is defined over a state space whose dimension is equal to the dimension of the underlying semi-discrete system. Besides a low dimensional semi-discretization it is important to solve the HJB equation efficiently to address the curse of dimensionality. We propose to apply a semi-Lagrangian scheme using spatially adaptive sparse grids. Sparse grids allow the discretization of the high(er) dimensional value functions arising in the numerical scheme since the curse of dimensionality of full grid methods arises to a much smaller extent. For additional efficiency an adaptive grid refinement procedure is explored. We present several numerical examples studying the effect of the parameters characterizing the sparse grid on the accuracy of the value function and optimal trajectories. Furthermore we analyze the behaviour of the trajectories in case of noise.

A sparse discontinuous Galerkin method for the Vlasov-Poisson system

Blanca Ayuso de Dios[1] *and Saverio Castelanelli*[2]

[1]Center of Uncertainty Quantification, Division of Mathematics & Computational Sciences & Engineering (MCSE), KAUST, Saudi Arabia; blanca.ayusodios@kaust.edu.sa
[2]Zurich Insurance Company Ltd., Switzerland; saverio.castelanelli@mathmods.eu

We consider the application of sparse grid techniques for discontinuous Galerkin (DG) approximations of some simple hyperbolic problems, with particular attention to the kinetic Vlasov-Poisson system. We describe the construction of the methods in the lowest order case and discuss their stability, error analysis and further properties. We include some simple numerical tests that show that the proposed sparse-DG method is indeed more efficient than the standard DG method, when comparing accuracy versus cost. This is joint work with Saverio Castelanelli (Zuerich).

Invited Talk

Multiple point evaluation on combined tensor product supports

Ralf Hiptmair

ETH Zürich, Germany; hiptmair@sam.math.ethz.ch

The presentation has its focus on the design of an efficient algorithm for a problem encountered in the context of semi-Lagrangian methods on sparse grids spaces.

We consider the multiple point evaluation problem for an n-dimensional space of functions $[-1,1[^d \mapsto \mathbb{R}$ spanned by d-variate basis functions that are the restrictions of simple (say linear) functions to tensor product domains. For arbitrary evaluation points this task is faced in the context of (semi-)Lagrangian schemes using adaptive sparse tensor approximation spaces for boundary value problems in moderately high dimensions.

We devise a fast algorithm for performing $m \geq n$ point evaluations of a function in this space with computational cost $O(m \log^d n)$. We resort to nested segment tree data structures built in a preprocessing stage with an asymptotic effort of $O(n \log^{d-1} n)$.

References

[1] R. Hiptmair, G. Phillips, and G. Sinha, *Multiple point evaluation on combined tensor product supports*, Numerical Algorithms, 62 (2012), pp. 317–337. DOI: 10.1007/s11075-012-9624-4.

Session

A slim dynamic data layout for more localized operations on spatially adaptive sparse grids

Gerrit Buse[1] *and Riko Jacob*[2]

[1]TU München, Germany; buse@in.tum.de
[2]ETH Zürich, Switzerland; rjacob@inf.ethz.ch

Spatially adaptive sparse grids (SASG) struggle in the face of modern hardware which reveals its full power only to those that make excessive use of caches and parallel computing resources. Current implementations of data structures for SASG however focus on programming convenience mostly and are therefore not contemporary any more. Introduced as a novum in scientific computing in the late 1990s, hash maps are to this day the most common data structure for SASG. Hash maps managed to take the leading position from sophisticated multi-dimensional tree structures, offering higher usability and far more flexibility by sticking close to the mathematical notation and by taking all responsibility concerning memory management from the programmer.

However, the price paid for this convenience raises nowadays the matter of reconsideration of the hash map as primary data structure for SASG. In the best case, an unordered map distributes its entries evenly across all bins and thus ensures access to all data items in (amortized) constant time. But even under the idealized assumption that key comparison takes only O(1) time, this promise loses its meaning when the limiting factor of data access is memory latency. Neither temporal nor spatial locality of accessed data can be ensured in algorithm implementations that use a hash map as underlying data structure.

We propose a novel data structure for SASG, that was conceived by Riko Jacob already in 2010, but has so far not appeared in a publication. The idea is a generalization of ideas presented by Riko Jacob and Gerrit Buse at the SGA 2012 workshop. A pseudorecursive enumeration scheme therein assigns consecutive indices to the points of a multi-dimensional regular sparse grid. Since the shape of regular grids is known, the index is implicit in the data structure and only reproduced on demand by algorithms for optimized stride calculations. For SASG of unknown shape, we make the index explicit and derive a key-value-based storage layout, in which the index serves as unique key to identify a grid point's data. A sorted list of key-value pairs now yields special properties: It represents a serialization of a multi-recursive breadth-first traversal of the SASG. For instance, if the dimension traversal order for a 3-D grid is (0,1,2), 0 is the fastest dimension and the traversal descends in this dimension first. A direct implication is that the 1-D subtrees with respect to the fastest dimension reside in compact, contiguous memory. As previously analyzed in the works about regular grids, this maximizes data locality during the application of sparse-grid-typical 1-D operators at least in this fast dimension.

In order to exploit these properties also for similar work done in the slower dimensions, we again use the metaphor of a work piece and a drill. When mounted in a vise, we need to approach the work piece from different angles. This means that our drill, the 1-D operator, needs to adapt, and in our particular case, we cannot expect to work on compact memory any more. Instead, we can also turn the work piece and always use the same drill. We choose this approach and encode the dynamics into the data structure, which performs a dimensional rotation on the data between the different phases of processing. The rotation corresponds to a cyclic shift of the dimension order, e.g., from (0,1,2) to (1,2,0). Obviously, it produces serialized 1-D subtrees with respect to another dimension, and we can apply our tool again in the very same fashion as for the previously fastest dimension. This principle was shown to work for regular sparse grids, and we now extend it to arbitrary SASG. The structured rotation from the regular grid case now becomes a recalculation of keys and a generalized sorting phase. We provide evidence for the efficiency of the approach in form of impressive speedups obtained for our realization of the classical hierarchization algorithm, which

we compare to a state-of-the-art implementation of the algorithm based on a hash map. Another major gain of the data structure is its extreme space efficiency. N data points require only 2N storage, orders of magnitude less than any hash map. We can therefore store much larger grids, for whose processing we also achieve impressive parallel efficiency.

Session

Adaptive sparse-grid methods for backward stochastic differential equations and applications in solving partial differential equations

Guannan Zhang[1], *Max Gunzburger*[2] *and Weidong Zhao*[3]

[1]Oak Ridge National Laboratory, United States; zhangg@ornl.gov
[2]Florida State University, United States; gunzburg@fsu.edu
[3]Shandong Unviersity, China; wdzhao@sdu.edu.cn

We propose adaptive sparse-grid schemes for the following high-dimensional backward stochastic differential equations (BSDEs),

$$\begin{cases} X_t = X_0 + \int_0^t b(s, X_s, Y_s, Z_s)ds + \int_0^t \sigma(s, X_s, Y_s, Z_s)dW_s, \\ Y_t = \xi + \int_t^T f(s, X_s, Y_s, Z_s)ds - \int_t^T Z_s dW_s, \end{cases}$$

This effort is mainly motivated by the relationship between BSDEs and a certain class of nonlinear parabolic partial differential equations (PDEs) described by the nonlinear Feynman-Kac theory, such that our approaches can be extended to solve PDEs. For time discretization of BSDEs, by taking conditional mathematical expectation and using Itô isometry theorem, classic time-stepping methods, such as Crank-Nicolson, multistep schemes, can be used directly. Furthermore, when solving BSDEs, approximating spatial derivatives for the case of PDEs is converted to approximating conditional mathematical expectations with Lévy kernels. As such, the BSDE can be solved independently at each spatial point without solving a linear system when using implicit time-stepping schemes. Hence, the spatial approximation can be constructed based on any function approximation approach, e.g. polynomial interpolation or spectral approximation, without concerns about conditioning and instability. However, by observing the fact that BSDEs used in practice usually involve a high-dimensional Lévy process, such that effective quadrature rule for approximating conditional mathematical expectations and approximation methods for spatial discretization are needed. For the quadrature rule, the sparse-grid Clenshaw-Curtis rule can be used for Lévy kernels defined on bounded domains; the sparse-grid Gauss-Hermite rule is preferable for uncorrelated Gaussian kernels. For the spatial discretization, global sparse-grid polynomial interpolation and adaptive piecewise hierarchical sparse-grid approach can be used to approximate smooth and irregular solutions, respectively. Various numerical examples on BSDEs and corresponding PDEs are presented to demonstrate effectiveness of our approach.

Multilevel quadrature methods for stochastic PDEs with lognormal diffusion coefficients

Markus Siebenmorgen[1], *Helmut Harbrecht*[2] *and Michael Peters*[3]

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This talk is dedicated to multilevel quadrature methods for the rapid solution of stochastic partial differential equations with a log-normal distributed diffusion coefficient. The key idea of these approaches is a sparse grid approximation of the occurring product space between the stochastic and the spatial variable. We develop the mathematical theory and present error estimates for the computation of the solution's statistical moments with focus on the mean and variance. Especially, the present framework covers the multilevel Monte Carlo method and the multilevel quasi Monte Carlo method as special cases. We show that the quasi Monte Carlo method based on a Halton sequence is applicable in arbitrary high stochastic dimension provided that the diffusion coefficient complies certain regularity assumptions. The theoretical findings are supplemented by numerical experiments.

Session

Multivariate integration in reproducing kernel Hilbert spaces

Jens Oettershagen[1] *and Michael Griebel*[2]

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[2]University of Bonn, Germany; griebel@ins.uni-bonn.de

We discuss the construction of sparse grid integration methods that are based on certain optimized univariate quadrature rules with slowly increasing number of nodes. This property is useful especially in Hilbert spaces of smooth or even analytic functions. We will also construct optimized index-sets tailored to the smoothness of the integrand by means of a dimension-adaptive approach.

Approximation of multivariate periodic functions by trigonometric polynomials based on rank-1 lattice sampling

Toni Volkmer

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We consider the approximation of periodic functions $f\colon \mathbb{T}^d \to \mathbb{C}$ belonging to Sobolev spaces of isotropic and dominating mixed smoothness, namely to the Hilbert spaces

$$\mathcal{H}^{\alpha,\beta}(\mathbb{T}^d) := \left\{ f \in \mathcal{C}(\mathbb{T}^d)\colon \|f|\mathcal{H}^{\alpha,\beta}(\mathbb{T}^d)\| := \sqrt{\sum_{\mathbf{k}\in\mathbb{Z}^d} \omega^{\alpha,\beta}(\mathbf{k})^2 |\hat{f}_{\mathbf{k}}|^2} < \infty \right\}$$

with $\beta \geq 0$, $\alpha > -\beta$, where $\hat{f}_{\mathbf{k}}$ are the Fourier coefficients of f and the weights $\omega^{\alpha,\beta}(\mathbf{k}) := \max(1, \|\mathbf{k}\|_1)^\alpha \prod_{s=1}^d \max(1, |k_s|)^\beta$ for $\mathbf{k} := (k_1, \ldots, k_d)^\top$. For the approximation of the function f, a trigonometric polynomial

$$p(\mathbf{x}) := \sum_{\mathbf{k}\in I} \hat{p}_{\mathbf{k}} \mathrm{e}^{2\pi \mathrm{i}\mathbf{k}\cdot\mathbf{x}}$$

with frequencies supported on an index set $I \subset \mathbb{Z}^d$, $|I| < \infty$, is used and the Fourier coefficients $\hat{p}_{\mathbf{k}} \in \mathbb{C}$ are going to be computed from sampling values of the function f. In general, this approximation causes an unavoidable error, the so-called truncation error $\|f - S_I f\|$, where $S_I f := \sum_{\mathbf{k}\in I} \hat{f}_{\mathbf{k}} \mathrm{e}^{2\pi\mathrm{i}\mathbf{k}\cdot\circ}$ is the Fourier partial sum of the Fourier coefficients $\hat{f}_{\mathbf{k}}$ of the function f for an arbitrary frequency index set $I \subset \mathbb{Z}^d$.

For instance, if we consider the Sobolev spaces of dominating mixed smoothness $\mathcal{H}^{0,\beta}(\mathbb{T}^d)$, $\beta > 0$, then we may use hyperbolic cross index sets $I_N^{d,0} := \{\mathbf{k} \in \mathbb{Z}^d\colon \omega^{0,1}(\mathbf{k}) := \prod_{s=1}^d \max(1, |k_s|) \leq N\}$ as frequency index sets I for the trigonometric polynomial p. In this case, the truncation error is

$$\|f - S_{I_N^{d,0}} f|L^2(\mathbb{T}^d)\| \leq N^{-\beta} \, \|f|\mathcal{H}^{0,\beta}(\mathbb{T}^d)\|.$$

For a function $f \in \mathcal{H}^{\alpha,\beta}(\mathbb{T}^d)$, we obtain

$$\|f - S_{I_N^{d,T}} f|\mathcal{H}^{r,t}(\mathbb{T}^d)\| \leq N^{-(\alpha-r+\beta-t)} \, \|f|\mathcal{H}^{\alpha,\beta}(\mathbb{T}^d)\|$$

for $N \geq 1$, $\beta \geq t \geq 0$, $\alpha + \beta > r + t$ and $T := -\frac{\alpha-r}{\beta-t}$, where the frequency index set $I_N^{d,T} := \{\mathbf{k} \in \mathbb{Z}^d\colon \omega^{-T,1}(\mathbf{k}) = \max(1, \|\mathbf{k}\|_1)^{-T} \prod_{s=1}^d \max(1, |k_s|) \leq N^{1-T}\}$.

We are interested in obtaining Fourier coefficients $\hat{p}_{\mathbf{k}}$ from sampling values such that the approximation error $\|f - p\|$ is identical or similar to the truncation error mentioned above, where $I = I_N^{d,T}$ and $p(\mathbf{x}) := \sum_{\mathbf{k} \in I_N^{d,T}} \hat{p}_{\mathbf{k}} \mathrm{e}^{2\pi \mathrm{i} \mathbf{k} \cdot \mathbf{x}}$. Recently an algorithm for the trigonometric interpolation on so-called generalized sparse grids for the class $\mathcal{H}^{\alpha,\beta}(\mathbb{T}^d)$ of functions as well as estimates for the approximation error were investigated in [1].

Here, we propose a different approach which is based on sampling the function f along a rank-1 lattice. Therefor, a suitable rank-1 lattice can be easily constructed for a given frequency index set I using a component-by-component method. The main advantage of our method, i.e., computing the Fourier coefficients $\hat{p}_{\mathbf{k}}$ from sampling values along the rank-1 lattice, is that it is based mainly on a one-dimensional fast Fourier transform, and that the arithmetic complexity of the algorithm depends only on the cardinality of the support of the trigonometric polynomial in the frequency domain. Namely, the arithmetic complexity of the algorithm is $\mathcal{O}(|I|^2 \log |I| + d|I|)$. We present upper bounds for the approximation error and achieve an optimal order of convergence when using suitable frequency index sets and rank-1 lattices. Numerical results are presented, which confirm the theoretical findings. We compare our results with the ones from [1].

This is joint work with Lutz Kämmerer and Daniel Potts

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Session

A new sparse collocation method for solving the vibrational Schrödinger equation

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We present a new Smolyak-inspired collocation method to compute vibrational energy levels of molecules. The key advantage of our collocation method is that it obviates the need to solve a generalized eigenvalue problem. This advantage is achieved by combining Lagrange-like functions with a Smolyak interpolant. Uncommon features of our method include: (1) we use a spectral basis; (2) we exploit the structure of the (nested) grid to develop an efficient algorithm for evaluating the matrix-vector products; (3) basis functions in level j are not also in level j+1 (although the space spanned by the functions in level j+1 does include the space spanned by the functions of level j); (4) we do not do a sum over product grids; (5) we choose points to reduce the size of the composite grid. Using these and similar ideas we are able to solve 12-D problems.

LSE approach to solving the electronic Schrödinger equation

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The local Schrödinger equation (LSE) method is a very accurate method for solving the electronic Schrödinger equation. It works by forming a basis from a recursion using the Hamiltonian and solving the electronic Schrödinger equation at a set of points. The LSE method does not have the limitation of requiring the basis be analytically integrable. The current strategy for this method is to sample points using Monte-Carlo. Using Boys theorem we see that the LSE method can be reformulated as a numerical integration problem, i.e. the Monte-Carlo sampling is actually numerical integration where the points have uniform weights. Using Monte-Carlo provides satisfactory results, however Monte-Carlo does not take into account the smoothness of the integrand. Recent results from Griebel and others in the mathematics literature show how one may construct accurate grids for performing cubature (multidimensional quadrature) with polynomial scaling. In this presentation the mechanics of the approach will be explained and preliminary results will be shown.

Efficient spectral Galerkin methods for electronic structure calculations

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In quantum chemistry the main interest is to find an approximation to the solution of the Schrodinger equation, which is a high-dimensional eigenvalue problem. In this work, we propose efficient spectral Galerkin methods for one-dimensional electronic Schrodinger equations. Furthermore, we apply the Slalter determinant which gives antisymmetric grids, suited to fermionic systems. Besides, the spectral Galerkin discretization results in a generalized linear eigenvalue problem, which is solved by the trace minimization scheme. Several numerical experiments are presented to show the costs, accuracy and convergence rates.

Invited Talk

Multilevel stochastic collocation methods for SPDEs and optimal points for Lagrange interpolation on hypercubes

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In this talk, we present results for two problems that deal with the approximation of functions in high, or at least, moderate dimension.

Multilevel methods for SPDEs seek to decrease computational complexity by balancing spatial and stochastic discretization errors, resulting in low (high) stochastic complexity whenever the spatial complexity is high (low). Multilevel techniques have been applied with great success to Monte Carlo methods (MLMC). In joint work with P. Jantsch, A. Teckentrup, and C. Webster, we extended the notion of multilevel methods to the stochastic collocation (SC) setting. In this talk, we present convergence and complexity analyses of a multilevel SC (MLSC) method, demonstrating its advantages compared to standard single-level SC approximations, and highlight conditions under which a sparse grid MLSC approach is preferable to MLMC.

We also discuss the computational construction of point sets in hypercubes that are optimal for total degree Lagrange polynomial interpolation on hypercubes, where optimality is defined as the minimization of the Lebesgue constant for the point set. We discuss what is known and not known about the dependence of the Lebesgue constant on the dimension and the polynomial degree. We then conjecture a growth rate for that constant and test the validity of the conjecture through some numerical experiments.

Session

A sparse interpolation algorithm for dynamical simulations in computational chemistry

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In this talk we present a new implementation of Smolyak's sparse grid interpolation algorithm designed for dynamical simulations of photo-induced molecular transformations.

A molecule conforms to a geometry that minimizes its potential energy, and many molecules have multiple potential energy minima. These geometries correspond to local minima of the molecule's potential energy surface, and one can simulate how a molecule transitions from one geometry to another by following the steepest descent path, or reaction path, on potential energy surfaces. Molecular vibrations and thermal fluctuations cause randomness in dynamics, so one must follow several paths simultaneously to more accurately simulate possible reaction paths. Current algorithms for reaction path following are too computationally burdensome for molecules of moderate size, but Smolyak's sparse interpolation algorithm offers a cheap surrogate for potential energy surfaces. While current implementations of Smolyak's algorithm are not designed to simultaneously follow multiple reaction paths efficiently, our implementation of Smolyak's algorithm achieves this efficiency by recursively defining Lagrange basis polynomials, vectorizing computations, and making use of an efficient reformulation of Smolyak's algorithm.

We will describe our new implementation of Smolyak's algorithm and compare performance times to MATLAB's Sparse Grid Interpolation Toolbox to demonstrate its computational savings. We will also present dynamical simulations for the photoisomerization of 2-butene that include as many as six degrees of freedom.

Session

Datadriven uncertainty quantification with adaptive sparse grids in underground flow simulations

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Non-intrusive stochastic collocation methods are commonly used in the quantification of uncertainties (UQ). Their main advantage is that they don't require any changes in the corresponding simulation code. They typically rely on building a surrogate model of a simulation that depends on a set of input parameters.The input space in the UQ context is usually a probability space describing the uncertainty linked with some simulation parameters. Conventional non-intrusive collocation methods require analytic descriptions of the probabilistic characteristics of the input. This is often not the case and the input is described by a set of samples drawn from some unknown distribution. We show in this talk that a sparse grid approach for both, estimating the unknown distribution of the input and its propagation through some model leads to a highly accurate representation of the uncertainty of the outcome. We present recent developments of UQ in subsurface flow simulations (CO2 storage). The respective real-world scenario requires custom-tailored criteria for adaptive refinement to reduce the number of sampling points as well as possible, for example. We evaluate the results we obtained by the stochastic collocation method combined with our density estimation approach using spatially adaptive sparse grids and compare them to previous methods in this context.

Multilevel sparse grid stochastic collocation methods

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Stochastic collocation methods for approximating partial differential equations with random input data (coefficients and forcing terms) suffer from the curse of dimensionality, whereby increases in the stochastic dimension cause an explosion of computational effort. In this talk, we propose and analyze a multilevel version of the stochastic collocation method, which – as in multilevel Monte Carlo (MLMC) methods – uses hierarchies of spatial approximations to reduce the overall computational complexity. In addition, our approach utilizes a sequence of multi-dimensional interpolants of increasing fidelity, which can then be used for approximating statistics of the solution as well as buildilng high-order surrogates featuring faster convergence rates. This work also provides a rigorous convergence and computational cost analysis of the multilevel method, demonstrating its advantages with regard to standard, single-level approximations as well as MLMC methods.

Session

Sparse-grid, reduced basis approximation of Bayesian inverse problems

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In this talk, we present a new algorithm for computational reduction in solving Bayesian inverse problems that have been addressed in [7, 4, 5, 2, 3, 6]. For the approximation of the high-dimensional integration, we use the dimension-adaptive sparse grid and reduced basis methods that has been developed in the work [1]. Moreover, we propose a goal-oriented error estimator for the reduced basis construction.

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Sparse grid interpolants as surrogate models in statistical inverse problems

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We consider statistical inverse problems where Bayes' rule is used to infer parameters from indirect

noisy data. The solution of inverse problems requires many forward problem evaluations which can become computationally expensive. Most practical inverse problems are large-scale, meaning that they involve dealing with high-dimensional problem spaces and large data sets. For these reasons, solving practical inverse problems demands different techniques to reduce the computational costs, such as employing more efficient sampling methods, which will lead to a reduction of the number of forward evaluations, and employing surrogate models to approximate the high-fidelity forward model, which will lead to a reduction of computational costs at each forward evaluation run. Driven by these motivations, this work investigates and examines the application of sparse grid interpolants (SGI) as surrogate models being used in Bayesian inverse problems. Compared to other classes of surrogate models, the SGI surrogate models have a very desirable feature–they are non-intrusive. They do not require access to the operators of the forward model but treat the forward model as a black box. To assess the applicability and quality of the SGI surrogate models, we present experiments based on examples from computational fluid dynamics, shape optimization, and heat conduction. A posterior distribution was obtained by sampling the forward simulations with the SGI surrogate model and Markov Chain Monte Carlo. For comparison purpose, another posterior distribution was also obtained with a projection-based reduced-order surrogate model. Even though the SGI surrogate models use the forward model as a black box, the experiments demonstrate the good capability of the SGI for inferring parameters from data containing large noise.

Session

On the optimised combination technique for eigenvalue problems

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We study the sparse grid combination technique for the numerical solution of d-dimensional eigenproblems on sparse grids. We investigate both the normal combination technique and the optimised combination technique for eigenvalue problems. We consider two applications, data analysis using spectral embeddings, and the numerical solution of the Schrödinger equation.

The combination technique for large scale gyrokinetic eigenvalue problems

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The simulation of microturbulences in hot fusion plasmas using the 5-D gyrokinetic equations is a crucial part in understanding the behavior of hot fusion plasmas. Identifying the microinstabilities by solving the gyrokinetic eigenvalue problem using the simulation code GENE is a computationally demanding task. There are two fundamental challenges that require significant research efforts: the curse of dimensionality, leading to an unfeasible high number of degrees of freedom, and the limited parallel efficiency of the current eigenvalue solver.

The sparse grid combination technique, combines several solutions of the eigenvalue problem from different grid-sizes. An optimization of the combination coefficients (Opticom) is then further improving the solution of the eigenvalue problem.

This approach not only reduces the computational effort of the gyrokinetic eigenvalue problem, it also introduces a certain tolerance to hardware faults, since single partial approximations can be omitted. Using the combination techniques allows on the one hand large scale parameter scans and on the other hand a study of scenarios using large grid size, which were not feasible before.

Optimal scaling parameters for sparse grid discretizations

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The combination technique constructs sparse grids using linear combinations of anisotropic full grids and has been successfully employed for, e.g., PDE solving, function approximation and data mining. The relative scaling of the anisotropic full grids depends on the application and is often known a priori. The optimized combination technique (OptiCom), however, determines the best possible scaling a posteriori and has first been introduced in the context of function regression.We use the OptiCom not for function regression but as a variable preconditioner for high-dimensional PDE problems. We discuss a new matrix-vector multiplication for the OptiCom that,

similarly to the unidirectional principle, exploits the structure of sum-of-tensor products operators. Using this matrix-vector multiplication, we can compute one iteration step of our OptiCom-preconditioned solver in log-linear runtime with respect to the number of degrees of freedom as opposed to quadratic costs typically associated with the OptiCom. A CG version is also presented.This is joint work with Peter Oswald (Jacobs University Bremen) and Michael Griebel (University of Bonn).

Session

Sparse grids and battleships in higher dimensions

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The game Battleships can serve as a nice example to explain some of the basic principles of sparse grids to undergraduates or even to a general audience. While sparse grids are not the optimal strategy for a generalized (continuous) version of the game which has been abstracted to arbitrary dimensions, they are not too far from optimal. Furthermore, they can be used to introduce Monte Carlo methods as well as some standard notions such as discrepancy. This presentation summarizes certain aspects from lectures and presentations, combining Battleships and sparse grids.

Sparse grid density estimation with data independent quantities

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Nonparametric density estimation is a fundamental problem of statistics and data mining. Even though kernel density estimation is arguably the most widely used method, its performance highly depends on the choice of the kernel bandwidth, and it can become computationally expensive for large data sets. We present an adaptive sparse-grid-based density estimation (SGDE) method which discretizes the estimated density function on basis functions centered at grid points rather than on kernels centered at the data points. Thus, the costs of evaluating the estimated density function are independent from the number of data points. We give details on how to estimate density functions on sparse grids and develop a cross validation technique for the parameter selection. We speedup the estimation process by splitting the computational procedure into an offline and an online phase. In the offline phase, data-independent auxiliary quantities (*a priori* grid optimization) are pre-computed and stored. In the online phase, the density for new, previously unseen data is estimated by reusing the pre-computed quantities. In our numerical examples, speedups of up to two orders of magnitude are achieved. We furthermore employ our method for the classification of astronomical objects to demonstrate that it is competitive to current kernel-based density estimation approaches not only with respect to runtime but also with respect to accuracy.

Session

Massively parallel simulation of time-dependent initial value problems with the sparse grid combination technique

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In this work we address some of the major challenges when applying the combination technique to time-dependent initial value simulations on large HPC systems. Our example application is the simulation of plasma turbulence, which is relevant for fusion energy research. We use the code GENE to solve the five dimensional gyrokinetic equations.

We present a parallelization concept which exploits the two-level parallelism of the combination technique. It is based on the manager-worker pattern and tailored to large HPC systems. The parallelization concept is promising to tackle the main exascale challenges scalability, load-balancing and resilience. Although being developed particularly for GENE, it is designed as general as possible. Thus, it enables the adaption of other application codes without major modifications.

For time-dependent initial value simulations it is necessary to synchronize the combination solution between the partial problems every several time steps to avoid divergence. In order to minimize the time of this synchronization step, we already presented efficient global communication schemes that exploit the hierarchical structure of the combination solution. In this talk we will elaborate on the many substeps that are necessary to apply this synchronization step to a complex application like GENE.

We applied the combination technique to initial value simulations with GENE on the supercomputer Hermit. We will compare the combination solution to the corresponding full grid solution with respect to approximation quality and use of computional resources. Furthermore we will examine how the frequency of the synchronization step influences the approximation quality and also the computational costs of the combination solution.

Overcoming the fault tolerance (exa)challenge using sparse grids in plasma physics simulations

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The first descriptions of the sparse grid combination technique in the nineties already revealed its inherent parallelization potential. Decomposing a sparse grid into anisotropic, independent full grids on which the solution is computed provides a second level of parallelism, the first being the usual domain decomposition. This key observation makes the combination technique a promising candidate for future exascale simulations. Whats more, the combination technique provides intuitive approaches to tackle the problem of fault tolerance in the context of large scale simulations. By incorporating ideas from adaptive sparse grids, multivariate extrapolation, and the generalized combination technique, it is possible to achieve full algorithm-based fault tolerance for high-dimensional applications. To illustrate the flexibility and performance of the approaches to fault tolerance, we simulate hot plasma fusion using the gyrokinetic simulation code GENE. The underlying PDE is five

dimensional and nonlinear, which gives rise to instabilities and turbulent transport effects. High-fidelity simulations can thus prove crucial to understand the driving mechanisms behind plasma fusion phenomena.

Cache-optimal component grid hierarchization outperforming the unidirectional algorithm

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The sparse grid combination technique provides a framework to solve high-dimensional numerical problems with standard solvers by assembling the sparse grid from many coarse and anisotropic full grids called component grids. Hierarchization is one of the most fundamental tasks for sparse grids. It describes the transformation from the full grid basis to the hierarchical basis. We present a cache-oblivious hierarchization algorithm for the component grids of the combination technique causing $|G|(1/B + \mathcal{O}(1/(M^{1/d}))$ cache misses. Here, G denotes the component grid, d the dimension, M the size of the cache and B the cache line size. This algorithm decreases the leading term of the cache misses by a factor of d compared to the unidirectional algorithm which is the common standard up to now. We complement this upper bound by a lower bound of $|G|(1/B + \mathcal{O}(1/(BM^{1/(d-1)}))$. For $B = 1$, a minor modification of the analysis of the algorithm shows that the upper and lower bound match.

Invited Talk

High-dimensional stochastic computing by adaptive-sparse polynomial dimensional decomposition

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This article presents two novel adaptive-sparse polynomial dimensional decomposition (PDD) methods for solving high-dimensional uncertainty quantification problems in computational science and engineering [1, 2]. The methods entail global sensitivity analysis for retaining important PDD component functions and sparse-grid dimension-reduction integration for estimating the PDD expansion coefficients. A unified algorithm, endowed with two distinct ranking schemes for grading component functions, was created for their numerical implementation. The fully adaptive-sparse PDD method is comprehensive and rigorous, leading to the second-moment statistics of a stochastic response that converges to the exact solution when the tolerances vanish. A partially adaptive-sparse PDD method, obtained through regulated adaptivity and sparsity, is economical and is, therefore, expected to solve practical problems with numerous variables. Compared with past developments, the adaptive-sparse PDD methods do not require its truncation parameter(s) to be assigned *a priori* or arbitrarily. The numerical results reveal that an adaptive-sparse PDD method achieves a desired level of accuracy with considerably fewer coefficients compared with existing PDD approximations. For a required accuracy in calculating the probabilistic response characteristics, the new bivariate adaptive-sparse PDD method is more efficient than the existing bivariately truncated PDD method by almost an order of magnitude. Finally, stochastic shape optimization of a jet engine bracket with 79 variables was performed, demonstrating the power of the new methods to tackle practical engineering problems [3].

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Session

Combination technique based k-th moment analysis of elliptic problems with random diffusion

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We consider the efficient deterministic solution of elliptic boundary value problems with random diffusion matrix. Assuming random perturbations with known k moments, we derive, to leading order in the random perturbations amplitude, deterministic equations for k moments of the random solution. The solutions k-th moment satisfies a k-fold tensor product boundary value problem on the k-fold product domain which can efficiently be discretized in sparse tensor product spaces. By defining the complement spaces via Galerkin projections, the related system of linear equations decouples and can be solved by standard multilevel finite element solvers. Numerical results for k = 2 are presented to validate and quantify our theoretical findings

Session

Using adaptive sparse grids to solve high-dimensional dynamic economic models

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We present a flexible and scalable method to compute global solutions of high-dimensional stochastic dynamic economic models. Within a time-iteration setup, we interpolate policy functions using an adaptive sparse grid algorithm with piecewise multi-linear (hierarchical) basis functions. As the dimensionality increases, sparse grids grow considerably slower than standard tensor product grids. In addition, the grid scheme we use is automatically refined locally and can thus capture steep gradients or even non-differentiabilities. To further increase the maximum problem size we can handle, our implementation is fully hybrid parallel, i.e. using a combination of MPI-CUDA/Thrust. This parallelization enables us to efficiently use high-performance computing architectures. Our code scales up nicely to more than sixteen thousand parallel MPI processes. To demonstrate the performance of our method, we apply it to high-dimensional international real business cycle models with capital adjustment costs and irreversible investment.

Improving the efficiency of data mining on spatially adaptive sparse grids

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The least-squares-based approach to data mining on spatially adaptive sparse grids is efficient in the sense that it scales linearly in the number of data points. This a significant advantage compared to many other approaches that show quadratic scaling. Still, solving large regression and classification tasks can take up huge amounts of time. For this reason, efficient algorithms are required.

During the last years, developments in hardware have made it more difficult to write algorithms that use all available computing resources. This is mainly due to the introduction of large vector units and the availability of processors with many cores. Additionally, the gap between the speed of the main memory and the speed of the execution units has widened. Thus, memory accesses have become more and more expensive.

In this talk, we will first introduce the standard, hardware-efficient streaming algorithm for solving regression problems on spatially adaptive sparse grids. Afterwards, we present algorithmic developments that focus on avoiding unnecessary computations of the streaming approach while still utilizing the computational resources efficiently. Overall, this results in speedups of up to 6x compared to previous algorithms for all datasets evaluated.

Session

Stochastic collocation for differential algebraic qquations arising from gas network simulation

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The gas transport within a single pipe segment is described by the so-called isothermal Euler equations. The equations arising from the conservation of mass and momentum together with the equations of state of a real gas form a coupled PDE. Additionally, we obtain algebraic equations by Kirchhoff's current law since at each connecting node of pipes, the sum of all incoming gas flows must equal the sum of all outgoing flows.

We use the method of stochastic collocation to quantify the uncertainties arising from the stochastic parameters of the DAEs. Due to the method's non-intrusiveness we can apply a commercial gas network simulator as black-box solver to compute a stationary solution for a given parameter set. To overcome the curse of dimensionality we use dimension-adaptive sparse grids with a piecewise polynomial hierarchical basis. Numerical results are provided to show convergence as well as the sensitivity of the network to local parameters which justifies the anisotropic approach.

Multi Index Monte Carlo: when sparsity meets sampling

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We propose and analyze a novel Multi Index Monte Carlo (MIMC) method for weak approximation of stochastic models that are described in terms of differential equations either driven by random measures or with random coefficients. The MIMC method is both a stochastic version of the combination technique introduced by Zenger, Griebel and collaborators and an extension of the Multilevel Monte Carlo (MLMC) method first described by Heinrich and Giles. Inspired by Giles's seminal work, instead of using first-order differences as in MLMC, we use in MIMC high-order mixed differences to reduce the variance of the hierarchical differences dramatically. This in turn yields new and improved complexity results, which are natural generalizations of Giles's MLMC analysis, and which increase the domain of problem parameters for which we achieve the optimal convergence, $O(TOL^{-2})$. Moreover, we motivate the systematic construction of optimal sets of indices for MIMC based on properly defined profits that in turn depend on the average cost per sample and the corresponding weak error and variance. Under standard assumptions on the convergence rates of the weak error, variance and work per sample, the optimal index set turns out to be of Total Degree (TD) type. In some cases, using optimal index sets, MIMC achieves a better rate for the computational complexity than does the corresponding rate when using Full Tensor sets. We also show the asymptotic normality of the statistical error in the resulting MIMC estimator and justify in this way our error estimate, which allows both the required accuracy and the confidence in our computational results to be prescribed...

Session

Convergence results for discretized regression applied to sparse grids

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Machine learning tasks are often tackled by support vector machines, radial basis function neural networks and other methods which employ a data-centered approach to explore given input data points and the manifold they reside on. For many applications a large amount of data ($n > 10^3$) is available and a straightforward application of the aforementioned techniques is not feasible.

Algorithms with non-data-based tensor-product grid discretizations directly allow for linear runtime with respect to n. However the curse of dimensionality (i.e. the size $\mathcal{O}(N^m)$ of the discretization space – where N denotes the amount of basis functions in one space direction and m denotes the space dimension) prohibits an application to higher-dimensional problems. To this end, sparse grid methods have been successfully employed in this context to reduce the amount of basis functions considerably.

For the specific setting of regression, there already exist upper bounds on the overall error consisting of bias and sampling error. However, these are not directly applicable for search spaces which are not dense in L_2. We will show how this framework can be altered to deal with the discretized setting. For the example of regression on sparse grids we will derive an explicit upper bound for the convergence rate by using well-known results on the interpolation error in sparse grid spaces.

Online data mining with sparse grids

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Sparse Grids are well-suited for handling large data sets when performing Data Mining. With the SGDE methods [2], the solutions need to be rebuild entirely when new data points are made available. Thus, we extend those methods to be able to handle live data streams.

We study the application of sparse grids to density estimation with data streams.When new data is received, the previous approximation needs to be updated to take into account the new information. This update is done in constant time for each new data point. It is necessary to find a balance between the old data and the new data in the result to ensure both stability and adaptivity. Also, we want to be able to adapt to a changing distribution of the density by slowly decreasing the impact of older data points until they are forgotten.

Using the density estimation, we also perform classification [1] on huge data sets with sparse grids. For benchmarking, we use synthetic data sets as well as real world data sets such as the DR10 from the Sloan Digital Sky Survey. We observe, that our methods qualify for lowering the memory usage drastically while maintaing the quality of the approximation in terms of error.

References

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Greedy sparse grids adaptivity in the context of online learning

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With the growing interest around Big Data, new challenges arise for data mining methods with adaptive sparse grids. In this setting the data is often plentiful but noisy and contains redundant information.

We consider the problem of online learning, where only a part of the input data is used for training at any given time. This situation arises, e.g., due to data availability or memory limitations.

The limited availability of data poses new challenges for learning algorithms and adaptivity, and we investigate the ways to adjust the strategies for space and dimension adaptive refinement of sparse grids.

As this is an area of active research, we discuss the current ideas and research directions as well as show the preliminary results. We analyse the new methods in terms of accuracy and processing speed.

Invited Talk

Quasi-optimal sparse grids for PDEs with random coefficients

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In this work we provide a convergence analysis for the quasi-optimal Stochastic Sparse Grid Collocation method, in which the construction of a sparse grid is recast into a knapsack problem: a profit is assigned to each hierarchical surplus and only the most profitable terms are added to the sparse grid.

We show how the convergence rate of the sparse grid approximation error with respect to the total number of points in the grid can be related to weighted summability properties of the sequence of profits. This argument is very general and can be applied to sparse grids built with any univariate family of points, both nested and non-nested.

As an example, we apply such quasi-optimal sparse grid to the solution of a particular elliptic PDE with uniformly distributed stochastic diffusion coefficients, namely the inclusions problem: we detail the convergence estimate obtained in this case, using polynomial interpolation on either nested (ClenshawCurtis) or non-nested (GaussLegendre) abscissas, verify its sharpness numerically, and compare the performance of the resulting quasi-optimal grids with a few alternative sparse grid construction schemes recently proposed in literature.

Some results and comparison with adaptive sparse grids and log-normally distributed random variables will also be shown.

Session

Computation of the response surface and post-processing in the tensor train data format

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We apply the Tensor Train (TT) approximation to construct the Polynomial Chaos Expansion (PCE) of a random field, and solve the stochastic elliptic diffusion PDE with the stochastic Galerkin discretization. We compare two strategies of the polynomial chaos expansion: sparse and full polynomial (multi-index) sets. In the full set, the polynomial orders are chosen independently in each variable, which provides higher flexibility and accuracy. However, the total amount of degrees of freedom grows exponentially with the number of stochastic coordinates. To cope with this curse of dimensionality, the data is kept compressed in the TT decomposition, a recurrent low-rank factorization. PCE computations on small sparse sets are extensively studied, but the TT representation requires specific treatment. We outline how to deduce the PCE from the covariance matrix, assemble the Galerkin operator, and evaluate some post-processing (mean, variance, Sobol indices), staying within the low-rank framework. The most difficult stages are the interpolation of a function in the TT format using a few number of samples, which is performed via the cross approximation method, and the solution of the discretized equation (linear system), for which the recently developed alternating minimal energy algorithm is applied. In the numerical experiments, we demonstrate that the full set encapsulated in the TT format is indeed preferable in cases when high accuracy and high polynomial orders are required.

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