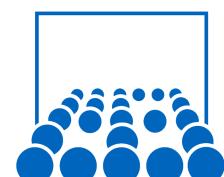


**2nd Workshop on**

**Sparse Grids and Applications**

**2012**

**PROGRAM and ABSTRACTS**



July 2 – 6, 2012

Munich, Germany



**2nd Workshop on**

**Sparse Grids and Applications**

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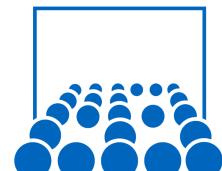
July 2 – 6, 2012  
Munich, Germany

**Organized by**

Chair of Scientific Computing, Department of Informatics, TUM  
and Focus Group HPC, Institute for Advanced Study, TUM

**Sponsored by**

Focus Group HPC, Institute for Advanced Study, TUM  
Munich, Germany



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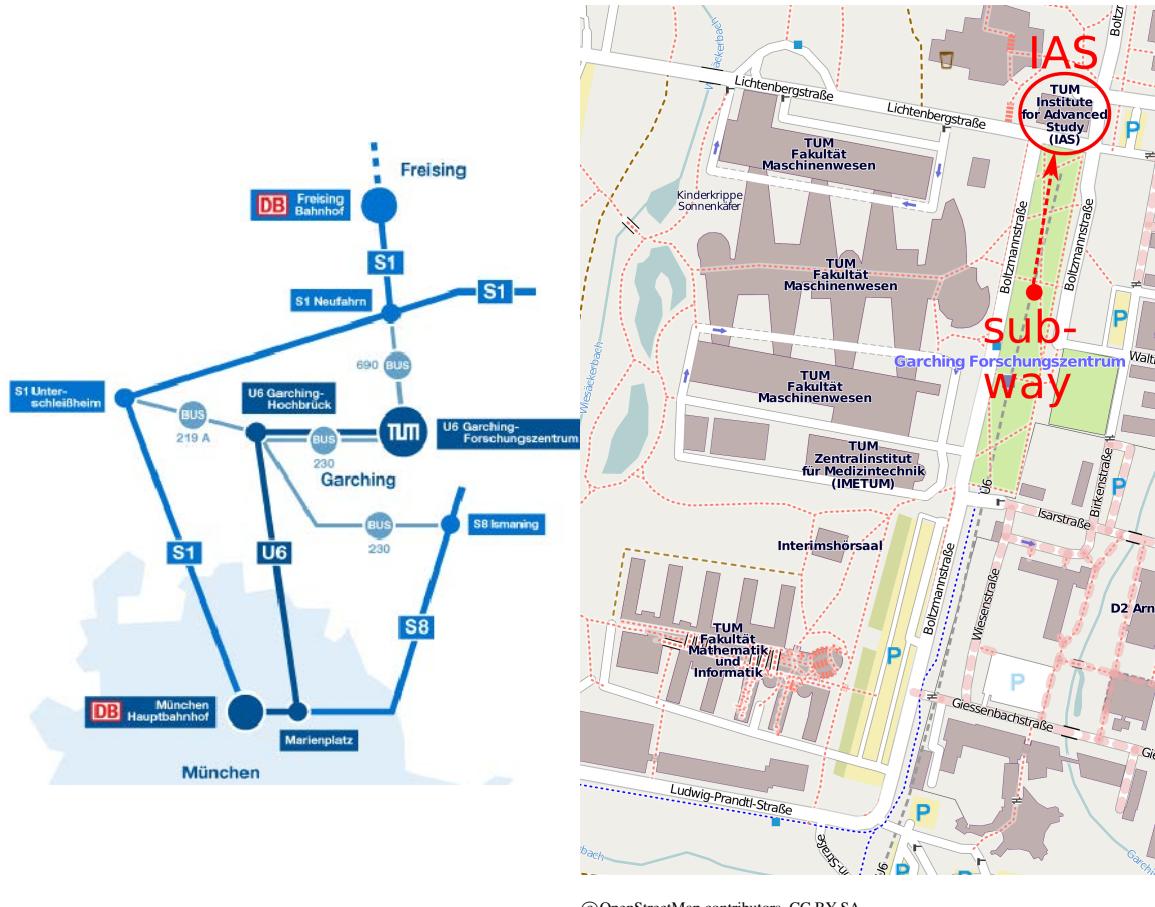
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# Sparse Grids and Applications, July 2 – 6, 2012

	Monday	Tuesday	Wednesday	Thursday	Friday
8:00 am	Registration				
8:30 am	Address of Welcome Peherstorfer, Butnaru Chair: Pflüger	Gerstner, Weiser Chair: Garcke	Hamaekers, Anderson Chair: Stevenson	Pflüger, Zaspel Chair: Reisinger	Garcke, Bohn Chair: Gerstner
9:00 am					
9:30 am					
10:00 am					
10:30 am	Coffee Break	Coffee Break	Coffee Break	Coffee Break	Coffee Break
11:00 am	Benk, Heinecke Chair: Pflüger	Jacob, Buse Chair: Garcke	Dinh, Chernov Chair: Stevenson	Wong, Kowitz Chair: Reisinger	Khakhtskyy, Harding Chair: Gerstner
11:30 am					
12:00 am					
12:30 am	Lunch Break	Lunch Break	Lunch Break	Lunch Break	Lunch Break
1:00 pm					
1:30 pm					
2:00 pm	Invited talk: Zenger Chair: Hegland	Invited talk: Harbrecht Chair: Hamaekers			Jakeman, Ottershagen, Kämmerer Chair: Harbrecht
2:30 pm		Coffee Break			Schieche, Chair: Harbrecht Chair: Hegland
3:00 pm					Coffee Break
3:30 pm					Webster, Sprungk Chair: Harbrecht
4:00 pm	Stevenson, Hullmann Chair: Hegland	Ayers, Shen Chair: Hamaekers			
4:30 pm					
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# Directions and Orientation



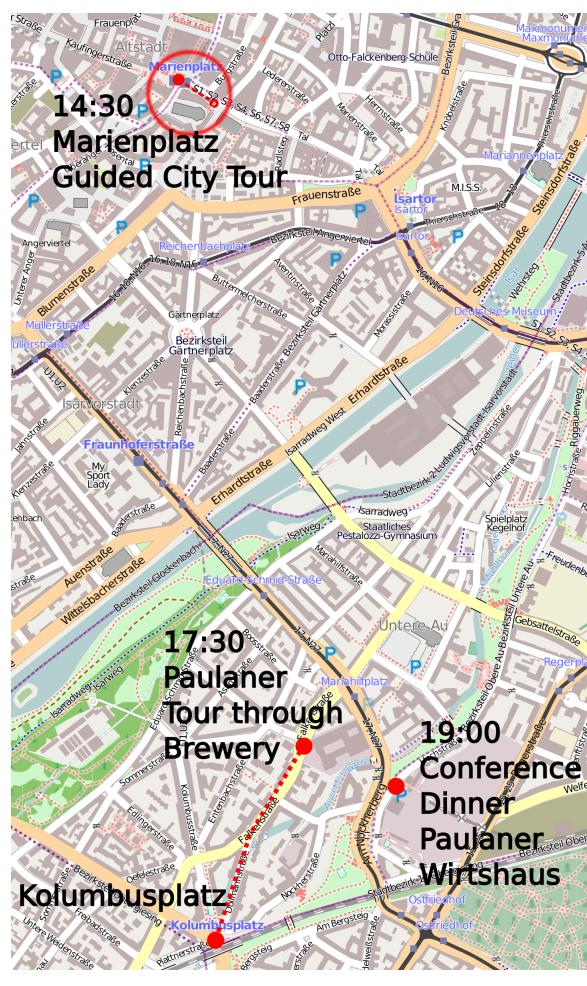
## Directions

From Munich main station (Hauptbahnhof), take any S-Bahn eastbound (via Marienplatz or Ostbahnhof). Change at station Marienplatz (second stop) to the U6 northbound to Garching-Forschungszentrum (via Fröttmaning, soccer stadium). Note that some trains stop earlier in Fröttmaning. You can wait in Fröttmaning for the next train to Garching-Forschungszentrum.

Disembark at the final destination Garching-Forschungszentrum. Leave the subway station in the direction of travel (exit Lichtenbergstraße). The IAS is straight ahead and right in front of you (about 200m).

Overall travel time approx.: 30-40 min.

## Social Event, Wednesday, July 04



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We will ask for your plans in attending these events during the first days of the workshop. You do not need to take part in all the events. There is the opportunity to come to join and leave the group between each event. To allow some planning on our side, you will have to sign up in a list we will put up for each event.

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

Christoph Kowitz: +49 174 6708910

### 14:30 Guided City Tour

- We will meet in front of the IAS at 13:40 and we will take the subway U6 from *Garching Forschungszentrum* at 13:53
- The subway takes approx. 30 min to Marienplatz
- The meeting point is on *Marienplatz* in front of the “*Spielzeugmuseum*”, which is the tower of the old (but newer looking) town hall, east of the main square
- After the tour we proceed to the brewery together

### 17:30 Tour of the Paulaner Brewery

- We proceed there together right after the city tour
- If you will not be at the city-tour, the meeting point is the entrance of the brewery at Falkenstr. 11
- You get there by leaving the subway U1 or U2 at Kolumbusplatz and walking northbound to Falkenstrasse

### 19:00 Conference Dinner

- We will proceed there right after the brewery-tour
- At Paulaner Wirtshaus am Nockherberg at Hochstraße 77
- We will sit outside in the *beergarden* if the weather is nice, otherwise inside

# ***PROGRAM***

8.15–8.45 **Registration**

8.45–9.00 **Address of Welcome**

9.00–10.20 **Session**

*Chair: Pflüger*

1. **A Sparse-Grid-Based Out-of-Sample Extension for Dimensionality Reduction and Clustering with Laplacian Eigenmaps – Benjamin Peherstorfer**
2. **An Investigation of Sparse Grid Interpolation in the Context of Reduced Order Models – Daniel Butnaru and Benjamin Peherstorfer**

10.20–11.00 **Coffee Break**

11.00–12.20 **Session**

*Chair: Pflüger*

1. **Expected Value Estimation in Financial Derivative Pricing with Sparse Grids – Janos Benk and Alexander Heinecke**
2. **A Cache-Aware and Vectorized Up-Down Implementation supporting Spatially Adaptive Sparse Grids – Alexander Heinecke**

12.20–13.30 **Lunch**

13.30–14.30 **Invited Talk**

*Chair: Hegland*

1. **Sparse Ideas on Sparse Grids Revisited – Christoph Zenger**

14.30–15.10 **Coffee Break**

15.10–16.30 **Session**

*Chair: Hegland*

1. **The adaptive wavelet-Galerkin method using tensor product wavelets – Rob Stevenson and Sebastian Kestler**
2. **Generalized sparse grid generating systems with the optimal diagonal scaling by means of Linear Programming – Alexander Hullmann**

9.00–10.20 Session

Chair: Garcke

1. Adaptive Sparse Grids and Multilevel Monte Carlo – *Thomas Gerstner and Stefan Heinz*
2. Numerical Integration used for inference in state-space models – *Constantin Weiser*

10.20–11.00 Coffee Break

11.00–12.20 Session

Chair: Garcke

1. Efficient Regular Sparse Grid Hierarchization by a Dynamic Memory Layout – *Riko Jacob*
2. Efficient Pseudo-Recursive Evaluation Schemes for Non-Adaptive Sparse Grids – *Gerrit Buse*

12.20–13.30 Lunch

13.30–14.30 Invited Talk

Chair: Hamaekers

1. Approximation of two-variate functions: singular value decomposition versus sparse grids – *Michael Griebel and Helmut Harbrecht*

14.30–15.10 Coffee Break

15.10–16.30 Session

Chair: Hamaekers

1. Breaking the Curse of Dimension for the Electronic Schrödinger Equation with Functional Analysis – *Paul Ayers*
2. Sparse Spectral-Galerkin Methods for High-Dimensional PDEs and Applications to the electronic Schrodinger equation – *Jie Shen*

9.00–10.20 Session

*Chair: Stevenson*

1. **Sparse grids for the electronic Schrödinger equation** – *Jan Hamaekers*
2. **Multidimensional Quadrature Approaches for Solving the Electronic Schrödinger Equation** – *James S. M. Anderson and Paul W. Ayers*

10.20–11.00 Coffee Break

11.00–12.20 Session

*Chair: Stevenson*

1.  **$n$ -Widths and  $\varepsilon$ -dimensions for high-dimensional sparse approximations** – *Dinh Dung and Tino Ullrich*
2. **Sparse space-time Galerkin BEM for the nonstationary heat equation** – *Alexey Chernov and Christoph Schwab*

12.20–13.30 Lunch

14.30–17.00 Guided city tour @ Marienplatz

17.30–19.00 Tour of brewery @ Nockherberg

19.00–22.00 Conference dinner @ Brewery Nockherberg

9.00–10.20 Session

Chair: Reisinger

1. ***SG<sup>++</sup> – Software for Spatially Adaptive Sparse Grids*** – *Dirk Pflüger*
2. ***Multi-GPU fluid simulations on sparse grids*** – *Peter Zaspel and Michael Griebel*

10.20–11.00 Coffee Break

11.00–12.20 Session

Chair: Reisinger

1. ***Modified applications of the combination technique in density estimation*** – *Matthias Wong*
2. ***An Opticom Method for Computing Eigenpairs*** – *Christoph Kowitz and Markus Hegland*

12.20–13.30 Lunch

13.30–14.30 Invited Talk

Chair: Harbrecht

1. ***The sparse grid combination technique for quasi-linear PDEs*** – *Christoph Reisinger*

14.30–15.10 Session

Chair: Harbrecht

1. ***Analysis and Application of Stochastic Collocation on Sparse Grids*** – *Bettina Schieche and Jens Lang*

15.10–15.50 Coffee Break

15.50–17.10 Session

Chair: Harbrecht

1. ***A hierarchical adaptive sparse grid stochastic wavelet collocation method for PDEs with random input data*** – *Clayton Webster, Max Gunzburger and Guannan Zhang*
2. ***Stochastic collocation for a groundwater problem*** – *Björn Sprungk and Oliver Ernst*

**9.00–10.20 Session**

*Chair: Gerstner*

1. **Using Hyperbolic Cross Approximation to measure and compensate Covariate Shift – Jochen Garcke and Thomas Vanck**
2. **Principal manifold learning with a dimension-adaptive sparse grid discretization – Bastian Bohn and Michael Griebel**

**10.20–11.00 Coffee Break**

**11.00–12.20 Session**

*Chair: Gerstner*

1. **Distributed data-mining with sparse grids using alternating direction method of multipliers – Valeriy Khakhutskyy**
2. **Robust solutions to hyperbolic PDE's with multiple grids – Brendan Harding and Markus Hegland**

**12.20–13.30 Lunch**

**13.30–15.30 Session**

*Chair: Hegland*

1. **Goal Orientated Adaptivity for Quantifying Uncertainty in Computationally Intensive Models – John Jakeman**
2. **Dimension-adaptive Sparse Grid Quadrature for Integrals with Boundary Singularities – Michael Griebel and Jens Oettershagen**
3. **Generated sets vs. sparse grids as sampling schemes for hyperbolic cross trigonometric polynomials – Lutz Kämmerer**

## ***ABSTRACTS***

# A Sparse-Grid-Based Out-of-Sample Extension for Dimensionality Reduction and Clustering with Laplacian Eigenmaps

*Benjamin Peherstorfer*

Technische Universität München, Germany; pehersto@in.tum.de

Spectral graph theoretic methods such as Laplacian Eigenmaps are among the most popular algorithms for dimensionality reduction and clustering. One drawback of these methods is, however, that they do not provide a natural out-of-sample extension. They only provide an embedding for the given training data. The most common out-of-sample extension for Laplacian Eigenmaps and other spectral methods is based on the Nyström method. This out-of-sample extension is based on the assumption that we can represent the similarity measure as a kernel function. They are then utilized to compute the embedding of out-of-sample points. We propose to use sparse grid functions to approximate the eigenfunctions of the Laplace-Beltrami operator. We then have an explicit mapping between ambient and latent space. Thus, out-of-sample points can be mapped as well. In contrast to full grids, sparse grids allow us to apply grid-based discretization methods in high dimensional settings. Hence, as the grid-based approximation of the eigenfunctions keeps the dimension of the eigenproblem independent of the number of training data points, large data sets can be treated more easily. We present clustering and dimensionality reduction results for synthetic and real-world examples to support the effectiveness of the sparse-grid-based explicit mapping.

## An Investigation of Sparse Grid Interpolation in the Context of Reduced Order Models

*Daniel Butnaru<sup>1</sup> and Benjamin Peherstorfer<sup>2</sup>*

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Reduced order models (ROMs) are used more and more in areas where the execution time of the full forward model becomes prohibitive, especially in real-time or repeated execution scenarios. Typically, ROMs are classified in the two big classes: data-fit and projection-based, each with particular characteristics concerning intrusiveness, cost and reuse possibilities. In this paper, we investigate if sparse grid interpolation can also play a role in constructing ROMs either as standalone or in combination with other methods. We present results for several simulation codes.

# Expected Value Estimation in Financial Derivative Pricing with Sparse Grids

*Janos Benk<sup>1</sup> and Alexander Heinecke<sup>2</sup>*

Technische Universität München, Germany

<sup>1</sup>benk@in.tum.de

<sup>2</sup>heinecke@in.tum.de

For correct decision making during the maturity of a financial derivative, the approximation of the expected value function of the payoff is essential. The expected value of one option can trigger e.g., the early exercise of the American option. Dynamic trading strategies require, among others, the expected value of the asset portfolio guiding optimal decisions which target high returns on the investment.

One approach, to approximate the expected value function, is to solve a regularization problem with Monte-Carlo points as input values. The solution of this regularization problem is the expected value function. In order to cope with higher-dimensional problems (e.g. basket-options), we use sparse grids for solving the given regularization problem.

Although we are employing sparse grids, there is still an enormous demand on computing power, especially in higher-dimensional settings. We present methods that tackle this challenge from different angles: we use spatially adaptive grids which helps to reduce the number of degrees of freedom. Furthermore, we implemented the needed algorithms in a hardware aware manner to leverage hardware architecture features like vector-extensions or even accelerator boards.

# A Cache-Aware and Vectorized Up-Down Implementation supporting Spatially Adaptive Sparse Grids

*Alexander Heinecke*

Technische Universität München, Germany; heinecke@in.tum.de

Solving partial differential equations (PDE) on spatially adaptive grids is a challenging task since a complex algorithm, the so called Up-Down scheme, has to be employed. This program is used to derive an application of matrix vector multiplications which are needed during the iterative solution process of a finite element discretized PDE. The Up-Down calculations use the sparse grid's underlying hierarchical basis functions and are carried out by nested recursions which are essential due to the grid's adaptivity.

Especially when solving parabolic problems with adaptive grids, the underlying grid structure has to be flexible in order to allow arbitrary grid modifications at any time, such as refining only a single grid point and not the whole sub-space the identified grid point is belonging to. The most widely used method to achieve these properties is using a hash based grid storage organization. However, all these approaches often suffer from poor spatial and temporal memory locality and are not vectorizable due to scalar and recursive kernels resulting from the Up-Down's dimensional splitting of finite elements operators.

In this work an Up-Down implementation is presented which significantly reduces the computing time as it reconsiders the dimensional splitting. The revised splitting method reduces the number grid storage traversals to one and allows a vectorization of the one-dimensional, recursive operators. Beside changes applied to classical Up-Down implementations, this work also includes runtime

measurements on contemporary x86-based machines featuring vector extensions and multi-level memory hierarchies.

## Invited Talk

# Sparse Ideas on Sparse Grids Revisited

*Christoph Zenger*

TU München, Germany; zenger@in.tum.de

The sparse grid approach can be considered as a special combination of some mathematical and algorithmic principles. These principles are the origin of both the strengths of the approach (e.g., to tackle to some extent the curse of dimensionality) and of the limitations (e.g., the restriction to problems with cartesian product structure). In this talk we discuss ideas (not results) to overcome some of the limitations in the context of the solution of partial differential equations by alternative algorithmic concepts.

# The adaptive wavelet-Galerkin method using tensor product wavelets

*Rob Stevenson<sup>1</sup> and Sebastian Kestler<sup>2</sup>*

<sup>1</sup>university of amsterdam, Netherlands; r.p.stevenson@uva.nl

<sup>2</sup>Universitaet Ulm, Germany; sebastian.kestler@uni-ulm.de

We present a new efficient approximate evaluation scheme to be used in an optimally converging adaptive sparse-grid method. One of its ingredients is a generalization to multi-tree index sets of the fast sparse-grid matrix vector multiplication routine introduced by R. Balder and Ch. Zenger in [1].

## References

- [1] R. Balder and C. Zenger. The solution of multidimensional real Helmholtz equations on Sparse Grids. *SIAM J. Sci. Comput.*, 17, 3:631–646, May 1996.

# Generalized sparse grid generating systems with the optimal diagonal scaling by means of Linear Programming

*Alexander Hullmann*

Institute for Numerical Simulation, University of Bonn, Germany; hullmann@ins.uni-bonn.de

Tensor products of one-dimensional multilevel systems can be used to represent multivariate functions. Then, by a proper truncation of the resulting series expansion, we can construct problem-dependent sparse grids, which allow us to efficiently approximate higher-dimensional problems for various norms and smoothness classes.

We discuss additive Schwarz preconditioners for the corresponding systems of linear equations. The problem of finding the optimal diagonal scaling for the generating system subspaces can be solved by means of Linear Programming. For e.g.  $H^1$ -elliptic problems, an optimally scaled regular sparse grid generating system exhibits a condition number of the order  $O(k^{d-2})$  for level  $k$  in  $d$  dimensions.

This is suboptimal compared to the  $O(1)$  condition numbers realized by prewavelet discretizations that directly rely on multiresolution norm equivalences. However, we will discuss an approach that likewise realizes  $O(1)$  condition numbers in the generating system without specifically discretizing the detail spaces via more complicated basis functions.

This is joint work with M. Griebel (University of Bonn) and P. Oswald (Jacobs University Bremen).

# Adaptive Sparse Grids and Multilevel Monte Carlo

*Thomas Gerstner<sup>1</sup> and Stefan Heinz<sup>2</sup>*

Universität Frankfurt, Germany

<sup>1</sup>[gerstner@math.uni-frankfurt.de](mailto:gerstner@math.uni-frankfurt.de)

<sup>2</sup>[heinz@math.uni-frankfurt.de](mailto:heinz@math.uni-frankfurt.de)

The Multilevel Monte Carlo method introduced by Michael Giles is a technique to reduce the computational complexity of estimating an expected value arising from a stochastic differential equation using Monte Carlo path simulations. In this method, path simulations with different timesteps are combined in such a way that the ratio of computational cost and error (variance) is minimized. This can reduces the complexity, up to a logarithmic factor, by one order of magnitude. It has many applications, particularly in computational finance.

In this talk, we will show that the Multilevel Monte Carlo method can be interpreted as a sparse grid method in dimension-samples space. We extend the method to deal with adaptivity and apply this adaptive Multilevel Monte Carlo method to the pricing of special financial products such as Asian, digital and barrier options.

# Numerical Integration used for inference in state-space models

*Constantin Weiser*

Johannes Gutenberg-University of Mainz, Germany; [constantin.weiser@uni-mainz.de](mailto:constantin.weiser@uni-mainz.de)

State-space models are a very general framework for modeling dynamic processes with at least one unobservable parameter. This class of models is widely used, especially by physicists and engineers. They are also more and more common in economics and finance.

The inference on the unobservable parameter is made using an iterated process of prediction and filtering. Every step uses the Bayes' rule, which includes a potentially high-dimensional integral. So the inference is done by a high number (up to several hundreds or thousands, depending on the length of the observed time series) of medium- to high-dimensional (depending on the complexity of the model) integrals. If maximum-likelihood estimation is used to determine the potentially unknown coefficients of the models, then the computation of millions of integrals may be necessary.

In general these integrals are not manageable analytically and if they are, then is this a result of hard and binding restrictions. One common known restricted model is the so-called "Kalman-Filter". There is a wide literature discussing less restricted methods, but they mostly use simulation-based approaches, like the particle-filter.

Because of the known problems with simulation based approaches, we establish a grid based approach for our work, especially the sparse-grid approach or to be more precise the "spatial adaptive sparse grid approach" as given by Dirk Pflüger and others. Furthermore a "rescaled sparse grid approach" to improve the efficiency is suggested.

First results show us that the new methods outperform the simulation-based ones in terms of convergence speed by orders of magnitude, although the programming is more difficult.

# Efficient Regular Sparse Grid Hierarchization by a Dynamic Memory Layout

*Riko Jacob*

ETH Zürich, Switzerland; jacob@in.tum.de

Algorithms on Sparse Grids, like hierarchization, are notorious for their bad memory access patterns [2, 3]. Following ideas from the theory of external memory algorithms [1, 3], we propose an algorithm that works with a dynamic layout of the variables. We consider the task of hierarchization, i.e., given the function values at the points of a sparse grid in  $d$ -dimensional space and level- $l$ , compute the coefficients of the hierarchical bases functions, so called hierarchical surpluses.

The classical hierarchization algorithm works dimension by dimension and computes in the current dimension hierarchical surpluses. Let us pictorially describe the situation by thinking of the sparse grid as a work piece that needs to be drilled from many different directions. Now there are two standard ways of doing this: either you mount the working piece to the bench and move a mobile drill around it, or you mount the drill on the bench and turn the working piece. We propose to shift to the analogue of the latter method: Instead of adapting the one-dimensional hierarchization procedure to the current dimension, we move the data. This scheme leads to an alternation of computing hierarchical surpluses in the first dimension (working) and rotating the data by  $(x_1, x_2, \dots, x_{d-1}, x_d) \mapsto (x_d, x_1, \dots, x_{d-2}, x_{d-1})$  such that again the first dimension is the direction to work on. These two phases are repeated  $d$  times to complete the hierarchization.

There are three advantages with this method:

- We can choose a memory layout that makes the access pattern of the working step cache-friendly
- Both phases are exactly the same for all  $d$  rounds. They can be phrased as sparse matrix multiplication. Computing these matrices once is sufficient.
- There is no need to store position information (like level and index) together with a variable (it is always implied by the position). This leads to a fairly small memory-footprint, in particular when compared to hash-based implementations.
- The algorithm can be easily and efficiently (both computation and memory access-wise) parallelized for multiple cores.

Data layouts for sparse grids have been considered [4]. The key property of the cache friendly layout we use here is to sort the points lexicographically, such that points that differ only in their first coordinate are stored adjacently.

The algorithm is implemented in C++ using OpenMP, compiled with gcc and run on a 4-core machine running linux. Preliminary runtime comparisons with the SG<sup>++</sup> framework [3, 6] show significant performance advantages of the proposed approach. Performance is roughly equal for small dimensions and high levels. For moderate dimensions and moderate levels there is an advantage of a factor of roughly 80, and for really high dimensions and low levels, the new approach is up to several thousand times faster. Further, the size (in number of variables) of grids that can be dealt with (in main memory) is roughly 10 times bigger (for high dimensions even more).

## Acknowledgments

I am grateful to Dirk Pflüger for introducing me to the topic and supplying me with the SG<sup>++</sup> source code. For many fruitful discussions I want to thank Gerrit Buse, Hans Bungartz and Dirk Pflüger.

## References

- [1] A. Aggarwal and J. S. Vitter. The input/output complexity of sorting and related problems. *Communications of the ACM*, 31(9):1116–1127, 1988.
- [2] H.-J. Bungartz and M. Griebel. Sparse grids. *Acta Numerica*, 13:147–269, 2004. URL <http://dx.doi.org/10.1017/S0962492904000182>.
- [3] A. Maheshwari and N. Zeh. A survey of techniques for designing i/o-efficient algorithms. In U. Meyer, P. Sanders, and J. Sibeyn, editors, *Algorithms for Memory Hierarchies*, volume 2625 of *Lecture Notes in Computer Science*, pages 36–61. Springer Berlin / Heidelberg, 2003. ISBN 978-3-540-00883-5. URL [http://dx.doi.org/10.1007/3-540-36574-5\\_3](http://dx.doi.org/10.1007/3-540-36574-5_3).
- [4] A. Murarasu, J. Weidendorfer, G. Buse, D. Butnaru, and D. Pflüger. Compact data structure and parallel algorithms for the sparse grid technique. In *16th ACM SIGPLAN Symposium on Principles and Practice of Parallel Programming*, 2011.
- [5] D. Pflüger. *Spatially Adaptive Sparse Grids for High-Dimensional Problems*. Verlag Dr. Hut, München, Aug. 2010. ISBN 9783868535556. URL <http://www5.in.tum.de/pub/pflueger10spatially.pdf>.
- [6] URL <http://www5.in.tum.de/SGpp/>.

## Efficient Pseudo-Recursive Evaluation Schemes for Non-Adaptive Sparse Grids

*Gerrit Buse*

Technische Universitaet Muenchen, Germany; buse@in.tum.de

In this work we propose novel algorithms for sparse grid evaluation, operating on non-adaptive, yet potentially anisotropic grid types. Besides regular grids this includes truncated grids as introduced in [2], as well as variants of both using boundary grid points.

The data structure we use resembles the implicit data structures proposed in [3], [1] in two ways. First, we employ a linear coefficient array as data container, in which the coefficients are densely packed in memory without any gaps. Second, we define a bijective mapping computable in  $\mathcal{O}(d)$  time (resp.  $\mathcal{O}(d + n)$  time for truncated grids) for level  $n$  grids in  $d$  dimensions, which uniquely identifies each coefficient's position in the array, depending on the level index vector pair.

Despite these similarities, our approach is based on a different idea and totally avoids random access into the grid. Instead, the coefficients form a sequence as seen when running over the grid using a multi-dimensional, recursive breadth first traversal, and accessing grid point data is done in an incremental fashion only. Our algorithms therefore rather think in terms of distances and strides than in absolute positions.

With this setup, we are able to combine two properties that typically favor efficient sparse grid algorithms.

1. Storing only the coefficients without any structural information saves a lot of memory (especially for large  $d$ ) and thus improves data locality.
2. Sparse grids are inherently recursive and some of the fastest algorithms are based on recursive grid traversals with optimized tensor product calculations, which—through our recursive data layout—become applicable for our algorithms, too.

On a modern Intel multicore CPU platform our implementation achieves competitive results for  $d$  up to 10, compared to results presented in [3]. As we show, this also holds for the results obtained on Nvidia Fermi GPUs, for which speedups of up to 4.5 over a 12 core Intel Westmere EP platform are observed for  $d \leq 10$ . However, due to very limited fast memory on the GPU these results do not scale when going to a higher dimensionality. In really high-dimensional settings in the order of hundreds of dimensions, our evaluation algorithm outperforms any other known algorithm on the CPU.

## References

- [1] Christian Feuersänger. Dünngitterverfahren für hochdimensionale elliptische partielle Differentialgleichungen. Diplomarbeit, Institut für Numerische Simulation, Universität Bonn, 2005. (pdf contains corrections).
- [2] Alin Murarasu, Gerrit Buse, Josef Weidendorfer, Dirk Pflüger, and Arndt Bode. fastsg: A fast routines library for sparse grids. In *Proceedings of the International Conference on Computational Science, ICCS 2012*, Procedia Computer Science, June 2012. accepted for publication.
- [3] Alin Murarasu, Josef Weidendorfer, Gerrit Buse, Daniel Butnaru, and Dirk Pflüger. Compact data structure and scalable algorithms for the sparse grid technique. In *Proceedings of the 16th ACM symposium on Principles and practice of parallel programming, PPoPP '11*, pages 25–34, New York, NY, USA, feb 2011. Cambridge University Press.

## Invited Talk

# Approximation of two-variate functions: singular value decomposition versus sparse grids

*Michael Griebel<sup>1</sup> and Helmut Harbrecht<sup>2</sup>*

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We compare the cost complexities of two approximation schemes for functions  $f \in H^p(\Omega_1 \times \Omega_2)$  which live on the product domain  $\Omega_1 \times \Omega_2$  of general domains  $\Omega_1 \subset \mathbb{R}^{n_1}$  and  $\Omega_2 \subset \mathbb{R}^{n_2}$ , namely the singular value / Karhunen-Loeve decomposition and the sparse grid representation. Here we assume that suitable finite element methods with associated *fixed* order  $r$  of accuracy are given on the domains  $\Omega_1$  and  $\Omega_2$ . Then, the sparse grid approximation essentially needs only  $\mathcal{O}(\varepsilon^{-\frac{\max\{n_1, n_2\}}{r}})$  unknowns to reach a prescribed accuracy  $\varepsilon$  provided that the smoothness of  $f$  satisfies  $p \geq r \frac{n_1 + n_2}{\max\{n_1, n_2\}}$ , which is an almost optimal rate. The singular value decomposition produces this rate only if  $f$  is analytical since otherwise the decay of the singular values is not fast enough. If  $p < r \frac{n_1 + n_2}{\max\{n_1, n_2\}}$ , then the sparse grid approach gives essentially the rate  $\mathcal{O}(\varepsilon^{-\frac{n_1 + n_2}{p}})$  while, for the singular value decomposition, we can only prove the rate  $\mathcal{O}(\varepsilon^{-\frac{2 \min\{r, p\} \min\{n_1, n_2\} + 2p \max\{n_1, n_2\}}{(2p - \min\{n_1, n_2\}) \min\{r, p\}}})$ . We derive the resulting complexities, compare the two approaches and present numerical results which demonstrate that these rates are also achieved in numerical practice.

## **Breaking the Curse of Dimension for the Electronic Schrödinger Equation with Functional Analysis**

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Most approaches for solving the electronic Schrödinger equation do not fully exploit the functional-analytic simplicity of the electronic wavefunction. Because of this, the cost of these methods explodes exponentially with increasing electron number, an effect that is often called the curse of dimension. Recent work in mathematics and computer science shows how, by exploiting the smoothness of molecular wavefunctions, one can design methods that achieve the same accuracy as full configuration interaction, but with polynomial cost. The mathematical background of this approach is presented, along with a detailed prescription for identifying the relevant Slater determinants and computational results for atomic ground states, atomic excited states, and molecular potential energy curves. In the basis-set limit, this truncated configuration interaction method is size-consistent.

## **Sparse Spectral-Galerkin Methods for High-Dimensional PDEs and Applications to the electronic Schrödinger equation**

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We shall present a new sparse spectral method for high-dimensional problems, and present, in particular, rigorous error estimates as well as efficient numerical algorithms for elliptic equations in both bounded and unbounded domains. As an application, we shall use the proposed sparse spectral method to solve the N-particle electronic Schrödinger equation.

# Sparse grids for the electronic Schrödinger equation

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We study tensor product multiscale many-particle spaces with finite-order weights and their application for the electronic Schrödinger equation. Any numerical solution of the electronic Schrödinger equation using conventional discretization schemes is impossible due to its high dimensionality. Therefore, typically Monte Carlo methods (VMC/DMC) or nonlinear model approximations like Hartree-Fock (HF), coupled cluster (CC) or density functional theory (DFT) are used. We present a new numerical method which combines the favorable properties of efficient Gaussian type orbitals basis sets, which are applied with good success in conventional electronic structure methods, and tensor product multiscale bases, which provide guaranteed convergence rates and allow for adaptive resolution. To this end, the approach is based on a modified adaptive sparse grid technique and a certain particle-wise decomposition with respect to one-particle functions obtained by a nonlinear rank-1 approximation. Sparse grids allow to overcome the exponential complexity exhibited by conventional discretization procedures. Here, we employ a multiscale Gaussian frame for the sparse grid spaces and we use Gaussian type orbitals to represent the rank-1 approximation. With this approach we are able to treat small atoms and molecules with up to six electrons.

# Multidimensional Quadrature Approaches for Solving the Electronic Schrödinger Equation

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Achieving multiHartree accuracy in electronic structure computations is a priority when developing an electronic structure method. The full configuration interaction (Full-CI) method reliably achieves this accuracy, but is very computationally expensive (exponential scaling). Full-CI is a robust method that can be used with any Hamiltonian. It does not take advantage of the inherent smoothness associated with the solutions to the electronic Hamiltonian. In the molecular electronic structure problem simplicity arises from every electron being identical, and that the electronic Hamiltonian only contains one- and two-body symmetric operators. Our modern grid-based approach takes into account these symmetries that are neglected in the Full-CI approach. Grid methods, often termed “basis set free” methods, have been seen as anathemas due to their reputation of exponential scaling. However, results from Griebel and others in the mathematics of complexity literature show how one may construct accurate grids for performing cubature (multidimensional quadrature) with polynomial scaling. Utilising these efficient grids for electronic structure gives rise to grid methods that scale polynomially while maintaining Full-CI accuracy. In this presentation the mechanics of the approach will be explained and recent results will be presented.

## **$n$ -Widths and $\varepsilon$ -dimensions for high-dimensional sparse approximations**

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We study linear hyperbolic cross approximations, Kolmogorov  $n$ -widths and  $\varepsilon$ -dimensions of periodic multivariate function classes with anisotropic smoothness in high-dimensional settings. Indeed, if  $f$  is a  $d$ -variate function and  $n$  the dimension of the linear approximation space, both parameters  $n$  and  $d$  play the same essential role in asymptotic estimations of convergence rates. We prove upper and lower bounds for the error measured in an isotropic Sobolev space, of linear approximations by trigonometric polynomials with frequencies from sparse hyperbolic cross spaces as well as corresponding  $n$ -widths and  $\varepsilon$ -dimensions of function classes with anisotropic smoothness. In the estimates we particularly care for the respective dependence on the dimension  $d$ . From the received results it follows that in some cases the curse of dimensionality can be really broken. In other cases we are able to state negative results as a consequence of the obtained lower bounds.

## **Sparse space-time Galerkin BEM for the nonstationary heat equation**

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We construct and analyze sparse tensorized space-time Galerkin discretizations for boundary integral equations resulting from the boundary reduction of nonstationary diffusion equations with either Dirichlet or Neumann boundary conditions. The approach is based on hierarchical subspace decompositions and a weighted sparse tensor product construction. We compare the convergence behavior of the proposed method to the standard full tensor product discretizations. In particular, we show for the problem of nonstationary heat conduction in a bounded two- or three-dimensional spatial domain that low order sparse space-time Galerkin schemes are competitive with high order full tensor product discretizations in terms of the asymptotic convergence rate of the Galerkin error in the energy norms, under similar regularity requirements on the solution.

## **$SG^{++}$ – Software for Spatially Adaptive Sparse Grids**

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We present our software toolbox  $SG^{++}$  and underlying ideas of its software design. We demonstrate the use for some use-cases. A special focus is put on the general structure of its modular design, on data structures and on parallelizations. We furthermore aim to gather feedback on the expectations the sparse grid community has at a general, spatially adaptive software package.

## **Multi-GPU flow simulations on sparse grids in presence of uncertainties**

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This talk outlines our latest results in implementing a fully multi-GPU based solver for fluid flows in presence of uncertain input data which is optimized for performance and further parallelized by different sparse grid techniques.

It is well-known that the direct numerical simulation of instationary incompressible fluid flows in three dimensions is a very computational intensive problem. This becomes even more problematic by introducing two-phase flow simulations. At the same time, we know that most of the relevant engineering applications face the challenge of having some uncertainties in the input parameters such as inflow velocities, geometries or material parameters. We thus should incorporate techniques to analyze these kind of perturbations. However, by using non-intrusive uncertainty quantification methods, we end up performing hundreds or thousands of compute-intensive fluid simulations.

Our goal is, to attack this extreme compute challenge by the combination of standard parallelizations, modern parallel compute architectures, i.e. GPUs, and different sparse grid techniques.

A GPU-based stochastic radial basis function collocation method is used as non-intrusive uncertainty quantification method. The applied two-phase flow solver is NaSt3DGPF, which now runs fully parallel on multi-GPU clusters. Furthermore, to achieve a clearly improved strong scaling, the sparse grid combination technique on GPUs is applied. Obviously, the overall stochastic collocation method can be even more optimized in performance by applying adaptive sparse grids for integration and the sampling of the stochastic space.

# Modified applications of the combination technique in density estimation

*Matthias Wong*

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The combination technique in dealing with high dimensional computational problems has continued to attract use since its invention in 1992. However, naive adoption of the technique could lead to problems. This paper investigates various ways in which the combination technique could be modified and used as applied to the problem of density estimation. In particular, we vary the use of the combination technique by applying the combination not merely to the solution but also to each iterative step. Moreover we advocate the choice of the combination coefficients which are optimal with respect to understood criterions. In this we choose coefficients which minimize the target functional. The approaches are inspired by the “opticom” techniques developed by Hegland, Gärcke and Challis. Numerical results are represented and conclusions are drawn regarding the applicability of these approaches to other problems.

## An Opticom Method for Computing Eigenpairs

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The coming large fusion experiment ITER will heavily benefit from numerical simulations. One model for simulating the hot plasmas occurring in such a device are the gyrokinetic equations, which can resolve the plasmas microturbulence. A linear analysis of these equations reveals the unstable modes driving the microturbulence. Due to the moderately high dimensionality of the problem, the computation of eigenvalues and eigenvectors for the linear analysis could heavily profit from sparse grids. Since the highly efficient and parallelized simulation code GENE is already at hand, a combination technique approach is used. Applying the classical combination technique to the gyrokinetic eigenvalue problem is not applicable due to the different scaling of the computed eigenvector. The opticom is the remedy to that problem, since it formulates the search for the optimal combination coefficient, i.e. the scaling factors for the different eigenvector solutions, as a minimization problem. Applying that technique with the search for a single eigenpair, the computation of the respective eigenvalue has to be reformulated into an optimization problem. This has been done using the approach of Osborne and allowed the computation of eigenpairs out of coarse resolution solutions. A few examples are shown, which prove the applicability of a combination approach to eigenvalue problems in general as well as for the gyrokinetic eigenvalue problem.

## Invited Talk

# The sparse grid combination technique for quasi-linear PDEs

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The sparse grid combination technique has been reported to give good numerical results for various linear and non-linear PDEs in moderate dimensions, e.g., in applications from financial derivative pricing or fluid dynamics. The numerical analysis of the method is invariably based on a certain expansion in the mesh widths, of the approximation error for the chosen discretisation on regular grids. It is this result which so far has been established only for simple model problems. We show here how a recently published error correction technique based on semi-discretisations can be extended to parabolic PDEs with a convex non-linearity in the gradient. We provide numerical results, highlight the relation to other methods, and discuss the possibility of extensions to more general equations.

# Analysis and Application of Stochastic Collocation on Sparse Grids

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Uncertain input data for partial differential equations (PDEs) are often reasonably described by a set of independent random variables. To discretize the resulting parameter space, Monte Carlo simulations, spectral methods of Galerkin type, or stochastic collocation on sparse grids can be used. We focus on the latter, because it decouples the problem into a set of deterministic equations, while being able to achieve high convergence rates.

We adaptively choose the collocation points on anisotropic sparse grids based on Gauss-Patterson quadrature nodes and Smolyak's algorithm. Moreover, we describe the random solution field in terms of hierarchical Lagrange polynomials. The hierarchical surpluses can naturally be used as error indicators, because they contain the amount of change in the solution with respect to new collocation points. The algorithm terminates when this change falls under a given tolerance.

Our experience includes elliptic, parabolic, and various flow problems with random parameters, where we have used up to 17 random dimensions so far. We observe that adaptive stochastic collocation performs quite well for all examples, but overestimates the interpolation error in some cases, leading to more collocation points than actually necessary. One reason for that is that the algorithm can only terminate properly, when the stochastic tolerance is not chosen smaller than deterministic discretization errors.

Our aim is to analyze and detect deterministic and stochastic errors. To this end, we use an adjoint approach to obtain more accurate error estimates than given by the error indicators. What we see is that adjoint stochastic collocation needs a few collocation points to capture deterministic errors, but a huge number to capture stochastic errors. We present results obtained with reduced order models of the adjoint problem, in order to evaluate this huge number of adjoint collocation points with moderate computational costs.

# A hierarchical adaptive sparse grid stochastic wavelet collocation method for PDEs with random input data

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Accurate predictive simulations of complex real world applications require numerical approximations to first, oppose the curse of dimensionality and second, converge quickly in the presence of steep gradients, sharp transitions, bifurcations or finite discontinuities in high-dimensional parameter spaces. In this talk we present a novel multidimensional multiresolution adaptive (MdMrA) sparse grid stochastic collocation method, that utilizes hierarchical multiscale piecewise Riesz basis functions constructed from interpolating wavelets. The basis for our non-intrusive method forms a stable multiscale splitting and thus, optimal adaptation is achieved. Error estimates and numerical examples will used to compare the efficiency of the method with several other techniques.

## Stochastic collocation for a groundwater problem

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We present an application of sparse grids in the context of stochastic collocation (SC) methods applied to an Uncertainty Quantification (UQ) problem. The problem we consider derives from a site assessment study for a radioactive waste repository known as WIPP (Waste Isolation Pilot Plant) in New Mexico (USA). The quantity of interest (QOI) is the travel time of radioactive particles released within the repository and transported through a conductive layer above the site in case of a future accidental breach.

When uncertainty in the hydraulic conductivity of the ambient rock formation is modelled as a lognormal random field, computing the travel time requires the solution of a stationary diffusion equation with random coefficient.

A simple, but usually inefficient, numerical treatment for models with random data is the Monte Carlo method (MC). In contrast with MC, SC methods attempt to exploit the smooth dependence of the solution of a PDE with random data on the random parameters.

We investigate how these techniques perform relative to MC for approximating the travel time. Our objective is to approximate its cumulative distribution function (cdf) rather than merely its mean or variance.

To this end, we apply the SC method and investigate to what extent it allows computational savings over MC at comparable accuracy. We gauge accuracy with the Kolmogorov-Smirnov test to verify whether the approximate cdf's of the QOI thus obtained are statistically indistinguishable, i.e., if the approximation error of the SC method is smaller than the sampling error of the MC method. We also investigate to what extent anisotropic SC methods lead to further acceleration of convergence.

# Using Hyperbolic Cross Approximation to measure and compensate Covariate Shift

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The concept of covariate shift in data analysis describes a displacement of the training and test distribution while the conditional remains the same. One can address this problem by using individual weights for each training datapoint, which emphasizes the training points close to the test data set so that these get a higher significance. We propose a new method for calculating such weights by minimizing a Fourier series approximation of distance measures like Pearson chi-squared or Kullback-Leibler. To be able to use the proposed approach for higher dimensional data, we employ the so-called hyperbolic cross approximation.

Results show that the new approach can compete with the latest methods and that on real life data an improved performance can be obtained.

# Principal manifold learning with a dimension-adaptive sparse grid discretization

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Manifold learning deals with the reconstruction of the underlying structure of given i.i.d. samples  $\mathbf{x}_i \in \mathbb{R}^d, i = 1, \dots, k$  drawn according to an unknown probability measure. The data points are assumed to stem from an  $m$ -dimensional submanifold  $\mathcal{M} \subset \mathbb{R}^d$ .

Among others, the most popular manifold learning methods are Isomap, Laplacian eigenmaps, self-organizing maps and regularized principal manifolds. The latter usually constructs a parameterization of the manifold as a weighted sum of kernel functions in an a-priori chosen reproducing kernel Hilbert space. This is similar to the construction of support vector machines for regression tasks. This method, although often used for practical applications, inherently suffers from the computational complexity with respect to the amount of input data. Formally, the inversion of a full  $k \times k$  matrix has to be computed. As one matrix vector multiplication requires  $\mathcal{O}(k^2)$  operations, the computational costs for an iterative solver are at least quadratic with respect to  $k$ .

To overcome this drawback, we employ a sparse grid discretization to parameterize the manifold and solve a regularized minimization problem using an expectation-maximization scheme. Our approach scales linearly in  $k$  and the ambient space dimension  $d$ . Constructing a sparse grid of level  $l$ , the number of grid points scales like  $\mathcal{O}(2^l l^{s-1})$ .

In real-world applications, the dimension  $s$  has to be estimated in a preprocessing step. A compression algorithm and a dimension-adaptive sparse grid discretization are employed, in order to make our algorithm feasible for too large a-priori estimates  $\tilde{s} > s$ .

We conclude with results for an application to real-world data and a comparison to other manifold learning methods.

# Distributed data-mining with sparse grids using alternating direction method of multipliers

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Sparse grids have been successfully used for the mining of large datasets with a moderate number of dimensions. Compared to the established machine learning techniques, like artificial neural networks or support vector machines, sparse grids produce an approximant that is easier to analyze and to interpret. Although the solution of high-dimensional data-mining problems using sparse grids was a subject of several studies previously [1, 2, 3], further improvements in this area are desired. Especially interesting in this context are the problems where dimensionality cannot be reduced using regular methods (e.g., PCA).

We investigate the opportunities for solving high-dimensional machine learning problems with sparse grids by splitting and solving it using the alternating direction method of multipliers (ADMM) [4] in parallel fashion. This method should allow one to reduce the size of problems that have to be solved and, therefore, to further reduce the impact of the curse of dimensionality. We show the first results of the new approach using a set of problems.

## References

- [1] C. Feuersänger. Sparse Grid Methods for Higher Dimensional Approximation. Rheinische Friedrich-Wilhelms-Universität Bonn, 2010.
- [2] J. Gärcke. Maschinelles Lernen durch Funktionsrekonstruktion mit verallgemeinerten dünnen Gittern. Rheinischen Friedrich-Wilhelms-Universität Bonn, 2004.
- [3] D. Pflüger. Spatially Adaptive Sparse Grids for High-Dimensional Problems. Verlag Dr. Hut, München, Aug. 2010.
- [4] S. Boyd, N. Parikh, E. Chu, B. Peleato, and J. Eckstein. Distributed Optimization and Statistical Learning via the Alternating Direction Method of Multipliers. Foundations and Trends in Machine Learning, 3(1):1–122, 2010.

## Robust solutions to hyperbolic PDE's with multiple grids

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As the largest supercomputers continue to grow exponentially in terms of total processors and flops the frequency of faults in these machines also increases. The need for applications to continue and recover in the event of a fault is becoming increasingly apparent. We will discuss the application of extrapolation and combination techniques to developing fault tolerant algorithms for solving PDE's. We focus on hyperbolic PDE's and in particular we study the scalar advection equation. It will be demonstrated how multiple grids can be used for fault recovery and still produce good results with the combination technique.

# Goal Orientated Adaptivity for Quantifying Uncertainty in Computationally Intensive Models

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Estimating the probability a system will fail and inferring the distributions of model parameters from experimental data are two tasks often undertaken when quantifying uncertainty in models of physical systems. Typically, probabilities of failure are estimated using importance sampling (IS) and the posterior distributions of model parameters are estimated using Monte-Carlo Markov Chain (MCMC) methods. Both IS and MCMC often require millions of samples to estimate the desired probabilistic quantities. When the model is computationally intensive to run these methods are infeasible. One approach used to circumvent this issue, is to construct a surrogate model of the expensive physics based model and run the sampling methods on the surrogate, which is cheap to evaluate. The surrogate is usually constructed in a manner that minimizes the the approximation error with respect to some ‘global’ measure. However this ‘global’ approach is inefficient. In the problems discussed here often only small regions of the input space are of interest. Local goal orientated adaptation, which respects, the localised nature of the problem can produce large reductions in the number of evaluations of the expensive physics model. In this talk we will discuss the use of locally adaptive sparse grids for the estimation of failure probabilities and Bayesian inference of parameter distributions.

# Dimension-adaptive Sparse Grid Quadrature for Integrals with Boundary Singularities

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Sparse grid quadrature is based on tensorproducts of univariate quadrature rules like Newton-Cotes formulae, Clenshaw-Curtis or Gauss-Legendre. In this talk we present new sparse grid quadrature schemes, that are based on certain univariate variable transformations. They yield an advantage over conventional methods, if the integrand possesses boundary singularities.

As an application we compute multivariate normal probabilities.

# Generated sets vs. sparse grids as sampling schemes for hyperbolic cross trigonometric polynomials

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The classical hyperbolic cross discrete Fourier transform suffers from growing condition numbers of their corresponding Fourier matrices. For that reason we change the spatial discretisation to generated sets which are generalisations of rank-1 lattices known from numerical integration. Our goal is to find spatial discretisations allowing the unique and stable reconstruction of multivariate trigonometric polynomials. We use nonlinear optimisation techniques to determine suitable generated sets. Allowing a mild oversampling, we get sampling schemes guaranteeing a fast and stable reconstruction of hyperbolic cross trigonometric polynomials with condition numbers of the corresponding reconstruction matrices near one. This talk draws the attention to stability problems that are somehow caused by the structure of sparse grids. Several reasonable examples confirm the theoretical results.

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