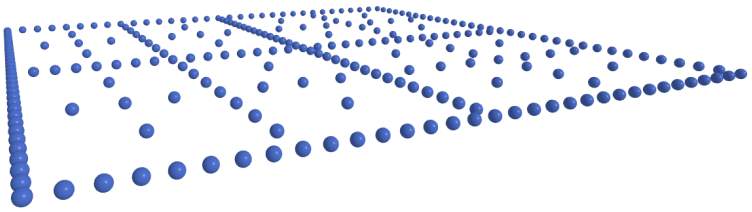
4th Workshop on

Sparse Grids and Applications

2016

PROGRAM and ABSTRACTS



U.S. DEPARTMENT OF ENERGY | Office of Science

October 4–7, 2016

Miami, Florida, USA

4th Workshop on

Sparse Grids and Applications

2016

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Miami, Florida, USA

Organized by

Department of Computational and Applied Mathematics
Oak Ridge National Laboratory

Sponsored by

Advanced Scientific Computing Research
Office of Science, US Department of Energy

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Program Overview

	October 4, 2016 (Tuesday)	October 5, 2016 (Wednesday)	October 6, 2016 (Thursday)	October 7, 2016 (Friday)
7:30-9:00	Breakfast (covered) and registration 8:50-9:00 Welcome and Overview	Breakfast (covered) and registration	Breakfast (covered) and registration	Breakfast (covered) and registration
9:00 - 9:35	**Jochen Garcke** Suboptimal feedback control of PDEs by solving HJB equations on adaptive sparse grids	**Christoph Pflaum** Ritz-Galerkin Discretization of PDE's with Variable Coefficients on Sparse Grids Using Prewavelets	**Tucker Carrington** A new sparse-grid collocation method for solving the Schroedinger equation	**Toni Volkmer** Sparse high-dimensional FFT with applications to data mining
9:35 - 10:10	**Lee Ricketson** Sparse grid techniques for particle–in–cell schemes	**Yingda Cheng** An Adaptive Multiresoluton Discontinuous Galerkin Method for Time-Dependent Transport Equations in Multi-dimensions	**Jingwei Hu** A Stochastic Galerkin Method for the Boltzmann Equation with High Dimensional Random Inputs Using Sparse Grids	**Bryan Quaifei** High-Order Adaptive Time Stepping for Vesicle Suspensions
10:10-10:45	Coffee Break(covered)	Coffee Break(covered)	Coffee Break(covered)	Coffee Break(covered)
10:45-11:20	**Abdellah Chkifa** A sparse grid collocation method based on LaVallée Poussin kernel.	**Miroslav Stoynov** A Dynamically Adaptive Sparse Grids Method for Quasi-Optimal Interpolation of Multidimensional Functions	**Yanzhao Cao** Backward SDE method for nonlinear filtering problems	**Soeren Wolfers** Multi-index approximation of multilinear problems with applications to kernel-based methods in UQ
11:20-11:55	**Jens Oettershagen** Optimal Integration in Reproducing Kernel Hilbert spaces	**Kilian Röhner** Spatial Refinement for Sparse Grid Classifiers based on Online Density Estimation	**Peng Chen** Adaptive sparse quadrature for high-dimensional integration with Gaussian distribution: application to Bayesian inverse problems	**Allessandro Alla** Nonlinear Model Reduction via Dynamic Mode Decomposition
11:55-12:30	**Fabian Franzelin** Preserving Positivity of Sparse Grid Surrogates	**Peter Jantsch** Lebesgue constant for weighted Leja sequences on unbounded domains	**Nick Dexter** Global Reconstruction of Solutions to Parametric PDEs via Compressed Sensing	**Constantin Weiser** Computationally Efficient Estimation of Multinomial and Panel Probit Models
12:30-13:45	Lunch Break (covered)	Lunch Break (covered)	Lunch Break (covered)	Lunch Break (covered)
13:45-14:45	**C. T. Kelley (invited)** Sparse Grids and Computational Chemistry	**Raul Tempone (invited)** Multi-Index approximation and smoothing techniques with sparse grids	**Tino Ullrich (invited)** Hyperbolic cross approximation--past, present and future	**Kenneth Judd (invited)** High-Dimensional Challenges in Economic Modeling
14:45-15:20	**Julian Valentin** Gradient-Based Topology Optimization with B-Splines on Sparse Grids	**Hoang Tran** Polynomial approximation via compressed sensing of high-dimensional functions on lower sets	**Rai Prashant** Low-rank approximation based quadrature for fast evaluation of quantum chemistry integrals	**Anh Tran** Comparison between Kaucher interval arithmetic, polynomial chaos expansion on Smolyak sparse grids, and Monte Carlo sampling in Molecular Dynamics simulation
15:20-15:50	Coffee Break(covered)	Coffee Break(covered)	Coffee Break(covered)	Closing remarks
15:50-16:25	**Bastian Bohn** Sparse grid regression in the noiseless setting	**David Pfander** Performance-Portable Close-to-Peak-Peformance Regression on Spatially Adaptive Sparse Grids Using Auto-Tuning	**Dirk Pflüger** Fault tolerance and silent fault detection with the sparse grid combination technique	
16:25-17:00	**Peter Schober** Solving Dynamic Portfolio Choice Models in Discrete Time Using Spatially Adaptive Sparse Grids	**Markus Siebenmorgen** Smoothing the payoff of European basket options	**Mario Heene** Massively parallel computation of high-dimensional PDEs with the Sparse Grid Combination Technique	
17:00-17:35	**Diane Guignard** A posteriori error estimate and adaptive sparse grid algorithm for random PDEs	**Lorenzo Tamellini** A sparse version of IGA solvers	**Guannan Zhang** A multilevel reduced-basis method for parameterized PDEs	

Directions and Orientation

Address of the venue

InterContinental Miami
100 Chopin Plaza, Miami, FL 33131
Phone: +1(305) 577-1000
`http://www.icmiamihotel.com`

By car from Miami International Airport

Take 836 East to I-95 South to Biscayne Boulevard (Exit 2A). Take the ramp down through two red lights. Turn left at the stop sign (get in the far right lane). Turn right at first red light (one half-block). The InterContinental Miami is on your right.

By Metrorail

For $2/person, guests can ride the rails to & from Miami International Airport MIA Mover all the way through to the InterContinental Miami. Board at the MIA Mover in the terminal, transfer to Metrorail and hop on the Metro Mover to the Bayfront Park Station. Public Transportation gets you here! Use the Trip Planner at `http://miamidade.gov/transit/mobile` or download the MDT Transit app for maps.

Parking

The daily parking rate is $42.00.

ABSTRACTS

Session, 9:00–10:10

Suboptimal feedback control of PDEs by solving HJB equations on adaptive sparse grids

Jochen Garcke[1], *Ilja Kalmikov*[2] *and Axel Kröner*[3]

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An approach to solve finite time horizon suboptimal feedback control problems for partial differential equations is proposed by solving dynamic programming equations on adaptive sparse grids. 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 value functions in (higher) space dimensions 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. The approach is illustrated for the wave equation and an extension to equations of Schrödinger type is indicated. We present several numerical examples studying the effect the parameters characterizing the sparse grid have on the accuracy of the value function and the optimal trajectory. closed-loop suboptimal control of PDEs and HJB equations and sparse grids and curse of dimensionality

Sparse grid techniques for particle-in-cell schemes

Lee Ricketson[1] *and Antoine Cerfon*[2]

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The kinetic equations governing plasma dynamics are six-dimensional PDEs for which the dominant computational concern is the curse of dimensionality. Motivated by this, the dominant scheme in many applications is particle-in-cell (PIC), which has the major advantage of reducing the dimensionality of the grid from six to three. The price to pay for this dimensionality reduction is the statistical error inherent to any particle method. Moreover, the statistical figure of merit is the number of particles per grid cell, meaning the curse of dimensionality persists. Since the number of grid cells can be very large, good statistical resolution requires overwhelmingly large particle populations. We propose to rectify this situation using the combination technique for sparse grids. In addition to accelerating grid computations, the cells in the relevant combination grids are much larger than for a comparable regular grid. In this way, we can achieve many more particles per cell for any given number of total particles. This results in dramatic reduction of statistical error. We present results from test cases that demonstrate the accuracy and efficiency of the new scheme.

Session, 10:45–12:30

A sparse grid collocation method based on LaVallée Poussin kernel

Moulay Abdellah Chkifa[1]

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In this talk, we present a new approach to polynomial approximation of functions in high dimension. We present a new non-intrusive collocation method that is based on Smolyack formula applied to polynomial approximations in one dimension that are based on Fejer and LaValle Poussin kernel. Smolyak formula allows us to transform a hierarchical collocation strategy in one dimension to a hierarchical collocation strategy in high dimension with possibly a straightforward computational formula and similar stability properties. We discuss the accuracy and stability of the introduced method versus the number of collocations needed and compare it to other existing strategies such as sparse hierarchical interpolation and sparse least squares. Numerical examples are provided to support the theoretical results and demonstrate the computational efficiency of the introduced method.

Optimal Integration in Reproducing Kernel Hilbert spaces

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

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We present a black box algorithm for the construction of integration algorithms in tensor products of reproducing kernel Hilbert spaces. Here, in a first step an optimization procedure is employed to compute both stable and optimally weighted sequences of nested quadrature rules. In a second step, quasi-optimal index sets are build to obtain (generalized) sparse grids that inherit certain optimality properties of the univariate quadrature rules.

Preserving Positivity of Sparse Grid Surrogates

Fabian Franzelin[1] *and Dirk Pflüger*[2]

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It is a challenging task to limit the range of values of a locally refined sparse grid surrogate $u^S G(x)$ to the range of some function $u(x)$ we want to approximate. If u(x) is a probability density function, for example, we want to preserve positivity and unit integrand. A common approach is to approximate $\log(u(x))$, which has been applied to the interpolation of functions with Gaussian shape in astrophysics [Griebel10] and in the context of density estimation [Pflueger10].

In this talk we present a different approach based on extending the grid of uSG such that we enforce a non-negative range of values everywhere on the input domain without enumerating the whole full grid. In our approach we search the smallest number of additional full grid points we need to add to the grid in order to achieve a non-negative range. We will theoretically derive which points we have to consider and present an algorithm that computes these points efficiently by evaluating

intersections of grid points with negative coefficients. We will present algorithms that compute the coefficients of the new grid points in linear time with respect to the number grid points.

This approach has two main advantages over the log-approach: (1) the surrogate is still just a linear combination of basis functions, and (2) computing its integral is easier than integrating exponentials. This makes it interesting for a large variety of applications. We will present results in the context of density estimation with locally adaptive sparse grids [Peherstorfer14] and uncertainty quantification [Franzelin16].

Invited Talk, 13:45–14:45

Sparse Grids and Computational Chemistry

C. T. Kelley

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Sparse grids can build efficient reduced order models of the potential energy surfaces (PESs) of molecules. A molecule with N-atoms has $3N - 6$ molecular coordinates (bond and torsion angles and bond lengths). The potential energy is a function of these coordinates and the discrete excitation state. An expensive electronic structure computation must be done to evaluate the energy. Therefore, to use the energy functional to drive dynamics or explore the intricate geometry of the PESs, one must use reduced order models.

We have used our sparse grid model to render PESs and explore their structures and to drive dynamic simulations. In this talk we will discuss the basic ideas of quantum chemistry simulations, describe the stages of model reduction, sparse grid interpolation being the final stage, and illustrate the ideas with our work on two molecules.

Session, 14:45–15:20

Gradient-Based Topology Optimization with B-Splines on Sparse Grids

Julian Valentin[1], *Daniel Hübner*[2], *Dirk Pflüger*[3] *and Michael Stingl*[4]

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We present sparse grids for gradient-based topology optimization using a homogenization approach. More precisely, we determine the shape of a cantilever such that its deformation under load gets minimized under a volume constraint. For each evaluation of the objective function, thousands of so-called elasticity tensors $E_k \in \mathbb{R}^{3\times3}$ have to be calculated using the method of finite elements. Each elasticity tensor calculation takes up several seconds, implying that it takes hours for one optimizer iteration for the high-dimensional optimization problem (tens of thousands of unknowns).

By replacing the elasticity tensors E_k with interpolants $\tilde{E}_k$, which can be precomputed during an offline phase, we can save a vast amount of time. The use of sparse grids commends itself since the number of parameters, on which the tensors depend, is infeasible for full grid approaches. However, most conventional sparse grid basis functions are not continuously differentiable, leading to kinks in corresponding approximations. Hierarchical B-splines are an alternative which allow to access the continuous derivatives explicitly and efficiently. Availability of gradients is of great use in many applications; in our case, we are able to use gradient-based optimization methods without having to approximate the derivatives artificially by finite differences.

Preserving positive the definiteness of the tensors is an additional requirement on the interpolation which posed a major challenge. Oscillations of the interpolants that arised due to overlapping supports of basis functions and the nature of B-splines crashed the optimizer. We remedy this issue by interpolating Cholesky factors on the sparse grids instead.

In this talk, we will also elaborate on the spatially adaptive sparse grids with boundary points we generated to interpolate the elasticity tensors. Finally, we will show results for two- and three-dimensional cantilevers.

Session, 15:50–17:35

Sparse grid regression in the noiseless setting

Bastian Bohn[1]

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One of the most important tasks in the field of machine learning is function regression. Here, many kernel-based methods have proven to be very successful in exploring given input data, e.g. support vector machines or radial basis function neural networks. However, when a large amount of data ($n > 10^3$) is available, these methods cannot be applied in a straightforward manner as their computational costs scale at least like n^2. Here, one has to consider other methods to reduce the cost complexity considerably. To this end, sparse grid methods can be employed if the dimension m of the domain is only moderately high ($m \leq 10$). Their runtime is only linear with respect to n. Spatial- and dimension-adaptive sparse grids allow to treat even higher-dimensional cases.

In this talk we examine the case of sparse grid regression for noiseless function evaluations. We extend the analysis of [CohenDavenportLeviatan13] to non-orthonormal bases and investigate the convergence behavior for a sparse grid regression algorithm based on tensor products of piecewise linear prewavelets. We will compare our results to the noisy case, where the asymptotic error bounds are considerably larger than in the noiseless case. Finally, we derive an appropriate balancing between the sparse grid discretization level and the number of data points in order to obtain a stable and optimally convergent method. We undermine our theoretical findings by several numerical results.

Solving Dynamic Portfolio Choice Models in Discrete Time Using Spatially Adaptive Sparse Grids

Peter Schober[1]

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I propose a dynamic programming approach to solve the Bellman equation in discrete time using spatially adaptive sparse grids. In doing so, I focus on Bellman equations arising in Finance, specifically dynamic portfolio choice models over the lifecycle.

Recent research trends aim at increasing the complexity of these models by adding more dimensions to the state space and/or including additional stochastic risk factors. This added complexity leads to models that, in most cases, cannot be solved analytically and therefore discrete time dynamic programming approaches are commonly employed.

Since the complexity of the dynamic programming approach (and other approaches) grows exponentially in the dimension of the state space, it suffers from the so called curse of dimensionality. Interpolating the value function using spatially adaptive sparse grids can break this curse to some extent. Following recent approaches proposed in the economics and computer science literature, I develop a spatially adaptive sparse grid interpolation scheme on the value function employing local basis functions. The addition of unspanned labor income or, comparably, non-hedgeable risk factors contributes to the dimensionality of the computation of the expectation of continuation. Hence, the computation of the expectation also suffers from the curse of dimensionality when numerical quadrature rules are applied. To address this issue, I complement my approach by the use of global polynomial-based numerical quadrature rules on sparse grids to compute expectations over the stochastic risk factors.

I study the numerical properties of my approach by replicating well-known dynamic portfolio choice models with varying state space dimensionality and stochastic risk factors.

A posteriori error estimate and adaptive sparse grid algorithm for random PDEs

Diane Guignard[1], *Fabio Nobile*[2] *and Marco Picasso*[3]

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In this talk, we consider a simple elliptic diffusion problem with a random coefficient that depends affinely on a finite number of random variables. This problem is solved using the stochastic collocation finite element method. A residual-based a posteriori error estimate that controls the two sources of error, the physical and stochastic spaces discretization, is first derived. The stochastic error estimator is then used to drive an adaptive sparse grid algorithm which aim at circumvent the so-called "curse of dimensionality" inherent to tensor grids. Several numerical examples are given to illustrate the performance of the adaptive procedure.

Session, 9:00–10:10

Ritz-Galerkin Discretization of PDE's with Variable Coefficients on Sparse Grids Using Prewavelets

Christoph Pflaum[1] *and Rainer Hartmann*[2]

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Sparse grids can be used to discretize elliptic differential equations of second order on a d-dimensional cube. Using the Ritz-Galerkin discretization, one obtains a linear equation system with $O(N(\log N)^{d-1})$ unknowns. The corresponding discretization error is $O(N^{-1}(\log N)^{d-1})$ in the H^1-norm. A major difficulty in using this sparse grid discretization is the complexity of the related stiffness matrix. To reduce the complexity of the sparse grid discretization matrix, we apply prewavelets and a discretization with semi-orthogonality. Stability and optimal convergence of this discretization is proved with respect to the H^1-norm for the Helmholtz equation with variable coefficients and arbitrary dimension d (see [1]). Furthermore, a recursive algorithm is presented, which performs a matrix vector multiplication with the stiffness matrix by $O(N(\log N)^{d-1})$ operations. Simulation results up to level 10 are presented for a 6-dimensional Helmholtz problem with variable coefficients. The simulation results show an optimal sparse grid convergence behavior. The condition number of the linear equation system is less than 10. This means only a few cg-iterations are need to obtain a small algebraic error. Furthermore, simulation results are presented for Poisson's equation on a 3-dimensional curvilinear bounded domain. Simulation results show optimal convergence behavior with respect to the L^2-norm.

[1] C. Pflaum and R. Hartmann, A Sparse Grid Discretization of the Helmholtz Equation with Variable Coefficients in High Dimensions, to appear in SINUM, 2016.

An Adaptive Multiresoluton Discontinuous Galerkin Method for Time-Dependent Transport Equations in Multi-dimensions

Yingda Cheng[1] *and Wei Guo*[2]

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In this talk, we present an adaptive multiresolution DG method for time-dependent transport equations. The scheme is constructed based on the standard weak form of DG method for hyperbolic equations and the multiwavelets of Alpert. We show that our scheme can naturally go back to a sparse grid DG method, saving computational cost, when the solution possess sufficient smoothness. When the solution is no longer smooth, the adaptive algorithm that uses the hierarchical surplus as the refinement or coarsening indicator, can automatically capture the local structures. We use the Hash table as the underlying data structure and can deal with equations in arbitrary dimensions. By using the DG framework, many nice properties are retained for the transport equations. The numerical scheme is validated by benchmark tests with smooth and nonsmooth solutions, and the standard Vlasov-Poisson (VP) system and oscillatory VP system.

Session, 10:45–12:30

A Dynamically Adaptive Sparse Grids Method for Quasi-Optimal Interpolation of Multidimensional Functions

Miroslav Stoyanov[1] *and Clayton Webster*[2]

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In this work we develop a dynamically adaptive sparse grids (SG) method for quasi-optimal interpolation of multidimensional analytic functions defined over a product of one dimensional bounded domains. The goal of such approach is to construct an interpolant in space that corresponds to the "best M-terms" based on sharp a priori estimate of polynomial coefficients. In the past, SG methods have been successful in achieving this, with a traditional construction that relies on the solution to a Knapsack problem: only the most profitable hierarchical surpluses are added to the SG. However, this approach requires additional sharp estimates related to the size of the analytic region and the norm of the interpolation operator, i.e., the Lebesgue constant. Instead, we present an iterative SG procedure that adaptively refines an estimate of the region and accounts for the effects of the Lebesgue constant. Our approach does not require any a priori knowledge of the analyticity or operator norm, is easily generalized to both affine and non-affine analytic functions, and can be applied to sparse grids built from one dimensional rules with arbitrary growth of the number of nodes. In several numerical examples, we utilize our dynamically adaptive SG to interpolate quantities of interest related to the solutions of parametrized elliptic and hyperbolic PDEs, and compare the performance of our quasi-optimal interpolant to several alternative SG schemes.

Spatial Refinement for Sparse Grid Classifiers based on Online Density Estimation

Kilian Röhner[1] *and Hans-Joachim Bungartz*[2]

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Online density estimation on sparse grids can be sped up by splitting the process into two phases. In the offline phase, the data-independent, yet grid-dependent system matrix is decomposed so that the density estimation can be calculated in an online phase with reduced complexity. The offline decomposition has to be done with a regular sparse grid because the data will only be available at process time in case of online learning. Then, in order to adapt to the data, we want to spatially refine the grid. A change of the underlying grid thus requires an update of the decomposition. We present an approach that allows for such a grid update in the decompositions. In classification, we can calculate such a density estimation for each class in order to use Bayes' theorem to construct a classifier. When improving our classifier in the online learning setting, we need to adapt to the data and spatially refine the grids from the density estimations with the task of classification in mind. We search for refinable grid points that will help us best identify the border of two classes in critical regions. Here, we make use of the sparse grid structure in order to identify these borders fast. With growing number of classes, the number of potential critical regions grows quadratically. We try to reduce the search for these regions by taking into account the likelihood that the corresponding classes are dominant. Using example datasets, we show that online adaptive methods often outperform classical approaches with regards to runtime and memory consumption. Also, they are

competitive with regard to accuracy, since we make up for the regular sparse grid decomposed during the offline phase that neglected the concrete data by spatially refining the model in the online phase.

Lebesgue constant for weighted Leja sequences on unbounded domains

Peter Jantsch[1], *Clayton Webster*[2] *and Guannan Zhang*[3]

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The standard Leja points are a nested sequence of points defined on a compact subset of the real line, and can be extended to unbounded domains with the introduction of a weight function $w : \mathbb{R} \to [0, 1]$. Due to a simple recursive formulation, such abcissas show promise as a foundation for high-dimensional approximation methods such as sparse grid collocation, deterministic least squares, and compressed sensing. Just as in the unweighted case of interpolation on a compact domain, we use results from potential theory to prove that the Lebesgue constant for the Leja points grows subexponentially with the number of interpolation nodes.

Invited Talk, 13:45–14:45

Multi-Index approximation and smoothing techniques with sparse grids

Raul Tempone[1]

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We present the Multi-Index Stochastic Collocation method (MISC) for computing statistics of the solution of a PDE with random data. MISC is a combination technique using mixed differences of spatial approximations and quadratures over random data. We provide (i) an optimal selection of the most effective mixed differences to include in MISC, (ii) a complexity analysis and (iii) a numerical study showing its effectiveness, comparing it with other related methods available in the literature.

Later, we will briefly address the problem of pricing basket options in a multivariate Black-Scholes or Variance Gamma model. From a numerical point of view, pricing such options corresponds to moderate and high dimensional numerical integration problems with non smooth integrands. Due to this lack of regularity, higher order numerical integration techniques may not be directly available, requiring the use of methods like Monte Carlo specifically designed to work for non-regular problems. We propose here to use the inherent smoothing property of the density of the underlying in the above models to mollify the payoff function using an exact conditional expectation. The resulting conditional expectation is unbiased and yields a smooth integrand, which is amenable to the efficient use of adaptive sparse grid cubature. Numerical examples indicate that the high-order method may perform orders of magnitude faster compared to Monte Carlo or Quasi-Monte Carlo in dimensions up to 25.

References:

[1] "Multi-Index Stochastic Collocation convergence rates for random PDEs with parametric regularity", by A. L. Haji Ali, F. Nobile, L. Tamellini, and R. Tempone. To appear in Foundations of Computational Mathematics, 2016.

[2] "Multi-Index Stochastic Collocation for random PDEs", by A. L. Haji Ali, F. Nobile, L. Tamellini, and R. Tempone. Computers and Mathematics with Applications, Vol. 306, pp. 95–122, July 2016.

[3] "Smoothing the payoff for efficient computation of basket option pricing", by C. Bayer, M. Siebenmorgen, and R. Tempone. *arXiv:1607.05572*. July 2016.

[4] "Sparse approximation of multilinear problems with applications to kernel-based methods in UQ", by F. Nobile, R. Tempone, and S. Wolfers. Preprint, August 2016.

[5] "Convergence of quasi-optimal sparse grid approximation of Hilbert-valued functions: application to random elliptic PDEs", by F. Nobile, L. Tamellini, and R. Tempone. Numerische Mathematik, Vol. 134, Issue 2, pp 343–388, October 2016.

Session, 14:45–15:20

Polynomial approximation via compressed sensing of high-dimensional functions on lower sets

Hoang Tran[1], *Abdellah Chkifa*[2], *Nick Dexter*[3], *and Clayton Webster*[4]

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This work proposes and analyzes a compressed sensing approach to polynomial approximation of complex-valued functions in high dimensions. Of particular interest is the setting where the target function is smooth, characterized by a rapidly decaying orthonormal expansion, whose most important terms are captured by a lower (or downward closed) set. By exploiting this fact, we present a novel weighted L^1 minimization procedure with a precise choice of weights, and a new version of iterative hard thresholding method, for imposing the downward closed preference. Theoretical results reveal that our computational approaches possess a provably reduced sample complexity compared to existing compressed sensing techniques presented in the literature. In addition, the recovery of the corresponding best approximation using these methods is established through an improved bound for the restricted isometry property. Numerical examples are provided to support the theoretical results and demonstrate the computational efficiency of the new weighted L^1 minimization strategy.

Session, 15:50–17:35

Performance-Portable Close-to-Peak-Peformance Regression on Spatially Adaptive Sparse Grids Using Auto-Tuning

David Pfander[1] *and Dirk Pflüger*[2]

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Modern hardware architectures offer high performance by employing multiple cores, multiple vector units, deeply-pipelined execution units and a sophisticated cache hierarchy. To reach short runtimes for increasingly larger problems, highly-optimized implementations have to make use of these performance-enhancing architectural details. However, to achieve a significant fraction of the peak performance of a hardware device, manually-optimized implementations are still common practice. This leads to two problems: A tedious development process and a loss of portability, especially if the implementation uses intrinsics or inline assembly. We propose an auto tuning approach that reduces the effort required by automatizing compute kernel variant testing. Because our compute kernels consist of code generators that emit portable code and by employing parameterized optimizations, our approach enables performance-portability with little extra effort. This approach was applied to the sparse grid regression method. The sparse grids regression method solves a penalized least squares problem and is algorithmically well-suited for large datasets with millions of data points as it scales linearly in the dataset size. To target a wider range of regression problems, we present compute kernels for sparse grids with two different basis functions: Linear basis function and modified linear basis function which extrapolate towards the boundary for an algorithmically inexpensive boundary treatment. Furthermore, our algorithms support spatially adaptive sparse grids to reduce the effort required to solve the regression problem and thereby enable larger problems as well as problems of higher dimension. Our experiments show that we reach up to 64% of the peak performance on graphics processor. This corresponds to 96% of the achievable peak performance if the instruction mix imposed by the algorithm is considered. On processors and accelerators the performance is slightly lower, but at least 50% of the reachable peak performance are achieved on every device under test. Our work investigates the challenges that have to be overcome to map numerical code to modern hardware and shows how these challenges can be overcome.

Smoothing the payoff of European basket options

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The pricing problem of European basket options in a Black-Scholes model leads in certain cases to the calculation of the integral

$$E\left[\left(\sum_{i=1}^{d} w_i e^{X_i} - K\right)^+\right],$$

where $X \sim \mathcal{N}(0, \Sigma)$ with a covariance matrix Σ and $d \gg 1$. Hence, we have to compute an integral over the integration domain $\mathbb{R}^d$ for an integrand with a kink. We provide a simple smoothing

technique which produces an analytic integrand and is able to reduce the dimensionality of the integration problem by 1. Moreover, this smoothing does not introduce any approximation error. In particular, we transform the d-dimensional random variable in such a way that it is feasible to apply the famous Black-Scholes formula with respect to a single coordinate. The resulting integration problem over $\mathbb{R}^{d-1}$ of an analytic function is then solved by an adaptive sparse grid approach. This leads, at least in considerably high dimensions, to better convergence results compared to those of standard Monte Carlo or quasi-Monte Carlo quadratures. The technique can be easily transferred to the more involved and practical relevant Variance Gamma model.

A Sparse Version of IGA Solvers

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Isogeometric Analysis (IGA) has been introduced by Hughes and coworkers in the early 2000 to bridge the gap between Computer Aided Design (CAD) and PDE-based engineering analysis. The core idea of IGA is to use the basis functions used by CAD designers to describe geometries – typically cubic splines or Non-Uniform Rational B-Splines (NURBS) – as a basis for the approximation of the solution of the PDE as well; the PDE is then solved with traditional approaches (hp-Galerkin, collocation). The main advantages of IGA over standard Finite Elements analysis (FEA) are the straightforward treatment of complex geometries, without need for mesh generation (although the CAD description of the geometry must be suitably generated), and the fact basis functions with high-order and high-degree of regularity (or even with varying degrees of smooothness) can be easily generated, thanks to the flexibility of the splines/NURBS bases. A well-established mathematical theory has been developed over the last two decades and nowadays IGA can be successfully applied to solid, fluid, and multiphysics problems, and even outperform FEA in certain circumstances; however, despite the effort of the IGA community, efficient algorithms for the assembly of Galerkin matrices (especially for higher order splines/NURBS) and local refinement technologies are still missing. Two- and tri-dimensional splines/NURBS are built by tensorization of univariate bases, hence sparsification of the method can be done quite easily, at-least for the h-version of IGA. The combination technique then allows to reuse existing IGA solvers. In this talk, we will discuss the potential of sparse-IGA methods and, if time allows, how sparse-IGA can be embedded into Multi-Index Monte Carlo / Multi-Index Stochastic Collocation schemes for the solution of PDEs with random coefficients.

Session, 9:00–10:10

A new sparse-grid collocation method for solving the Schroedinger equation

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I shall present a new collocation method for solving the Schroedinger equation. Collocation has several important advantages over the Galerkin method. Most importantly, it obviates the need for quadrature. The kinetic energy matrix-vector product is evaluated by transforming a vector labelled with (nondirect product) grid indices to a vector labelled by (nondirect product) basis indices. Both the transformation and application of the kinetic energy operator scale favourably. Some ideas of general interest: 1) a general scheme for pruning bases and grids when using sparse-grid methods; 2) nested functions and grids in which the difference between the number of points (and functions) in level i+1 and level i is very small (e.g. one); 3) collocation without a "mass matrix"; 4) collocation with spectral Lagrange-type functions; 5)"hierarchical" functions built from non-polynomial general bases.

A Stochastic Galerkin Method for the Boltzmann Equation with High Dimensional Random Inputs Using Sparse Grids

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We propose a stochastic Galerkin method using sparse grids for the Boltzmann equation with high dimensional random inputs. The method uses locally supported piecewise polynomials as an orthonormal basis of the random space. By a sparse grid technique, only a moderate number of basis functions are required to achieve good accuracy in high dimensional random spaces. We discover a sparse structure of a set of basis-related coefficients, which allows us to accelerate the computation of the collision operator. Regularity of the solution of the Boltzmann equation in the random space and an accuracy result of the stochastic Galerkin method are proved in multidimensional case. The efficiency of the method is illustrated by numerical examples with uncertainties from the initial data, boundary data and collision kernel.

Session, 10:45–12:30

Backward SDE method for nonlinear filtering problems

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A nonlinear filtering problem can be classified as a stochastic Bayesian optimization problem of identifying the state of a system with a noise perturbation given noisy observations of the system. Well known numerical simulation methods include unscented Kalman filters and particle filters. In this talk, we attempt to construct efficient numerical methods using forward backward stochastic differential equations. The backward SDEs for nonlinear filtering problems are the counter parts of Fokker-Planck equations for SDEs with no observation constraints. We will describe the process of deriving such backward SDEs as well as the corresponding high order numerical algorithms for nonlinear filtering problems.

Adaptive sparse quadrature for high-dimensional integration with Gaussian distribution: application to Bayesian inverse problems

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In this work, we present convergence analysis of an adaptive sparse quadrature for high/infinite-dimensional integration with respect to Gaussian distributed random variables. Under certain assumptions on the univariate quadrature and the regularity of the integrand, we demonstrate the dimension-independent convergence property of the proposed algorithm. We apply this algorithm to infinite-dimensional Bayesian inverse problems in combination of a Hessian-based parametrization of the uncertain parameter.

Global Reconstruction of Solutions to Parametric PDEs via Compressed Sensing

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We present a novel theoretical framework for solving parametric PDEs via compressed sensing over tensor-products of Hilbert spaces. This work builds on the existing theory for the recovery of compressible solutions via ℓ^1-minimization, and guarantees convergence in terms of the errors of the best s-term approximation and the residual in a given polynomial subspace. Compared to other approaches that only recover a functional of the solution, e.g. evaluation at a single point, our

approach recovers the solution globally over the physical domain. We also provide extensions to the fixed point continuation algorithms and the Bregman iterations for solving the basis pursuit problem in this context. We conclude with numerical results demonstrating the efficacy of our approach in high-dimensions and comparisons with sparse grids and stochastic Galerkin approximations.

Invited Talk, 13:45–14:45

Hyperbolic cross approximation–past, present and future

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Hyperbolic cross approximation is a special type of multivariate approximation. Recently, driven by applications in engineering, biology, medicine and other areas of science, new challenging problems have appeared. In this plenary talk I will survey on classical as well as contemporary methods developed in multivariate approximation theory in the last decades. We will focus on (non)linear approximation, preasymptotics for high-dimensional problems, sparse grid sampling recovery and numerical integration. The respective algorithms are known to work very well in moderate space dimensions and have potential for applications in really high dimensions. It is now well understood that this theory is important both for theoretical study and for practical applications. Nevertheless, both theoretical analysis and construction of practical algorithms turn out to be very difficult problems. Motivated by recently discovered deep connections between hyperbolic cross approximation (and related sparse grids) and other areas of mathematics (such as probability, discrepancy and numerical integration) we will put emphases on the presentation of ideas and methods rather than just listing known results in this area. We will also focus on very recent results which sometimes highlight new interesting directions of research and I hope to stimulate further active research in this fascinating and challenging area of approximation theory and numerical analysis.

Session, 14:45–15:20

Low-rank approximation based quadrature for fast evaluation of quantum chemistry integrals

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A new method is proposed for a fast evaluation of high-dimensional integrals of potential energy surfaces (PES) that arise in many areas of quantum dynamics. Our approach decomposes the integrand into suitable low-rank tensor formats using a set of integrand evaluations. The high dimensional integration problem is then reduced to a relatively short sum of products of easy-to-evaluate low-dimensional integrals, each of which can be estimated using appropriate (sparse) quadrature rules. The decomposition is achieved by suitable version of alternating least squares algorithm depending on the type of tensor format considered. This approach also eradicates a force-constant evaluation as the hotspot of many quantum dynamics simulations and also delays the curse of dimensionality. In this work, we specifically consider canonical and tensor train formats for approximation. This general method is applied to two applications in quantum chemistry.

The first application is anharmonic vibrational zero-point and transition energy calculations of molecules using the second-order diagrammatic vibrational many-body Green's function theory with a harmonic-approximation reference. In this application, not only the PES but also Green's functions are high dimensional, both of which are thus subjected to a low-rank decomposition. Our approach achieves an accuracy comparable to Monte-Carlo techniques with a several orders of magnitude speedup, i.e. with a drastically lower number of PES evaluations.

The second application involves estimation of anharmonic state counts and partition functions for molecules via classical phase space integrals in both cartesian and curvilinear coordinates. Here, the integrand is the volume of a hypersphere whose radius is a function of the PES. The radius is approximated in a rank one canonical tensor format in order to avoid exponential increase in the rank of the integrand obtained by the application of hypersphere volume function. As in the first application, we again obtain orders of magnitude speedup as compared to the benchmark Monte Carlo evaluations.

Session, 15:50–17:00

Fault tolerance and silent fault detection with the sparse grid combination technique

Dirk Pflüger[1], *Alfredo Parra Hinojosa*[2], *Mario Heene*[3], *Hans-Joachim Bungartz*[4] *and Markus Hegland*[5]

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Future exascale systems are expected to have a mean time between failures in the range of minutes. Classical approaches such as checkpointing and then recomputing the missing solution will be therefore out of scope. Algorithm-based fault tolerance (ABFT) in contrast aims to continue without recomputations and with only minor extra computational effort. To achieve this, numerical schemes have to be adapted.

The project EXAHD within Germany's priority program "Software for Exascale Computing" (SPPEXA) develops new fault tolerant algorithms for future high-performance computing (HPC) systems. The target application is the solution of high-dimensional PDEs, for example for the simulation of hot fusion plasmas.

EXAHD exploits the hierarchical extrapolation scheme provided by the sparse grid combination technique. Using the hierarchical ansatz, we show how to mitigate hard faults. Furthermore, even soft faults (for example due to silent data corruption) can often be detected and handled. We have implemented a fault-tolerance software layer for HPC systems and can show results for massively parallel experiments.

Massively parallel computation of high-dimensional PDEs with the Sparse Grid Combination Technique

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The problem sizes for the solution of higher-dimensional PDEs, such as the simulation of plasma turbulence in a fusion device, are often very limited due to the exponential increase in the degrees of freedom with the dimensionality. With the Sparse Grid Combination Technique (SGCT) we can mitigate this so-called curse of dimensionality and push the computational limits of high-dimensional simulations significantly.

Offering a second level of parallelism, the SGCT minimizes the need for global communication and ensures scalability on future (exascale) HPC systems. In this work we present our scalable parallelization concept, our distributed sparse grid data-structures, and our efficient algorithms to handle the remaining global communication. We provide experimental results that demonstrate the scalability of our algorithms to 180,225 cores on the supercomputer Hazel Hen. Furthermore, we present our experiences gained within the project EXAHD of Germany's priority program "Software for Exascale Computing" (SPPEXA) through applying the SGCT to large-scale plasma turbulence simulations with GENE.

A multilevel reduced-basis method for parameterized partial differential equations

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An important approximation scheme for alleviating the overall computational complexity of solving parameterized PDEs is known as multilevel methods, which have been successfully used in the Monte Carlo and collocation setting. In this effort, we propose to improve the multilevel methods with the use of reduced-basis (RB) techniques for constructing the spatial-temporal model hierarchy of PDEs. Instead of approximating the solution manifold of the PDE, the key ingredient is to build approximate manifolds of first-order differences of PDE solutions on consecutive levels. To this end, we utilize a hierarchical finite element (FE) framework to formulate an easy-to-solve variational FE system for the first-order differences. Moreover, by deriving a posteriori error estimates for the RB solutions, we also intend to develop a greedy-type adaptive strategy in order to construct a good set of snapshots. The main advantage of our approach lies in the fact that the manifold of the first-order differences becomes progressively linear as the physical level increases. Thus, much fewer expensive snapshots are required to achieve a prescribed accuracy, resulting in significant reduction of the offline computational cost of greedy algorithms. Furthermore, our approach combines the advantages of both multilevel Monte Carlo and multilevel collocation methods, in the sense that it can generate snapshots anywhere in the parameter domain but also features fast convergence.

Session, 9:00–10:10

Sparse high-dimensional FFT with applications to data mining

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We consider the (approximate) reconstruction of a high-dimensional (e.g. $d = 10$) periodic signal from samples using a trigonometric polynomial $p_I \colon \mathbb{T}^d \simeq [0,1)^d \to \mathbb{C}$,

$$p_I(\boldsymbol{x}) := \sum_{\boldsymbol{k} \in I} \hat{p}_{\boldsymbol{k}} \, \mathrm{e}^{2\pi \mathrm{i} \boldsymbol{k} \cdot \boldsymbol{x}}, \quad \hat{p}_{\boldsymbol{k}} \in \mathbb{C},$$

where $I \subset \mathbb{Z}^d$ is a suitable and unknown frequency index set. For this setting, we present a method which adaptively constructs the index set I of frequencies belonging to the non-zero or (approximately) largest Fourier coefficients in a dimension incremental way. This method computes projected Fourier coefficients from samples along suitable rank-1 lattices $\Lambda(\boldsymbol{z}, M) := \{\frac{j}{M}\boldsymbol{z} \mod \mathbf{1} \colon j = 0, \ldots, M-1\} \subset \mathbb{T}^t$, $\boldsymbol{z} \in \mathbb{Z}^t$, $t \in \{1, \ldots, d\}$, and then determines the frequency locations. For the computation, only one-dimensional fast Fourier transforms (FFTs) and simple index transforms are used. When we assume that the signal has sparsity $s \in \mathbb{N}$ in frequency domain and the frequencies $\boldsymbol{k}$ are contained in the cube $[-N, N]^d \cap \mathbb{Z}^d$, $N \in \mathbb{N}$, our method requires $\mathcal{O}(d\, s^2 N)$ samples and $\mathcal{O}(d\, s^3 + d\, s^2 N \log(s\, N))$ arithmetic operations in the case $\sqrt{N} \lesssim s \lesssim N^d$.

We discuss applications of this method to regression / classification. Given a set of data $S := \{(\boldsymbol{y}_\ell, f_\ell)\}_{\ell=1,\ldots,L}$ with nodes $\boldsymbol{y}_\ell \in \mathbb{R}^d$ and function values / class labels $f_\ell \in \mathbb{R}$, we employ the regularization network approach and consider the regularized least squares problem

$$\frac{1}{L} \sum_{\ell=0}^{L-1} (f_\ell - p_I(\boldsymbol{y}_\ell))^2 + \lambda \Phi(p_I) \to \min,$$

with regularization parameter $\lambda \geq 0$ and e.g. with $\Phi(p_I) := \|\nabla p_I\|_2^2$. Now, we use a modified version of our dimension-incremental method for the proposed task. For evaluating our ansatz function p_I at the data nodes $\boldsymbol{y}_\ell$ in a fast way, we apply Taylor's formula in combination with rank-1 lattices $\Lambda(\boldsymbol{z}, M)$. Using suitable heuristics, we obtain a dimensionally adaptive and dimensionality reducing algorithm, which selects appropriate attributes / features from the given data and yields a sparse low-dimensional approximant p_I.

This is joint work with Daniel Potts.

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High-Order Adaptive Time Stepping for Vesicle Suspensions

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I will present an adaptive high-order accurate time-stepping numerical scheme for the flow of vesicles suspended in a Stokesian fluid. The scheme can be summarized as an approximate implicit spectral deferred correction (SDC) method that is built on a linearized low-order time stepping method. Invariant properties of vesicle flows are used to estimate the local truncation error which in turn adjusts the time step size. Two-dimensional results for single-vesicle flows, constricted geometry flows, converging flows, and flows in a Couette apparatus will be presented.

Session, 10:45–12:30

Multi-index approximation of multilinear problems with applications to kernel-based methods in UQ

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We provide a novel framework for the sparse approximation of multilinear problems and show that several problems in Uncertainty Quantification fit within this framework. In these problems, the value of a multilinear map has to be approximated using approximations of different accuracy and computational work of the arguments of this map. We propose and analyze a generalized version of Smolyak's algorithm, which provides sparse approximation formulas with convergence rates that mitigate the curse of dimension that appears in multilinear approximation problems with a large number of arguments. We apply the general framework to response surface approximation and optimization under uncertainty for parametric partial differential equations using kernel-based approximation. The theoretical results are supplemented by numerical experiments.

Nonlinear Model Reduction via Dynamic Mode Decomposition

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We propose a new technique for obtaining reduced order models for nonlinear dynamical systems. Specifically, we advocate the use of the recently developed Dynamic Mode Decomposition (DMD), an equation-free method, to approximate the nonlinear term. DMD is a spatio-temporal decomposition of a data matrix that correlates spatial features while simultaneously associating the activity with periodic temporal behavior. With this decomposition, one can obtain a fully reduced dimensional surrogate model and avoid the evaluation of the nonlinear term in the online stage. This allows for a reduction in the computational cost, and, at the same time, accurate approximations of the problem. We present a suite of numerical tests to illustrate our approach and to show the effectiveness of the method in comparison to existing approaches.

Computationally Efficient Estimation of Multinomial and Panel Probit Models

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Multinomial probit models are widely used for the analysis of individual choices in empirical economic research. Unlike simpler models like multinomial or nested logit models, they allow for a completely flexible or arbitrarily parameterized substitution pattern between alternatives. Maximum likelihood estimation of multinomial and panel probit models is complicated by the fact that the likelihood function contains an analytical intractable integral, which needs to be approximated. Since the 1990s, the Geweke-Hajivassiliou-Keane (GHK) simulator has been the method of choice for tackling this approximation problem. Using simulators based on pseudo or quasi random number generators, they are now implemented in standard software like Stata, the NLOGIT addition to LIMDEP or the mlogit package in R. While these simulation estimators perform better than many alternative approaches, the computational burden of an accurate approximation of choice probabilities can be substantial and often prohibitive. Less accurate approximations lead to convergence problems of the likelihood maximization algorithm and to biased parameter estimates. We revisit the problem of an accurate approximation of multinomial and/or longitudinal probit likelihoods using different newer approaches of numerical integration. Namely we substitute the (pseudo/quasi) random numbers by efficient tailored sparse grid quadrature rules. Within a simulation study we compare their performance in terms of choice probability approximation as well as parameter estimation and find dramatic improvements over the standard GHK approach. They reduce the computational burden by orders of magnitude, allowing a much more widely applicable, reliable, and convenient application of these models in empirical research.

Invited Talk, 13:45–14:45

High-Dimensional Challenges in Economic Modeling

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Economies are complex dynamical systems. Any plausible model will be of very high dimension when you consider the variety of products and actors operating in different social and physical environments. An important feature of economics is that people's decisions are based on beliefs of future economic conditions, implying that people are not particles. The aim of the mathematical models is to solve for the decisions of the agents, which will depend on a high-dimensional state space. The forward-looking nature of economic decisions implies that one needs to solve nonlinear partial differential equations where some future terminal time is the ?initial? condition. Fortunately, economic dynamics are similar to diffusion processes and the unknown decision rules are well-behaved functions. In particular, we use many tools from high-dimensional methods, such as sparse grids, and Smolyak interpolation and quadrature, and we are beginning to deploy methods from machine learning. In many problems, we do not know what part of the state space is relevant, but we have developed extensions of standard approximation methods to handle that problem. Our methods make extensive use of parallel computing. I will present an example of an integrated model of stochastic climate and stochastic economic processes which we solved using 80K cores in four hours, and for which we have demonstrated linear scaling even beyond 80K cores. The application also highlights weaknesses of the existing work on climate change and economics. This work clearly shows that economic problems present novel challenges for high-dimensional mathematics and massively parallel computing, and that those tools can significantly improve the realism of economic analysis.

Session, 14:45–15:20

Comparison between Kaucher interval arithmetic, polynomial chaos expansion on Smolyak sparse grids, and Monte Carlo sampling in Molecular Dynamics simulation

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The accuracy of the interatomic potential models play an essential role in the molecular dynamics (MD) predictions. These interatomic potentials, which characterizes the interactions between atoms and molecules, are the main source of model-form uncertainty in MD and usually referred to as epistemic uncertainty. Another type of uncertainty, which comes from the thermal fluctuation of the MD simulation, typically induced by a thermostat, is referred to as aleatory uncertainty. In this work, we compare the effectiveness of three uncertainty quantification methods, namely Kaucher interval arithmetic, polynomial chaos expansion on Smolyak sparse grids, and Monte Carlo sampling methods in the application of Lennard-Jones potentials for liquid argon coupled with Langevin thermostat. The example is chosen such that both aleatory and epistemic uncertainty are included. Computational cost and accuracy are discussed between these three methods.

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