Institut für Numerische Simulation

Rheinische Friedrich-Wilhelms-Universität Bonn

6th Workshop on High-Dimensional Approximation

Book of Abstracts

Date:	2015-09-14/2015-09-18
Location:	Bonn, Germany
Sponsor:	University of Bonn
	Hausdorff Center for Mathematics
	Fraunhofer SCAI
Scientific Committee:	Albert Cohen (U Pierre et Marie Curie, France)
	Jochen Garcke (U Bonn & Fraunhofer SCAI, Germany)
	Michael Griebel (U Bonn & Fraunhofer SCAI, Germany)
	Wolfgang Hackbusch (Max Planck Institut Leipzig, Germany)
	Markus Hegland (ANU, Australia)
	Frances Kuo (UNSW, Australia)
	Christoph Schwab (ETH Zürich, Switzerland)
	Ian Sloan (UNSW, Australia)
	Henryk Wozniakowski (Columbia U, USA & Warsaw U, Poland)
	Harry Yserentant (TU Berlin, Germany)
Local Organizers:	Bastian Bohn
	Barbara Fuchs
	Jochen Garcke
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Contents

General Information

The 6th Workshop on High-Dimensional Approximation covers current research on all numerical aspects of high-dimensional problems. The scope ranges from high-dimensional approximation theory over computational methods to engineering and scientific applications.
This international workshop is the sixth in a series which were previously held at The Australian National University in Canberra (HDA05, HDA07, and HDA2013), at the University of New South Wales in Sydney (HDA09), and at the University of Bonn (HDA2011). This time the workshop returns to University of Bonn to be held from 14. – 18. September 2015.

Workshop Venue

The workshop is hosted by the

Institute for Numerical Simulation,
University of Bonn,
`http://www.ins.uni-bonn.de`,

in cooperation with the

Hausdorff Center for Mathematics,
University of Bonn,
`http://www.hcm.uni-bonn.de`

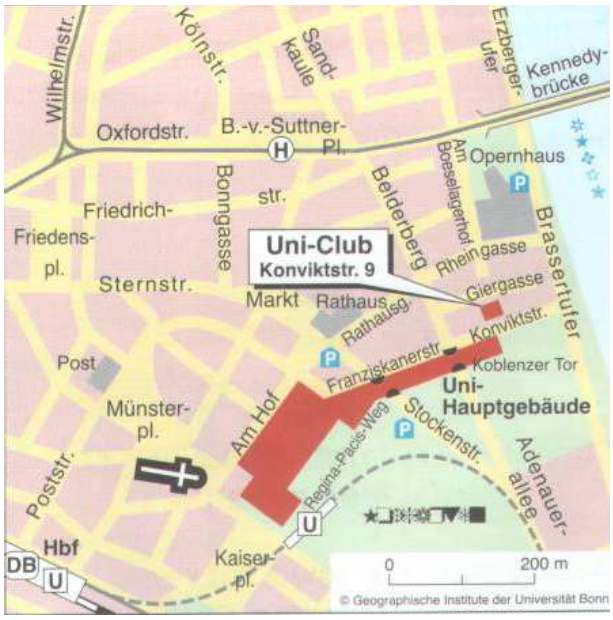
and the

Fraunhofer Institute for Algorithms and
Scientific Computing SCAI,
Sankt Augustin,
`http://www.scai.fraunhofer.de`.

The workshop takes place at the

Universitätsclub Bonn,
`http://www.uniclub-bonn.de`.
Konviktstraße 9, 53115, Bonn.

Our registration desk will be open Monday, September 14th, from 08:00-09:00 a.m. Before and after the workshop, you can contact us by email at `hda2015@ins.uni-bonn.de`.
We will have a data-projector, a flipchart and laptops running Windows 7 with Acrobat-Reader and Power Point (2010) in the conference room. Please bring your talk (.pdf or .ppt) along with you on a USB-stick. If you need any other hard- or software (e.g. video adapter cable for your own MacBook) to present your talk, please make sure to bring them yourself.
Network access (WLAN) for reading email etc. is available throughout the university club. Each participant has a personlized account for the university network. Please refer to the separate flyer for detailed information about the login procedure.



Icebreaker Reception

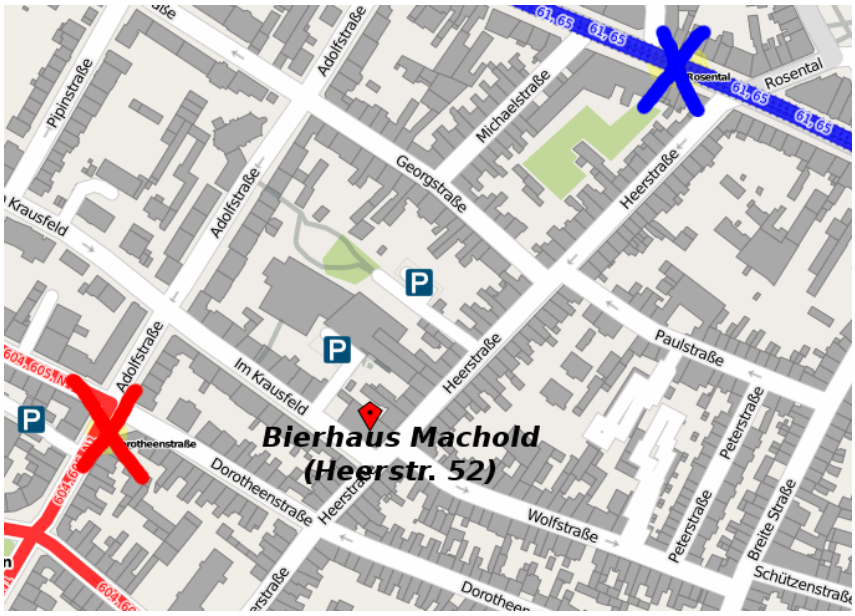
Sunday, 2015-09-13, 1900: Icebreaker Reception in the local brewery "Bönnsch", Sterntorbrücke 4, 53111 Bonn, `http://www.boennsch.de`. Please inform us at `hda2015@ins.uni-bonn.de` for planning purposes if you want to join.

Excursion

Wednesday, 2015-09-16, 1600: Guided Tour through the "Arithmeum", Lennéstr. 2, 53113 Bonn, `http://www.arithmeum.uni-bonn.de`.

Conference Dinner

Wednesday, 2015-09-16, 1900: Conference Dinner in the "Bierhaus Machold", Heerstr. 52, 53111 Bonn, `http://www.bierhaus-machold.com`.



It is approximately a 20 minute footwalk from the university club (or the Arithmeum) to the Bierhaus Machold. If you want to use public transport instead, the closest bus stop is "Dorotheenstrasse" (red X) where the busses 604 and 605 stop and the closest tramway stop is "Rosental" (blue X) where tram 61 stops. The busses leave from "Friedensplatz" and Bonn central station and the tram leaves from "Stadthaus" and Bonn central station.

Accomodation Tax

Note that the city of Bonn collects a tax (5% of the accomodation costs) per guest for private overnight stays. To confirm that your stay in Bonn is due to business reasons and therefore excluded from that tax, you need to fill out a business accomodation form and give it to the hotel you are staying in together with the confirmation of attendance at the HDA. Both, the accomodation form and the attendance confirmation can be found in your conference materials.

HCM-invited speakers

For this year's Workshop on High-Dimensional Approximation

- Albert Cohen
- Paul Constantine
- Metin Demiralp

were invited by the Hausdorff Center for Mathematics in Bonn to give an extended 50-minute talk. These talks are scheduled right after lunch on monday, tuesday and thursday.

Scientific Committee

- Prof. Albert Cohen (U Pierre et Marie Curie, France)
- Prof. Jochen Garcke (U Bonn & Fraunhofer SCAI, Germany)
- Prof. Michael Griebel (U Bonn & Fraunhofer SCAI, Germany)
- Prof. Wolfgang Hackbusch (Max Planck Institute Leipzig, Germany)
- Prof. Markus Hegland (ANU, Australia)
- Prof. Frances Kuo (UNSW, Australia)
- Prof. Christoph Schwab (ETH Zürich, Switzerland)
- Prof. Ian Sloan (UNSW, Australia)
- Prof. Henryk Wozniakowski (Columbia U, USA & Warsaw U, Poland)
- Prof. Harry Yserentant (TU Berlin, Germany)

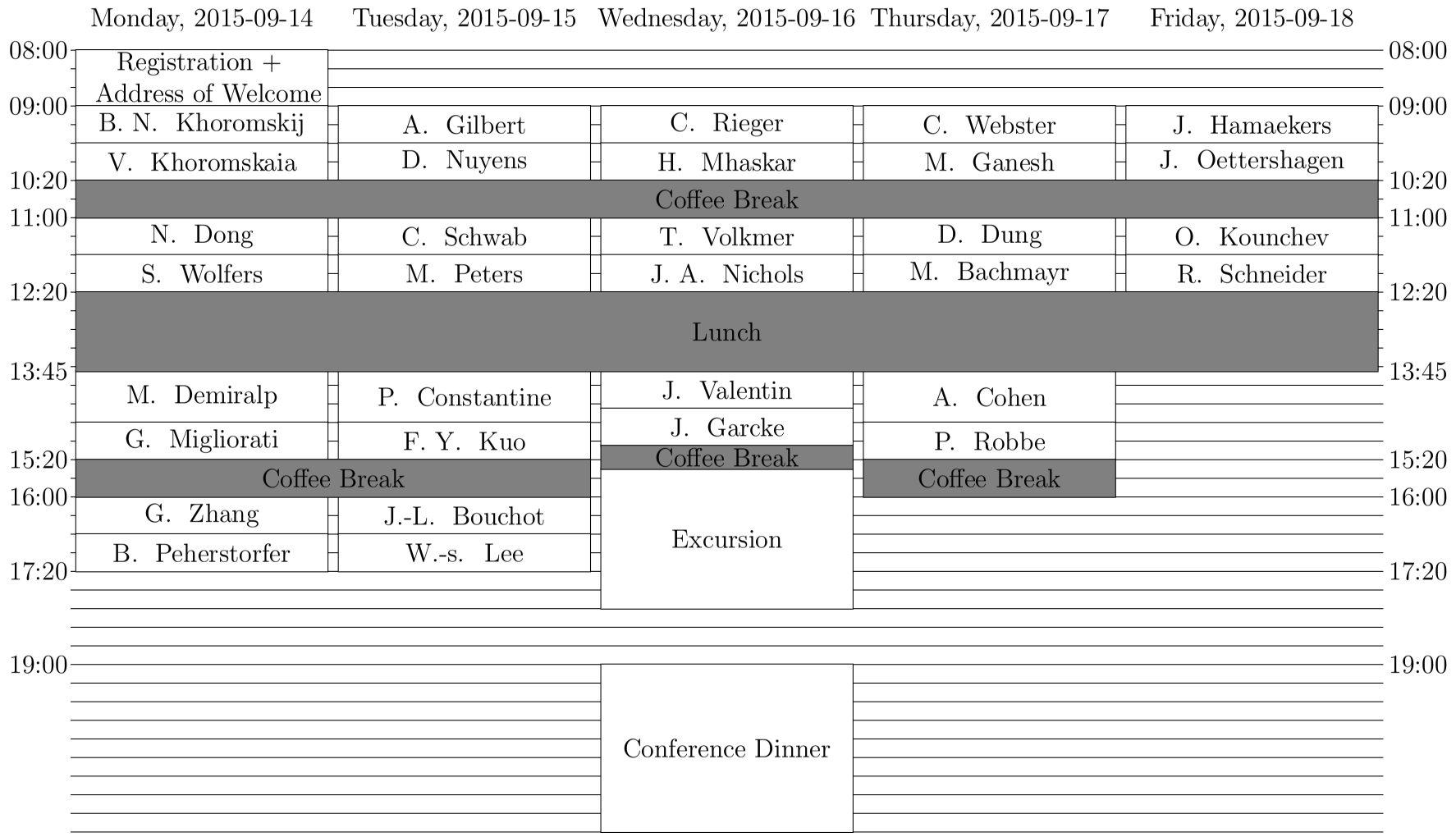
Local Organizers

- Bastian Bohn
- Barbara Fuchs
- Prof. Jochen Garcke

Acknowledgements

Special thanks to the Hausdorff Center for Mathematics for financial support.

Timetable


Monday, 2015-09-14
Tuesday, 2015-09-15
Wednesday, 2015-09-16
Thursday, 2015-09-17
Friday, 2015-09-18
08:00
09:00
10:20
11:00
12:20
13:45
15:20
16:00
17:20
19:00
Registration + Address of Welcome
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V. Khoromskaia
A. Gilbert
D. Nuyens
C. Rieger
H. Mhaskar
C. Webster
M. Ganesh
J. Hamaekers
J. Oettershagen
Coffee Break
N. Dong
S. Wolfers
C. Schwab
M. Peters
T. Volkmer
J. A. Nichols
D. Dung
M. Bachmayr
O. Kounchev
R. Schneider
Lunch
M. Demiralp
G. Migliorati
P. Constantine
F. Y. Kuo
J. Valentin
J. Garcke
A. Cohen
P. Robbe
Coffee Break
Coffee Break
Coffee Break
G. Zhang
B. Peherstorfer
J.-L. Bouchot
W.-s. Lee
Excursion
Conference Dinner

Detailed Program

Monday, 09:00–09:40, B. N. Khoromskij. *Towards tensor approximation of multi-dimensional PDEs with highly oscillating data.*

Monday, 09:40–10:20, V. Khoromskaia. *Calculation of Bethe-Salpeter excitation energies by using tensor-based Hartree-Fock solver and low-rank factorizations.*

Monday, 11:00–11:40, N. Dong. *Multivariate integration over the Euclidean space for analytic functions.*

Monday, 11:40–12:20, S. Wolfers. *Chebyshev nodes in multiple dimensions.*

Monday, 13:45–14:40, M. Demiralp. *High dimensional model representation theory from beginning to its most recent form.*

Monday, 14:40–15:20, G. Migliorati. *Stability and accuracy of discrete least squares on multivariate polynomial spaces with evaluations at random or low-discrepancy point sets.*

Monday, 16:00–16:40, G. Zhang. *A reduced-basis approach for parameterized backward SDEs and application to a class of quasilinear parabolic PDEs.*

Monday, 16:40–17:20, B. Peherstorfer. *Multifidelity Monte Carlo.*

Tuesday, 09:00–09:40, A. Gilbert. *Implementing the Multivariate Decomposition Method for infinite-dimensional integration.*

Tuesday, 09:40–10:20, D. Nuyens. *Construction of quasi-Monte Carlo methods for parameterised PDE problems.*

Tuesday, 11:00–11:40, C. Schwab. *Higher order Quasi-Monte Carlo Bayesian estimation for high-dimensional problems.*

Tuesday, 11:40–12:20, M. Peters. *Multilevel quadrature for elliptic PDEs with random data.*

Tuesday, 13:45–14:40, P. Constantine. *Active subspaces for dimension reduction and approximation.*

Tuesday, 14:40–15:20, F. Y. Kuo. *Quasi-Monte Carlo methods with circulant embedding for elliptic PDEs with lognormal random coefficients.*

Tuesday, 16:00–16:40, J.-L. Bouchot. *A multi-level compressed sensing Petrov-Galerkin method for the approximation of parametric PDEs.*

Tuesday, 16:40–17:20, W.-s. Lee. *A sparse sampling method to estimate parameters in multivariate exponential sums.*

Wednesday, 09:00–09:40, C. Rieger. *Nonstandard kernels for high-dimensional reconstruction problems.*

Wednesday, 09:40–10:20, H. Mhaskar. *A unified framework for harmonic analysis of functions on directed graphs and changing data.*

Wednesday, 11:00–11:40, T. Volkmer. *Fast and exact reconstruction of arbitrary multivariate high-dimensional algebraic polynomials in Chebyshev form.*

Wednesday, 11:40–12:20, J. A. Nichols. *A simple pathwise approach to anomalous diffusion.*

Wednesday, 13:45–14:25, J. Valentin. *Gradient-based optimization with hierarchical B-Splines on sparse grids.*

Wednesday, 14:25–15:05, J. Garcke. *Towards optimal feedback control of the wave equation by solving Hamilton-Jacobi Bellman equations on sparse grids.*

Thursday, 09:00–09:40, C. Webster. *Compressed sensing approaches for polynomial approximation of Hilbert-valued functions on lower sets.*

Thursday, 09:40–10:20, M. Ganesh. *A new class of constructive high-dimensional approximations: Algorithm, analysis and application.*

Thursday, 11:00–11:40, D. Dung. *Collocation linear methods for parametric and stochastic elliptic PDEs.*

Thursday, 11:40–12:20, M. Bachmayr. *Summability in polynomial expansions of affinely parametrized linear elliptic PDEs.*

Thursday, 13:45–14:40, A. Cohen. *Sparse approximation of elliptic PDEs with lognormal coefficients.*

Thursday, 14:40–15:20, P. Robbe. *A practical Multilevel quasi-Monte Carlo method for simulating elliptic PDEs with random coefficients.*

Friday, 09:00–09:40, J. Hamaekers. *Discrete Fourier transform on generalized sparse grids.*

Friday, 09:40–10:20, J. Oettershagen. *Numerical integration of multivariate analytic funtions.*

Friday, 11:00–11:40, O. Kounchev. *New polynomial models in Linear Algebra and tensor approximations.*

Friday, 11:40–12:20, R. Schneider. *Hierarchical tensor representation with application to molecular dynamics.*

Monday, 2015-09-14

Towards tensor approximation of multi-dimensional PDEs with highly oscillating data

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The breaking through approach to low-parametric representation of multivariate functions and operators is based on the principle of separation of variables [4]. The method of quantized tensor approximation (QTT) is proven to provide the logarithmic data-compression on a wide class of discrete functions (vectors) and operators (matrices) [1]. This allows to reformulate the standard discretization schemes for steady-state and dynamical PDEs by using the low-rank quantized tensor approximation and then solve the resultant high-dimensional systems with the logarithmic complexity in the initial problem size. Several applications of the QTT-based tensor numerical methods will be discussed.
We demonstrate how the grid-based QTT tensor approximation applies to the integration of multidimensional or/and highly-oscillating functions, say, many-electron integrals, integrals with the large lattice sum of interaction potentials [2], [3] or with the complicated high-frequency oscillators [5].
Finally, we discuss the low-rank QTT tensor representation of the discrete FEM elliptic operators and their inverse. As the particular applications, we consider matrices, arising from FEM approximation of PDEs with highly oscillating coefficients (homogenization theory) and the reduced basis approximation of the Hartree-Fock equation for large lattice-structured systems.

[1] B.N. Khoromskij. *$O(d \log N)$-Quantics Approximation of N-d Tensors in High-Dimensional Numerical Modeling.* J. Constr. Approx. v. 34(2), 257-289 (2011); (Preprint 55/2009 MPI MiS, Leipzig 2009).
[2] V. Khoromskaia and B. N. Khoromskij. *Grid-based lattice summation of electrostatic potentials by assembled rank-structured tensor approximation.* Comp. Phys. Communications, 185 (2014), pp. 3162-3174.
[3] V. Khoromskaia, and B.N. Khoromskij. *Tensor Approach to Linearized Hartree-Fock Equation for Lattice-type and Periodic Systems.* E-preprint arXiv:1408.3839, 2014 (submitted).
[4] Boris N. Khoromskij. *Tensor Numerical Methods for High-dimensional PDEs: Basic Theory and Initial Applications.* ESAIM: Proceedings and Surveys, Eds. N. Champagnat, T. Leliévre, A. Nouy. January 2015, Vol. 48, p. 1-28. http://dx.doi.org/10.1051/proc/201448001.
[5] B.N. Khoromskij, and A. Veit. *Efficient computation of highly oscillatory integrals by using QTT tensor approximation.* E-preprint arXiv:1408.5224, 2014 (submitted).
http://personal-homepages.mis.mpg.de/bokh; *bokh@mis.mpg.de*

Calculation of Bethe-Salpeter excitation energies by using tensor-based Hartree-Fock solver and low-rank factorizations

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vekh@mis.mpg.de
Co-Author(s): P. Benner, B. N. Khoromskij

The Bethe-Salpeter equation (BSE) is a reliable model for estimating the absorption spectra in molecules and solids on the basis of accurate calculation of the excitation energies from first principles. The necessary prerequisites for generation of the matrices in the BSE system are ab-initio Hartree-Fock calculations giving as a result the large 4th order tensor of two-electron integrals (TEI), a full set of molecular orbitals and the respective eigenvalues. This first step is efficiently implemented by using fast calculations by tensor-based Hartree-Fock solver [1,2,4], which provides TEI in a low-rank factorized form.

The challenging BSE problem includes calculation of the BSE operator in terms of two-electron integrals tensor represented in molecular orbital basis, and introduces a complicated algebraic task of solving the arising large matrix eigenvalue problem. The direct diagonalization of the BSE matrix is practically intractable due to $O(N^6)$ complexity scaling in the size of the atomic orbitals basis set, N. We present a new approach [3] to the computation of Bethe-Salpeter excitation energies which can lead to relaxation of the numerical costs up to $O(N^3)$. First the diagonal plus low-rank tensor approximations to the fully populated submatrices in the BSE matrix is constructed, enabling easier partial eigenvalue solver for a large auxiliary system but with a simplified block structure. Then a small subset of eigenfunctions from the auxiliary BSE problem is selected to solve the Galerkin projection of the initial spectral problem onto the reduced basis set.

The numerical tests on BSE calculations for a number of molecules confirm ε-rank bounds for the blocks of BSE matrix. They show that the reduced BSE eigenvalue problem with small matrices enables calculation of the low part of the excitation spectra for molecules up to small amino acids (Glycine, C2H5NO2) with sufficient accuracy [3,4].

[1] V. Khoromskaia, B.N. Khoromskij and R. Schneider. *Tensor-structured Calculation of the Two-electron Integrals in a General Basis.* SIAM J. Sci. Comp., **35** (2), A987-A1010, 2013.

[2] V. Khoromskaia. *Black-Box Hartree-Fock Solver by Tensor Numerical Methods.* Comp. Methods Appl. Math., Vol. 14 (2014) No.1, pp. 89-111.

[3] P. Benner, V. Khoromskaia and B.N. Khoromskij. *A Reduced Basis Approach for Calculation of the Bethe-Salpeter Excitation Energies using Low-rank Tensor Factorizations.* arXiv:1505.02696v1, 2015.

[4] V. Khoromskaia and B.N. Khoromskij. *Tensor Numerical Methods in Quantum Chemistry: from Hartree-Fock to Excitation Energies.* Physical Chemistry Chemical Physics, accepted, 2015, DOI: 10.1039/c5cp01215e .

Multivariate integration over the Euclidean space for analytic functions

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In this talk we study multivariate integration over $\mathbb{R}^s$ for weighted analytic functions, whose Fourier transform decays exponentially fast. We prove that the exponential convergence rate can be achieved by using a classical quasi-Monte Carlo method. More specific, we prove two convergence rates of $\mathcal{O}(\exp(-N^{\frac{1}{D(s)+B(s)}}))$ and $\mathcal{O}(\exp(-N^{\frac{1}{B(s)}}(\ln N)^{-\frac{D(s)}{B(s)}}))$, where $D(s)$ and $B(s)$ are respectively defined by the exponential decay of the Fourier transform and of the integrand, for two different function classes. We discuss work in progress to obtain a stronger convergence rate with less dependence on the dimension. Some numerical results demonstrate the theory
This talk is based on a joint work with D. Nuyens.

Chebyshev nodes in multiple dimensions

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Co-Author(s): B. Zwicknagl

Chebyshev nodes are well-known for their near-optimal polynomial interpolation and quadrature properties on intervals. In particular, the associated Lebesgue constant grows only logarithmically, whereas that associated to equispaced nodes grows exponentially. Generalizations of Chebyshev nodes to domains in multiple dimensions have so far only been studied on hyper-cubes. In this talk, we consider more general domains and study the properties of node sets that are similar to Chebyshev nodes in the sense that they are distributed more densely near the boundary of the domain.

High dimensional model representation theory from beginning to its most recent form

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High Dimensional Model Representation (HDMR) was proposed by Sobol at the beginning of 1990s. He proposed a decomposition with components ascending in multivariance such that the components were being evaluated under certain vanishing integral impositions. The multivariate integration domain was defined as unit hypercube whose one corner is located at the origin while its edges reside in the positive semiaxes. Sobol had not specified any weight function other than the unit constant weight function which remains 1 everywhere in the integration domain.
The first extension to Sobol's proposal had come from Rabitz group which brought two basic changes to somehow generalize the issue: (1) The geometry became not limited to the Sobol's unit hypercube. However, only orthogonal geometries considered to avoid incompatibilities in the components determinations; (2) The weight function utilization became available. However, it was considered as a product of univariate weight functions each of which depends on a different independent variable (this limitation has been relaxed by the works in Demiralp group later). The works of Rabitz group have also made available new varieties for HDMR which were somehow based on delta distribution issues. They called these types of HDMR "Cut–HDRM" and "MultiCut–HDMR". They also proposed "Random Sampling HDMR" later.
Another group which has taken important steps to develop a theory on HDMR has been the research team of the author of this abstract. Demiralp group first defined not an additive but a purely product type representaion which was named "Factorized HDMR" or briefly "FHDMR". While plain HDMR truncation approximants work well for dominantly additive functions, FHDMR could reproduce the target function at univariate level truncation if the target is a product of univariate functions. Same group has later defined a new HDMR which can work exact in both cases of pure additivity and pure multiplicativity while it also works well for mixtures. This has been called "Hybrid HDMR (HHDMR)".
There has been many milestone type steps after the development of FHDMR and HHDMR in Demiralp group works. Logarithmic HDMR, Transformational HDMR, Generalized HDMR, Multivariate weight utilization in HDMR, Index HDMR are some examples to this end. However, the most fruitful one for the present times appears to be EMPR (Enhanced Multivariance Products Representation) which uses given univariate support functions to enhance the HDMR expansion terms' multivariance to its maximum value. EMPR brings a lot of flexibilities to control the truncation approximation qualities of the representation. The support functions can also be optimally chosen to get maximum approximation efficiency. Even by using bivariate EMPR on the functions and/or arrays it is possible to generate representations over certain tridiagonal rectangular core matrices. These issues are under intense study for the moment and each development seems to take us to new original ideas.
The talk will focus all these issues as the time length of the presentation allows.

Stability and accuracy of discrete least squares on multivariate polynomial spaces with evaluations at random or low-discrepancy point sets

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We review some of the results achieved in the analysis of the stability and accuracy of discrete least squares on multivariate polynomial spaces, with evaluations at random points [1] or at low-discrepancy point sets [2]. Afterwards we present convergence estimates in probability for several noise models, recently proven in [3] using arguments from the theory of large deviations.

[1] A.Chkifa, A.Cohen, G.Migliorati, F.Nobile, R.Tempone: Discrete least squares polynomial approximation with random evaluations - application to parametric and stochastic elliptic PDEs, ESAIM:M2AN 49(3):815-837, 2015.
[2] G.Migliorati and F.Nobile: Analysis of discrete least squares on multivariate polynomial spaces with evaluations at low-discrepancy point sets, J.Complexity 31(4):517-542, 2015.
[3] G.Migliorati, F.Nobile and R.Tempone: Convergence estimates in probability and in expectation for discrete least squares with noisy evaluations at random points, submitted, available as MATHICSE report 3.2015.

A reduced-basis approach for parameterized backward SDEs and application to a class of quasilinear parabolic PDEs

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Co-Author(s): W. Zhao

This effort is motivated by the relationship between backward SDEs and a class of quasilinear PDEs, described by the nonlinear Feynman-Kac theory, such that our approach can be applied to solving quasilinear parabolic PDEs with deterministic or random parameters, where we aim at approximating the parameterized viscosity solution of the PDEs. In the SDE setting, the temporal-spatial differential operator in the PDE is described by the dynamics of the underlying stochastic process, and the key task in developing numerical schemes is to approximate the conditional mathematical expectation of the solution and the forcing term with respect to the stochastic process. In this effort, we utilize the empirical interpolation method (EIM) to approximate the involved expectation operator, such that we can obtain the off-line online decomposition of computational cost. The main feature of the SDE approach is that the approximate solution can be computed independently at each spatial grid point without solving linear systems when using implicit time-stepping schemes. This feature will lead to a significantly reduction by avoiding the off-line cost of approximating the Jacobian of the nonlinear operator using the EIM. In addition, our approach can provide a reduced-basis approximation to not only the solution of the PDE, but also its gradient. Various numerical examples on backward SDEs and the corresponding quasilinear PDEs with parameterized coefficients are presented to demonstrate effectiveness of our approach.

Multifidelity Monte Carlo

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Our multifidelity Monte Carlo (MFMC) method aims at accelerating the Monte Carlo estimation of statistics of outputs of computationally expensive high-fidelity models by exploiting surrogate models. Surrogate models such as projection-based reduced models, data-fit models and simplified models do not necessarily give rise to a collection of models that follow a known hierarchy of error and computational costs. Thus, classical acceleration methods for Monte Carlo that are based on the notion of such a hierarchy are often not applicable. In contrast, our MFMC method provides a framework to combine an arbitrary number of surrogate models of any type. Each of the surrogate models is viewed as an information source, where the collective information provided by all surrogate models is greater than the information provided by a single surrogate model or the high-fidelity model alone. An optimization problem balances the number of model evaluations across the high-fidelity and surrogate models with respect to correlation strength and computational costs. We show mathematically and demonstrate numerically that combining the high-fidelity model with surrogate models of different approximation quality and costs is often more beneficial than combining the high-fidelity model with accurate surrogate models only. In this sense, surrogate models that inform different aspects of the high-fidelity model are better than surrogate models that are accurate but lack a rich diversity. Our MFMC method establishes accuracy guarantees by occasional recourse to the high-fidelity model and provides an unbiased estimator of the statistics of the high-fidelity model, even in the absence of error bounds and error estimators for the surrogate models. Numerical experiments with linear and nonlinear examples show that speedups by orders of magnitude are obtained compared to Monte Carlo estimation that invokes a single model only.

Tuesday, 2015-09-15

Implementing the Multivariate Decomposition Method for infinite-dimensional integration

A. Gilbert
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Co-Author(s): F. Kuo, D. Nuyens, L. Plaskota, I. Sloan, G. Wasilkowski

This talk is on implementing the Multivariate Decomposition (MDM) algorithm to approximate the integral of functions of infinitely-many variables. It is assumed that the functions considered can be decomposed into a sum of finitely-many functions which only depend on a finite number of variables (for example, the ANOVA or anchored decomposition).
Loosely speaking, the MDM first chooses a collection of decomposition terms which contribute most to the integral, this collection is referred to as the "active set". Quadrature rules are then applied to each term in the active set and the final estimate of the integral is taken to be the sum over all such approximations.
Numerical results for constructing the active set and the quadrature approximations will be given.

Construction of quasi-Monte Carlo methods for parameterised PDE problems

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Co-Author(s): F. Y. Kuo

We present a practical view on solving parameterised PDE problems using quasi-Monte Carlo methods. We discuss and demonstrate some code to construct higher-order interlaced polynomial lattice rules which can be tuned to the PDE as well as some easier methods based on plain lattice rules.

Higher order Quasi-Monte Carlo Bayesian estimation for high-dimensional problems

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Co-Author(s): J. Dick, R. Gantner, T. LeGia

We analyze Quasi-Monte Carlo quadratures in Bayesian estimation of solutions to countably-parametric operator equations with holomorphic dependence on the parameters considered in [Cl. Schillings and Ch. Schwab: Sparsity in Bayesian Inversion of Parametric Operator Equations. Inverse Problems, **30**, (2014)].
Such problems arise in numerical uncertainty quantification and in Bayesian inversion of operator equations with distributed uncertain inputs, such as uncertain coefficients, uncertain domains or uncertain source terms and boundary data. We show that the parametric Bayesian posterior densities belong to a class of weighted Bochner spaces of functions of countably many variables, with a particular structure of the QMC quadrature weights: up to a (problem-dependent, and possibly large) finite dimension J product weights can be used, and beyond this dimension, weighted spaces with the so-called SPOD weights recently introduced in [F.Y. Kuo, Ch. Schwab, I.H. Sloan, Quasi-Monte Carlo finite element methods for a class of elliptic partial differential equations with random coefficients. SIAM J. Numer. Anal. 50 (2012), 3351–3374] are used to describe the solution regularity. We establish error bounds for higher order, Quasi-Monte Carlo quadrature for the Bayesian estimation based on [J. Dick, Q.T. LeGia and Ch. Schwab, Higher order Quasi-Monte Carlo integration for holomorphic, parametric operator equations, Report 2014-23, SAM, ETH Zürich]. It implies, in particular, regularity of the parametric solution and of the countably-parametric Bayesian posterior density in SPOD weighted spaces. This, in turn, implies that the Quasi-Monte Carlo quadrature methods in [J. Dick, F.Y. Kuo, Q.T. Le Gia, D. Nuyens, Ch. Schwab, Higher order QMC Galerkin discretization for parametric operator equations, SINUM (2014)] are applicable to these problem classes, with dimension-independent convergence rates $\mathcal{O}(N^{-1/p})$ of N-point HoQMC approximated Bayesian estimates where $0 < p < 1$ depends only on the sparsity class of the uncertain input in the Bayesian estimation. Hybridized versions of the fast component-by-component (CBC for short) construction [R. N. Gantner and Ch. Schwab Computational Higher Order Quasi-Monte Carlo Integration, Report 2014-25, SAM, ETH Zürich] allow efficient Bayesian estimation with up 10^3 parameters.

Multilevel quadrature for elliptic PDEs with random data

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This talk is dedicated to multilevel quadrature methods for the solution of elliptic partial differential equations with random data, like a random diffusion coefficient or a random domain. The key idea of these approaches is a sparse grid approximation of the occurring product space between the stochastic and the spatial variable. In particular, the present framework covers the multilevel Monte Carlo method and the multilevel quasi-Monte Carlo method as special cases. The presented theory is supplemented by numerical experiments.

Active subspaces for dimension reduction and approximation

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Active subspaces are an emerging set of tools for approximating a scalar-valued function of several variables by a function of a few linear combinations of the variables. The linear combinations' weights are the principal eigenvectors from the average outer product of the function's gradient with itself. The low-dimensional map from the linear combinations of variables to the reals is constructed as a conditional average. I will present mean-squared error estimates for this construction in terms of the eigenvalues of the aforementioned matrix. I will describe a Monte Carlo method for estimating both the eigenvectors and the conditional average, and I'll show mean-squared error bounds for these estimates. I will discuss current challenges and mention several applications from science and engineering. For more information, visit activesubspaces.org ¡http://activesubspaces.org¿.

Quasi-Monte Carlo methods with circulant embedding for elliptic PDEs with lognormal random coefficients

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In a recent paper (J. Comp. Phys., 2011), the authors proposed a new practical method for computing functionals of the solution of certain classes of elliptic partial differential equations with random coefficients. This method combined circulant embedding/FFT methods for sampling the random field with quasi-Monte Carlo methods. It was capable of handling fluid flow problems in random heteogeneous media with high stochastic dimension, as demonstrated by detailed numerical experiments. In this talk I will present our follow-up work which provides the first convergence analysis for this method.

A multi-level compressed sensing Petrov-Galerkin method for the approximation of parametric PDEs

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In this talk we review the use of compressed sensing and its weighted version in the context of high-dimensional parametric and stochastic PDEs. We see that under some rather weak summability and ellipticity assumptions, the Chebysheff polynomial chaos expansion of the solution map shows some weighted compressibility property and derive a compressed sensing framework for its approximation. We further extend our approach with a multi-level scheme solution map shows some compressibility property. We further derive a multi-level scheme to speed up the calculations, leading to a method that has a computational cost in the order of a single PDE solve at the finest level and yet still provide reliable recovery guarantees

A sparse sampling method to estimate parameters in multivariate exponential sums

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We consider the interpolation of an n-variate exponential sum

$$F(x_1, \ldots, x_n) = \sum_{j=1}^{t} c_j e^{f_{j,1}x_1 + f_{j,2}x_2 + \cdots + f_{j,n}x_n}.$$

That is, to recover parameters $c_j, f_{j,k}$ from the evaluations of $F(x_1, \ldots, x_n)$.
We present a parametric method that can interpolate $F(x_1, \ldots, x_n)$ from $(n+1)\cdot t$ evaluations. In order to solve for the multivariate parameters, the target function $F(x_1, \ldots, x_n)$ is evaluated at the additional points defined by the *identification shifts*. Since the total number of parameters c_j and $f_{j,k}$ is exactly $(n+1)\cdot t$, our method can interpolate $F(x_1, \ldots, x_n)$ from the minimum possible number of evaluations.
In general, our method can be used in exponential analysis problems where additional evaluations of the same exponentials are required. One of such applications is to recover the correct frequencies from the aliased results caused by different subsamplings.
Our method can be embedded in any Prony-like algorithm, such as the least square Prony, ESPRIT, matrix pencil, etc., thus can be viewed as a new class of tools exposing an additional range of possibilities in exponential analysis.

Wednesday, 2015-09-16

Nonstandard kernels for high-dimensional reconstruction problems

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In this talk, we present certain non-standard kernels which naturally arise in high dimensional reconstruction problems. Numerically feasible reconstruction processes usually exhibit special structures which have to be exploited. One example for such a structure are highly non-Euclidean metrics as they arise in machine learning applications. We present a systematic framework to introduce smoothness spaces with reproducing kernels in such a context. The fact that such spaces have a reproducing kernel which can at least be numerically approximated enables us to use the rich toolbox of kernel-based methods from machine learning in this general context. Finally, we give a priori error bounds for the reconstruction error.
This is partly based on joint work with M. Griebel and B. Zwicknagl (both Bonn University).

A unified framework for harmonic analysis of functions on directed graphs and changing data

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Diffusion geometry is a recent powerful tool for analyzing high dimensional, unstructured data by embedding it on a low dimensional manifold. We present a general framework for studying harmonic analysis of functions in the settings of various emerging problems in the theory of diffusion geometry. The starting point of the now classical diffusion geometry approach is the construction of a kernel whose discretization leads to an undirected graph structure on an unstructured data set. We study the question of constructing such kernels for directed graph structures, and argue that our construction is essentially the only way to do so using discretizations of kernels. We then use our previous theory to develop harmonic analysis based on the singular value decomposition of the resulting non–self–adjoint operators associated with the directed graph. Next, we consider the question of how functions defined on one space evolves to another space in the paradigm of changing data sets recently introduced by Coifman and Hirn. While the approach of Coifman and Hirn require that the points on one space should be in a known one–to–one correspondence with the points on the other, our approach allows the identification of only a subset of landmark points. We introduce a new definition of distance between points on two spaces, construct localized kernels based on the two spaces and the landmark points, and study the evolution of smoothness of a function on one space to its lifting to the other space via the landmarks. We develop novel mathematical tools that enable us to study these seemingly different problems in a unified manner.

Fast and exact reconstruction of arbitrary multivariate high-dimensional algebraic polynomials in Chebyshev form

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We consider a multivariate high-dimensional algebraic polynomial in Chebyshev form

$$p(\boldsymbol{x}) = \sum_{\boldsymbol{k}\in I} \hat{p}_{\boldsymbol{k}}\, T_{\boldsymbol{k}}(\boldsymbol{x}) = \sum_{\boldsymbol{k}\in I} \hat{p}_{\boldsymbol{k}} \prod_{t=1}^{d} T_{k_t}(x_t), \quad \hat{p}_{\boldsymbol{k}} \in \mathbb{R}, \tag{1}$$

where $I \subset \mathbb{N}_0^d$ is an arbitrary non-negative index set of finite cardinality, $d \in \mathbb{N}$ is the dimension and $T_{\boldsymbol{k}} : [-1,1]^d \to [-1,1]$, $T_{\boldsymbol{k}}(\boldsymbol{x}) := \prod_{t=1}^{d} T_{k_t}(x_t)$, are multivariate Chebyshev polynomials for $\boldsymbol{k} := (k_1, \ldots, k_d)^\top \in \mathbb{N}_0^d$ built from a tensor product of univariate Chebyshev polynomials of the first kind $T_k : [-1,1] \to [-1,1]$, $T_k(x) := \cos(k \arccos x)$, $k \in \mathbb{N}_0$. In particular, if we choose the index set I as a d-dimensional ℓ_1-ball of refinement $n \in \mathbb{N}_0$, $I = \{\boldsymbol{k} \in \mathbb{N}_0^d \colon \|\boldsymbol{k}\|_1 \le n\}$, then any algebraic polynomial of total degree $\le n$ in d variables restricted to the domain $[-1,1]^d$ can be represented by a polynomial p from (1).
In this talk, we describe a fast method for the evaluation of a polynomial p from (1) with arbitrarily chosen index set $I \subset \mathbb{N}_0^d$ and arbitrary coefficients $\hat{p}_{\boldsymbol{k}} \in \mathbb{R}$, $\boldsymbol{k} \in I$, at the nodes of an arbitrary d-dimensional rank-1 Chebyshev lattice

$$\mathrm{CL}(\boldsymbol{z}, M) := \left\{ \boldsymbol{x}_j := \cos\left(\frac{j}{M}\pi \boldsymbol{z}\right) : j = 0, \ldots, M \right\} \subset [-1,1]^d,$$

which is characterized by the generating vector $\boldsymbol{z} \in \mathbb{N}_0^d$ and the size parameter $M \in \mathbb{N}_0$. This method only uses a single one-dimensional discrete/fast cosine transform of type I (1d-DCT-I) of length M and simple index transforms, yielding an arithmetic complexity of $\mathcal{O}(M \log M + d\, 2^d |I|)$.
Moreover, we discuss conditions on rank-1 Chebyshev lattices $\mathrm{CL}(\boldsymbol{z}, M)$, such that the exact reconstruction of polynomials p from (1) based on samples $p(\boldsymbol{x}_j)$, $j = 0, \ldots, M$, is possible for an arbitrarily chosen index set $I \subset \mathbb{N}_0^d$ of finite cardinality. For building such a rank-1 Chebyshev lattice $\mathrm{CL}(\boldsymbol{z}, M)$ suitable for reconstruction, we give an algorithm which is based on a component-by-component approach and we show numerical results. Using such a suitable rank-1 Chebyshev lattice $\mathrm{CL}(\boldsymbol{z}, M)$, we present a method for the fast and exact reconstruction of the coefficients $\hat{p}_{\boldsymbol{k}}$, $\boldsymbol{k} \in I$, from the samples $p(\boldsymbol{x}_j)$ at the rank-1 Chebyshev lattice nodes $\boldsymbol{x}_j$, $j = 0, \ldots, M$. We only apply a single 1d-DCT-I of length M to the samples and perform simple index transforms as well as multiplications with scaling factors. The arithmetic complexity for the reconstruction method is $\mathcal{O}(M \log M + d\, 2^d |I|)$.
This is joint work with Daniel Potts.

A simple pathwise approach to anomalous diffusion

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Anomalous diffusion, where mean-squared displacement is proportional to t^α, is typically difficult to compute numerically due to the non-locality of the fractional differential operator, or in another sense, the non-Markovian nature of the underlying stochastic process. We can however take advantage of the semi-Markovian nature of the process, when viewed as a series of jumps in the random walk setting, to calculate individual paths. This, coupled with recent discoveries in discrete power-law distributions, allow us to formulate a remarkably simple algorithm for producing paths for particles undergoing anomalous diffusion.

Gradient-based optimization with hierarchical B-Splines on sparse grids

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Optimization problems occur nearly everywhere in theoretical and practical applications, e.g., in inverse problems, which ask for model parameter values to match simulated with observed experimental data. How to solve these problems especially in high dimensions with as few evaluations as possible is thus of great interest.
In this talk, we want to solve bound-constrained optimization problems for a continuous objective function $f\colon [0,1]^d \to \mathbb{R}$. We assume evaluations of the objective function to be expensive, as they can depend on the results of a complex simulation. As d increases, the problem suffers from the well-known curse of dimensionality. Sparse grids have proven themselves as a tool to ease the curse at least to some extent. A standard approach would be to use sparse grid interpolants as a surrogate for the objective function to drastically reduce the cost of evaluating the objective function to the cost of evaluating the interpolant, which is much cheaper. Common optimization algorithms can then be applied to the interpolant.
In many applications, gradient-based optimization techniques can exploit the availability of the gradient or the Hessian of the function to be optimized. However, conventional basis functions for sparse grids, e.g., piecewise linear or polynomial basis functions, share the shortcoming of not having continuous derivatives. This makes the use of gradient-based methods on these sparse grid interpolants very limited.
We consider in this talk p times continuously differentiable B-splines as sparse grid basis functions, which feature many analytically and numerically nice properties. We observe that when ordered in a hierarchical manner, they form a basis of the spline space, which consists of all piecewise polynomials with some additional smoothness conditions. After explaining the Novak-Ritter criterion we used to generate our spatially adaptive sparse grid, we elaborate on our algorithm for optimizing the B-spline interpolant. Finally, we present numerical results for some artificial test functions as well as for an example application.

Towards optimal feedback control of the wave equation by solving Hamilton-Jacobi Bellman equations on sparse grids

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In this talk we derive sub-optimal controllers in feedback form for finite time horizon optimal control problems for the wave equation by solving Hamilton-Jacobi Bellman (HJB) 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 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 higher dimensional value functions arising in the numerical scheme since the curse of dimensionality of full grid methods arises to a much smaller extent. For additional efficiency, an adaptive grid refinement procedure is explored. We present several numerical examples studying the effect of the parameters characterizing the sparse grid on the accuracy of the value function and optimal trajectories.

Thursday, 2015-09-17

Compressed sensing approaches for polynomial approximation of Hilbert-valued functions on lower sets

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This talk proposes and analyzes compressed sensing approaches for uniformly recovering polynomial approximations of Hilbert-valued functions. A typical example in this setting involves the solution to parametric PDEs, wherein the sets of best s-terms are often downward closed, and we seek to exploit this fact by studying ℓ_1 minimization estimates under this additional assumption. In addition, a direct application of standard compressed sensing algorithms to parametric PDEs only allows recovery at a single point in physical space. As such, to simultaneously approximate the solution in the entire physical domain, we also provide an extension of l_1 minimization to multi-dimensional Hilbert-valued functions. Numerical tests will be provided that support the new theory.

A new class of constructive high-dimensional approximations: Algorithm, analysis and application

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Efficient computation of statistical moments for functions defined on high dimensional spaces is crucial for understanding of various random physical processes. Such physical quantities of interest (QoI) are typically modeled by stochastic partial differential equations and hence are computationally expensive to evaluate at each realization point in high dimensions. Monte Carlo (MC) and its high-order variants (such as QMC) provide direct approximations to high dimensional moment integrals. Analysis of such approximations do not yield information on the error in approximating the QoI in high dimensional spaces. We develop, analyze, and implement a new framework to compute stochastic moments through a novel class of approximations of the QoI in high dimensional spaces.

Collocation linear methods for parametric and stochastic elliptic PDEs

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We consider the elliptic problem with random/parametrized input

$$-\operatorname{div}(a(x,y)\nabla u(x,y)) \;=\; f(x) \quad x\in D,\; y\in[-1,1]^\infty, \quad u|_{\partial D} \;=\; 0, \tag{2}$$

where $D\subset\mathbb{R}^m$ is a bounded domain with a Lipschitz boundary ∂D, $f\in L_2(D)$, and the diffusions a is affinely dependent with respect to random/parametrized variable y, more precisely,

$$a(x,y) \;=\; \overline{a}(x) \;+\; \sum_{j=1}^{\infty} y_j\,\psi_j(x), \tag{3}$$

and satisfies the uniform ellipticity assumption. We propose collective collocation linear methods for solving (2), based on spatial finite element approximation on D and stochastic Lagrange polynomial interpolation on $[-1,1]^\infty$. Under very light assumptions on the expansion (3) and standard assumptions on finite element approximation in the energy norm for the domain D, we show that our method gives the same convergence rate as that by a finite element approximation for solving the corresponding elliptic problem without random/parametrized input in the domain D. The stochastic infinite-variate part completely disappears from the convergence rate and influences only the constant.

Summability in polynomial expansions of affinely parametrized linear elliptic PDEs

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We consider elliptic partial differential equations with diffusion coefficients that affinely depend on countably many parameters. We study the summability properties of polynomial expansions of the function mapping parameter values to solutions of the PDE, considering both Taylor and Legendre series. Our results considerably improve on previously known estimates of this type, and in particular, they take into account structural features of the affine parametrization of the coefficient. We demonstrate that the new bounds are sharp in certain model cases and we illustrate them by numerical experiments.

Sparse approximation of elliptic PDEs with lognormal coefficients

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Elliptic partial differential equations with diffusion coefficients of lognormal form, that is $a = \exp(b)$ where b is a gaussian random field, are considered. We study the ℓ_p summability properties of the Hermite polynomial expansion of the solution in terms of the countably many scalar parameters appearing in a given representation of b. These summability results have direct consequences on the approximation rates of best n-term truncated Hermite expansions. Our results significantly improve on the state of the art estimates established by Hoang and Schwab for this problem. In particular, they take into account the support properties of the basis functions involved in the representation of b, in addition to the size of these functions. One interesting conclusion from our analysis is that in certain relevant cases, the Karhunen-Loeve representation of b might not be the best choice in terms of the resulting sparsity and approximability of Hermite expansion.

A practical Multilevel quasi-Monte Carlo method for simulating elliptic PDEs with random coefficients

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The efficient numerical simulation of models described by partial differential equations (PDEs) is an important task in engineering and science. Often, the coefficients in such models are not known exactly or are subject to uncertainty. Because the uncertainty propagates through the solution, this typically leads to very high dimensional quadrature problems when computing the statistics of certain quantities of interest. Recently, the Multilevel Monte Carlo method (MLMC), a combination of Monte Carlo sampling and a multigrid idea, has been successfully applied to these problems, showing significant gains. In this presentation, we investigate how the classical MLMC method can be improved even further by combining it with quasi-Monte Carlo (QMC) integration. Specifically, we introduce a Multilevel quasi-Monte Carlo estimator (MLQMC) based on randomized rank-1 lattice rules. The error analysis of this estimator results in an optimal number of samples at each level that is a significant improvement over the classical amount of work. Numerical results illustrate the superiority of the new MLQMC method over the standard MLMC estimator. We show that for certain problems, one can achieve a cost almost inversely proportional to the requested tolerance on the root-mean-square error. This is much better than the classical method, for which the cost is inversely proportional to the square of the requested tolerance.

Friday, 2015-09-18

Discrete Fourier transform on generalized sparse grids

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

Numerical integration of multivariate analytic funtions

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We discuss tensor products of certain, maximally nested univariate quadrature methods (e.g. Leja rules) that are taylored to analytic function spaces. We prove exponential convergence rates in the finite-dimensional setting and super-algebraic rates in the infinite-dimensional setting.

New polynomial models in Linear Algebra and tensor approximations

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We introduce several new functional (including polynomial) models for linear operators in finite-dimensional linear spaces, where the linear operator is either differentiation or multiplication. For example, we provide a new polynomial model for the Jordan normal form and models for general linear operators, which are not available even in advanced references on linear algebra, cf. [1,2,3,6].
These new models provide unitary equivalent operators to a very wide class of tensors. We provide criteria for solubility of linear equations with tensors. On the other hand these new models hint a natural tensor generalization for the notion of rank of a matrix, and one may consider a natural approximations to the tensors by lower rank tensors.
The majority of these models are suggested by the solution to the pseudo-positive Moment problem, cf. [4,5].

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Hierarchical tensor representation with application to molecular dynamics

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Hierarchical Tucker tensor format, introduced by Hackbusch and coworkers, and a particular case of Tensor Trains (TT) (Tyrtyshnikov) have been introduced for high dimensional problems. The parametrization has been known in quantum physics as tensor network states.
We consider an application of this approach for computing meta-stable states in molecular dynamics. This requires the computation of the first eigenfunctions of the transfer operator. In the Langevin dynamics, these are the eigenfunctions of the corresponding Fokker Planck. The transfer operator becomes symmetric in L_2 w.r.t. to the Gibbs measure, or equilibrium distribution. Based on a tensor product basis in high dimensions, the hierarchical tensor representation (TT tensor) is obtained by alternating directional search (ALS). Since there the operator is in general not available in tensor form, corresponding matrix elements are computed by Monte Carlo sampling. This is joint work with F. Nüsken and F. Noe (FU Berlin).

Participants