Workshop on Stochastic Partial Differential Equations

August 24-28, 2009

TU Darmstadt

Organization
S. Dahlke
S. Larsson
K. Ritter
R. Schilling
W. Stannat
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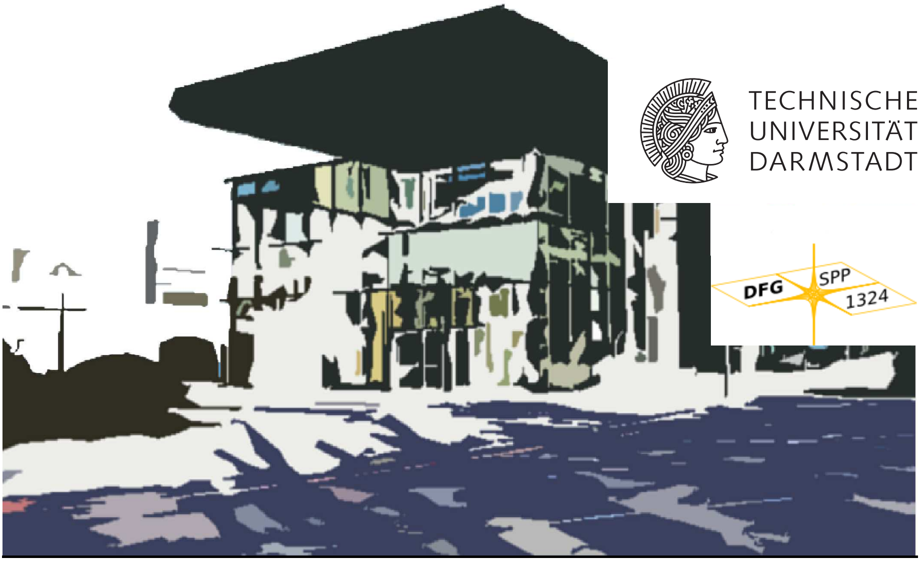
Short Courses
M. Röckner
I. Gyöngy

Keynote Speakers
M. Kovács
G. Pavliotis
J. Printems
M. Romito



August 27, 2009

Contents

1 General Information

1.1 Accommodation

The participants are recommended to stay in one of the following hotels, located in walking distance (5 - 15 minutes) to the lecture venue.

- WELCOME HOTEL DARMSTADT
  Karolinenplatz 4
  64289 Darmstadt
  Tel: +49-6151-3914-0
  Fax: +49-6151-3914-444

- HOTEL BOCKSHAUT
  Kirchstraße 7-9
  64283 Darmstadt
  Tel: +49-6151-9967-0
  Fax: +49-6151-9967-29

- HOTEL ERNST LUDWIG
  Ernst Ludwig Straße 14
  64289 Darmstadt
  Tel: +49-6151-9266 or +49-6151-26011

For a way description to the lecture venue or to public transportation please see the map in section 1.4.

1.2 Registration

On Monday morning, starting from 8:30, registration is possible in the lobby of the lecture hall. If you want to register another day please contact the secretary of the *AG Stochastik*, Mrs. Frohn, building S2|15, room 338 (Department of Mathematics).

1.3 Lecture Hall

The venue of the workshop is the lecture hall 024 in the Institut für Kernphysik, IKP (Nuclear Physics Department) of the TU Darmstadt, building S2|14, located at Schlossgartenstraße 9, next to the building of the Department of Mathematics.

1.4 Map & Points of Interest

The map can be found on the last page.

1.5 Public Transportation

The closest bus and tram stops to the venue of the workshop are **Schloss** (trams: S2, S3, S9) and **Willy-Brandt-Platz** (trams: S4, S5, S6, S7, S8). Both stops are within 10 minutes walking distance to the lecture hall.

1.6 Food & Beverage

Cheap and plain food can be purchased at the TU Darmstadt Refectory, building S1|11, (see map), Monday to Friday 11:15 to 14:00. Additionally there are lots of good restaurants and bistros near TU Darmstadt.

Name	Address	Phone	Cuisine	Opening Hours
Ratskeller	Marktplatz 8	26444	German	10:00 - 24:00
Pizzeria da Nino	Alexanderstr. 29	24220	Italian	18:00 - 23:00
Haroun‘s	Friedensplatz 6	23487	Oriental	11:00 - 01:00
Vis à Vis	Furhmannstr. 2	9670806	Bistro	10:00 - 16:00
Central Station	Carree		Bistro	10:00 - 01:00

1.7 WiFi & Computer Access

You have access to the TUD WiFi during your stay. user name and password to access WLAN *TUD* are enclosed in your personal file.

- SSID of the network: TUD
- authentification: WPA2-Enterprise
- encryption: CCMP or AES
- type of authentification: EAP-TTLS
- authentification protocol: PAP, sometimes plaintext
- outer identity: anonymous@tu-darmstadt.de
- inner identity: user name

Alternatively, you can have computer access in the room K313, located in the third floor in the Department of Mathematics, S2|15 (see map). All computers run Debian 4.0. In order to run a browser just click the menu to the lower left, select *Internet* and a suitable browser, e.g. *Iceweasel*. For login information please ask the technical support.

1.8 Conference Dinner

On Tuesday, August 25th there will be a conference dinner at the Welcome Hotel (see map) at 19:30.

1.9 Excursion

On Wednesday, August 26th there will be an excursion to *Kirchberghäuschen, Bensheim*. We will start around 15:00 in front of the lecture hall. A short bustrip will take us to *Fürstenlager, Auerbach*, the former summer residence of Hessian dukes, which is now embedded into a large park at the slope of the Odenwald. We start for a short walk to Kirchberghäuschen, where we have a great view over vineyards and the Rhine Valley. Kirchberghäuschen is a small restaurant which offers local food and wine. The bus will return for Darmstadt around 19:30.

1.10 Contact Information

If there are any needs or questions concerning the workshop, please feel free to contact one of the local organizers or the technical support:

- Prof. Dr. Klaus Ritter
  Office: S2-15, Room 340
  Phone: +49 (0) 6151 - 16 2288
- Prof. Dr. Wilhelm Stannat
  Office: S2-15, Room 341
  Phone: +49 (0) 6151 - 16 3183
- Ferdinand Ebert
  Technical Support

Acknowledgements

Financial support by DFG, through SPP 1342 and IRTG 1529, is gratefully acknowledged.

2 Programme

	Monday	Tuesday	Wednesday	Thursday
08:30	Registration			
09:00–10:00	Röckner	Röckner	Romito	Pavliotis
10:00	Peszat	Szepessy	Crisan	Geiß
10:30	*Coffee Break*	*Coffee Break*	*Coffee Break*	*Coffee Break*
11:00	Xiong	Lord	Blömker	Schmalfuß
11:30	Gyöngy	Gyöngy	Printems	von Schwerin
12:00				Marheineke
12:30–14:00	*Lunch Break*	*Lunch Break*	*Lunch Break*	*Lunch Break*
14:00	Röckner	Kovacs		Cyron
14:30				Hakansson
15:00	Voß	Kim	Excursion	Henkel
15:30	Gruhlke	Hausenblas		Carelli
16:00	*Coffee Break*	*Coffee Break*		*Coffee Break*
16:30	Gyöngy	Lindner		Zouraris
17:00		Jentzen		Ritter
17:30	Weber			

Monday, 24 August 2009

Time	Speaker	*Title of Talk*
9:00-10:00	Röckner	*A Concise Course on Stochastic Partial Differential Equations I*
10:00-10:30	Peszat	*Regularity of solutions to linear SPDEs with Levy noise*
10:30-11:00		–Coffee Break–
11:00-11:30	Xiong	*Joint continuity for the solutions to a class of nonlinear SPDE*
11:30-12:30	Gyöngy	*On Numerical Solutions of Stochastic Partial Differential Equations I*
12:30-14:00		–Lunch Break–
14:00-15:00	Röckner	*A Concise Course on Stochastic Partial Differential Equations II*
15:00-15:30	Voß	*Sampling Conditioned Hypoelliptic Diffusions*
15:30-16:00	Gruhlke	*Transition Path Sampling - Non-gradient case*
16:00-16:30		–Coffee Break–
16:30-17:30	Gyöngy	*On Numerical Solutions of Stochastic Partial Differential Equations II*
17:30-18:00	Weber	*Sharp interface limits for invariant measures*

Tuesday, 25 August 2009

Time	Speaker	*Title of Talk*
09:00-10:00	Röckner	*A Concise Course on Stochastic Partial Differential Equations III*
10:00-10:30	Szepessy	*Stochastic molecular dynamics*
10:30-11:00		–Coffee Break–
11:00-11:30	Lord	*Numerical solution of the stochastic Swift-Hohenberg Equation*
11:30-12:30	Gyöngy	*On Numerical Solutions of Stochastic Partial Differential Equations III*
12:30-14:00		–Lunch Break–
14:00-15:00	Kovacs	*Strong, weak and a posteriori error analysis of the finite element method for parabolic and hyperbolic stochastic equations*
15:00-15:30	Kim	*An* L_2*-theory of stochastic PDEs driven by Lèvy processes*
15:30-16:00	Hausenblas	*SPDEs driven by Levy processes and their numerical approximation*
16:00-16:30		–Coffee Break–
16:30-17:00	Stoevesandt	*Analysing Multipoint Correlations in Numerical Simulations*
17:00-17:30	Lindner	*Weak order for the discretization of the stochastic heat equation driven by impulsive noise*
17:30-18:00	Jentzen	*Taylor expansions for stochastic partial differential equations*

Wednesday, 26 August 2009

Time	Speaker	*Title of Talk*
09:00-10:00	Romito	*Markovian approach to stochastic PDE*
10:00-10:30	Crisan	*Solving the Zakai equation using cubature methods*
10:30-11:00		–Coffee Break–
11:00-11:30	Blömker	*Local Shape of Random invariant Manifold*
11:30-12:00	Millet	*On the splitting method for the stochastic Schrödinger equation*
12:00-13:00	Printems	*Weak order for the discretization of the stochastic heat equationdriven by impulsive noise*
13:00-15:00		–Lunch Break–
15:00-19:30		–Excursion–

Thursday, 27 August 2009

Time	Speaker	*Title of Talk*
09:00-10:00	Pavliotis	*Asymptotic Problems for non-Markovian Langevin equations*
10:00-10:30	Geiß	*On the L_p-variation of BSDEs and fractional smoothness*
10:30-11:00		–Coffee Break–
11:00-11:30	Schmalfuß	*Random dynamical systems with SPDE driven by a fractional Brownian motion*
11:30-12:00	von Schwerin	*Adaptive Multi Level Monte-Carlo Simulation of Stochastic Ordinary Differential Equations*
12:00-12:30	Marheineke	*SPDE-models for nonwoven production processes*
12:30-14:00		–Lunch Break–
14:00-14:30	Cyron	*A finite element approach to the Brownian dynamics of polymers*
14:30-15:00	Hakansson	*Conjugate gradient and GMRES methods for parametrized linear random algebraic equations*
15:00-15:30	Henkel	*Pointwise Approximation of a Stochastic Heat Equation with Additive Space-Time White Noise*
15:30-16:00	Carelli	*Domain decomposition strategies for the stochastic heat equation*
16:00-16:30		–Coffee Break–
16:30-17:00	Zouraris	*Finite element approximations for a fourth-order SPDE*
17:00-17:30	Ritter	*Multi-level Monte Carlo Methods for SPDEs*

3 List of Talks

3.1 Short Courses

István Gyöngy
On Numerical Solutions of Stochastic Partial Differential Equations
University of Edinburgh, UK

First lecture

In the first part of this series of lectures, stochastic evolution equations with monotone operators are considered. A general framework to investigate various numerical approximations is introduced that can be used to study finite difference, wavelets and finite elements space discretizations. Rate of convergence estimates are obtained. The results can be applied to a class of quasilinear stochastic PDEs of parabolic type. In particular, rate of convergence estimates for finite difference schemes to linear SPDEs are deduced from the abstract setting.

Second lecture

In the second part, splitting-up approximations for linear SPDEs are studied and moment estimates for the error are obtained. We also show that our estimates are sharp.

Third lecture

In the third part, accelerated numerical schemes for PDEs and SPDEs are presented. In particular, sufficient conditions are given under which the convergence of finite difference approximations for stochastic PDEs of parabolic type can be accelerated to any given order of convergence by Richardson's method.

The first part of these lectures is based on joint work with Annie Millet. The second and third parts are based on joint results with Nicolai Krylov.

Michael Röckner
A Concise Course on Stochastic Partial Differential Equations
Universität Bielefeld, Germany

First lecture

The first lecture will consist of an introduction to stochastic integration with respect to Brownian motion, in particular on Hilbert spaces. We shall try to keep prerequisites to a minimum as far as this is possible.

Second lecture

The second lecture will present the main existence and uniqueness result for stochastic differential equations (SDE) under monotonicity conditions within the so-called "variational approach". We shall also briefly recall the special finite dimensional case, where the proof is based on the Euler approximation. If time permits, we shall also compare this with other approaches ("semigroup approach", "martingale approach").

Third lecture

The third lecture will be devoted to examples and applications to stochastic partial differential equations of evolutionary type. These include the stochastic heat equation, the stochastic p-Laplace equation and the stochastic porous media equation. In particular, the latter has been analyzed recently in a number of papers in regard to various aspects. If there is time left, I shall give a short overview about the respective results.

The lectures will be based on the following **reference**:

C.Prevot, M. Röckner: *A Concise Course on Stochastic Partial Differential Equations*, Lecture Notes in Mathematics, 1905, Springer, Berlin 2007.

3.2 Keynote Speakers

Mihaly Kovacs
Strong, weak and a posteriori error analysis of the finite element method for parabolic and hyperbolic stochastic equations
University of Otago, New Zealand

We consider the heat and wave equations driven by additive noise. We discretize the equations in space by the standard continuous finite element method and derive various error estimates under sharp regularity assumptions. We use the operator semigroup framework for stochastic PDEs proposed by Da Prato and Zabczyk in the analysis. The first kind of estimate measures the error in the mean square norm and shows the so called strong convergence. Here, appropriate error estimates for the deterministic problem give error estimates for the stochastic equations in a more or less straightforward fashion. In case of the semilinear stochastic heat equation the possibility of truncating the expansion of the noise is also discussed. In the second type of error analysis the error is measured in the weak sense of probability measures and implies the so called weak convergence. The analysis in this case is considerably more complicated and uses more advanced results both from infinite dimensional stochastic analysis as well as from functional analysis. Here, the linear stochastic heat equation is discussed. Finally, we consider a posteriori type error estimates for the stochastic heat equation.

Grigorios Pavliotis
Asymptotic Problems for non-Markovian Langevin equations
Imperial College London, UK

In this talk we will present some recent results on the long time asymptotics of the generalized Langevin equation (gLE). In particular, we study the ergodic properties of the gLE and we also prove a homogenization (central limit) theorem. The analysis is based on the approximation of the gLE by a high (and possibly infinite) dimensional degenerate Markovian system, and on the analysis of the spectrum of the generator of this Markov process.

Jacques Printems
Weak order for the discretization of the stochastic heat equation driven by impulsive noise
Université Paris-Est, France

First, I will recall some known results concerning weak and strong order of convergence of numerical schemes applied to some SPDEs driven by space-time noise. I will also give some examples of the typical difficulties encountered. Then I will consider two semi-discrete schemes for SPDEs of Burger's type in the additive case and give some results of rate of convergence for the weak error.

Marco Romito
Markovian approach to stochastic PDE
University of Florence, Italy

The analysis of solutions to some stochastic dissipative PDE (notably, the Navier-Stokes equations) for which well-posedness is an open problem can be explored using the idea of Markov solutions. Under appropriate assumptions on the driving noise such solutions have some remarkable properties, such as regularity (with respect to initial condition) and unique ergodicity. Such properties seem to be closely related to the topology where the equations are locally solvable.
It turns out that Markov solutions essentially provide a useful framework to clearly state and recover several properties of solutions, such as convergence to the invariant measure (including the case of mild degeneracy of the noise) or stability with respect to small parameters.
We shall discuss some examples that try to clarify the whole picture.

3.3 Further Speakers

Dirk Blömker
Local Shape of Random invariant Manifolds
Universität Augsburg, Germany

We consider an SPDE of Burgers type with simple multiplicative noise. Near a change of stability, we investigate the local shape of the random invariant manifold around the deterministic fixed-point. This approach is compared to the approximation of SPDEs via amplitude equations. Joint work with Wei Wang (Adelaide/Nanjing).

Erich Carelli
Domain decomposition strategies for the stochastic heat equation
Universität Tübingen, Germany

We consider the numerical approximation of solutions of the stochastic, Hilbert space valued heat equation

$$dX_t + AX_t dt = Q^{1/2} dW_t \qquad \forall t \in (0,T) \text{ and } X_0 \in H, \tag{3.1}$$

with an elliptic operator $A : D(A) \to H$, and $Q : H \to H$ is the covariance operator of the driving Wiener process. We apply different domain decomposition algorithms based on explicit and implicit time stepping, paired with finite element and backward Euler discretisation to solve the problem, and give optimal strong and weak rates of convergence.

Dan Crisan
Solving the Zakai equation using cubature methods
Imperial College London, UK

In the last decade, a new class of numerical methods for approximating weak solutions of SDEs have been introduced by Kusuoka, Lyons, Ninomiya and Victoir. These methods are based on the work of Kusuoka and Stroock who established refined gradient upper bounds for the associated semigroup using Malliavin Calculus techniques. In this talk, I will present an application of these methods to the numerical solution of the Zakai equation and its application to stochastic filtering. The talk is based on joint work with S. Ghazali.
Further information: `http://www.ma.ic.ac.uk/~dcrisan/weakapprx.pdf`

Christian Cyron
A finite element approach to the Brownian dynamics of polymers
TU Müchen, Germany

For several decades Brownian dynamics of polymers has attracted rising interest among physicists, chemists, material scientists and engineers. Many processes of crucial importance especially in biophysics are well-known to be governed by the Brownian dynamics of polymers.
Computer simulations have become increasingly popular in order to study this dynamics. For such simulations Brownian dynamics is usually modeled by means of a stochastic partial differential equation. The polymers subject to this dynamics are

usually modeled as a chain of beads and rods in order to account for structural mechanics. So called bead-spring- and bead-rod-models together with an explicit time integration scheme are especially popular. However, there is a number of drawbacks of such models, especially with respect to numerical stability and a missing sound theoretical foundation.
In this talk we introduce a new approach for the numerical simulation of Brownian dynamics of polymers by means of the so called finite element method. We show the extensions necessary for non-linear finite beam elements in order capture Brownian polymer dynamics and discuss the advantages of this approach over other model, especially bead-spring- and bead-rod-models. We demonstrate the efficiency of the method by means of several numerical examples with respect to biophysics. Finally we give a brief outlook how the finite element approach for Brownian polymer dynamics could be exploited to understand phenomena such as mechanics of the cytoskeleton or cell motility.

Stefan Geiß

On the L^p-variation of BSDEs and fractional smoothness

University of Jyväskylä, Finland

We consider the L^p-variation of BSDEs and relate this to a generalized version of fractional smoothness which takes care about the propagation of singularities over time.

Daniel Gruhlke

Transition Path Sampling - Non-gradient case

Universität Bonn, Germany

Transition path sampling is concernd with sampling from the distribution of the solution of an SDE, conditioned on the value of its endpoint. The case where the drift of this SDE is given by a gradient of a potential is studied in detail in works of M. Hairer, A. Stuart and J. Voss. The main idea is to find a process on path space which has the wanted distribution as (unique) invariant measure.
The used techniques do not apply in the non-gradient case which is left as an open problem, but a Dirichlet form approach allows us to construct a process on path-space which is reversible with respect to the distribution of the SDE (conditioned on the value of endpoint) even in the non-gradient setting.

Par Hakansson
Conjugate gradient and GMRES methods for parametrized linear random algebraic equations
University of Southampton, UK

We present preconditioned conjugate gradient methods for solving linear random algebraic equations that arise from discretization of stochastic partial differential equations (SPDE) [1]. Hence, by finding solution to SPDEs we can look into uncertainty propagation in mechanical problems. The random dimension is parametrized in a polynomial chaos basis. Preconditioned iterative schemes are presented for equations with symmetric positive definite and general nonsymmetric coefficient matrices. We show that for the special case of symmetric positive definite coefficient matrices, the proposed formulation of the conjugate gradient algorithm has a mathematical equivalence with the Ghanem-Spanos polynomial chaos projection scheme. We illustrate and solve a problem in computing the residual at accurate PC-order needed to safely determine convergence of solution. Numerical results are presented for a steady-state stochastic diffusion equation to illustrate the performance of the proposed numerical methods [2].

References

[1] R. Ghanem and P. Spanos, Stochastic Finite Elements: A Spectral Approach, Springer-Verlag, 1991

[2] CE Powell and HC Elman, Block-diagonal preconditioning for spectral stochastic finite-element systems, IMA J Numer Anal 29: 350-375 (2009)

Erika Hausenblas
SPDEs driven by Levy processes and their numerical approximation
Universität Salzburg, Austria

First, I would like to introduce Levy processes, respective Poisson random measures, and stochastic integration with respect to Levy processes, in particular, stochastic integration in Banach spaces.
The second part of the talk will be about existence and uniqueness of SPDEs. Here, I will point out the techniques which are used and present some results.
In the third and last part of the talk I will speak abut the numerical approximation of SPDEs, in particular, of SPDEs driven by Levy processes.
The talk will be based on the following works [1–3]:

[1] E. Hausenblas: Existence, uniqueness and regularity of parabolic SPDEs driven by Poisson random measure. *Electron. J. Probab.*, **10**, (2005), 1496–1546.

[2] E. Hausenblas: Finite element approximation of stochastic partial differential equations driven by Poisson random measures of jump type. *SIAM J. Numer. Anal.* **46** (2007/08), 437–471.

[3] E. Hausenblas, T. Dunst: Numerical experiments concerning Finite element approximation of stochastic partial differential equations driven by Poisson random measures . *In preparation*, (2009).

Daniel Henkel

Pointwise Approximation of a Stochastic Heat Equation with Additive Space-Time White Noise

TU Darmstadt, Germany

We consider a stochastic heat equation on the spatial domain $(0,1)$ with additive space-time white noise, and we study approximation of the mild solution at a fixed time point with respect to the average L_2-distance. In this talk we consider algorithms, which use a total of N evaluations of one-dimensional components of the driving Wiener process W and we present upper and lower error bounds in terms of N. In particular we compare uniform with non-uniform time discretizations.

Arnulf Jentzen

Taylor expansions for stochastic partial differential equations

J. W. Goethe Universität Frankfurt, Germany

Taylor expansions of the solution of a stochastic partial differential equation (SPDE) of evolutionary type and their first applications to numerical analysis are presented. The key instruments for deriving such Taylor expansions are the semigroup approach, i.e. to understand the SPDE as a mild integral equation, and an appropriate recursion technique.

Kyeong-Hun Kim
An L_2-theory of stochastic PDEs driven by Lèvy processes
Korea University, Republic of Korea

In this talk, we consider the following stochastic PDE driven by Lèvy processes:

$$du = (D_i(a^{ij}u_{x^j} + b^i u) + cu_{x^i} + du + f)dt + (\sigma^{ik}u_{x^i} + \nu^k u + g^k)dZ_t^k.$$

Here $i, j = 1, 2, ..., n$ and $k = 1, 2, ...$ All the coefficients of the equation are random and depend also on space and time variables. We present the uniqueness and existence results in L_2-spaces.

Felix Lindner
Weak order for the discretization of the stochastic heat equation driven by impulsive noise
TU Dresden, Germany

We study the approximation of the distribution of X_T, where $(X_t)_{t\in[0,T]}$ is a Hilbert space-valued stochastic process that solves a linear parabolic stochastic partial differential equation written in abstract form as

$$dX_t + AX_t\,dt = Q^{1/2}\,dZ_t, \quad X_0 = x_0 \in H, \quad t \in [0, T],$$

driven by an impulsive space time noise whose covariance operator Q is given. $A^{-\alpha}$ is assumed to have finite trace for some $\alpha > 0$ and $A^\beta Q$ is assumed to be bounded for some $\beta \geq 0$.
A discretized solution $(X_h^n)_{n\in\{0,1,...,N\}}$ is defined via finite element methods in space (parameter $h > 0$) and implicit Euler schemes in time (parameter $\Delta t = T/N$). For suitable functions φ defined on H, it is shown that

$$|\mathbb{E}\varphi(X_h^N) - \mathbb{E}\varphi(X_T)| = O(h^\gamma + \Delta t^{\gamma/2})$$

where $\gamma < 1 - \alpha + \beta$.
This work is based on a paper by A. Debussche and J. Printems.

Gabriel Lord
Numerical solution of the stochastic Swift-Hohenberg Equation
Heriot–Watt University, UK

Nicole Marheineke
SPDE-models for nonwoven production processes
TU Kaiserslautern, Germany

For the simulation of production processes of technical textiles a hierarchy of SPDE-models is presented. The models range from highly complex three-dimensional fluid-solid interactions to one-dimensional fiber dynamics with stochastic aerodynamic drag and further to efficiently handable stochastic surrogate models for fiber lay-down. The hierarchy is theoretically and numerically analyzed in this talk.

Szymon Peszat
Regularity of solutions to linear SPDEs with Levy noise
Polish Academy of Sciences, Cracow, Poland

Conditions for the existence of a cadlag version of a solution to an infinite dimensional linear stochastic differential equation driven by a Levy noise will be given. Examples of equations with non cadlag solutions will be presented as well.

Klaus Ritter
Multilevel Monte-Carlo Methods for SPDEs
TU Darmstadt, Germany

We study infinite-dimensional integration wrt the distribution of the mild solution X of an spde at the final time point T, i.e. computation of the expected value $E(f(X(T)))$ for certain functionals f. In this talk we focus on Lipschitz functionals and we combine the multi-level technique with results for pathwise approximation of X to obtain new algorithms and corresponding error bounds for the integration problem. The theoretical analysis is complemented by numerical experiments.
This is a joint work with Simone Graubner (TU Darmstadt) and Thomas Müller-Gronbach (University of Passau).

Björn Schmalfuß
Random dynamical systems with SPDE driven by a fractional Brownian motion
Universität Paderborn, Germany

We consider an spde with a fractional Brownian motion. At first we show that such an equation generates a random dynamical system. Based on this property we then formulate conditions ensuring that the generated random dynamical system has a random attractor or a random unstable manifold.

Anders Szepessy
Stochastic molecular dynamics
Royal Institute of Technology, Stockholm, Sweden

Starting from the Schrödinger equation for nuclei-electron systems I will show two stochastic molecular dynamics effects derived from a Gibbs distribution:

- When the ground state has a large spectral gap a precise Langevin equation for molecular dynamics approximates observables from the Schrödinger equation.
- If the gap is smaller in some sense, the temperature also gives a precise correction to the ab initio ground state potential energy.

The two approximation results holds with a rate depending on the spectral gap and the ration of nuclei and electron mass.
I will also give an example of course-graining this stochastic Langevin molecular dynamics equation to obtain a continuum stochastic partial differential equation for phase transitions.

Erik von Schwerin
Adaptive Multi Level Monte Carlo Simulation of Stochastic Ordinary Differential Equations
King Abdullah University of Science and Technology, Saudi Arabia

This work generalizes a multilevel Forward Euler Monte Carlo method introduced in [1] for the approximation of expected values depending on the solution to an Ito stochastic differential equation. The work [1] proposed and analyzed a Forward Euler Multilevel Monte Carlo method based on a hierarchy of uniform time discretizations and control variates to reduce the computational effort required by a standard, single level, Forward Euler Monte Carlo method. This work introduces and analyzes an adaptive hierarchy of non uniform time discretizations, generated by adaptive algorithms introduced in [2, 3]. These adaptive algorithms apply either deterministic time steps or stochastic time steps and are based on adjoint weighted a posteriori error expansions first developed in [4]. Under sufficient regularity conditions, both our analysis and numerical results, which include one case with singular drift and one with stopped diffusion, exhibit savings in the computational cost to achieve an accuracy of $O(\mathrm{TOL})$, from $O\left(\mathrm{TOL}^{-3}\right)$ to $O\left(\left(\mathrm{TOL}^{-1}\log(\mathrm{TOL})\right)^2\right)$.
This is a joint work with H. Hoel, R. Tempone and A. Szepessy.

References

[1] Giles, M. B., Multilevel Monte Carlo path simulation, *Oper. Res*, **56**, no. 3, 607-617, (2008).

[2] Moon, K-S. ; von Schwerin, E. Szepessy, A.; and Tempone, R., An adaptive algorithm for ordinary, stochastic and partial differential equations, *Recent advances in adaptive computation, Contemp. Math*, **383**, 325-343, (2005).

[3] Moon, K-S.; Szepessy, A.; Tempone, R. and Zouraris, G. E., Convergence rates for adaptive weak approximation of stochastic differential equations, *Stoch. Anal. Appl.*, **23**, no. 3, 511-558, (2005).

[4] Szepessy, A.; Tempone, R. and Zouraris, G. E.: Adaptive weak approximation of stochastic differential equations, *Comm. Pure Appl. Math*, **54**, no. 10, 1169-1214, (2001).

Jochen Voß

Sampling Conditioned Hypoelliptic Diffusions

University of Leeds, UK

A well-known method to sample from a given target distribution on a finite dimensional space is to simulate the solution of a stochastic differential equation (SDE) which has the target distribution as its invariant measure. Assuming ergodicity of the SDE, the solution of the SDE at a "large" time can be used as an approximation to a sample from the target distribution.
If the target distribution lives on an infinite dimensional space, the situation is less clear, but it transpires that often one can still employ the same idea. We show how one can use SDEs with values in the space of continuous functions to sample from certain target distributions on this space. In the cases we consider, the sampling equation turn out to be stochastic partial differential equations (SPDEs).
In order to derive an implementable MCMC method from these results, one needs to discretise the resulting SPDEs. We give some preliminary results comparing different discretisation schemes for these equations.

Hendrik Weber

Sharp interface limit for invariant measures

Universität Bonn, Germany

The invariant measure of a 1-dimensional Allen-Cahn equation with an additive space-time white noise is studied. This measure is absolutely continuous with respect to a Brownian bridge with a density which can be interpreted as a potential energy term. We consider the sharp interface limit in this setup. In the right scaling this corresponds to a Gibbs type measure on a growing interval with decreasing temperature. Our main result is that in the limit we still see exponential convergence towards a curve of minimizers of the energy if the interval does not grow too fast. In the original scaling the limit measure is concentrated on configurations with precisely one jump. This jump is distributed uniformly.

Jie Xiong
Joint continuity for the solutions to a class of nonlinear SPDE
University of Tennessee, US

For a superprocess in a random environment in one dimensional space, a nonlinear stochastic partial differential equation is derived for its density by Dawson-Vaillancourt-Wang (2000). The joint continuity was left as an open problem. In this talk, we will give an affirmative answer to this problem.

Georgios Zouraris
Finite element approximations for a fourth-order SPDE
University of Crete, Greece

We consider an initial and Dirichlet boundary value problem for a fourth-order SPDE driven by an additive space-time white noise. Discretizing the space-time white noise a modeling error is introduced and an regularized problem is obtained. The solution of the regularized problem is approximated combining a finite element method in space with the backward Euler method in time. We derive error estimates for the modeling error and for the approximation error to the solution of the regularized problem.

4 Registrants

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Points of interest:

1. Department of Mathematics including Computer Pool
2. Lecture Hall
3. Welcome Hotel
4. Hotel Bockshaut
5. Hotel Ernst Ludwig
6. Darmstadt City (Carree)
7. Bus stop, Willy-Brandt Platz
8. Bus stop, Schloss
9. Refectory