Institut für Numerische Simulation
Rheinische Friedrich-Wilhelms-Universität Bonn

Sixth International Workshop

Meshfree Methods for Partial Differential Equations

Book of Abstracts

Date:	October 04–06, 2011
Location:	Bonn, Germany
Sponsor:	Sonderforschungsbereich 611
Organizers:	Prof. Ivo Babuška (University of Texas, Austin, USA)
	Prof. Ted Belytschko (Northwestern University, USA)
	Prof. Jiun-Shyan Chen (University of California, Los Angeles, USA)
	Prof. Michael Griebel (Universität Bonn, Germany)
	Prof. Wing Kam Liu (Northwestern University, USA)
	Prof. Marc Alexander Schweitzer (Universität Stuttgart, Germany)
	Prof. Harry Yserentant (Technische Universität Berlin, Germany)
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Universität Bonn SFB 611

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The numerical treatment of partial differential equations with meshfree discretization techniques has been a very active research area in recent years. While the fundamental theory of meshfree methods has been developed and considerable advances of the various methods have been made, many challenges in the mathematical analysis and practical implementation of meshfree methods remain.

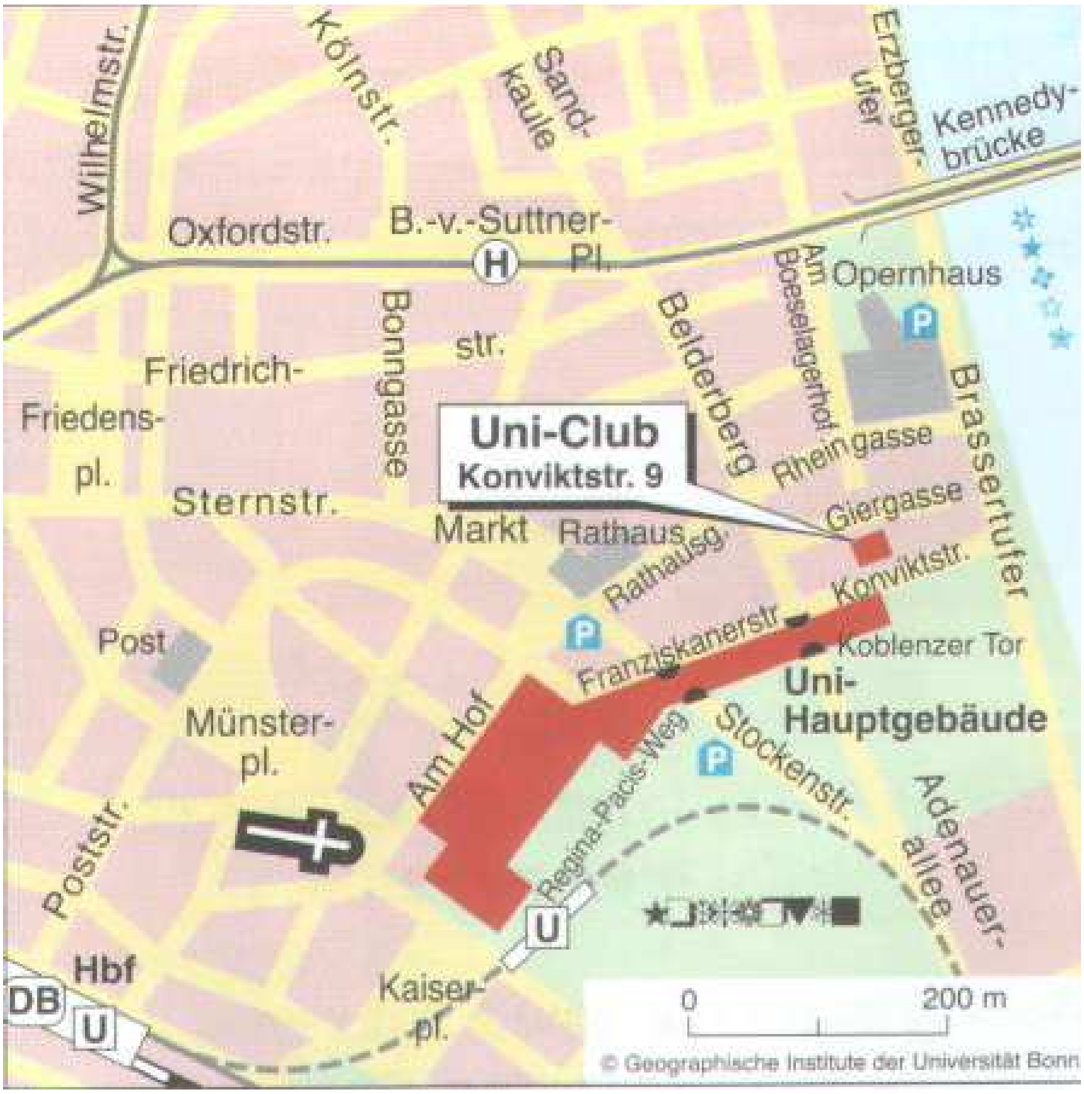
Meshfree methods, particle methods, and generalized finite element methods have undergone substantial development since the mid 1990s. The growing interest in these methods is in part due to the fact that they are very flexible numerical tools and can be interpreted in a number of ways. For instance, meshfree methods can be viewed as a natural extension of classical finite element and finite difference methods to scattered node configurations with no fixed connectivity. Furthermore, meshfree methods have some advantageous features which are especially attractive when dealing with multiscale phenomena: A-priori knowledge about particular local behavior of the solution can be introduced easily in the meshfree approximation space, and an enrichment of a coarse scale approximation with fine scale information is possible in a seamless fashion. The implementation of meshfree methods and their parallelization however requires special attention, for instance with respect to numerical integration.

This symposium aims to promote collaboration among engineers, mathematicians, and computer scientists and industrial researchers to address the development, mathematical analysis, and application of meshfree and particle methods especially to multiscale phenomena. While contributions in all aspects of meshfree methods are invited, some of the key topics to be featured are

- Coupling of meshfree methods, finite element methods, particle methods, and finite difference methods
- Coupling of multiple scales, e.g. continuum models to discrete models
- Application of meshfree, generalized/extended finite element methods
- Parallel computation in meshfree methods
- Mathematical theory of meshfree, generalized finite element, and particle methods
- Fast and stable domain integration methods
- Enhanced treatment of boundary conditions
- Identification and characterization of problems where meshfree methods have clear advantage over classical approaches

Workshop venue
The workshop is hosted by the Institut für Numerische Simulation, Universität Bonn, http://www.ins.uni-bonn.de, in cooperation with the Sonderforschungsbereich 611 „Singuläre Phänomene und Skalierung in mathematischen Modellen“, Universität Bonn, http://sfb611.iam.uni-bonn.de, funded by the Deutsche Forschungsgemeinschaft, http://www.dfg.de, and the Universitätsclub Bonn, http://www.uniclub-bonn.de.

Contact Information



Our registration desk will be open Tuesday from 8.00 – 8.45 a.m. Before and after the workshop, please use the email meshfree@ins.uni-bonn.de, Phone ++49-228-733427 and Fax ++49-228-737527.

We will have overhead-projectors, data-projectors (resolution 1024×768), flip-charts and laptops running Windows XP, MS Office, Acrobat-Reader in the conference rooms.

Computing facilities are located on the second floor of the university club. 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.

Conference dinner Wednesday, October 05: Conference dinner at the restaurant "Em Höttche", Markt 4, starting at 19:00. Please bring your dinner ticket with you!

Program Committee

- Prof. Ivo Babuška (University of Texas, Austin, USA)
- Prof. Ted Belytschko (Northwestern University, USA)
- Prof. Jiun-Shyan Chen (University of California, Los Angeles, USA)
- Prof. Michael Griebel (Universität Bonn, Germany)
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- Prof. Marc Alexander Schweitzer (Universität Stuttgart, Germany)
- Prof. Harry Yserentant (Technische Universität Berlin, Germany)

Local Organizers

- Prof. Michael Griebel
- Prof. Marc Alexander Schweitzer
- Dr. Christian Rieger

Acknowledgement
Special thanks also to the Sonderforschungsbereich 611 and the Deutsche Forschungsgemeinschaft for funding the financial support.

Timetable

Time	Tuesday 04.10.2011	Wednesday 05.10.2011	Thursday 06.10.2011
8:00–8:30	Registration		
8:30–8:45	Opening Remarks		
08:45–09:30	Liu	Arnold	
09:30–10:15	Oliver	Emmrich	Schweitzer
10:15–10:45		Coffee Break	
10:45–11:30	Nistor	Chen	Lipton
11:30–12:00	Nogueira	Chinchaladze	Gáspár
12:00–12:30	Bompadre	Colominas	Rainer
12:30–14:30		Lunch Break	
14:30–15:00	Ganzenmüller	Liu	Schönewald
15:00–15:30	Simkins	Fackeldey	Seibold
15:30–16:00		Coffee Break	
16:30–17:00	Ye	Daum	Davydov
17:00–17:30	Yas'ko		Govorukhin
19:00		Dinner	

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Tue 10:45–11:30, Wolfgang Paul Hall, V. Nistor. *Quasi-optimal rates of convergence for GFEM on polygons*.

Tue 11:30–12:00, Wolfgang Paul Hall, X. Nogueira. *Compressible flow applications of a finite volume method based on Moving Least Squares*.

Tue 12:00–12:30, Wolfgang Paul Hall, A. Bompadre. *Error analysis of meshfree approximation methods based on optimization*.

Tue 14:00–14:30, Wolfgang Paul Hall, G. C. Ganzenmüller, S. Hiermaier, M. O. Steinhauser. *Thermodynamically consistent coupling of Smooth Particle Hydrodynamics and Molecular Dynamics*.

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Wed 8:45–9:30, Wolfgang Paul Hall, A. Arnold. *ESPResSo - Extensible Simulation Package for Research on Soft matter*.

Wed 9:30–10:15, Wolfgang Paul Hall, E. Emmrich. *Analysis of the peridynamic model in nonlocal elasticity*.

Wed 10:45–11:30, Wolfgang Paul Hall, J. S. Chen. *A General Framework of Domain Integration in Meshfree Methods*.

Wed 11:30–12:00, Wolfgang Paul Hall, N. Chinchaldze. *Cubature of the solution of the thin wedge-shaped shells deflections problem by approximate quasi-interpolant*.

Wed 12:00–12:30, Wolfgang Paul Hall, I. Colominas. *Meshless approximations for the development of high order finite volume methods*.

Wed 14:00–14:30, Wolfgang Paul Hall, W. K. Liu. *Immersed Molecular Electrokinetic Finite Element Method for Nano-Devices in Biotechnology and Drug Delivery*.

Wed 14:30–15:00, Wolfgang Paul Hall, K. Fackeldey. *Meshfree Methods in Drug Design*.

Wed 16:00–16:30, Wolfgang Paul Hall, F. Daum. *Solution of Poisson's equation in high dimensions*.

Thu 9:30–10:15, Wolfgang Paul Hall, M. A. Schweitzer. *TBA*.

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Thu 11:30–12:00, Wolfgang Paul Hall, C. Gáspár. *Some Regularized Versions of the Method of Fundamental Solutions*.

Thu 12:00–12:30, Wolfgang Paul Hall, S. Rainer. *Meshfree exponential integrators*.

Thu 14:00–14:30, Wolfgang Paul Hall, A. Schönewald. *A Smoothed Point Interpolation Method for Structural Dynamics*.

Thu 14:30–15:00, Wolfgang Paul Hall, B. Seibold. *Characteristic particle methods for traffic flow simulations on highway networks*.

Thu 16:00–16:30, Wolfgang Paul Hall, O. Davydov,D. T. Oanh. *RBF-FD Methods for Elliptic Equations*.

Thu 16:30–17:00, Wolfgang Paul Hall, V. Govorukhin. *A meshfree method for the analysis of planar flows of a inviscid fluids*.

1 Tuesday 04.10.2011

1.1 Immersed Molecular Electrokinetic Finite Element Method for Nano-Devices in Biotechnology and Drug Delivery

Tue 8:45–9:30, Wolfgang Paul Hall

Wing Kam Liu*
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The lecture opens with a discussion on modern uses of multiscale analysis, uncertainty quantification techniques, and validation experiments for the design of nanodevices in biotechnology and medicine. The 3D immersed molecular electrokinetic finite element method (IMEFEM) will be presented for the modeling of micro fluidic electrokinetic assembly of nano wires and filaments and bio-molecules. This transformative bio-nanotechnology is being developed to enable drug delivery systems to achieve desired therapeutic effects and for the design and optimization of an electric field enabled nanotip DNA sensor. For the Nanodiamond-based drug delivery device we will discuss the multiscale analysis, quantum and molecular mechanics, immersed finite element and meshfree methods, uncertainty quantification, validation experiments. In addition, we will describe the mathematical formulation of pH control interactions among chemically functionalized nanodiamond, doxorubicin hydrochloride drugs and biocompatible parylene polymer. For the nanotip, we will discuss the underlying mechanics and physical parameters influencing the bio-sensing efficiency of the nanotip, such as the threshold of applied electric field, nano/microfluidics, bio-molecule deformation, and nanoscale Brownian motion. Through multiscale analysis, we will provide guidelines for nanodevice design, including fundamental mechanisms driving the system performance and optimization of distinct parameters for the high-sensitivity device throughput.

1.2 TBA

Tue 9:30–10:15, Wolfgang Paul Hall

Marcel Oliver*
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1.3 Quasi-optimal rates of convergence for GFEM on polygons

Tue 10:45–11:30, Wolfgang Paul Hall

Anna Mazzucato, Victor Nistor*, Qingqin Qu
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We construct a sequence S_n of Generalized Finite Element (GFEM) spaces on a polygonal domain Ω that provide optimal rates of convergence for the approximate solutios of the Poisson equation -Delta u = f with Dirichlet boundary conditions. The proof is based on the usual regularity results for u in weighted Sobolev (or Babuska-Kondratiev) spaces. This leads to the optimal rates of convergence $||u - u_n||_1 \leq Cdim(S_n)^{-m/2}||f||_{m-1}$ where $u_n \in S_n$ are the Finite Element approximations of the solution. The integer m is the order of the polynomials used and f is assumed to be in $H^{m-1}(\Omega)$. No extraneous assumptions on the solution u are made. In particular, it is not assumed that u is in any high regularity Sobolev space (only that u is in H^1 as the weak solution of the equation). The grading used is similar to the one used by Babuska-Kellogg-Pitkaranta, Apel, and others in the framework of the usual FEM. This is joint work with Anna Mazzucato and Qingqin Qu

1.4 Compressible flow applications of a finite volume method based on Moving Least Squares

Tue 11:30–12:00, Wolfgang Paul Hall

Xesús Nogueira*
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Finite volume solvers have been (and still are) the standard method to compute compressible flows in industry. Recently, a a high-order finite volume method based on Moving Least Squares (MLS) approximants have been developed by the authors. MLS is used to compute the derivatives of the reconstruction step of a finite volume method. This numerical methodology allows to increase the accuracy of any existing finite volume code in a simple way.

In this contribution we show several applications of a high-order finite volume method based on Moving Least Squares (MLS) approximations. . The high accuracy in the computation of derivatives makes possible the application of this numerical method in aeroacoustics problems, DNS and LES of compressible turbulent flows.

1.5 Error analysis of meshfree approximation methods based on optimization

Tue 12:00–12:30, Wolfgang Paul Hall

Agustin Bompadre*
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Approximation methods are used to solve numerically PDEs in Material Science. Finite Element Methods are the most usual technique used in this context.

In this talk, we discuss meshfree approximation methods, which are approximation methods that do not need a meshing of the domain. We give a set of sufficient conditions to guarantee the convergence of approximates based on meshfree methods. We review the Local Maximum-Entropy approximation scheme, which is a meshfree approximation method based on an optimization principle, and we show that the general error bounds apply to this method.

1.6 Thermodynamically consistent coupling of Smooth Particle Hydrodynamics and Molecular Dynamics

Tue 14:00–14:30, Wolfgang Paul Hall

G. C. Ganzenmüller*, S. Hiermaier, M. O. Steinhauser
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It is straightforward from a computational perspective to devise ad-hoc coupling schemes, based on momentum exchange only, between classical Molecular Dynamics (MD) and Smooth Particle Hydrodynamics (SPH), as both methodologies use mesh-independent solution strategies. However, a thermodynamic inconsistency with respect to temperature arises at the interface, where SPH particles meet MD particles. SPH – being a continuum method – lacks thermal fluctuations based on the equipartition theorem, and temperature is only associated with the particles' internal energy. In MD, on the other hand, temperature manifests itself as thermal fluctuations of the particles' velocities only. Here, we introduce a new strategy, based on Dissipative Particle Dynamics with conserved Energy [1], which includes macroscopic heat transfer between MD and SPH particles and couples SPH temperature with MD kinetic temperature by means of a thermodynamically consistent fluctuation-dissipation theorem. We validate our coupling scheme by showing that the particle velocity distribution is consistent with the theoretical Maxwell-Boltzmann result, while total energy is conserved within numerical errors. The correct dynamics of shock-wave propagation is demonstrated with a system, where a shock-wave front is passed from SPH regions to MD regions and back. As an important example application in Biophysics, we present results for shock-wave induced damage of a lipid bilayer membrane in a multiscale system: here, the aqueous environment of the lipid bilayer is inexpensively modelled with SPH, while the bilayer itself is represented using MD particles with almost atomistic detail. Thus, our strategy serves as a scale-bridging technique between continuum mechanics and the microscopic world.

[1] J. B. Avalos and A. D. Mackie, âĂIJDissipative particle dynamics with energy conservation,âĂİ Europhysics Letters (EPL), vol. 40, no. 2, pp. 141-146, 1997.

1.7 Meshfree Modeling of Fracture in Laminated Composites

Tue 14:30–15:00, Wolfgang Paul Hall

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A problem of increasing importance in the aerospace industry is in detailed modeling of explicit fracture in laminated composite materials. For design applications, the simulation must be capable of initiation and propagation of changes in the problem domain. Further, these changes must be able to be incorporated within a design-scale simulation. The use of a visibility condition, coupled with the local and dynamic nature of meshfree shape function construction allows one to initiate and explicitly open and propagate holes inside a previously continuous problem domain. The method to be presented naturally couples to a hierarchical multi-scale material model incorporating external knowldege bases to achieve the goal of a practical explicit fracture modeling capability for full-scale problems.

In the area of women's health, the extreme mechanical deformation of various organs, muscles and connective tissues ocurring during vaginal childbirth are believed to be the root cause of several significant medical conditions. These conditions include incontinence and organ prolapse - a potentially life threatening condition. The urogynecology community is interested in performing epidemiological studies of these deformations in women. To perform such a study, the medical images of hundreds or thousands of patients must be transformed into a geometric model suitable for mechanical analysis. Currently, a surface triangulation of an organ is extracted from a stack of two-dimensional images that have been manually segmented. From this surface tesselation, three-dimensional finite element models are developed. This latter step is often quite tedious and manually intensive. An approach based on meshfree methods for generating an analysis-suitable geometry will be discussed. The goal of processing hundreds of models precludes manual intervention, so a completely automated method is mandatory.

1.8 Approximation of Stochastic Partial Differential Equations by Kernel-based Collocation Methods

Tue 16:00–16:30, Wolfgang Paul Hall

Qi Ye*
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In this talk we will use the kernel-based collocation approximating method (meshfree approximation method) to estimate the solution of high dimensional stochastic partial differential equations. Using an implicit scheme, we can transfer stochastic parabolic equations into stochastic elliptic equations. We mainly focus on how to approximate the numerical solution of the elliptic equations for each time step. The estimator of the elliptic equations is a linear combination of reproducing kernels not only done with related differential operators and boundary operators but also centered at chosen collocation points. Its random coefficients are computed by a random linear equations system.

1.9 Vortex-Source Method for the 3D Incompressible Irrotational Flow

Tue 16:30–17:00, Wolfgang Paul Hall

Mykola Yaśko*
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Method of weighted residual is used for developing of the boundary integral representation for the velocity of the three-dimensional inviscid irrotational flow. It is shown that the velocity in an arbitrary point of domain can be expressed through its values on the boundary. The boundary integral equations of the second kind for the solving of the boundary-valued problems of the first and second kind are received.

It is marked that the given integral equation allows the effective numerical solving. Examples of numerical computation for sphere and ellipsoid are given for demonstration of efficiency of the offered method.

2 Wednesday 05.10.2011

2.1 ESPResSo - Extensible Simulation Package for Research on Soft matter

Wed 8:45–9:30, Wolfgang Paul Hall

Axel Arnold*
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Many properties of soft matter, such as polymers or colloidal particles, arise on length scales that are inaccessible to particle-based simulations on atomistic scale, even for future generations of supercomputers. On the other hand, atomistic details often do not play a role in the macroscopic behavior of the system and can therefore be coarse-grained away , which drastically reduces the amount of degrees of freedom. Complex fluid dynamics is an extreme example, in which the particles are replaced by a continuum approach. However, many properties of soft matter still require to investigate systems as built up of individual particles, although these no longer need to be atoms, but can be made up of hundreds of atoms or molecules. Typical examples are treating the monomers of a polymer as particles, or even whole colloidal particles of micrometer size. Under these circumstances, it is possible to ignore the solvent, e. g. water, in simulations of solutions, which often adds by far most of the degrees of freedom. However, it also mediates the interactions between the remaining particles, such as colloids or polymers, which has to be taken into account. Electrostatic interactions become truly long-ranged with an effective dielectric constant, which requires accurate algorithms for their calculation. If the system dynamics is important, the hydrodynamic interactions need to be modeled. Modelling these long-ranged interactions is therefore one of the main challenges of coarse- grained simulation of soft matter.

In this talk, I will present ESPResSo, the Extensible Simulation Package for Research on Soft Matter, which is a simulation package specifically designed for studying coarse-grained soft matter models. It has many state-of-the-art algorithms for electrostatics and hydrodynamic interactions, especially a recently developed GPU-lattice-Boltzmann hydrodynamics solver, which is used to mediate hydrodynamic interactions between embedded particles.

2.2 Analysis of the peridynamic model in nonlocal elasticity

Wed 9:30–10:15, Wolfgang Paul Hall

Etienne Emmrich*
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Peridynamics is a rather new nonlocal continuum theory that avoids spatial derivatives. It is believed to be suited for the description of fracture and other material failure. From the mathematical point of view, the peridynamic model exhibits several difficulties: nonlocality, nonlinearity, time delay, and multiscale behaviour. The analysis and numerical analysis of the peridynamic model is, therefore, still at the very beginning.

In this talk, we give a survey of results known so far. In particular, we focus on existence of solutions to the linearized model and to a viscous regularization of the nonlinear model. The latter relies on nonlinear evolution equations of second order with nonconvex potentials.

2.3 A General Framework of Domain Integration in Meshfree Methods

Wed 10:45–11:30, Wolfgang Paul Hall

Jiun-Shyan Chen*
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The rate of convergence in the Galerkin based numerical methods for solving PDEs is determined by the order of completeness in the approximation functions and the order of accuracy in the domain integration of the weak form. In this work, we first show that the integration conditions for the n-th order exactness of Galerkin method can be expressed in the form of divergence theorem of the n-th order moment of the approximation functions (termed the n-th order divergence condition herein). We show that with the n-th order polynomial reproducing conditions introduced in the construction of the trial functions and the n-th order divergence condition imposed in the construction of test functions, n-th order patch tests can be exactly passed with arbitrary point distribution in meshfree methods. This approach can be used as a correction of the existing meshfree methods to achieve higher order convergence rates, which cannot be done without the proper integration conditions imposed even if the approximation functions posses sufficient order of completeness. Examples include a corrected direct nodal integration to achieve quadratic rate of convergence in L2 norm, and a corrected stabilized conforming nodal integration to achieve cubic rate of convergence in L2 norm when linear and quadratic basis functions are used, respectively, in the reproducing kernel approximation.

2.4 Cubature of the solution of the thin wedge-shaped shells deflections problem by approximate quasi-interpolant

Wed 11:30–12:00, Wolfgang Paul Hall

Natalia Chinchaladze*
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of Iv. Javakhishvili Tbilisi State University
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In 1991 Maz'ya proposed a new approximation method called approximate approximations, mainly directed to the numerical solution of partial differential equations. We apply this method to the solution of the problem of shell deflections in the case when the shell thickness is equal to zero along a part of the boundary. The convergence of the obtained series is proved, some numerical results are given.

2.5 Meshless approximations for the development of high order finite volume methods

Wed 12:00–12:30, Wolfgang Paul Hall

Ignasi Colominas*
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Many of finite volume solvers are stacked at convergence orders of two due to the difficult for the computation of derivatives on unstructured grids. In this context, the use of meshfree methods is a very efficient choice to easily improve the accuracy of finite volume numerical schemes. A finite volume method using Moving Least Squares approximants for the computation of derivatives have been developed by the authors *Luiscmame,cmamexes* , and it has been succesfully used for the computation of turbulent flows and aeroacoustics. But MLS is not the only choice. In this work we present a study of the properties of the different numerical schemes obtained by using different meshless techniques. We focus on wave propagation problems, and we analyze the dispersion and dissipation curves of the different schemes when solving the 1D advection equation.

2.6 Archetype-Blending Multiresolution Theory for Materials Design

Wed 14:00–14:30, Wolfgang Paul Hall

Wing Kam Liu*
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In the not too distant future, an integrated multiscale analysis system is desirable for the design of a reliable engineering structure to sustain harsh environmental conditions within a predetermined lifetime. A multiresolution mathematical theory that may overcome the limitations of conventional approaches is being developed for the design of higher strength, toughness, extended fatigue life and lower weight materials. Our vision for deriving the governing equations of life cycle functional materials design is to treat large experimental and computational data sets as the building blocks. The derivation of the mathematical model will involve processing, testing, imaging, characterization, verification and validation, and uncertainty qualification. While materials science and experimental observation will heavily influence the model, it will ultimately be the new predictive science mathematical theory that will unify these ideas and lead to a solution.

We envision that the data set mathematical foundation will start with linking spatial and temporal scales for continuous resolution of a microstructure. We want to be able to zoom into a microstructure in the same way that modern satellite technology allows us to zoom into images anywhere, anytime, and with any resolution. Hence, the separation of data by scales is done through the use of computer imaging and materials science knowledge. The quantification and variability of microstructured data sets are performed through the use of statistical and decision making theories, whereas the understanding of scale linking is done via processing, testing and characterization of the data set samples. We then have refined data in order of scale, and these data sets are mapped into the resolution axis, which is an extension of the length scale theory in mechanics of materials, a variable length and temporal scale theory. Note that the data is in 4 dimensions, (x, y, z, t), so the spatial and temporal resolution axes are the 5th and 6th dimensions. Now the microstructure is shown in continuous resolution. To represent the stochastic nature of the data, another dimension will be added for each parameter with an axis as the variance of that parameter.

A new Archetype-Blending Multiresolution Continuum Mathematical theory, which is based on a bottom-up reinterpretation of multiresolution quantities, is being developed. In this scheme, we depart from the assumption of micromorphism and replace it with a nonlocal sweep of the heterogeneous neighborhood (i.e. anholonomic conformation) of a material-point (i.e. archetype) to construct a blended (and holonomic) multiscale manifold, while exploiting the same multiscale variational principle as that of the multiresolution continuum. The resulting holonomic multiscale manifold thus permits the derivation of multiscale compatibility conditions that govern our newly developed topologically based fracture criterion, which stems from the integral law of compatibility, appositely for large deformations. Applications of the proposed archetype-blending theory are materials generic. The approach aims at constructing on-the-fly fully coupled multiscale constitutive laws, while only requiring the definition of archetype behaviors to any degree of complexity. Our current efforts span metals and alloys, polymer composites, ceramics and biomaterials.

2.7 Meshfree Methods in Drug Design

Wed 14:30–15:00, Wolfgang Paul Hall

Konstantin Fackeldey*
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In the last few years, the simulation of molecules for the development and design of Drugs have become more and more important. The complex shape and the flexibility of the proteins is a challenging task, since their corresponding phase space is high dimensional. However, the dynamics of a system in thermodynamic equilibrium does not visit all states by the same amount. More precisely, subsets in the phase space can be found in which the system is not stable but metastable. This is the starting point for conformation dynamics, where by a Robust Perron Cluster Analysis (PCCA+) these metastabilities are detected and their transition probabilities are determined. Even though, that this course of action reduces the number of degrees of freedom dramatically, the "reduced" state space is still high dimensional. Thus we use meshfree methods in order to detect the metastablities as a linear combination of basis functions.

2.8 Solution of Poisson's equation in high dimensions

Wed 16:00–16:30, Wolfgang Paul Hall

Fred Daum*
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We compute the gradient of the solution to Poisson's equation for state vectors with high dimensions (d = 3 to 30) using particle methods. The algorithm is similar to Coulomb's law in electromagnetics. We show numerical results for difficult nonlinear filter problems that are roughly ten orders of magnitude faster than standard particle filters for the same accuracy. The key parameters in this problem include: initial uncertainty of the state vector, signal-to-noise ratio of the measurements, stability of the plant model and dimension of the state vector. We derive a flow of particles to compute Bayes' rule, rather than using a pointwise multiplication; this solves the well known and important problem of particle degeneracy. The particle flow is computed as the solution of a linear first order highly underdetermined PDE, similar to the Gauss divergence law. We show roughly a dizen distinct methods to solve this PDE.

3 Thursday 06.10.2011

3.1 TBA

Thu 9:30–10:15, Wolfgang Paul Hall

Marc Alexander Schweitzer*
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3.2 Optimal Local Basis Functions and Exponential Convergence for Multi-scale Generalized Finite Element Methods

Thu 10:45–11:30, Wolfgang Paul Hall

Robert Lipton*, Ivo Babuska
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Modern structures such as airplane wings exhibit complicated sub structures and make use of composite materials in their construction. The high cost of experimental tests for these hierarchical structures is driving a trend toward virtual testing. This requires the development of multi-scale numerical methods capable of handling large degrees of freedom spread across different length scales. In this talk we introduce optimal local basis functions for use in multi-scale finite element methods. The optimal local basis delivers a global basis with exponential convergence with respect to the dimension of the global approximation space. This convergence is shown to hold for problems with rough coefficients. This is joint work with Ivo Babuska.

3.3 Some Regularized Versions of the Method of Fundamental Solutions

Thu 11:30–12:00, Wolfgang Paul Hall

Csaba Gáspár*
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A powerful and popular meshfree solution technique of partial differential equations is the method of fundamental solutions. The method is often applied together with the method of particular solutions. Here the solution of the original boundary value problem is expressed as a sum of a particular solution (no boundary condition is prescribed) and a homogeneous solution (supplied with a modified boundary condition). The homogeneous solution is approximated in a form similar to the method of radial basis function, where the applied radial basis function is the fundamental solution of the original partial differential operator. The main drawback of this approach is that one has to introduce a set of fictitious source points located outside of the domain of the partial differential equation. The proper choice of the locations of the source points is crucial. If they are too far from the boundary, the resulting algebraic system becomes extremely ill-conditioned. If they are too close to the boundary, numerical singularities are generated in the approximate solution.

To overcome the above difficulties, the original problem is approximated by another higher order partial differential equation, the fundamental solution of which is continuous at the origin. To solve this new problem, the method of fundamental solution can directly be applied. Due to the continuity of the fundamental solution, the source points are allowed to be located on the boundary. No numerical singularities are generated, and, in addition to this, the condition number of the resulting algebraic system remains moderate. The problem is thus converted to a boundary interpolation problem. The approach remains applicable to the Stokes system and also to problems with variable coefficients, though in the latter case, the fundamental solution is not available in an explicit form in general. In this situation, the above mentioned boundary interpolation can be performed by using quadtree-based multigrid tools, which are useful also in obtaining particular solutions. In the talk, error estimations are also derived and the method is demonstrated through various numerical examples.

Keywords: method of fundamental solutions, regularization, radial basis functions, quadtree, multigrid

3.4 Meshfree exponential integrators

Thu 12:00–12:30, Wolfgang Paul Hall

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For the numerical solution of time-dependent partial differential equations, a class of meshfree exponential integrators is proposed. These methods are of particular interest in situations where the solution of the differential equation concentrates on a small part of the computational domain which may vary in time. For the space discretization, radial basis functions with compact support are suggested. The time integration is performed with exponential integrators or splitting methods. The proposed integrators are fully adaptive in space and time. Theoretical aspects as well as numerical examples that illustrate the robustness and the good stability properties of these methods are discussed.

3.5 A Smoothed Point Interpolation Method for Structural Dynamics

Thu 14:00–14:30, Wolfgang Paul Hall

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In this work, the smoothed point interpolation method for dynamic problems in structural mechanics is discussed. The generalized Galerkin weak form is applied to the Euler's partial differential equation of motion. Therefor, the problem area is divided into smoothing subdomains based on a smoothed strain field. The procedure is discussed, taking into account edge-based, cell-based, and node-based methods, combined with appropriate T-schemes for the selection of the support nodes. The approximating shape functions are computed by the meshfree radial point interpolation method. The mass matrix is computed, employing the integration points and smoothing domains, which have already been computed for the construction of the stiffness matrix, keeping the computational effort to a minimum.

The presented method offers a variety of excellent properties: Most importantly, the incompatibility problem of the radial point interpolation method can be dealt with, upper and lower bound properties can be found, and the locking phenomenon can be overcome. Furthermore, the spatial integration is performed only on the boundaries of the smoothing domains, which reduces the computation times compared to standard integration methods as the Gauss quadrature scheme, for instance, considerably.

Different numerical examples, e.g. the dynamic analyses of a clamped truss and a bending beam, are evaluated to illustrate the convergence and the efficiency of the proposed method.

3.6 Characteristic particle methods for traffic flow simulations on highway networks

Thu 14:30–15:00, Wolfgang Paul Hall

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Vehicular traffic flow on highways is frequently modeled by macroscopic PDEs on networks. Popular models consist of hyperbolic conservation laws on the edges (roads), augmented by specific coupling conditions on the vertices (ramps and intersections). A challenge in the simulation of network flows is that often times only few degrees of freedom can be attributed to each edge. Hence, numerical approaches are required that evolve solutions very accurately with very few computational nodes. In order to derive such methods, we start with a class of characteristic particle methods that evolve scalar one-dimensional conservation laws solutions exactly, or exactly except right around shocks. We then demonstrate how these particle methods can be extended to nonlinear flow models on networks.

3.7 RBF-FD Methods for Elliptic Equations

Thu 16:00–16:30, Wolfgang Paul Hall

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We investigate low order RBF-based generalised finite difference methods (RBF-FD) on irregular centres. This approach is genuinely meshless and can compete in accuracy with the linear finite element method that requires solving linear systems of comparable bandwidth/density . Algorithms and numerical results for stencil support selection, adaptive refinement and optimal shape parameter will be discussed. The results are obtained jointly with Dang Thi Oanh.

3.8 A meshfree method for the analysis of planar flows of a inviscid fluids

Thu 16:30–17:00, Wolfgang Paul Hall

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The variant of vortex particles-in-cells method is suggested for computing 2D inviscid incompressible flows in a closed domain with possible flow through it. The governing equations are the 2D Euler equations in terms of stream function and vorticity or geophysical models of the atmosphere. In the talk development of a method originally presented in [1] is considered. The approach is based on vorticity field approximation using its values at a set of fluid particles and the stream function computation using the Galerkin method. The flow domain is divided into rectangular cells. Vorticity in every cell is interpolated by a third order polynomial that is constructed by the method of least squares with the use of the particles currently located in a cell. The resultant piecewise continuous polynomial approximation of vorticity is employed to derive analytically GalerkinâĂŹs coefficients of stream function expansion.

Use of various integrators for calculation of dynamics of fluid particles is studied on a number of test problems. On the basis of these calculations optimum methods are suggested. Parallel realization of a method is prezented, speedup possibilities are experimentally studied at various parameters of a method. The performance of the method is illustrated by results of flows trough channel problem investigation [1, 2] and analysis of the multipoles vortex patch dynamics in geophysical flows.

References [1] Govorukhin, V. N.; IlâĂŹin, K.I. Numerical study of an inviscid incompressible flow through a channel of finite length. Int. J. Numer. Methods Fluids 60, No. 12, 1315-1333 (2009). [2] Govorukhin, V.N.; Morgulis, A.B.; Vladimirov, V.A. Planar inviscid flows in a channel of finite length: washout, trapping and self-oscillations of vorticity. J. Fluid Mech. 659, 420-472 (2010).

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