2nd Workshop on Computational Mathematics

May 25-26, 2012

Department of Applied Mathematics,

The Hong Kong Polytechnic University, Hong Kong

Sponsors:

AMSS-PolyU Joint Research Institute
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Department of Applied Mathematics, PolyU

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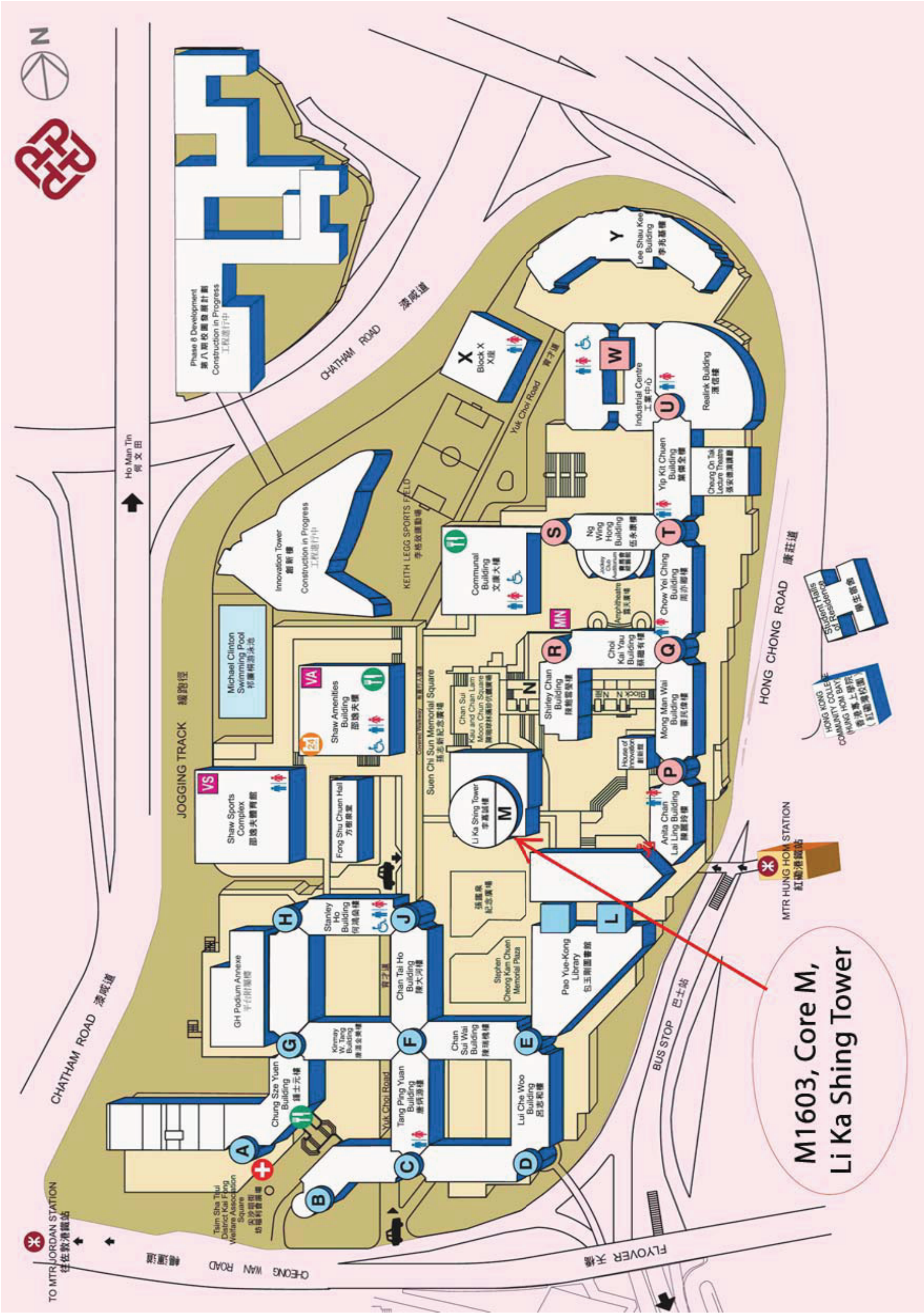

M1603, Core M,
Li Ka Shing Tower
Li Ka Shing Tower
M
Phase 8 Development
Construction in Progress
CHATHAM ROAD
Ho Man Tin
Innovation Tower
Construction in Progress
KEITH LEGG SPORTS FIELD
Yuk Choi Road
Block X
Industrial Centre
Realink Building
Lee Shau Kee Building
Yip Kit Chuen Building
Cheung On Tak Lecture Theatre
Ng Wing Hong Building
Communal Building
Chow Yei Ching Building
Amphitheatre
Choi Kai Yau Building
Shirley Chan Building
Mong Man Wai Building
House of Innovation
Anita Chan Lai Ling Building
HONG CHONG ROAD
Student Halls of Residence
HONG KONG COMMUNITY COLLEGE (HUNG HOM BAY)
MTR HUNG HOM STATION
Michael Clinton Swimming Pool
JOGGING TRACK
Shaw Amenities Building
Shaw Sports Complex
Suen Chi Sun Memorial Square
Fong Shu Chuen Hall
Stanley Ho Building
Chan Tai Ho Building
Pao Yue-Kong Library
Stephen Cheong Kam Chuen Memorial Plaza
GH Podium Annexe
Kinmay W. Tang Building
Chan Sui Wai Building
Chung Sze Yuen Building
Tang Ping Yuan Building
Lui Che Woo Building
Yuk Choi Road
BUS STOP
FLYOVER
CHEONG WAN ROAD
TO MTR JORDAN STATION
Tsim Sha Tsui District Kai Fong Welfare Association Square

Friday, 25 May 2012

09:00	**Registration**	M1607
09:10-09:30	**Opening Ceremony** Group Photo	M1603
09:30-10:50	**Plenary Session:** Chair: Ian H. Sloan 09:30 C. T. Kelley *Hybrid Monte-Carlo Deterministic Algorithm for Neutron Transport* 10:10 Amiya Kumar Pani *Optimal* $\boxed{L^\infty - L^2}$*-error Analysis of Semidiscrete Galerkin Methods for Linear Parabolic Problems with Nonsmooth Initial Data: An Alternate Approach and Some Ramifications*	M1603
10:50-11:10	**Coffee Break**	M1607
11:10-12:30	**Plenary Session:** Chair: C. T. Kelley 11:10 Ian H. Sloan *Spherical Designs and Approximate Spherical Designs as Tools for Numerical Integration* 11:50 Eiichi Bannai *Some Problems Related to Spherical Designs*	M1603
12:30-14:20	**Lunch**	
14:30-15:20	**Invited Session:** Chair: Amiya Kumar Pani 14:30 Mingyu Xu *Numerical Simulations and Convergence for Backward Stochastic Differential Equations* 15:00 Congpei An *Regularized Least Squares Approximation over the Unit Sphere by Using Spherical Designs*	M1603
15:20-15:40	**Coffee Break**	M1607
15:40-17:40	**Local Speakers Session:** Chair: Graeme Fairweather 15:40 Liqun Qi *The Quantum Eigenvalue Problem* 16:10 Man-Kam Kwong *Proving the Monotonicity of the Period Function of an ODE Using Maple* 16:40 Xiaojun Chen *Computational Existence Proofs for Spherical $t-$Designs* 17:00 Yanping Lin *Immersed Finite Element Methods for Interface Problems* 17:20 Zhonghua Qiao *Adaptive Time Stepping and Energy Stable Schemes*	M1603
18:00-20:30	**Dinner**	

Saturday, 26 May 2012

09:30-10:50	**Plenary Session:** Chair: Dongwoo Sheen 09:30 Graeme Fairweather *An ADI Extrapolated Crank-Nicolson Orthogonal Spline Collocation Method for Nonlinear Reaction-Diffusion Systems* 10:10 Jie Shen *Fast Spectral-Galerkin Methods for High-Dimensional PDEs and Applications to the Electronic Schrodinger Equation*	M1603
10:50-11:10	**Coffee Break**	M1607
11:10-12:30	**Plenary Session:** Chair: Jie Shen 11:10 Shuhuang Xiang *On Orthogonal Polynomial Expansions and Interpolant Approximations* 11:50 Dongwoo Sheen *A Quadrilateral Morley Element for Biharmonic Equations*	M1603
12:30-14:20	**Lunch**	
14:30-15:00	Visit AMA	
15:00-16:00	Open Discussion	HJ610

Regularized Least Squares Approximation over the Unit Sphere by Using Spherical Designs

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Abstract

We consider polynomial approximation on the unit sphere by a class of regularized discrete least squares methods, with novel choices for the regularizing operator and the point sets of the discretisation. We allow different kinds of rotationally invariant regularization operators, including the zero operator (in which case the approximation includes interpolation, quasi-interpolation and hyperinterpolation); powers of the negative Laplace-Beltrami operator (which can be suitable when there are data errors); and regularizers that yield filtered polynomial approximations, which (even for exact data) can exhibit improved uniform approximation compared to the unregularized case. As node sets we use spherical t-designs, which are point sets on the sphere which when used as equal-weight quadrature rules integrate all spherical polynomials up to degree t exactly. For $t \in [L, 2L)$, the error analysis corresponding to different choices on regularization operators are discussed. Finally, the numerical illustrates the theoretical results, and show that well chosen regularizers and well conditioned spherical t-designs can provide good polynomial approximation on the sphere, with or without the presence of data errors.

This is a joint work Prof. Xiaojun Chen, Prof. Ian H. Sloan and Prof. Rob. S. Womersley.

Reference

(1) C. An, Error Analysis of Regularized Least Squares Approximation over the unit Sphere, Preprint.
(2) C. An, X. Chen, I. H. Sloan and R. S. Womersley, Regularized Spherical Least-squares Approximations on the Sphere Using Spherical Designs, SIAM J. Numer. Anal., to appear.
(3) C. An, X. Chen, I. H. Sloan and R. S. Womersley, Well Conditioned Spherical Designs for Integration and Interpolation on the Two-Sphere, SIAM J. Numer. Anal. 48 (2010), pp. 2135-2157.

Some Problems Related to Spherical Designs

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Abstract

We discuss some results and conjectures related to spherical t-designs. The following two topics will be discussed, among others.

(i) Spherical designs of harmonic index t. We call a finite subset X on the unit sphere S^{n-1} a design of harmonic index t, if $\sum_{x \in X} f(x) = 0$ for all homogeneous harmonic polynomials $f(x)$ of degree exactly t. Please note that this is a weaker condition than design of strength t (usual spherical t-designs) and design of index t. We discuss whether there is any natural Fisher type lower bounds for size $|X|$. We observe some interesting configurations which attain possible putative lower bounds. (This is joint work with Makoto Tagami of Niigata Institute of Technology.)

(ii) Many existence proofs of spherical t-designs as well as of other t-designs (e.g., interval t-designs) are known. Most of them use either topological techniques or the continuity property of real numbers. We want to discuss the existence of so called "rational" t-designs. Some recent progress on this topic will be surveyed.

Computational Existence Proofs for Spherical $t-$Designs

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Abstract

Spherical $t-$designs provide quadrature rules for the sphere which are exact for polynomials up to degree t. In this talk, we propose a computational algorithm based on interval arithmetic which, for given t, upon successful completion will have proved the existence of a $t-$design with $(t+1)^2$ nodes and will have computed narrow interval enclosures which are known to contain these nodes with mathematical certainty. Since there is no theoretical result which proves the existence of a t-design with $(t+1)^2$ nodes for arbitrary t, our method contributes to the theory because it was tested successfully for $t = 1, 2, ..., 100$, i.e., for all t considered so far. The $t-$design is usually not unique; our method aims at finding a well-conditioned one. The method relies on computing an interval enclosure for the zero of a highly nonlinear system of dimension $(t+1)^2$. We therefore develop several special approaches which allow us to use interval arithmetic efficiently in this particular situation. The computations were all done using the MATLAB toolbox INTLAB. At the end of this talk, applications of well conditioned spherical designs for integration, interpolation and regularized least squares approximations on the two-sphere are discussed.

This is a joint work with Congpei An, Andreas Frommer, Bruno Lang, Ian Sloan and Womersley.

Reference

(1) C. An, X. Chen, I. Sloan and R.S. Womersley, Well conditioned spherical designs for integration and interpolation on the two-sphere, SIAM J. Numerical Analysis, 48(2010), 2135-2157.
(2) C. An, X. Chen, I.H. Sloan and R.S. Womersley, Regularized least squares approximations on the sphere using spherical designs, to appear in SIAM J. Numerical Analysis.
(3) X. Chen, A. Frommer and B. Lang, Computational existence proofs for spherical $t-$designs, Numerische Mathematik, 117(2011), 289-305.
(4) X. Chen and R.S. Womersley, Existence of solutions to systems of underdetermined equations and spherical designs, SIAM J. Numerical Analysis, 44(2006), 2326-2341.
(5) X. Chen, R. Womersley and J. Ye, Minimizing the condition number of a Gram matrix, SIAM J. Optimization, 21(2011), 127-148.

An ADI Extrapolated Crank-Nicolson Orthogonal Spline Collocation Method for Nonlinear Reaction-Diffusion Systems

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Abstract

A new numerical technique is presented for the solution of a class of two-component nonlinear reaction-diffusion problems in a rectangle. In this method, orthogonal spline collocation (OSC) with piecewise polynomials of degree $r \geq 3$ is used for the spatial discretization, and the time-stepping is performed using an algebraically linear alternating direction implicit (ADI) method based on an extrapolated Crank-Nicolson OSC method. At each time step, this technique reduces the multidimensional problem to sets of independent linear OSC two-point boundary value problems in the coordinate directions. The efficacy of the method is demonstrated using well-known examples of reaction-diffusion models arising in chemistry and biology. Moreover, it is demonstrated numerically that the method is second-order accurate in time and of optimal accuracy in space in various norms, and possesses superconvergence properties.

Hybrid Monte-Carlo Deterministic Algorithm for Neutron Transport

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Abstract

Neutron transport in power reactors is modeled with a linear Boltzmann equation in phase space (space + momentum). The neutron transport equation is an integro-differential whose solution is the intensity of radiation. The quantities of interest are integrals of the intensity over some of the variables (the angles of direction of motion). The two most common methods of solution are Monte Carlo approximation (accurate and very expensive) and various deterministic discretization approaches (less expensive, but subject to solution artifacts from the discretization).

We are developing algorithms that will combine good physical modeling properties of Monte-Carlo simulation with the computational efficiency of deterministic modeling. Our approach changes the Boltzmann equation to a coupled system of a linear equation in phase space of a very simple form, and a nonlinear equation in space only (not momentum) which can be solved with a Newton-Krylov approach. In our hybrid approach we solve the Boltzmann equation with a Monte Carlo simulation.

The Monte Carlo error affects the nonlinear solver in many ways. The termination criteria for both the linear and nonlinear iterations must take the Monte Carlo error into account. The line search may fail, and one must use knowledge of the Monte Carlo simulation to address line search failures. Finally, the quality of the final result will be affected. In this talk we discuss our recent progress and describe some unsolved problems.

Proving the Monotonicity of the Period Function of an ODE Using Maple

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Abstract

A special case (when $\gamma = -1$) of the following initial value problem arises in the construction of a class of rotational flow with radial symmetry for the 2-dimensional Euler-Poisson system.

$$r''(t) + r^{\gamma}(t) - \frac{1}{r^3(t)} = 0, \qquad r(0) = \alpha, \quad r'(0) = 0 \quad (-3 < \gamma < 1).$$

All solutions of this differential equation are periodic. Let $T(\alpha)$ denote the period of the solution as a function of the initial amplitude α. It is desirable to know if $T(\alpha)$ is increasing for $\alpha > 1$.

A result of S.N. Chow and D. Wang (1986) provides a sufficient condition to answer the question, for $\gamma = -1$, in the affirmative. However, verifying the criterion needs the help of a symbolic manipulation software such as Maple.

The Chow-Wang criterion is extended to handle the case for more general γ.

Immersed Finite Element Methods for Interface Problems

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Abstract

We will report some of recent results on immersed finite element methods for interface problems. Other related problems will also be mentioned.

Optimal $L^\infty - L^2$-error Analysis of Semidiscrete Galerkin Methods for Linear Parabolic Problems with Nonsmooth Initial Data: An Alternate Approach and Some Ramifications

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Abstract

In this talk, starting with some earlier results, we propose and analyze an alternate approach of optimal L^2- error estimates for semidiscrete Galerkin approximations to a second order linear parabolic initial and boundary value problem with rough initial data. Our analysis is based on energy arguments without using parabolic duality. Further, it follows the spirit of the proof technique used for deriving optimal error estimates for finite element approxima- tions to parabolic problems with smooth initial data and hence, it unifies both theories, that is, one for smooth initial data and other for nonsmooth data. Moreover, the proposed technique is also extended to a semidiscrete mixed method for linear parabolic integro-differential equations with nonsmooth data for which there are some problems in deriving optimal L^2-error estimates.

This is a joint work with Deepjyoti Goswami.

The Quantum Eigenvalue Problem

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Abstract

The quantum eigenvalue problem arises in the study of the geometric measure of the quantum entanglement. In this talk, we convert the quantum eigenvalue problem to a Z-eigenvalue problem of a real symmetric tensor. In this way, the theory and algorithms for Z-eigenvalues can be applied to the quantum eigenvalue problem. In particular, this gives an upper bound for the number of quantum eigenvalues. We show that the quantum eigenvalues appear in pairs, i.e., if a real number λ is a quantum eigenvalue of a square symmetric tensor Ψ, then $-\lambda$ is also a quantum eigenvalue of Ψ. When Ψ is real, we show that the entanglement eigenvalue of Ψ is always greater than or equal to the Z-spectral radius of Ψ, and that in several cases the equality holds.

We also show that the ratio between the entanglement eigenvalue and the Z-spectral radius of a real symmetric tensor is bounded above in a real symmetric tensor space of fixed order and dimension.

Adaptive Time Stepping and Energy Stable Schemes

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Abstract

In this talk, we first give a brief review on the recent development of the energy stable numerical schemes for the nonlinear diffusion equations. And then we will introduce an adaptive time-stepping strategy, which is based on the energy variation. This strategy has been successfully applied to the nonlinear diffusion equations. It can not only resolve the steady state solution efficiently, but also resolve the dynamics of the system accurately. Finally, we will show the application of the proposed method in complex fluids simulations.

A Quadrilateral Morley Element for Biharmonic Equations

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Abstract

We begin with a brief review on the recent development in finite element methods for biharmonic problems. Biharmonic problems arise from bending of clamped thin isotropic elastic plates and creeping flow of a viscous incompressible fluid. Conforming finite elements are expensive to implement, in general, in solving the fourth-order PDEs. This, together with the Stokes and elasticity problems, has been one of the major driving engines that lead to study nonconforming finite elements.

We will propose a Morley-type finite element for quadrilateral meshes to solve biharmonic problems. For each quadrilateral the element is defined by the span of P_2 plus two functions from P_3. Error estimates and numerical results will be presented.

Fast Spectral-Galerkin Methods for High-Dimensional PDEs and Applications to the Electronic Schrodinger Equation

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Abstract

Many scientific, engineering and financial applications require solving high-dimensional PDEs. However, traditional tensor product based algorithms suffer from the so called "curse of dimensionality". We shall construct a new sparse spectral method for high-dimensional problems, and present, in particular, rigorous error estimates as well as efficient numerical algorithms for elliptic equations in both bounded and unbounded domains. As an application, we shall use the proposed sparse spectral method to solve the N-particle electronic Schrodinger equation.

Spherical Designs and Approximate Spherical Designs as Tools for Numerical Integration

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Abstract

Spherical designs are point sets on the sphere which when used as equal-weight integration rules integrate exactly all polynomials up to some degree. As a result those integration rules have a nice convergence property for functions in certain Sobolev spaces. In this talk we introduce the new concept of approximate spherical design – a sequence of points sets on the sphere is a sequence of approximate spherical designs if the corresponding equal-weight integration rules have the same asymptotic error behaviour in Sobolev spaces as sequences of true spherical designs. Many good point sets for integration belong to (or are suspected to belong to) families of approximate spherical designs. The talk describes joint work with Robert Womersley, Ed Saff and Johann Brauchart.

On Orthogonal Polynomial Expansions and Interpolant Approximations

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Abstract

In this talk, we will consider asymptotics on the coefficients of $f(x)$ expanded in forms of ultraspherical or Jacobi polynomial series, which imply the rate of the decay of the coefficients and derive the truncated error bounds. Moreover, from which we show that the Chebyshev coefficient α_n decays a factor of $\sqrt{n}$ faster than the Legendre coefficient u_n. Furthermore, by using the Chebyshev expansion for $f(x)$ of finite regularity, we give optimal orders for Cleshaw-Curtis, Féjer and Gauss quadrature, and present the aliasing error between the coefficients, which also show the equal accuracy of these quadrature for non-analytic functions. In addition, we consider Legendre approximation with interpolation. In particular, we are interested in the barycentric Lagrange formula at the Gauss-Legendre points. Explicit barycentric weights, in terms of Gauss-Legendre points and corresponding quadrature weights, are presented that allow a fast evaluation of the Legendre interpolation formula. Finally, we present an application for Clenshaw-Curtis-Filon-type quadrature to Volterra integral equations containing highly oscillatory Bessel kernels.

This is a joint work with Bornemann, Brunner, Chen, Cho and Wang.

Numerical Simulations and Convergence for Backward Stochastic Differential Equations

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Abstract

Non-linear backward stochastic differential equations (BSDEs in short) were firstly introduced by Pardoux and Peng (1990), who proved the existence and uniqueness of the adapted solution, under smooth square integrability assumptions on the coefficient and the terminal condition, and when the coefficient $g(t,\omega,y,z)$ is Lipschitz in (y,z) uniformly in (t,ω). For many nonlinear cases of g, we cannot find the solution explicitly. Here we study different algorithms for backward stochastic differential equations (BSDE in short) basing on random walk framework for 1-dimensional Brownian motion. Implicit and explicit schemes for are introduced. Then we prove the convergence of different algorithms and give simulation results for different types of BSDEs. And we will give some simulations for Brownian motion and BSDEs.