Abstracts

Fractional Cahn-Hilliard equation(s): analysis, properties and approximation

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ABSTRACT

The classical Cahn-Hilliard equation [1] is a nonlinear, fourth order in space, parabolic partial differential equation which is often used as a diffuse interface model for the phase separation of a binary alloy. Despite the widespread adoption of the model, there are good reasons for preferring models in which fractional spatial derivatives appear [2, 3]. We consider two such Fractional Cahn-Hilliard equations (FCHE). The first [4] corresponds to considering a gradient flow of the free energy functional in a negative order Sobolev space $H_{-\alpha}$, $\alpha \in [0, 1]$ where the choice $\alpha = 1$ corresponds to the classical Cahn-Hilliard equation whilst the choice $\alpha = 0$ recovers the Allen-Cahn equation.It is shown that the equation preserves mass for all positive values of fractional order and that it indeed reduces the free energy. The well-posedness of the problem is established in the sense that the H_1-norm of the solution remains uniformly bounded.We then turn to the delicate question of the L_∞ boundedness of the solution and establish an L_∞ bound for the FCHE in the case where the non-linearity is a quartic polynomial. As a consequence of the estimates, we are able to show that the Fourier-Galerkin method delivers a spectral rate of convergence for the FCHE in the case of a semi-discrete approximation scheme. Finally, we present results obtained using computational simulation of the FCHE for a variety of choices of fractional order α. We then consider an alternative FCHE [3, 5] in which the free energy functional involves a fractional order derivative.

(joint work with Zhiping Mao)

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Energy preserving method for nonlinear Schrödinger equations

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ABSTRACT

The Schrödinger equation is at heart of Bose Einstein Condensates with the celebrated Gross Pitaevskii equation. Such dispersive partial differential equations have many preserved quantities such as the mass, the energy or the momentum. It is therefore crucial to build numerical schemes that preserve these invariants. I will review in this talk some ways to perform numerical integration in time of nonlinear Schrödinger equations and will focus on energy preserving method for various nonlinearities. I will present the pros and cons of the various methods.

Droplets and supersolids - novel physics of dipolar Bose-Einstein condensates

Blair Blakie

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ABSTRACT

We study the physics of a single component dipolar condensate in the regime where the long-ranged magnetic dipole-dipole interactions dominate over the contact interactions. At the meanfield level this system is unstable to mechanical collapse, however beyond meanfield corrections arising from quantum fluctuations can stabilise the system into a self-bound droplet state. Theoretically these corrections can be included in the Gross-Pitaevskii theory as a higher order nonlinearity. When the system is suitably confined by an external potential it can be favourable for several droplets to form and realise a regularly spaced droplet array. Furthermore, such a modulated ground state may maintain global phase coherence and meet the requirements for being a supersolid, I.e. a crystalline phase of matter with a non-zero superfluid density. This area of research has been very active due to three prominent experiments recently realising the supersolid phase of matter. In this talk I will overview the basic physics of this system and some of the numerical challenges related to predicting its ground states and excitations.

The formation of compact objects at finite temperatures in a self-gravitating bosonic system

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ABSTRACT

We study self-gravitating bosonic systems, candidates for dark-matter halos, by carrying out a suite of direct numerical simulations (DNSs) designed to investigate the formation of finite-temperature, compact objects in the three-dimensional (3D) Fourier-truncated Gross-Pitaevskii-Poisson equation (GPPE). This truncation allows us to explore the collapse and fluctuations of compact objects, which form at both zero temperature and finite temperature. We show that the statistically steady state of the GPPE, in the large-time limit and for the system sizes we study, can also be obtained efficiently by fine-tuning the temperature in an auxiliary stochastic Ginzburg-Landau-Poisson equation (SGLPE). We show that, over a wide range of model parameters, this system undergoes a thermally driven first-order transition from a collapsed, compact, Bose-Einstein condensate to a tenuous Bose gas without condensation. By a suitable choice of initial conditions in the GPPE, we also obtain a binary condensate that comprises a pair of collapsed objects rotating around their center of mass.

Ground states of Bose-Einstein condensates with higher order interaction

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ABSTRACT

We analyze the ground state of a Bose-Einstein condensate in the presence of higher-order interaction (HOI), modeled by a modified Gross–Pitaevskii equation (MGPE). Due to the appearance of HOI, the ground state structures become very rich and complicated. We establish the existence and non-existence results under different parameter regimes, and obtain their limiting behaviors and/or structures with different combinations of HOI and contact interactions.

A free boundary approach to Gross-Pitaevski equations

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ABSTRACT

We propose an idea to solve the Gross-Pitaevskii Equation for dark structures inside an infinite constant background density, without the introduction of artificial boundary conditions. We map the unbounded physical domain into the bounded domain $(-1, 1)^3$, and discretize the rescaled equation by equispaced 4th-order finite differences. This results in a free boundary approach, which can be solved in time by the Strang splitting method. Numerical results confirm existing ones based on the Fourier pseudospectral method and point out some weaknesses of the latter such as the need of a quite large computational domain, and thus a consequent critical computational effort, in order to provide reliable time evolution of the vortical structures, of their reconnections, and of integral quantities like mass, energy, and momentum. The free boundary approach reproduces them correctly, in both finite and infinite domains at a very reasonable computational cost.

We show the versatility of this method by carrying out one-and three-dimensional simulations and by using it also in the case of Bose-Einstein Condensates, for which vanishing boundary conditions can be used.

Reduction dynamics for soliton stripes, vortices, and vortex rings in quantum superfluids

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ABSTRACT

Motivated by recent experimental advances in the imaging and manipulation of Bose-Einstein condensates (BECs), we showcase some results pertaining the reduction of the original (higher dimensional) dynamics into a much more manageable low-dimensional dynamical system. In particular, we will show how a "soup" of interacting trapped BEC vortices in (quasi-)2D geometries is reduced to a set of couple ODEs that is able to predict bifurcations in the original PDE and the experiment. We will also present a dynamical reduction, based on adiabatic invariants, for a wide variety of solitonic stripes embedded in 2D space (including dark, bright, dark-bright stripes). Finally, we will also explore some extensions of the dynamical reduction for 3D vortex rings which are formed when a vortex filament (a "twister") is looped back onto itself creating a close ring that carries vorticity.

Incompressible Schrödinger and Ginzburg–Landau systems in computer graphics

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ABSTRACT

There has been increasing attention in the Ginzburg–Landau ground state problems in computer graphics, where one of the central interests is finding a globally coherent pattern on a curved surface with optimal placement of topological defects. Examples of these patterns range from stripe patterns, guiding fields for materials in fabrications, to spinor fields that describe isometric deformations. In the first half of this talk, I will use a gauge-invariant framework of complex line bundles to provide an overview of the applications of Ginzburg–Landau systems beyond its condensed matter physics origin. In the second half of the talk, I will present a method for classical fluid animations via the incompressible Schrödinger flow, which is the time-dependent spinor Schrödinger equation subject to the constraint that its hydrodynamical form is an incompressible flow. The incompressibility constraint removes the quantum Bohm pressure in the closely related Gross–Pitaevskii equations and the Madelung equations, leaving a fluid system near the one governed by the classical incompressible Euler equation. The spinorial component of the system boosts the vortex dynamics from the Euler fluid with a Landau–Lifschitz gyromagnetic force, enabling complex vortex phenomena even at a coarse computational grid. I will also explain that the incompressible Schrödinger flow is a symplectic Hamiltonian system described through the Bloch-sphere-valued Clebsch variables.

Finite-element tools for the 2D/3D simulation of phase-change materials

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ABSTRACT

The coupling between thermal convection and melting is a key phenomenon in many applications, ranging from geophysical flows (Earth's mantle formation, magma oceans) to the energy storage or passive temperature control devices using phase-change materials (PCMs). We present numerical simulations of a heated cavity filled with a pure PCM and consider both lateral and basal heating. The former case is well documented in the literature, while the latter (equivalent to the Rayleigh-Benard convection with melting) was less studied for confined geometries.

We present a new single domain numerical approach to solve the 2D/3D Navier-Stokes-Boussinesq equations for phase-change systems with natural convection. The key ingredients of the method are the use of an adaptive finite element method with a new regularization of the functions representing the variation of thermodynamic properties at the solid-liquid interface, and a fully linearized Newton algorithm for the time integration of the system of equations. The advantage of our adaptivity method is to allow accurate and simultaneous tracking of different interfaces in the system.

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Uniform error bounds of an exponential wave integrator Fourier pseudospectral method for the long time dynamics of the nonlinear Klein-Gordon equation

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ABSTRACT

In this talk, an exponential wave integrator Fourier pseudospectral (EWI-FP) method is presented and analyzed for the nonlinear Klein-Gordon equation (NKGE) with a cubic nonlinearity whose strength is characterized by ε^2 with $0 < \varepsilon \leq 1$ a dimensionless parameter. We mainly focus on the long-time resolutions of the EWI-FP method for the NKGE with weak nonlinearity. Over the long-time interval $[0, T_0/\varepsilon^\beta]$, the uniform error bounds of the EWI-FP discretization in terms of ε is carried out at the order of $O(h^m + \varepsilon^{2-\beta}\tau^2)$ with mesh size h, time step τ and m an integer depending on the regularity of the solution.

Uniform error estimate of a nested Picard integrator Fourier pseudospectral method for the nonlinear Schrödinger equation with wave operator

Yichen Guo

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ABSTRACT

In this seminar, an uniformly accurate nested Picard iterative integrator Fourier pseudospectral (NPI-FP) method is proposed for the nonlinear Schrödinger equation (NLS) with wave operator (NLSW). The NLSW is NLS perturbed by the wave operator with strength described by a parameter $\varepsilon \in (0, 1]$. The error bound is established at $O(h^m + \tau^2)$ independent of ε with mesh size h, time step τ for both well-prepared and ill-prepared initial data , and we will prove the temporal estimate for semi-discrete scheme.

Glitching pulsars: probing the interaction of incompressible quantum superfluids with compressible dissipative nuclear fluids under strong gravitational fields

Ahmad A. Hujeirat

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ABSTRACT

In this talk I will review the mechanisms underlying the glitch phenomena observed in pulsars, briefly describe the internal structures of neutron star within the framework of General Relativity, explain why their supranuclear dense cores must be in superfluid phase and why they must end as invisible gravitational BECs on the cosmological time scale. Moreover, recent arguments that favor dark BECs over classical black holes will be reviewed, and their connection to dark matter and dark energy in cosmology will be discussed.

Variational quantum algorithms for nonlinear problems

Dieter Jaksch

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ABSTRACT

I will discuss how nonlinear problems including nonlinear partial differential equations can be efficiently solved by variational quantum computing. This is achieved by utilizing multiple copies of variational quantum states to treat nonlinearities efficiently and by introducing tensor networks as a programming paradigm. I will demonstrate the key concepts of the algorithm using the nonlinear Schrödinger equation as a canonical example. I will present numerical results showing that the variational quantum ansatz can be exponentially more efficient than matrix product states and present experimental proof-of-principle results obtained on an IBM Q device.

A dynamical systems approach to deep learning: optimization, approximation and beyond

Qianxiao Li

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ABSTRACT

In this talk, we discuss a dynamical systems approach to deep learning through a continuous-time approximation, where deep residual neural networks are regarded as discretizations of differential equations. From this perspective, the learning problem can be formulated as a mean-field optimal control problem. We will discuss the mathematical basis for this formulation, including necessary and sufficient conditions for optimality, as well as learning algorithms one can derive from this viewpoint. We will also discuss the approximation properties of such idealized deep networks, including sufficient conditions for universal approximation, which is related to the problem of controllability. This approach connects deep learning on the one hand and dynamical systems and control on the other, and opens up new ways to attack the pertinent problems in modern machine learning research.

An efficient and accurate parallel simulator for streamer discharges in three dimensions

Bo Lin

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ABSTRACT

An efficient and accurate MPI-based parallel simulator is proposed for streamer discharges in three dimensions. It adopts the fluid model with SP3 approximation to the photoionization. Firstly, A new second-order semi-implicit scheme is proposed for the temporal discretization, which relaxes the dielectric relaxation time restriction. Secondly, a multigrid preconditioned FGMRES solver is introduced, which dramatically improves the efficiency of elliptic solver. Last but not least, all the methods are implemented using MPI, and the good parallel efficiency of the code is demonstrated. The interaction of two streamers is studied.

Quantum turbulence exploration using the Gross-Pitaevskii equation

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ABSTRACT

We solve numerically the Gross-Pitaevskii (GP) equation to simulate the dynamics of Quantum Turbulence (QT) in a periodic box. This intends to model the behaviour of superfluid helium, thus a viscous free flow. As in classical turbulence, the initial condition may be crucial in computing properties of QT. In this work, we discuss several accurately prepared intial data, based on near solutions of GP equation or related to classical flows. We then compare their effect on energy spectra and structure functions. Simulations are performed with a spectral code solving the GP equation using MPI-OpenMP parallel programming.

This is joint work with I. Danaila, L. Danaila, M. Kobayashi, C. Lothodé, Ph. Parnaudeau and M. Brachet

Continuum models of transportation networks with differential equations

Peter A. Markowich

King Abdullah University of Science and Technology, Saudi Arabia

ABSTRACT

An overview is presented of recent analytical and numerical results for the elliptic - parabolic system of partial differential equations proposed by Hu and Cai, which models the formation of biological transportation networks. The model describes the pressure field using a Darcy type equation and the dynamics of the conductance network under pressure force effects. Randomness in the material structure is represented by a linear diffusion term and conductance relaxation by an algebraic decay term. We first introduce micro- and mesoscopic models and show how they are connected to the macroscopic PDE system. Then, we provide an overview of analytical results for the PDE model, focusing mainly on the existence of weak and mild solutions and analysis of the steady states. The analytical part is complemented by extensive numerical simulations. We propose a discretization based on finite elements and study the qualitative properties of network structures for various parameter values.

Matter waves in disordered potentials: from localization to thermalization and condensation

Christian Miniatura[1,2,3,4]

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ABSTRACT

Because of their high degree of control and tunability, quantum gases have become versatile model systems to study effects originating from many different fields of physics such as condensed matter, quantum information, quantum hydrodynamics and even high-energy physics. The physics of disordered systems has not escaped the trend with the observation of coherent backscattering and Anderson localization [1, 2]. When interactions are additionally present, disordered gases offer even richer phenomena [3, 4]. Another important, yet poorly understood problem, is the long-time limit of the out-of equilibrium dynamics of weakly interacting quantum gases in disordered potentials, for which two main scenarios exist. In the first one, an atomic cloud is prepared as a spatially narrow wave packet whose spreading is followed in time. In this configuration, the nature of the system's dynamics at asymptotically long times remains debated, though theoretical works suggest that the cloud keeps expanding indefinitely. In the second one, the cloud is prepared in a plane-wave state at constant density (global excitation) and the interesting dynamics takes place in momentum space. At long times, a thermalization process is expected due to atomic collisions but the precise nature of the equilibrated state, resulting from the complicated interplay between interactions and disorder, is largely unknown. In the absence of disorder, thermalization has been extensively studied for waves, and in particular for optical waves, obeying the nonlinear Schrödinger equation within the framework of weak turbulence (WT) theory [5, 6]. It was found that the system generically equilibrates to a thermal Rayleigh-Jeans distribution maximizing entropy [7, 8], a problem recently extended to WT in confining potentials [9].

For strongly disordered systems, this thermalization process needs further analysis since the density of states (DoS) is dramatically altered at low energies where a possible condensation process would occur. This is the question we address in the present talk [10]. By considering a weakly-interacting plane matter wave released in a two-dimensional (2D) speckle potential, we show that the equilibrium momentum distribution achieved by the matter wave at long times is a thermal Rayleigh-Jeans distribution. This result is analogous to WT, except that the system state is made random by the disorder and not imposed as such at the beginning. Furthermore, we find that in contrast to usual 2D WT, the equilibrium distribution also exhibits, for specific values of the disorder strength and of the initial velocity, a large-scale coherent structure. This condensate coexists with the background of thermalized atoms and disappears at vanishing disorder [10].

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Relaxation dynamics of many-body open quantum systems

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ABSTRACT

We will first present an overview about the use of Matrix Product States to study many-body open quantum systems. Later we will discuss the relaxation dynamics of strongly interacting systems under the effect of dephasing, and show the emergence of different relaxation regimes and aging.

Dynamical modelling of phase transitions

Nikolaos Proukakis

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ABSTRACT

The non-equilibrium crossing of an incoherent–coherent phase transition in different geometries and dimensionalities is a broadly-applicable and challenging topic of potential technological interest. In this talk I discuss how this can be modelled via stochastic Gross-Pitaevskii-type equations. I will specifically focus on the Bose-Einstein Condensation phase transition in an elongated 3D ultracold atomic system and a ring-shaped trap, comparing in both cases findings to experimental measurements. I will then discuss the corresponding phase transition problem in 2D homogeneous systems for both closed systems (ultracold atoms) and driven-dissipative systems (exciton-polaritons), demonstrating that both are of the Berezinskii-Kosterlitz-Thouless type.

Extreme vortex states and the hydrodynamic blow-up problem

Bartosz Protas

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ABSTRACT

In the presentation we will discuss our research program focused on a systematic search for extreme, potentially singular, behaviors in the Navier-Stokes system and in other models of fluid flow. Enstrophy and enstrophy-like quantities serve as convenient indicators of the regularity of solutions to such system – as long as these quantities remains finite, the solutions are guaranteed to be smooth and satisfy the equations in the classical (pointwise) sense. However, there are no available estimates with finite a priori bounds on the growth of enstrophy in 3D Navier-Stokes flows and hence the regularity problem for this system remains open. While the 1D Burgers and the 2D Navier-Stokes system are known to be globally well posed, the question whether the corresponding estimates on the instantaneous and finite-time growth of various enstrophy-like quantities is quite relevant. We demonstrate how new insights concerning such questions can be obtained by formulating them as variational PDE optimization problems which can be solved computationally using suitable discrete gradient flows. More specifically, such an optimization formulation allows one to identify "extreme" initial data which, subject to certain constraints, leads to the most singular flow evolution which can then be compared with upper bounds obtained using rigorous methods of mathematical analysis. In order to quantify the maximum possible growth of enstrophy in 3D Navier-Stokes flows, we consider a family of such optimization problems in which initial conditions with prescribed enstrophy E_0 are sought such that the enstrophy in the resulting Navier-Stokes flow is maximized at some time T. By solving these problems for a broad range of values of E_0 and T, we demonstrate that the maximum growth of enstrophy is in fact finite and scales in proportion to $E_0^{3/2}$ as E_0 becomes large. Thus, in such worst-case scenario the enstrophy still remains bounded for all times and there is no evidence for formation of singularity in finite time. We also analyze properties of the Navier-Stokes flows leading to the extreme enstrophy values and show that this behavior is realized by a series of vortex reconnection events.

[Joint work with Diego Ayala, Dongfang Yun and Di Kang]

Generating synthetic spin-orbit coupling in cold atoms using periodic driving

Han Pu

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ABSTRACT

Synthetic spin-orbit coupling (SOC) in cold atoms has received much attention over the past decade, and has been one of the most active frontiers in cold atom research. The most common way of generating SOC is through Raman transition in atoms. However, the Raman beams may lead to heating of the atomic system. Here we show that SOC can also be generated by subjecting the atom to a periodically oscillating magnetic field without additional laser beams. This can lead to some exotic type of SOC and, in the mean time, circumvent the Raman-induced heating problem.

Dark matters from particles with unusual statistics

Mirza Satriawan

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ABSTRACT

We review and study the proposal that dark matters are possibly a form of particles with non Bose-Fermi statistics. In particular we consider the case that dark matters are a condensation of particles with infinite statistics. Two cases of infinite statistics are considered, indistinguishable and distinguishable infinite statistics. In addition partial results for the case of parastatistics are also discussed.

On a dissipative Gross-Pitaevskii-type model for exciton-polariton condensates

Jesus Sierra

University of Vienna, Austria

ABSTRACT

We study a generalized dissipative Gross-Pitaevskii-type model arising in the description of exciton-polariton condensates. We derive global in-time existence results and various a-priori estimates for this model posed on the one-dimensional torus. Moreover, we analyze in detail the long-time behavior of spatially homogenous solutions and their respective steady states and present numerical simulations in the case of more general initial data. We also study the convergence to the corresponding adiabatic regime, which results in a single damped-driven Gross-Pitaveskii equation.

Recent development of state-to-state quantum reactive scattering theory

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ABSTRACT

Development about efficient and accurate theory is fundamental problem in theoretical chemistry field. To development new theories and improve the numerical efficiency for calculating state-to-state quantum reactive scattering information using time-dependent quantum wave packet method, plays an important role in molecular reaction dynamics field. In past several years, we have developed several quantum reactive scattering theories, which are able to accurately and efficiently calculate state-to-state reactive scattering differential cross sections, by solving the long-standing so-called “coordinate problem”. For the first time, we would be able to accurately calculate state-to-state information of all of the product channels. Besides our theoretical developments, several cooperated work with the experiment will be briefly discussed.

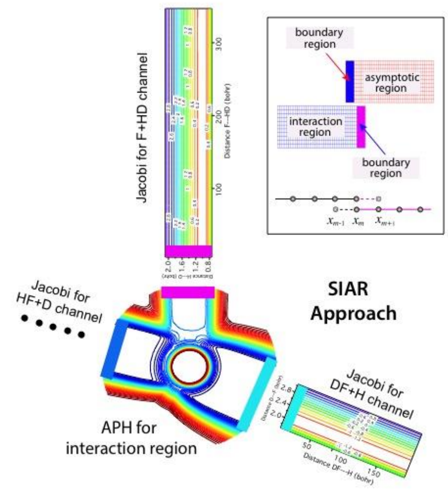

Fig 1. IARD scheme for a state-to-state calculation

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Computing ground states of spin 2 Bose-Einstein condensates by the normalized gradient flow

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ABSTRACT

In this talk, we will propose an efficient and accurate numerical method to compute the ground state of spin-2 Bose-Einstein condensates via the normalized gradient flow (NGF). The key idea is to find proper additional conditions to uniquely solve out the five projection constants in the corresponding projection step of NGF. Numerical results will be reported to show the efficiency of our method and to demonstrate some interesting phenomena.

Fast algorithms for deep learning based PDE solvers

Haizhao Yang

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ABSTRACT

In this talk, we introduce two fast algorithms for solving nonlinear and high-dimensional PDEs and eigenvalue problems. One is motivated by the two grid method in traditional nonlinear solvers and one is motivated by the self-paced learning in machine learning.