Abstracts

Computational methods for the dynamics of the nonlinear Schroedinger/Gross-Pitaevskii equations and applications

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ABSTRACT

In this tutorial, I begin wtih the nonlinear Schroedinger/Gross-Pitaevskii equations (NLSE/GPE) for modeling Bose-Einstein condensation (BEC), nonlinear optics, quantum physics and chemistry, etc., and review some dynamical properties of NLSE/GPE including conserved quantities, dispersion relation, center-of-mass dynamics, soliton solutions and semiclassical limits. Different numerical methods will be presented including finite different time domain (FDTD) methods and time-splitting spectral method, and their error estimates and comparison will be discussed. Extensions to NLSE/GPE with an angular momentum rotation term and/or non-local dipole-dipole interaction as well as multi-component will be presented. Finally, applications to soliton interactions, collapse and explosion of BEC, quantum transport and quantized vortex interaction will be investigated.

References

[1] W. Bao and Y. Cai, Mathematical theory and numerical methods for Bose-Einstein condensation, Kinet. Relat. Mod., 6 (2013), pp. 1-135.

[2] X. Antoine W. Bao and C. Besse, Computational methods for the dynamics of the nonlinear Schrodinger/Gross-Pitaevskii equations, Comput. Phys. Commun., 184 (2013), pp. 2621-2633.

[3] W. Bao, Q. Tang and Z. Xu, Numerical methods and comparison for computing dark and bright solitons in the nonlinear Schrodinger equation, J. Comput. Phys., 235 (2013), pp. 423-445.

[4] W. Bao, D. Jaksch and P. A. Markowich, Numerical solution of the Gross-Pitaevskii equation for Bose-Einstein condensation, J. Comput. Phys., 187 (2003), pp. 318-342. 1221.

Solving PDEs with finite elements: an introduction to free software FreeFem++

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ABSTRACT

This tutorial provides a hands-on introduction to the foundations and implementation of numerical algorithms to solve various PDE problems in 1D/2D/3D domains with the finite element method.

The free software FreeFem++ (www.freefem.org) offers an ideal framework to start a scientific computing activity: all the technicalities of the finite-element implementation are hidden from the user and the syntax is very close to mathematical formulations.

This graduate-level presentation of FreeFem++ will enable a fast progress in mastering numerical methods and the software. For advanced users, the tutorial will be a great opportunity to test FreeFem++ in solving their own problems.

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Level: Graduate

Features: Numerical methods: Theory and Examples, Computer Implementation

Prerequisites: basic programming skills, elementary calculus

Participants are advised to bring their laptops and install FreeFem++ (www.freefem.org)

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Tutorial Description:
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Each following part of the tutorial contains a short theoretical presentation of the numerical method, directly followed by its implementation in the form of computer programs:

Part 1: Installing Freefem++ and solving the 2D Poisson/Laplace problem
-- general presentation of FreeFem++
-- install FreeFem++ on each computer
-- building a 2D finite element mesh
-- weak formulation of the Poisson problem
-- solving the problem, visualize the solution
-- boundary conditions
-- more complicated meshes

Part 2: Solving stationary linear PDEs in 2D domains
-- heat equation
-- linear elasticity equations
-- adding source terms (identifying sub-domains)
-- imposing mixed boundary conditions
-- using macros

Part 3: Solving time-dependent PDEs in 2D domains
-- time-integration schemes
-- unsteady heat equation
-- wave equation
-- matrix formulation and optimization of programs
-- mesh adaptivity

Part 4: Some advanced features
-- solving non-linear PDEs with the Newton method
-- example of 2D applications: Stokes or Navier-Stokes equations
-- example of 3D applications: deformation eigen-modes of a 3D beam

Tensor networks for strongly correlated quantum systems

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ABSTRACT

The theoretical description of strongly correlated many-body quantum systems suffers from the curse of dimensionality: the number of degrees of freedom required to describe the system increases exponentially with system size. Tensor networks are a powerful approach to efficiently truncate the system description in a physically meaningful way. It allows compressing quantum states and quantum operators into tensor networks and, in many cases, carrying out all required operations without ever decompressing these networks. In these tutorials, I will introduce the basics of tensor network theory as used for describing ground states and quantum dynamics of well-controlled strongly correlated quantum systems. I will first discuss the basic notions of matrix product states and operators and describe the most widely used algorithms like density matrix renormalization group (DMRG) for finding ground states and its dynamical version which allows finding the evolution of a quantum system. I will provide examples of how of the most important applications of these algorithms in recent years. I will then move to more advanced topics like projected entangled pair states (PEPS) and describe the challenges faced in numerical applications of these tools. Finally, I will described possible connections of tensor networks to nascent quantum technologies like quantum simulation and computing.

Numerical methods for solving Schrodinger equation about chemical reaction

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ABSTRACT

A series of numerical methods used for solving schrodinger equation, which describe a chemical reaction process, such as, DVR method, Lagrange mesh, FE-DVR, higher-order difference method, DAF and methods for time-propagation etc. will be reviewed. The current applications and numerical challenges of solving the Schrodinger equation for describing a state-to-state chemical reaction will be emphasised.

References

[1] Sun, Z. G.; Guo, H.; Zhang, D. H. Journal of Chemical Physics. 2010, 132, 084112.

[2] Zhao, H. L.; Hu, X. X. Journal of Chemical Physics 2019, 150, 134105.

[3] Yuan, D. F.; . . . ; Wang X. A.; Sun, Z. G.; Zhang, D. H.; Yang, X. M. 2019, Science, 362, 1289

[4] Yang, T. G.; . . . ; Sun, Z. G.; Yang, X. M.; Alexander, M.; Neumark, D. 2019, Nature Chemistry