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Abstracts

Seminars on Modelling and Numerical Simulation
of Non-Equilibrium Processes

18–21 January 2022

1 Jingrun Chen

University of Science and Technology of China, China
Numerical methods for Landau-Lifshitz-Glibert equation

Abstract

Magnetic materials possess intrinsic magnetic order, termed as magnetization, whose dynamics is described by the Landau-Lifshitz-Gilbert (LLG) equation. Though phenomenological, this equation has been extensively used for magnetization dynamics at the nanoscale with satisfactory model accuracy. Mathematically, LLG equation is a system of nonlinear equations of parabolic type with possibly degeneracy and a pointwise nonconvex constraint. This presentation discusses two lines of work for this equation. One line of work is an improvement of Gauss-Seidel Projection Method (the seminal work proposed by Wang, Garcia-Cervera, and E in 2001). Our improvement reduces the number of linear systems of equations at each step by more than half without sacrificing the stability. The temporal accuracy is first-order. The other line is a semi-implicit scheme with second-order accuracy in time. The convergence rate is proved under the condition the temporal stepsize is proportional to the spatial gridsize. Interestingly, all rigorous results for quadratic convergence in the literature require severer conditions that ours. Both methods are verified to be unconditionally stable for real micromagnetics simulations.

2 Xin Liu

Academy of Mathematics and Systems Science, CAS, China
A penalty-free infeasible approach for a class of nonsmooth optimization problems over the Stiefel manifold

Abstract

Transforming into an exact penalty function model with convex compact constraints yields efficient infeasible approaches for optimization problems with orthogonality constraints. For smooth and 2,1-norm regularized cases, these infeasible approaches adopt simple and orthonormalization-free updating scheme and show their high efficiency in the test examples. However, to avoid orthonormalization while enforcing the feasibility of the final solution, these infeasible approaches introduce a quadratic penalty term, where an inappropriate penalty parameter can lead to numerical inefficiency. Inspired by penalty-free approaches for smooth optimization problems, we proposed a proximal first-order algorithm for a class of optimization problems with orthogonality constraints and nonsmooth regularization term. The consequent algorithm, named sequential linearized proximal gradient method (SLPG), alternatively takes tangential steps and normal steps to improve the optimality and feasibility respectively. In SLPG, the orthonormalization process is invoked only once at the last step if high precision in feasibility is needed, showing that main iterations in SLPG are orthonormalization-free. Besides, both the tangential steps and normal steps do not involve the penalty parameter, and thus SLPG is penalty-free and avoids the inefficiency by inappropriate penalty parameter. We analyze the global convergence properties of SLPG where the tangential steps are inexactly computed. By inexactly computing tangential steps, for smooth cases and 2,1-norm regularized cases, SLPG has a closed-form updating scheme, which leads to its cheap tangential steps. Numerical experiments illustrate the numerical advantages of SLPG when compared with existing first-order methods.

3 Di Fang

University of California, Berkeley, USA
Time-dependent Hamiltonian simulation of highly oscillatory dynamics

Abstract

Highly oscillatory dynamics are ubiquitous in nature and practical applications, resulting from either the large operator norm of the Hamiltonian, or the rapid change of the Hamiltonian itself when the Hamiltonian is time-dependent, or both. We develop a simple algorithm, called quantum Highly Oscillatory Protocol (qHOP) that can handle both oscillatory sources simultaneously. To our knowledge, this is the first quantum algorithm that is both insensitive to the rapid changes of the time-dependent Hamiltonian and exhibits commutator scaling. Furthermore, we prove that our method achieves superconvergence for the digital simulation of the Schrödinger equation that has wide applications in electronic structure theory, molecular dynamics and quantum machine learning.