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Solving Boltzmann and Fokker-Planck Equations Using Sparse Representation

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14. ABSTRACT

The main objectives of this project is to develop efficient and accurate spectral methods for fractional PDEs and highdimensional problems.
Fractional partial differential equations (FPDEs) appear in the investigation of transport dynamics in complex systems which are governed by the anomalous diffusion and non-exponential relaxation patterns. The main difficulties for dealing with fractional differential equations are: (i) fractional derivatives are non-local operators; (ii) fractional PDEs in space are usually derived in unbounded domains and their solutions exhibit slow algebraic decay at infinity; (iii) when truncated to finite domains, fraction derivatives involve singular weight functions and the solutions of FPDEs are usually singular near the boundary.
We developed several efficient approaches to deal with these problems.
The main difficulty for solving high-dimensional problems is how to break the curse of dimensionality. We continued our work in developing fast sparse spectral methods for solving a class of moderately high dimensional elliptic equations in bounded and unbounded domains.
Many complex nonlinear systems can be described as gradient flows. We developed a class of extremely efficient numerical methods for solving a large class of gradient flows.

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Accurate and Efficient Spectral Methods for Higher-dimensional and Fractional Differential Equations

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Abstract

The main objectives of this project is to develop efficient and accurate spectral methods for fractional PDEs and high-dimensional problems.

Fractional partial differential equations (FPDEs) appear in the investigation of transport dynamics in complex systems which are governed by the anomalous diffusion and non-exponential relaxation patterns. The main difficulties for dealing with fractional differential equations are: (i) fractional derivatives are non-local operators; (ii) fractional PDEs in space are usually derived in unbounded domains and their solutions exhibit slow algebraic decay at infinity; (iii) when truncated to finite domains, fraction derivatives involve singular weight functions and the solutions of FPDEs are usually singular near the boundary. We developed several efficient approaches to deal with these problems.

The main difficulty for solving high-dimensional problems is how to break the curse of dimensionality. We continued our work in developing fast sparse spectral methods for solving a class of moderately high dimensional elliptic equations in bounded and unbounded domains.

Many complex nonlinear systems can be described as gradient flows. We developed a class of extremely efficient numerical methods for solving a large class of gradient flows.

1 Efficient and accurate spectral methods for fractional PDEs

We developed fast and accurate spectral methods for solving a class of fractional PDEs.

1.1 Riesz fractional differential equations

Riesz derivatives are special two-sided fractional derivatives with equal coefficients, and they are very useful thanks to its similarity to the fractional Laplace operator. We developed efficient and accurate spectral Petrov-Galerkin methods for Riesz fractional PDEs with homogeneous Dirichlet BCs or fractional integral BCs. The methods are based on a new class of generalized Jacobi functions which are tailored to Riesz fractional derivatives. We derived useful properties of these generalized Jacobi functions, and in particular their optimal approximation results in non-uniformly weighted Sobolev spaces. By using various orthogonal properties of Jacobi polynomials and generalized Jacobi functions, we developed efficient Petrov-Galerkin methods for a class of Riesz fractional PDEs, and derived rigorous error estimates. In particular, it is shown that the errors decay exponentially fast as long as the data (right-hand side function) is smooth, despite that fact that the solution has singularities at the endpoints.

1.2 Tempered fractional differential equations on unbounded domains

Solutions of normal diffusion equations usually exhibits heavy tails, i.e., power law decays at infinity. The tempered fractional derivatives are introduced recently to "temper" the power law decay. It has been argued that tempered anomalous diffusion models have advantages over the normal dissuasion models in some applications of geophysics and finance.

We presented efficient spectral methods using the generalized Laguerre functions for solving the tempered fractional differential equations on the half line and on the whole line. Our numerical methods and analysis are based on an important observation that the tempered fractional derivative, when restricted to the half line, is intrinsically related to the generalized Laguerre functions.

1.3 Hermite spectral methods for fractional PDEs in unbounded domains

Fractional diffusion equations are naturally derived on unbounded domains. Their solutions usually decay very slowly at infinity and it is not clear how to derive transparent boundary conditions at truncated boundaries. By using the key fact that Hermit functions are eigenfunctions of Fourier transform, we developed efficient Hermite-colocation and Hermite-Galerkin methods for solving a class of fractional PDEs defined through Fourier transforms, and derived corresponding error estimates. In particular, the cost of our spectral methods for solving fractional PDEs on unbounded domains is of the same order as that for regular PDEs. We applied these methods for solving fractional advection-diffusion equations and fractional non- linear Schrödinger equations. The analysis and numerical results presented in this paper indicate that the proposed Hermite-collocation and Hermite-Galerkin methods are an effective approach to deal with fractional PDEs on unbounded domains directly.

1.4 Spacer-time spectral methods for fractional PDEs

We developed a new space-time spectral method for nonlinear fractional sub-diffusion equation. Our new scheme is based on a set of Fourier-like basis functions in the spatial variable and GJFs in time variable. The Fourier-like basis functions are discrete eigenfunctions of the Laplace operator, and lead to diagonal stiffness and mass matrices; The GJFs are chosen to match the leading singularity of the underlying problem so that they provide better performance than polynomial basis. We also presented error analysis for typical linear and nonlinear problems, and numerical results to validate our algorithms and error estimates.

1.5 Efficient spectral methods for PDEs with weakly singular solutions and their applications to FPDEs

Solutions for many problems of interest, particularly those pf fractional PDEs, exhibit singular behaviors at domain corners or points where boundary condition changes type. For this type of problems, direct spectral methods with usual polynomial basis functions do not lead to a satisfactory convergence rate.

1.5.1 Müntz-Galerkin methods

We developed the Müntz-Galerkin methods for problems with singular solutions for which direct spectral method with usual polynomial basis functions do not lead to a satisfactory convergence rate. Assuming that we have a singular expansion for the solution near a singular point in the form, our Müntz-Galerkin method is based on Müntz polynomials defined from the singular expansion. To overcome the poor conditioning of the Müntz polynomials, we explored relations between Jacobi polynomials and Müntz polynomials, and developed efficient implementation procedures for the Müntz-Galerkin method. We developed a framework to analyze the approximation errors of Müntz polynomials and derived the optimal error estimates for the Müntz-Galerkin method. As examples of applications, we employed the Müntz-Galerkin method to solve the Poisson equation with mixed Dirichlet-Neumann boundary conditions, and showed that the Müntz-Galerkin method leads to much improved rates of convergence compared to classical spectral methods.

1.5.2 Enriched spectral methods

We developed enriched spectral-Galerkin methods (ESG) for solving PDEs with weakly singular solutions. While the general idea of ESG is very simple — adding leading singular functions to the usual spectral approximation space, one has to overcome several obstacles to efficiently and accurately implement this in practical situations. Successful implementations of ESG rely on three ingredients: (i) determine a few leading singular terms for the underlying problem; (ii) homogenize the boundary conditions for the singular functions and use the modified Gram-Schimdt process to orthogonalize them; and most importantly (iii) use ESG-II, which is based on a special property of the spectral methods, to approximate the solution in the enriched spectral space. The computational cost of ESG is essentially $k + 1$ solvers, with k being the number of used leading singular terms, of the usual spectral-Galerkin method for which fast solvers are in general available. Theoretical estimates indicate that the accuracy of ESG can be as high as needed by increasing k.

2 High dimensional problems

We continued our work in developing efficient sparse spectral methods for solving a class of moderately high dimensional elliptic equations in bounded and unbounded domains.

2.1 Orthonormal mapped Chebyshev functions for high dimensional problems in unbounded domains

We studied approximation properties of orthonormal mapped Chebyshev functions (OMCFs) in unbounded domains. The OMCFs, unlike the usual mapped Chebyshev functions which are associated with weighted Sobolev spaces, are associated with the usual (non-weighted) Sobolev spaces, and lead to particularly simple stiffness and mass matrices for higher-dimensional problems.

We established error estimates by the usual tensor product OMCFs and hyperbolic cross OMCFs. In particular, our error estimates and numerical results indicate that the convergence rates for anisotropic problems with limited regularity, the hyperbolic cross OMCFs depend only weakly on the dimensions, making them suitable for higher-dimensional problems. On the other hand, for problems with isotropically smooth solutions, the convergence rates by the hyperbolic cross OMCFs, while still being exponential, depend strongly on the dimensions.

2.2 Nodal sparse spectral-element methods

We developed sparse grid spectral element methods using nodal bases for multi-dimensional elliptic PDEs. We use Chebyshev-Gauss-Lobatto sparse grid points to interpolate data, and use Lagrange bases in sparse grid approximation space to form linear algebraic system using a pseudo-spectral approach. The two sparse grid methods, sgSEM-N and sgSEM-Nm distinguish from each other on how many edge DoFs used. sgSEM-Nm uses less edge DoFs than sgSEM-N to get a better conditioned Schur system. Preliminary numerical methods show that the iteration numbers of sgSEM-N and sgSEM-Nm using CG with a simple block-diagonal preconditioner for the corresponding Schur-complement are similar.

Since the main cost in a spectral element method is usually associated with solving the Schur-complement system, and sgSEM-Nm uses less edge DoFs, particularly in higher-dimensions and with larger numbers of elements, it can be expected that sgSEM-Nm, with a better preconditioner, can potentially be much more effective than sgSEM-N and sgSEM-N-F.

3 Efficient numerical methods for gradient flows and phase-field models

We developed several accurate and efficient numerical methods for gradient flows and phase-field models. In particular, we developed the so called Scalar Auxiliary Variable (SAV) approach for a large class of gradient flows, including those with non-local or fractional free energies. These schemes are unconditionally stable about a modified energy, linear and second-order accurate, while offers the following additional advantages:

- It greatly simplifies the implementation and is much more efficient: at each time step of the SAV schemes, the computation of the scalar auxiliary variable r^{n+1} and the original unknowns are totally decoupled and only requires solving linear systems with constant coefficients.
- It applies to a larger class of gradient flows. In particular, it offers an effective approach to deal with gradient flows with non-local free energy.

Furthermore, we can even construct higher-order stiffly stable schemes with all the above attributes by combining SAV approach with higher-order BDF schemes. And when coupled with a suitable time adaptive strategy, the SAV schemes are extremely efficient and applicable to a large class of gradient flows. This approach has received much attention since it first appeared, and a paper summarizing the concepts and applications of SAV has just been accepted by *SIAM Review*.

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