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Fast algorithms for spectral collocation with non-periodic boundary conditions

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Abstract

We present a method for the numerical solution of partial differential equations using spectral collocation. By employing a structured representation of linear operators we are able to use fast algorithms without being restricted to periodic boundary conditions. The underlying ideas are introduced and developed in the context of linearly implicit methods for stiff equations. We show how different boundary conditions may be applied and illustrate the technique on the Allen–Cahn equation and the diffusion equation.

Keywords: Pseudospectral methods; Chebyshev collocation; Fast algorithms; Fast direct solver; Semi-separable; Boundary conditions

1. Introduction

An important factor in the rise in popularity of spectral methods is the availability of fast transform methods. Due to the global nature of the basis functions employed, matrix representations of differential operators in the spatial domain are not sparse and are costly to work with. Working in a transformed domain returns us to a sparse representation.

In a number of situations, staying in the spatial domain may be highly desirable. The most common reason for favoring a transform-free method is to facilitate enforcing boundary conditions. If we wish to work

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on a non-periodic problem and specify Dirichlet or Neumann boundary conditions, it is natural to work in physical space. However, if we do so our Chebyshev derivative operator will be a full matrix and the size of problem we can tackle will be severely reduced.

In this paper, we introduce a new method for efficiently solving spectral discretizations of partial differential equations (PDEs) while staying in the spatial domain. We will develop our ideas in the context of linearly implicit (LI) methods. This approach is currently the most popular choice for PDEs with low-order non-linear terms and higher-order linear terms.

A recent paper by Kassam and Trefethen [9] includes a survey of methods being applied to treat problems of this kind and indicates that LI methods may not always be the best choice. As such, we also discuss how the ideas we propose here can be used to similar advantage in integrating factor (IF) and exponential time differencing (ETD) methods. These methods are of recent vintage but show great promise.

Linearly implicit (also known as implicit–explicit or IMEX) methods are widely used and have a history going back at least to 1980. In these early papers we find a full description of the method [15] and some results on stability [33]. More recent treatments include [2,3]. The defining feature of LI methods is that they employ an implicit discretization of leading order *linear* terms and an explicit discretization of the remaining, typically *non-linear* terms. Thus, if the inversion of the resulting linear system can be accomplished at a low cost then one obtains an efficient method in which the leading order timestepping stability constraint has been eliminated. Unfortunately, the solution to such linear systems is costly for Chebyshev collocation and quite generally for spectral discretizations when remaining in the spatial domain.

Here, by employing an appropriate representation of the differential operator on the spatial domain, we can use an implicit time discretization of the leading order linear operators and apply direct, fast, non-iterative methods to solve the resulting linear system at each timestep. This allows us to remove the highest order timestepping constraint while retaining nearly linear scaling in the number of collocation points.

We illustrate this strategy in the particular case of functions on a finite interval, discretized by collocation on the Gauss–Lobatto points.

2. Basic strategy

The basis of our approach is a representation of differential operators. In transform methods no explicit representation of the derivative operator is needed, as the coefficients of the derivative are generated through recursion. In the spatial domain, the derivative has a matrix representation and classically this is what is used in physical space numerical methods.

However, the matrix representation of the derivative is not sparse, symmetric or even normal (see [17]). It is computationally expensive to work with such matrices. The matrix of the derivative is also ill-conditioned, so even a brute force solution of a discretized differential equation using *iterative* methods will be very expensive.

In our approach we represent the Chebyshev derivative operator not with a matrix, but with a *hierarchically semi-separable representation* (also known as a *rebus*). This is a representation closely related to the fast multipole method (FMM) in the form developed by Starr and Rokhlin [31] and by Yarvin and Rokhlin [34]. Similar developments along these lines have since been made by Beylkin, Coult and Mohlenkamp in [7] and Beylkin and Sandberg in [10]. The formulation we adopt here was introduced by Chandrasekaran and Gu in [13]. We place this representation in historical context in Section 3 and proceed to review the definition and properties of the representation below in Section 4.

Our approach to solving the PDEs is as follows. Starting from the governing equations, we discretize the time dependence using an implicit discretization of the leading order linear terms. This avoids high stability restrictions on the allowable time step. Then, we introduce the rebus representation of the spectral derivative operator and use fast algorithms to generate the needed higher order linear operator for a timestep.