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Spectral integration of linear boundary value problems

Divakar Viswanath

Department of Mathematics, University of Michigan, United States

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ABSTRACT

Spectral integration was deployed by Orszag and co-workers (1977, 1980, 1981) to obtain stable and efficient solvers for the incompressible Navier–Stokes equation in rectangular geometries. Since then several variations of spectral integration have appeared in the literature. In this article, we derive yet more versions of spectral integration. These new versions of spectral integration rely exclusively on banded matrices as opposed to banded matrices bordered with dense rows. In addition, we derive a factored form of spectral integration which relies only on bi- and tri-diagonal matrices. Key properties, such as the accuracy of spectral integration even when Green's functions are not resolved by the underlying grid and the accuracy of spectral integration in spite of ill-conditioning of underlying linear systems are investigated. Timed comparisons show that reducing spectral integration to bi- and tri-diagonal systems leads to significant speed-ups.

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1. Introduction

One of the earliest methods for solving the incompressible Navier–Stokes equation was proposed in a pioneering paper by Orszag [1]. In that paper, Orszag tackled the problem of numerically integrating wall-bounded shear flows using Chebyshev series expansions. The Chebyshev polynomial is defined by $T_n(y) = \cos(n \arccos y)$ for $-1 \leq y \leq 1$. If $u(y) = \alpha_0 T_0/2 + \sum_{j=1}^{\infty} \alpha_j T_j$ is the Chebyshev series of $u(y)$, we denote the Chebyshev coefficient α_n by $\mathcal{T}_n(u)$. The points $y_j = \cos(j\pi/M)$, $j = 0, \ldots, M$, are the Chebyshev grid points. The discrete cosine transform may be used to pass back and forth between the physical domain function values $u(y_j)$, $0 \leq j \leq M$, and the coefficients in the Chebyshev expansion $\alpha_0 T_0/2 + \sum_{j=1}^{M-1} \alpha_j T_j + \alpha_M T_M/2$, if $\alpha_j = 0$ for $j > M$.

The method proposed by Orszag in [1] is certainly complete. However, it is much too expensive. It does not appear to have been implemented and therefore its effectiveness cannot be gaged. Nevertheless, Orszag and co-workers [2,3] derived an effective algorithm for the integration of the incompressible Navier–Stokes equations in rectangular geometries that has been widely used along with a few other popular modifications for more than two decades [4].

The method of spectral integration was introduced by Gottlieb and Orszag as a reformulation of the tau-equations [5, p. 119]. It forms the basis of widely used methods for the solution of the incompressible Navier–Stokes equations [4,2]. Below and throughout this paper, D denotes d/dy. The Chebyshev tau equations for a boundary value problem such as

$$\left(D^2 - a^2\right) u = f(y), \quad u(\pm 1) = 0, \tag{1.1}$$

are obtained by expanding the solution u in a truncated Chebyshev series and equating the Chebyshev coefficients of $T_0, \ldots, T_{M-2}$ in the expansion of $\left(D^2 - a^2\right) u$ to those of f, and enforcing the boundary conditions to get two more equations. As Gottlieb and Orszag noted the tau equations are dense and not well-conditioned. Their method of rewriting gives a tridiagonal system bordered by dense rows corresponding to the boundary conditions.

E-mail address: divakar@umich.edu.

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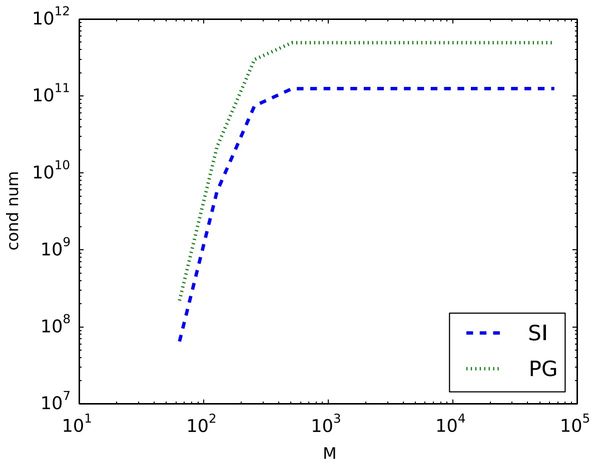

Fig. 1.1. Plot of the infinite-norm condition number vs the number of grid point M for two methods, spectral integration (SI) and Petrov–Galerkin (PG). The methods are applied to the 4th order problem $(D^2 - \alpha^2)(D^2 - \beta^2)u = f$ with $\alpha = 10^3$ and $\beta = 10^4$. The condition number indeed converges to a constant as M increases but the constant is very large.

In Section 2, we derive a variety of spectral integration methods. All the methods of Section 2 work with purely banded matrices and no bordering rows. Later in this introduction, and in Section 4, we argue that eliminating bordering by dense rows leads to a more efficient solver. The main reason for greater efficiency is that bi- and tri-diagonal solvers are included in the LAPACK library for which highly optimized implementations, such as Intel MKL, are available. Optimized implementations, such as Intel MKL, are continually updated to keep up with changes in computer architecture. A hand coded implementation, which would be required for banded matrices bordered by dense rows, is unlikely to be as well optimized and even more unlikely to stay up-to-date with changes in computer architecture.

A property brought to light by Greengard [6] is that condition numbers of spectral integration matrices, corresponding to boundary value problems such as (1.1), are bounded in the limit $M \to \infty$. As noted by Rokhlin [7], any integral formulation has this property because the integral operators that are discretized are compact. In contrast, the tau equations discretize (1.1) in its differential form and therefore suffer from ill-conditioning. In particular, their condition number goes to ∞ as $M \to \infty$. This property of spectral integration has been noted by other authors as well and spectral integration has been deemed to be well-conditioned [5,8].

Although this may be a useful property, it is by itself inadequate to understand the robustness of spectral integration as applied to the Navier–Stokes equations in the turbulent regime. Fig. 1.1 depicts a scenario, typical of the incompressible Navier–Stokes equations in rectangular geometries [9], where the constant the condition number converges to as M increases is greater than 10^{11}. These matrices cannot be considered well-conditioned. The figure shows condition numbers (computed using the `dgbcon` and `dpbcon` routines in LAPACK) for a version of spectral integration derived in Section 2 and for the Petrov–Galerkin method of Shen [10–12], which uses Legendre polynomials. Plots of condition numbers would look the same for any version of spectral integration. Even though the condition number implies a loss of 11 digits of accuracy, we show in Section 4 that such systems are solved with almost machine precision. In Section 3, we give a partial explanation of this phenomenon. Contrary to what the condition numbers suggest the Petrov–Galerkin method is the most accurate.

Iterative methods have been championed for the solution of linear systems that arise after the discretization of integral formulations [7]. In this instance, iterative methods would be of little use because the constants the condition numbers converge to are so large. It is not enough for a method to be $\mathcal{O}(M)$. The constant in front of the M can make a big difference. In Section 4, we find that the speed-up between even highly optimized implementations can approach and exceed a factor of 2.

A number of numerical examples are included in Section 4. The example in Section 4.1 shows that the forms of spectral integration derived in Section 2 match the accuracy of earlier computations [6,13]. One of the forms of spectral integration derived in Section 2 allows for piecewise Chebyshev grids. The example in Section 4.2 shows that this method reduces the number of grid points from 1024 in an earlier computation [14] to only 161, while reducing the relative error from 10^{-4} to 10^{-10}.

Piecewise Legendre grids, which are analogous to piecewise Chebyshev grids, have been considered by Diamessis et al. [15] in the context of stratified flow. The patching conditions which occurs between subdomains are handled by Diamessis et al. using a penalty term. In our method they are handled explicitly.

In Section 4.3, we give a timed comparison between the two different versions of spectral integration in Section 2 and the Petrov–Galerkin method [10]. All our implementations use highly optimized library functions for solving linear systems and for computing the discrete cosine transform. Even so, spectral integration relying on pentadiagonal systems is found to consume 50% more time than spectral integration using tridiagonal systems. The reason is that solving two tridiagonal systems using the optimized MKL library is much cheaper than solving one pentadiagonal system. Some of the issues that arise in such optimized implementations are discussed. Explicit comparison to spectral integration with dense bordered

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