Journal of Computational Physics 287 (2015) 254–268

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

A preconditioned numerical solver for stiff nonlinear reaction–diffusion equations with fractional Laplacians that avoids dense matrices

Alex Simmons, Qianqian Yang*, Timothy Moroney

School of Mathematical Sciences, Queensland University of Technology, GPO Box 2434, Brisbane, QLD 4001, Australia

ARTICLE INFO

Article history:
Received 13 June 2014
Received in revised form 25 November 2014
Accepted 6 February 2015
Available online 11 February 2015

Keywords:
Fractional Laplacian
Nonlinear
Jacobian-free Newton–Krylov
Backward differentiation formula
Banded preconditioner
Contour integral method

ABSTRACT

The numerical solution of fractional partial differential equations poses significant computational challenges in regard to efficiency as a result of the spatial nonlocality of the fractional differential operators. The dense coefficient matrices that arise from spatial discretisation of these operators mean that even one-dimensional problems can be difficult to solve using standard methods on grids comprising thousands of nodes or more. In this work we address this issue of efficiency for one-dimensional, nonlinear space-fractional reaction–diffusion equations with fractional Laplacian operators.

We apply variable-order, variable-stepsize backward differentiation formulas in a Jacobian-free Newton–Krylov framework to advance the solution in time. A key advantage of this approach is the elimination of any requirement to form the dense matrix representation of the fractional Laplacian operator. We show how a banded approximation to this matrix, which can be formed and factorised efficiently, can be used as part of an effective preconditioner that accelerates convergence of the Krylov subspace iterative solver. Our approach also captures the full contribution from the nonlinear reaction term in the preconditioner, which is crucial for problems that exhibit stiff reactions. Numerical examples are presented to illustrate the overall effectiveness of the solver.

1. Introduction

Recently there has been a great deal of interest in the applied mathematics community concerning fractional calculus and its applications to modelling anomalous diffusion. Fractional derivatives are becoming widely used and accepted in models of diffusion-type processes where the underlying particle motion deviates from Brownian motion [2]. A typical application area is transport in porous media, where models of seepage flow [19], seawater intrusion [1] and wood drying [31], to name just three, make use of fractional derivatives. In other areas too, we see fractional models becoming established, such as in drug delivery [41], heart physiology [5,29], elasticity [30], quantum mechanics [17], bioengineering [21], optimal image processing [7] and magnetic resonance imaging analysis [22,9]. Analytical solution methods exist only for a small number of simple, mostly linear, fractional differential equations. To obtain solutions to more complex problems, numerical methods are required.

* Corresponding author. Tel.: +61 7 3138 2890; fax: +61 7 3138 2310.
E-mail address: q.yang@qut.edu.au (Q. Yang).

http://dx.doi.org/10.1016/j.jcp.2015.02.012
0021-9991/

In this paper we are concerned with fractional reaction–diffusion equations of the form

$$\frac{\partial u(x,t)}{\partial t} = -\kappa \left(-\nabla^2\right)^{\alpha/2} u(x,t) + S(u(x,t)) \tag{1}$$

on the finite domain $0 \le x \le L$, with homogeneous Dirichlet boundary conditions and initial condition $u(x,0) = u_0(x)$. The operator $\left(-\nabla^2\right)^{\alpha/2}$ denotes the fractional Laplacian operator of order $\alpha \in (1,2]$, which is defined through its spectral representation.

Definition 1. (See [13].) Suppose the Laplacian $(-\nabla^2)$ has a complete set of orthonormal eigenfunctions φ_n corresponding to eigenvalues λ_n^2 on a bounded region $\mathcal{D}$, i.e., $(-\nabla^2)\varphi_n = \lambda_n^2 \varphi_n$; $\mathcal{B}(\varphi) = 0$ on $\partial\mathcal{B}$, where $\mathcal{B}(\varphi)$ is one of the standard three homogeneous boundary conditions. Let

$$\mathcal{F}_\gamma = \left\{ f = \sum_{n=1}^{\infty} c_n \varphi_n, c_n = \langle f, \varphi_n \rangle \,\middle|\, \sum_{n=1}^{\infty} |c_n|^2 |\lambda|_n^\gamma < \infty, \gamma = \max(\alpha, 0) \right\}$$

then for any $f \in \mathcal{F}_\gamma$, $(-\nabla^2)^{\alpha/2} f$ is defined by

$$(-\nabla^2)^{\alpha/2} f = \sum_{n=1}^{\infty} c_n (\lambda_n^2)^{\alpha/2} \varphi_n.$$

Using the matrix transfer technique proposed by Ilić et al. [14], the fractional PDE (1) is spatially discretised by first finding the matrix representation $\mathbf{A}$ of the standard Laplacian using finite differences or other such methods. The matrix representation of the fractional Laplacian is then given by $\mathbf{A}^{\alpha/2}$. For example, using finite differences with N uniform divisions of width $h = L/N$, the semidiscrete form of (1) is the system of ODEs

$$\dot{\mathbf{u}} = -\kappa \mathbf{A}^{\alpha/2} \mathbf{u} + \mathbf{S}(\mathbf{u}) =: \mathbf{F}(\mathbf{u}), \quad \mathbf{u}(\mathbf{x}, 0) = \mathbf{u}_0(\mathbf{x}) \tag{2}$$

where $\mathbf{A} = \text{tridiag}(-1, 2, -1)/h^2$.

Aside from the usual challenges of nonlinearity and stiffness, Eq. (2) poses an additional challenge that is not present in standard (non-fractional) reaction–diffusion problems: $\mathbf{A}^{\alpha/2}$ is dense, even though $\mathbf{A}$ itself is sparse (indeed, tridiagonal, in our problem). Hence, it is natural to consider numerical methods for solving (2) that do not require explicit formation of $\mathbf{A}^{\alpha/2}$ and instead deal only with $\mathbf{A}$. This becomes essential when solving problems on grids with many thousands of nodes, where the memory and computational expenses associated with forming and working with $\mathbf{A}^{\alpha/2}$ can be prohibitive, even in this one-dimensional setting.

There are a number of mature initial value problem solvers for stiff systems of nonlinear ODEs

$$\dot{\mathbf{u}} = \mathbf{F}(\mathbf{u}) \tag{3}$$

that can be configured to never form the Jacobian matrix $\mathbf{J} = \partial\mathbf{F}/\partial\mathbf{u}$, that is, to work Jacobian-free. CVODE, part of the SUNDIALS Suite of Non-linear and Differential/Algebraic Equation Solvers [12], is an excellent example. Such solvers appear very attractive in the present context because they avoid the need to work with dense matrices. They also tend to provide variable-order, variable-stepsize integration with sophisticated local error control among other desirable features.

In order to work Jacobian-free, these solvers typically employ some form of Newton–Krylov iteration [16] to resolve the solution at each timestep. In addition to providing the right hand side function $\mathbf{F}$, the user of these solvers is also expected to provide a means of dealing with the stiffness in the problem. This is provided in the form of a preconditioner: a matrix or a routine that approximates the action of the inverse of the Jacobian (or related matrix) on an arbitrary vector.

While at first this last requirement appears to run counter to the idea of working Jacobian-free, in many cases a much simplified approximation to the Jacobian suffices for preconditioning purposes, provided it captures the dominant source of stiffness in the problem. In the present application, we seek a sparse approximation to the Jacobian that suffices for the purpose of preconditioning. A key contribution of this paper is demonstrating how to efficiently construct such a matrix.

A number of authors have also proposed efficient methods for solving (1), and other similar fractional PDEs. Yang et al. [39] considered a time- and space-fractional variation of (1) in two dimensions with no reaction term, and used the matrix transfer technique with finite difference and finite element discretisations in space. The solution was advanced in time by computing a matrix function vector product $f(\mathbf{A})\mathbf{b}$ where $f(\mathbf{A}) = (\mathbf{I} + \gamma\kappa\mathbf{A}^{\alpha/2})$, and this was carried out using a Krylov subspace projection method preconditioned with deflation.

Burrage et al. [6] considered (1) and its higher-dimensional generalisations. They used the matrix transfer technique with finite element discretisation in space, and a first order implicit/explicit Euler discretisation in time. They investigated several methods for computing the resulting matrix function vector products, including the contour integral method of Hale et al. [11], which is discussed in Section 2.2, the extended Krylov subspace method and the preassigned poles and interpolation nodes method.

Bueno-Orovio et al. [4] solved (1) and its higher-dimensional generalisations using Fourier spectral methods, with a first order, fully implicit backward Euler temporal discretisation. Fixed point iteration was used to solve the resulting nonlinear systems in Fourier space to advance the solution in time.