Semi-Implicit Spectral Collocation Methods for Reaction-Diffusion Equations on Annuli

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In this article, we develop numerical schemes for solving stiff reaction-diffusion equations on annuli based on Chebyshev and Fourier spectral spatial discretizations and integrating factor methods for temporal discretizations. Stiffness is resolved by treating the linear diffusion through the use of integrating factors and the nonlinear reaction term implicitly. Root locus curves provide a succinct analysis of the A-stability of these schemes. By utilizing spectral collocation methods, we avoid the use of potentially expensive transforms between the physical and spectral spaces. Numerical experiments are presented to illustrate the accuracy and efficiency of these schemes. © 2010 Wiley Periodicals, Inc. *Numer Methods Partial Differential Eq* 27: 1113–1129, 2011

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I. INTRODUCTION

Reaction-diffusion equations are an important type of partial differential equations that model a wide variety of physical, chemical, and biological processes. For example, tumor growth can be modeled by reaction-diffusion systems on spheres [1, 2]. In developmental biology, reaction-diffusion equations have been used to model tissue development through the spatial and temporal distribution of morphogens [3]. Protein trafficking in cells involves the diffusion of monomer, dimers, and tetramers and their association and disassociation. This process can be modeled by reaction-diffusion equations inside the cytoplasm, which in the simplest case can be treated as a two-dimensional annulus.

The development of efficient numerical methods for reaction-diffusion equations and particularly for stiff systems has been an active area of research. Exponential time differencing methods [4, 5], integrating factor methods [3, 6], and operator splitting methods [7] have all been extensively investigated. Combined with *a posteriori* error estimates, reaction-diffusion systems can be solved adaptively through operator splitting methods [8].

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The geometry of domains is an important consideration when developing efficient numerical methods for stiff reaction-diffusion systems. Numerical methods that assume Cartesian geometry may not be extended directly to polar coordinate systems. For polar domains like annuli, spectral methods are a natural choice to exploit the periodicity in the azimuthal direction. Spectral methods, finite difference methods, and finite element methods constitute the three major types of numerical methods [9, 10]. Spectral methods have been successfully applied to various types of scientific computing problems, see, e.g., [11] for an application of the spectral element methods to geophysics problems. However, the spectral Galerkin methods based on Fourier expansions [9, 12] may become very complicated or even untenable, when they are applied to treat nonlinear reaction terms. The transforms between the physical and spectral spaces could compromise the efficiency of these methods when they are used in time-dependent problems, although the fast Fourier transform can be used.

Integrating factor methods have been investigated to decouple operators of different natures in differential equations [13–15]. An operator integration factor splitting method was developed for time-dependent problems in [13] and then applied to incompressible fluid flow. In [14], an integration factor splitting method was investigated and used for the shallow water equations. Integrating factor finite difference methods were developed in [3, 6] for solving reaction-diffusion equations in Cartesian geometries. In this paper, we combine integrating factor methods and spectral collocation methods (Chebyshev in the radial direction and Fourier in the azimuthal direction) to develop numerical schemes for reaction-diffusion problems on annuli. Special considerations arising due to a polar singularity [16] do not arise on annular domains. The use of integrating factors is shown to improve stability without compromising accuracy. Integrating factors also enable us to decouple linear and nonlinear terms and require the solution of a number of small independent nonlinear systems rather than a single large fully coupled nonlinear system. Spectral collocation methods both provide spectral accuracy and avoid expensive transforms between the physical and spectral spaces. The use of Chebyshev polynomials in the radial direction enables us to resolve radial boundary layers with moderate computational efforts. Recognizing the 2nd Dalquist barrier, we restrict our attention to the integration schemes that are second order in time.

The rest of this paper is organized as follows. In Section II, we present semi-implicit spectral collocation schemes for reaction-diffusion equations on annuli with homogeneous Dirichlet boundary conditions. Section III briefly discusses other related numerical methods. Implementation strategies for enforcing more complicated boundary conditions and numerical results are presented in Section IV. The paper is concluded with some remarks in Section V.

II. SEMI-IMPLICIT SPECTRAL COLLOCATION SCHEMES

A. Development of Semi-implicit Spectral Collocation Schemes

We consider the following initial and boundary value problem for a nonlinear scalar reaction-diffusion equation

$$u_t = D\Delta u + f(u) + g(r, \theta, t), \quad (r, \theta) \in \Omega, \quad t \in (0, T], \quad (2.1)$$

where (r, θ) are the polar coordinates, $\Omega = \{(r, \theta) : r_a \leq r \leq r_b, \theta \in [0, 2\pi)\}$ is an annulus with $0 < r_a < r_b$, $T > 0$ is the final time, u the unknown concentration, $D > 0$ a constant diffusion, Δ the spatial Laplacian operator, f an autonomous nonlinear reaction term, and g a known source. Recall that the Laplacian operator in cylindrical coordinates is

$$\Delta u = u_{rr} + r^{-1}u_r + r^{-2}u_{\theta\theta}. \quad (2.2)$$

FIG. 1. An annulus with a spectral grid (Chebyshev in the radial direction and Fourier in the azimuthal direction).

For ease of presentation, we consider the homogeneous Dirichlet boundary conditions

$$u|_{\Gamma_a} = u|_{\Gamma_b} = 0, \quad \forall t \in (0, T], \quad (2.3)$$

where Γ_a and Γ_b are the inner and outer circles, respectively. As shown in the numerical examples in Section IV, our schemes can be extended to other types of boundary conditions and systems of reaction-diffusion equations. An initial condition

$$u(r, \theta, 0) = u_0(r, \theta), \quad \forall (r, \theta) \in \Omega \quad (2.4)$$

is specified to close the system.

A two-stage discretization approach is adopted to establish our numerical schemes: first a spatial discretization and then a temporal discretization. We apply the Chebyshev spectral collocation method in the radial direction and the Fourier spectral collocation method in the angular direction, see Fig. 1.

Let N_r be a positive integer and $s_i = \cos(i\pi/N_r)$, $0 \leq i \leq N_r$ the Chebyshev collocation nodes on the reference interval $[-1, 1]$. Let $\mathbf{D}_{C,N_r}^{(1)}$ and $\mathbf{D}_{C,N_r}^{(2)}$ be the $(N_r - 1) \times (N_r - 1)$ first and second order Chebyshev differentiation matrices corresponding to the homogeneous Dirichlet boundary conditions on the reference interval [10]. We define

$$\mathbf{A}_1 = \frac{2}{r_b - r_a} \mathbf{D}_{C,N_r}^{(1)}, \quad \mathbf{A}_2 = \frac{4}{(r_b - r_a)^2} \mathbf{D}_{C,N_r}^{(2)}. \quad (2.5)$$

For convenience, we denote

$$r_i = \frac{r_b + r_a}{2} + \frac{r_b - r_a}{2} s_i, \quad 0 \leq i \leq N_r,$$

and define a diagonal matrix

$$\mathbf{R} = \text{diag}(r_1, \dots, r_{N_r-1}). \quad (2.6)$$

Let N_θ be an even positive integer and $\theta_j = 2j\pi/N_\theta$, $1 \leq j \leq N_\theta$. We define

$$\mathbf{B} = \mathbf{D}_{F,N_\theta}^{(2)} \quad (2.7)$$

as the second order $N_\theta \times N_\theta$ Fourier differentiation matrix [10].

Given the homogeneous Dirichlet boundary conditions and the periodicity of the solution in the angular direction, we consider the unknowns

$$\mathbf{U} = \mathbf{U}(t) = \left[U(r_i, \theta_j, t) \right]_{(N_r-1) \times N_\theta}$$

at the interior grid points (r_i, θ_j) , $1 \leq i \leq N_r - 1$, $1 \leq j \leq N_\theta$ for $t \in [0, T]$. We denote $\mathbf{U}_n = \mathbf{U}(t_n)$. Similarly, we define

$$\mathbf{G} = \mathbf{G}(t) = \left[\mathbf{g}(r_i, \theta_j, t) \right]_{(N_r-1) \times N_\theta}$$

and $\mathbf{G}_n = \mathbf{G}(t_n)$.

We approximate the Laplacian operator (2.2) at the grid points to obtain

$$\Delta u \approx \mathbf{A}_2 \mathbf{U} + \mathbf{R}^{-1} \mathbf{A}_1 \mathbf{U} + \mathbf{R}^{-2} \mathbf{U} \mathbf{B}.$$

After this semi-discretization in space, we end up with a system of ordinary differential equations (ODEs) for the unknowns at the grid points,

$$\frac{d\mathbf{U}}{dt} = D(\mathbf{A}_2 \mathbf{U} + \mathbf{R}^{-1} \mathbf{A}_1 \mathbf{U} + \mathbf{R}^{-2} \mathbf{U} \mathbf{B}) + \mathbf{F}(\mathbf{U}) + \mathbf{G}(t), \quad t \in (0, T], \quad (2.8)$$

where $\mathbf{F}(\mathbf{U})$ is of the same size as $\mathbf{U}$ and evaluated componentwise and pointwise at the grid points.

We rewrite the $(N_r - 1) \times N_\theta$ matrix of unknowns $\mathbf{U}$ column by column to obtain an $(N_r - 1)N_\theta$ -dimensional vector $\mathcal{U}$. That is, using the notation [17], $\mathcal{U} = \text{vec}(\mathbf{U})$. The ODE system (2.8) is rewritten as

$$\frac{d\mathcal{U}}{dt} = \mathcal{L}\mathcal{U} + \mathcal{F}(\mathcal{U}) + \mathcal{G}(t), \quad (2.9)$$

where

$$\mathcal{L} = D(\mathbf{I}_{N_\theta} \otimes (\mathbf{A}_2 + \mathbf{R}^{-1} \mathbf{A}_1) + \mathbf{B}^T \otimes \mathbf{R}^{-2}). \quad (2.10)$$

Let N_t be a positive integer, $\Delta t = T/N_t$, and $t_n = n\Delta t$ ($0 \leq n \leq N_t$). We apply an integrating factor method to Eq. (2.9). Multiplying both sides by $e^{-t\mathcal{L}}$ and then integrating on $[t_n, t_{n+1}]$, we obtain

$$\mathcal{U}_{n+1} = e^{\Delta t \mathcal{L}} \mathcal{U}_n + e^{\Delta t \mathcal{L}} \int_0^{\Delta t} e^{-\tau \mathcal{L}} \left[\mathcal{F}(\mathcal{U}(t_n + \tau)) + \mathcal{G}(t_n + \tau) \right] d\tau. \quad (2.11)$$

A family of numerical schemes can be established through different approximations of the above integral. Similar (second and even higher order) numerical schemes based on finite difference spatial discretizations for reaction-diffusion systems in Cartesian geometry are derived in [3, 6]. However, we shall consider mainly the following second order methods (in polar geometry) based on integrating factors. The reasons for doing so are presented at the end of next subsection.

- The second order explicit Adams-Bashforth scheme reads as follows

$$\mathcal{U}_{n+2} = e^{\Delta t \mathcal{L}} \left[\mathcal{U}_{n+1} + \frac{3}{2} \Delta t \left(\mathcal{F}(\mathcal{U}_{n+1}) + \mathcal{G}_{n+1} \right) \right] - \frac{1}{2} \Delta t e^{2\Delta t \mathcal{L}} \left(\mathcal{F}(\mathcal{U}_n) + \mathcal{G}_n \right). \quad (2.12)$$

- The second order backward differentiation formula (BDF) is

$$\mathcal{U}_{n+2} - \frac{2}{3}\Delta t \mathcal{F}(\mathcal{U}_{n+2}) = \frac{2}{3}\Delta t \mathcal{G}_{n+2} + \frac{4}{3}e^{\Delta t \mathcal{L}}\mathcal{U}_{n+1} - \frac{1}{3}e^{2\Delta t \mathcal{L}}\mathcal{U}_n. \quad (2.13)$$

- The trapezoidal-rule approximation of the integral leads to

$$\mathcal{U}_{n+1} - \frac{\Delta t}{2}\mathcal{F}(\mathcal{U}_{n+1}) = \frac{\Delta t}{2}\mathcal{G}_{n+1} + e^{\Delta t \mathcal{L}}\left[\mathcal{U}_n + \frac{\Delta t}{2}\left(\mathcal{F}(\mathcal{U}_n) + \mathcal{G}_n\right)\right]. \quad (2.14)$$

Schemes (2.12) and (2.13) need a starter scheme, e.g., an Euler scheme or a 2nd order Runge-Kutta scheme, but scheme (2.14) does not. All these three schemes have global temporal truncation errors $\mathcal{O}(\Delta t^2)$.

B. Absolute Stability of Semi-implicit Spectral Collocation Schemes

To analyze linear A-stability of the above integrating factor schemes, we consider the following model scalar equation

$$u_t = \lambda u + \mu u, \quad (2.15)$$

where λ is considered to be an eigenvalue of $\mathcal{L}$ and μ an eigenvalue of the Jacobian obtained from linearizing $\mathcal{F}(\mathcal{U})$ around a steady state u_0 . It is assumed that $\lambda \leq 0$.

Remark 1. The discrepancy between linear and nonlinear absolute stability of reaction-diffusion equations is briefly discussed in [3]. Further details about nonlinear absolute stability can be found in [18].

When applied to the model equations [Eq. (2.15)], the second order explicit Adams-Bashforth scheme (2.12) yields

$$u_{n+2} = e^{\lambda \Delta t} \left[u_{n+1} + \frac{3}{2}\Delta t \mu u_{n+1} \right] - e^{2\lambda \Delta t} \frac{1}{2}\Delta t \mu u_n,$$

with an auxiliary polynomial

$$\left(z^2 - e^{\lambda \Delta t} z \right) - w \left(\frac{3}{2}e^{\lambda \Delta t} z - \frac{1}{2}e^{2\lambda \Delta t} \right),$$

where $w = \mu \Delta t$. The root z of the above polynomial should stay inside the unit disk for the scheme to be A-stable. To this end, we consider the root locus curve [19] defined by

$$w = \frac{z^2 - e^{\lambda \Delta t} z}{\frac{3}{2}e^{\lambda \Delta t} z - \frac{1}{2}e^{2\lambda \Delta t}}, \quad z = e^{i\theta}, \quad \theta \in [0, 2\pi). \quad (2.16)$$

The domain of absolute stability $\mathcal{D}_a$ for this scheme consists of $w \in \mathbb{C}$ that is interior to the above closed curve. But the domain does not contain the negative complex plane $\mathbb{C}^-$, as shown in Fig. 2. Therefore, the second order integrating factor Adams-Bashforth scheme (2.12) is not A-stable.

For the 2nd order integrating factor BDF scheme (2.13), the auxiliary polynomial is

$$\left(z^2 - \frac{4}{3}e^{\lambda \Delta t} z + \frac{1}{3}e^{2\lambda \Delta t} \right) - w \frac{2}{3}z^2.$$

FIG. 2. The absolute stability domains for the 2nd order explicit Adams-Bashforth scheme (2.12) with $\lambda\Delta t = -0.01, -0.5, -1$. Each domain is bounded by the corresponding closed curve. [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

The root locus curve is described by

$$w = \frac{e^{2i\theta} - \frac{4}{3}e^{\lambda\Delta t}e^{i\theta} + \frac{1}{3}e^{2\lambda\Delta t}}{\frac{2}{3}e^{2i\theta}}, \quad \theta \in [0, 2\pi). \quad (2.17)$$

The domain of absolute stability $\mathcal{D}_a$ is the exterior of this closed curve. It is interesting to see that

$$\begin{aligned} \operatorname{Re}(w) &= \frac{3}{2} - 2e^{\lambda\Delta t} \cos \theta + \frac{1}{2}e^{2\lambda\Delta t} \cos(2\theta) \\ &= \frac{1}{2}(1 - e^{2\lambda\Delta t}) + (1 - e^{\lambda\Delta t} \cos \theta)^2 \geq 0, \end{aligned}$$

for any w on the root locus curve, since $0 < e^{\lambda\Delta t} \leq 1$. Therefore, $\mathbb{C}^- \subset \mathcal{D}_a$, as shown in Fig. 3, and the second order semi-implicit backward differentiation scheme (2.13) is A-stable.

Applying the trapezoid scheme (2.14) to the model equation [(Eq. 2.15)], we obtain

$$u_{n+1} = \frac{\Delta t}{2} \mu u_{n+1} + e^{\lambda\Delta t} \left[u_n + \frac{\Delta t}{2} \mu u_n \right]$$

with an auxiliary polynomial

$$z - e^{\lambda\Delta t} = w \left(\frac{z}{2} + \frac{e^{\lambda\Delta t}}{2} \right),$$

where $w = \mu\Delta t$ again. The root locus curve is now (see Fig. 4)

$$w = 2 \frac{z - e^{\lambda\Delta t}}{z + e^{\lambda\Delta t}} = 2 \frac{z - a}{z + a}, \quad z = e^{i\theta}, \quad \theta \in [0, 2\pi), \quad (2.18)$$

FIG. 3. The absolute stability domains for the 2nd order semi-implicit backward differentiation scheme (2.13) with $\lambda \Delta t = -0.01, -0.5, -1$. Each domain is the exterior of the corresponding closed curve. [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

where for convenience we denote $a = e^{\lambda \Delta t}$. The above fractional linear transform maps the open disk $|z| < a$ to the negative complex plane $\mathbb{C}^-$. So the semi-implicit trapezoid scheme (2.14) is A-stable.

It is known that the second order Chebyshev differentiation matrix has negative eigenvalues [20], although it is nonsymmetric. The eigenvalue with the largest magnitude is about $-0.047N^4$ [21]. The Laplacian is a positive definite operator, the eigenvalues of $\mathcal{L}$ are all real and negative. These facts combined imply that (2.9) is a strongly stiff system.

The integrating factor method can be combined with virtually any standard ODE solvers to develop numerical schemes for reaction-diffusion equations. We do not do so, since the

FIG. 4. The absolute stability domains for the 2nd order semi-implicit trapezoid scheme (2.14) with $\lambda \Delta t = -0.1, -0.5, -1$. Each domain is the exterior of the corresponding circle. [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

well-known Dahlquist second barrier [19, 22] reveals that an A-stable linear multistep method must be implicit and its order cannot exceed two. More facts along this line are

- The explicit Runge-Kutta methods are not A-stable;
- Neither the (explicit) Adams-Bashforth nor the (implicit) Adams-Moulton methods are A-stable, although the A-stability domains for the latter are slightly larger;
- The first order BDF is actually the implicit Euler method, it is A-stable but only first order accurate. The second order BDF is A-stable. The BDF with order three or higher are not A-stable;
- The trapezoidal method is an A-stable single-step second-order implicit method.

Therefore, the integrating factor 2nd order trapezoid scheme (2.14) will be our main tool for solving reaction-diffusion systems. For comparison, we also discuss two integrating factor 2nd order schemes: the explicit Adams-Bashforth scheme (2.12) and the implicit backward differentiation scheme (2.13).

III. OTHER RELATED NUMERICAL METHODS

A. Direct Spectral Collocation Methods

Besides the semi-implicit schemes discussed in the previous section, single or multiple step methods, e.g., the explicit or implicit Euler method, the implicit trapezoid method, the Runge-Kutta methods, or the Adams-Bashforth methods, can also be applied directly to the ODE system (2.9), without invoking an integrating factor. We shall consider only the following three direct schemes and compare them with the integrating factor schemes (2.12)–(2.14).

- The direct second order Adams-Bashforth scheme reads as

$$\begin{aligned} \mathcal{U}_{n+2} = & \left(\mathcal{I} + \frac{3}{2} \Delta t \mathcal{L} \right) \mathcal{U}_{n+1} + \frac{3}{2} \Delta t (\mathcal{F}(\mathcal{U}_{n+1}) + \mathcal{G}_{n+1}) \\ & - \frac{1}{2} \Delta t (\mathcal{L} \mathcal{U}_n + \mathcal{F}(\mathcal{U}_n) + \mathcal{G}_n), \end{aligned} \quad (3.1)$$

where $\mathcal{I}$ is the identity matrix with the size of $\mathcal{L}$, and $\mathcal{F}(\mathcal{U}_n), \mathcal{F}(\mathcal{U}_{n+1})$ are evaluated componentwise and pointwise. This two-step scheme needs a starter scheme.

- The direct 2nd order backward differentiation scheme is

$$\begin{aligned} & \left(\mathcal{I} - \frac{2}{3} \Delta t \mathcal{L} \right) \mathcal{U}_{n+2} - \frac{2}{3} \Delta t \mathcal{F}(\mathcal{U}_{n+2}) \\ & = \frac{2}{3} \Delta t \mathcal{G}_{n+2} + \frac{4}{3} \mathcal{U}_{n+1} - \frac{1}{3} \mathcal{U}_n. \end{aligned} \quad (3.2)$$

This is also a two-step scheme that needs a starter scheme.

- The direct trapezoid scheme reads as

$$\begin{aligned} & \left(\mathcal{I} - \frac{\Delta t}{2} \mathcal{L} \right) \mathcal{U}_{n+1} - \frac{\Delta t}{2} \mathcal{F}(\mathcal{U}_{n+1}) \\ & = \left(\mathcal{I} + \frac{\Delta t}{2} \mathcal{L} \right) \mathcal{U}_n + \frac{\Delta t}{2} \mathcal{F}(\mathcal{U}_n) + \frac{\Delta t}{2} (\mathcal{G}_{n+1} + \mathcal{G}_n). \end{aligned} \quad (3.3)$$

Notice that the nonlinear discrete system in (2.13) or (2.14) is actually a decoupled system of $(N_r - 1) \times N_\theta$ equations, one equation per grid node, since the nonlinear term $\mathcal{F}(\mathcal{U}_{n+1})$ is evaluated componentwise and pointwise. By contrast, the $(N_r - 1) \times N_\theta$ equations in (3.2) and (3.3) are coupled, due to the term $\mathcal{L}\mathcal{U}_{n+1}$. More work has to be done to solve the coupled nonlinear system in (3.2) or (3.3). However, (3.2) or (3.3) does not involve matrix exponentials, whereas (2.13) and (2.14) do. The matrix exponential $e^{\Delta t \mathcal{L}}$ or $e^{2\Delta t \mathcal{L}}$ can be precomputed though.

B. Semi-implicit Finite Difference Schemes

Semi-implicit schemes based on finite difference discretizations in the radial and angular directions can also be developed for Eq. (2.1). For ease of presentation, we consider again homogeneous Dirichlet boundary conditions on both inner and outer circles.

Let N_r, N_θ, N_t be positive integers. Let $r_a = r_0 < r_1 < \dots < r_{i-1} < r_i < \dots < r_{N_r} = r_b$ be a uniform partition in the radial direction with $h_r = (r_b - r_a)/N_r$, $\theta_j = 2\pi j/N_\theta, 0 \leq j \leq N_\theta$ a uniform partition in the angular direction with $h_\theta = 2\pi/N_\theta$, and $t_n = n\Delta t (0 \leq n \leq N_t)$ a uniform partition of $[0, T]$ with $\Delta t = T/N_t$.

For simplicity of presentation, we consider a scalar reaction-diffusion equation. For the finite difference spatial discretizations, we still have

$$\Delta u \approx \mathbf{A}_2 \mathbf{U} + \mathbf{R}^{-1} \mathbf{A}_1 \mathbf{U} + \mathbf{R}^{-2} \mathbf{U} \mathbf{B},$$

but now $\mathbf{A}_1, \mathbf{A}_2, \mathbf{B}$ are completely different. To be specific, we have

$$\mathbf{A}_1 = \frac{1}{2h_r} \begin{bmatrix} 0 & 1 & & \\ -1 & 0 & 1 & \\ \cdots & \cdots & \cdots & \cdots \\ & -1 & 0 & 1 \\ & & -1 & 0 \end{bmatrix}, \quad \mathbf{A}_2 = \frac{1}{h_r^2} \begin{bmatrix} -2 & 1 & & \\ 1 & -2 & 1 & \\ \cdots & \cdots & \cdots & \cdots \\ & 1 & -2 & 1 \\ & & 1 & -2 \end{bmatrix}, \quad (3.4)$$

and

$$\mathbf{B} = \frac{1}{h_\theta^2} \begin{bmatrix} -2 & 1 & & & 1 \\ 1 & -2 & 1 & & \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ & & 1 & -2 & 1 \\ 1 & & & 1 & -2 \end{bmatrix}. \quad (3.5)$$

Here $\mathbf{A}_1$ and $\mathbf{A}_2$ are $(N_r - 1) \times (N_r - 1)$ matrices, $\mathbf{B}$ is an $N_\theta \times N_\theta$ matrix. The diagonal matrix $\mathbf{R}$ has the same form (2.6), but the nodes r_i are uniformly distributed. Similar finite difference schemes for the Cartesian geometry can be found in [3, 6]. Finite difference approximations based on nonuniform grids are possible but significantly more complicated. They are not discussed in this paper.

One can repeat the numerical schemes (2.12)–(2.14) for the above finite difference discretizations, the only change is to replace the spectral differentiation matrices in (2.5) and (2.7) by the finite difference matrices in (3.4) and (3.5). The overall errors of the semi-implicit finite difference schemes are $\mathcal{O}(h_r^2 + h_\theta^2 + \Delta t^2)$, when $h_r, h_\theta, \Delta t$ are small enough.

TABLE I. Abbreviations for the numerical schemes tested.

IF	With integrating factors (semi-implicit)
AB	Adams-Bashforth temporal discretization
BD	Backward differentiation temporal discretization
TZ	Trapezoid temporal discretization
2	2nd order in time (by design)
FD	Finite difference spatial discretization
SC	Spectral collocation spatial discretization

IV. IMPLEMENTATION ISSUES AND NUMERICAL EXPERIMENTS

In this section, we present numerical experiments on three examples to demonstrate the strength of our numerical schemes. Implementation strategies on how to enforce more complicated boundary conditions are also discussed.

The Chebyshev and Fourier differentiation matrices can be generated using the algorithms discussed in [10]. Our semi-implicit numerical schemes (2.12) – (2.14) rely on matrix exponentials of the discrete Laplacian in polar coordinates. Among the algorithms for computing matrix exponentials, the scaling and squaring algorithm based on a Padé approximation [23, 24] is widely used and has been implemented in Matlab (function `expm`). For the spectral collocation spatial discretization, the exponential matrices are small, although dense, and can be precomputed before the time-stepping iterations in our numerical schemes.

For convenience, we abbreviate the numerical schemes as described in Table I. In the following three numerical examples, we use

$$\log_2 \frac{E(2\Delta t)}{E(\Delta t)}$$

to measure temporal convergence rates, where $E(\Delta t)$, $E(2\Delta t)$ are respectively the errors when time steps Δt and $2\Delta t$ are used.

Example 1. (A 2-Species Nonlinear System). We consider a 2-species nonlinear system

$$\begin{cases} (u_1)_t = D\Delta u_1 + f_1(u_1, u_2) + g_1(r, \theta, t), \\ (u_2)_t = D\Delta u_2 + f_2(u_1, u_2) + g_2(r, \theta, t) \end{cases}$$

on the annulus $\Omega = \{(r, \theta) : r \in [1, 2], \theta \in [0, 2\pi)\}$ during a finite time period $[0, T]$. Homogeneous Dirichlet boundary conditions are imposed on both inner and outer circles

$$u_1|_{r=1} = u_1|_{r=2} = u_2|_{r=1} = u_2|_{r=2} = 0, \quad \forall t \in (0, T].$$

An exact solution is specified as

$$\begin{cases} u_1(r, \theta, t) = (C_1 e^{\alpha t} + C_2 e^{\delta t}) \ln((r-1)(2-r)+1), \\ u_2(r, \theta, t) = C_3 e^{\alpha t} \ln((r-1)(2-r)+1). \end{cases}$$

The reaction terms are

$$\begin{cases} f_1(u_1, u_2) = \alpha u_1 + \beta u_2, \\ f_2(u_1, u_2) = \gamma u_1 + \delta(u_2 - u_2^3). \end{cases}$$

TABLE II. Example 1: Errors $\|u(\cdot, \cdot, T) - U_{N_r}(\cdot, \cdot)\|_{l^\infty}$ and convergence rates in Δt for the Adam-Bashforth and trapezoid schemes (with and without an integrating factor): $N_r = 31, T = 1$.

$T/\Delta t$	IF.AB2.SC	rate	AB2.SC	rate	IF.TZ2.SC	rate	TZ2.SC	rate
50	NaN	US	NaN	US	6.2673E-3	–	5.0391E-2	–
100	1.6309E-3	–	NaN	US	1.6409E-3	1.93	1.8184E-3	–
200	4.1281E-4	1.98	7.4528E-1	–	4.1529E-4	1.98	4.1758E-4	2.12
400	1.0356E-4	1.99	1.0353E-4	–	1.0418E-4	1.99	1.0421E-4	2.00
800	2.5944E-5	1.99	2.5939E-5	1.99	2.6100E-5	1.99	2.6105E-5	1.99
1600	6.5220E-6	1.99	6.5206E-6	1.99	6.5608E-6	1.99	6.5622E-6	1.99

Here “NaN” stands for “Not a Number” and “US” for “unstable”.

The source terms $g_i(r, \theta, t), i = 1, 2$ and initial conditions are derived accordingly.

In numerical runs, we set $T = 1, D = 10^{-3}, \alpha = -0.1, \beta = 0, \gamma = 10, \delta = -100, C_1 = 1, C_2 = 0.1, C_3 = 1$. For the nonlinear reaction terms, the Jacobian matrix of the linearization is

$$\begin{bmatrix} \alpha & \beta \\ \gamma & \delta \end{bmatrix} = \begin{bmatrix} -0.1 & 0 \\ 1 & -100 \end{bmatrix},$$

which has two negative eigenvalues $\mu_{\min} = -100, \mu_{\max} = -0.1$. The reaction stiffness ratio [18] is 1000. We set $N_\theta = 2$ for an angular discretization, since the problem is independent of θ . A choice of $N_r = 31$ is fine enough for a radial discretization, so that temporal errors dominate and are relatively easy to measure. For $N_r = 31$, all eigenvalues of $\mathcal{L}$ are negative. In particular, the smallest and largest eigenvalues are $\lambda_{\min} \approx -175.9, \lambda_{\max} = -0.0887$. The diffusion stiffness ratio is about 1983. This problem is strongly stiff in both diffusion and reaction. We want to point out that diffusion stiffness results from a numerical discretization of the Laplacian operator, while reaction stiffness is mainly due to different reaction rates.

As shown in Table II, the Adams-Bashforth schemes (with and without the integrating factor) are not A-stable and their numerical solutions blow up for larger time steps. The integrating factor improves stability and allows relatively large time steps. The trapezoidal schemes (with and without the integrating factor) are both A-stable. Even though their numerical errors are comparable, the integrating factor trapezoidal scheme (2.14) has advantages in solving decoupled nonlinear systems of just order two at the grid points. For the direct trapezoidal scheme (3.3), one has to solve a nonlinear system of size $(N_r - 1) \times N_\theta \times 2$ that is coupled on the whole spatial mesh. The integrating factor decouples nonlinearity to each grid point.

For the trapezoidal schemes IF.TZ2.SC and TZ2.SC, we employ the Newton’s method with 10 iterations for solving the order 2 nonlinear systems at individual grid points. An implication of the 2nd order convergence of the Newton’s method is that the number of significant digits approximately doubles after each iteration. Ten iterations will be enough for reaching machine precision for most problems. Certainly, more sophisticated criteria can be set and checked to avoid unnecessary iterations if one solves large size nonlinear systems. Here the integrating factor decouples nonlinearity to individual nodes and we solve an order two nonlinear system at each node. It is more efficient to use a fixed number of iterations in this case.

Example 2. (More on Boundary Conditions). In this example, we show how to handle more complicated boundary conditions. The domain is again the annulus $\Omega = \{(r, \theta) : r \in [1, 2], \theta \in [0, 2\pi)\}$. The reaction term is linear, $f(u) = \alpha u$, and the exact solution is specified as

$$u(r, \theta, t) = e^{\beta t}(e^{r-1} - r)$$

with $\beta < 0$. The source term is computed accordingly

$$g(r, \theta, t) = (\beta - \alpha)e^{\beta t}(e^{r-1} - r) - De^{\beta t}(e^{r-1} + r^{-1}(e^{r-1} - 1)).$$

A no-flux (Neumann) condition is imposed on the inner circle, whereas a time-dependent nonhomogeneous Dirichlet condition is specified on the outer circle:

$$\frac{\partial u}{\partial r} \Big|_{r=1} = 0, \quad u|_{r=2} = e^{\beta t}(e - 2), \quad \forall t \in (0, T].$$

To close the system, an initial condition is specified as

$$u(r, \theta, 0) = e^{r-1} - r, \quad \forall (r, \theta) \in \Omega.$$

Remark 2. When modeling protein trafficking inside live cells, a no-flux condition is needed to ensure that no proteins penetrate the inner boundary of the cytoplasm back to the nucleus.

For this problem, the unknowns

$$\mathbf{U} = \mathbf{U}(t) = \left[U(r_i, \theta_j, t) \right]_{(N_r+1) \times N_\theta}$$

are defined for all grid points. In (2.5), we use the unmodified $(N_r + 1) \times (N_r + 1)$ first and second order Chebyshev differentiation matrices $\mathbf{A}_1$ and $\mathbf{A}_2$ that involve no boundary conditions [10]. For the Chebyshev spectral collocation method, nodes are labeled backwards (from 1 to -1 , for the reference interval $[-1, 1]$). Since the 1st order radial derivative of the unknown function vanishes on the inner circle for any θ_j , $1 \leq j \leq N_\theta$, we have

$$0 = \sum_{k=0}^{N_r-1} \mathbf{A}_1(N_r, k) \mathbf{U}_{n+1}(k, j) + \mathbf{A}_1(N_r, N_r) \mathbf{U}_{n+1}(N_r, j),$$

which implies that

$$\mathbf{U}_{n+1}(N_r, j) = - \sum_{k=0}^{N_r-1} \frac{\mathbf{A}_1(N_r, k)}{\mathbf{A}_1(N_r, N_r)} \mathbf{U}_{n+1}(k, j).$$

But due to the Dirichlet boundary condition at $r = 2$, $\mathbf{U}_{n+1}(1, j)$, $\forall j \in \{1, \dots, N_\theta\}$ is known. For scheme (2.14), our Matlab implementation of the above boundary conditions reads

```

...
BCN = (-1/A1(Nr+1,Nr+1))*A1(Nr+1,1:Nr);
...
Un1(1,:) = exp(beta*tn1)*(exp(1)-2);
Un1(Nr+1,:) = BCN*Un1(1:Nr,:);
...

```

where $\mathbf{Un1}$ is the matrix of unknowns at all grid points for the new time step $\mathbf{tn1}$. For schemes (2.12) and (2.13), one only needs to replace $\mathbf{tn1}$ by $\mathbf{tn2}$.

In numerical runs, we take $D = 10^{-4}$, $\alpha = 1$, $\beta = -0.1$, $T = 1$. We also set $N_\theta = 2$, since the problem is independent of θ . The errors at the grid points measured in the discrete max norm for

TABLE III. Example 2: Errors $\|u(\cdot, \cdot, T) - \mathbf{U}_{N_r}(\cdot, \cdot)\|_{l^\infty}$ and convergence rates in Δt for schemes (2.12)–(2.14) with $N_r = 10, T = 1$.

Δt	IF . AB2 . SC	Rate	IF . BD2 . SC	Rate	IF . TZ2 . SC	Rate
1/100	7.700E-7	–	1.239E-6	–	8.749E-9	–
1/200	1.927E-7	1.998	3.122E-7	1.989	2.186E-9	2.000
1/400	4.821E-8	1.999	7.835E-8	1.994	5.465E-10	2.000
1/800	1.205E-8	1.999	1.962E-8	1.997	1.366E-10	1.999
1/1600	3.015E-9	1.999	4.911E-9	1.998	3.419E-11	1.998

all three integrating factor schemes (2.12)–(2.14) are listed in Table III. A second order convergence rate $\mathcal{O}(\Delta t^2)$ is clearly exhibited for all three schemes. With only 11 grid points in the radial direction, all three schemes produce fairly accurate numerical solutions. One can also observe that the errors from the trapezoid scheme are smaller than those of the Adams-Bashforth and backward differentiation schemes.

The integrating factor Adams-Bashforth and backward differentiation schemes (2.12) and (2.13) maintain a second order convergence rate, even though the explicit Euler method is used as a starter scheme. Clearly, one can use the second order Runge-Kutta method as a starter scheme to improve the overall errors. Here we use the explicit Euler method instead in order to verify that a first order starter scheme does not affect the second order convergence of the above two 2-step schemes.

Example 3. (A Nonlinear Equation. Comparison with Finite Difference Methods). As previously discussed, one could apply finite differences or spectral collocations for the spatial discretization. The following example shows that for certain problems, especially the ones with boundary layers, the performance of the spectral collocation method is superior.

We consider an annulus $\Omega = \{(r, \theta) : r \in [1, 3], \theta \in [0, 2\pi)\}$ and a time period $[0, T] = [0, 1]$. The reaction-diffusion equation has a nonlinear reaction $f(u) = u - u^3$ and a constant diffusion $D > 0$. An exact solution is specified as

$$u(r, \theta, t) = e^{\beta t} (1 - (r - 2)^{2p}) (\sin(q\theta) + 1),$$

where $\beta < 0$ is a small constant depicting temporal decay and $p > 0$ is a parameter characterizing steepness of the solution near the inner and outer circular boundaries. Steep boundary layers in the exact solution near the inner and outer boundaries can be observed in Fig. 5. The source term and initial condition are derived accordingly. Homogeneous Dirichlet boundary conditions are imposed.

In numerical runs, the parameters are set as $D = 10^{-3}, \beta = -0.2, p = 5, q = 1$. Four integrating factor schemes were tested: the 2nd order Adams-Bashforth or the trapezoid rule for temporal discretizations; finite differences or spectral collocations for spatial discretizations. Namely, IF . AB2 . FD, IF . AB2 . SC, IF . TZ2 . FD, and IF . TZ2 . SC, see Table I for abbreviations. For the trapezoid schemes, the Newton's method with 10 iterations was employed to solve a nonlinear scalar equation at each grid point.

As observed in Fig. 6 and Table IV, the spectral collocation methods are fairly accurate for $N_r = 31, N_\theta = 4$. Both the Adams-Bashforth and the trapezoidal schemes exhibit a second order convergence in time. However, for the finite difference discretizations, $N_r = 31$ is not fine enough to resolve the radial steep fronts, and the numerical errors are not convergent for small time steps. With an increase to $N_r = 301$ (see Table V), there are some improvements in accuracy initially

FIG. 5. Example 3: Boundary layers near the inner circle $r = 1$ and the outer circle $r = 3$ exhibited in the exact solution (at the final time $T = 1$). [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

FIG. 6. Example 3: Left: Errors of finite differences vs spectral collocations for $N_r = 31$; Right: Errors of finite differences for $N_r = 31$ vs $N_r = 301$. [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

TABLE IV. Example 3: Comparison of numerical schemes with finite difference or spectral collocation spatial discretizations.

$T/\Delta t$	IF . AB2 . FD	Rate	IF . TZ2 . FD	Rate	IF . AB2 . SC	Rate	IF . TZ2 . SC	Rate
10	1.3170E-3	—	1.2326E-3	—	2.7213E-3	—	3.0083E-3	—
20	1.2532E-3	0.07	1.2320E-3	0.00	1.5256E-3	0.83	8.6854E-4	1.79
40	1.2372E-3	0.01	1.2318E-3	0.00	6.4087E-4	1.25	2.2723E-4	1.93
80	1.2331E-3	0.00	1.2318E-3	0.00	2.1360E-4	1.58	5.7504E-5	1.98
160	1.2321E-3	0.00	1.2318E-3	0.00	6.2049E-5	1.78	1.4420E-5	1.99
320	1.2319E-3	0.00	1.2318E-3	0.00	1.6744E-5	1.88	3.6079E-6	1.99
640	1.2318E-3	0.00	1.2318E-3	0.00	4.3507E-6	1.94	9.0216E-7	1.99
1280	1.2318E-3	0.00	1.2318E-3	0.00	1.1089E-6	1.97	2.2555E-7	1.99

Errors $\|u(\cdot, \cdot, T) - \mathbf{U}_{N_t}(\cdot, \cdot)\|_{l^\infty}$ and convergence rates in Δt for $N_r = 31, N_\theta = 4$.

(for $\Delta t = 1/10, 1/20, 1/40$), for the numerical solutions obtained from finite differences. But temporal errors are still subordinate for small time steps ($\Delta t < 1/40$). Further refining spatial discretizations will result in significant increase of computational costs. In this regard, compact finite difference schemes [6] are needed, even though such schemes in polar coordinates are not straightforward. Another approach will be adaptive finite difference spatial discretizations. For the spectral collocation methods, compact schemes are also possible and helpful, but not really needed, since the sizes of the spatial discretization matrices $\mathbf{A}_1, \mathbf{A}_2, \mathbf{B}$ are relatively small.

The spatial discretization matrices $\mathbf{A}_1, \mathbf{A}_2, \mathbf{B}$ are sparse for finite differences but dense for spectral collocations. However, in the integrating factor schemes, $e^{\Delta t \mathcal{L}}, e^{2\Delta t \mathcal{L}}$ will be dense anyway for either finite differences or spectral collocations. There will be no significant differences in computational costs, while accuracies of numerical solutions could be quite different, as shown in this example.

V. DISCUSSION AND CONCLUDING REMARKS

In this paper, we have developed a family of semi-implicit numerical schemes for stiff reaction-diffusion equations on annuli. Among them, the integrating factor trapezoidal scheme (2.14) based on spatial spectral collocations has proven to be very reliable due to its A-stability and small discretization and truncation errors. Compact schemes for stiff reaction-diffusion equations in Cartesian coordinates have been investigated by [6] and shown to be very efficient in terms of computational costs (storage and operations count). For reaction-diffusion equations on polar domains, developing compact schemes is possible but not straightforward.

TABLE V. Example 3: Numerical results of finite difference schemes.

$T/\Delta t$	IF . AB2 . FD	Rate	IF . TZ2 . FD	Rate
10	2.721257E-3	—	2.328785E-3	—
20	1.304860E-3	1.06	6.724436E-4	1.79
40	5.175824E-4	1.33	1.837373E-4	1.87
80	1.837168E-4	1.49	1.837241E-4	0.00
160	1.837189E-4	0.00	1.837208E-4	0.00
320	1.837195E-4	0.00	1.837199E-4	0.00
640	1.837196E-4	0.00	1.837197E-4	0.00
1280	1.837197E-4	0.00	1.837197E-4	0.00

Errors $\|u(\cdot, \cdot, T) - \mathbf{U}_{N_t}(\cdot, \cdot)\|_{l^\infty}$ and convergence rates in Δt for $N_r = 301, N_\theta = 4$.

As demonstrated by the numerical experiments presented in this paper, spectral spatial discretizations can provide accurate results with relatively few collocation nodes. The clustering of Chebyshev nodes near boundaries offers needed spatial resolution for resolving various types of boundary conditions, particularly those which give rise to boundary layers.

Integrating factors allow us to efficiently resolve behaviors on different time scales. Numerical difficulties arising due to stiffness are endemic amongst reaction-diffusion problems. The use of integrating factors enables time step sizes to be adjusted more flexibly and future work will address the use of *a posteriori* error estimates and adaptive time-stepping.

Improved models of cellular processes will ultimately require the solution of reaction-diffusion equations in general three-dimensional domains. Even the first step, namely solving reaction-diffusion equations on spherical annuli, remains a challenging computational task. Numerical methods based on spherical harmonic functions [1] or double Fourier series [25] require expensive transforms between the physical and spectral spaces, and treating the nonlinear reaction term using a double Fourier series method can be complicated. More efficient numerical methods need to be developed. This is currently under investigation and will be reported in our future work.

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