

Smoothing Schemes for the System of Advection–Diffusion–Reaction Equations & Applications

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Abstract

There has been a resurgence of work in modeling and computational analysis for advection-diffusion-reaction phenomenon since the mid 1980's. Many new applications & models have been discovered, which use parabolic partial differential equations (PDE) under initial, boundary, or forcing conditions with irregularities. New computational techniques must be developed, both on serial & parallel. We focus now on computational difficulties with irregular initial or boundary data or forcing terms.

Abstract...

Computing accurate approximations under conditions of large advection or when there are significantly different diffusion parameters also presents difficulties. The problem is that high frequencies are amplified in the error - and usually, numerical schemes and their theory are designed for sufficient regularity; computational experiments indicate major problems to achieve accuracy. Moreover, “high frequency” depends a lot on the relative interplay between the mesh sizes and advection & diffusion rates.

Abstract...

We will discuss initial damping schemes for linear homogeneous and inhomogeneous as well as semilinear parabolic problems with nonsmooth data. A new family of parallel Padé schemes is developed for high accuracy and robust performance. Up-to-date applications arise naturally in atmospheric science, computer graphic imaging, electrochemistry, financial engineering, mathematical biology, combustion, pattern formation, and environmental science.

Computational Difficulties

- *Advection* (first order spatial derivatives)- could be large compared with diffusion;
- *Diffusion* (second order spatial derivatives), *widely varying diffusion coefficients*;
- *Reaction* term non-smooth;
- *Low regularity* for initial or boundary data, incompatibility in boundary data- spurious oscillations are amplified.

Typical PDE System

$$\frac{\partial u}{\partial t} + \vec{v} \cdot \nabla u = D \nabla^2 u + f(t, u)$$

u = vector of reactants (or species, temperature ...)

D = Matrix of Diffusivities- often widely varying

\vec{v} = drift velocity ($\vec{v} \cdot \nabla u =$ convection flux)

f = nonlinear reaction kinetics

→ Initial data is not smooth

& there are irregularities in f or boundary data

& widely different diffusivities

& relatively large advection

Applications & PDE Models

- Turing System, A. Turing (1952). "A Chemical Basis for Morphogenesis." To model patterns in nature. Turing's only paper on the subject- was totally ignored until the 1980's.
- P. Gray & S.K. Scott (1983, 1985). Sustained oscillations and exotic patterns in isothermal chemical reactions with feedback. Many applications to pattern formation in biology, as well. Shows a surprising variety of patterns. There are stationary states, sustained oscillations and chaotic behavior.

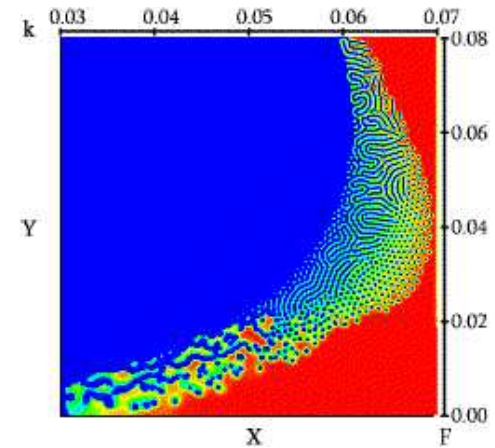
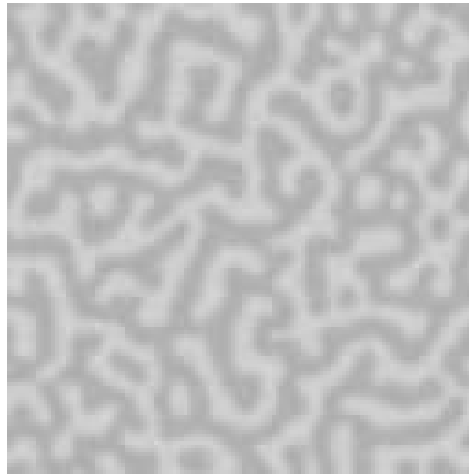
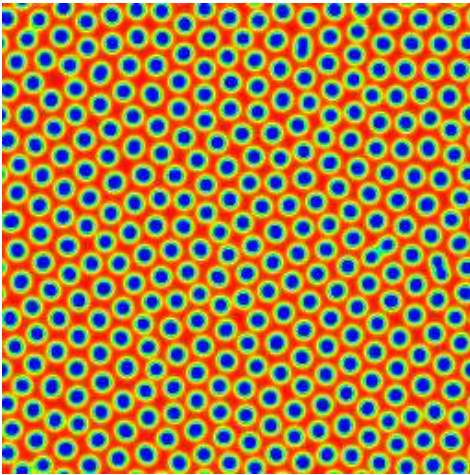
An Example with Gray-Scott

Gray-Scott System

$$\begin{aligned}u_t &= D_u \nabla^2 u - uv^2 + F(1 - u) \\v_t &= D_v \nabla^2 v + uv^2 - (F + k)v\end{aligned}$$

Models an autocatalytic reaction $U + 2V \rightarrow 3V$; in-flow of U with rate A , out-flow of V with rate B ($B > A$ means additional reaction $V \rightarrow$ inert product). A typical range of diffusivity is $D_u = 2 \times 10^{-5}$ and $D_v = 10^5$, with F and k being control parameters.

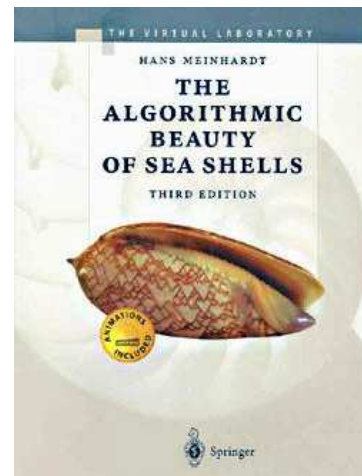
Some Gray-Scott patterns:



Spots or stripes (u, v graphs, left and center) occur only for parameter values in the red region of parameter space (right).

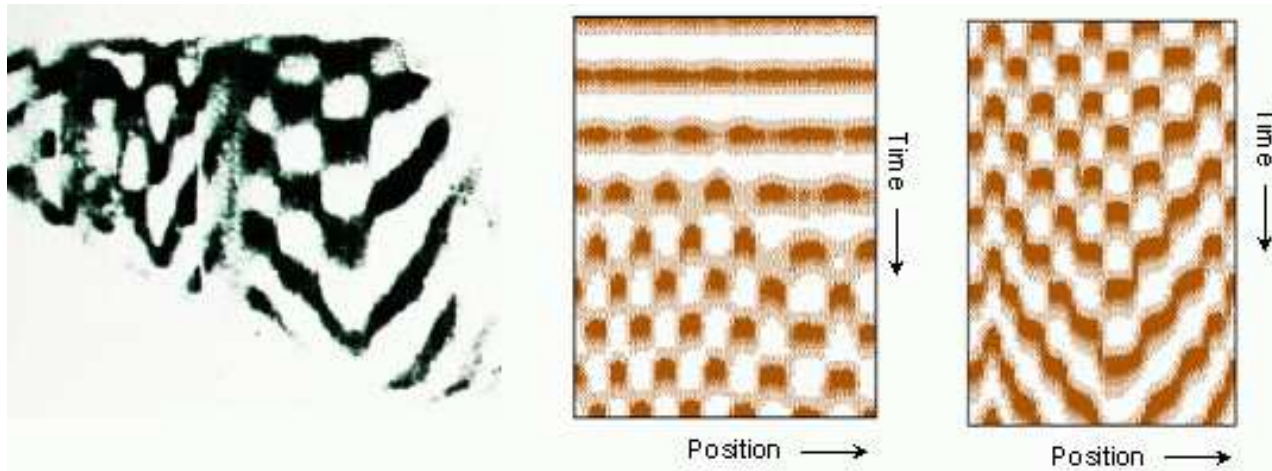
Applications...Sea Shells

- H. Meinhardt (1995). "The Algorithmic Beauty of Sea Shells", Springer-Verlag. Contains parabolic reaction-diffusion systems of PDE modeling pattern formation in sea shells with realistic data. These models are a bit different from Gray-Scott.



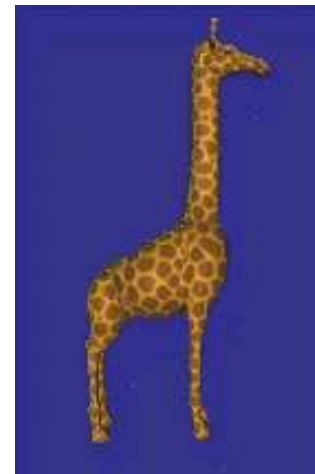
Applications...Sea Shells

A Meinhardt Pattern:



Applications...Computer Animation

- Computer Graphics- simulation of animals- e.g. spots and stripes and realistic looking textures (G. Turk, Computer Graphics 1991). The relatively good success of solving these equations and playing with the control parameters to simulate nature's pattern.



Other Applications...Chemistry

- FitzHugh-Nagumo Equation. A standard simple example from mathematical biology, typically neuron and cardiac modeling.
- Of course, the Belousov - Zhabotinsky chemical reaction: Provided one of the earliest experimental demonstrations of self-organizing process.
- Combustion Modelling. Strong singularities in forcing term. Can be extremely difficult due to highly singular aspects of the models.

Electrochemical Kinetics

- Mixed diffusion coupled with homogeneous reactions and convection.

“Complicated boundary conditions are typical for electrochemical kinetic simulations... most of the electrode reactions involve at least two reactants of variable concentrations that need to be included in the model equations... electrochemical transient methods consist in applying various time-dependent polarization impulses to the electrodes.”

Electrochemical Kinetics...

- “... Electrochemical initial boundary value problems often involve initial conditions that are inconsistent with the boundary conditions... A similar difficulty also arises if temporal discontinuities in the boundary conditions occur at later times, as for example in the case of double or cyclic potential step transients.” (L.K. Bieniasz & C. Bureau, *Electroanalytical Chem.*, 2000)
- Next slide: Contains an example of a system of PDE modeling in Electrochemical Kinetics...

Electrochemical Kinetics

Nonlinear Reaction

$$\begin{aligned}\frac{\partial c_M}{\partial t} &= \frac{\partial^2 c_M}{\partial x^2} - \kappa_p c_M c_{P_2} - \kappa_p c_M c_{P_1}, \\ \frac{\partial c_{MR}}{\partial t} &= \frac{\partial^2 c_{MR}}{\partial x^2} - 2(\kappa_p/\xi) c_{MR}^2, \\ \frac{\partial c_{P_0}}{\partial t} &= \frac{\partial^2 c_{P_0}}{\partial x^2} + (\kappa_p/\gamma) c_{P_1}, \\ \frac{\partial c_{P_1}}{\partial t} &= \frac{\partial^2 c_{P_1}}{\partial x^2} + \kappa_p c_M c_{P_1} - (\kappa_p/\gamma) c_{P_1} + (\kappa_p/\gamma) c_{P_2}, \\ \frac{\partial c_{P_2}}{\partial t} &= \frac{\partial^2 c_{P_2}}{\partial x^2} + (\kappa_p/\xi) c_{MR}^2 + \kappa_p c_M c_{P_2} - (\kappa_p/\gamma) c_{P_2},\end{aligned}$$

Atmospheric Transport of Chemical Species...

- Chemical species in the troposphere: a phenomenon that can involve chemical kinetics, diffusion, and advection with many species, giving rise to very difficult numerical problems. Specific computational challenges include: 1) large spatial regions, 2) huge variations in time scales, and 3) nonlinear systems of reaction-diffusion-advection equations, which to date do not have highly developed computational or theoretical analysis.

Atmospheric Science...

- Air quality studies: For example, Sandu, Verwer, Blom, Spee and Carmichael (Atm. Env., 1997) work with nonlinear reaction-diffusion systems for atmospheric chemical reaction modeling and give an example of 45 chemical reactions between 17 species. Discontinuities arise in the derivatives of the solution and the solver must cover a large range of reaction times. Others deal with models for photochemical dispersion to enhance the understanding of chemical composition of the atmosphere.

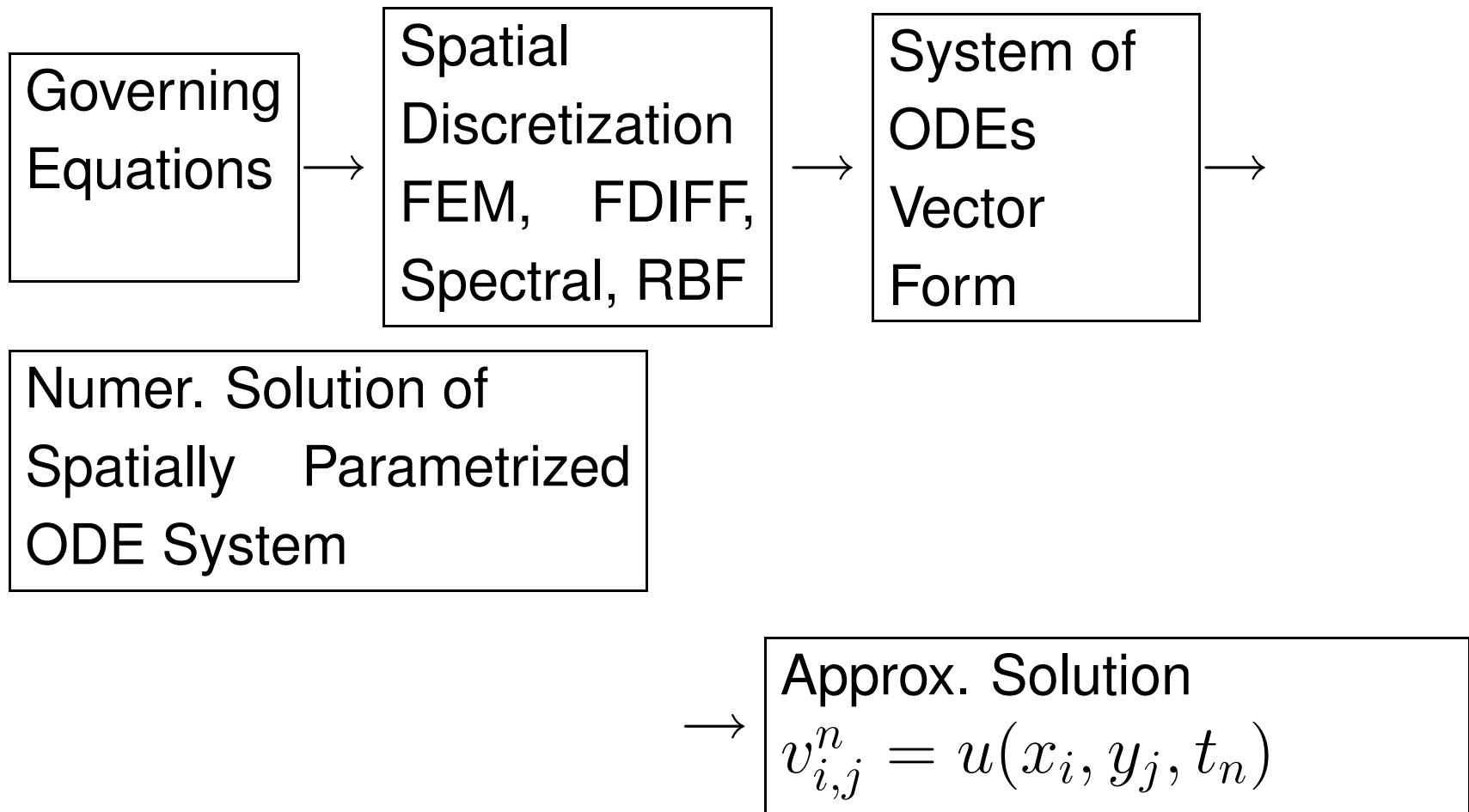
Applications...Chemical Kinetics

- Slepchenko, Schaff and Choi (J. Comp. Phys., 2000) present a problem of a biochemical processes involving Calcium oscillations and Calcium buffering, with applications to cell dynamics and drug absorption. The physical phenomena involved include chemical kinetics, membrane fluxes and diffusion, as well as nonlinear reaction-diffusion systems with large variation in diffusion rates.
- Zhornitskaya and Bertozzi (SIAM J. Numerical Analysis, 2000) treat the problem of numerical simulation of lubrication–type equations for thin liquid films and fluid interfaces driven by surface tension.

Applications...Fluid Drop Simulation

- Patzek, Basaran, Benner (*J. Comp. Phys.*, 1991 & 1995) examine the problem of fluid drops in free space with an eye on applications to containerless material processing in ultralow gravity or modeling of ink drops, etc.
- Various approaches in advection-reaction-diffusion equations for free boundary problems can be found in models of fluid droplets: e.g. fluid filaments, ink jet printing simulation, fiber spinning and control of flow for kevlar, lycra, or fiber-optic materials.

Scheme Overview - MOL



Padé Approximations of Matrix Exponentials

Introduction

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- Parabolic PDE have a smoothing property, where for positive time the solution is infinitely differentiable even if the initial data is nonsmooth.
- Numerical schemes used to solve these equations are also expected to have an analogous smoothing property i.e., optimal order convergence with nonsmooth data.
- Nonsmooth data can appear in the form of initial data that is only in $L_2(\Omega)$ or $H_s(\Omega)$ for low s ; it can occur from mismatched initial and boundary conditions.

The Luskin-Rannacher and Rannacher Schemes

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- Higher order schemes (Rannacher (1984)): $2m$ steps of $(m - 1, m)$ -Padé at the start, followed by diagonal (m, m) -Padé. This theoretically gives $2m^{th}$ order accuracy.
- The original Luskin-Rannacher and Rannacher damping schemes (1982-1984) indeed work fine in general, but lack robustness under difficult conditions. Numerical experiments have been weak; this problem has not been known at all until recently.

Our New Family of Schemes...

Homogeneous Case

- Inversion of higher order matrix polynomials has been a major problem for higher order schemes due to ill-conditioned systems. We introduce methods based on partial fraction decomposition of matrix rational functions for both parallel computation and better serial computation.

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- Our new family of schemes is the same as Luskin-Rannacher for Crank-Nicolson (order 1). It differs in the Padé initial damping scheme in higher order versions.

The New Schemes...

Homogeneous Case

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- We change the damping schemes from $2m$ steps of $(m - 1, m)$ -Padé to only 2 steps (independent of m) of $(0, 2m - 1)$ -Padé.
- The Luskin-Rannacher results have been dormant, essentially only touched on theoretically in papers by A. Hansbo in 1999 and Khaliq and Wade in 2001. The original authors did only basic numerics and missed the subtlety in the practical performance.

The New Schemes...

Homogeneous Case

- The Rannacher convergence result gives only theoretical error estimates, but does not guarantee elimination of oscillations. Such problems indeed are observed for more difficult problems (not actually tested by Rannacher). For some sizes or combinations parameter values (depending also on the step sizes) the error can be totally swamped by spurious oscillations.

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- It is especially difficult to deal with systems that have widely varying diffusions due to multiple scales. The result is bad performance for mid-range step sizes.

The New Schemes...

Homogeneous Case

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- Two interesting developments, (i) Positivity and (ii) Efficient splitting of Padé schemes have occurred in the past decade.
- The notion of a positive scheme is a refinement of L_0 -stability. A positive scheme (for test equation $y' + \lambda y = 0$) has a positive symbol on the positive real axis and is monotonely decreasing to 0. It should be a good approximation to $e^{-\lambda}$, which represents the amplification factor per time step on this simple test equation.

The New Schemes...

Homogeneous Case

- Gallopoulos and Saad (1988) and Khaliq, Twizell and Voss (1993) showed that higher diagonal Padé schemes can be implemented as solving several well-conditioned backward Euler type problems (in parallel). Even in serial, there is a significant advantage.

The New Schemes...

Homogeneous Case

- Gallopoulos and Saad (1988) and Khaliq, Twizell and Voss (1993) showed that higher diagonal Padé schemes can be implemented as solving several well-conditioned backward Euler type problems (in parallel). Even in serial, there is a significant advantage.
- The new family utilizes diagonal Padé schemes damped initially by positivity-preserving $(0, 2m - 1)$ -Padé schemes, which have better shaped approximations to $e^{-\lambda}$. (See graph next.)

Graph of Symbols— Positivity

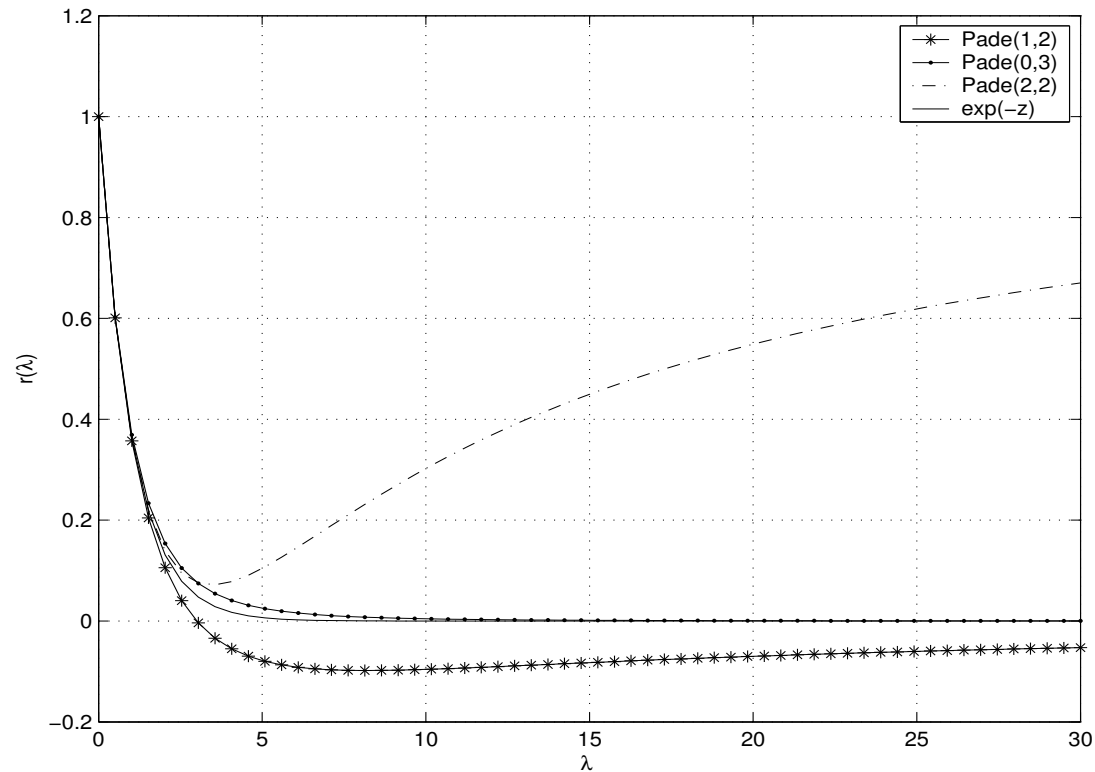


Figure 1: Amplification symbols $\{(\lambda, r(\lambda)) : \lambda \geq 0\}$ to design fourth order schemes.

The Abstract PDE...

General Set-Up

Consider the initial value problem

$$\begin{aligned}u_t + Au &= f \quad \text{in } \Omega, \quad t \in (0, \bar{t}] = J, \\u &= v \quad \text{on } \partial\Omega, \quad t \in J, \quad u(\cdot, 0) = v \quad \text{in } \Omega,\end{aligned}$$

Ω is a bounded domain in \mathbf{R}^d with lipschitz boundary and

$$A := - \sum_{j,k=1}^d \frac{\partial}{\partial x_j} \left(a_{j,k}(x) \frac{\partial}{\partial x_k} \right) + \sum_{j=1}^d b_j(x) \frac{\partial}{\partial x_j} + b_0(x)$$

Standard Assumptions

1. $a_{j,k}$, b_j , and b_0 are to be C^∞ functions on $\bar{\Omega}$,
 $a_{j,k} = a_{k,j}$, $b_0 \geq 0$ and

$$\sum_{j,k=1}^d a_{j,k} \xi_j \xi_k \geq c_0 |\xi|^2, \text{ with } c_0 > 0, \text{ on } \bar{\Omega}, \forall \xi \in \mathbf{R}^d.$$

2. $-A$ is the inf. generator of a unif. bdd., strongly continuous, analytic semigroup $\{e^{-tA}\}_{t \geq 0}$ which is the solution operator for the homogeneous part.

Padé Schemes...

1. Use (m, n) –Padé approximation for e^{-z} .

$R_{m,n}(z) := P_{m,n}(z)/Q_{m,n}(z)$, where

$$P_{m,n}(z) = \sum_{j=0}^m \frac{(m+n-j)!m!}{(m+n)!j!(m-j)!} (-z)^j,$$

and $Q_{m,n}(z) = \sum_{j=0}^n \frac{(m+n-j)!n!}{(m+n)!j!(n-j)!} (z)^j.$

Padé Schemes... Cases of Interest

- $R_{m,n}(z) = e^{-z} + O(|z|^{m+n+1})$ as $z \rightarrow 0$.
- Backward Euler, $R_{0,1}(z) = (1 + z)^{-1}$;
Crank-Nicolson, $R_{1,1}(z) = (1 - \frac{1}{2}z)(1 + \frac{1}{2}z)^{-1}$.
- $R_{1,2}(z) = (1 - \frac{1}{3}z)(1 + \frac{2}{3}z + \frac{1}{6}z^2)^{-1}$,
 $R_{0,3}(z) = (1 + z + \frac{1}{2}z^2 + \frac{1}{6}z^3)^{-1}$, &
 $R_{2,2}(z) = (1 - \frac{1}{2}z + \frac{1}{12}z^2)(1 + \frac{1}{2}z + \frac{1}{12}z^2)^{-1}$.
- $R_{1,2}$ is the damping device of Rannacher.
- $R_{0,3}$ is positivity preserving, to be used as a damping device.

Properties of Padé Symbols

$$\begin{aligned}r_s(z) &= e^{-z} + O(|z|^{2m}), \\r_m(z) &= e^{-z} + O(|z|^{2m+1}).\end{aligned}$$

Lemma 0.1 *For each $m > 0$ there exists $\beta > 0$ and $c > 0$ such that*

$$|r_s(z)| \leq c|z|^{-(2m-1)}, \quad |\arg(z)| \leq \beta.$$

Lemma 0.2 *For each $m > 0$, $L > 0$, and $\theta \in (0, \pi/2)$ there exists $\delta > 0$ such that*

$$|r_m(z)| \leq \begin{cases} e^{-\delta|z|}, & |z| \leq L, |\arg(z)| \leq \theta; \\ e^{-\delta|z|^{-1}}, & |z| \geq L, |\arg(z)| \leq \theta. \end{cases}$$

The New Schemes PSP(m)...

Homogeneous Case

- Accurate with Order $2m$
- Luskin-Rannacher & Rannacher schemes

$$\mathbf{SP}(\mathbf{m}) \quad v_{n+1} = \begin{cases} R_{m-1,m}(kA)v_n, & 1 \leq n < p = 2m; \\ R_{m,m}(kA)v_n, & n \geq p = 2m. \end{cases}$$

- New Schemes

$$\mathbf{PSP}(\mathbf{m}) \quad v_{n+1} = \begin{cases} R_{0,2m-1}(kA)v_n, & 0 \leq n < p = 2; \\ R_{m,m}(kA)v_n, & n \geq p = 2. \end{cases}$$

Example... (Rannacher) SP(2)

4th Order

$$v_1 = \left(I - \frac{1}{3}kA\right)\left(I + \frac{2}{3}kA + \frac{1}{6}k^2A^2\right)^{-1}v_0,$$

$$v_2 = \left(I - \frac{1}{3}kA\right)\left(I + \frac{2}{3}kA + \frac{1}{6}k^2A^2\right)^{-1}v_1,$$

$$v_3 = \left(I - \frac{1}{3}kA\right)\left(I + \frac{2}{3}kA + \frac{1}{6}k^2A^2\right)^{-1}v_2,$$

$$v_4 = \left(I - \frac{1}{3}kA\right)\left(I + \frac{2}{3}kA + \frac{1}{6}k^2A^2\right)^{-1}v_3,$$

$$v_{n+1} = \left(I - \frac{1}{2}kA + \frac{1}{12}k^2A^2\right)\left(I + \frac{1}{2}kA + \frac{1}{12}k^2A^2\right)^{-1}v_n$$

$(n \geq 4).$

Example... (New Scheme) PSP(2)

4th Order

$$v_1 = \left(I + kA + \frac{1}{2}k^2 A^2 + \frac{1}{6}k^3 A^3\right)^{-1} v_0,$$

$$v_2 = \left(I + kA + \frac{1}{2}k^2 A^2 + \frac{1}{6}k^3 A^3\right)^{-1} v_1,$$

$$v_{n+1} = \left(I - \frac{1}{2}kA + \frac{1}{12}k^2 A^2\right) \left(I + \frac{1}{2}kA + \frac{1}{12}k^2 A^2\right)^{-1} v_n$$

$(n \geq 2).$

We use the partial fraction splitting method described next to implement these algorithms in parallel, and even in the serial case. Complex arithmetic is necessary.

Convergence Theorem...

Homogeneous Case

R. Rannacher (1984), in the self-adjoint Hilbert space case, and A. Hansbo (1999), in the Banach space case, have shown optimal order estimates for nonsmooth initial data for the original SP schemes in the following sense: For $n \geq 2$ and $0 < k \leq k_0$, and $v \in X$:

$$\| (e^{-t_n A} - R_{m,m}^{n-2m}(kA) R_{m-1,m}^{2m}(kA)) v \| \leq c t_n^{-2m} k^{2m} \|v\|$$

Parallel Implementation...

Homogeneous Case

Gallopoulos and Saad (1988) and Khaliq, Twizell, Voss (1993), we can implement the main schemes as well as the damping subdiagonal schemes in a partial fraction decomposition that allows efficient and accurate computations on serial or parallel machines.

$$R_{m,n}(z) = \sum_{i=1}^{q_1} \frac{w_i}{z - c_i} + 2 \sum_{i=q_1+1}^{q_1+q_2} \Re \left(\frac{w_i}{z - c_i} \right),$$

where $R_{m,n}$ has q_1 real poles and $2q_2$ nonreal poles $\{c_i\}$, with $q_1 + 2q_2 = n$, and where $w_i = P_{m,n}(c_i)/Q'_{m,n}(c_i)$.

Parallel Implementation...

Homogeneous Case

If $m = n$ it works out as

$$R_{m,m}(z) = (-1)^m + \sum_{i=1}^{q_1} \frac{w_i}{z - c_i} + 2 \sum_{i=q_1+1}^{q_1+q_2} \Re \left(\frac{w_i}{z - c_i} \right).$$

Parallel Implementation...

Homogeneous Case

The scheme for $v_{s+1} = e^{-\Delta t A} v_s$ is:

Algorithm 1

1. For $i = 1, \dots, q_1 + q_2$, solve $(\Delta t A - c_i I) y_i = v_s$;

2a. (If $m < n$) Compute

$$v_{s+1} = \sum_{i=1}^{q_1} w_i y_i + 2 \sum_{i=q_1+1}^{q_1+q_2} \Re(w_i y_i);$$

2b. (If $m = n$) Compute

$$v_{s+1} = (-1)^m v_s + \sum_{i=1}^{q_1} w_i y_i + 2 \sum_{i=q_1+1}^{q_1+q_2} \Re(w_i y_i).$$

Parallel Implementation...

Example (0, 3)–Padé

$$q_1 = q_2 = 1$$

$$c_1 = -1.596071637983322,$$

$$c_2 = -0.7019641810083392 - i1.807339494452022,$$

$$w_1 = 1.475686517795721,$$

$$w_2 = -0.7378432588978604.$$

$$v_{s+1} = w_1 y_1 + 2\Re(w_2 y_2),$$

$$(kA - c_1 I)y_1 = v_s \ \& \ (kA - c_2 I)y_2 = v_s$$

Parallel Implementation...

Example (1, 2)–Padé

$$q_1 = q_2 = 1$$

$$c = -2.0 - i1.414213562373095$$

$$w = -1.0 + i3.535533905932738$$

$$v_{s+1} = 2\Re(wy),$$

where $(kA - cI)y = v_s$.

Parallel Implementation...

Example (2, 2)–Padé

$$q_1 = q_2 = 1$$

$$c = -3.0 - i1.732050807568877$$

$$w = -6.0 + i10.39230484541326$$

$$v_{s+1} = v_s + 2\Re(wy),$$

where $(kA - cI)y = v_s$.

Convergence New Scheme...

Homogeneous Case

Theorem 0.3 *For any integer $m > 0$ there exists $c > 0$ such that for integers $n \geq 2$ and $v \in X$*

$$\| (e^{-t_n A} - r_m(kA)^{n-2} r_s(kA)^2) v \| \leq c t_n^{-2m} k^{2m} \|v\|.$$

Note: The new scheme requires only 2 damping steps, independent of m .

The New Schemes...Inhomogeneous Case

- B.A. Wade A.Q.M.Khaliq, M. Yousuf, J. Vigo-Aguiar have recently extended the same idea to the development of a class of smoothing schemes for the inhomogeneous linear case, using positivity-preserving Padé schemes for damping.

The New Schemes...Inhomogeneous Case

- B.A. Wade A.Q.M.Khaliq, M. Yousuf, J. Vigo-Aguiar have recently extended the same idea to the development of a class of smoothing schemes for the inhomogeneous linear case, using positivity-preserving Padé schemes for damping.
- We also use partial fraction decomposition to construct a parallel version both and at the same time a better serial implementation for improved accuracy and computational efficiency with higher order methods.

The New Schemes...Inhomogeneous Case

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The New Schemes...Inhomogeneous Case

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- Then we seek to approximate this solution operator to preserve efficiency and performance under low regularity in the problems data.
- We must choose the right Padé approximations with identical denominators throughout.
- We must build in the partial fraction splitting for parallelizability and serial efficiency as well.

The New Schemes...Inhomogeneous Case

By Duhamel's principle, the exact solution can be written as

$$u(t) = E(t)v + \int_0^t E(t-s)f(s, u(s))ds,$$

where $E(t) = e^{-tA}$ is the solution operator of the corresponding homogeneous problem with $f = 0$.

The exact solution has the recurrence formula

$$u(t_{n+1}) = e^{-kA}u(t_n) + k \int_0^1 e^{-kA(1-\tau)} f(u(t_n + \tau k), t_n + \tau k) d\tau,$$

where $0 < k \leq k_0$, for some k_0 , is the time step and $t_n = nk$.

The New Schemes...Inhomogeneous Case

The smoothing scheme is called **IPSP(m)**, m is a positive integer and $p \geq 2$ is the number of special starting steps with the subdiagonal damping scheme.

For $0 < k \leq k_0$ & $t_n := nk$:

$$v_{n+1} = \begin{cases} R_{0,2m-1}(kA)v_n + k \sum_{i=1}^m P_i(kA)f(t_n + \tau_i k), & 0 \leq n < p; \\ R_{m,m}(kA)v_n + k \sum_{i=1}^m P_i(kA)f(t_n + \tau_i k), & n \geq p. \end{cases}$$

The New Schemes...Inhomogeneous Case

The rational functions $\{P_i(z)\}_{i=1}^s$ are obtained by solving

$$\sum_{i=1}^s \tau_i^l P_i(z) = \frac{l!}{(-z)^{l+1}} \left(r(z) - \sum_{j=0}^l \frac{(-z)^j}{j!} \right), \quad l \leq s-1.$$

where s is the number of quadrature points τ_i , used to approximate the integral term. The rational function

$r_s(z) = R_{0,2m-1}(z)$, for the starting scheme, and $r_m(z) = R_{m,m}(z)$ for the main scheme.

Self-Adjoint, Hilbert Space (Inhomogeneous Case)

Theorem. Assume A is a self-adjoint operator on a Hilbert space \mathcal{H} and the time discretization scheme is accurate of order $q = 2m$, where m is a positive integer. Suppose $f^{(l)}(t) \in \dot{H}^{2q-2l}$ for $l < q$, $t \geq 0$. Then there exists a constant $C = C(t)$ such that for $0 < k \leq \bar{k}$

$$\|v_n - u(t_n)\| \leq Ck^q \left(t_n^{-q} \|v\| + t_n \sum_{l=0}^{q-1} \mathcal{S}_l + \int_0^{t_n} \|f^{(q)}\| ds \right),$$

where $0 < n \leq \bar{n}$, $\mathcal{S}_l = \sup_{s \leq t_n} |f^{(l)}(s)|_{2q-2l}$

Parallel Padé Schemes— Inhomogeneous Case

Following Khaliq, Twizell, Voss (1993):

- If $n < m$, we utilize

$$R_{n,m}(z) = \sum_{i=1}^{q_1} \frac{w_i}{z - c_i} + 2 \sum_{i=q_1+1}^{q_1+q_2} \Re \left(\frac{w_i}{z - c_i} \right)$$

- If $n = m$, then we utilize

$$R_{m,m}(z) = (-1)^m + \sum_{i=1}^{q_1} \frac{w_i}{z - c_i} + 2 \sum_{i=q_1+1}^{q_1+q_2} \Re \left(\frac{w_i}{z - c_i} \right)$$

where $R_{m,n}$ has q_1 real poles and $2q_2$ nonreal poles, with $q_1 + 2q_2 = m$

and $w_i = P_{m,n}(c_i)/Q'_{m,n}(c_i)$.

Parallel Padé Schemes...

The corresponding $\{P_j(z)\}_{j=1}^s$ takes the form

$$P_j(z) = \sum_{i=1}^{q_1} \frac{w_{ij}}{z - c_i} + 2 \sum_{i=q_1+1}^{q_1+q_2} \Re \left(\frac{w_{ij}}{z - c_i} \right), \quad j = 1, 2, \dots, s.$$

Note that the rational functions $P_j(z)$ for the $(0, 2m - 1)$ -Padé are not the same as for the (m, m) -Padé. By construction, for each j , the poles of $P_j(z)$ and the corresponding Padé scheme are the same.

Algorithm

To compute $v_{s+1} = e^{-kA}v_s + k \int_0^1 e^{-kA(1-\tau)} f(t_s + \tau k) d\tau$
we have constructed the following algorithm

1. For $i = 1, \dots, q_1 + q_2$, solve

$$(kA - c_i I) y_i = w_i v_s + \sum_{j=1}^s k w_{ij} f(t_s + \tau_j k);$$

2a. (If $n < m$) Compute $v_{s+1} = \sum_{i=1}^{q_1} y_i + 2 \sum_{i=q_1+1}^{q_1+q_2} \Re(y_i);$

2b. (If $n = m$) Compute

$$v_{s+1} = (-1)^m v_s + \sum_{i=1}^{q_1} y_i + 2 \sum_{i=q_1+1}^{q_1+q_2} \Re(y_i).$$

Numerical Experiments–

Homogeneous Case

- We show a standard example with high frequencies, a second example that is a convection–diffusion problem with nonsmooth initial data.
- The spatial discretization in all experiments will be a second order central difference scheme on a uniform mesh of size h , chosen h sufficiently small. All the numerical schemes are implemented in serial using the split versions described earlier, for accuracy.

A Homogeneous PDE with High Frequencies

- A standard example with difficulty from high frequencies through parameter q (Cash (1984)):

$$\begin{aligned}\frac{\partial u}{\partial t} &= d \frac{\partial^2 u}{\partial x^2}, & x \in (0, 1), \quad t > 0, \\ u(x, 0) &= A \sin(\pi x) + A \sin(q\pi x), & x \in [0, 1], \\ u(0, t) &= u(1, t) = 0\end{aligned}$$

- $u(x, t) = Ae^{-\pi^2 dt} \sin(\pi x) + Ae^{-q^2 \pi^2 dt} \sin(q\pi x)$,
where $A = 10^5$.

PDE with High Frequencies

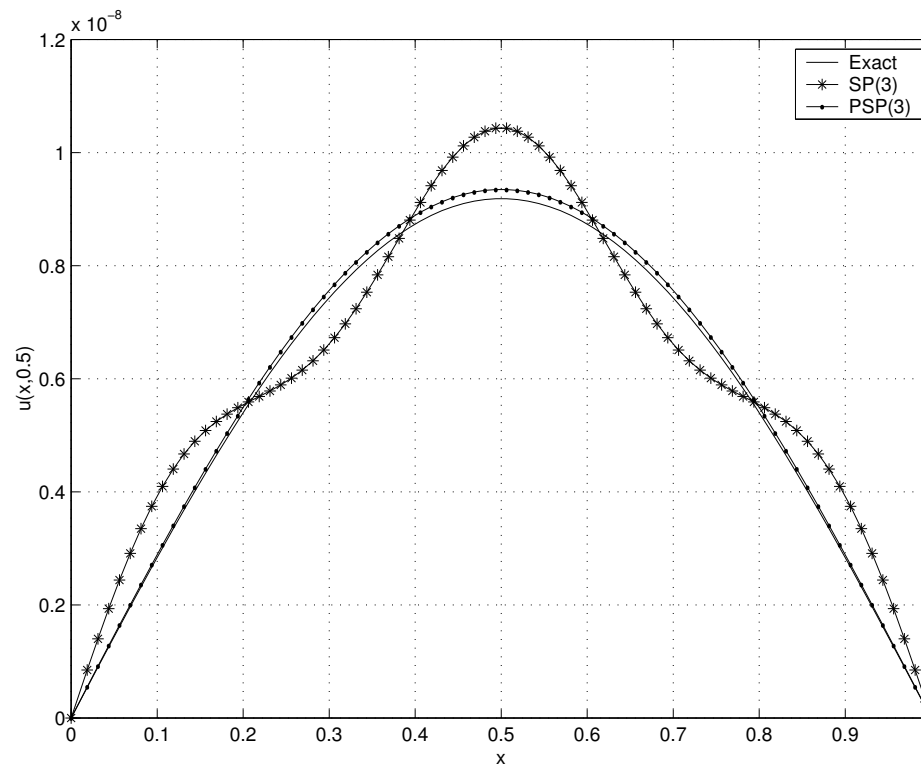


Figure 2: The Rannacher sixth order scheme SP(3) vs. the new scheme PSP(3); with $d = 3.75$, $t = 0.5$, $q = 5$, $k = 0.05$, and $h = 0.00625$.

PDE with High Frequencies

Table 1: Convergence properties of SP(2) and PSP(2) in the max norm; with $d = 2.25$, $q = 6$, $t = 0.5$, and $h = 0.0001$.

k	SP(2) Error	PSP(2) Error	SP(2) Order	PSP(2) Order
0.1	1.058×10^{-5}	1.498×10^{-5}	—	—
0.05	1.289×10^{-6}	1.155×10^{-6}	3.04	3.70
0.025	5.293×10^{-8}	9.744×10^{-8}	4.61	3.57
0.01251	3.393×10^{-9}	7.294×10^{-9}	3.96	3.74
0.00625	2.163×10^{-10}	5.024×10^{-10}	3.97	3.86
0.003125	1.252×10^{-11}	3.415×10^{-11}	4.11	3.88

A Convection-Diffusion PDE

Following Kohler and Voss (1999):

$$\begin{aligned}\frac{\partial u}{\partial t} &= d \frac{\partial^2 u}{\partial x^2} - \beta \frac{\partial u}{\partial x}, & x \in (0, 0.5), t > 0, \\ u(x, 0) &= v(x), & x \in [0, 0.5], \quad u(0, t) = u(0.5, t) = 0,\end{aligned}$$

where

$$v(x) = \begin{cases} 20x - 2, & 0.1 \leq x \leq 0.15; \\ -20x + 4, & 0.15 \leq x \leq 0.2; \\ 0, & \text{else.} \end{cases}$$

Convection-Diffusion Convergence

Table 2: Convergence properties of SP(2) and PSP(2) in the max norm; with $\beta = 2.0$, $d = 1.8$, $t = 0.2$.

k	SP(2) Error	PSP(2) Error	SP(2) Order	PSP(2) Order
0.1	1.493×10^{-5}	1.874×10^{-5}	—	—
0.05	1.026×10^{-5}	2.430×10^{-6}	0.54	2.95
0.025	3.237×10^{-7}	5.020×10^{-8}	4.99	5.60
0.01253	2.084×10^{-8}	3.993×10^{-9}	3.96	3.65
0.00625	4.879×10^{-10}	3.183×10^{-10}	5.42	3.65
0.003125	1.635×10^{-11}	2.289×10^{-11}	4.90	3.80

Convection-Diffusion Graphs

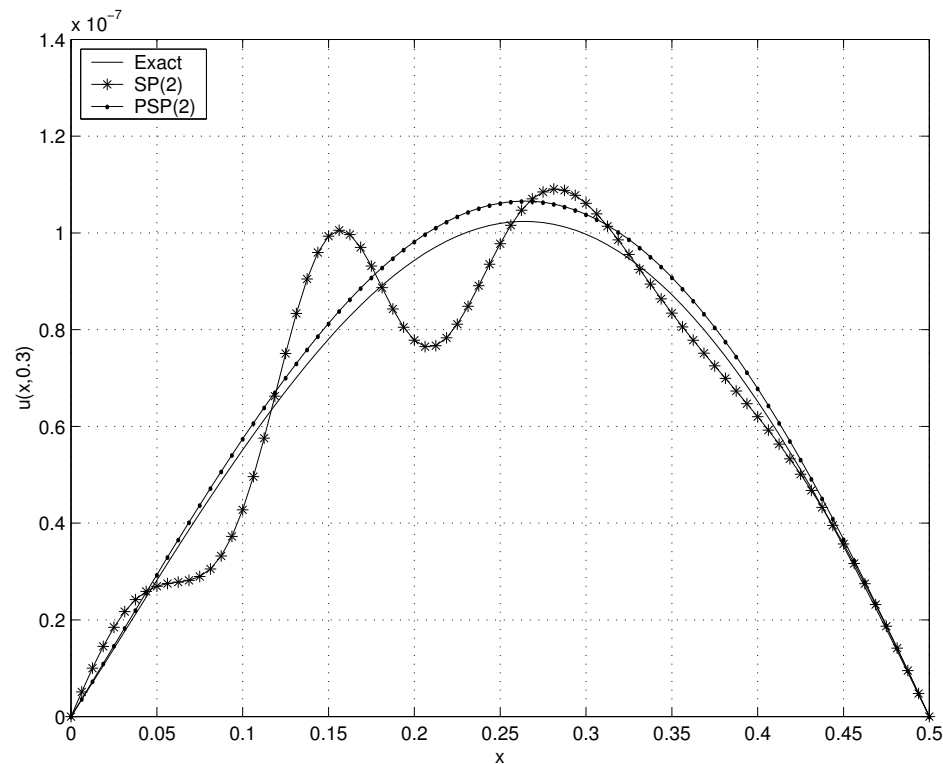


Figure 3: Comparison of SP(2) with PSP(2), a view of Table II, row 4; with $\beta = 2.0$, $d = 1.8$, $t = 0.2$, $k = 0.0125$.

Convection-Diffusion Graphs

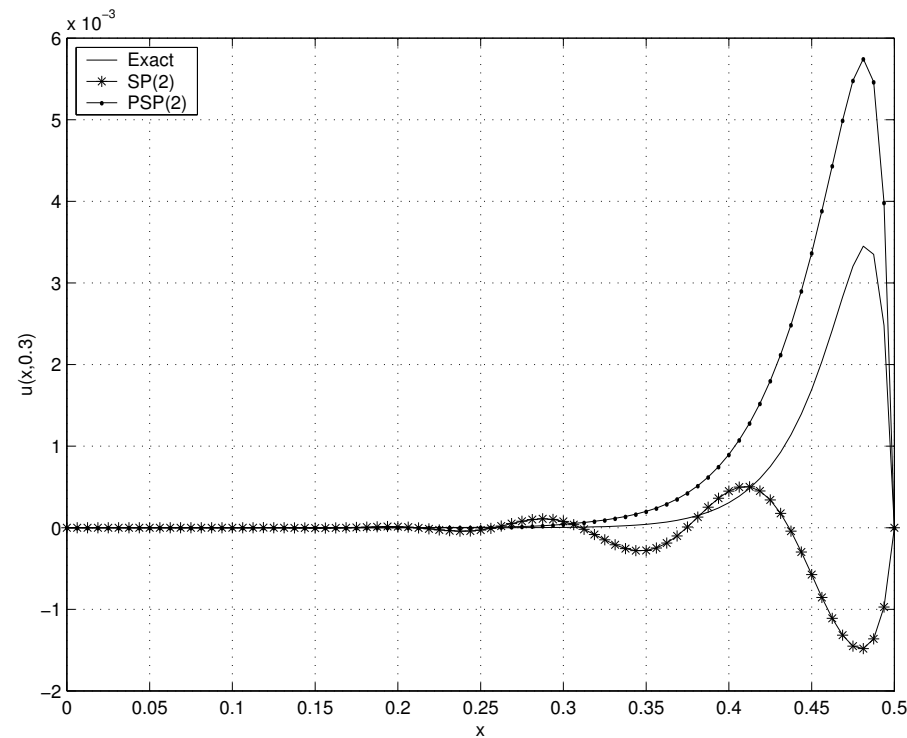


Figure 4: Comparison of the fourth order schemes SP(2) and PSP(2) under a high convection to diffusion ratio; with $\beta = 2.0$, $d = 0.015$, $t = 0.3$, $k = 0.05$, and $h = 0.00625$.

A Nonlinear Biochemistry Problem

$$\frac{\partial u}{\partial t} = d \frac{\partial u^2}{\partial x^2} - \frac{u}{1+u}, \quad x \in [0, 1], \quad t > 0,$$
$$u(x, 0) = 1, \quad u(0, t) = u(1, t) = 0,$$

- We implemented our new fourth order smoothing scheme for semilinear problems.
- We compare it with the fourth order exponential time differencing Runge-Kutta type schemes proposed by Cox & Matthews (modified by Kassam & Trefethen (2005)).

A Nonlinear Biochemistry Problem

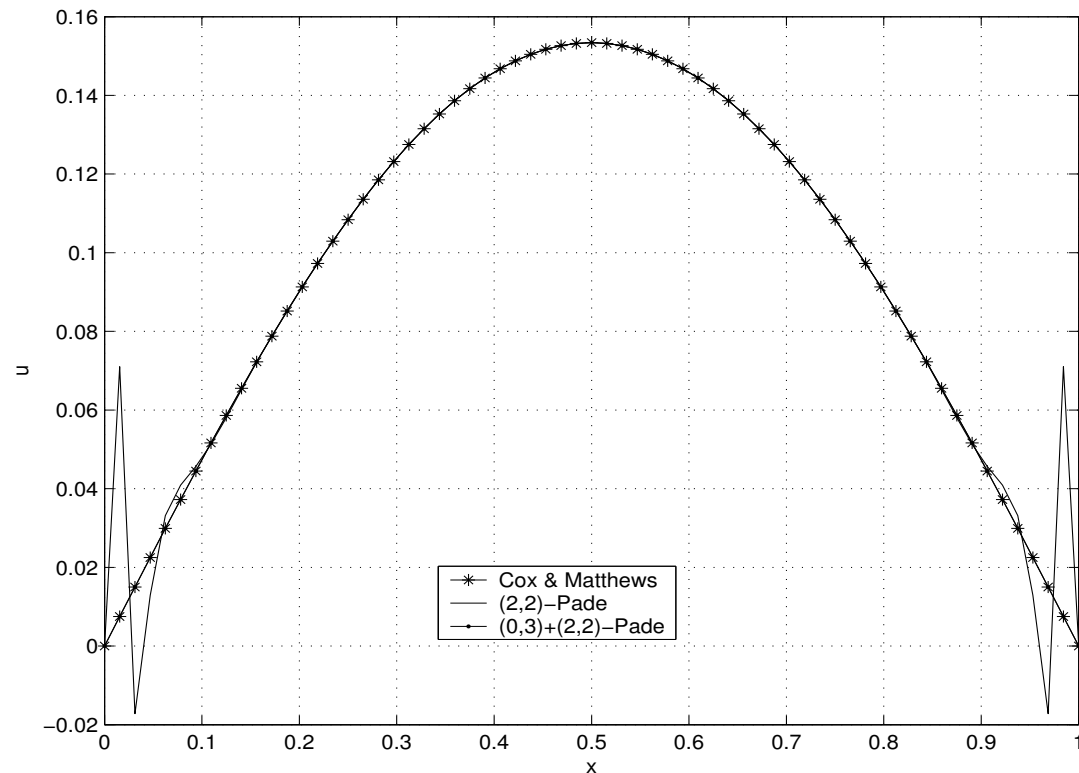


Figure 5: Graph of (2,2)-Padé, (0,3)+(2,2)-Padé and Cox & Matthews schemes using the values $h = 0.078125$ and $k = 0.00625$ at $t = 0.2$

Computing–Time Comparison

h	k	(2,2)-Padé	(0,3)+(2,2)-Padé	Cox-Matthews
0.03125000	0.025000	0.020	0.030	0.0300
0.01562500	0.012500	0.020	0.040	0.2100
0.00781250	0.006250	0.060	0.080	2.4830
0.00390625	0.003125	0.190	0.300	51.726
0.00195313	0.001563	0.681	0.951	832.13

Table 3: Time comparison table at $t = 0.2$.

Allen-Cahn Equation

$$\begin{aligned}\frac{\partial u}{\partial t} &= \epsilon \frac{\partial u^2}{\partial x^2} + u(1 - u^2) & x \in [-1, 1] \\ u(x, 0) &= 0.53x + 0.47 \sin(-1.5\pi x) & t > 0 \\ u(-1, t) &= -1, \quad u(1, t) = 1\end{aligned}$$

Kassam and Trefethen (2005)

Chebyshev spectral method is used to approximate spatial derivative and our Padé Runge-Kutta type time stepping scheme to solve the corresponding problem in time.

Allen-Cahn Equation

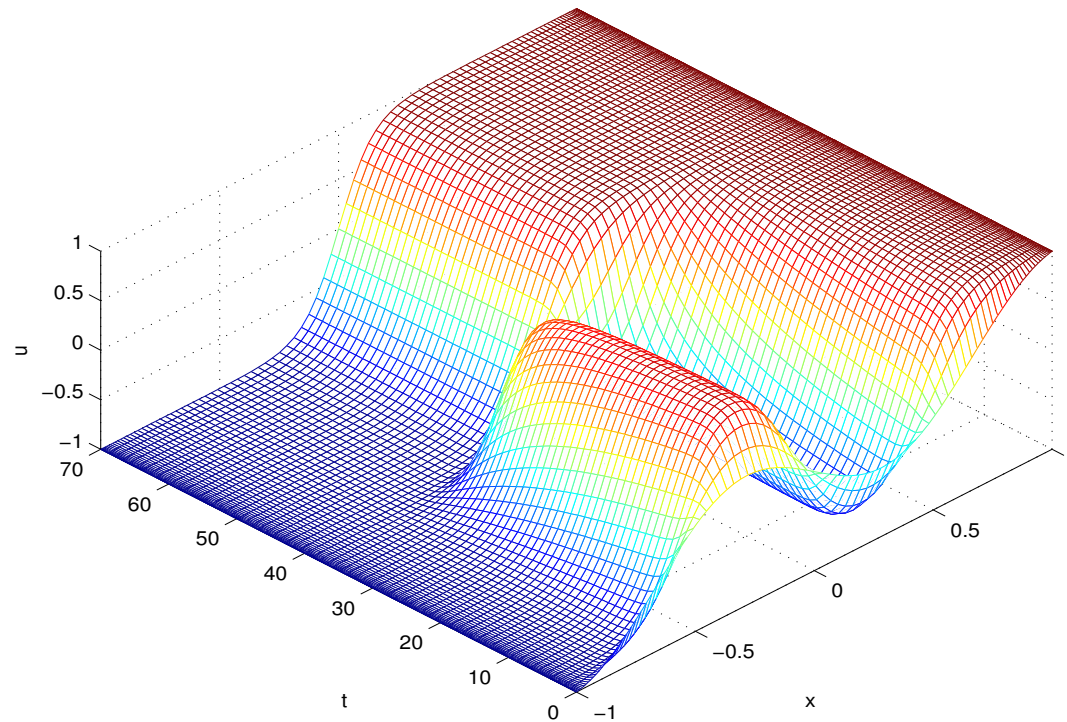


Figure 6: Time evolution graph of Allen-Cahn equation using Kassam-Trefethen method with $n = 50$, $t = 70$, $\epsilon = 0.01$

Allen-Cahn Equation

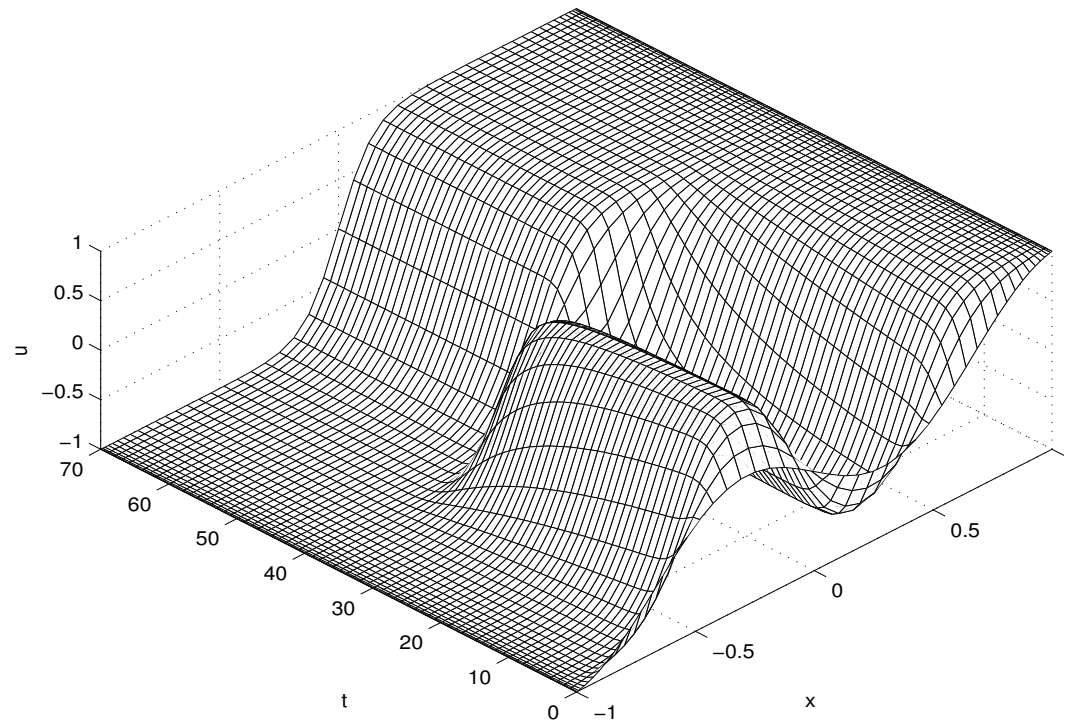


Figure 7: Time evolution graph of Allen-Cahn equation using fourth order (2,2)-Padé scheme with $n = 50$, $t = 70$, $\epsilon = 0.01$