

Hermite Collocation and SSPRK Schemes for the Numerical Treatment of a Generalized Kolmogorov-Petrovskii-Piskunov Equation

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Abstract—In this study we develop high order numerical methods to capture the spatiotemporal dynamics of a generalized Kolmogorov-Petrovskii-Piskunov (KPP) equation characterized by density dependent non-linear diffusion. Towards this direction we consider third order Strong Stability Preserving Runge-Kutta (SSPRK) temporal discretization schemes coupled with the fourth order Hermite cubic Collocation (HC) spatial discretization method. We numerically investigate their convergence properties to reveal efficient HC-RK pairs for the numerical treatment of the generalized KPP equation. The Hadamard product is used to characterize the collocation discretized non-linear equation terms. Several numerical experiments are included to demonstrate the performance of the methods.

Index Terms—Generalized Kolmogorov-Petrovskii-Piskunov Equation, Hermite Collocation, Strong Stability Preserving Runge-Kutta, Hadamard product.

I. INTRODUCTION

To incorporate density-dependent active motility to, for instance, biological migration models, described by the Fisher ([1]) or the KPP ([2]) classical equations, is by considering a density-dependent diffusion coefficient $D(u)$ (cf. [3], [4], [5] and the references therein). Assuming that $D(u)$ depends linearly in u , that is $D(u) = \lambda_0 u + \lambda_1$ (cf. [6]), the generalized KPP equation we consider here takes the form:

$$u_t = \mathcal{L}[u] := [(\lambda_1 u + \lambda_0)u_x]_x + \sum_{k=1}^M \lambda_{k+1} u^k, \quad (1)$$

where $u \equiv u(x, t)$ and $\lambda_i \in \mathbf{R}$, for all $i = 0, \dots, M$. For the corresponding Cauchy problem we also assume an initial density distribution $u(x, 0) = f(x)$, while for its numerical treatment we also impose Neumann boundary conditions

$$u_x(a, t) = 0 \quad \text{and} \quad u_x(b, t) = 0 \quad (2)$$

away enough from the wave front.

We point out that, the classical KPP problem has been extensively investigated in the literature (see for example [7] - [14] and the references therein) as its contribution to model development in mathematical biology, chemistry, genetics and many, many more important scientific areas, is fundamental.

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Aiming at the development of high order numerical schemes for the investigation of the spatiotemporal dynamics of the generalized KPP equation (1), and encouraged of our earlier results presented in [15] for the generalized Fisher equation, in Section 2 we adapt the Hermite Collocation (HC) method, a fourth order scheme, to discretize in space. In Section 3, explicit (to avoid solving nonlinear systems) third order Strong Stability Preserving (SSP) Runge-Kutta time discretization schemes are coupled with the HC method. Their efficiency and convergence properties are numerically investigated in Section 4.

II. HERMITE COLLOCATION (HC) SPATIAL DISCRETIZATION METHOD

Assuming sufficiently smooth solutions of equation (1), a uniform partition of $[a, b]$ into N subintervals, with spacing $h = (b - a)/N$ and nodes $x_j := a + jh$, $j = 1, \dots, N + 1$, the Hermite Collocation method seeks $O(h^4)$ approximations in the form:

$$U(x, t) = \sum_{j=1}^{N+1} [\alpha_{2j-1}(t)\phi_{2j-1}(x) + \alpha_{2j}(t)\phi_{2j}(x)] \quad (3)$$

where $\phi_{2j-1}(x)$ and $\phi_{2j}(x)$ are the Hermite cubic nodal basis functions centered over node x_j , described by

$$\phi_{2j-1}(x) = \begin{cases} \phi\left(\frac{x_j-x}{h}\right) & , \quad x \in I_{j-1} \\ \phi\left(\frac{x-x_j}{h}\right) & , \quad x \in I_j \\ 0 & , \quad \text{otherwise} \end{cases}, \quad (4)$$

$$\phi_{2j}(x) = \begin{cases} -h\psi\left(\frac{x_j-x}{h}\right) & , \quad x \in I_{j-1} \\ h\psi\left(\frac{x-x_j}{h}\right) & , \quad x \in I_j \\ 0 & , \quad \text{otherwise} \end{cases}$$

with $\phi(s) = (1 - s)^2(1 + 2s)$, $\psi(s) = s(1 - s)^2$ for $s \in [0, 1]$.

Equations (3) and (4) directly imply that each Hermite basis function (except the boundary ones) is supported only over two consecutive elements. Hence, over each element $I_j = [x_j, x_{j+1}]$, $j = 1, \dots, N$, there are only 4 non-zero basis functions, and therefore I_j is an element of 4 degrees of freedom (d.o.f.). As an immediate consequence, for $\bar{x} \in I_j$, we may write

$$U(\bar{x}, t) = \sum_{\ell=2j-1}^{2j+2} \alpha_\ell(t)\phi_\ell(\bar{x})$$

which combined with equation (4) yields the well celebrated Hermite interpolation properties described by

$$\alpha_{2j-1}(t) = U(x_{2j-1}, t) \quad , \quad \alpha_{2j}(t) = U_x(x_{2j-1}, t) \quad . \quad (5)$$

Substitution of the approximate solution (3) into equations (1) and (2) yields the residuals

$$\mathcal{R}(x, t) := U_t(x, t) - \mathcal{L}[U(x, t)] \quad (6)$$

$$\mathcal{B}(x, t) := U_x(x, t) \quad . \quad (7)$$

For the evaluation of the unknown parameters $\alpha_i \equiv \alpha_i(t)$, $i = 1, \dots, 2(N+1)$ the Collocation method produces a system of ordinary differential equations (ODEs) by forcing the residual $\mathcal{R}(x, t)$ to vanish at $2N$ interior collocation points and the boundary residual $\mathcal{B}(x, t)$ at 2 boundary collocation points, namely

$$\mathcal{R}(\sigma_i, t) = 0 \quad , \quad i = 1, \dots, 2N \quad (8)$$

$$\mathcal{B}(a, t) = 0 \quad \text{and} \quad \mathcal{B}(b, t) = 0 \quad . \quad (9)$$

Collocation at the Gauss points (cf. [16]) adopts the two roots of the Legendre polynomial of degree 2 in each element I_j , $j = 1, \dots, N$ to produce the needed interior collocation points. Namely, the $2N$ interior Gaussian collocation points for the element I_j , $j = 1, \dots, N$ are given by

$$\sigma_{2j-1} = x_j + \frac{h}{2} \left(1 - \frac{1}{\sqrt{3}}\right) \quad \text{and} \quad \sigma_{2j} = x_j + \frac{h}{2} \left(1 + \frac{1}{\sqrt{3}}\right) \quad . \quad (10)$$

Combination, now, of equations (6), (8) and (10) yields the two elemental collocation equations in the form

$$U_t(\sigma_i, t) = \mathcal{L}[U(\sigma_i, t)] \quad , \quad i = 2j - 1, 2j \quad (11)$$

or, equivalently, by using (5) and expanding,

$$\begin{aligned} \sum_{\ell=2j-1}^{2j+2} \dot{\alpha}_\ell(t) \phi_\ell(\sigma_i) &= \left(\lambda_0 + \lambda_1 \sum_{\ell=2j-1}^{2j+2} \alpha_\ell(t) \phi_\ell(\sigma_i) \right) \\ &\cdot \sum_{\ell=2j-1}^{2j+2} \alpha_\ell(t) \phi_\ell''(\sigma_i) \\ &+ \lambda_1 \left(\sum_{\ell=2j-1}^{2j+2} \alpha_\ell(t) \phi_\ell'(\sigma_i) \right)^2 \quad (12) \\ &+ \sum_{k=1}^M \lambda_{k+1} \left(\sum_{\ell=2j-1}^{2j+2} \alpha_\ell(t) \phi_\ell(\sigma_i) \right)^k \end{aligned}$$

where, of course, $\dot{\alpha}_\ell(t) = \frac{d}{dt} \alpha_\ell(t)$ and $\phi_\ell'(x) = \frac{d}{dx} \phi_\ell(x)$.

To express, now, the above elemental equations (12) in matrix form, and avoid lengthy algebraic manipulations, let us first observe that

$$\sum_{\ell=2j-1}^{2j+2} \alpha_\ell(t) \phi_\ell^{(m)}(\sigma_i) |_{i=2j-1, 2j} = C_j^{(m)} \boldsymbol{\alpha}_j \quad , \quad (13)$$

where

$$C_j^{(m)} = \begin{bmatrix} A_j^{(m)} & B_j^{(m)} \end{bmatrix} \quad , \quad m = 0, 1, 2 \quad (14)$$

$$\boldsymbol{\alpha}_j = \begin{bmatrix} \alpha_{2j-1}(t) & \alpha_{2j}(t) & \alpha_{2j+1}(t) & \alpha_{2j+2}(t) \end{bmatrix}^T \quad (15)$$

with

$$\begin{aligned} A_j^{(m)} &= \begin{bmatrix} \phi_{2j-1}^{(m)}(\sigma_{2j-1}) & \phi_{2j}^{(m)}(\sigma_{2j-1}) \\ \phi_{2j-1}^{(m)}(\sigma_{2j}) & \phi_{2j}^{(m)}(\sigma_{2j}) \end{bmatrix} \\ &= \frac{1}{h^m} \begin{cases} \begin{bmatrix} s_1^{(m)} & h s_2^{(m)} \\ s_3^{(m)} & -h s_4^{(m)} \end{bmatrix} \quad , \quad m = 0, 2 \\ \begin{bmatrix} s_1^{(m)} & h s_2^{(m)} \\ s_1^{(m)} & h s_4^{(m)} \end{bmatrix} \quad , \quad m = 1 \end{cases} \quad (16) \end{aligned}$$

$$\begin{aligned} B_j^{(m)} &= \begin{bmatrix} \phi_{2j+1}^{(m)}(\sigma_{2j-1}) & \phi_{2j+2}^{(m)}(\sigma_{2j-1}) \\ \phi_{2j+1}^{(m)}(\sigma_{2j}) & \phi_{2j+2}^{(m)}(\sigma_{2j}) \end{bmatrix} \\ &= \frac{1}{h^m} \begin{cases} \begin{bmatrix} s_3^{(m)} & h s_4^{(m)} \\ s_1^{(m)} & -h s_2^{(m)} \end{bmatrix} \quad , \quad m = 0, 2 \\ \begin{bmatrix} s_3^{(m)} & h s_4^{(m)} \\ s_3^{(m)} & h s_2^{(m)} \end{bmatrix} \quad , \quad m = 1 \end{cases} \quad (17) \end{aligned}$$

and

	$m = 0$	$m = 1$	$m = 2$
$s_1^{(m)}$	$\frac{9+4\sqrt{3}}{18}$	-1	$-2\sqrt{3}$
$s_2^{(m)}$	$\frac{3+\sqrt{3}}{36}$	$\frac{\sqrt{3}}{6}$	$-1 - \sqrt{3}$
$s_3^{(m)}$	$\frac{9-4\sqrt{3}}{18}$	1	$2\sqrt{3}$
$s_4^{(m)}$	$-\frac{3-\sqrt{3}}{36}$	$-\frac{\sqrt{3}}{6}$	$-1 + \sqrt{3}$

Using, now, the symbol \circ to denote the Hadamard matrix product, it may easily verified, after some algebraic manipulations, that the matrix form of the elemental equations in (12) may be written as

$$\begin{aligned} C_j^{(0)} \dot{\boldsymbol{\alpha}}_j &= \lambda_0 C_j^{(2)} \boldsymbol{\alpha}_j + \lambda_1 \left(C_j^{(0)} \boldsymbol{\alpha}_j \right) \circ \left(C_j^{(2)} \boldsymbol{\alpha}_j \right) \\ &+ \lambda_1 \left(C_j^{(1)} \boldsymbol{\alpha}_j \right) \circ \left(C_j^{(1)} \boldsymbol{\alpha}_j \right) \\ &+ \sum_{k=1}^M \lambda_{k+1} \left(C_j^{(0)} \boldsymbol{\alpha}_j \right)^{\circ k} \quad . \quad (18) \end{aligned}$$

Moreover, recall the relations in (5) and observe that

$$\alpha_2(t) = U_x(x_1, t) \equiv U_x(a, t)$$

and

$$\alpha_{2N+2}(t) = U_x(x_{N+1}, t) \equiv U_x(b, t) \quad ,$$

which, combined with the boundary residual equations in (7) and (9), yield

$$\alpha_2(t) = \alpha_{2N+2}(t) = 0 \quad , \quad (19)$$

hence, also,

$$\dot{\alpha}_2(t) = \dot{\alpha}_{2N+2}(t) = 0 \quad . \quad (20)$$

A careful assembly of all elemental and boundary collocation equations, described above, leads to the non-linear

doing so one may obtain

$$\alpha^0 = \begin{bmatrix} \alpha_1(0) \\ \alpha_3(0) \\ \alpha_4(0) \\ \vdots \\ \alpha_{2N-1}(0) \\ \alpha_{2N}(0) \\ \alpha_{2N+1}(0) \end{bmatrix} = \begin{bmatrix} U(x_1, 0) \\ U(x_2, 0) \\ U_x(x_2, 0) \\ \vdots \\ U(x_{N-1}, 0) \\ U_x(x_{N-1}, 0) \\ U(x_N, 0) \end{bmatrix} = \begin{bmatrix} f(x_1) \\ f(x_2) \\ f'(x_2) \\ \vdots \\ f(x_{N-1}) \\ f'(x_{N-1}) \\ f(x_N) \end{bmatrix} \quad (24)$$

IV. NUMERICAL RESULTS

Several different model problems are used in this section for the assessment of the HC-SSPRK schemes. The spatial absolute error

$$\mathcal{E}_n := \|U(x, t_n) - u(x, t_n)\|_2$$

is used in all experiments to measure the accuracy of the numerical approximations in each time step $t = t_n$, while their infinity norm over all time steps

$$\mathcal{E}_\infty = \max_n \{\mathcal{E}_n\}$$

is adapted to evaluate the overall accuracy of the numerical space-time integration. The order of convergence (O.o.C) of the Collocation method, as well as the computational time needed to reach time level $t = 2$, are also used to demonstrate the preservation of the expected accuracy and the efficiency of the methods.

Model Problem I

The first model problem, used to investigate the performance of the HC-RK methods, is described by

$$\begin{aligned} u_t &= [(1 - 2u)u_x]_x + \frac{1}{2}u - u^2 \\ u_x(-\pi, t) &= 0, \quad u_x(\pi, t) = 0 \\ u(x, 0) &= \frac{1}{2} - \frac{1}{6} \left(1 + \sin \frac{x}{2}\right) \end{aligned}$$

and admits the exact solution (cf. [6])

$$u(x, t) = \frac{1}{2} - \frac{1}{3} \left(1 + \sin \frac{x}{2}\right) \left(1 + e^{\frac{t}{2}}\right)^{-1}.$$

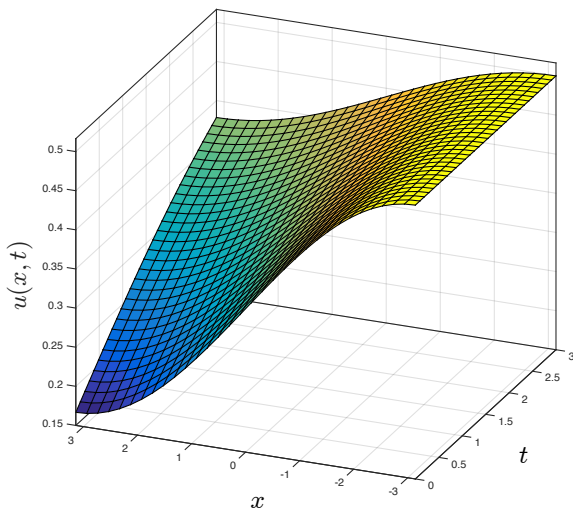


Fig. 1: Plot of the exact/numerical solution

The results obtained from all experiments for this model problem, are reported by means of Table I and Figure 2 that follow.

TABLE I Computational Performance of HC-RK schemes

	Error Norm \mathcal{E}_∞	Collocation's O.o.C.	Time (sec) needed to reach $t = 2$	
h	SSP(4,3)/(3,3)	SSP(4,3)/(3,3)	SSP(4,3)	SSP(3,3)
1/4	2.91e-07	-	0.07	0.21
1/8	1.97e-08	3.88	0.26	0.76
1/16	1.28e-09	3.94	1.19	3.37
1/32	8.01e-11	3.99	5.22	15.74
1/64	5.05e-12	3.98	28.38	88.38

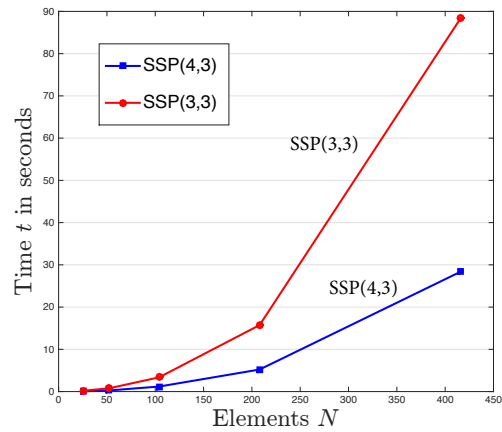


Fig. 2: Time comparison in seconds between SSPRK(4,3)-(3,3) and RK4.

The CFL conditions, imposed on time stepping, are numerically found to satisfy

$$\begin{aligned} \Delta t &\leq \frac{1}{5} h^2 \quad \text{for SSPRK(4,3)} \\ \Delta t &\leq \frac{1}{10} h^2 \quad \text{for SSPRK(3,3)} \end{aligned}$$

and, apparently, favor the SSPRK(4,3) scheme. Under these restrictions both time discretization schemes remain strongly stable, as it is depicted in Figure 3 for SSPRK(4,3), and at

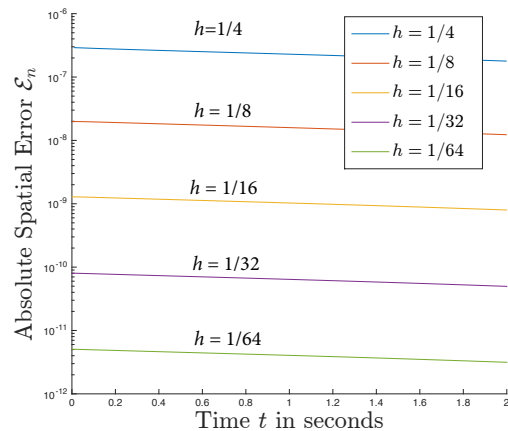


Fig. 3: Spatial absolute error as a function of time for the HC-SSPRK(4,3)

the same time, produce identical high accuracy error results while preserving the $O(h^4)$ order of convergence of the HC

method (see Table I). However, due to the CFL condition, the SSPRK(4,3) outperforms HC-SSRK(3,3) (see Table I and Figure 2) method despite the fact that it needs the calculation of an extra stage.

Model Problem II

The second model problem, used to investigate the performance of the HC-RK methods, is described by

$$u_t = \frac{1}{100}u_{xx} + \frac{1}{4}u(1 - u^3)$$

$$u_x(-10, t) = 0, \quad u_x(5, t) = 0$$

$$u(x, 0) = 1 + (2^{3/2} - 1)e^{(-15\sigma_1 x)^{-2/3}}$$

and admits the exact solution (cf. [11])

$$u(x, t) = 1 + (2^{3/2} - 1)e^{(-\frac{3}{2}\sigma_1(10x+2\lambda_1 t))^{-2/3}}$$

where $\sigma_1 = \lambda - \sqrt{\lambda^2 - \frac{1}{4}}$ and $\lambda = \frac{7\sqrt{2}}{16\sqrt{5}}$.

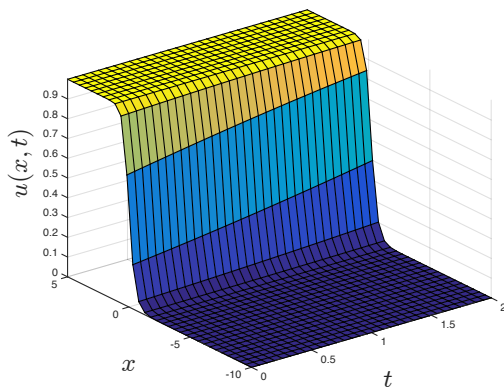


Fig. 4: Plot of the exact/numerical solution

The results obtained from all experiments for this model problem, are reported my means of Table II and Figure 5 that follow.

TABLE II Computational Performance of HC-RK schemes

h	Error Norm	Collocation's	Time (sec) needed	
	\mathcal{E}_∞	O.o.C.	to reach $t = 2$	
	SSP(4,3)/(3,3)	SSP(4,3)/(3,3)	SSP(4,3)	SSP(3,3)
1/4	2.17e-04	-	0.10	0.17
1/8	1.42e-05	3.93	0.51	0.83
1/16	8.84e-07	4.00	2.85	4.57
1/32	5.52e-08	4.00	18.60	29.48
1/64	3.45e-09	4.00	134.71	208.29

The CFL conditions, imposed on time stepping, are numerically found to satisfy

$$\Delta t \leq \frac{1}{8} h^2 \quad \text{for SSPRK(4,3)}$$

$$\Delta t \leq \frac{1}{16} h^2 \quad \text{for SSPRK(3,3)}$$

and, apparently, favor the SSPRK(4,3) scheme. Under these restrictions both time discretization schemes remain stable, as it is depicted in Figure 6 for SSPRK(4,3), and at the same time, produce identical high accuracy error results while preserving the $O(h^4)$ order of convergence of the HC method (see Table II). However, due to the CFL condition, the SSPRK(4,3) outperforms HC-SSRK(3,3) (see Table II and Figure 5) method despite the fact that it needs the calculation of an extra stage.

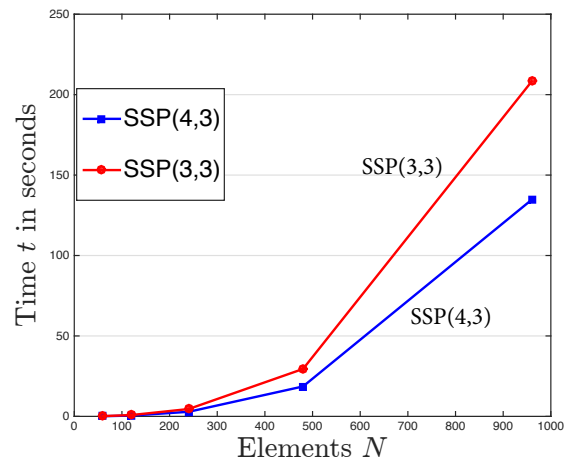


Fig. 5: Time comparison in seconds between SSPRK(4,3)-(3,3) and RK4.

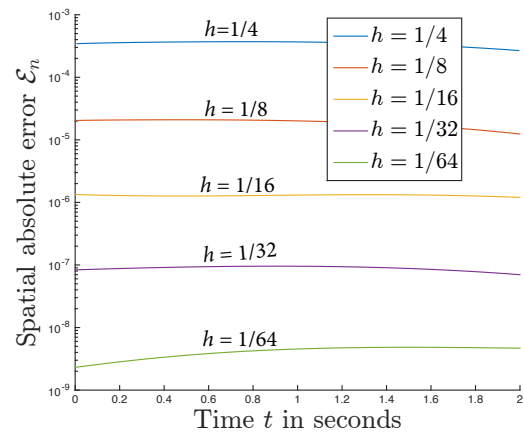


Fig. 6: Spatial absolute error as a function of time for the HC-SSPRK(4,3)

Model Problem III

The third model problem, used to investigate the performance of the HC-RK methods, is described by

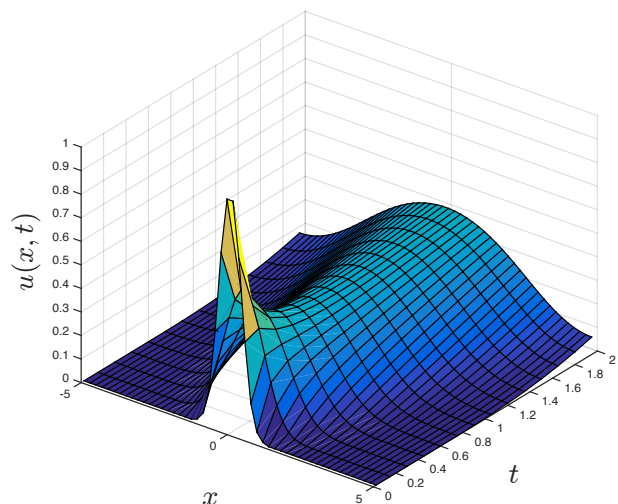


Fig. 7: Plot of the numerical solution

$$u_t = \left[\left(\frac{1}{10}u + 1 \right) u_x \right]_x + u - u^2 - 2u^3$$

$$u_x(-5, t) = 0, \quad u_x(5, t) = 0$$

$$u(x, 0) = \frac{1}{0.4\sqrt{\pi}} e^{-\left(\frac{x}{0.4}\right)^2}.$$

The results obtained from all experiments for this model problem, are reported my means of Table III and Figure 8 that follow.

TABLE III Computational Performance of HC-RK schemes

	Error Norm \mathcal{E}_∞	Collocation's <i>O.o.C.</i>	Time (sec) needed to reach $t = 2$	
h	SSP(4,3)/(3,3)	SSP(4,3)/(3,3)	SSP(4,3)	SSP(3,3)
1/4	1.72e-05	-	0.18	0.27
1/8	1.26e-06	3.77	0.78	1.20
1/16	8.17e-08	3.94	3.93	6.17
1/32	5.15e-09	3.98	23.03	36.14
1/64	3.24e-10	3.98	147.29	252.05

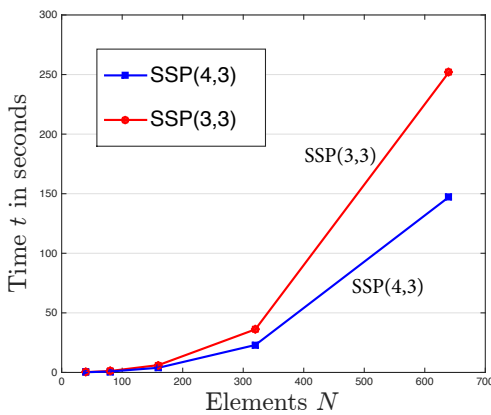


Fig. 8: Time comparison in seconds between SSPRK(4,3)-(3,3) and RK4.

The CFL conditions, imposed on time stepping, are numerically found to satisfy

$$\Delta t \leq \frac{1}{10} h^2 \quad \text{for SSPRK(4,3)}$$

$$\Delta t \leq \frac{1}{20} h^2 \quad \text{for SSPRK(3,3)}$$

and favor consistently the SSPRK(4,3) scheme. Under these restrictions both time discretization schemes produce identical high accuracy error results while preserving the $O(h^4)$ order of convergence of the HC method (see Table III). However, due to the CFL condition, the SSPRK(4,3) outperforms HC-SSRK(3,3) (see Table III and Figure 8) method despite the fact that it needs the calculation of an extra stage.

CONCLUSION

In this work, the fourth order *HC* is coupled to third order *SSPRK* schemes for the treatment of a generalized Fisher equation. Numerical results presented, imply that HC-SSPRK(4,3) method is a very competitive, effective and stable space-time integration scheme. For stiff parabolic problems and problems with large derivative variations other type time integration schemes and adaptive grids will be used in future work.

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