Runge-Kutta and Discontinuous Hermite Collocation for biological invasion problems modeled by non linear parabolic equations

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European Union
European Social Fund

OPERATIONAL PROGRAMME
EDUCATION AND LIFELONG LEARNING
investing in knowledge society
MINISTRY OF EDUCATION & RELIGIOUS AFFAIRS
MANAGING AUTHORITY

NSRF
2007-2013
programme for development
EUROPEAN SOCIAL FUND

Co-financed by Greece and the European Union

Non Linear Parabolic PDEs

$$\frac{\partial u}{\partial t} = \mathcal{L}(u) + \mathcal{G}(u) \tag{1}$$

Let,

$$\mathcal{L}(u) := \text{the parabolic linear operator and}$$
$$\mathcal{G}(u) := \text{the non linear operator of the PDE.}$$

A careful assembly of all interior elemental and boundary collocation equations in (1), leads to the system:

$$C^{(0)}\dot{\mathbf{a}} = L(\mathbf{a}) + G(\mathbf{a})$$

where $L(\mathbf{a})$ and $G(\mathbf{a})$ are the discrete analogues of $\mathcal{L}(u)$ and $\mathcal{G}(u)$. Finally, assuming that $\tilde{L}(\mathbf{a}) = \left[C^{(0)}\right]^{-1} L(\mathbf{a})$ and $\tilde{G}(\mathbf{a}) = \left[C^{(0)}\right]^{-1} G(\mathbf{a})$ we get the system of ODEs below:

$$\dot{\mathbf{a}} = \tilde{L}(\mathbf{a}) + \tilde{G}(\mathbf{a}) \tag{2}$$

Butcher form:

$$
\begin{aligned}
\mathbf{a}^{(i)} &= \mathbf{a}^n + \Delta t \sum_{j=1}^{m} a_{ij} \left(\tilde{L}(\mathbf{a}^{(j)}) + \tilde{G}(\mathbf{a}^{(j)}) \right) \\
\mathbf{a}^{n+1} &= \mathbf{a}^n + \Delta t \sum_{j=1}^{m} b_j \left(\tilde{L}(\mathbf{a}^{(j)}) + \tilde{G}(\mathbf{a}^{(j)}) \right)
\end{aligned}
$$

$$
\begin{array}{c|c} A & d \\ \hline b^T & \end{array} = \begin{array}{ccc|c} a_{11} & \cdots & a_{1m} & d_1 \\ \vdots & & \vdots & \vdots \\ a_{m1} & \cdots & a_{mm} & d_m \\ \hline b_1 & \cdots & b_m & \end{array}
$$

Time Discretization Schemes - Diagonally Implicit Runge-Kutta

Diagonally-Implicit RK (DIRK), is a class of Runge-Kutta Methods determined by the properties:

- $a_{ij} = 0$ for every $j > i$
- $a_{ii} = \lambda$, for every $i = 1, \ldots, m$

Constant λ is chosen for improving the stability properties of method.
DIRK methods are simpler and computationally more efficient than full-implicit or implicit methods, while they present their stability properties (under some necessary conditions).

DIRK(2,3)

$$
\begin{aligned}
\mathbf{a}^{(1)} = \mathbf{a}^n &\quad + \quad \lambda \Delta t \left(\tilde{L}(\mathbf{a}^{(1)}) + \tilde{G}(\mathbf{a}^{(1)}) \right) \\
\mathbf{a}^{(2)} = \mathbf{a}^n &\quad + \quad \Delta t \left[(1 - 2\lambda) \left(\tilde{L}(\mathbf{a}^{(1)}) + \tilde{G}(\mathbf{a}^{(1)}) \right) + \lambda \left(\tilde{L}(\mathbf{a}^{(2)}) + \tilde{G}(\mathbf{a}^{(2)}) \right) \right] \\
\mathbf{a}^{n+1} = \mathbf{a}^n &\quad + \quad \frac{\Delta t}{2} \left[\left(\tilde{L}(\mathbf{a}^{(1)}) + \tilde{G}(\mathbf{a}^{(1)}) \right) + \left(\tilde{L}(\mathbf{a}^{(2)}) + \tilde{G}(\mathbf{a}^{(2)}) \right) \right]
\end{aligned}
$$

Generally DIRK(2,3) is second order method except the case of $\lambda = \frac{1}{2} \pm \frac{\sqrt{3}}{2}$ where becomes third order method.

DIRK(2,3)

$$\mathbf{a}^{(1)} = \mathbf{a}^n + \lambda\Delta t \left(\tilde{L}(\mathbf{a}^{(1)}) + \tilde{G}(\mathbf{a}^{(1)})\right)$$

$$\mathbf{a}^{(2)} = \mathbf{a}^n + \Delta t \left[(1-2\lambda)\left(\tilde{L}(\mathbf{a}^{(1)}) + \tilde{G}(\mathbf{a}^{(1)})\right) + \lambda\left(\tilde{L}(\mathbf{a}^{(2)}) + \tilde{G}(\mathbf{a}^{(2)})\right)\right]$$

$$\mathbf{a}^{n+1} = \mathbf{a}^n + \frac{\Delta t}{2} \left[\left(\tilde{L}(\mathbf{a}^{(1)}) + \tilde{G}(\mathbf{a}^{(1)})\right) + \left(\tilde{L}(\mathbf{a}^{(2)}) + \tilde{G}(\mathbf{a}^{(2)})\right)\right]$$

Generally DIRK(2,3) is second order method except the case of $\lambda = \frac{1}{2} \pm \frac{\sqrt{3}}{2}$ where becomes third order method.

Strong Stability Preserving Runge-Kutta Schemes are highly stable methods, especially for nonlinear hyperbolic problems with discontinuous solution.
If the solution of a PDE is nonsmooth, stability in L_2 norm is not sufficient because the presence of oscillations prevents the approximation from converging uniformly.
SSPRK methods require stability in the maximum norm or in the TV semi-norm in order to ensure that the numerical scheme does not allow oscillations to form.

$$||\mathbf{a}||_{TV} = \sum_{j=0}^{N} |\mathbf{a}_{j+1} - \mathbf{a}_j|$$

Shu-Osher $(\alpha - \beta)$ form:

$$\begin{aligned}
\mathbf{a}^{(0)} &= \mathbf{a}^n \\
\mathbf{a}^{(i)} &= \sum_{k=0}^{i-1} \left[\alpha_{i,k} \mathbf{a}^{(k)} + \Delta t \beta_{i,k} \left(\tilde{L}(\mathbf{a}^{(k)}) + \tilde{G}(\mathbf{a}^{(k)}) \right) \right] \\
\mathbf{a}^{n+1} &= \mathbf{a}^{(m)}
\end{aligned}$$

where,

$$\alpha = \begin{bmatrix} \alpha_{1,0} & & & \\ \alpha_{2,0} & \alpha_{2,1} & & \\ \vdots & \vdots & \ddots & \\ \alpha_{m,0} & \alpha_{m,1} & \cdots & \alpha_{m,m-1} \end{bmatrix}, \; \beta = \begin{bmatrix} \beta_{1,0} & & & \\ \beta_{2,0} & \beta_{2,1} & & \\ \vdots & \vdots & \ddots & \\ \beta_{m,0} & \beta_{m,1} & \cdots & \beta_{m,m-1} \end{bmatrix}$$

SSP(3,3)

$$\begin{aligned}
\mathbf{a}^{(1)} &= \mathbf{a}^n + \Delta t \left(\tilde{L}(\mathbf{a}^n) + \tilde{G}(\mathbf{a}^n) \right) \\
\mathbf{a}^{(2)} &= \frac{3}{4}\mathbf{a}^n + \frac{1}{4}\mathbf{a}^{(1)} + \frac{1}{4}\Delta t \left(\tilde{L}(\mathbf{a}^{(1)}) + \tilde{G}(\mathbf{a}^{(1)}) \right) \\
\mathbf{a}^{n+1} &= \frac{1}{3}\mathbf{a}^n + \frac{2}{3}\mathbf{a}^{(2)} + \frac{2}{3}\Delta t \left(\tilde{L}(\mathbf{a}^{(2)}) + \tilde{G}(\mathbf{a}^{(2)}) \right)
\end{aligned}$$

SSP(4,3)

$$\begin{aligned}
\mathbf{a}^{(1)} &= \mathbf{a}^n + \frac{1}{2}\Delta t \left(\tilde{L}(\mathbf{a}^n) + \tilde{G}(\mathbf{a}^n) \right) \\
\mathbf{a}^{(2)} &= \mathbf{a}^{(1)} + \frac{1}{2}\Delta t \left(\tilde{L}(\mathbf{a}^{(1)}) + \tilde{G}(\mathbf{a}^{(1)}) \right) \\
\mathbf{a}^{(3)} &= \frac{2}{3}\mathbf{a}^n + \frac{1}{3}\mathbf{a}^{(2)} + \frac{1}{6}\Delta t \left(\tilde{L}(\mathbf{a}^{(2)}) + \tilde{G}(\mathbf{a}^{(2)}) \right) \\
\mathbf{a}^{n+1} &= \mathbf{a}^{(3)} + \frac{1}{2}\Delta t \left(\tilde{L}(\mathbf{a}^{(3)}) + \tilde{G}(\mathbf{a}^{(3)}) \right)
\end{aligned}$$

SSP(3,3)

$$\begin{aligned}
\mathbf{a}^{(1)} &= \mathbf{a}^n + \Delta t \left(\tilde{L}(\mathbf{a}^n) + \tilde{G}(\mathbf{a}^n) \right) \\
\mathbf{a}^{(2)} &= \frac{3}{4}\mathbf{a}^n + \frac{1}{4}\mathbf{a}^{(1)} + \frac{1}{4}\Delta t \left(\tilde{L}(\mathbf{a}^{(1)}) + \tilde{G}(\mathbf{a}^{(1)}) \right) \\
\mathbf{a}^{n+1} &= \frac{1}{3}\mathbf{a}^n + \frac{2}{3}\mathbf{a}^{(2)} + \frac{2}{3}\Delta t \left(\tilde{L}(\mathbf{a}^{(2)}) + \tilde{G}(\mathbf{a}^{(2)}) \right)
\end{aligned}$$

SSP(4,3)

$$\begin{aligned}
\mathbf{a}^{(1)} &= \mathbf{a}^n + \frac{1}{2}\Delta t \left(\tilde{L}(\mathbf{a}^n) + \tilde{G}(\mathbf{a}^n) \right) \\
\mathbf{a}^{(2)} &= \mathbf{a}^{(1)} + \frac{1}{2}\Delta t \left(\tilde{L}(\mathbf{a}^{(1)}) + \tilde{G}(\mathbf{a}^{(1)}) \right) \\
\mathbf{a}^{(3)} &= \frac{2}{3}\mathbf{a}^n + \frac{1}{3}\mathbf{a}^{(2)} + \frac{1}{6}\Delta t \left(\tilde{L}(\mathbf{a}^{(2)}) + \tilde{G}(\mathbf{a}^{(2)}) \right) \\
\mathbf{a}^{n+1} &= \mathbf{a}^{(3)} + \frac{1}{2}\Delta t \left(\tilde{L}(\mathbf{a}^{(3)}) + \tilde{G}(\mathbf{a}^{(3)}) \right)
\end{aligned}$$

Time Discretization Schemes - IMplicit EXplicit Runge-Kutta (IMEX RK)

A first possibility is the discretization of equation (2) by DIRK, an advantage is that these schemes have good stability properties, and a drawback that they require solving several nonlinear systems of equations (resulting from operator $G(\mathbf{a})$).
A second possibility, is the discretization of equation (2) by SSPRK, such schemes are fast and simple but the approximation converge only under an appropriate time restriction.
A third possibility, is the discretization of each operator separately by using IMEX methods.

$$
\begin{aligned}
\mathbf{a}^{(i)} &= \mathbf{a}^n + \Delta t \sum_{j=1}^{i-1} \tilde{a}_{ij} \tilde{L}(\mathbf{a}^{(j)}) + \Delta t \sum_{j=1}^{i} a_{ij} \tilde{G}(\mathbf{a}^{(j)}) \\
\mathbf{a}^{n+1} &= \mathbf{a}^n + \Delta t \sum_{i=1}^{m} \tilde{b}_i \tilde{L}(\mathbf{a}^{(i)}) + \Delta t \sum_{i=1}^{m} b_i \tilde{G}(\mathbf{a}^{(i)})
\end{aligned}
$$

where $A = (a_{ij})$, $a_{ij} = 0$ for every $j \geq i$ and $\tilde{A} = (\tilde{a}_{ij}) : \; m \times m$ are lower triangular matrices, while $b, \tilde{b} \in \mathbb{R}^m$

IMEX RK(3,3,2)

$$\begin{aligned}
\mathbf{a}^{(1)} &= \mathbf{a}^n + \lambda\Delta t\tilde{L}(\mathbf{a}^{(1)}) \\
\mathbf{a}^{(2)} &= \mathbf{a}^n + \Delta t\tilde{G}(\mathbf{a}^{(1)}) + \Delta t(1-2\lambda)\tilde{L}(\mathbf{a}^{(1)}) + \lambda\Delta t\tilde{L}(\mathbf{a}^{(2)}) \\
\mathbf{a}^{(3)} &= \mathbf{a}^n + \frac{\Delta t}{4}\left[\tilde{G}(\mathbf{a}^{(1)}) + \tilde{G}(\mathbf{a}^{(2)}\right] + \Delta t(\frac{1}{2}-\lambda)\tilde{L}(\mathbf{a}^{(1)}) + \lambda\Delta t\tilde{L}(\mathbf{a}^{(3)}) \\
\mathbf{a}^{n+1} &= \mathbf{a}^n + \frac{\Delta t}{6}\left[\tilde{G}(\mathbf{a}^{(1)}) + \tilde{G}(\mathbf{a}^{(2)}) + 4\tilde{G}(\mathbf{a}^{(3)})\right] \\
&+ \frac{\Delta t}{6}\left[\tilde{L}(\mathbf{a}^{(1)}) + \tilde{L}(\mathbf{a}^{(2)}) + 4\tilde{L}(\mathbf{a}^{(3)})\right]
\end{aligned}$$

IMEX RK(3,3,2)

$$
\begin{aligned}
\mathbf{a}^{(1)} &= \mathbf{a}^n + \lambda \Delta t \tilde{L}(\mathbf{a}^{(1)}) \\
\mathbf{a}^{(2)} &= \mathbf{a}^n + \Delta t \tilde{G}(\mathbf{a}^{(1)}) + \Delta t (1 - 2\lambda) \tilde{L}(\mathbf{a}^{(1)}) + \lambda \Delta t \tilde{L}(\mathbf{a}^{(2)}) \\
\mathbf{a}^{(3)} &= \mathbf{a}^n + \frac{\Delta t}{4} \left[\tilde{G}(\mathbf{a}^{(1)}) + \tilde{G}(\mathbf{a}^{(2)}) \right] + \Delta t (\frac{1}{2} - \lambda) \tilde{L}(\mathbf{a}^{(1)}) + \lambda \Delta t \tilde{L}(\mathbf{a}^{(3)}) \\
\mathbf{a}^{n+1} &= \mathbf{a}^n + \frac{\Delta t}{6} \left[\tilde{G}(\mathbf{a}^{(1)}) + \tilde{G}(\mathbf{a}^{(2)}) + 4\tilde{G}(\mathbf{a}^{(3)}) \right] \\
&+ \frac{\Delta t}{6} \left[\tilde{L}(\mathbf{a}^{(1)}) + \tilde{L}(\mathbf{a}^{(2)}) + 4\tilde{L}(\mathbf{a}^{(3)}) \right]
\end{aligned}
$$

Classical Fisher's equation

$$u_t = [Du_x]_x + \lambda_2 u - \lambda_3 u^2$$

Replacing the constant diffusion coefficient D by a density-dependent $D(u)$ and assuming that the diffusivity depends linearly on density, namely $D(u) = \lambda_0 u + \lambda_1$, the **Generalized Fisher's equation** takes the form:

$$u_t = [(\lambda_0 u + \lambda_1) u_x]_x + \lambda_2 u - \lambda_3 u^2 \quad (3)$$

$$u_x(a,t) = 0 \ , \ u_x(b,t) = 0$$
$$u(x,0) = f(x)$$

The linear operator of (3) is $\mathcal{L}(u) = \lambda_1 \frac{\partial^2 u}{\partial x^2} + \lambda_2 u$

and the non linear is $\mathcal{G}(u) = \lambda_0 u \frac{\partial^2 u}{\partial x^2} + \lambda_0 \left(\frac{\partial u}{\partial x} \right)^2 - \lambda_3 u^2$,

so equation (3) can take the form :

$$\frac{\partial u}{\partial t} = \mathcal{L}(u) + \mathcal{G}(u)$$

The Hermite Collocation method seeks $\mathcal{O}(h^4)$ approximations in the form:

$$U(x,t) = \sum_{j=1}^{N+1} \left[a_{2j-1}(t)\phi_{2j-1}(x) + a_{2j}(t)\phi_{2j}(x)\right]$$

and if $x \in I_j$ element we may write:

$$U(x,t) = \sum_{k=2j-1}^{2j+2} a_k(t)\phi_k(x)$$

Applying all interior elemental & boundary collocation equations in $\mathcal{L}(u)$ is trivial that:

$$L(\mathbf{a}) = \lambda_1 C^{(2)}\mathbf{a} + \lambda_2 C^{(0)}\mathbf{a}$$

To express, now, the discrete operator of $\mathcal{G}(u)$ in matrix form we will use the following propotition for the general nonlinear term:

$$\frac{\partial^m}{\partial x^m}U(x,t)\frac{\partial^n}{\partial x^n}U(x,t) = \left(C^{(m)}\mathbf{a}\right) \circ \left(C^{(n)}\mathbf{a}\right)$$

where, the symbol $\circ$ denote the Hadamard matrix product.
So, the discrete operator $G(\mathbf{a})$ takes the form:

$$G(\mathbf{a}) = \lambda_0 \left(C^{(0)}\mathbf{a}\right)\circ\left(C^{(2)}\mathbf{a}\right)+\lambda_0 \left(C^{(1)}\mathbf{a}\right)\circ\left(C^{(1)}\mathbf{a}\right)-\lambda_3 \left(C^{(0)}\mathbf{a}\right)\circ\left(C^{(0)}\mathbf{a}\right)$$

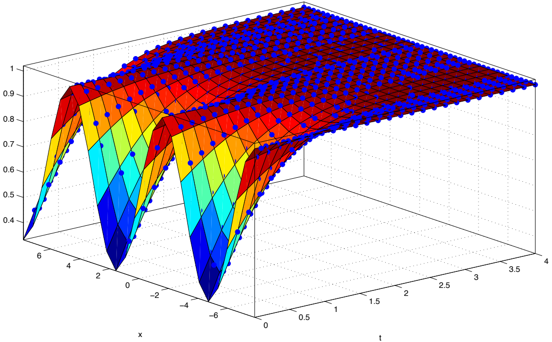
Hence, equation (3) may be written as:

$$C^{(0)}\dot{\mathbf{a}} = L(\mathbf{a}) + G(\mathbf{a})$$
$$\dot{\mathbf{a}} = \tilde{L}(\mathbf{a}) + \tilde{G}(\mathbf{a})$$

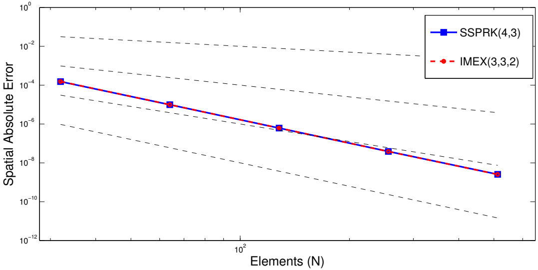
$$u_t = [(1-u)u_x]_x + 2u - 2u^2 \quad , \qquad -5\pi/2 \le x \le 5\pi/2, \quad 0 \le t \le T$$

$$u_x(\frac{-5\pi}{2}, t) = 0, \quad u_x(\frac{5\pi}{2}, t) = 0 \quad , \qquad u(x,0) = \frac{1}{3}\left[2 + \sin(-x)\right]$$

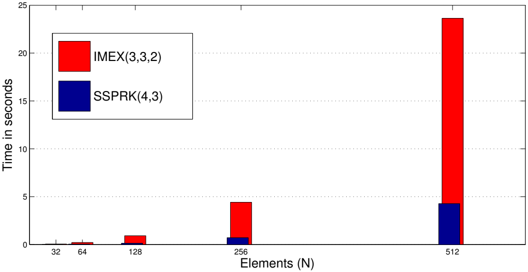
and admits the exact solution $u(x,t) = \frac{1}{3}\left[\frac{e^{-t}(3e^{2t}+1+2\sin(-x))}{e^{t}+e^{-t}}\right]$.



	Error Norm $\mathcal{E}_\infty$		*Collocation's o.o.c*		*Time to reach* $t = 2$	
N	SSP(4,3)	IMEX	SSP(4,3)	IMEX	SSP(4,3)	IMEX
32	1.53e-04	1.55-04	-	-	0.01	0.06
64	9.85e-06	9.86e-06	3.95	3.97	0.05	0.22
128	6.20e-07	6.19e-07	3.99	3.99	0.14	0.92
256	3.88e-08	3.85e-08	4.00	3.99	0.72	4.42
512	2.56e-09	2.55e-09	3.93	3.92	4.28	23.63

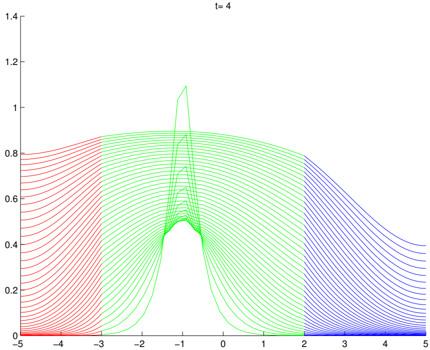


Spatial Absolute Error
Elements (N)
SSPRK(4,3)
IMEX(3,3,2)

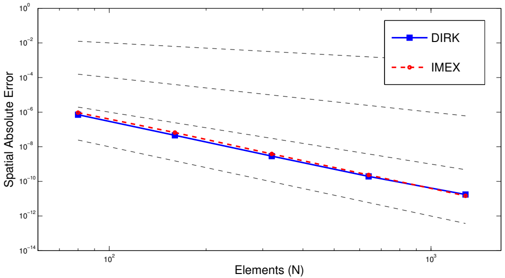


Time in seconds
Elements (N)
IMEX(3,3,2)
SSPRK(4,3)
32
64
128
256
512

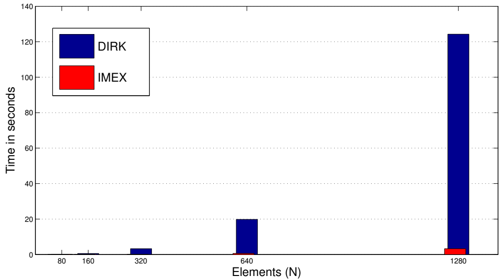
$$u_t = [Du_x]_x + u - u^2, \quad -5 \le x \le 5 \quad , \qquad 0 \le t \le T$$
$$u_x(-5,t) = 0, \quad u_x(5,t) = 0 \quad , \qquad u(x,0) = f(x)$$
$$D = \begin{cases} \gamma & , \quad x \in [-5,-3) \cup [2,5] \\ 1 & , \quad x \in [-3,2) \end{cases}$$



	$Error\ Norm\ \mathcal{E}_\infty$		$Collocation's\ o.o.c$		$Time\ to\ reach\ t = 2$	
N	DIRK	IMEX	DIRK	IMEX	DIRK	IMEX
80	7.13e-07	9.39e-07	-	-	0.18	0.04
160	4.60e-08	6.61e-08	3.95	3.82	0.58	0.06
320	2.90e-09	3.86e-09	3.98	4.09	3.27	0.17
640	1.94e-10	2.36e-10	3.89	4.02	19.80	0.60
1280	1.74e-11	1.47e-11	3.47	4.00	124.28	3.26
2560	-	-	-	-	891.34	19.63



DIRK
IMEX
Spatial Absolute Error
Elements (N)
10^{0}
10^{-2}
10^{-4}
10^{-6}
10^{-8}
10^{-10}
10^{-12}
10^{-14}
10^{2}
10^{3}



DIRK
IMEX
Time in seconds
Elements (N)
140
120
100
80
60
40
20
0
80
160
320
640
1280

Biological invasion problems
(2+1) Dimensions

$$\frac{\partial u}{\partial t} = \nabla\left[D\nabla(u)\right] \quad , \quad u := u(x,y,t)$$

$$(x,y) \in [a,b]^2 \quad , \quad 0 \leq t \leq T$$

$$u(x,y,0) = f(x,y) \quad , \quad \frac{\partial u}{\partial \eta} = 0$$

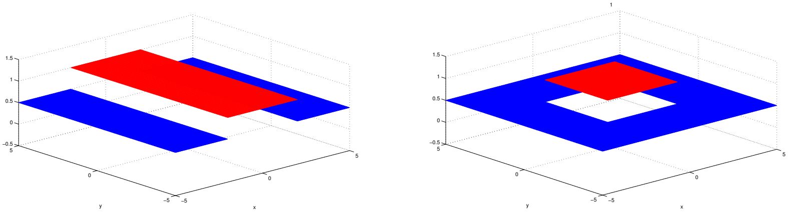


Figure : Stripes Problem (left) and Rectangular Problem (right).

$$D = \begin{cases} \gamma & , \quad (x,y) \in [-4,-2] \times [-4,4] \\ 1 & , \quad (x,y) \in (-2,2) \times (-2,2) \\ \gamma & , \quad (x,y) \in [2,4] \times [-4,4] \end{cases}$$

Two dimensional Collocation matrices in Stripes problem can be formed as the cronecker product of 1D DHC and HC matrices.

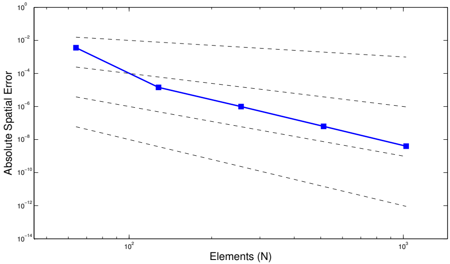
System of ODEs:

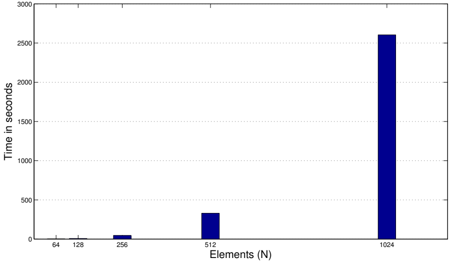
$$\begin{aligned} \left(\tilde{C}_x^{(0)} \otimes C_y^{(0)}\right) \dot{\mathbf{a}} &= \left(D_x \tilde{C}_x^{(2)} \otimes C_y^{(0)}\right) \mathbf{a} + \left(D_x \tilde{C}_x^{(0)} \otimes C_y^{(2)}\right) \mathbf{a} \\ A_{00} \dot{\mathbf{a}} &= (A_{20} + A_{02})\, \mathbf{a} \\ A_{00} \dot{\mathbf{a}} &= B \mathbf{a} \end{aligned}$$

where, $D_x = diag(\gamma, \ldots, \gamma, 1, \ldots, 1, \gamma, \ldots, \gamma) \in \mathbb{R}^{N_x}$

DIRK method for 2D Stripes Problem

N	$Error\ Norm\ \mathcal{E}_\infty$	$o.o.c.$	$Time\ to\ reach\ t = 1$
64	3.61e-03	-	2.14
128	1.44e-05	7.96	7.86
256	9.89e-07	3.86	47.98
512	6.31e-08	3.96	330.72
1024	3.97e-09	3.98	2604.38
2048	-	-	23836.24


Absolute Spatial Error
Elements (N)


Time in seconds
3000
2500
2000
1500
1000
500
0
64
128
256
512
1024
Elements (N)

Thank you

Thank you!!