Second and third order methods for the time integration of multi-D advection diffusion reaction PDEs

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Outline of the talk

- Motivation
- Convergence Analysis and New methods
- Convergence results for 2D-Problems of Adv-Diff-React
- Numerical experiments and Boundary Correction Technique
- Concluding Remarks and Future Work

Motivation

- Semi-spatial discretizations (Finite Differences) of an Advect-Diff-React PDE-problem gives rise to a family of ODEs

$$y_h'(t) = f_h(t, y_h(t)), \quad y_h(0) = u_{0,h}^*,$$
$$0 \le t \le t_{end}, \quad y_h, f_h \in \mathbb{R}^{m(h)}, \; h \to 0^+.$$

- $h \to 0^+$ measures the spatial mesh-width $(m(h) \to \infty)$
- The exact PDE-solution $u_h(t)$ satisfies the perturbed ODEs

$$u_h'(t) = f_h(t, u_h(t)) + \sigma_h(t), \quad u_h(0) = u_{0,h}^*$$

- Some properties of the PDE problem should be preserved in the spatial discretization: Energy, Positivity, TVD, etc.
- There is Stiffness in the ODE systems when some diffusion is present or when some reaction term is stiff in the PDE.

Motivation

- The time integrator is based on the two-stage Radau IIA method by Ehle (1969) and Axelsson (1969)

$$e = \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad A = \begin{pmatrix} 5/12 & -1/12 \\ 3/4 & 1/4 \end{pmatrix}, \quad c = Ae.$$

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$$Y_n = e \otimes y_n + \tau (A \otimes I_m) F(et_n + c\tau, Y_n), \quad y_{n+1} = Y_{n,2}$$

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$$Y_n := (Y_{n,i})_{i=1}^2 \approx (y(t_n + c_i \tau))_{i=1}^2,$$

$$F(et_n + c\tau, Y_n) := (f(t_n + c_i\tau, Y_{n,i}))_{i=1}^2,$$

Motivation

References for the integrator are

- *An iterated Radau method for time-dependent PDEs*, J. Comput. Appl. Math. 231 (2009)
  S. Perez-Rodriguez, S. Gonzalez-Pinto and B. Sommeijer
- *A variable time-stepsize code for advection-diffusion-reaction PDEs*, Appl. Numer. Math. (2010)
  S. Gonzalez-Pinto and S. Perez-Rodriguez.
- *Second and third order methods for the time integration of multidimensional adv-dif-react PDEs*, submitted public. in 2010,
  S Gonzalez-Pinto, D Hernandez-Abreu & S Perez-Rodriguez

Motivation

- The method consists of giving 3 iterations with some Inexact Newton Iteration of splitting type for the Radau IIA formula.
  It is A-stable for 2D Adv-Dif-React (ADR)
  It is A$(\pi/4)$-stable for 3D-(ADR).
  It is A$_0$-stable for any multidimensional (ADR).
- It has order three in time in ODE sense,

$$\|u_h(t_n) - y_n\| = \mathcal{O}(\tau^3) + \mathcal{O}(h^r), \quad n = 0, 1, \ldots, N = t_{end}/\tau$$

$$(h > 0 \quad \text{fixed}, \ \tau \to 0^+), \quad r = 2 \quad \text{typically.}$$

- The method has given good results (compared with VODPK and RKC) on practical 2D-3D problems:
  - 2D-Radiation Diffusion (Hundsdorfer-Verwer, 2003), 2D-Brusselator (Hairer-Wanner, 1996)
  - 3D-Combustion Model (Sommeijer et al. (1997)), 3D-Burgers (Verwer et al. (2004))

Motivation

- Is our method a third order method in time when both $h \to 0^+$ and $\tau \to 0^+$??
- Do the Boundary Conditions play any role in the order of convergence ??
- If so, how can be avoided the order reduction ??

Motivation

- Consider the 2D-diffusion reaction problem (Hundsdorfer-Verwer p. 367, Springer 2003)
- $$u_t = \alpha(u_{xx} + u_{yy}) + \alpha^{-1}u^2(1-u),$$
$$(x,y) \in \Omega \equiv (0,1)^2,\ t \in [0,1],\ \alpha = 1/10$$
- Dirichlet Boundary Conditions and Initial condition are prescribed by the exact Solution
$$u(x,y,t) = \left(1 + \exp\left(\frac{1}{2\alpha}(x+y-t)\right)\right)^{-1}.$$
- Spatial semi-discretization made by using central differences of order two.

Motivation

$$\varepsilon_2(h,\tau) = -\log_{10} \|u_h(t_{end}) - y_{met}(t_{end})\|$$

$$p = \frac{\varepsilon_2(h/2,h) - \varepsilon_2(h,2h)}{\log_{10} 2}, \qquad \tau = 2h$$

$$\text{Global errors estimated} = \mathcal{O}(\tau^p) + \mathcal{O}(h^2)$$

$\tau = 2h$	$h = 1/20$	$1/40$	$1/80$	$1/160$	$1/320$
$\varepsilon_2(h,\tau)(p)$	$3.2(0.6)$	$3.4(0.6)$	$3.6(0.7)$	$3.8(0.8)$	$4.0(0.9)$

- $p \nearrow 1$. It seems that for $\tau = \mathcal{O}(h)$ we get

$$\text{Global errors} = \mathcal{O}(h).$$

Motivation

- Goal is to estimate the Global Errors ($h \to 0^+,\ \tau \to 0^+$)

$$\text{Global errors } = \mathcal{O}(\tau^{p_1}) + \mathcal{O}(h^r) + \mathcal{O}(\tau^{p_2} h^s)$$

$$p_1 > 0,\ p_2 > 0,\ r > 0, \quad s \in \mathbb{R}, \quad p_1,\ p_2,\ s = ??$$

- The PDE problems are assumed to be semilinear, with ODEs counterpart

$$u'_h(t) = f_h(t, u_h(t)) + \sigma_h(t),\ u_h(0) = u^*_{0,h},$$

$$f_h(t, u_h(t)) := J_h u_h(t) + g_h(t)$$

$$\|\sigma_h(t)\| = \mathcal{O}(h^r), \quad J \equiv J_h := \left(\sum_{j=1}^{d} J_{j,h}\right),$$

$$J_{j,h} = V_h \Lambda_{j,h} V_h^{-1},\ \text{Cond}(V_h) = \mathcal{O}(1), \quad \text{Jordan's Form}$$

Our method, step $(t_n, y_n) \longrightarrow (t_n+\tau, y_{n+1})$

$$\text{Predictor:} \quad Y_n^0 \equiv (Y_{n,i}^0)_{i=1}^2 = e \otimes y_n,$$

$$q \text{ Iter: } (I \otimes \Pi) E^\nu = ((I-L)S^{-1} \otimes I_m) D_n^{\nu-1} + (L \otimes I_m) E^\nu,$$

$$Y_n^\nu = Y_n^{\nu-1} + (S \otimes I_m) E^\nu, \; (\nu = 1, \ldots, q)$$

$$\text{Corrector:} \quad y_{n+1} = Y_{n,2}^q$$

$$D_n^{\nu-1} := e \otimes y_n - Y_n^{\nu-1} + \tau (A \otimes I_m) F(e t_n + c\tau, Y_n^{\nu-1})$$

$$\Pi := \prod_{j=1}^d (I_m - \gamma \tau J_j) = I_m - \gamma \tau J + \mathcal{O}(\tau^2), \quad \textbf{AMF} - \textbf{factoriz.}$$

Our method above has as coefficients

$$T = \gamma S (I_2 + L) S^{-1}, \quad \gamma = \frac{\sqrt{6}}{6}, \quad q = 3$$

$$S = \begin{pmatrix} 1 & \frac{5-2\sqrt{6}}{9} \\ 0 & 1 \end{pmatrix}, \quad L = \begin{pmatrix} 0 & 0 \\ \frac{3\sqrt{6}}{4} & 0 \end{pmatrix}$$

Convergence Analysis

The iterations can be reformulated in a simpler way as,

$$[I_{2m} - T \otimes (\tau P)](Y_n^{\nu} - Y_n^{\nu-1}) = D_n^{\nu-1}, \quad (\nu = 1, \ldots, q)$$

$$P = (\gamma\tau)^{-1}(I - \textstyle\prod_{j=1}^{d}(I - \gamma\tau J_j)) = \sum_j J_j + (-\gamma\tau)\sum_{j<k} J_j J_k$$

$$+(-\gamma\tau)^2 \textstyle\sum_{j<k<l} J_j J_k J_l + \ldots + (-\gamma\tau)^{(d-1)} J_1 J_2 \cdots J_d.$$

More general methods denoted by AMF-qIt are given by

$$\text{Predictor:} \quad Y_n^0 = e \otimes y_n,$$

$$q \text{ Iter: } [I_{2m} - T_\nu \otimes (\tau P)](Y_n^{\nu} - Y_n^{\nu-1}) = D_n^{\nu-1}, \quad (\nu = 1, \ldots, q)$$

$$\text{Corrector:} \quad y_{n+1} = Y_{n,2}^q$$

$$T_\nu = \gamma S_\nu (I_2 + L_\nu) S_\nu^{-1}, \quad \gamma = \frac{\sqrt{6}}{6}$$

$$S_\nu = \begin{pmatrix} 1 & s_\nu \\ 0 & 1 \end{pmatrix}, \quad L_\nu = \begin{pmatrix} 0 & 0 \\ l_\nu & 0 \end{pmatrix}$$

Convergence Analysis

- The global errors (time-space) satisfy the recursion,

$$\epsilon_{n+1} = R_q(\tau J_1, \dots, \tau J_d) \cdot \epsilon_n + l_n, \quad n = 0, 1, 2, \dots, t_{end}/\tau - 1.$$

- Where $R_q(\tau J_1, \dots, \tau J_d)$ is the stability function of the method. It just depends on the coefficients and on q

The local errors $l_n = u_h(t_{n+1}) - y_{met}(t_{n+1}; t_n, u_h(t_n))$, satisfy

$$l_n = l_n^{[1]} + l_n^{[2]} + l_n^{[3]}$$

$$l_n^{[1]} = \tau^3 H_q^{[1]} \left(v_3 \otimes u_h^{(3)}(t_n + \theta\tau) \right), \quad v_3 = (2/81,\ 0)^T$$

$$l_n^{[2]} = H_q^{[2]}((A - T_1) \otimes \tau P + A \otimes \tau(P - J)) \sum_{l \geq 1} \frac{\tau^l}{l!} c^l \otimes u_h^{(l)}(t_n)$$

$$l_n^{[3]} = \mathcal{O}(\tau \cdot \sigma_h(t_n)) = \mathcal{O}(\tau h^r),$$

The matrices $H_q^{[k]}$ depend on the matrices $\tau J_j,\ j = 1(d)$

Convergence Analysis. New methods

- Order of convergence two just in one iteration, requires

$$(A - T_1)c = 0.$$

- We consider 3 methods with
$\gamma = 1/\sqrt{6} = \det A, \quad T_\nu = \gamma S_\nu (I_2 + L_\nu) S_\nu^{-1},$

$$S_\nu = \begin{pmatrix} 1 & s_\nu \\ 0 & 1 \end{pmatrix}, \quad L_\nu = \begin{pmatrix} 0 & 0 \\ l_\nu & 0 \end{pmatrix}$$

- **AMF-3It**: $q = 3, \quad s_\nu = \frac{5-2\sqrt{6}}{9}, \quad l_\nu = \frac{3\sqrt{6}}{4}, \ (\nu = 1, 2, 3).$
$T_\nu = T$ constant. It is required $e_2^T(I - A^{-1}T) = 0^T$
but $(A - T)c \neq 0$
- **AMF-1It**: $q = 1, \quad s_1 = -\frac{3+2\sqrt{6}}{9}, \quad l_1 = \frac{3}{4}(-12 + 5\sqrt{6}).$
- **AMF-2It**: $q = 2, \quad T_2 = T, \quad s_2 = \frac{5-2\sqrt{6}}{9}, \quad l_2 = \frac{3\sqrt{6}}{4}$

Convergence Analysis. H-Assumptions

The **H**-assumptions must be satisfied whenever$(\tau \to 0^+,\ h \to 0^+)$

$$P = \sum_j J_j + (-\gamma\tau) \sum_{j<k} J_j J_k + \ldots + (-\gamma\tau)^{(d-1)} J_1 J_2 \cdots J_d$$

(H1) $u_h^{(j)}(t) = \mathcal{O}(1),\ j = 1(4), \quad \sigma_h(t) = \mathcal{O}(h^r)$

(H2) $(R_q(\tau J, \tau P))^n = \mathcal{O}(1),\ n = 0, 1, \ldots, t_{end}/\tau - 1$

(H3) $H_q(\tau J, \tau J) = \mathcal{O}(1),\ H_q^{[k]}(\tau J, \tau P)(I \otimes \tau J) = \mathcal{O}(1),\ k = 1, 2$

Results for 2D-problems & spatial errors $\mathcal{O}(h^2)$

	Time-Indep. (Dirichl. BC)	Time-Dep. (Dirich. BC)
AMF-1It	$\mathcal{O}(\tau^2) + \mathcal{O}(h^2)$	$\mathcal{O}(\tau^2) + \mathcal{O}(h^2) + \mathcal{O}(\rho)$
AMF-2It	$\mathcal{O}(\tau^3) + \mathcal{O}(h^2) + \mathcal{O}(\tau^2\rho)$	$\mathcal{O}(\tau^3) + \mathcal{O}(h^2) + \mathcal{O}(\rho)$
AMF-3It	$\mathcal{O}(\tau^2) + \mathcal{O}(h^2)$	$\mathcal{O}(\tau^2) + \mathcal{O}(h^2) + \mathcal{O}(\rho)$

- Global errors in the weighted Euclidean norm for AMF-qIt methods.

$$\rho := \min\{1, \tau^2 h^{-1}\}$$

- This implies that for Time-Dependent BC, taking $\tau = \mathcal{O}(h)$, it holds

$$\textbf{Global errors} = \mathcal{O}(h), \quad h \to 0^+.$$

for the three methods.

Numerical Experiments

2D-problem revisited (Hundsdorfer-Verwer p. 367, Springer 2003)

$$u_t = \alpha(u_{xx} + u_{yy}) + \alpha^{-1}u^2(1-u),$$

$$(x,y) \in \Omega \equiv (0,1)^2,\ t \in [0,1],\ \alpha = 1/10$$

Boundary Conditions of Dirichlet-type and Exact Solution given by

$$u(x,y,t) = \left(1 + \exp(\frac{1}{2\alpha}(x+y-t))\right)^{-1}$$

The spatial semi-discretization $(1 \le i,\ j \le N-1,\ h = N^{-1})$

$$u'_{ij}(t) = \alpha h^{-2}(u_{i-1,j}+u_{i+1,j}+u_{i,j-1}+u_{i,j+1}-4u_{ij})+\frac{1}{\alpha}(u_{ij})^2(1-u_{ij})$$

Dirichlet-BC: $u_{ij}(t) = u(x_i, y_j, t)$; $\quad$ for $i = 0, N$ or $j = 0, N$

Numerical Experiments

$$\varepsilon_2(h,\tau) = -\log_{10}\|u_h(t_{end}) - y_{met}(t_{end})\|,$$

$$p = \frac{\varepsilon_2(h/2,h) - \varepsilon_2(h,2h)}{\log_{10} 2}$$

$\tau = 2h$	$h = 1/20$	$1/40$	$1/80$	$1/160$	$1/320$
AMF-1It	$2.30(1.7)$	$2.80(1.2)$	$3.16(1.0)$	$3.47(1.0)$	$3.77(1.0)$
AMF-2It	$3.33(0.4)$	$3.45(0.6)$	$3.63(0.8)$	$3.86(0.9)$	$4.12(0.9)$
AMF-3It	$3.23(0.6)$	$3.40(0.6)$	$3.57(0.7)$	$3.79(0.8)$	$4.04(0.9)$

The three methods have global errors of order $\mathcal{O}(h)$, as predicted by the theory

Boundary Correction Technique (B.C.T.)

It is inspired in some ideas by M.H. Carpenter et al., SIAM J. Sci. Comput., 16 (1995). Consider the 2D-problem

$$u_t = \alpha(u_{xx} + u_{yy}) + \alpha^{-1}u^2(1-u), \quad (x,y) \in (0,1)^2,\ t \in [0,1],$$

$$\alpha = 0.1, \quad u(x,y,t) = \left(1 + \exp\left(\frac{1}{2\alpha}(x+y-t)\right)\right)^{-1}$$

The spatial semi-discretization $(1 \le i,\ j \le N-1,\ h = N^{-1})$

$$u'_{ij}(t) = \alpha h^{-2}(u_{i-1,j} + u_{i+1,j} + u_{i,j-1} + u_{i,j+1} - 4u_{ij}) + \frac{1}{\alpha}(u_{ij})^2(1-u_{ij})$$

Replace the BC of Dirichlet-type by **its derivative w.r.t. time**

$$u'_{ij}(t) = (2\alpha)^{-1}u_{ij}(1-u_{ij}), \text{ for } i = 0, N \text{ or } j = 0, N$$

We get an IVP of $(N+1)^2$ equations with $(N+1)^2$ unknowns

2D-problems (BCT) & spatial errors $\mathcal{O}(h^2)$

	Time-Indep. (Dirichl) or **(B.C.T.)**	$\tau = \mathcal{O}(h^{0.75})$
AMF-1It	$\mathcal{O}(\tau^2) + \mathcal{O}(h^2)$	$\mathcal{O}(h^{1.5})$
AMF-2It	$\mathcal{O}(\tau^3) + \mathcal{O}(h^2) + \mathcal{O}(\tau^2 \rho)$	$\mathcal{O}(h^2)$
AMF-3It	$\mathcal{O}(\tau^2) + \mathcal{O}(h^2)$	$\mathcal{O}(h^{1.5})$

- Global errors in the weighted Euclidean norm for AMF-qIt methods.

$$\rho := \min\{1, \tau^2 h^{-1}\}$$

Numerical results with the B.C.T.

	AMF-1It		AMF-2It		AMF-3It	
h	ε_2 (p)	NDE	ε_2 (p)	NDE	ε_2 (p)	NDE
$1/20$	1.2 (1.5)	5	1.4 (2.4)	15	1.6 (2.2)	25
$1/40$	1.7 (1.5)	8	2.2 (2.7)	24	2.2 (3.4)	40
$1/80$	2.1 (1.5)	13	3.0 (2.6)	39	3.2 (3.4)	65
$1/160$	2.6 (1.6)	22	3.8 (2.5)	66	4.3 (2.8)	110
$1/320$	3.0 (1.5)	38	4.5 (2.4)	114	5.1 (2.3)	190
$1/640$	3.5 (1.5)	64	5.2 (2.3)	192	5.8 (2.1)	320
$1/1280$	4.0 $(--)$	107	5.9 $(--)$	321	6.5 $(--)$	535

$$\tau = 2 \cdot h^{0.75}, \quad \varepsilon_2 = -\log_{10} \| u_h(t_{end}) - y_{met}(t_{end}) \|$$

p is the estimated global order of convergence (PDE) halving h

Concluding Remarks and Future Work

- We get uniform convergence for 2D-problems **(BCT)**

$$\textbf{GE} = \mathcal{O}(\tau^2) + \mathcal{O}(h^2), \quad \text{(AMF-1it or AMF-3it)}$$
$$\textbf{GE} = \mathcal{O}(\tau^3) + \mathcal{O}(h^2), \quad \text{If } \tau = \mathcal{O}(h^{0.75}) \text{ (AMF-2it)}$$

- $(A - T_1)c = 0$ crucial to reach order two in 1 iteration
- Our methods are competitive with classical ones of order 2, such as the Douglas method or the Trapezoidal Splitting (Hundsdorfer, 1998)
- The convergence results can be generalized to dD-problems. Main objection is the stability requirement
  $(R(\tau J_1, \ldots, \tau J_d))^n = \mathcal{O}(1), \quad n = 1, 2, \ldots, t_{end}/\tau.$
  The stability wedge for the eigenvalues of each J_k is limited to (Hudsdorfer, 1998), $\mathcal{W}(\alpha),\ \alpha = \pi/(2(d-1))$
- The convergence framework can be easily extended to most of one-step methods