Representation and estimation of local errors for splitting methods involving two or three parts

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Numerical Analysis of Evolution Equations
8th NAI Workshop, Innsbruck (Austria), October 14–17, 2014

- Evolution equation for $u = u(t)$ (linear):

$$\frac{d}{dt}u(t) = H\,u(t), \quad H\,u = A\,u + B\,u\ [+C\,u]; \quad u(0) \text{ given}$$

- Example: Linear Schrödinger equation

$$\mathrm{i}\,\partial_t\psi(x,t) = \underbrace{-\tfrac{1}{2}\Delta_x\psi(x,t)}_{\sim A\psi} + \underbrace{V(x)\,\psi(x,t)}_{\sim B\psi}, \quad x \in \mathbb{R}^3$$

- Semi-discretization in time
- Approach: Exponential splitting:
  Separately integrate A- B- $[C]$-parts (for efficiency)
- $\rightsquigarrow$ Use efficient and accurate space discretization for Δ,
  of spectral type (FFT, ..., perfect for periodic boundary conditions)
- Analogous for nonlinear case
- Example: Cubic nonlinear Schrödinger equation

$$\mathrm{i}\,\partial_t\psi(x,t) = \underbrace{-\tfrac{1}{2}\Delta_x\psi(x,t)}_{\sim A\psi} + \underbrace{\kappa\,|\psi(x,t)|^2\,\psi(x,t)}_{\sim B(\psi)}, \quad x \in \mathbb{R}^3$$

- Nonlinear terms may be split up to enable easy separate integration.
- In particular, for *systems* of evolution equations, single components may be 'frozen' over substeps.
- Handling of non-autonomous eqs. via 'freezing time' over substeps

  Example:

  $$\tfrac{d}{dt}u(t) = Au(t) + B(t,u(t))$$

  Rewrite as

  $$\tfrac{d}{dt}\boldsymbol{u}(t) = \boldsymbol{A}\boldsymbol{u}(t) + \boldsymbol{B}(\boldsymbol{u})(t) + \boldsymbol{C}(\boldsymbol{u})(t),$$

  with ($v \leftrightsquigarrow t$)

  $$\boldsymbol{u} = \begin{pmatrix} u \\ v \end{pmatrix}, \quad \boldsymbol{A}\boldsymbol{u} = \begin{pmatrix} Au \\ 0 \end{pmatrix}, \quad \boldsymbol{B}(\boldsymbol{u}) = \begin{pmatrix} B(v,u) \\ 0 \end{pmatrix}, \quad \boldsymbol{C}(\boldsymbol{u}) = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

  Integration of $\boldsymbol{C}$-part updates time t.

- See numerical examples below. $(\longrightarrow)$

Higher-order multi-stage schemes and local error

⇝ *s-stage scheme, order p*

- Standard low-order schemes: Lie-Trotter ($p = 1$), Strang ($p = 2$).
- Higher-order s-stage splitting scheme (linear case), with stepsize t:

  $\mathrm{e}^{t(A+B[+C])}u =: \mathcal{E}(t)u \approx \mathcal{S}(t)u$, where

  $$\mathcal{S}(t) = \mathcal{S}_s(t) \cdots \mathcal{S}_1(t) = \big([\mathrm{e}^{tC_s}]\mathrm{e}^{tB_s}\mathrm{e}^{tA_s}\big) \cdots \big([\mathrm{e}^{tC_1}]\mathrm{e}^{tB_1}\mathrm{e}^{tA_1}\big)$$

  with stepsize t, and

  $$\textstyle\sum_j a_j = \sum_j b_j \ [= \sum_j c_j] = 1 \quad \text{(basic consistency requirement)}$$

- *Defect* of splitting operator (think of t as continuous variable):

  $\mathcal{D}(t)u := \big(\frac{d}{dt}S(t) - (A+B[+C])\mathcal{S}(t)\big)u;\quad \mathcal{D}(0) = 0$ by consistency

- $\Rightarrow$ Basic *local error* representation via V.O.C.,

  $$\mathcal{L}(t)u := \big(\mathcal{S}(t) - \mathcal{E}(t)\big)u = \int_0^t \mathcal{E}(t-\tau)\mathcal{D}(\tau)\,d\tau \cdot u$$

- *Goal:* Exact representation of local error for scheme of order p,
  for the purpose of rigorous analysis.

Higher-order multi-stage schemes and local error

$\rightsquigarrow$ *For order p: structure of leading term in Taylor expansion of local error*

- Assume conditions for order p are satisfied (for s appropriately large)
- $\Rightarrow$ Local error operator $\mathcal{L}(t)$ satisfies (formally, at first)

$$\begin{aligned}\mathcal{L}(t) &= \tfrac{t^{p+1}}{(p+1)!}\,\tfrac{d^{p+1}}{dt^{p+1}}\mathcal{L}(0) + \mathcal{O}(t^{p+2}) \\ &= \tfrac{t^{p+1}}{(p+1)!}\,\tfrac{d^{p}}{dt^{p}}\mathcal{D}(0) + \mathcal{O}(t^{p+2})\end{aligned}$$

- Here,

$$\tfrac{d^{p+1}}{dt^{p+1}}\mathcal{L}(0) = \tfrac{d^{p}}{dt^{p}}\mathcal{D}(0) = \text{L.C. of iterated commutators of } A, B, [C]$$

- Example: For $C = 0$ and $p = 3$, $\frac{d^4}{dt^4}\mathcal{L}(0) = \frac{d^3}{dt^3}\mathcal{D}(0)$ is a L.C. of

$$[A,[A,[A,B]]], \quad [B,[A,[A,B]]] = [A,[B,[A,B]]], \quad [B,[B,[A,B]]]$$

(elements from basis of free Lie algebra generated by A, B).

Analogously for $C \neq 0$, with 18 independent commutators

$$[A,[A,[A,B]]], \quad \ldots, \quad [[[B,C],C],C]$$

- $\rightsquigarrow$ Data commutators acting on current approximation u determine behavior of leading local error term.

Exact representation of local error

⇝ *Multiple V.O.C. integral in terms of higher-order defects*

- Let $\delta(\mathcal{X}) = \frac{d}{dt}\mathcal{X} - H\,\mathcal{X}$, $\delta_j(\mathcal{X}_j) = \frac{d}{dt}\mathcal{X}_j - H_j\,\mathcal{X}_j$ $(H_j = A_j + B_j + C_j)$
- *'Canonical' notation:* $\mathcal{S}^{(0)} := \mathcal{S}$, $\mathcal{S}^{(1)} := \mathcal{D} = \delta(\mathcal{S}^{(0)})$ ($\mathcal{D}$ = defect)
- Assume order p $\Rightarrow$ several derivatives of defect vanish at $t = 0$

  $\Rightarrow$ $\mathcal{L}(t)$ expands into multiple (iterated) V.O.C. integral

  $$\mathcal{L}(t) = \int_0^t \int_0^{\tau_1} \cdots \int_0^{\tau_{p-1}} \mathcal{E}(t-\tau_p)\mathcal{S}^{(p)}(\tau_p)\,d\tau_p \cdots d\tau_1$$

  with higher-order defects $\mathcal{S}^{(p)} := \delta^p(\mathcal{S}^{(0)})$.
- $\mathcal{S}^{(p)} = \mathcal{S}^{(p)}(t)$ has multinomial Leibniz representation

  $$\boxed{\mathcal{S}^{(p)} = \sum_{\boldsymbol{k}\in\mathbb{N}_0^s,\ |\boldsymbol{k}|=p} \binom{p}{\boldsymbol{k}} \mathcal{S}_s{}^{(k_s)} \cdots \mathcal{S}_1{}^{(k_1)}}$$
- Here: $\mathcal{S}_j{}^{(k)}$ recursively defined by $\mathcal{S}_j{}^{(0)} = \mathcal{S}_j$, and

  $$\mathcal{S}_j{}^{(k+1)} = \delta_j(\mathcal{S}_j{}^{(k)}) + [\mathcal{S}_j{}^{(k)}, \underline{H}_j], \quad k \geq 0$$

  $\underline{H}_j$ ... linear combinations of the H_ℓ.

Exact representation of local error

$\rightsquigarrow$ *Recursive representation of higher-order defect stages* $\mathcal{S}_j^{(k)}$ *(general case* $A+B+C$*)*

- Omitting details, we have

$$\mathcal{S}_j^{(k)} = \sum_{\ell=0}^{k} \binom{k}{\ell} \mathcal{W}_j^{(k-\ell)} \mathcal{V}_j^{(\ell)}, \quad j = 1 \ldots s$$

- $\mathcal{V}_j^{(\ell)}$ and $\mathcal{W}_j^{(\ell)}$ are solutions of recursively defined evolution equations,

$$\tfrac{d}{dt}\mathcal{V}_j^{(k)} = A_j \mathcal{V}_j^{(k)} + \sum_{\ell=1}^{k} \binom{k}{\ell} A_j^{[\ell]} \mathcal{V}_j^{(k-\ell)},$$

$$\tfrac{d}{dt}\mathcal{W}_j^{k} = \mathcal{W}_j^{(k)} B_j + C_j \mathcal{W}_j^{(k)} + \sum_{\ell=1}^{k} \binom{k}{\ell} \big(\mathcal{W}_j^{(k-\ell)} B_j^{[\ell]} + C_j^{[\ell]} \mathcal{W}_j^{(k-\ell)}\big),$$

  with

  - $\mathcal{V}_j^{(0)} = \mathrm{e}^{tA_j}$, $\mathcal{W}_j^{(0)} = \mathrm{e}^{tC_j}\,\mathrm{e}^{tB_j}$,
  - initial values $\mathcal{V}_j^{(k)}(0), \mathcal{W}_j^{(k)}(0)$ defined recursively,
  - $A_j^{[\ell]}, B_j^{[\ell]}, C_j^{[\ell]}$ ... iterated commutator expressions.

- Special case of splitting into two operators ($C = 0$, or $A = 0$) simplifies in appropriate way.

- Theory enables to prove rigorous a priori local error estimates under minimal regularity requirements.

- Defect $\mathcal{D}(t)u$ is usually a computable quantity (⟶)

  Can be used to design an a posteriori error estimate of the form

$$\widetilde{\mathcal{L}}(t)u := \tfrac{t}{p+1}\mathcal{D}(t)u \approx \mathcal{L}(t)u$$

- ... based on the idea (with $f(\tau) = \mathcal{E}(t-\tau)\mathcal{D}(\tau)$):

$$\mathcal{L}(t) = \int_0^t f(\tau)\,d\tau \approx \int_0^t \tfrac{\tau^p}{p!} f^{(p)}(0)\,d\tau = \tfrac{t^{p+1}}{(p+1)!} f^{(p)}(0) \approx \tfrac{t}{p+1} f(t)$$

- Analysis of *deviation* $\widetilde{\mathcal{L}}(t,u) - \mathcal{L}(t,u)$ is an extension of the a priori local error analysis. Error estimate is asymptotically correct,

$$\widetilde{\mathcal{L}}(t)u - \mathcal{L}(t)u = \mathcal{O}(t^{p+2})$$

  provided all occurring expressions are well-defined and bounded.

- Nonlinear case:

$$\tfrac{d}{dt}u = H(u) = A(u) + B(u)\ [+C(u)]; \quad u(0)\ \text{given},$$

  splitting by separate integrations over substeps.

- Here:
  - Leading error term analogous as before, involving commutators of the nonlinear vector fields $A(u)$, $B(u)$, $[C(u)]$
  - Exact integral representation of local error:

    So far worked out in detail for
    - $p = 1$ (Lie-Trotter)
    - $p = 2$ (Strang)
  - T.b.d.: Exact local error representation for multi-stage schemes

- Defect-based local error estimator

$$\widetilde{\mathcal{L}}(t,u) = \tfrac{t}{p+1}\mathcal{D}(t,u) \approx \mathcal{L}(t,u)$$

  can also be constructed. $(\longrightarrow)$

Defect-based local error estimator

$\rightsquigarrow$ *Practical evaluation of the defect. Example: nonlinear,* $s = 3$

- Consider splitting substeps:

$$\begin{aligned} u_1 &= \mathcal{E}_A(a_1 t, u), & v_1 &= \mathcal{E}_B(b_1 t, u_1), & w_1 &= \mathcal{E}_C(c_1 t, v_1) = \mathcal{S}_1(t, u) \\ u_2 &= \mathcal{E}_A(a_2 t, w_1), & v_2 &= \mathcal{E}_B(b_2 t, u_2), & w_2 &= \mathcal{E}_C(c_2 t, v_2) = \mathcal{S}_2(t, w_1) \\ u_3 &= \mathcal{E}_A(a_3 t, w_2), & v_3 &= \mathcal{E}_B(b_3 t, u_3), & w_3 &= \mathcal{E}_C(c_3 t, v_3) = \mathcal{S}_3(t, w_2) \end{aligned}$$

$$\mathcal{S}(t,u) = w_3 = \mathcal{S}_3(t, \mathcal{S}_2(t, \mathcal{S}_1(t,u)))$$

- $\rightsquigarrow$ Defect via Horner-type evaluation:

$$\begin{aligned} \mathcal{D}(t,u) = {} & \partial_2 \mathcal{E}_C(c_3 t, v_3) \cdot \partial_2 \mathcal{E}_B(b_3 t, u_3) \cdot \\ & \cdot \big\{ b_3 B(u_3) + \partial_2 \mathcal{E}_A(a_3 t, w_2) \cdot \\ & \cdot \big\{ a_3 A(w_2) + c_2 C(w_2) + \\ & + \partial_2 \mathcal{E}_C(c_2 t, v_2) \cdot \partial_2 \mathcal{E}_B(b_2 t, u_2) \cdot \\ & \cdot \{ b_2 B(u_2) + \partial_2 \mathcal{E}_A(a_2 t, w_1) \cdot \\ & \cdot \big\{ a_2 A(w_1) + c_1 C(w_1) + \\ & + \partial_2 \mathcal{E}_C(c_1 t, v_1) \cdot \partial_2 \mathcal{E}_B(b_1 t, u_1) \cdot \\ & \cdot \{ b_1 B(u_1) + \partial_2 \mathcal{E}_A(a_1 t, u) \cdot a_1 A(u) \} \} \} \} \big\} \\ & - A(w_3) - B(w_3) - (1 - c_3) C(w_3) \end{aligned}$$

Here, $\partial_2 \mathcal{E}(\cdot, v)$ = Fréchet derivative of flow $\mathcal{E}(\cdot, v)$ w.r.t. initial value v.

Numerical examples

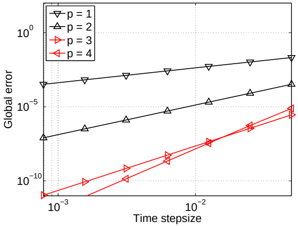
⇝ *Gross-Pitaevskii (GPE) type equation*

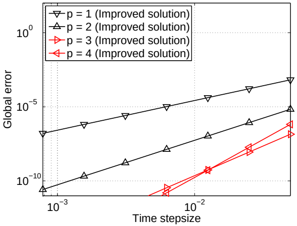
- GPE in 1D under harmonic potential, with additional inhomogeneity:

$$\mathrm{i}\partial_t \psi(x,t) = -\tfrac{1}{2}\partial_{xx}\psi(x,t) + \tfrac{1}{2}x^2\psi(x,t) + |\psi(x,t)|^2\psi(x,t) + r(x,t), \quad (x,t) \in (-8,8)\times(0,1)$$

  True solution = ground state of linear Schrödinger equation

- Splitting applied (orders $p = 1,2,3,4$, plus improvement by error estimator):
  - A ∼ Laplace operator (Fourier spectral discretization)
  - B ∼ potential + cubic nonlinearity
  - C ∼ inhomogeneity (integrate w.r.t. t)
- left / right: L_2 error of splitting / error of improved solution





- Two-component system, diffusion plus nonlinear reaction:

$$\begin{cases} \partial_t u(x,t) = (d_u \partial_{xx} - c_u) u(x,t) + c_u - u(x,t)\big(v(x,t)\big)^2 \\ \partial_t v(x,t) = (d_v \partial_{xx} - c_v) v(x,t) + u(x,t)\big(v(x,t)\big)^2 \end{cases}$$

$$d_u = 0.001, \quad d_v = 0.0001, \quad c_u = 0.04, \quad c_v = 0.1,$$

$$u(x,0) = \mathrm{e}^{-2x^2}, \; v(x,0) = 0.1 + \mathrm{e}^{-4x^2}, \quad (x,t) \in (-1.5\pi, 1.5\pi) \times (0,1)$$

  subject to periodic boundary conditions.

- Splitting applied (orders $p = 1, 2, 3, 4$, plus improvement by error estimator):
  - $A \sim$ diffusive part (Fourier spectral discretization)
  - $B, C \sim$ nonlinear reaction terms split into 2 parts

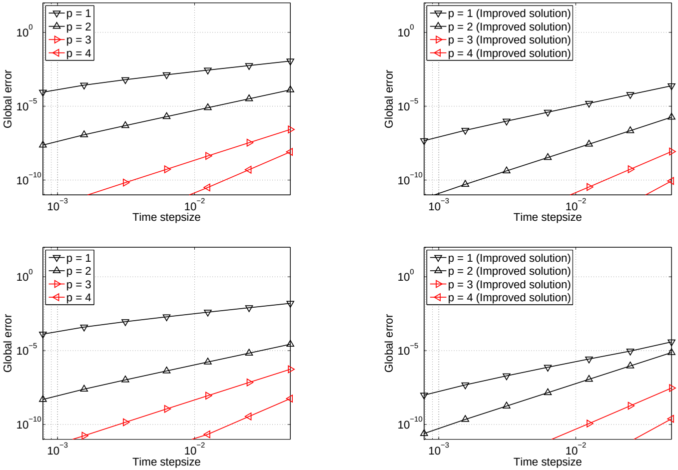
  Splitting of reaction terms according to

$$B : \begin{cases} \partial_t u(x,t) = -u(x,t)\big(v(x,t)\big)^2 \\ \partial_t v(x,t) = 0 \end{cases} \qquad C : \begin{cases} \partial_t u(x,t) = 0 \\ \partial_t v(x,t) = u(x,t)\big(v(x,t)\big)^2 \end{cases}$$

  ⇝ exact solutions to the subproblems easy to determine.

top / bottom: component 1 / component 2

left / right: L_2 error of splitting / error of improved solution



Partitioned Runge-Kutta

⇝ *Nonlinear wave equations, splitting into 2 parts*

- Problem class: nonlinear wave equation

$$\partial_t^2 u(t) = F(u(t)), \quad t \geq 0, \quad u(0), \partial_t u(0) \text{ given}$$

- With $v := \partial_t u$ ⇝ partitioned system

$$\partial_t u(t) = v(t)$$
$$\partial_t v(t) = F(u(t))$$

- More generally:

$$\begin{aligned} \partial_t u(t) &= G(v(t)) \\ \partial_t v(t) &= F(u(t)) \end{aligned} \quad \Leftrightarrow \quad \partial_t \begin{pmatrix} u \\ v \end{pmatrix} = \underbrace{\begin{pmatrix} G(v) \\ 0 \end{pmatrix}}_{A(u,v)} + \underbrace{\begin{pmatrix} 0 \\ F(u) \end{pmatrix}}_{B(u,v)}$$

- Here, second-order Strang splitting is equivalent to symplectic partitioned Runge-Kutta: $(u_0, v_0) \mapsto (u_1, v_1) = (\widetilde{u}(t), \widetilde{v}(t))$ via

$$\begin{aligned} u_{1/2} &= u_0 + \tfrac{t}{2} G(v_0) \\ v_1 &= v_0 + t F(u_{1/2}) \\ u_1 &= u_{1/2} + \tfrac{t}{2} G(v_1) \end{aligned}$$

- Defect of $(u_1, v_1) = (\widetilde{u}(t), \widetilde{v}(t))$:

$$\mathcal{D}(t, u_0, v_0) = \begin{pmatrix} \partial_t \widetilde{u}(t) - G(\widetilde{v}(t)) \\ \partial_t \widetilde{v}(t) - F(\widetilde{u}(t)) \end{pmatrix} = \mathcal{O}(t^2)$$

- Computable, derivative-free expression for $\partial_t \widetilde{u}(t), \partial_t \widetilde{v}(t)$ is obtained by differentiation of Runge-Kutta equations.
- $\rightsquigarrow$ Defect-based local error estimate:

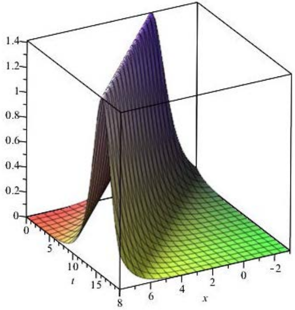
$$\widetilde{\mathcal{L}}(t, u_0, v_0) := \tfrac{t}{3}\mathcal{D}(t, u_0, v_0) \approx \mathcal{L}(t, u_0, v_0)$$

- Analogous for higher-order schemes ($s > 2$, $p > 2$)
- For efficiency:
  Evaluate Runge-Kutta step and error estimate simultaneously
- Use local error estimate for adaptive stepsize selection

- Focusing Klein-Gordon equation (Cauchy problem, 1D):

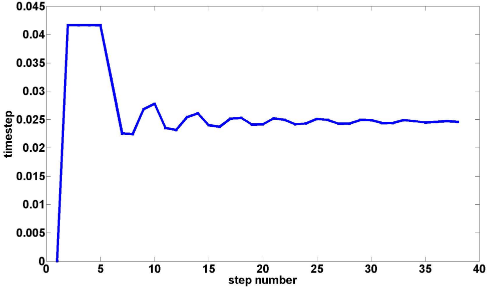
$$\partial_t^2 u = \partial_x^2 u - u + u^3, \quad u = u(x,t),\ x \in \mathbb{R},\ t \geq 0$$

- Travelling wave solution $u(x,t)$:

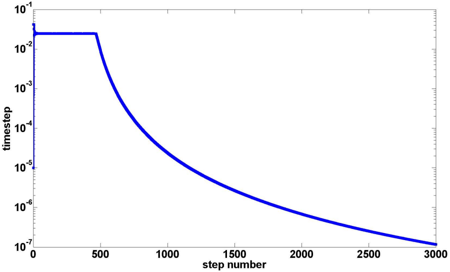


- Spatial discretization of $\partial_x^2 u$ by Fourier-spectral method, realized via [I]FFT
- Time integration by Runge-Kutta

- Algorithmic settings:
  - Symplectic partitioned Runge-Kutta, $s = p = 4$
  - Local error tolerance: $\texttt{tol} = 1\text{e-}8$
  - Stepsize control using defect-based local error estimator
- Sequence of stepsizes chosen ($0 \leq t \leq 1$):



- Integrate up to $t > 10$
- Stepsize chosen by controller:



- Integration stalls, stepsize $\rightarrow 0$
- What has happened?

  $\rightsquigarrow$ Analysis shows that solution is orbitally unstable – this is correctly diagnosed by local error estimator.

Discussion

$\rightsquigarrow$

- Reliable and asymptotically correct local error estimator:
  - enables adaptivity in time, given local error tolerance `tol`;
  - in particular: splitting error is under control.
- Accurate global a posteriori error estimate also comes for free (via defect integration using simple auxiliary scheme)
- Some open questions:
  - Details of adaptive strategy
  - Combination with adaptivity in space
  - Coping with order reductions under more general (non-periodic) boundary conditions
  - ...