Round-off Error Analysis of Explicit One-Step Numerical Integration Methods

RAIM 2017, LIP, ÉNS Lyon

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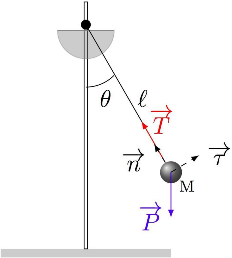
Ordinary differential equations (ODEs)

$$y'(t) = f(y, t).$$



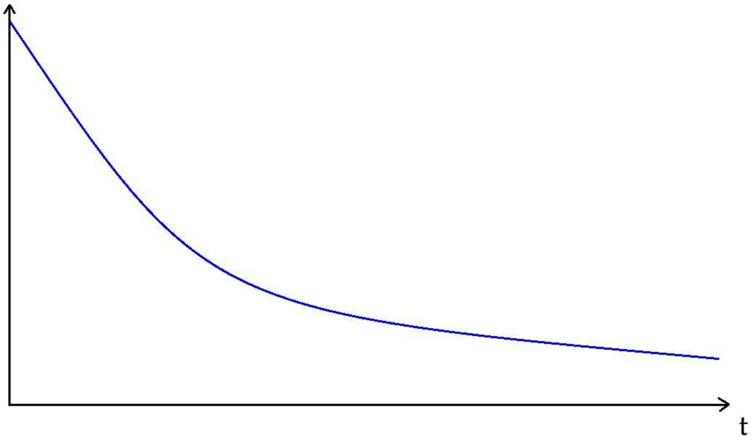
Motion of pendulum

Car shock absorber

SpaceX Falcon 9 space rocket

Exact resolution is hard ⇒ numerical methods.

Numerical integration



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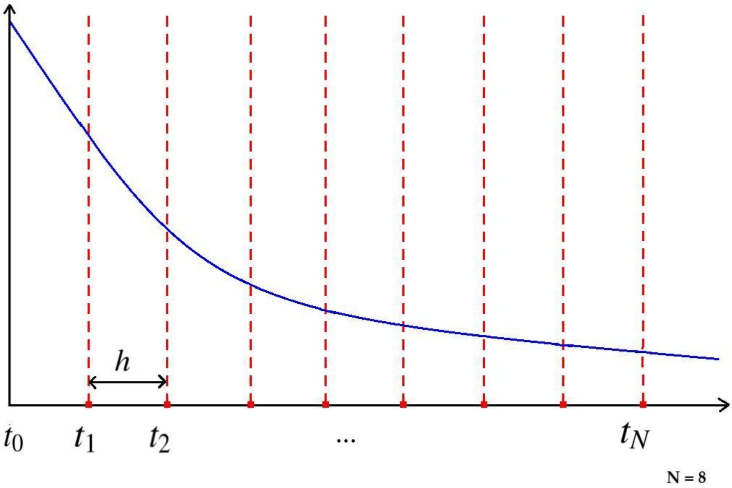

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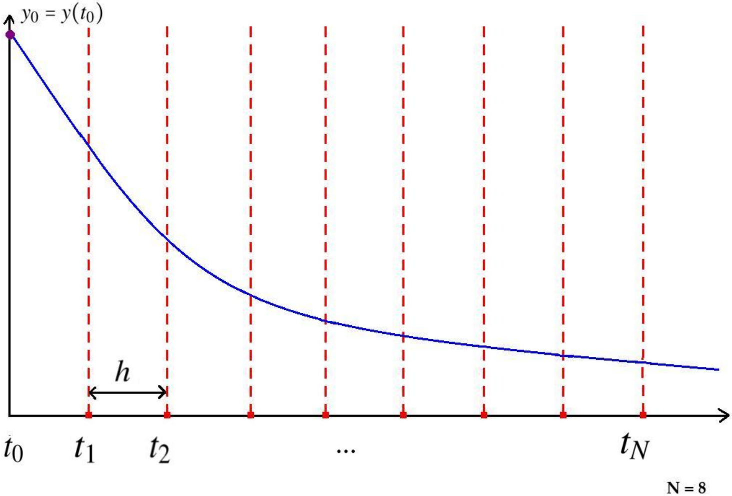

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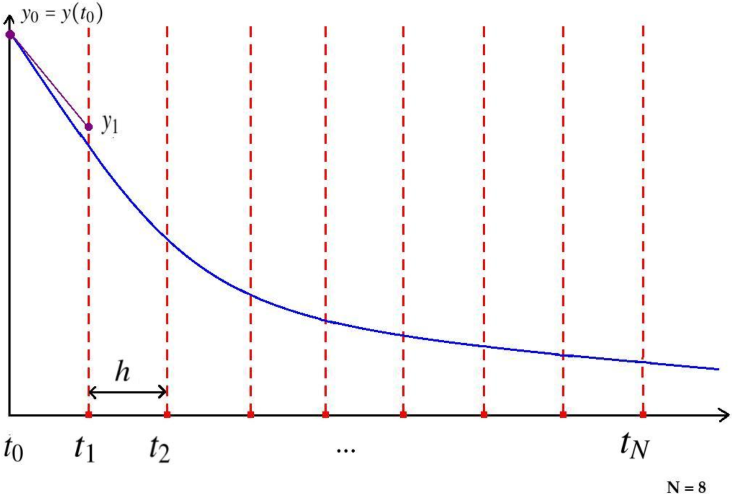

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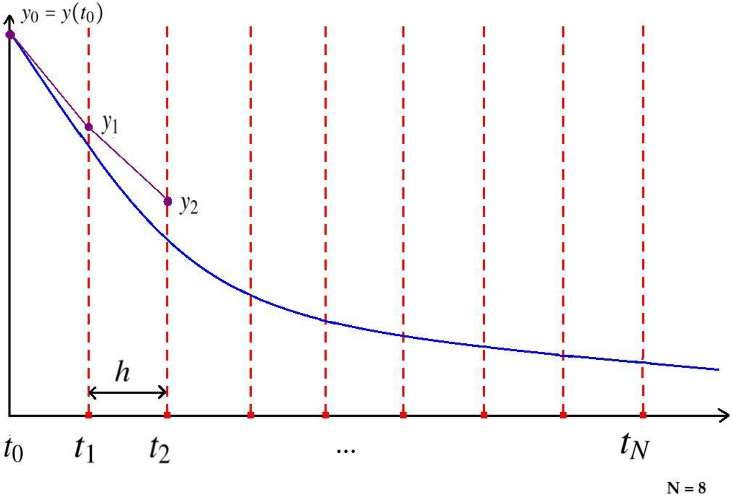

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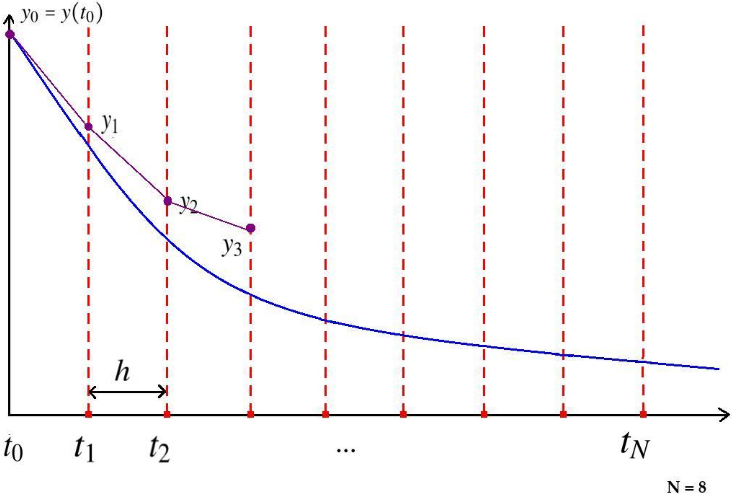

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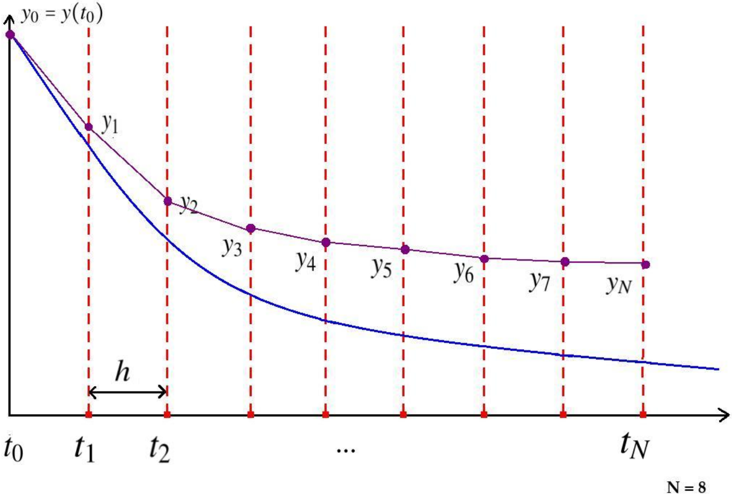

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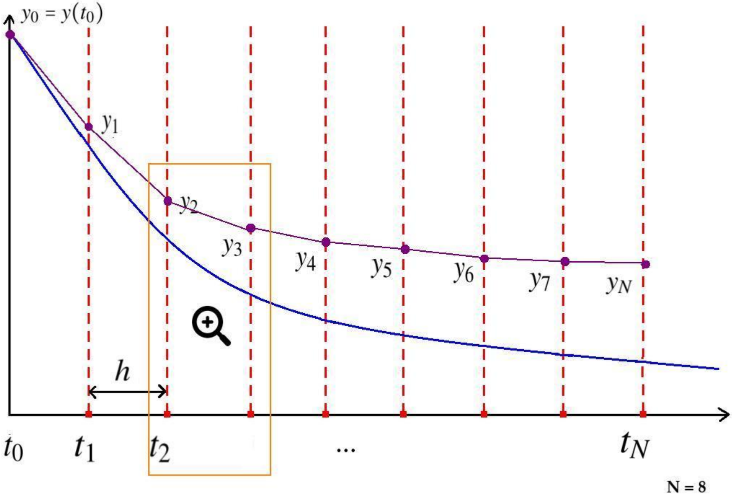
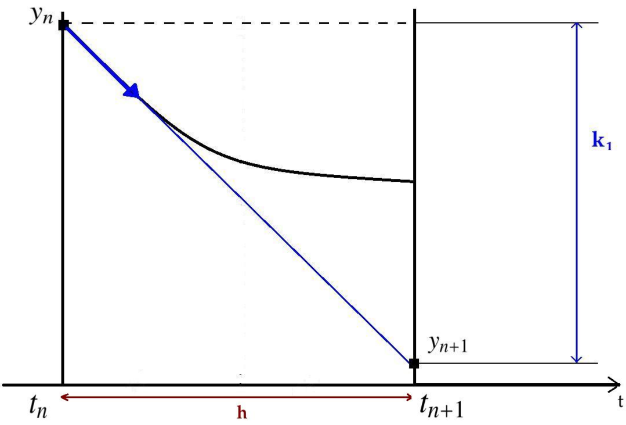
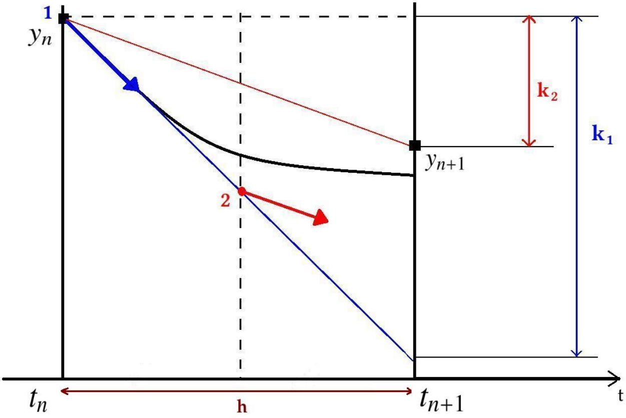


Euler method



$$k_1 = hf(t_n, y_n)$$
$$y_{n+1} = y_n + k_1 + O(h^2)$$

RK2 method



$$k_1 = h \times f(t_n, y_n) \qquad k_2 = h \times f(t_n + \frac{h}{2}, y_n + \frac{k_1}{2})$$
$$y_{n+1} = y_n + k_2 + O(h^3)$$

Working assumptions

- FP arithmetic;
  - neither underflow nor overflow,
  - radix 2 double precision, $u = 2^{-53}$

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  - first-order,
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  - $y : \mathbb{R} \to \mathbb{R}$,
- Methods.
  - explicit,
  - one step,
  - constant step.

RK methods on linear problems: linear stability

$$\begin{cases} y_0 \in \mathbb{R} \\ y_{n+1} = R(h,\lambda) y_n \end{cases}$$

(R polynomial in $h\lambda$)

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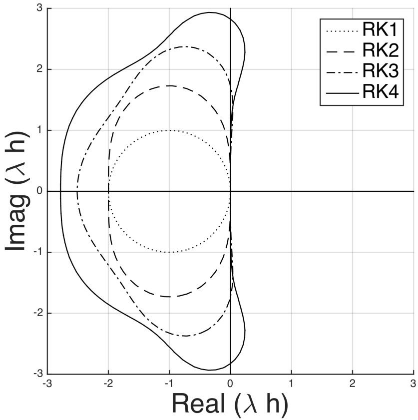
(R polynomial in $h\lambda$)

Stable $\Leftrightarrow$ $|R(h,\lambda)| < 1$:



RK methods on linear problems: FP implementation

$$\begin{cases} y_0 \in \mathbb{R} \\ y_{n+1} = R(h,\lambda) y_n \end{cases} \qquad \begin{cases} \widetilde{y_0} \simeq y_0 \\ \widetilde{y_{n+1}} = \widetilde{R}(\widetilde{h}, \widetilde{\lambda}, \widetilde{y_n}) \end{cases}$$

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Euler:

- $R(h,\lambda) = 1 + h\lambda$;
- $\widetilde{R}(\widetilde{h}, \widetilde{\lambda}, \widetilde{y_n}) = \widetilde{y_n} \oplus \widetilde{h} \otimes \widetilde{\lambda} \otimes \widetilde{y_n}$.

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RK4:

- $R(h,\lambda) = 1 + h\lambda + \frac{1}{2}(h\lambda)^2 + \frac{1}{6}(h\lambda)^3 + \frac{1}{24}(h\lambda)^4$;
- $\widetilde{R}(\widetilde{h}, \widetilde{\lambda}, \widetilde{y_n}) =$

$$\begin{aligned} &\widetilde{y_n} \oplus \widetilde{h} \oslash 6 \otimes \widetilde{\lambda} \otimes \widetilde{y_n} \oplus \widetilde{h} \oslash 3 \otimes \widetilde{\lambda} \otimes \widetilde{y_n} \oplus \widetilde{h} \otimes \widetilde{h} \oslash 6 \otimes \widetilde{\lambda} \otimes \widetilde{\lambda} \otimes \widetilde{y_n} \oplus \widetilde{h} \oslash 3 \otimes \widetilde{\lambda} \otimes \widetilde{y_n} \otimes \\ &\widetilde{h} \otimes \widetilde{h} \oslash 6 \otimes \widetilde{\lambda} \otimes \widetilde{\lambda} \otimes \widetilde{y_n} \oplus \widetilde{h} \otimes \widetilde{h} \otimes \widetilde{h} \oslash 12 \otimes \widetilde{\lambda} \otimes \widetilde{\lambda} \otimes \widetilde{\lambda} \otimes \widetilde{y_n} \oplus \widetilde{h} \oslash 6 \otimes \widetilde{\lambda} \otimes \widetilde{y_n} \\ &\oplus \widetilde{h} \otimes \widetilde{h} \oslash 6 \otimes \widetilde{\lambda} \otimes \widetilde{\lambda} \otimes \widetilde{y_n} \oplus \widetilde{h} \otimes \widetilde{h} \otimes \widetilde{h} \oslash 12 \otimes \widetilde{\lambda} \otimes \widetilde{\lambda} \otimes \widetilde{\lambda} \otimes \widetilde{y_n} \\ &\oplus \widetilde{h} \otimes \widetilde{h} \otimes \widetilde{h} \otimes \widetilde{h} \oslash 24 \otimes \widetilde{\lambda} \otimes \widetilde{\lambda} \otimes \widetilde{\lambda} \otimes \widetilde{\lambda} \otimes \widetilde{y_n}. \end{aligned}$$

($>$ 60 flops!)

State-of-the-art

Roundoff errors in numerical methods (N = nb of iterations):

- probabilistic result: error in $\sqrt{N}$ [Henrici,1963];
- in practice (implicit RK): error in N [Hairer&al, 2008];
- interval analysis [Bouissou-Martel, 2006];
- numerical integration (fine-grained): Newton-Cotes, Gauss-Legendre, ... [Fousse, 2006].

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Our approach:

- fined-grained analysis;
- use of mathematical properties of the methods (stability).

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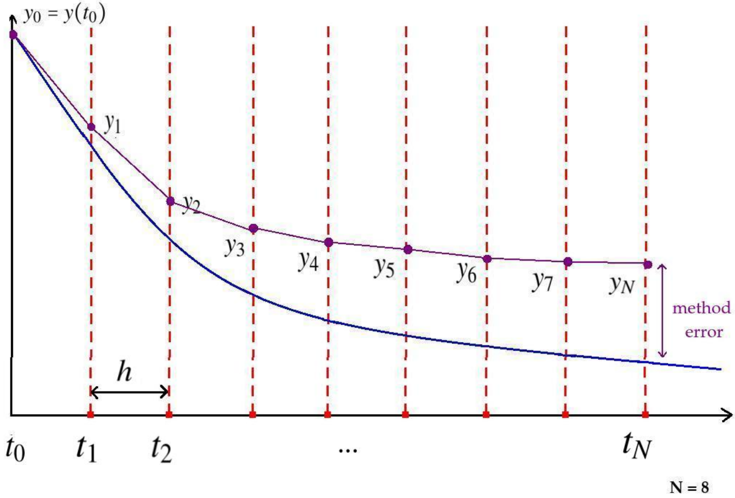
Method error vs roundoff error



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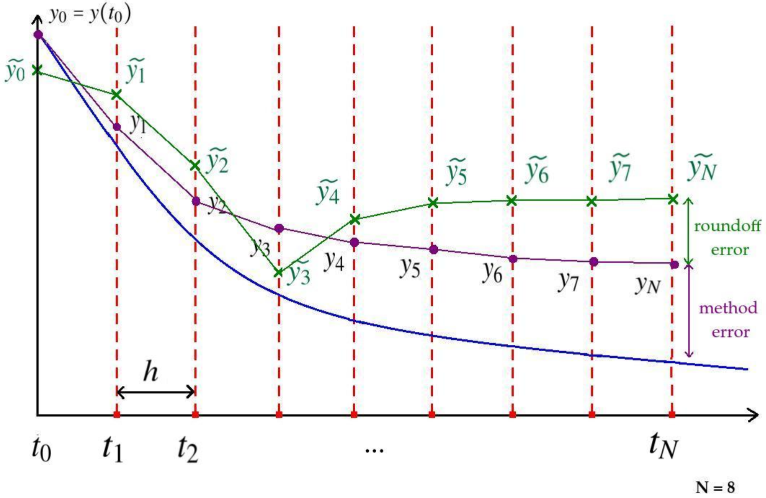
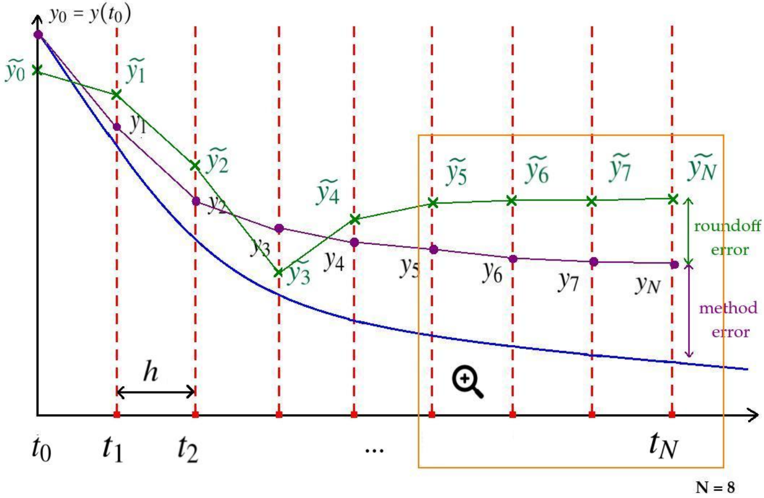
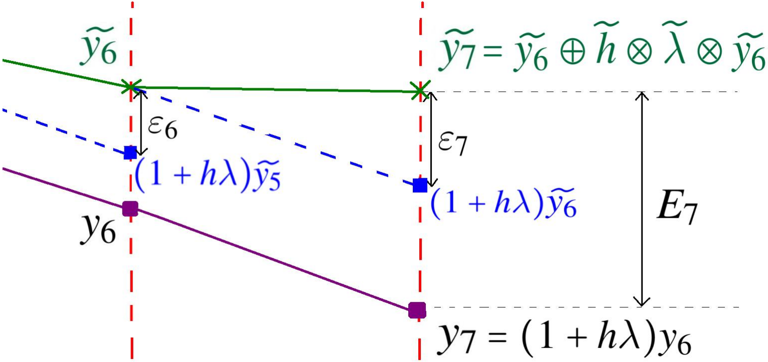


Method error vs roundoff error



Local roundoff error vs global roundoff error



Local error:

$$\varepsilon_0 = |\widetilde{y_0} - y_0|$$
$$\forall n \in \mathbb{N}^*,\ \varepsilon_n = |\widetilde{R}(\widetilde{h}, \widetilde{\lambda}, \widetilde{y_{n-1}}) - R(h, \lambda)\widetilde{y_{n-1}}|.$$

Global error:

$$\forall n \in \mathbb{N},\ E_n = \widetilde{y_n} - y_n.$$

From local to global roundoff error

Local error:

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Global error:

$$\forall n \in \mathbb{N},\ E_n = \widetilde{y_n} - y_n.$$

Theorem 1: Global absolute error of RK methods

Let $C \in \mathbb{R}_+^*$. *Suppose* $\forall n \in \mathbb{N}^*, \varepsilon_n \leqslant C|\widetilde{y_{n-1}}|$. *Then,* $\forall n \in \mathbb{N}$,

$$|E_n| \leqslant (C + |R(h,\lambda)|)^n \left(\varepsilon_0 + n\frac{C|y_0|}{C + |R(h,\lambda)|}\right).$$

Relative roundoff errors

Relative error:

$$\left|\frac{\widetilde{y_n} - y_n}{y_n}\right| \leqslant \left(\frac{C + |R(h,\lambda)|}{|R(h,\lambda)|}\right)^n \left(\frac{\varepsilon_0}{|y_0|} + n\frac{C}{C + |R(h,\lambda)|}\right).$$

Relative roundoff errors

Relative error:

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If $C \ll |R(h,\lambda)|$, then:

$$\left|\frac{\widetilde{y_n} - y_n}{y_n}\right| \lesssim \frac{\varepsilon_0}{|y_0|} + n\frac{C}{|R(h,\lambda)|}.$$

In practice (Euler, RK2, RK4): $C \leq 200u$ and $200u \ll |R(h,\lambda)|$.

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Technical lemma for local roundoff errors

Local error of stable Euler's method ($-2 \leq h\lambda < 0$):

$$\varepsilon_{n+1} = |\widetilde{y_n} \oplus (\widetilde{h} \otimes \widetilde{\lambda} \otimes \widetilde{y_n}) - (1 + h\lambda)y_n|.$$

Technical lemma for local roundoff errors

Local error of stable Euler's method ($-2 \leq h\lambda < 0$):

$$\varepsilon_{n+1} = |\underbrace{\widetilde{y_n}}_{X_1} \oplus (\underbrace{\widetilde{h} \otimes \widetilde{\lambda}}_{X_2} \otimes \underbrace{\widetilde{y_n}}_{y}) - (\underbrace{1}_{\alpha_1} + \underbrace{h\lambda}_{\alpha_2}) \underbrace{\widetilde{y_n}}_{y}|.$$

Lemma 2

Let $y \in \mathbb{R}$. *Let* $C_1, C_2 \in \mathbb{R}_+$. *Let* $\alpha_1, \alpha_2 \in \mathbb{R}$. *Let* $X_1, X_2 \in \mathbb{F}$ *s.t.* $|X_1 - \alpha_1 y| \leqslant C_1 |y|$ *and* $|X_2 - \alpha_2| \leq C_2$.

Then:

$$|X_1 \oplus (X_2 \otimes y) - (\alpha_1 + \alpha_2) y| \leqslant |y| \left(C_1 + C_2 + u\left(|\alpha_1| + 2|\alpha_2| + C_1 + 2C_2\right) + u^2 \left(C_2 + |\alpha_2|\right)\right).$$

Technical lemma for local roundoff errors

Local error of stable Euler's method ($-2 \leq h\lambda < 0$):

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Then:

$$|X_1 \oplus (X_2 \otimes y) - (\alpha_1 + \alpha_2) y| \leqslant |y| \left(C_1 + C_2 + u\left(|\alpha_1| + 2|\alpha_2| + C_1 + 2C_2\right) + u^2\left(C_2 + |\alpha_2|\right)\right).$$

$$|\underbrace{\widetilde{y_n}}_{X_1} - \underbrace{1}_{\alpha_1} \underbrace{\widetilde{y_n}}_{y}| \leq \underbrace{0}_{C_1} |\underbrace{\widetilde{y_n}}_{y}|, \qquad |\underbrace{\widetilde{h} \otimes \widetilde{\lambda}}_{X_2} - \underbrace{h\lambda}_{\alpha_2}| \leq \underbrace{6u}_{C_2}$$

(Gappa [Melquiond]).

Local roundoff errors of higher-order methods

Stable RK4 method:

	C	
$\widetilde{y_n}$	0	
$\circ\left[\widetilde{h\frac{1}{6}\lambda}\right]$	$2u$	$(Gappa)$
$\circ\left[\widetilde{y_n + h\frac{1}{6}\lambda y_n}\right] = \widetilde{y_n} \oplus \widetilde{h} \oslash 6 \otimes \widetilde{\lambda} \otimes \widetilde{y_n}$	$4u$	$(Lemma\,2)$
$\circ\left[\widetilde{h\frac{1}{3}\lambda}\right]$	$4u$	$(Gappa)$
$\circ\left[\widetilde{hh\frac{1}{6}\lambda\lambda}\right]$	$12u$	$(Gappa)$
$\circ\left[\widetilde{hhh\frac{1}{12}\lambda\lambda\lambda}\right]$	$28u$	$(Gappa)$
$\circ\left[\widetilde{hhhh\frac{1}{24}\lambda\lambda\lambda\lambda}\right]$	$53u$	$(Gappa)$
$\ldots$	$\ldots$	$(7 \times Lemma\,2)$
$\circ\left[\widetilde{y_n + \cdots + hhhh\frac{1}{24}\lambda\lambda\lambda\lambda y_n}\right]$	$194u$	$(Lemma\,2)$

Local roundoff errors of classical methods

Lemma 3: Local error of Euler method

Suppose $-2 \leqslant h\lambda \leqslant -2^{-100}$ *and* $2^{-60} \leqslant h \leqslant 1$. *Then:*
$\forall n \in \mathbb{N}, \quad \varepsilon_{n+1}^{Euler} \leqslant 11.01u\,|\widetilde{y_n}|$.

Lemma 4: Local error of RK2 method

Suppose $-2 \leqslant h\lambda \leqslant -2^{-100}$ *and* $2^{-60} \leqslant h \leqslant 1$. *Then:*
$\forall n \in \mathbb{N}, \quad \varepsilon_{n+1}^{RK2} \leqslant 28.01u\,|\widetilde{y_n}|$.

Lemma 5: Local error of RK4 method

Suppose $-3 \leqslant h\lambda \leqslant -2^{-100}$ *and* $2^{-60} \leqslant h \leqslant 1$. *Then:*
$\forall n \in \mathbb{N}, \quad \varepsilon_{n+1}^{RK4} \leqslant 194u\,|\widetilde{y_n}|$.

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Global roundoff errors of classical methods

Bounds on global errors:

- Euler: $C = 11.01u$

$$|E_n| \leqslant (11.01u + |R(h,\lambda)|)^n \left(\varepsilon_0 + n\frac{11.01u|y_0|}{11.01u + |R(h,\lambda)|}\right);$$

- RK2: $C = 28.01u$

$$|E_n| \leqslant (28.01u + |R(h,\lambda)|)^n \left(\varepsilon_0 + n\frac{28.01u|y_0|}{28.01u + |R(h,\lambda)|}\right);$$

- RK4: $C = 194u$

$$|E_n| \leqslant (194u + |R(h,\lambda)|)^n \left(\varepsilon_0 + n\frac{194u|y_0|}{194u + |R(h,\lambda)|}\right).$$

$\Rightarrow$ no compensation ☹ but reasonable bounds ☺.

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General methodology

$$y_{n+1} = \sum_{i=0}^{M} \alpha_i y_n \qquad \widetilde{y_{n+1}} = \oplus_{i=0}^{M} \widetilde{\alpha_i} \otimes \widetilde{y_n} \qquad (\alpha_i = h\lambda, \frac{h\lambda}{3}, \frac{h\lambda}{6}, \frac{h^4\lambda^4}{24} \dots)$$

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Methodology to bound roundoff errors:

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Methodology to bound roundoff errors:

1) bound $\varepsilon_0 = |\widetilde{y_0} - y_0|$;
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3) bound local errors by M applications of Lemma 2;

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Methodology to bound roundoff errors:

1) bound $\varepsilon_0 = |\widetilde{y_0} - y_0|$;
2) bound the error on each term α_i (Gappa + stability);
3) bound local errors by M applications of Lemma 2;
4) bound the global error by instantiating Theorem 1.

Conclusion and perspectives

Conclusion:

- fine and mechanical analysis of roundoff errors;
- results on useful and classical methods (Euler, RK2, RK4);
- linear growth of roundoff errors;
- no compensation (for explicit one-step methods).

Perspectives:

- overflows and underflows;
- formalization in Coq (proof assistant):
  - based on the Flocq library [Boldo-Melquiond],
  - based on the gappa and interval tactics [Melquiond],
- more general ODEs: complex, matricial, non-linear;
- more general methods: multi-step, variable step, implicit.