

# Adaptive numerical solvers

## for Ordinary Differential Equations

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<https://github.com/poliprojects/apc-project>

# Introduction

# Ordinary differential equations (ODE)

Given  $I = [t_0, t_F] \subset \mathbb{R}$ ,  $f(t, \mathbf{y}) : I \times \mathbb{R}^n \rightarrow \mathbb{R}^n$ ,  $f \in C^1$ , and  $t_0 \in I, \mathbf{y}_0 \in \mathbb{R}^n$ :

## Initial Value Problem (IVP):

find a  $C^1$  function  $\mathbf{y}(t) : I \rightarrow \mathbb{R}^n$  that solves

$$\begin{cases} \mathbf{y}'(t) = f(t, \mathbf{y}(t)) & \text{with } t \in I \\ \mathbf{y}(t_0) = \mathbf{y}_0 \end{cases}$$

(first order ODE)

Existence and uniqueness guaranteed under *Lipschitz continuity* of  $f$

# Iterative methods

- Discretization of time into  $N$  intervals:  $t_0, t_1, \dots, t_N = t_F$  through a discretization step  $h$ :  $t_{n+1} = t_n + h$ , with  $n = 0, 1, \dots, N$
- $\mathbf{y}(t_n)$  is numerically approximated by  $\mathbf{u}_n$ :

$$\mathbf{u}_0 = \mathbf{y}_0, \mathbf{u}_1, \dots, \mathbf{u}_N \in \mathbb{R}^n$$

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- In **single-step methods**,  $\mathbf{u}_{n+1}$  depends directly only on the one previous step  $\mathbf{u}_n$ :

$$\mathbf{u}_{n+1} = \mathbf{u}_n + h \phi(t_n, h, \mathbf{u}_n, \mathbf{u}_{n+1}, f)$$

- In **explicit** methods,  $\mathbf{u}_{n+1}$  does not appear in  $\phi$
- In **implicit** methods,  $\mathbf{u}_{n+1}$  appears in  $\phi$   
 $\implies$  nonlinear equations

# Runge-Kutta methods

- Family of **single-step** methods
- Weighted average of  $s$  evaluations (**stages**) of  $f$ :

$$\mathbf{u}_{n+1} = \mathbf{u}_n + h \sum_{i=1}^s b_i \mathbf{K}_i \quad \text{with}$$

$$\mathbf{K}_i = f(t_0 + c_i h, \mathbf{u}_n + \sum_{j=1}^s a_{ij} \mathbf{K}_j)$$

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- *Butcher tableau*:

$c_1$	$a_{11}$	$\dots$	$a_{1s}$
$\vdots$		$\ddots$	
$c_s$	$a_{s1}$		$a_{ss}$
	$b_1$	$\dots$	$b_s$

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$$\text{with } c_i = \sum_j a_{ij}$$

- $O(sn^2)$  if  $f$  linear
- Explicit if  $[a_{ij}]_{ij}$  is lower triangular



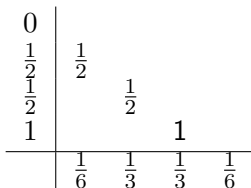
# Examples of RK variants (1)

- **Forward Euler (FE)** (explicit):

$$a = 0, \quad b = 1, \quad c = 0$$

$$\mathbf{u}_{n+1} = \mathbf{u}_n + hf(t_n, \mathbf{u}_n)$$

- **RK4 (standard)** (explicit):



## Examples of RK variants (2)

- Heun (explicit):

$$\begin{array}{c|cc}
 0 & & \\
 1 & 1 & \\
 \hline
 & \frac{1}{2} & \frac{1}{2}
 \end{array}$$

- Iserles-Nørsett (implicit):

$$\begin{array}{c|cccc}
 \frac{1}{3} & & & & \\
 \frac{2}{3} & & & & \\
 \frac{3}{3} & & & & \\
 \frac{21+\sqrt{57}}{48} & & & & \\
 \frac{21-\sqrt{57}}{48} & & & & \\
 \hline
 & \frac{9+3\sqrt{57}}{16} & \frac{9+3\sqrt{57}}{16} & -\frac{1+3\sqrt{57}}{16} & -\frac{1+3\sqrt{57}}{16}
 \end{array}$$

# Convergence analysis for RK

- **Convergence**  $\rightarrow$  absolute error:  $\|y_n - u_n\| \simeq O(h^q)$
- **Consistence**  $\rightarrow$  truncation error:  $\max_n \|\tau_n(h)\| \simeq O(h^q)$
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- Under reasonable Lipschitz continuity assumptions on  $\phi$ , a single-step method which is consistent is also convergent
- Runge-Kutta is consistent iff  $\sum_i b_i = 1 \implies$  **convergent**
- Steep limitations on order of convergence:
  - ▶ Maximum order is the number of stages
  - ▶ If  $s \geq 5$ , equality cannot be achieved in explicit variants

order	5	6	7	8
minimum $s$	6	7	9	11

# Adaptive methods

- Step  $h$  is **updated** at every iteration adaptively, i.e. based on the trend of the solution
  - ▶ Small  $h$  near steep slopes, large  $h$  near flat points
  - ▶ A *a posteriori* **estimate of error** is needed
  - ▶ Compute two-round solution with  $\frac{h}{2}$ , with single-round solution with  $h$
- No need for input of “correct” step
- Computational gain

# Consistency of adaptive methods

Forward Euler:

- Truncation errors:

$$e_h = h^2/2y''(\xi), \quad e_{h/2} = h^2/8y''(\eta) \cdot 2 + o(h^2)$$

- Error estimate:

$$|u_{h/2} - u_h| \simeq |e_{h/2}| \simeq h^2/4|y''(\hat{\eta})| + o(h^2) \stackrel{\downarrow}{<} \frac{\varepsilon}{2} \quad (\text{tolerance})$$

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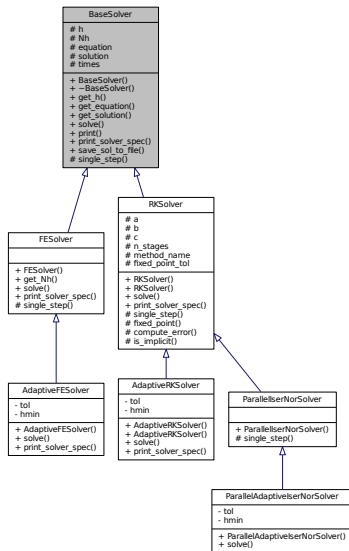
Runge-Kutta:

- ...

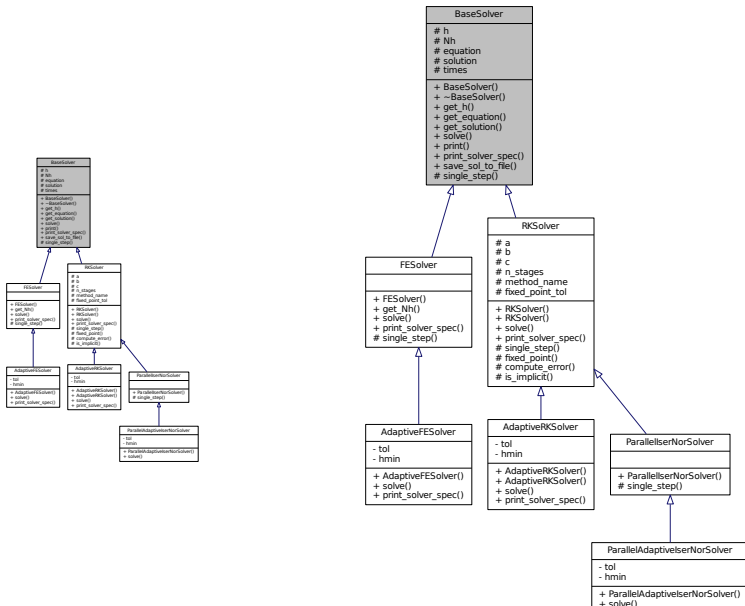
# Code structure



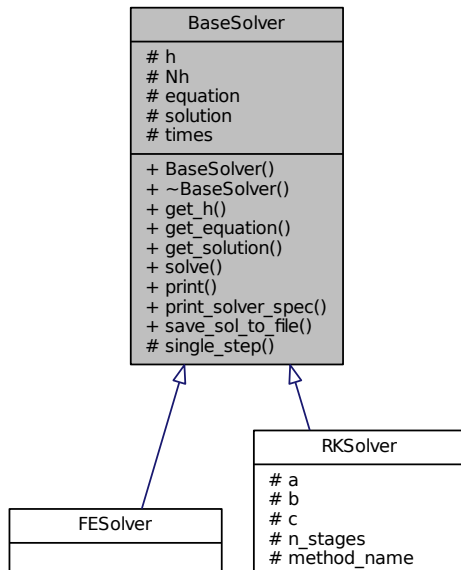
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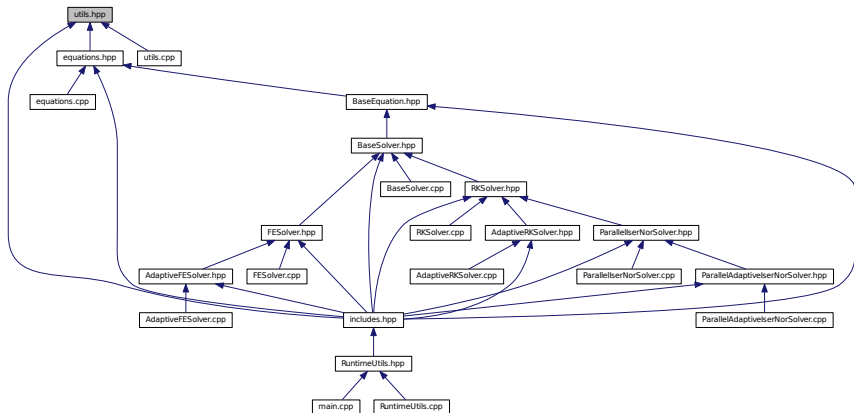
# Base classes



# Adaptive classes

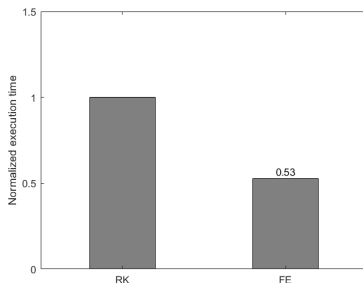


# Dependencies



# Implementation choices

- Seven test functions are provided
- Separate FE class is much more efficient than RK specialized class:



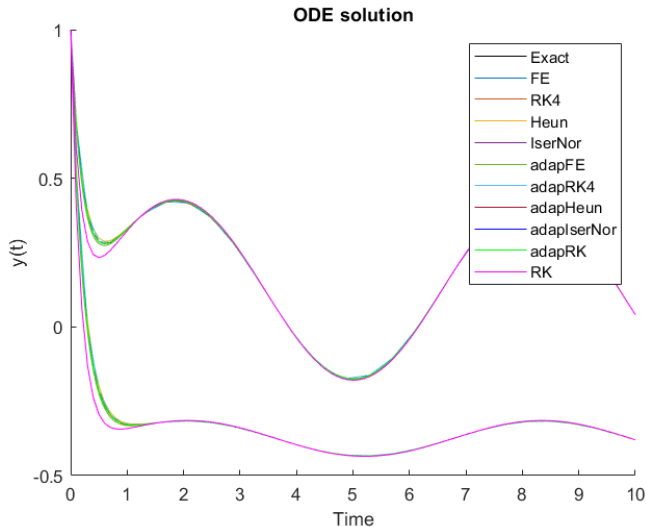
- Adaptive `single_step()` class methods are not efficient

# Parallel Iserles-Nørsett

- Exploits block-diagonal structure of Butcher array
- Runs in parallel on 2 processors, each dealing with one independent 2-by-2 block
- Fixed point algorithm was used for nonlinear equations

# Results

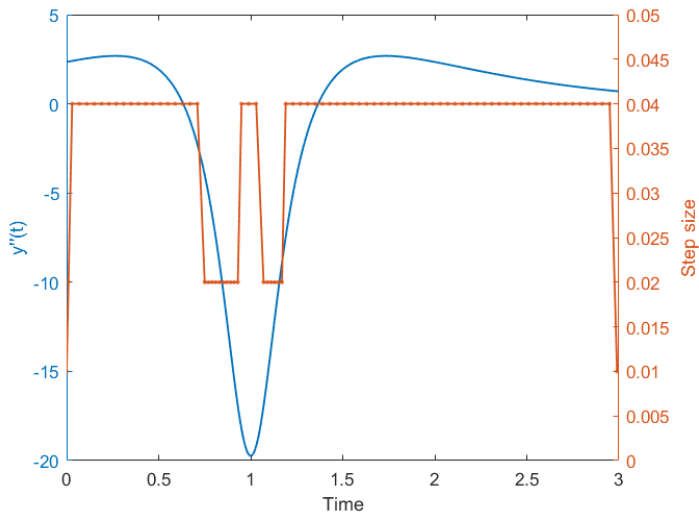
# Comparison between methods



(components of test #4)



# Trend of step in adaptive methods



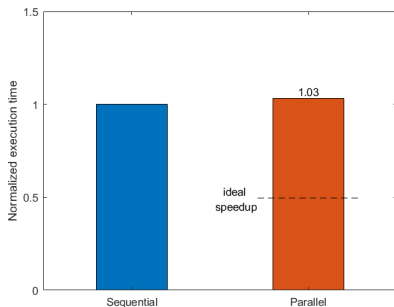
(test #7, adaptive Heun method)

# Actual efficiency of parallelism

Speedup is heavily dependent on the problem function:

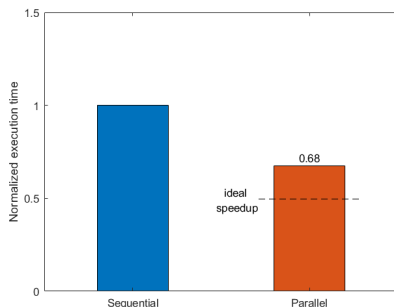
Test #5

$$f(t, y(t)) = -16y(t)$$



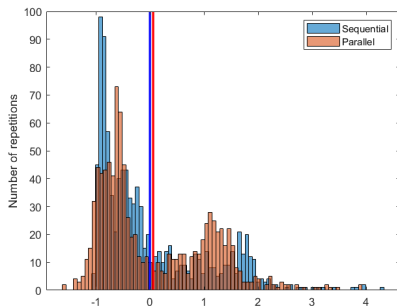
Test #6

$$f(t, y(t)) = \exp_2(-\frac{y(t)}{4}) + 6 + 10t$$

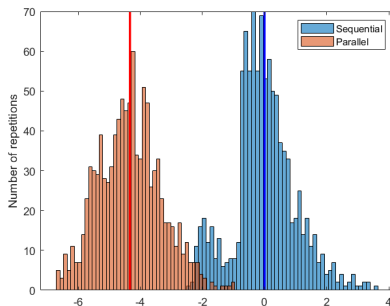


# Multiple run results

Test #5



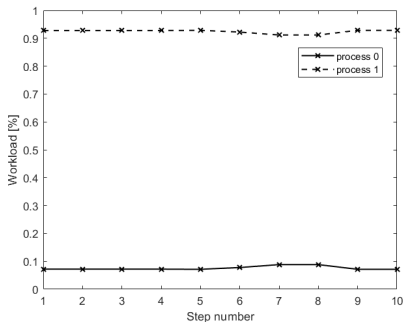
Test #6



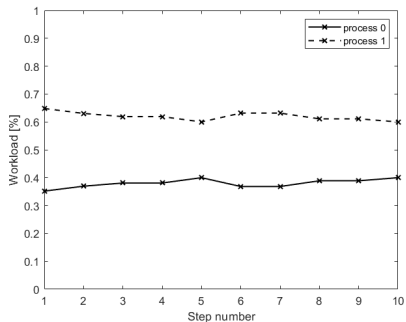
Why?

# Workload distribution

Test #5



Test #6

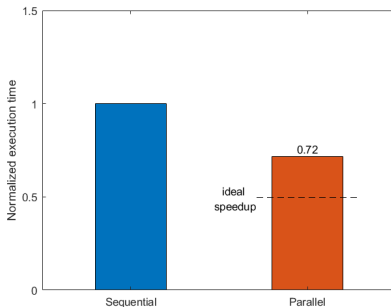
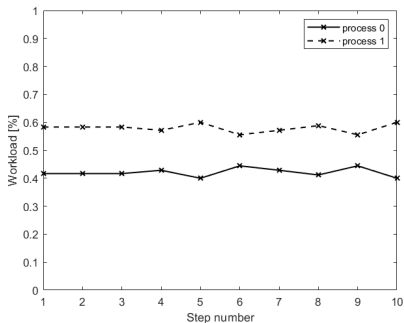


⇒ load imbalance





# A vectorial example

- Efficiency still depends on the function
- Here fixed point iterations are well-balanced among processors:

Test #4: 
$$\mathbf{f}(t, \mathbf{y}(t)) = \begin{bmatrix} -3 & -1 \\ 1 & -5 \end{bmatrix} \mathbf{y}(t) + \begin{bmatrix} \sin(t) \\ -2t \end{bmatrix}$$



# Bibliography

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-  Quarteroni, Saleri, *Calcolo scientifico*
-  Quarteroni, Sacco, Saleri, Gervasio, *Matematica numerica*
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