

# 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  $f$

# Runge-Kutta methods

- Family of **single-step** methods ( $\mathbf{u}_{k+1}$  depends directly only on  $\mathbf{u}_k$ )
- Weighted average of  $s$  evaluations (**stages**) of  $f$ :

$$\mathbf{u}_{k+1} = \mathbf{u}_k + h \sum_{i=1}^s b_i \mathbf{K}_i \quad \text{with}$$
$$\mathbf{K}_i = f(t_0 + c_i h, \mathbf{u}_k + \sum_{j=1}^s a_{ij} \mathbf{K}_j)$$

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- *Butcher tableau*:

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

with  $c_i = \sum_j a_{ij}$

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with  $c_i = \sum_j a_{ij}$

- $O(sn^2)$  if  $f$  linear
- Explicit if the upper triangular part of  $[a_{ij}]_{ij}$  is null

# Examples of explicit RK variants

- Forward Euler:  $a = 0$ ,  $b = 1$ ,  $c = 0$
- RK4:

0				
$\frac{1}{2}$	$\frac{1}{2}$			
$\frac{1}{2}$		$\frac{1}{2}$		
1			1	
	$\frac{1}{6}$	$\frac{1}{3}$	$\frac{1}{3}$	$\frac{1}{6}$

- Heun:

0		
1	1	
	$\frac{1}{2}$	$\frac{1}{2}$

# Convergence analysis for RK

- **Convergence**  $\rightarrow$  absolute error:  $\|\mathbf{y}(t_k) - \mathbf{u}_k\| \simeq O(h^q)$
- **Consistence**  $\rightarrow$  truncation error:  $\max_k \|\boldsymbol{\tau}_k(h)\| \simeq O(h^q)$
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- 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 posteriori **estimate of error** is needed
  - ▶ Compare two-round solution computed with step  $\frac{h}{2}$ , with single-round solution computed with step  $h$
- No need for input of “correct” step

# Error computation for adaptive methods

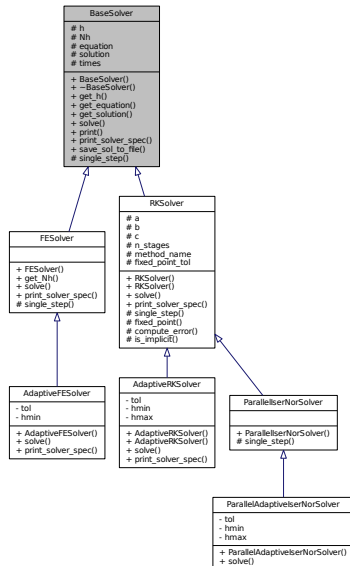
- Relative error in infinity norm is used:

$$\frac{\|\mathbf{u}_{h/2} - \mathbf{u}_h\|_\infty}{\|\mathbf{u}_{k-1}\|_\infty} < \frac{\varepsilon}{2} \quad (\text{tolerance})$$

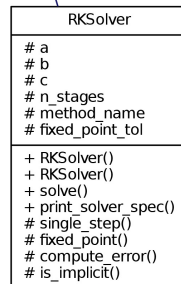
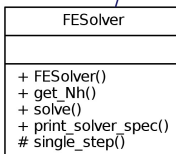
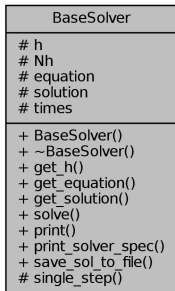
- This guarantees consistency (  $\implies$  convergence )
- At each iteration  $h$  can be doubled, halved, or unchanged
- $h_{min}$  and  $h_{max}$  are required for some methods

# Code structure

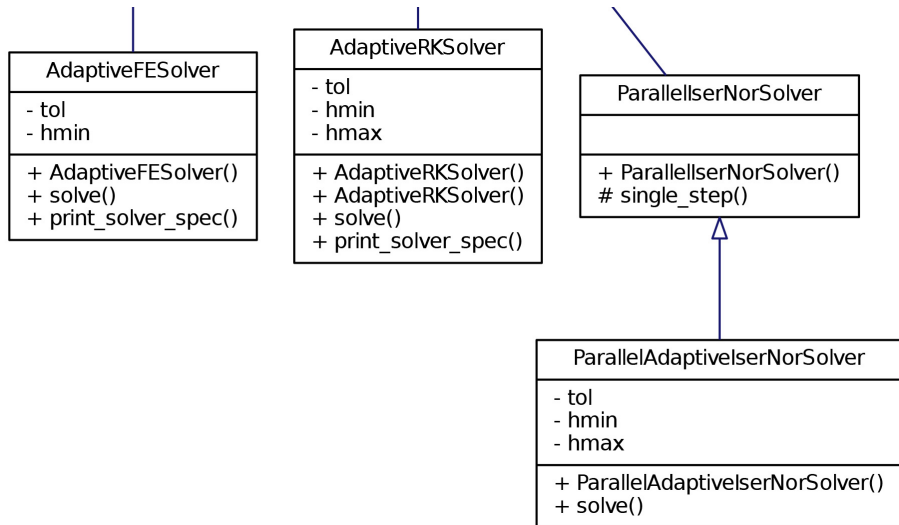
# Code structure



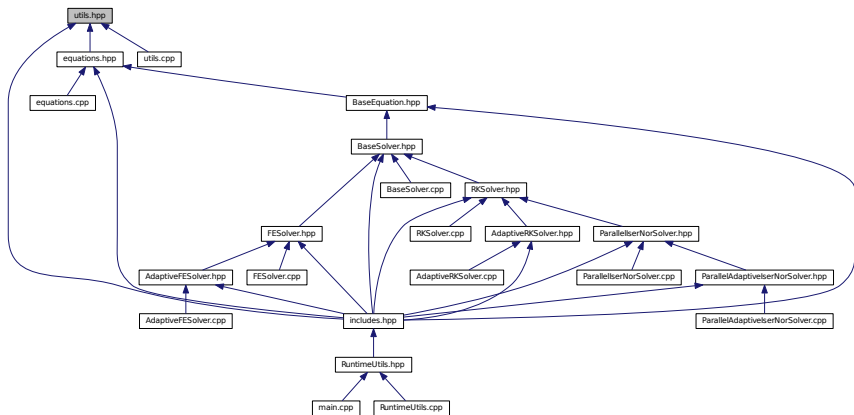
# Base classes



# Adaptive classes



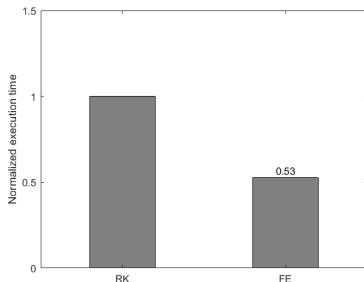
## Dependencies





# 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
- **Fixed point** algorithm was used for implicit methods

# Parallel Iserles-Nørsett

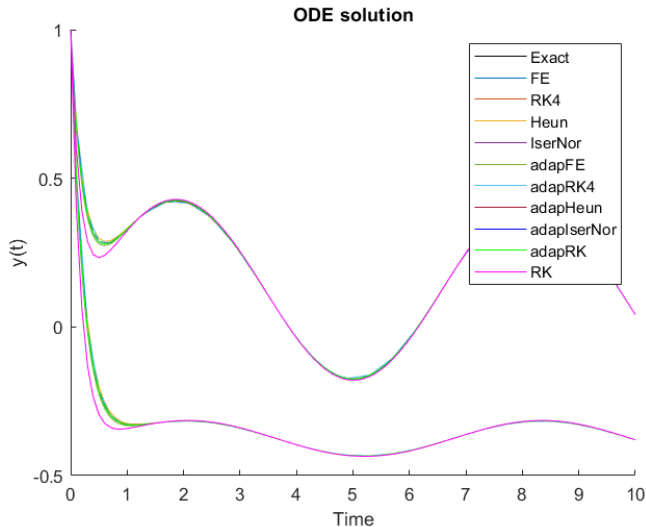
- **Implicit** method:

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

- Parallelization exploits **block-diagonal** structure of Butcher array
- The method runs in parallel on **2 processors**, each dealing with one independent 2-by-2 block

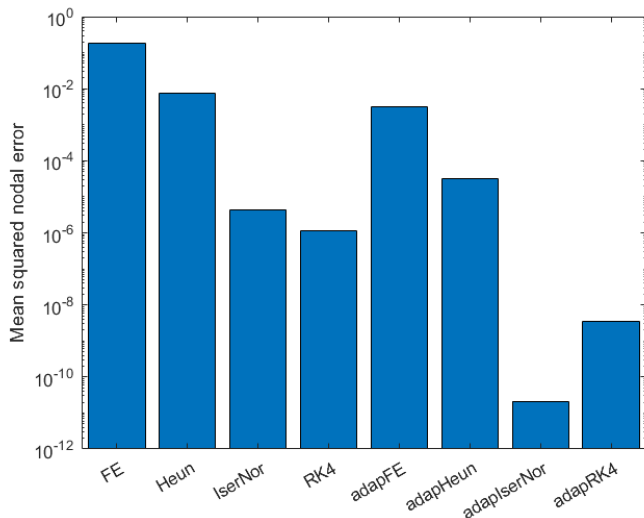
# Results

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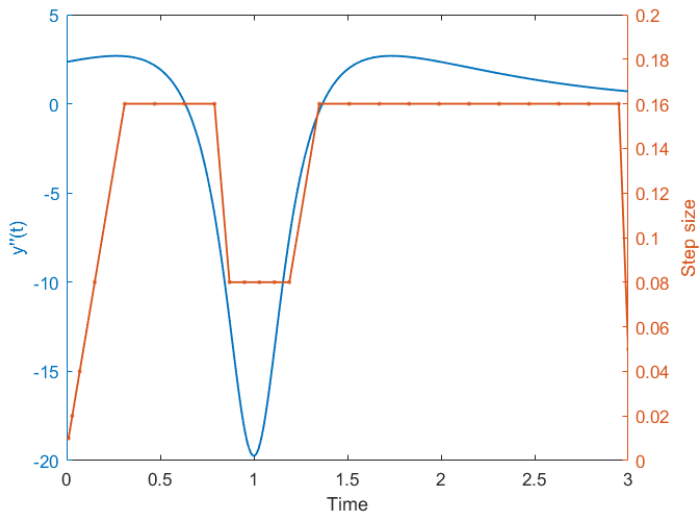
(components of test #4)

# Comparison between methods



(logarithm of relative Mean Square Errors in the nodes, test #1)

# Trend of step size in adaptive methods



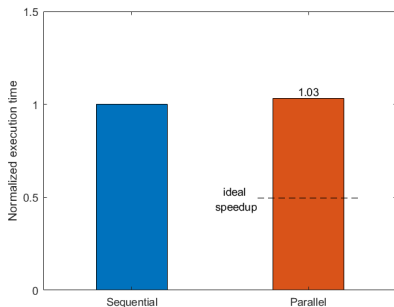
(test #7, adaptive RK4 method)

# Actual efficiency of parallelism

Speedup is heavily dependent on the problem function:

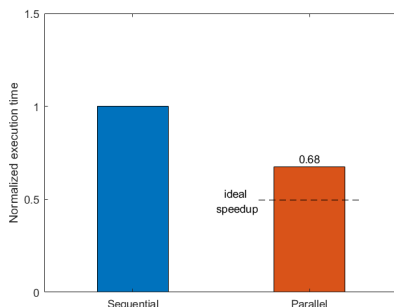
Test #5

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



Test #6

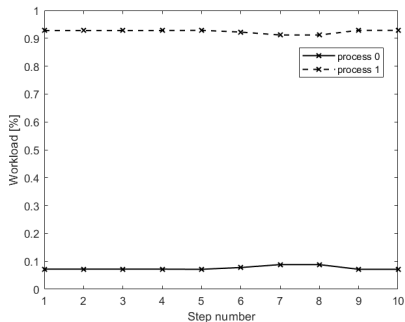
$$f(t, y(t)) = \exp_2\left(-\frac{y(t)}{4}\right) + 6 + 10t$$



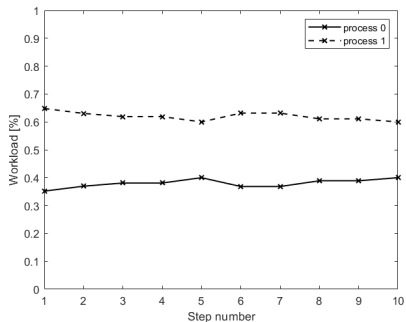
Why?

# Workload distribution

Test #5



Test #6



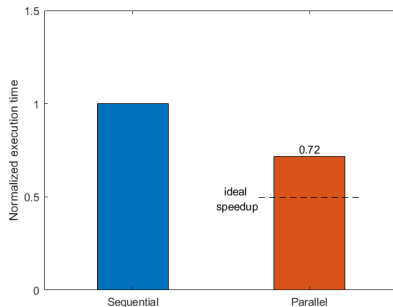
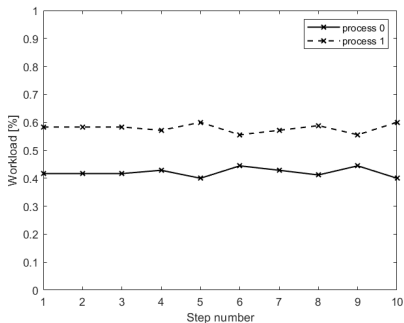
⇒ load imbalance







# 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

-  Podhaisky, *Parallel two-step Runge-Kutta methods*
-  Quarteroni, Saleri, *Calcolo scientifico*
-  Quarteroni, Sacco, Saleri, Gervasio, *Matematica numerica*
-  Solodushkin, Iumanova, *Parallel Numerical Methods for Ordinary Differential Equations: a Survey*