Computational Physics 2022

Sommersemester, 3th April, 2022 – 14th Juli, 2022

1) Introduction
2) Numbers and errors
3) Differentiation and integration
4) Ordinary differential equations
5) Molecular dynamics simulations
6) Partial differential equations
7) Iteration processes
8) Matrixdiagonalisation & Eigenvalue problems
9) Minimization
10) Random numbers
11) Monte Carlo (MC) Simulations
12) Perkolation
13) Stochastic Dynamics

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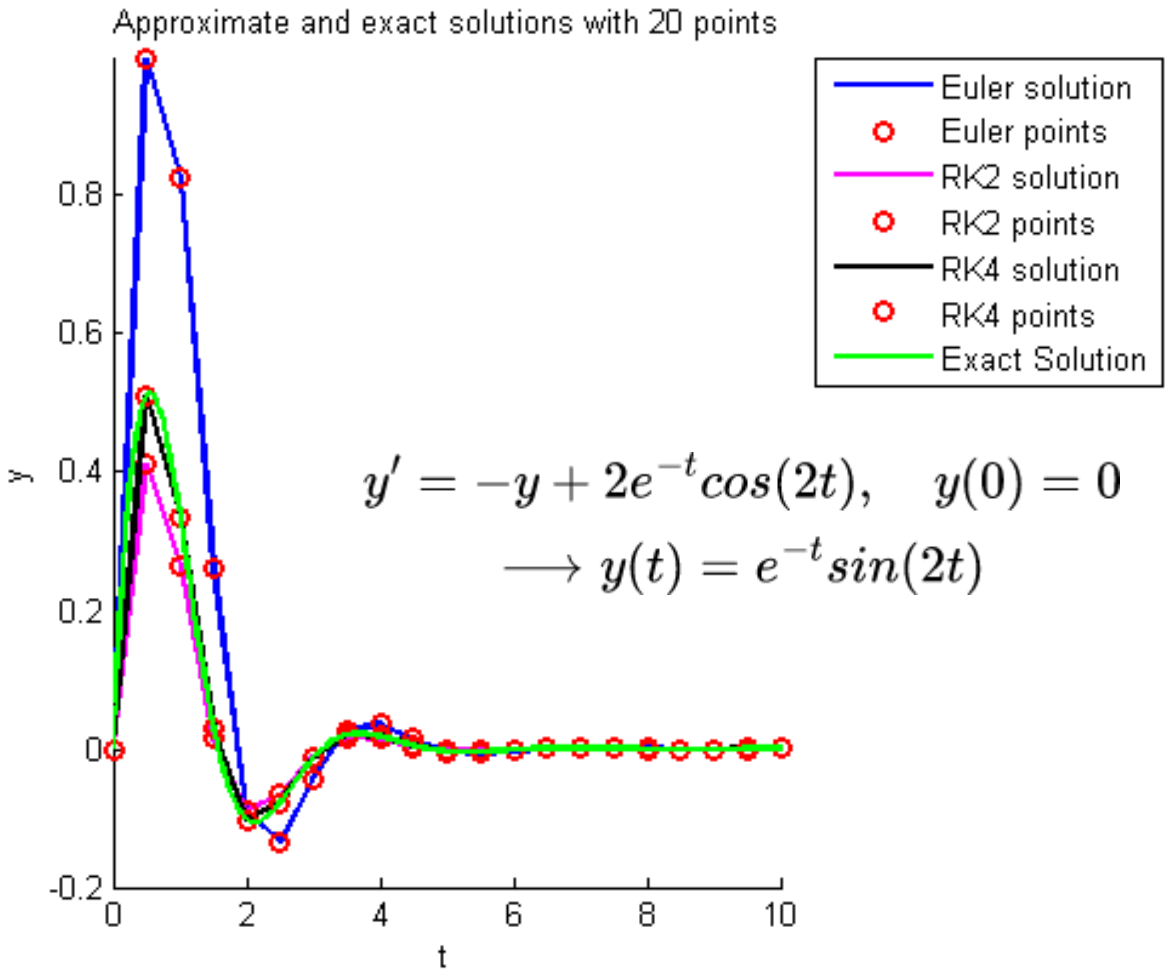
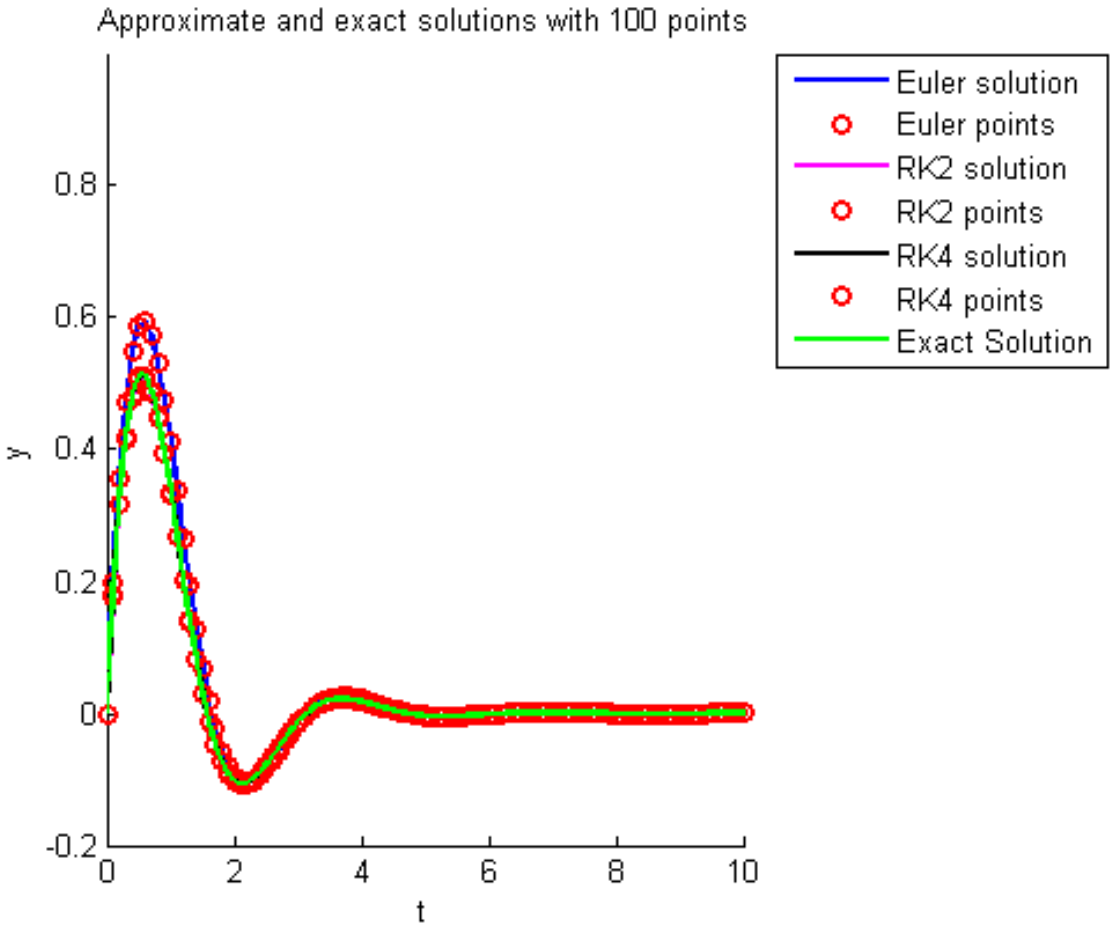
RK family: Example



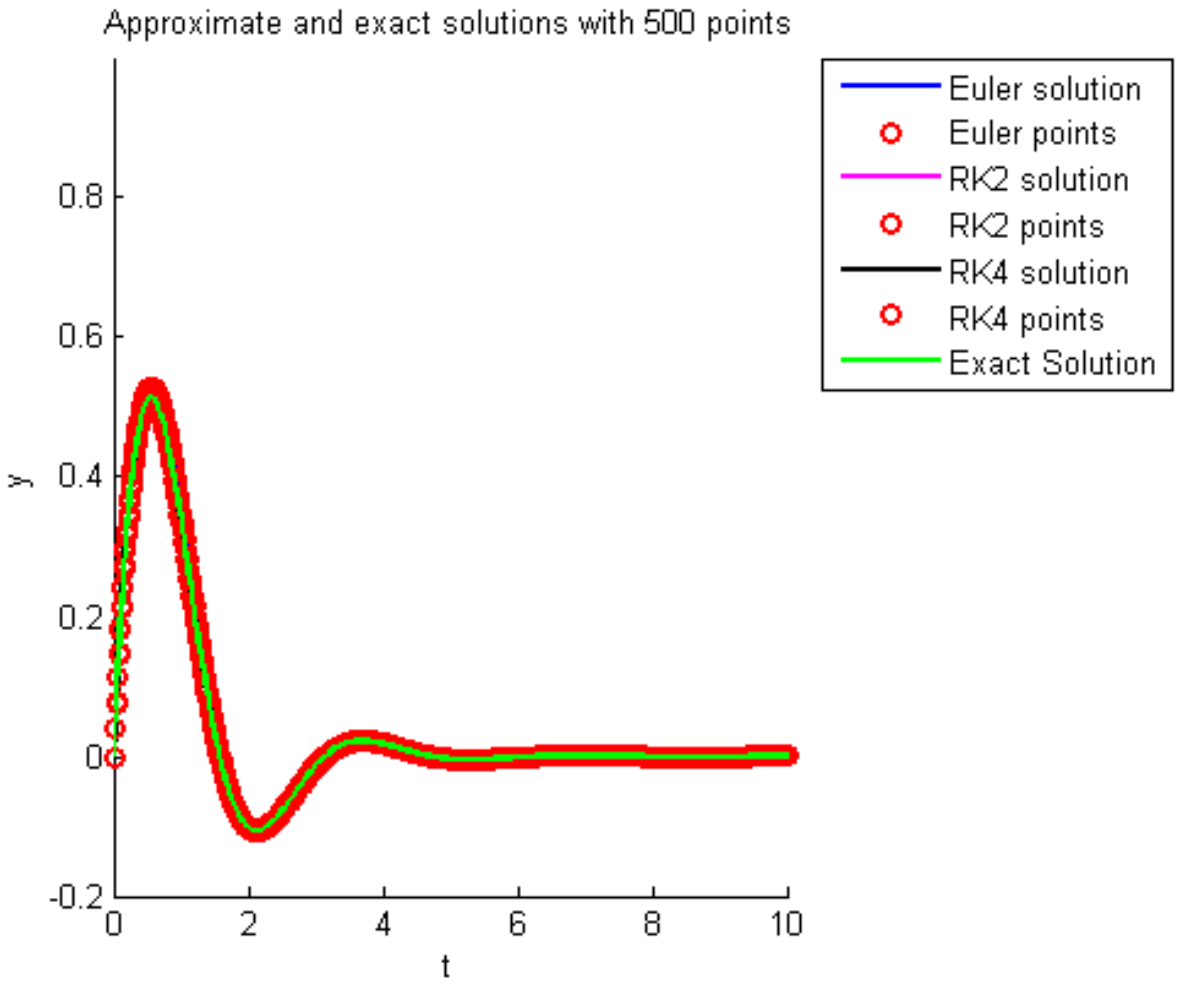
$$y' = -y + 2e^{-t}cos(2t), \quad y(0) = 0$$
$$\longrightarrow y(t) = e^{-t}sin(2t)$$

http://www.math.iit.edu/~fass/matlab/html/EulerRKConvergenceDemo.html

RK family


Approximate and exact solutions with 100 points
Euler solution
Euler points
RK2 solution
RK2 points
RK4 solution
RK4 points
Exact Solution
y
t
0.8
0.6
0.4
0.2
0
-0.2
0
2
4
6
8
10

RK family


Approximate and exact solutions with 500 points
Euler solution
Euler points
RK2 solution
RK2 points
RK4 solution
RK4 points
Exact Solution
0.8
0.6
0.4
0.2
0
-0.2
y
0
2
4
6
8
10
t

Simplectic algorithms

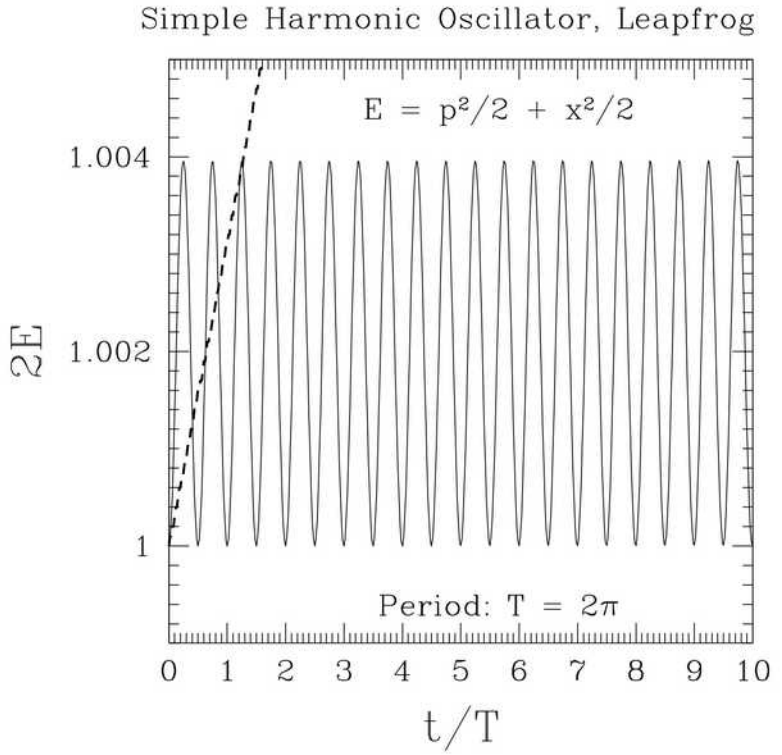
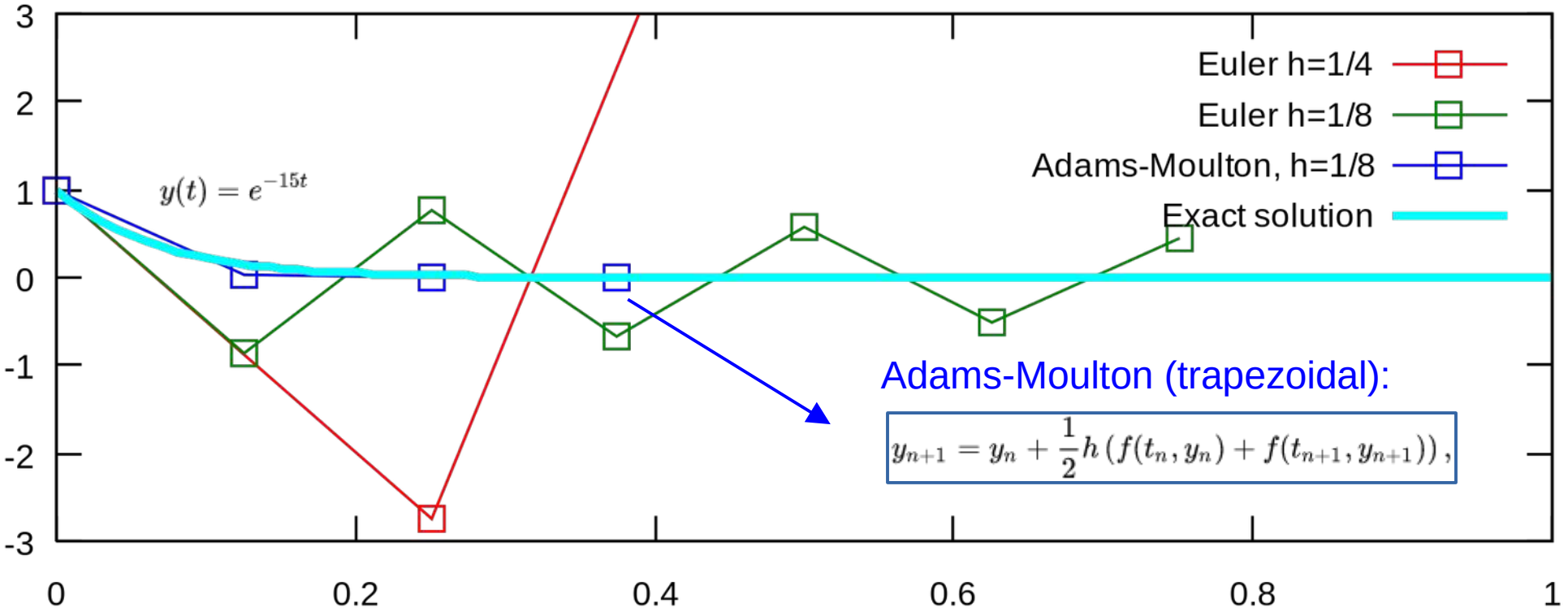


FIG. 5: Variation of (twice) the energy E as a function of time for the simple harmonic oscillator using the velocity Verlet algorithm (solid line) and second order Runge-Kutta (RK2) (dashed line). This for $m = k = 1$, with initial conditions, $x = 1, v = 0$ and a timestep of $h = 0.02T$, where the period T is 2π. Since velocity Verlet is symplectic, $2E$ never deviates much from its exact value of 1, but the energy in RK2 deviates more and more at long times.

Stiff equations

https://en.wikipedia.org/wiki/Stiff_equation

$$y'(t) = -15y(t), \quad t \geq 0, y(0) = 1.$$



Adams-Moulton (trapezoidal):

$$y_{n+1} = y_n + \frac{1}{2}h\left(f(t_n, y_n) + f(t_{n+1}, y_{n+1})\right),$$