Numerical Simulation/Integration, Three Examples

- simplest (but not recommended) implementation is a single step of an Euler integrator:

$$\boxed{f(s,a) := s + \Delta t \; f_\mathrm{c}(s,a)}$$

- more accurate are N steps of an Euler integrator:

$$
\begin{aligned}
&x_0 := s\\
&\text{for } i = 0 \text{ to } N-1 \text{ do}\\
&\qquad x_{i+1} := x_i + (\Delta t/N) f_\mathrm{c}(x_i, a)\\
&f(s,a) := x_N
\end{aligned}
$$

- more efficient are higher order **Runge Kutta (RK)** methods, e.g. a single RK4 step:

$$
\begin{aligned}
v_1 &:= f_\mathrm{c}(s,a)\\
v_2 &:= f_\mathrm{c}(s + (\Delta t/2)\; v_1, a)\\
v_3 &:= f_\mathrm{c}(s + (\Delta t/2)\; v_2, a)\\
v_4 &:= f_\mathrm{c}(s + \Delta t \; v_3, a)\\
f(s,a) &:= s + (\Delta t/6)\; (v_1 + 2v_2 + 2v_3 + v_4)
\end{aligned}
$$

Euler vs 4th Order Runge Kutta Method (RK4) for Test Problem

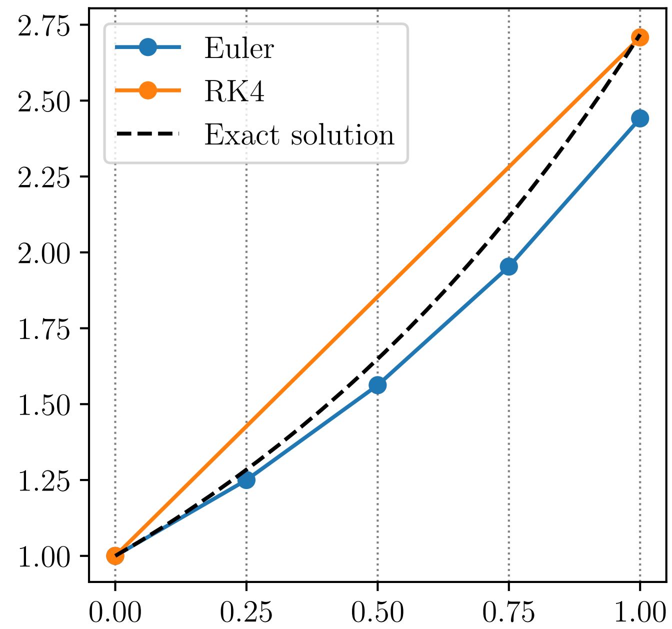
Aim: solve $\dot{s} = s + a$ for $\Delta t = 1, s = 1, a = 0$. Exact solution is $f(s, a) = e = 2.718$.

- Four Euler steps give

$$
\begin{aligned}
x_0 &:= 1 \\
x_1 &:= x_0 + 1/4 x_0 \quad [= (1 + 1/4) x_0] \\
x_2 &:= (1 + 1/4) x_1 \\
x_3 &:= (1 + 1/4) x_2 \\
x_4 &:= (1 + 1/4) x_3 \\
f_{\text{Euler}}(s, a) &:= x_4 \quad [= (1{+}1/4)^4 = 2.441], \text{ error} > 10\%
\end{aligned}
$$

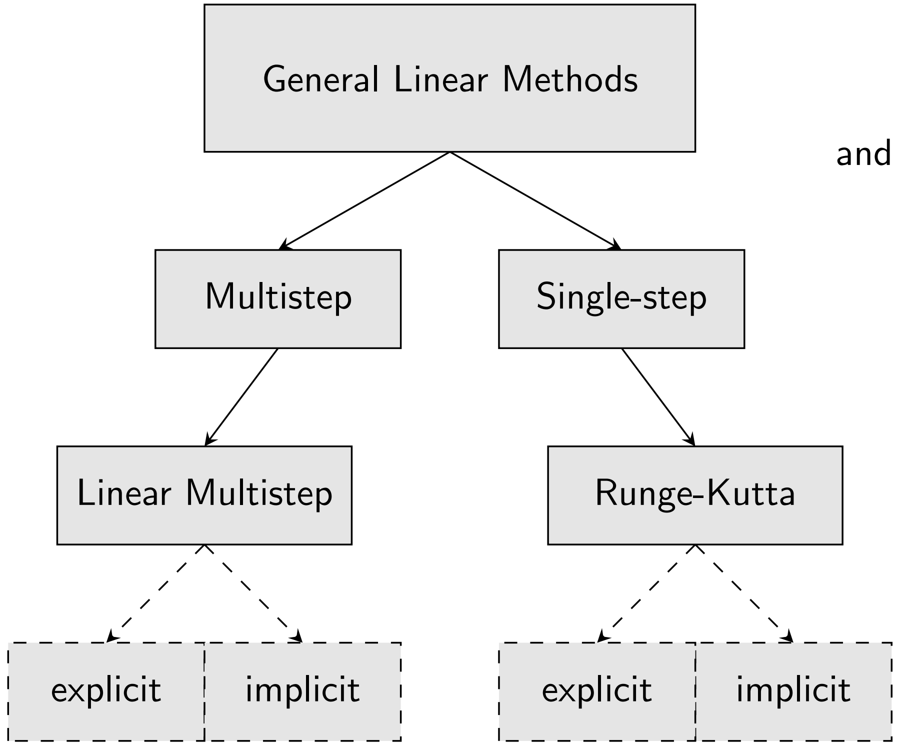
- One RK4 step gives

$$
\begin{aligned}
v_1 &:= 1 \\
v_2 &:= 1 + 1/2 v_1 \quad [= 6/4] \\
v_3 &:= 1 + (1/2) v_2 \quad [= 7/4] \\
v_4 &:= 1 + v_3 \quad [= 11/4] \\
f_{\text{RK4}}(s, a) &:= 1{+}(1/6)\ (v_1{+}2v_2{+}2v_3{+}v_4)\ [= 2.708]
\end{aligned}
$$



RK4 is 27x more accurate than Euler for same number $M = 4$ of function evaluations

Classes of Numerical Simulation Methods



and others ...

Fourth order RK method most efficient for typically desired accuracies

- each integration method is characterized by
  - integration order P and
  - number of internal stages S
- can increase accuracy by more integration steps N
- total number of function evaluations is $M = N \cdot S$
- integration error proportional to M^{-P}
- for small M, low order methods are most accurate, e.g., Euler with $P = 1$
- for large M, high order methods are more accurate
- humans typically want errors smaller than 10%, but rarely smaller than 10^{-6}
- accidentally, this favours the RK4 method $(P = 4)$