First differential approximation (FDA) for ODE systems with parameters

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FDA

In the 60s of the last century, N. N. Yanenko [1] formulated a method for differential approximation of a difference scheme. The main idea of this method is to replace the study of the properties of a difference scheme with the study of a problem with differential equations occupying an intermediate position between the original differential problem and its difference scheme. In the works of N. N. Yanenko and his students, as a result, concepts such as the approximation viscosity of the difference scheme and the first differential approximation (FDA) of the difference scheme were formulated.

There are a large number of numerical methods for solving ODE.

The FDA allows to obtain information about the quality of the selected numerical method for a specific system using only symbolic calculations.
We consider a first-order ODE system resolved with respect to the first derivatives and present an algorithm to calculate the FDA. The algorithm is a set of simple operations with formal power series.

Consider Jacobi oscillator as an example. By definition, the Jacobi functions $p = \operatorname{sn} t$, $q = \operatorname{cn} t$, $r = \operatorname{dn} t$ are a particular solution of a nonlinear autonomous system with the initial conditions are $p = 0$, $q = r = 1$, $k = 1/2$ for $t = 0$. This autonomous system has two quadratic integrals of motion:

$$\begin{cases} p_t - qr = 0, \\ q_t + pr = 0, \\ r_t + k^2 pq = 0, \\ p^2 + q^2 = C_1, \\ k^2 p^2 + r^2 = C_2. \end{cases} \tag{1}$$

Consider the original Runge-Kutta method of 4 orders for Jacobi oscillator (1)

$$
\begin{cases}
\dfrac{\widehat{p}-p}{h} - qr + h\left(\frac{k^2pq^2}{2} + \frac{pr^2}{2}\right) + \\
\quad + h^2\left(-\frac{k^2qr(2p-q)(2p+q)}{6} + \frac{qr^3}{6}\right) + \ldots = 0, \\
\dfrac{\widehat{q}-q}{h} + pr + h\left(-\frac{k^2p^2q}{2} + \frac{qr^2}{2}\right) + \\
\quad + h^2\left(\frac{k^2pr(p-2q)(p+2q)}{6} - \frac{pr^3}{6}\right) + \ldots = 0, \\
\dfrac{\widehat{r}-r}{h} + k^2pq + h\left(\frac{k^2r(q-p)(p+q)}{2}\right) + \\
\quad + h^2\left(\frac{k^4pq(p-q)(p+q)}{6} - \frac{2k^2pqr^2}{3}\right) + \ldots = 0.
\end{cases}
\tag{2}
$$

Here, for the compactness of formulas, p, q, r are denoted by $p(t), q(t), r(t)$, $\widehat{p}, \widehat{q}, \widehat{r}$ are denoted by $p(t+h), q(t+h), r(t+h)$, and according to the degree of h, the first two terms are given. Let's add the first two integrals to the system (2).

$$\begin{cases} \dfrac{(\widehat{p}^2+\widehat{q}^2)-(p^2+q^2)}{h}=0, \\ \dfrac{(k^2\widehat{p}^2+\widehat{r}^2)-(k^2p^2+r^2)}{h}=0, \end{cases} \tag{3}$$

Substitute Taylor series expansion at the point t for the functions $p(t), q(t), r(t), p(t+h), q(t+h), r(t+h)$ in the system (2), (3)

$$
\begin{cases}
p_t - qr + h\left(\frac{k^2pq^2}{2} + \frac{pr^2+p_{tt}}{2}\right) + \mathcal{O}(h^2) = 0, \\
q_t + pr + h\left(-\frac{k^2p^2q}{2} + \frac{qr^2+q_{tt}}{2}\right) + \mathcal{O}(h^2) = 0, \\
r_t + k^2pq + h\left(-\frac{k^2r(p-q)(p+q)}{2} + \frac{r_{tt}}{2}\right) + \mathcal{O}(h^2) = 0, \\
2\,(pp_t + qq_t) + h\big(pp_{tt} + p_t^2 + qq_{tt} + q_t^2\big) + \mathcal{O}(h^2) = 0, \\
2k^2pp_t + 2rr_t + h\big(k^2\,(pp_{tt} + p_t^2) + rr_{tt} + r_t^2\big) + \mathcal{O}(h^2) = 0.
\end{cases}
\tag{4}
$$

$$
\begin{cases}
p_t - qr + h^4\left(-\frac{k^4 qr\left(3p^4+3p^2q^2-2q^4\right)}{240} - \right. \\
\qquad \left. - \frac{k^2 qr^3(p-q)(p+q)}{80} + \frac{qr^5}{120}\right) + \mathcal{O}(h^5) = 0, \\
q_t + pr + h^4\left(-\frac{k^4 pr\left(2p^4-3p^2q^2-3q^4\right)}{240} + \right. \\
\qquad \left. + \frac{k^2 pr^3(p-q)(p+q)}{80} - \frac{pr^5}{120}\right) + \mathcal{O}(h^5) = 0, \\
r_t + k^2pq + h^4\left(-\frac{k^6 pq\left(2p^4-3p^2q^2+2q^4\right)}{240} + \right. \\
\qquad \left. + \frac{k^4 pqr^2(p-q)(p+q)}{80} + \frac{k^2pqr^4}{80}\right) + \mathcal{O}(h^5) = 0, \\
h^4\left(\frac{k^4 pqr(p-q)(p+q)\left(p^2+q^2\right)}{24}\right) + \mathcal{O}(h^5) = 0, \\
h^4\left(\frac{k^2 pqr(kp-r)(kp+r)\left(k^2p^2+r^2\right)}{24}\right) + \mathcal{O}(h^5) = 0.
\end{cases}
\tag{5}
$$

https://github.com/blinkovua/sharing-blinkov/tree/master/FDA_ODE

```
from fde_ode import *

init((p(t), q(t), r(t)), t, h)

def RungeKutta4(f, y):
    k1 = f(y)
    k2 = f(y + h*k1/2)
    k3 = f(y + h*k2/2)
    k4 = f(y + h*k3)
    return expand((k1 + 2*k2 + 2*k3 + k4)/6)

def f(y):
    return Matrix([\
        clip_n(y[1]*y[2]),\
        clip_n(-y[0]*y[2]),\
        clip_n(-k**2*y[0]*y[1]),\
    ])

set_clip(7, 6, Rational(0, 1))
```

```
r = RungeKutta4(f, Matrix([p(t), q(t), r(t)]))

prnlatex(F1, k)
F1 = clip((T(p(t+h))-T(p(t)))/h - T(m[0]))
prn(F1)
prn(F1, k)
prnlatex(F1, k)

f1 = NF(F1, [p(t).diff(t), q(t).diff(t), r(t).diff(t)],\
    [F1, F2, F3], head=False)
...
F4 = clip(((T(p(t+h))**2 + T(q(t+h))**2) -\
             (T(p(t))**2 + T(q(t))**2))/h)
...
f4 = NF(F4, [p(t).diff(t), q(t).diff(t), r(t).diff(t)],\
    [f1, f2, f3], head=True)
...
```

The implicit midpoint method is of second order. It is the simplest method in the class of collocation methods known as the Gauss-Legendre method. It is a symplectic integrator (6)

$$
\begin{array}{c|c}
\frac{1}{2} & \frac{1}{2} \\
\hline
 & 1
\end{array}
\tag{6}
$$

$$
\begin{cases}
\dfrac{p_{n+1} - p_n}{h} - \dfrac{q_{n+1} + q_n}{2}\dfrac{r_{n+1} + r_n}{2} = 0, \\
\dfrac{q_{n+1} - q_n}{h} + \dfrac{p_{n+1} + p_n}{2}\dfrac{r_{n+1} + r_n}{2} = 0, \\
\dfrac{r_{n+1} - r_n}{h} + k^2\dfrac{p_{n+1} + p_n}{2}\dfrac{q_{n+1} + q_n}{2} = 0.
\end{cases}
\tag{7}
$$

Theorem (Cooper, 1983; [12]). The midpoint finite-difference scheme (7) not only approximates the system, but also preserves all linear and quadratic integrals of this system.

$$
\left\{
\begin{array}{l}
p_t - qr + h^2 \left(-\frac{k^2 qr(p-q)(p+q)}{12} + \frac{qr^3}{12} \right) + \mathcal{O}(h^3) = 0, \\
q_t + pr + h^2 \left(\frac{k^2 pr(p-q)(p+q)}{12} - \frac{pr^3}{12} \right) + \mathcal{O}(h^3) = 0, \\
r_t + k^2 pq + h^2 \left(\frac{k^4 pq(p-q)(p+q)}{3} - \frac{k^2 pqr^2}{3} \right) + \mathcal{O}(h^3) = 0, \\
\mathcal{O}(h^\infty) = 0, \\
\mathcal{O}(h^\infty) = 0.
\end{array}
\right.
\tag{8}
$$

Elliptic functions and finite difference method

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The implicit midpoint rule

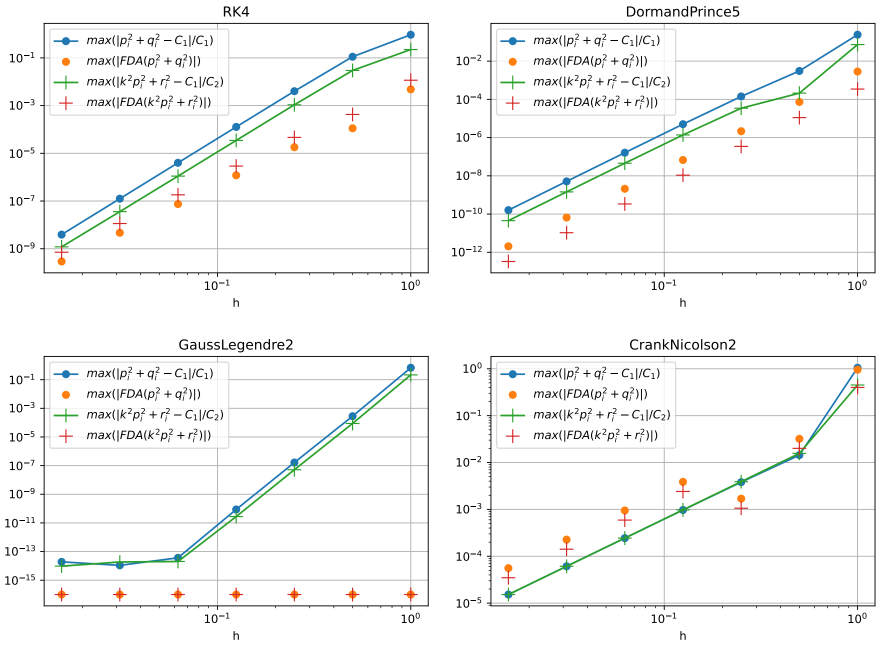
$$\frac{dx}{dt} = F(x) \quad \Rightarrow \quad \frac{x_{n+1} - x_n}{\Delta t} = \frac{F(x_{n+1}) + F(x_n)}{2}$$

Theorem (Cooper, 1987)

The implicit midpoint rule automatically inherits each quadratic conservation law.

If the field of algebraical integrals of dynamic system is generated by quadratic forms, then the implicit midpoint rule is total conservative.

Ref.: *Sanz-Serna J.M.* // SIAM Review. 2016. Vol. 58, No. 1, pp. 3–33.



RK4
DormandPrince5
GaussLegendre2
CrankNicolson2
$max(|p_i^2+q_i^2-C_1|/C_1)$
$max(|FDA(p_i^2+q_i^2)|)$
$max(|k^2p_i^2+r_i^2-C_1|/C_2)$
$max(|FDA(k^2p_i^2+r_i^2)|)$
h
10^{-1}
10^{0}

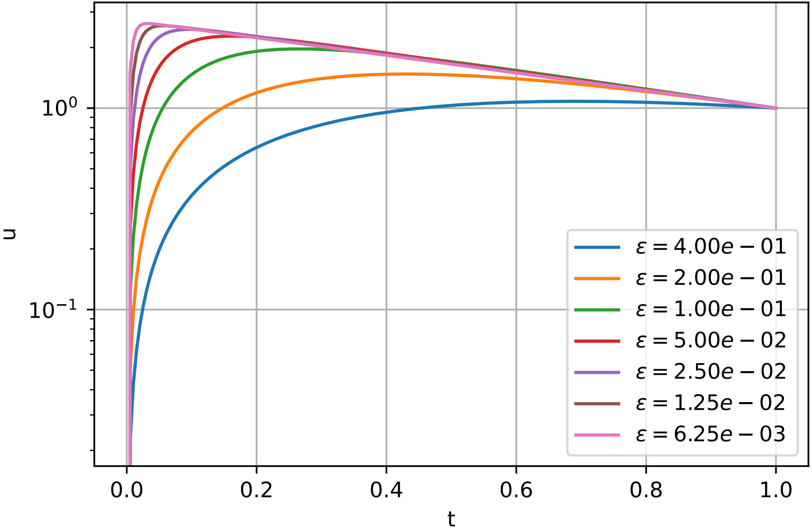
We consider the simple boundary-value problem [6] CHAPTER 12

$$\varepsilon u_{tt} + \left(\varepsilon^2 + 1\right) u_t + \left(1 - \varepsilon^2\right) u = 0. \tag{9}$$

where ε is a small dimensionless positive number. It is assumed that the equation and boundary conditions have been made dimensionless.

$u(0) = 0, u(1) = 1$

$$u = \frac{\left(-e^{\frac{t}{\varepsilon}} + e^{t(\varepsilon+2)}\right) e^{-\varepsilon t+\varepsilon-t+1-\frac{t}{\varepsilon}+\frac{1}{\varepsilon}}}{-e^{\frac{1}{\varepsilon}} + e^{\varepsilon+2}} \tag{10}$$



u
t
10^0
10^{-1}
0.0
0.2
0.4
0.6
0.8
1.0
$\varepsilon = 4.00e - 01$
$\varepsilon = 2.00e - 01$
$\varepsilon = 1.00e - 01$
$\varepsilon = 5.00e - 02$
$\varepsilon = 2.50e - 02$
$\varepsilon = 1.25e - 02$
$\varepsilon = 6.25e - 03$

Gauss-Legendre method FDA

$$\left\{\begin{array}{l} u_t - u_1 + h^2\left(\frac{\varepsilon^2(u-u_1)}{12} - \ldots - \frac{u+u_1}{12\varepsilon^2}\right) + \mathcal{O}(h^4) = 0, \\ {u_1}_t + \varepsilon\,(-u + u_1) + \frac{u+u_1}{\varepsilon} + \\ \qquad\quad + h^2\left(-\frac{\varepsilon^3(u-u_1)}{12} - \ldots + \frac{u+u_1}{12\varepsilon^3}\right) + \mathcal{O}(h^4) = 0. \end{array}\right. \tag{11}$$

Crank-Nicolson method FDA

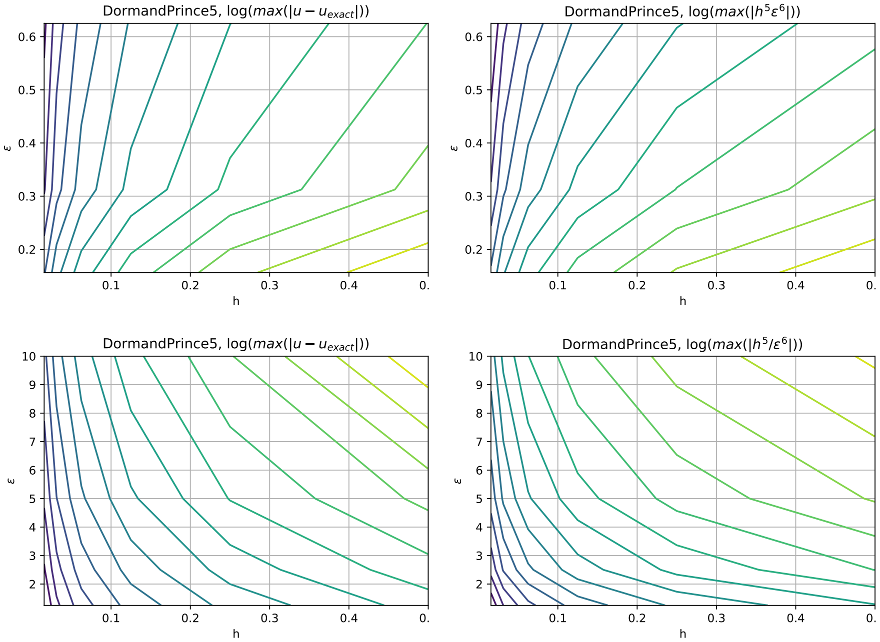
$$\left\{\begin{array}{l} u_t - u_1 + h^2\left(\frac{\varepsilon^2(u-u_1)}{12} - \ldots - \frac{u+u_1}{12\varepsilon^2}\right) + \mathcal{O}(h^4) = 0, \\ \varepsilon\,(-u + u_1) + {u_1}_t + \frac{u+u_1}{\varepsilon} + \\ +h^2\left(-\frac{\varepsilon^3(u-u_1)}{12} - \ldots + \frac{u+u_1}{12\varepsilon^3}\right) + \mathcal{O}(h^4) = 0. \end{array}\right. \tag{12}$$

"original" Runge-Kutta method FDA

$$\begin{cases} u_t - u_1 + h^4 \left(-\frac{\varepsilon^4 (u-u_1)}{120} + \ldots + \frac{u+u_1}{120\varepsilon^4} \right) + \mathcal{O}(h^5) = 0, \\ u_{1\,t} + \varepsilon \left(-u + u_1 \right) + \frac{u+u_1}{\varepsilon} + \\ \qquad\qquad + h^4 \left(\frac{\varepsilon^5 (u-u_1)}{120} + \ldots + - \frac{u+u_1}{120\varepsilon^5} \right) + \mathcal{O}(h^5) = 0. \end{cases} \tag{13}$$

Dormand-Prince 5 order FDA

$$\begin{cases} u_t - u_1 + h^5 \left(-\frac{\varepsilon^5 (u-u_1)}{3600} + \ldots + \frac{u+u_1}{3600\varepsilon^5} \right) + \mathcal{O}(h^6) = 0, \\ u_{1\,t} + \varepsilon \left(-u + u_1 \right) + \frac{u+u_1}{\varepsilon} + \\ \qquad\qquad + h^5 \left(\frac{\varepsilon^6 (u-u_1)}{3600} + \ldots - \frac{u+u_1}{3600\varepsilon^6} \right) + \mathcal{O}(h^6) = 0. \end{cases} \tag{14}$$


DormandPrince5, log($max(|u-u_{exact}|)$)
DormandPrince5, log($max(|h^5\varepsilon^6|)$)
DormandPrince5, log($max(|u-u_{exact}|)$)
DormandPrince5, log($max(|h^5/\varepsilon^6|)$)
ε
h
0.1
0.2
0.3
0.4
0.

Van der Pol oscillator

$$u_{tt} - \mu(1 - u^2)u_t + u = 0 \tag{15}$$

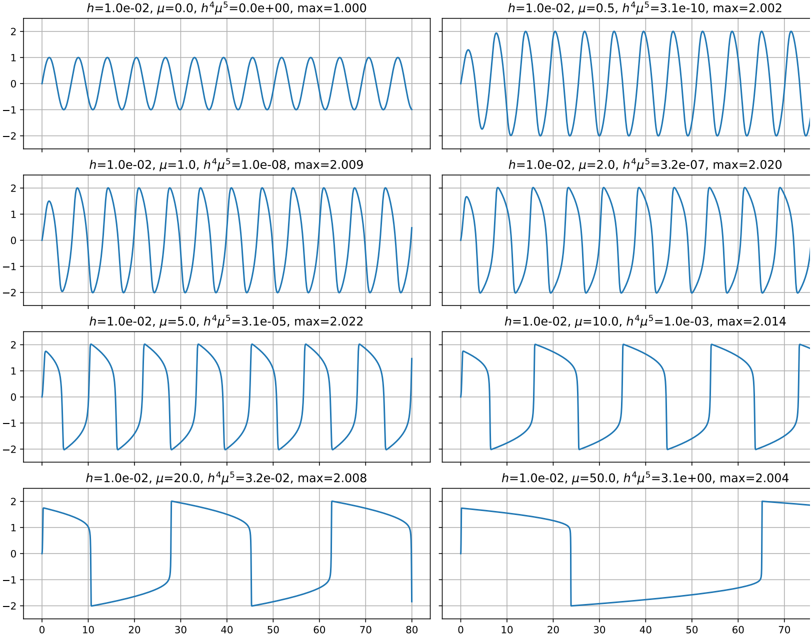
"original" Runge-Kutta method FDA

$$\begin{cases} -u_1 + u_t + h^4 \left(\frac{\mu^4 u_1 (u-1)^4 (u+1)^4}{120} + \ldots + \frac{u_1}{120} \right) + \mathcal{O}(h^5) = 0, \\ \mu u_1 \left(u - 1\right)\left(u + 1\right) + u + u_{1\,t} + \\ \qquad + h^4 \left(-\frac{\mu^5 u_1 (u-1)^5 (u+1)^5}{120} - \ldots - \frac{u}{120} \right) + \mathcal{O}(h^5) = 0. \end{cases} \tag{16}$$

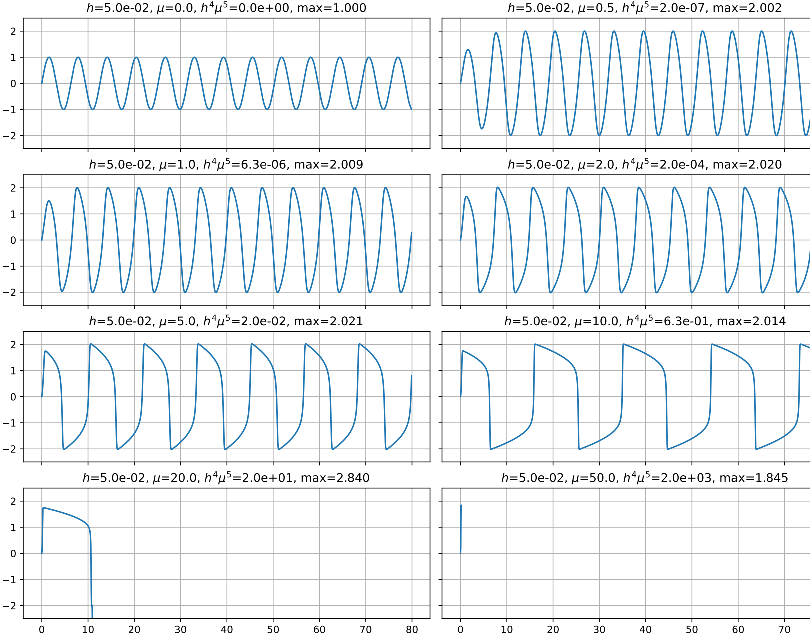
Dormand-Prince 5 order FDA

$$\begin{cases} -u_1 + u_t + h^5 \left(\frac{\mu^5 u_1 (u-1)^5 (u+1)^5}{3600} + \ldots + \frac{u}{3600} \right) + \mathcal{O}(h^6) = 0, \\ \mu u_1 \left(u - 1\right)\left(u + 1\right) + u + u_{1\,t} + \\ \qquad + h^5 \left(-\frac{\mu^6 u_1 (u-1)^6 (u+1)^6}{3600} - \ldots + \frac{u_1}{3600} \right) + \mathcal{O}(h^6) = 0. \end{cases} \tag{17}$$

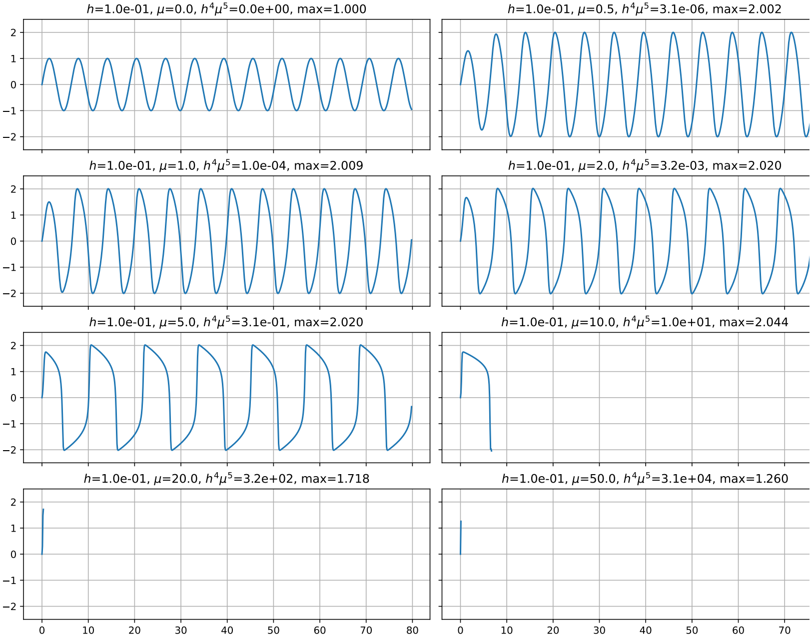
"original" Runge-Kutta $h = 0.01$



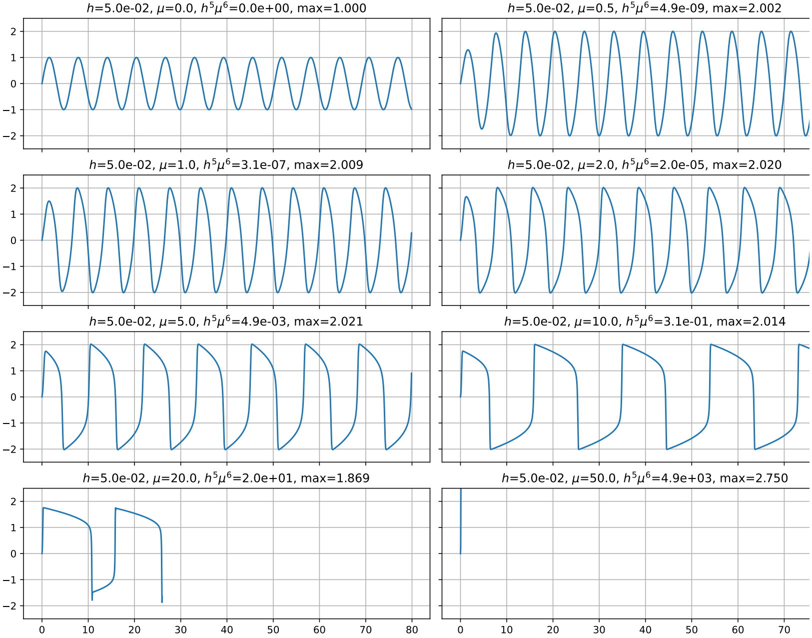
"original" Runge-Kutta $h = 0.05$



"original" Runge-Kutta $h = 0.1$



Dormand-Prince $h = 0.05$



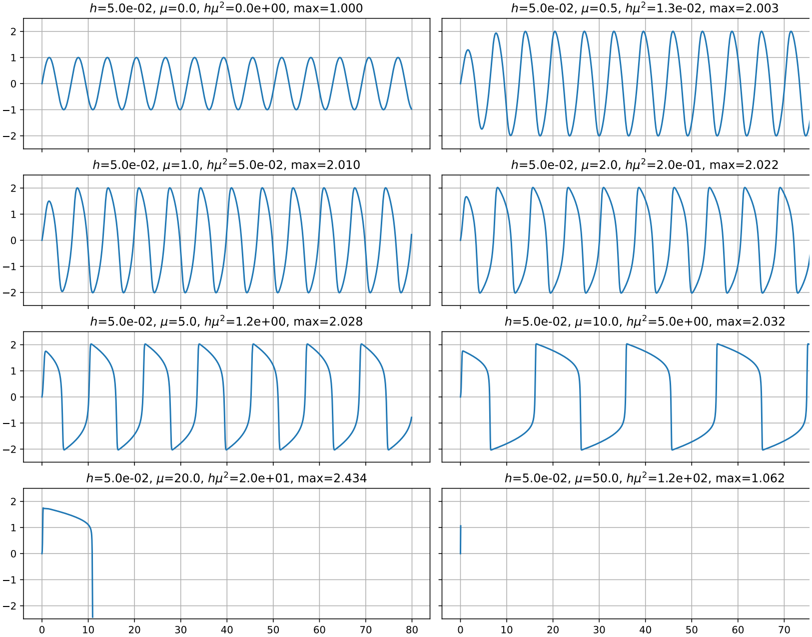
Gauss-Legendre method FDA

$$\begin{cases} -u_1 + u_t + h\left(-\frac{\mu u_1(u-1)(u+1)}{2} - \frac{u}{2}\right) + \mathcal{O}(h^2) = 0, \\ \mu u_1\,(u-1)\,(u+1) + u + u_{1\,t} + h\left(\frac{\mu^2 u_1(u-1)^2(u+1)^2}{2} + \right. \\ \qquad \left. + \frac{\mu u\left(u^2-2u_1^2-1\right)}{2} - \frac{u_1}{2}\right) + \mathcal{O}(h^2) = 0. \end{cases} \tag{18}$$

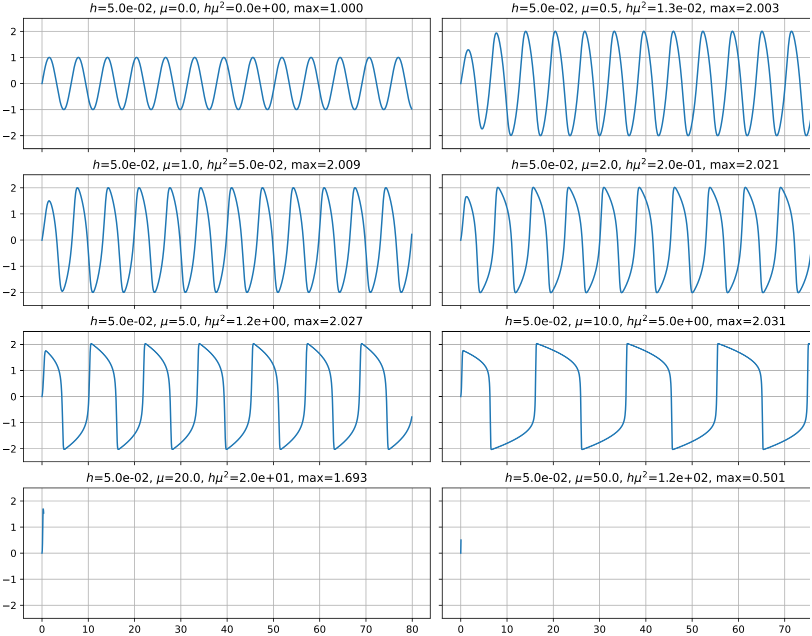
Crank-Nicolson method FDA

$$\begin{cases} -u_1 + u_t + h\left(-\frac{\mu u_1(u-1)(u+1)}{2} - \frac{u}{2}\right) + \mathcal{O}(h^2) = 0, \\ \mu u_1\,(u-1)\,(u+1) + u + u_{1\,t} + h\left(-\frac{\mu^2 u_1(u-1)^2(u+1)^2}{3} - \right. \\ \qquad \left. - \frac{\mu u\left(u^2-2u_1^2-1\right)}{3} + \frac{u_1}{3}\right) + \mathcal{O}(h^2) = 0. \end{cases} \tag{19}$$

Gauss-Legendre $h = 0.05$



Crank-Nicolson $h = 0.05$



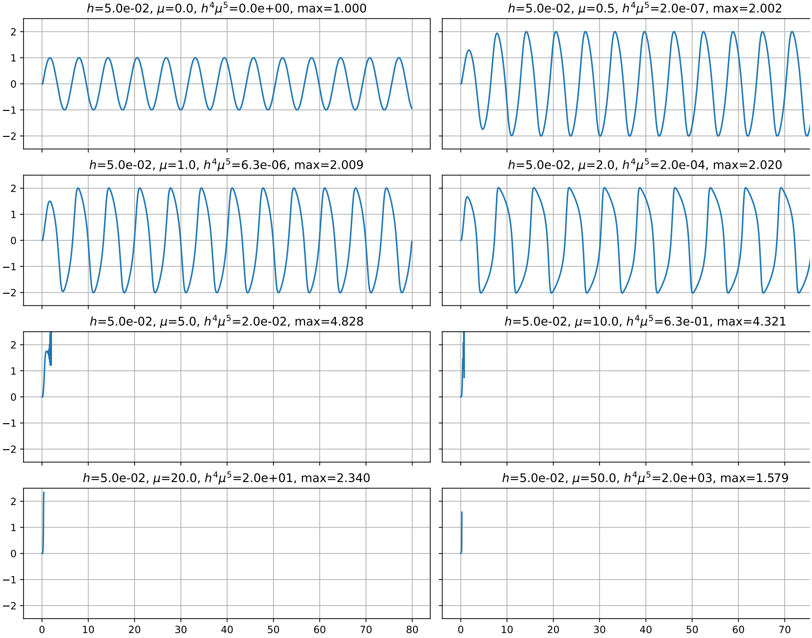
Adams-Bashforth 4 step FDA

$$
\begin{cases}
-u_1 + u_t + h^4\left(\frac{251\mu^4 u_1(u-1)^4(u+1)^4}{720} + \ldots + \frac{251 u_1}{720}\right) + \mathcal{O}(h^5) = 0,\\
\mu u_1\,(u-1)\,(u+1) + u + u_{1\,t} + \\
\qquad + h^4\left(-\frac{251\mu^5 u_1(u-1)^5(u+1)^5}{720} - \ldots - \frac{251 u}{720}\right) + \mathcal{O}(h^5) = 0.
\end{cases}
\tag{20}
$$

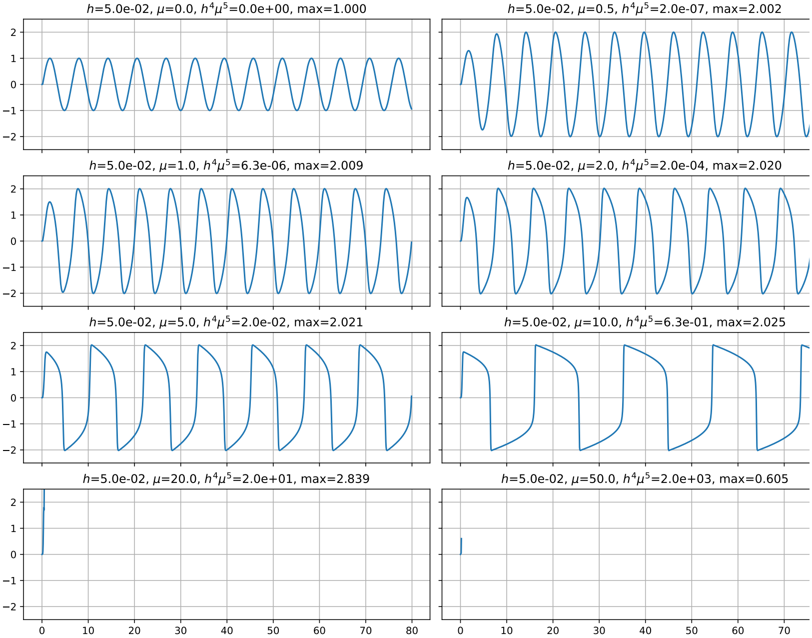
Adams-Moulton 4 step FDA

$$
\begin{cases}
-u_1 + u_t + h^4\left(-\frac{19\mu^4 u_1(u-1)^4(u+1)^4}{720} + \ldots - \frac{19 u_1}{720}\right) + \mathcal{O}(h^5) = 0,\\
\mu u_1\,(u-1)\,(u+1) + u + u_{1\,t} + \\
\qquad + h^4\left(\frac{19\mu^5 u_1(u-1)^5(u+1)^5}{720} - \ldots + \frac{19 u}{720}\right) + \mathcal{O}(h^5) = 0.
\end{cases}
\tag{21}
$$

Adams-Bashforth 4 step $h = 0.05$



Adams-Moulton 4 step $h = 0.05$



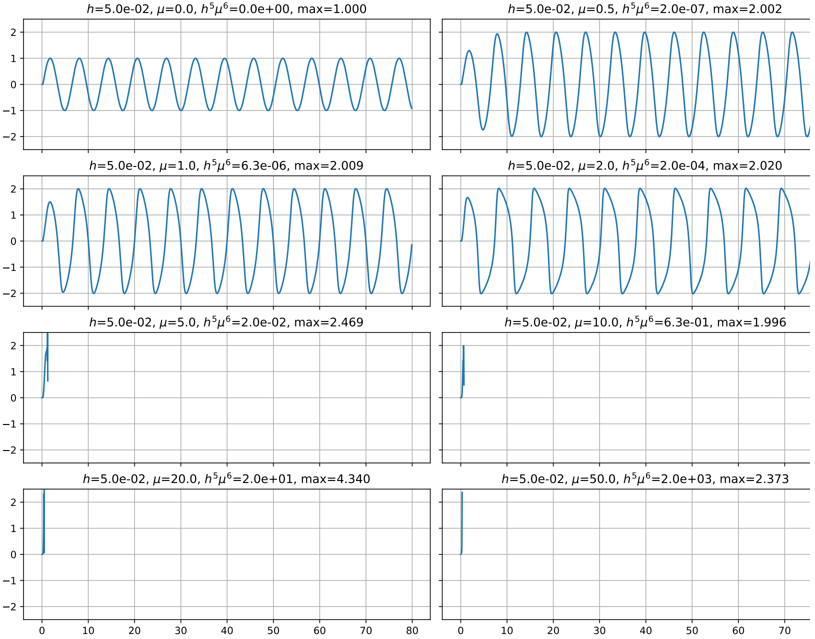
Adams-Bashforth 5 step FDA

$$\begin{cases} -u_1 + u_t + h^5\left(-\frac{95\mu^5 u_1 (u-1)^5 (u+1)^5}{288} + \ldots - \frac{95u}{288}\right) + \mathcal{O}(h^6) = 0, \\ \mu u_1 \left(u-1\right)\left(u+1\right) + u + u_{1\,t} + \\ \qquad + h^5\left(\frac{95\mu^6 u_1 (u-1)^6 (u+1)^6}{288} - \ldots - \frac{95u_1}{288}\right) + \mathcal{O}(h^6) = 0. \end{cases} \tag{22}$$

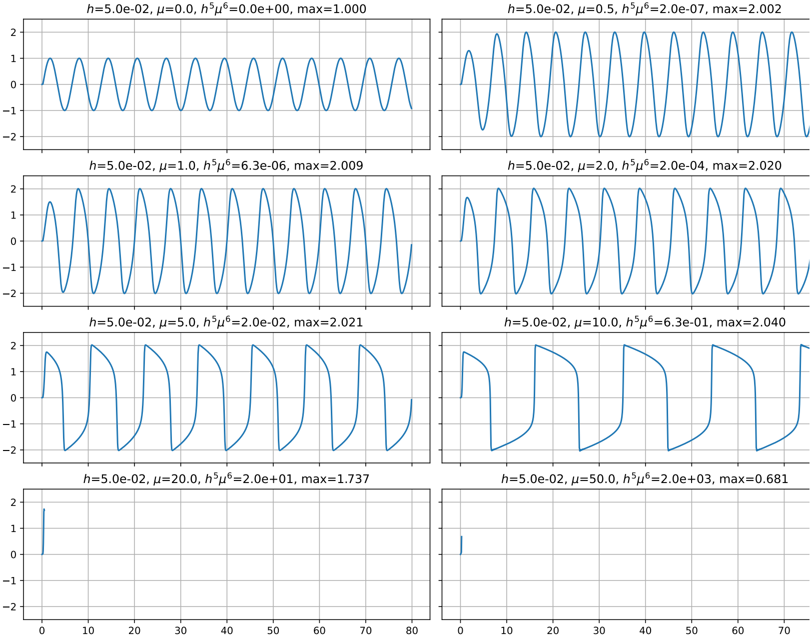
Adams-Moulton 5 step FDA

$$\begin{cases} -u_1 + u_t + h^5\left(\frac{3\mu^5 u_1 (u-1)^5 (u+1)^5}{160} + \ldots + \frac{3u}{160}\right) + \mathcal{O}(h^6) = 0, \\ \mu u_1 \left(u-1\right)\left(u+1\right) + u + u_{1\,t} + \\ \qquad + h^5\left(-\frac{3\mu^6 u_1 (u-1)^6 (u+1)^6}{160} - \ldots + \frac{3u_1}{160}\right) + \mathcal{O}(h^6) = 0. \end{cases} \tag{23}$$

Adams-Bashforth 5 step $h = 0.05$



Adams-Moulton 5 step $h = 0.05$



Conclusion

The most interesting FDA application for ODE are systems with parameters.

As a result, an explicit form of dependence of the error of numerical methods on the parameters of the system is obtained.

For ODE systems having the first integrals, the FDA allows you to estimate the error of performing the first integrals of the system.

The use of the FDA allows you to evaluate under what restrictions on parameters and step the selected numerical method can be applied.

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