1. Expansion of the 3rd order 3-step SSPx method (special form)

We are solving numerically the equation

$$u' = F(u).$$

Let t_0 be the initial time, and correspondingly $u_0 = u(t_0)$. Expanding the exact solution gives

$$\begin{aligned} u(t_0 + \Delta t) = u_0 + \Delta t F(u_0) + \frac{(\Delta t)^2}{2} F'(u_0) F(u_0) \\ + \frac{(\Delta t)^3}{6} \left[F''(u_0)(F(u_0))^2 + (F'(u_0))^2 F(u_0)\right] + o((\Delta t)^3). \end{aligned} \tag{1.1}$$

The special method takes the form

$$\begin{aligned} u_1 &= u_0 + a_1 \Delta t F(u_0), \\ \widetilde{u} &= (1 - w_1) u_0 + w_1 u_1, \\ u_2 &= \widetilde{u} + a_2 \Delta t F(u_1), \\ \bar{u} &= (1 - w_2) u_0 + w_2 u_2, \\ u_3 &= \bar{u} + a_3 \Delta t F(u_2). \end{aligned}$$

We now expand the numerical scheme:

$$\widetilde{u} = u_0 + w_1 a_1 \Delta t F(u_0),$$

$$\begin{aligned} u_2 &= u_0 + w_1 a_1 \Delta t F(u_0) + a_2 \Delta t F(u_0 + a_1 \Delta t F(u_0)) \\ &= u_0 + \underbrace{w_1 a_1 \Delta t F(u_0) + a_2 \Delta t (F(u_0) + a_1 \Delta t F(u_0) F'(u_0) + 2^{-1} (a_1 \Delta t F(u_0))^2 F''(u_0))}_{:=h} + o((\Delta t)^3). \end{aligned}$$

Remark 1.1. The o symbol implicitly has dependence on $F(u_0)$ and its derivatives, which means the approximation could be bad if F and its derivatives are very big.

So that

$$h = (w_1 a_1 + a_2) \Delta t F(u_0) + a_1 a_2 (\Delta t)^2 F(u_0) F'(u_0) + 2^{-1} a_1^2 a_2 (\Delta t)^3 (F(u_0))^2 F''(u_0) \tag{1.2}$$

Then,

$$\bar{u} = u_0 + w_2 h + o((\Delta t)^3).$$

Finally,

$$\begin{aligned} u_3 &= u_0 + w_2 h + a_3 \Delta t F(u_0 + h) + o((\Delta t)^3) \\ &= u_0 + w_2 h + a_3 \Delta t (F(u_0) + h F'(u_0) + 2^{-1} h^2 F''(u_0)) + o((\Delta t)^3) \\ &= u_0 + w_2 \left\{(w_1 a_1 + a_2) \Delta t F(u_0) + a_1 a_2 (\Delta t)^2 F(u_0) F'(u_0) + 2^{-1} a_1^2 a_2 (\Delta t)^3 (F(u_0))^2 F''(u_0)\right\} \\ &\quad + a_3 \Delta t \left\{F(u_0) + ((w_1 a_1 + a_2) \Delta t F(u_0) + a_1 a_2 (\Delta t)^2 F(u_0) F'(u_0)) F'(u_0) \right. \\ &\quad\quad \left. + 2^{-1} (w_1 a_1 + a_2)^2 (\Delta t)^2 (F(u_0))^2 F''(u_0)\right\} + o((\Delta t)^3). \end{aligned}$$

Comparing with expression 1.1, we obtain the following conditions in order for the method to be 3$^{\text{rd}}$ order:

$$w_2(w_1 a_1 + a_2) + a_3 = 1 \qquad (F(u_0)\Delta t), \tag{1.3}$$

$$w_2 a_1 a_2 + a_3 (w_1 a_1 + a_2) = \frac{1}{2} \qquad (F'(u_0)(\Delta t)^2), \tag{1.4}$$

$$a_1 a_2 a_3 = \frac{1}{6} \qquad (F(u_0)(F'(u_0))^2 (\Delta t)^3), \tag{1.5}$$

$$\frac{1}{2} w_2 a_1^2 a_2 + a_3 \frac{1}{2} (w_1 a_1 + a_2)^2 = \frac{1}{6} \qquad ((F(u_0))^2 F''(u_0)(\Delta t)^3). \tag{1.6}$$

Let us set $B := w_1 a_1 + a_2$. The system then yields

$$w_2 B + a_3 = 1, \tag{1.7}$$

$$w_2 + 6a_3^2 B = 3a_3, \tag{1.8}$$

$$a_1 a_2 a_3 = \frac{1}{6}, \tag{1.9}$$

$$w_2 a_1 + 6a_3^2 B^2 = 2a_3. \tag{1.10}$$

Then $B = (1 - a_3)/w_2$. Substituting in 1.8 and 1.9 we have:

$$w_2^2 + 6a_3^2(1 - a_3) = 3a_3 w_2,$$
$$w_2^3 a_1 + 6a_3^2(1 - a_3)^2 = 2a_3 w_2^2.$$

From the first we solve for w_2:

$$w_2 = \frac{3a_3 \pm \sqrt{9a_3^2 - 24a_3^2(1 - a_3)}}{2}.$$

In order for w_2 to be a real number, we need $a_3 \geq 5/8$. We also want $a_3 \leq 1$, otherwise the method has no gain.

We obtain

$$a_1 = \frac{2a_3(w_2(a_3))^2 - 6a_3^2(1 - a_3)^2}{(w_2(a_3))^3}$$

Let's first focus on the $-$ sign in w_2. From 5/8 to 1, w_2 is a decreasing function of a_3. a_1, instead, is increasing in a_3. $a_1(5/8) = 14/15$, and $a_1(2/3) = 1$. So $\max(a_1, a_2, a_3) \geq 1$ if $a_3 \geq 2/3$, hence it suffices to focus on the interval $a_3 \in [5/8, 2/3) = I$. Clearly, on I, $\max(a_1(a_3), a_3) = a_1(a_3)$, as $2/3 < 14/15$. Also, since $a_1 a_2 a_3 = \frac{1}{6}$, on I

$$\frac{5}{8}\frac{14}{15} a_2 \leq \frac{1}{6} \implies a_2 \leq \frac{2}{7} \implies \max(a_1, a_2, a_3) = a_1.$$

This means that the optimum is achieved for $a_3 = \frac{5}{8}$, $a_1 = \frac{14}{15}$, $a_2 = \frac{2}{7}$. We find w_1 from 1.3:

$$w_2(w_1 a_1 + a_2) + a_3 = 1 \implies w_1 = {a_1}^{-1}(w_2^{-1}(1 - a_3) - a_2) = \frac{15}{14}\left(\frac{16}{15}\frac{3}{8} - \frac{2}{7}\right) = \frac{6}{49}.$$

Then, $\min a_{\max} = \frac{14}{15}$, which means $\Delta t_{\max} \leq \frac{15}{14}\Delta t$. The gain is very small $\sim 7\%$.

Let's now focus on the $+$ case. We have that w_2 is an increasing function of a_3, and letting

$$A := \frac{1}{3}\left\{1 + \frac{(4 + 3\sqrt{2})^{1/3}}{2^{2/3}} - \frac{1}{(2(4 + 3\sqrt{2}))^{1/3}}\right\} \approx 0.6265,$$

we have that $w_2(A) = 1$. We need only to focus on the interval $a_3 \in [5/8, A] = J$. There, a_1 as a function of a_3 is decreasing, and it is such that $a_3(5/8) = \frac{14}{15}$. Also, since $A < \frac{14}{15}$, we will have that $\max(a_1(a_3), a_3) = a_1(a_3)$ on the interval J. By the same reasoning as the previous case, $\max(a_1, a_2, a_3) = a_1$ on J. Hence one just needs to optimize a_1, and as it is a decreasing function fo a_3, the optimum is achieved for the following choice of parameters:

$$\begin{aligned}
a_1 &= a_1(A) \approx 0.9245, \\
a_2 &= \frac{1}{6}(a_1 a_3)^{-1} \approx 0.2877, \\
a_3 &= A \approx 0.6265, \\
w_1 &= a_1^{-1}(w_2^{-1}(1 - a_3) - a_2) \approx 0.0927, \\
w_2 &= 1.
\end{aligned}$$

The gain is $\Delta t_{\max} \leq (a_{\max})^{-1}\Delta t \sim (0.9245)^{-1}\Delta t \sim 1.082\Delta t$.

2. Expansion for the second ansatz for the method: particular case $a_1 = a_3$

The second ansatz for the method takes the form

$$u_1 = u_0 + a_1 \Delta t F(u_0), \tag{2.1}$$

$$\widetilde{u} = (1 - w_1)u_0 + w_1 u_1, \tag{2.2}$$

$$u_2 = \widetilde{u} + a_2 \Delta t F(u_1), \tag{2.3}$$

$$\bar{u} = (1 - w_2)\widetilde{u} + w_2 u_2, \tag{2.4}$$

$$u_3 = \bar{u} + a_3 \Delta t F(u_2). \tag{2.5}$$

The calculations go through as in the previous case, with h as before, in 1.2. We have that, in this case,

$$\overline{u} = (1 - w_2)(u_0 + a_1 w_1 \Delta t F(u_0)) + w_2 u_0 + w_2 h = u_0 + a_1 w_1 \Delta t F(u_0) - a_1 w_1 w_2 \Delta t F(u_0) + w_2 h.$$

Since $\overline{u}$ only enters in the first term in Equation 2.5, we obtain the following system:

$$w_1 a_1 + w_2 a_2 + a_3 = 1 \qquad (F(u_0)\Delta t), \tag{2.6}$$

$$w_2 a_1 a_2 + a_3(w_1 a_1 + a_2) = \frac{1}{2} \qquad (F'(u_0)(\Delta t)^2), \tag{2.7}$$

$$a_1 a_2 a_3 = \frac{1}{6} \qquad (F(u_0)(F'(u_0))^2(\Delta t)^3), \tag{2.8}$$

$$\frac{1}{2} w_2 a_1^2 a_2 + a_3 \frac{1}{2}(w_1 a_1 + a_2)^2 = \frac{1}{6} \qquad ((F(u_0))^2 F''(u_0)(\Delta t)^3). \tag{2.9}$$

Let us make the assumption $a_1 = a_3 := a$. We then obtain the system

$$\begin{aligned}
w_1 a + w_2 a_2 + a &= 1, \\
a(w_2 a_2 + w_1 a + a_2) &= \frac{1}{2}, \\
a^2 a_2 &= \frac{1}{6}, \\
\frac{1}{2} w_2 a^2 a_2 + a \frac{1}{2}(w_1 a + a_2)^2 &= \frac{1}{6}.
\end{aligned}$$

Upon requiring $a \neq 0$, this is equivalent to

$$w_1 a + w_2 a_2 + a = 1, \tag{2.10}$$

$$a(1 - a + a_2) = \frac{1}{2}, \tag{2.11}$$

$$a^2 a_2 = \frac{1}{6}, \tag{2.12}$$

$$\frac{1}{2} w_2 a^2 a_2 + a \frac{1}{2}(w_1 a + a_2)^2 = \frac{1}{6}. \tag{2.13}$$

From the first three equations we have that a needs to satisfy the equation of degree 3:

$$a^2 - a^3 + a^2 a_2 = a/2 \implies a^2 - a^3 + 1/6 = a/2 \implies a^3 - a^2 + a/2 - 1/6 = 0.$$

The only positive real solution of this equation is (according to Mathematica):

$$A = \frac{1}{3}\left\{1 + \frac{(4 + 3\sqrt{2})^{1/3}}{2^{2/3}} - \frac{1}{(2(4 + 3\sqrt{2}))^{1/3}}\right\} \approx 0.6265,$$

(it is a number that already showed up before). From here, we obtain $a_2 = \frac{a^{-2}}{6} \approx 0.4246$. Substituting $w_2 a_2$ from 2.10 into 2.13, we obtain an equation for w_1, which is

$$\frac{1}{2} A^2 (1 - A - w_1 A) + \frac{A}{2}(w_1 A + a_2)^2 = \frac{1}{6}.$$

Solving the resulting quadratic equation for w_1 we obtain a unique $w_1 \in [0,1]$, $w_1 \approx 0.3982$. Plugging those parameters back into Equation 2.10, we obtain a value for $w_2 \approx 0.3735$.

Now, $A^{-1} \approx 1.596$, which is bigger than $\sqrt{2}$.

In this case, A turns out to be **the optimum**, by using Lagrange multipliers (I have a messy Mathematica file with the computations, if needed I can tidy it up).

3. Expansion for the third ansatz for the method, with 6 parameters

In this case, the method becomes

$$
\begin{aligned}
u_1 &= u_0 + a_1 \Delta t F(u_0), && (3.1)\\
\widetilde{u} &= (1-w_1)u_0 + w_1 u_1, && (3.2)\\
u_2 &= \widetilde{u} + a_2 \Delta t F(u_1), && (3.3)\\
\bar{u} &= (1-w_2-w_3)u_0 + w_2 u_2 + w_3 u_1, && (3.4)\\
u_3 &= \bar{u} + a_3 \Delta t F(u_2). && (3.5)
\end{aligned}
$$

Calculating the relevant system, it becomes

$$
\begin{aligned}
w_2(w_1 a_1 + a_2) + w_3 a_1 + a_3 &= 1 && (F(u_0)\Delta t), && (3.6)\\
w_2 a_1 a_2 + a_3(w_1 a_1 + a_2) &= \frac{1}{2} && (F'(u_0)(\Delta t)^2), && (3.7)\\
a_1 a_2 a_3 &= \frac{1}{6} && (F(u_0)(F'(u_0))^2(\Delta t)^3), && (3.8)\\
\frac{1}{2} w_2 a_1^2 a_2 + a_3 \frac{1}{2}(w_1 a_1 + a_2)^2 &= \frac{1}{6} && ((F(u_0))^2 F''(u_0)(\Delta t)^3). && (3.9)
\end{aligned}
$$

The constraint 3.8 implies that at least one of $\{a_1, a_2, a_3\}$ be greater or equal to $(a_1 a_2 a_3)^{1/3}$. Indeed, if all $a_i < (a_1 a_2 a_3)^{1/3}$, $i = 1,2,3$, then multiplying these inequalities together we would get $a_1 a_2 a_3 < a_1 a_2 a_3$, a contradiction. Hence

$$
\max\{a_1, a_2, a_3\} \geq (a_1 a_2 a_3)^{\frac{1}{3}} \implies \max\{a_1, a_2, a_3\} \geq (1/6)^{\frac{1}{3}}. \tag{3.10}
$$

Hence $a_{\max} \geq (1/6)^{\frac{1}{3}}$.

Let's now set $a_1 = a_2 = a_3$ in addition to the constraints 3.6 – 3.9. This will give 6 equations for 6 unknowns. Hence we solve the system:

$$
\begin{aligned}
w_2(w_1 a_1 + a_2) + w_3 a_1 + a_3 &= 1,\\
w_2 a_1 a_2 + a_3(w_1 a_1 + a_2) &= \frac{1}{2},\\
a_1 a_2 a_3 &= \frac{1}{6},\\
\frac{1}{2} w_2 a_1^2 a_2 + a_3 \frac{1}{2}(w_1 a_1 + a_2)^2 &= \frac{1}{6},\\
a_1 &= a_2,\\
a_1 &= a_3.
\end{aligned}
$$

There is exactly one real solution to this system such that $0 < w_1, w_2, w_3 < 1$. Namely:

$$
\begin{aligned}
a_1 &= a_2 = a_3 = (1/6)^{1/3} \approx 0.5503,\\
w_1 &= \frac{1}{2}\left(-1+\sqrt{9-2\cdot 6^{2/3}}\right) \approx 0.2739,\\
w_2 &= \frac{1}{2}\left(-1+6^{2/3}-\sqrt{9-2\cdot 6^{2/3}}\right) \approx 0.3769,\\
w_3 &= \frac{1}{2}\left(2\cdot 6^{1/3}-6^{1/3}\right) \approx 0.1661.
\end{aligned}
$$

Hence this is the optimum in this case, and the improvement is $a_{\max}^{-1} \approx 1.817$.

4. Can any Runge-Kutta method be written as combination of midpoint steps?

I assume here that "combination of s generalized midpoint steps" means a method of the form

$$
\begin{aligned}
y_{j+1} &= \bar{y}_j + \alpha_{j+1}\Delta t F(y_j), && j = 0,\dots,s,\\
\bar{y}_{j+1} &= \sum_{k=0}^{j+1} \beta_{jk} y_k, && j = 0,\dots,s-1.
\end{aligned} \tag{4.1}
$$

with the starting values $\bar{y}_0 = y_0 = y(t_n)$, and we let $y(t_{n+1}) := y_s$.

By an s-stage Runge-Kutta method, we denote a method such that

$$
\begin{aligned}
k_{i+1} &= F\left(x_0 + \Delta t \sum_{j=1}^{i} a_{i+1,j} k_j\right), i = 0,\dots,s-1\\
x(t_{n+1}) &= x_0 + \Delta t \sum_{j=1}^{s} b_j k_j.
\end{aligned} \tag{4.2}
$$

Here, similarly, $x_0 := x(t_n)$.

Let us first remark that an s-stage Runge-Kutta method has $s + s(s-1)/2$ free parameters, whereas a combination of s generalized midpoint steps has $s + s(s+1)/2 - 1$ free parameters.

Proposition 4.1. *An s-stage Runge-Kutta method (as in (4.2)) such that $a_{j+1,j} \neq 0$ for all $j = 1,\dots,s$ can be written as a particular combination of s generalized midpoint steps, as in (4.1).*

Remark 4.2. Notice that the coefficients β in this proposition need not lie in the interval $[0,1]$. If we were to require this, it would result in a condition on the coefficients a.

Proof. In the definition of Runge-Kutta method, we make the following assumption about notation.

We let, for every $j = 1,\dots,s$,

$$a_{s+1,j} := b_j,$$

so that the method becomes,

$$
\begin{aligned}
k_{i+1} &= F\left(x_0 + \Delta t \sum_{j=1}^{i} a_{i+1,j} k_j\right), i = 0,\dots,s-1\\
x(t_{n+1}) &= x_0 + \Delta t \sum_{j=1}^{s} a_{s+1,j} k_j.
\end{aligned} \tag{4.3}
$$

Let us now suppose throughout the rest of the proof that $a_{j+1,j} \neq 0$ for all $j = 1,\dots,s$.

We now set up an induction argument.

We denote by $\mathrm{IND}(j)$ the following hypothesis. $\mathrm{IND}(j-1)$ holds if and only if

$$y_k = x_0 + \Delta t \left(\sum_{i=1}^{k} a_{1+k,i} k_i\right) \tag{4.4}$$

holds for $k = 1, \dots, j-1$, $j \le s$.

We now check that IND(1) holds trivially. In fact, it is equivalent to

$$y_0 = x_0.$$

We now check that, supposing IND$(j-1)$, it is possible to deduce IND(j) for some choice of α_j and of $\{\beta_{j-2,q}\}_{q\in\{0,\dots,j-1\}}$. In this step, we assume that the coefficient $\alpha_1, \dots, \alpha_{j-1}$ as well as $\{\beta_{l,p}, (l,p)$ such that $l \in \{0,\dots,j-3\}, p \in \{0,\dots,l+1\}\}$ have already been chosen.

Now,

$$y_j = \bar{y}_{j-1} + \alpha_j \Delta t F(y_{j-1}) = \sum_{q=0}^{j-1} \beta_{j-2,q} y_q + \alpha_j \Delta t F(y_{j-1}).$$

By the induction hypothesis,

$$\begin{aligned}\sum_{q=0}^{j-1} \beta_{j-2,q} y_q &= \sum_{q=0}^{j-1} \beta_{j-2,q} \left(x_0 + \Delta t \sum_{i=1}^{q} a_{q+1,i} k_i \right) \\ &= x_0 \sum_{q=0}^{j-1} \beta_{j-2,q} + \Delta t \sum_{q=0}^{j-1} \sum_{i=1}^{q} a_{q+1,i} k_i \\ &= x_0 \sum_{q=0}^{j-1} \beta_{j-2,q} + \Delta t \sum_{i=1}^{j-1} \sum_{q=i}^{j-1} a_{q+1,i} k_i.\end{aligned}$$

Now we impose the relation (4.4) for $k = j$, and we obtain

$$x_0 + \Delta t \left(\sum_{i=1}^{j} a_{1+j,i} k_i \right) \stackrel{!}{=} x_0 \sum_{q=0}^{j-1} \beta_{j-2,q} + \Delta t \sum_{i=1}^{j-1} \sum_{q=i}^{j-1} a_{q+1,i} k_i + \alpha_j \Delta t F(y_{j-1}) \tag{4.5}$$

We have that, equating the coefficients of the k-terms, a sufficient condition for (4.5) to hold is

$$\begin{cases} \sum_{q=0}^{j-1} \beta_{j-2,q} = 1, \\ \sum_{q=i}^{j-1} \beta_{j-2,q} a_{q+1,i} = a_{j+1,i}, \qquad \text{for } i = 1, \dots, j-1 \\ \alpha_j = a_{j+1,j}. \end{cases} \tag{4.6}$$

This is a linear system of $j+1$ equations in $j+1$ unknowns. The system can be rewritten as $Ax = b$, where $\det A = \prod_{k=1}^{j} a_{k,k+1}$. We see that there exists a unique solution to the system in the conditions of the Proposition.

The induction step is therefore proved, and this proves the Proposition. □

Remark 4.3. We remark that, solving system (4.6) successively for $j = 1, \dots, s$, one can obtain explicitly the form of the coefficients α and β.

In particular, we have the following Proposition.

Proposition 4.4. *A 3-stage Runge-Kutta method to solve the problem $y' = F(y)$ is a particular case of combination of 3 generalized midpoint steps.*

Proof. We begin by setting the equations: $F(y_j) = k_{j+1}$, for $j = 1, \dots, s$, and derive some conditions on the coefficients.

$$\begin{aligned} &F(y_0) = k_1 \implies y_0 = x_0, \\ &F(y_1) = k_2 \implies y_0 + \alpha_1 \Delta t F(y_0) = x_0 + \Delta t (a_{21} F(y_0)) \implies \alpha_1 = a_{21}, \\ &F(y_2) = k_3 \implies \beta_{00} y_0 + \beta_{01} y_1 + \alpha_2 \Delta t F(y_1) = x_0 + \Delta t (a_{31} k_1 + a_{32} k_2) \\ &\qquad \implies a_{32} = \alpha_2, \beta_{00} + \beta_{01} = 1, \alpha_1 \beta_{01} = a_{31}. \end{aligned}$$

We then solve:

$$\alpha_1 = a_{21},\ \beta_{01} = a_{31}/(a_{21}),\ \beta_{00} = 1 - a_{31}/(a_{21}),\ \alpha_2 = a_{32}. \tag{4.7}$$

Finally, we require $y_3 = x_3$, and we have

$$\begin{aligned}
&\beta_{10}y_0 + \beta_{11}y_1 + \beta_{12}y_2 + \alpha_2\Delta tF(y_2)\\
&= \beta_{10}y_0 + \beta_{11}(y_0 + \alpha_1\Delta tF(y_0)) + \beta_{12}(\beta_{00}y_0 + \beta_{01}(y_0 + \alpha_1\Delta tF(y_0)) + \alpha_2\Delta tF(y_2)) + \alpha_3\Delta tF(y_2)\\
&= x_0 + b_1F(y_0) + b_2F(y_1) + b_3F(y_2).
\end{aligned}$$

Hence it suffices that

$$\begin{aligned}
\beta_{10} + \beta_{11} + \beta_{12} &= 1,\\
\beta_{11}\alpha_1 + \beta_{12}\beta_{01}\alpha_1 &= b_1,\\
\beta_{12}\alpha_2 &= b_2\\
\alpha_3 &= b_3.
\end{aligned} \tag{4.8}$$

So, if the coefficients $a_{i+1,i}$ are all nonzero, these equations can all be satisfied simultaneously. □

Remark 4.5. We remark that the relations (4.7) and (4.8) are exactly the relations obtained in the general case, i.e. (4.6).

5. Remarks on 4th order SSPx

A 4^{th} order SSPx takes the form

$$u_1 = u_0 + a_1\Delta tF(u_0), \tag{5.1}$$
$$\bar{u}_1 = (1 - w_1)u_0 + w_1u_1, \tag{5.2}$$
$$u_2 = \bar{u}_1 + a_2\Delta tF(u_1), \tag{5.3}$$
$$\bar{u}_2 = (1 - w_2 - w_3)u_0 + w_2u_1 + w_3u_2, \tag{5.4}$$
$$u_3 = \bar{u}_2 + a_3\Delta tF(u_2), \tag{5.5}$$
$$\bar{u}_3 = (1 - w_4 - w_5 - w_6)u_0 + w_4u_1 + w_5u_2 + w_6u_3, \tag{5.6}$$
$$u_4 = \bar{u}_3 + a_4\Delta tF(u_3). \tag{5.7}$$

The conditions for reaching 4^{th} order are the following:

$$a_1a_2a_3a_4 = \frac{1}{24}, \tag{5.8}$$

$$\begin{aligned}
&\frac{1}{2}a_4\left(a_3\left(a_2 + a_1w_1\right)^2 + a_1^2a_2w_3 + 2\left(a_1a_3w_1 + a_2\left(a_3 + a_1w_3\right)\right)\left(a_3 + a_2w_3 + a_1\left(w_2 + w_1w_3\right)\right)\right)\\
&+ \frac{1}{2}a_1a_2a_3\left(a_1 + 2a_2 + 2a_1w_1\right)w_6 = \frac{1}{6},
\end{aligned} \tag{5.9}$$

$$\frac{1}{6}\left(a_4\left(a_3 + a_2w_3 + a_1\left(w_2 + w_1w_3\right)\right)^3 + a_1^3a_2w_5 + \left(a_3\left(a_2 + a_1w_1\right)^3 + a_1^3a_2w_3\right)w_6\right) = \frac{1}{24}, \tag{5.10}$$

$$\frac{1}{2}\left(a_4\left(a_3 + a_2w_3 + a_1\left(w_2 + w_1w_3\right)\right)^2 + a_1^2a_2w_5 + \left(a_3\left(a_2 + a_1w_1\right)^2 + a_1^2a_2w_3\right)w_6\right) = \frac{1}{6}, \tag{5.11}$$

$$a_1a_3a_4w_1 + a_2\left(a_1a_4w_3 + a_3\left(a_4 + a_1w_6\right)\right) = \frac{1}{6}, \tag{5.12}$$

$$a_2a_4w_3 + a_3\left(a_4 + \left(a_2 + a_1w_1\right)w_6\right) + a_1\left(a_4w_2 + a_4w_1w_3 + a_2w_5 + a_2w_3w_6\right) = \frac{1}{2}, \tag{5.13}$$

$$a_4 + a_2w_5 + a_3w_6 + a_2w_3w_6 + a_1\left(w_4 + w_1w_5 + w_2w_6 + w_1w_3w_6\right) = 1. \tag{5.14}$$

We can reduce the system in the following way.

(1) From Equation (5.12), we obtain w_6 in terms of w_1 and w_3 (such equation is linear in w_6): $w_6 = F_1(w_1, w_3)$.

(2) From Equation (5.9), we obtain w_2 in terms of w_1 and w_3 (and w_6, but we substitute from point (1)): $w_2 = F_2(w_1, w_3)$.
(3) From Equation (5.13), we obtain w_5 in terms of w_2, w_3, w_1, w_6. Upon substitution, $w_5 = F_3(w_1, w_3)$.
(4) From Equation (5.14), we obtain w_4 in terms of w_1, w_2, w_3, w_5, w_6. Upon substitution, $w_4 = F_4(w_1, w_3)$.
(5) We finally substitute into Equations (5.10) and (5.11). We obtain a nonlinear system of two equations in two unknowns.

Unlike the 3$^{\text{rd}}$ order method, there does not seem to be a solution when $a_1 = a_2 = a_3 = a_4 = 24^{-\frac{1}{4}}$.

Recall that the optimal $a_{\max}$ we obtained from the 3$^{\text{rd}}$ order 3-step method was $(1/6)^{1/3} \sim 0.55$. The best $a_{\max}$ I could obtain (by a very rough heuristic search) now is 9/10. The corresponding values of a_1, a_2, a_3, a_4 are the following:

$$a_1 = 9/10, a_2 = 4/5, a_3 = 1/10, a_4 = 125/216.$$

For these values, there is a 4$^{\text{th}}$ order 4 steps SSPx algorithm. The improvement on timestep is quite small, and I need to optimize this result. All these calculations are in the Mathematica file.