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Search of Symmetric Composition Methods of Symmetric Integrators

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Abstract

Composition methods are useful when solving Ordinary Differential Equations (ODEs) as they increase the order of accuracy of a given basic numerical integration scheme. We will focus on symmetric composition methods involving some basic second order symmetric integrator with different step sizes [17]. The introduction of symmetries into these methods simplifies the order conditions and reduces the number of unknowns. Several authors have worked in the search of the coefficients of these type of methods: the best method of order 8 has 17 stages [24], methods of order 8 and 15 stages were given in [29, 39, 40], 10-order methods of 31, 33 and 35 stages have been also found [24, 34]. In this work some techniques that we have built to obtain 10-order symmetric composition methods of symmetric integrators of $s = 31$ stages (16 order conditions) are explored. Given some starting coefficients that satisfy the simplest five order conditions, the process followed to obtain the coefficients that satisfy the sixteen order conditions is provided.

Keywords: numerical methods for ODEs, symmetric numerical methods, symmetric composition, same basic integrator.

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1. Introduction

We will consider the next Initial Value Problem (IVP):

$$y'(t) = f(t, y(t)), \quad y(a) = y_0 \quad (1.1)$$

where $T = [a, b]$ is a finite interval and $y : [a, b] \rightarrow \mathbb{R}^m$ and $f : [a, b] \times \mathbb{R}^m \rightarrow \mathbb{R}^m$ are continuous functions. When f satisfies the Lipschitz condition in the second variable, the problem (1.1) has a unique solution in the interval T .

The above problem can be solved numerically, using a discretization of the time interval $T = [a, b]$ as follows:

$$a = t_0 < t_1 < \dots < t_{m-1} < t_m = b \quad (1.2)$$

We will denote $\Delta t = t_{j+1} - t_j$, $\forall j = 0, \dots, m-1$, by $h = \Delta t$ which is called the *time step size*. Note that we are considering a constant time step size and therefore:

$$\begin{cases} t_{j+1} = t_j + h, & \forall j = 0, \dots, m-1, \\ t_j = t_0 + j \cdot h, & \forall j = 0, \dots, m \end{cases} \quad (1.3)$$

The numerical methods to solve (1.1) give an approximation of the analytical solution on each time level defined above:

$$y(t_j) \approx y_j, \quad \forall j = 1, \dots, m \quad (1.4)$$

starting from $y(a) = y_0$.

Many researches have been focused on developing convenient numerical methods with good accuracy, good stability requirements or with the ability to preserve some conservation properties. In this work we are interested in composition methods, which are particularly useful when integrating numerically differential equations that have some special structure which is necessary to preserve. A composition method is the result of composing different methods or the same method several times. We will work with composition methods in which the same method is composed several times using different step sizes. This basic method will be second order accurate and symmetric. And also the composition will be developed symmetrically (this is described in depth in Section 3). Hence, we will work with symmetric composition methods of basic second order symmetric integrators, centering our attention in the search of a technique to find the coefficients of a 10-order and $s = 31$ stages method of this type.

The present work is organised as follows: in Section 2, a review about different numerical methods to solve Initial Value Problems (IVPs) is done. In Section 3, we introduce symmetric composition methods of symmetric integrators, providing some examples of these type of methods and showing some numerical results. In Section 5, we introduce the first technique we have used to find the coefficients of some 10-order and $s = 31$ stages methods. Our second technique is described in Section 6. Finally, in Section 7, some conclusions and the main research goals for the future are provided.

2. Review of some numerical methods for Initial Value Problems

In this section we will review some of the numerical methods used to solve the problem (1.1). The simplest numerical methods to obtain a solution of the problem (1.1) are the Euler's methods:

- The explicit Euler method which is given by: $y_{n+1} = y_n + hf_n$, being $f_n = f(t_n, y_n)$.
- And the implicit Euler method: $y_{n+1} = y_n + hf_{n+1}$, being $f_{n+1} = f(t_{n+1}, y_{n+1})$.

Both methods are *one-step methods*, as only the differential equation and the numerical approximation at the previous time level are used to calculate the numerical approximation y_{n+1} at the present time level t_{n+1} . Another well known one-step method is the trapezoidal method, which is second order accurate and unconditionally stable and it is given by the formula:

$$y_{n+1} = y_n + \frac{h}{2} (f_n + f_{n+1}) \quad (2.1)$$

Multistage methods constitute a variation of the one-step methods. They are one-step methods that use the evaluation of the derivative in some intermediate points of the step, being the Runge-Kutta methods an example of multistage methods. The general s -stage Runge-Kutta method for the initial value problem (1.1) has the following form [7, 16, 27]:

$$y_{n+1} = y_n + h \sum_{i=1}^s b_i k_i \quad (2.2)$$

where:

$$k_i = f(t_n + c_i h, y_n + h \sum_{j=1}^s a_{ij} k_j), \quad i = 1, 2, \dots, s \quad (2.3)$$

Constants a_{ij}, b_i, c_i are generally displayed in a table called Butcher array which can also be written in matrix form, Table 1. Vectors \mathbf{b} and \mathbf{c} are s -dimensional and the matrix A has dimension $s \times s$:

$$\mathbf{b} = [b_1, b_2, \dots, b_s]^T, \quad \mathbf{c} = [c_1, c_2, \dots, c_s]^T, \quad A = [a_{ij}]$$

$$\begin{array}{c|c} \mathbf{c} & A \\ \hline & \mathbf{b}^T \end{array}$$

Table 1: Butcher array in matrix form.

The Runge-Kutta methods can be explicit, implicit or half-implicit depending on the structure of the matrix $A = (a_{ij})$. If A is strictly lower triangular, the method is explicit. If A is lower triangular, the method is half-implicit and for a not lower triangular A , the method is implicit. Gauss s -stage and $2s$ order formulae are an example of implicit Runge-Kutta methods [5]. Note that for implicit Runge-Kutta methods the equation for k_i (2.3) involves all the k_j values. So in the

case of implicit Runge-Kutta methods we have to solve an extended system of equations. If each y_n is a real number, then we have a system of s equations with s unknowns for each time step. If each y_n is a vector of dimension N , then we have a system of $N \cdot s$ equations in $N \cdot s$ unknowns.

The estimates for the local truncation error of Runge-Kutta methods are not computationally cheap. This is one of the reasons why many studies have focused on the search of Runge-Kutta methods of orders p and $p + 1$, sharing the same set of coefficients c_i, a_{ij} . This process is known as embedding and the resulting Runge-Kutta methods are called embedded Runge-Kutta methods. The Butcher array of an embedded Runge-Kutta method is given by Table 2.

\mathbf{c}	A
	\mathbf{b}^T
	$\hat{\mathbf{b}}^T$
	\mathbf{E}^T

Table 2: Butcher array of the embedded Runge-Kutta methods.

The notation of the Table 2 has to be interpreted to mean that the method defined by \mathbf{c} , A and \mathbf{b}^T is of order p and the one defined by \mathbf{c} , A and $\hat{\mathbf{b}}^T$ is of order $(p + 1)$. In the embedded Runge-Kutta methods the constants k_i given by (2.3) are the same for both methods (for the method of order p and order $(p + 1)$). The vector \mathbf{E}^T is the difference $\hat{\mathbf{b}}^T - \mathbf{b}^T$. We will denote by \hat{y}_{n+1} and y_{n+1} the solutions of orders $(p + 1)$ and p respectively:

$$\hat{y}_{n+1} = y_n + h \sum_{i=1}^s \hat{b}_i k_i, \quad y_{n+1} = y_n + h \sum_{i=1}^s b_i k_i \quad (2.4)$$

In this context, the local truncation error can be estimated as the difference of the two values \hat{y}_{n+1} and y_{n+1} :

$$\hat{y}_{n+1} - y_{n+1} = h \sum_{i=1}^s E_i k_i \quad (2.5)$$

where $E_i = \hat{b}_i - b_i$. It is widely accepted that the Runge-Kutta embedding technique is an efficient method to find the numerical solution of nonstiff problems [32]. There are also some embedded Runge-Kutta methods implemented in MATLAB [1, 2, 31]: it is the case of the ode45 and the ode23. The function ode45 is based on the embedded Runge-Kutta method proposed in [12], which is known as DOPRI(5,4). It is a method of 7-stages, though in practice it operates as if it only had 6-stages, because the last coefficient of the vector $\hat{\mathbf{b}}^T$ is zero. The function ode23 is also based on another embedded Runge-Kutta proposed in [4]. It is a method of 4-stages, but again it is the type of method known as FSAL (First Same as Last) because of the last coefficient of the vector $\hat{\mathbf{b}}^T$ is zero. So, in practice it is a 3-stage method.

The multistep methods constitute another variation of the one-step methods. They use k previous approximations $y_n, y_{n+1}, \dots, y_{n+k-1}$ of the exact solution in the points $t_n, t_n + h, \dots, t_n + (k - 1)h$ to calculate y_{n+k} in the point $t_{n+k} = t_n + kh$. A multistep method can be written as follows:

$$\sum_{j=0}^k \alpha_j y_{n+j} = h \phi(f_{n+k}, f_{n+k-1}, \dots, f_n, t_n; h) \quad (2.6)$$

being $f_{n+j} = f(t_{n+j}, y_{n+j})$.

When the relationship among the values y_{n+j}, f_{n+j} for $j = 0, 1, \dots, k$ is linear, the multistep method (2.6) is linear and it can be written as:

$$\sum_{j=0}^k \alpha_j y_{n+j} = h \sum_{j=0}^k \beta_j f_{n+j} \quad (2.7)$$

where α_j, β_j are constants, $\alpha_k \neq 0$ and α_0 and β_0 non simultaneously zero. The method (2.7) is explicit when $\beta_k = 0$, and implicit when $\beta_k \neq 0$. The method is one-step when $k = 1$. Three classical linear multistep methods are the Adams Bashforth and Adams Moulton methods [20] and the Backward Differentiation Formula (BDF). Because of their good stability properties the BDFs are the most used [15, 18] and they are given by the expression:

$$\sum_{j=0}^k \hat{\alpha}_j y_{n+j} = h f_{n+k} \quad (2.8)$$

When solving ODEs, sometimes the accuracy is not the only requirement asked to the numerical method. For example, when we are working with a stiff problem, the numerical method used must be accurate and it also needs an extensive stability region [11]. Stiffness is a delicate and important concept when solving ODEs. Various authors [25, 27] say that there is no a rigorous definition of stiffness. It depends on the ODE, on its initial conditions, on the numerical method used for its resolution and on the time interval in which the ODE is solved. Another definition of stiffness is given in [26], which says that stiffness occurs when different magnitude eigenvalues exist in the solution, where this difference in the magnitude could happen in the real part or in the imaginary part of the eigenvalues. Because of this requirement, in the last years many researches have been focused on developing convenient numerical methods for stiff problems and a lot of improvements have been made on the basis of the BDF. One of the modifications done to the BDFs are the NDFs (Numerical Differentiation Formulae). It is a computationally cheap modification that consists of anticipating a difference of order $(k+1)$ multiplied by a constant $\kappa\gamma_k$ in the BDF formula of order k . This term has a positive effect on the local truncation error, making the NDFs more accurate than the BDFs and not much less stable. This modification was proposed by Shampine [32] but only for orders $k = 1, 2, 3, 4$, because it is inefficient for orders greater than 4. Other modifications have consisted in combining two multistep methods, using superfuture points (points that are outside the actual time step) or using derivatives of superior order [19]. The blended method [33] consists in a linear combination of the Adams Moulton method of order $(k+1)$ and the k -order BDF method, improving the stability properties of the method. In [8] and [9] Cash introduces methods using superfuture points to solve stiff IVPs. These methods are known as extended BDF (EBDF) and modified extended BDF (MEBDF). They consist of applying the BDF predictors twice and one implicit multistep corrector. Both methods use superfuture points to gain stability and they are A-stable up to order 4 and $A(\alpha)$ -stable up to order 9. In [10] a code based on the MEBDF is described and in [21] Matrix free MEBDF (MF-MEBDF) methods are introduced to optimize the computations of the EBDF. A different variation of the BDFs was introduced by Fredebeul [14], the A-BDF method. In this method the implicit and explicit BDF are used in the same formula, with a free parameter, being $A(\alpha)$ -stable up to order 7. Enright methods [13], Second derivative BDF

method (SDBDF) [19] or the *New Efficient Second Derivative Multistep Methods* [23] are examples of methods using the second derivative.

Another direction followed in the search of new methods consist of composing methods. Runge-Kutta methods with the same step size have been composed leading to the Butcher group [6], cyclic composition of multistep methods [35] and composition of low order Runge-Kutta methods has been carried out increasing the stability [22]. In this work we will consider the composition of a given basic one-step method with different step sizes. The aim of these type of compositions is to increase the order of accuracy of the method while preserving some properties of the basic initial method [29, 37, 38]. An s-stage composition method Ψ_h is given by:

$$\Psi_h = \Phi_{\gamma_s h}^{(s)} \circ \Phi_{\gamma_{s-1} h}^{(s-1)} \circ \dots \circ \Phi_{\gamma_1 h}^{(1)} \quad (2.9)$$

being each $\Phi_{\gamma_i h}^{(i)}$ a basic integration method that takes a step of size $\gamma_i h$, being γ_i and h real numbers.

When we take the same p -order base method Φ_h in (2.9), the following expression is obtained:

$$\Psi_h = \Phi_{\gamma_s h} \circ \Phi_{\gamma_{s-1} h} \circ \dots \circ \Phi_{\gamma_1 h} \quad (2.10)$$

Taking a basic p -order accurate Φ_h one-step method, the composition method (2.10) is $(p+1)$ -order accurate if the following equalities are satisfied:

$$\begin{cases} \gamma_1 + \dots + \gamma_s = 1 \\ \gamma_1^{p+1} + \dots + \gamma_s^{p+1} = 0 \end{cases} \quad (2.11)$$

From (2.11) it can be concluded that this type of composition allows an increase of order only when p is even (for odd p the second condition of (2.11) becomes impossible to satisfy). But this can be overcome by replacing the composition (2.10) by the following formula:

$$\Psi_h = \Phi_{\alpha_s h} \circ \Phi_{\beta_s h}^* \circ \Phi_{\alpha_{s-1} h} \circ \Phi_{\beta_{s-1} h}^* \circ \dots \circ \Phi_{\alpha_1 h} \circ \Phi_{\beta_1 h}^* \quad (2.12)$$

in which each Φ_h method is composed by its adjoint method Φ_h^* . The adjoint method Φ_h^* of a method Φ_h is the inverse map of the original method with reversed time step:

$$\Phi_h^* := \Phi_{-h}^{-1} \quad (2.13)$$

For example, the implicit Euler method is the adjoint of the explicit Euler method.

In the composition of a method with its adjoint (2.12), the condition to obtain a $(p+1)$ -order accurate new method becomes:

$$\begin{cases} \beta_1 + \alpha_1 + \dots + \beta_s + \alpha_s = 1 \\ (-1)^p \beta_1^{p+1} + \alpha_1^{p+1} + (-1)^p \beta_2^{p+1} \dots + (-1)^p \beta_s^{p+1} + \alpha_s^{p+1} = 0 \end{cases} \quad (2.14)$$

being possible also for odd p to obtain a $(p+1)$ -order new method.

3. Symmetric Composition Methods of Symmetric Integrators

3.1. General theory and some methods

In the previous section we have defined a composition method and we have seen the possibility that it gives to increase the order of the initial method. In this work we are interested in composition methods in which the same basic method is used in the composition, being this method symmetric. A method is symmetric if its adjoint is itself (self-adjoint method):

$$\Phi_h^* = \Phi_h \quad (3.1)$$

For example, the trapezoidal method is symmetric.

An interesting special case of (2.10) is the *symmetric composition* obtained by taking:

$$\gamma_i = \gamma_{s-i+1}, \quad i = 1, \dots, \left\lfloor \frac{s}{2} \right\rfloor \quad (3.2)$$

in which the composition is done symmetrically. The symbol $\lfloor s/2 \rfloor$ indicates the integer part of $s/2$.

So we will center this work in symmetric composition methods of symmetric integrators. Which means that:

- Composition methods which involve the same base method with different step sizes.
- The composition will be done in a symmetric way, choosing the coefficients as shown in (3.2).

In addition we will restrict our attention to symmetric composition methods of symmetric integrators of order $p = 2$.

The introduction of the symmetry condition (3.2) in the method simplifies considerably the order conditions, see [30]. We list here the order conditions through order ten:

$$\sum_{k=1}^s \gamma_k = 1, \quad (3.3)$$

$$\sum_{k=1}^s \gamma_k^3 = 0, \quad (3.4)$$

$$\sum_{k=1}^s \gamma_k^5 = 0, \quad \sum_{k=1}^s \gamma_k^3 \left(\sum_{l=1}^k \gamma_l \right)^2 = 0, \quad (3.5)$$

$$\begin{aligned} \sum_{k=1}^s \gamma_k^7 = 0, \quad \sum_{k=1}^s \gamma_k^5 \left(\sum_{l=1}^k \gamma_l \right)^2 = 0, \\ \sum_{k=1}^s \gamma_k^3 \sum_{l=1}^k \gamma_l \sum_{m=1}^k \gamma_m^3 = 0, \quad \sum_{k=1}^s \gamma_k^3 \left(\sum_{l=1}^k \gamma_l \right)^4 = 0, \end{aligned} \quad (3.6)$$

$$\begin{aligned}
\sum_{k=1}^s \gamma_k^9 &= 0, & \sum_{k=1}^s \gamma_k^7 \left(\sum_{l=1}^k \gamma_l \right)^2 &= 0, \\
\sum_{k=1}^s \gamma_k^5 \sum_{l=1}^k \gamma_l \sum_{m=1}^k \gamma_m^3 &= 0, & \sum_{k=1}^s \gamma_k^3 \sum_{l=1}^k \gamma_l \sum_{m=1}^k \gamma_m^5 &= 0, \\
\sum_{k=1}^s \gamma_k^3 \left(\sum_{l=1}^k \gamma_l \right)^2 \sum_{m=1}^k \gamma_m^3 \sum_{n=1}^m \gamma_n &= 0, & \sum_{k=1}^s \gamma_k^5 \left(\sum_{l=1}^k \gamma_l \right)^4 &= 0, \\
\sum_{k=1}^s \gamma_k^3 \left(\sum_{l=1}^k \gamma_l \right)^3 \sum_{m=1}^k \gamma_m^3 &= 0, & \sum_{k=1}^s \gamma_k^3 \left(\sum_{l=1}^k \gamma_l \right)^6 &= 0,
\end{aligned} \tag{3.7}$$

Summation with a prime indicates that the last term γ_i^j is taken as $\gamma_i^j/2$. The number of conditions for a second order symmetric composition method of symmetric integrators is 1 (condition (3.3)); for 4-order there are two order conditions (3.3) and (3.4); for 6-order four conditions (3.3), (3.4) and (3.5); for 8-order eight conditions (3.3)-(3.6); for 10-order sixteen conditions (3.3)-(3.7).

The minimal number of stages for an order $p = 2k$, $p \leq 10$, composition scheme subject to (3.2) is $2^k - 1$. For the minimal number of stages, the number of free parameters and algebraic constraints is the same and Newton's method can be used to find solutions. However, a number of numerical comparisons have shown that it is better to take $2^k + 1$ stages and use the additional free parameters to optimize the coefficients. One of the suggested choices is to minimize $\|\gamma\|_1$, which corresponds to the total distance travelled in the integration interval.

For order 8, the eight order conditions (3.3)-(3.6) have to be satisfied. This means that the minimal number of stages s is 15. The coefficients $\gamma_1, \gamma_2, \dots, \gamma_8$ have to be calculated. There are hundreds of solutions of this system, but the best 8-order methods have been found by [29, 39, 40]. By choosing $s = 17$ one degree of freedom is obtained when solving the system of equations. This makes possible an improvement on the method. A good method of this type is given in [29]. But the best known (in the sense of minimizing $\|\gamma\|_1$) 8-order and $s = 17$ stages method has been found by Kahan & Li [24], and it is given by:

$$\begin{aligned}
\gamma_1 &= \gamma_{17} = 0.13020248308889008087881763 \\
\gamma_2 &= \gamma_{16} = 0.56116298177510838456196441 \\
\gamma_3 &= \gamma_{15} = -0.38947496264484728640807860 \\
\gamma_4 &= \gamma_{14} = 0.15884190655515560089621075 \\
\gamma_5 &= \gamma_{13} = -0.39590389413323767733623154 \\
\gamma_6 &= \gamma_{12} = 0.18453964097831570709183254 \\
\gamma_7 &= \gamma_{11} = 0.25837438768632204729397911 \\
\gamma_8 &= \gamma_{10} = 0.29501172360931029887096624 \\
\gamma_9 &= -0.60550853383003451169892108
\end{aligned} \tag{3.8}$$

To obtain a 10-order method, sixteen order conditions have to be satisfied, being the minimal number of stages $s = 31$. The first 10-order and $s = 31$ and $s = 33$ stages methods were given by

Kahan & Li [24]. The 33-stages and 10-order Kahan & Li's method's coefficients are the following:

$$\begin{aligned}
 \gamma_1 &= \gamma_{33} = 0.12313526870982994083 \\
 \gamma_2 &= \gamma_{32} = 0.77644981696937310520 \\
 \gamma_3 &= \gamma_{31} = 0.14905490079567045613 \\
 \gamma_4 &= \gamma_{30} = -0.17250761219393744420 \\
 \gamma_5 &= \gamma_{29} = -0.54871240818800177942 \\
 \gamma_6 &= \gamma_{28} = 0.14289765421841842100 \\
 \gamma_7 &= \gamma_{27} = -0.31419193263986861997 \\
 \gamma_8 &= \gamma_{26} = 0.12670943739561041022 \\
 \gamma_9 &= \gamma_{25} = 0.17444734584181312998 \\
 \gamma_{10} &= \gamma_{24} = 0.44318544665428572929 \\
 \gamma_{11} &= \gamma_{23} = -0.81948900568299084419 \\
 \gamma_{12} &= \gamma_{22} = 0.13382545738489583020 \\
 \gamma_{13} &= \gamma_{21} = 0.64509023524410605020 \\
 \gamma_{14} &= \gamma_{20} = -0.71936337169922060719 \\
 \gamma_{15} &= \gamma_{19} = 0.20951381813463649682 \\
 \gamma_{16} &= \gamma_{18} = -0.26828113140636051966 \\
 &\gamma_{17} = 0.83647216092348048955
 \end{aligned} \tag{3.9}$$

Subsequently, a better 10-order and $s = 33$ stages method was calculated by Hairer, Lubich and Wanner [17]:

$$\begin{aligned}
 \gamma_1 &= \gamma_{33} = 0.09040619368607278492161150 \\
 \gamma_2 &= \gamma_{32} = 0.53591815953030120213784983 \\
 \gamma_3 &= \gamma_{31} = 0.35123257547493978187517736 \\
 \gamma_4 &= \gamma_{30} = -0.31116802097815835426086544 \\
 \gamma_5 &= \gamma_{29} = -0.52556314194263510431065549 \\
 \gamma_6 &= \gamma_{28} = 0.14447909410225247647345695 \\
 \gamma_7 &= \gamma_{27} = 0.02983588609748235818064083 \\
 \gamma_8 &= \gamma_{26} = 0.17786179923739805133592238 \\
 \gamma_9 &= \gamma_{25} = 0.09826906939341637652532377 \\
 \gamma_{10} &= \gamma_{24} = 0.46179986210411860873242126 \\
 \gamma_{11} &= \gamma_{23} = -0.33377845599881851314531820 \\
 \gamma_{12} &= \gamma_{22} = 0.07095684836524793621031152 \\
 \gamma_{13} &= \gamma_{21} = 0.23666960070126868771909819 \\
 \gamma_{14} &= \gamma_{20} = -0.49725977950660985445028388 \\
 \gamma_{15} &= \gamma_{19} = -0.30399616617237257346546356 \\
 \gamma_{16} &= \gamma_{18} = 0.05246957188100069574521612 \\
 &\gamma_{17} = 0.44373380805019087955111365
 \end{aligned} \tag{3.10}$$

Very good 10-order and $s = 31$, $s = 33$ and $s = 35$ stages methods have been given in [34] by

Sofroniou and Spaletta. Their 10-order and $s = 31$ stages method's coefficients are the following:

$$\begin{aligned}
 \gamma_1 &= \gamma_{31} = 0.14998070054317051502516939497857 \\
 \gamma_2 &= \gamma_{30} = 0.091208635101489291996105121514462 \\
 \gamma_3 &= \gamma_{29} = 0.50623124887796194535266557555255 \\
 \gamma_4 &= \gamma_{28} = 0.094789715925889154094231454089204 \\
 \gamma_5 &= \gamma_{27} = -0.19520875735034504160990960439871 \\
 \gamma_6 &= \gamma_{26} = -0.38816256756251756192331854792644 \\
 \gamma_7 &= \gamma_{25} = -0.27450555650873276528931810649505 \\
 \gamma_8 &= \gamma_{24} = 0.14264675556451861069659069043321 \\
 \gamma_9 &= \gamma_{23} = 0.067102518966825349346877396037809 \\
 \gamma_{10} &= \gamma_{22} = -0.19643186370792190448674783323248 \\
 \gamma_{11} &= \gamma_{21} = 0.29602854892160888804740587728740 \\
 \gamma_{12} &= \gamma_{20} = 0.18917810251470701571585847859316 \\
 \gamma_{13} &= \gamma_{19} = 0.19394700133244324371285167850479 \\
 \gamma_{14} &= \gamma_{18} = 0.10120067580762238380456506324802 \\
 \gamma_{15} &= \gamma_{17} = -0.58186926782264021140090352527182 \\
 &\gamma_{16} = 0.60772821879184217383575377417062
 \end{aligned} \tag{3.11}$$

Their 10-order and $s = 33$ stages method's coefficients:

$$\begin{aligned}
 \gamma_1 &= \gamma_{33} = 0.070711261586085399079302771810203 \\
 \gamma_2 &= \gamma_{32} = 0.090342080937267568345577914389234 \\
 \gamma_3 &= \gamma_{31} = 0.14103133297152486103524322594476 \\
 \gamma_4 &= \gamma_{30} = 0.40206004554029767537357060971803 \\
 \gamma_5 &= \gamma_{29} = -0.30239722849131075165735249848238 \\
 \gamma_6 &= \gamma_{28} = -0.22462355658241460137093154363351 \\
 \gamma_7 &= \gamma_{27} = 0.061496988956063121940380707068411 \\
 \gamma_8 &= \gamma_{26} = 0.11346847775740802675296685287062 \\
 \gamma_9 &= \gamma_{25} = 0.23654672241381781124636015203490 \\
 \gamma_{10} &= \gamma_{24} = 0.27211409645898977643699556260890 \\
 \gamma_{11} &= \gamma_{23} = 0.076129418470277234386530906651024 \\
 \gamma_{12} &= \gamma_{22} = -0.18543093454238185309165565783301 \\
 \gamma_{13} &= \gamma_{21} = -0.46495110925607623804616342747217 \\
 \gamma_{14} &= \gamma_{20} = 0.10423014962104084592532590279051 \\
 \gamma_{15} &= \gamma_{19} = 0.13621181452383232935841998116651 \\
 \gamma_{16} &= \gamma_{18} = -0.27010275720513252644976102610064 \\
 &\gamma_{17} = 0.48632639368142264147037913293721
 \end{aligned} \tag{3.12}$$

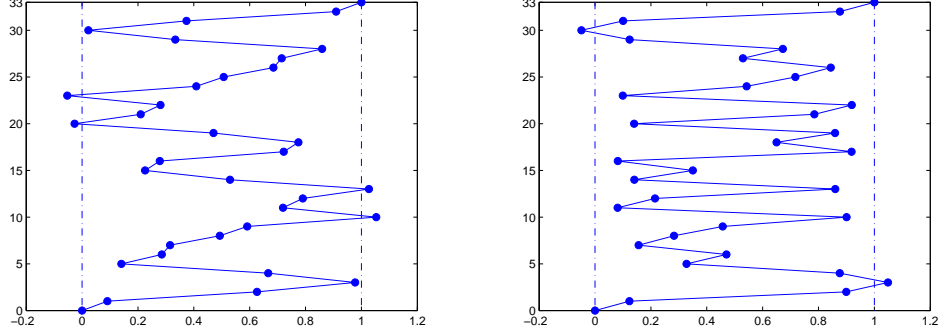


Figure 1: Cumulative weight plot for $s = 33$ stage and 10th order methods: left, Hairer; right, Kahan and Li.

Their 10-order and $s = 35$ stages method's coefficients:

$$\begin{aligned}
 \gamma_1 &= \gamma_{35} = 0.078795722521686419263907679337684 \\
 \gamma_2 &= \gamma_{34} = 0.31309610341510852776481247192647 \\
 \gamma_3 &= \gamma_{33} = 0.027918383235078066109520273275299 \\
 \gamma_4 &= \gamma_{32} = -0.22959284159390709415121339679655 \\
 \gamma_5 &= \gamma_{31} = 0.13096206107716486317465685927961 \\
 \gamma_6 &= \gamma_{30} = -0.26973340565451071434460973222411 \\
 \gamma_7 &= \gamma_{29} = 0.074973343155891435666137105641410 \\
 \gamma_8 &= \gamma_{28} = 0.11199342399981020488957508073640 \\
 \gamma_9 &= \gamma_{27} = 0.36613344954622675119314812353150 \\
 \gamma_{10} &= \gamma_{26} = -0.39910563013603589787862981058340 \\
 \gamma_{11} &= \gamma_{25} = 0.10308739852747107731580277001372 \\
 \gamma_{12} &= \gamma_{24} = 0.41143087395589023782070411897608 \\
 \gamma_{13} &= \gamma_{23} = -0.0048663605831352617621956593099771 \\
 \gamma_{14} &= \gamma_{22} = -0.39203335370863990644808193642610 \\
 \gamma_{15} &= \gamma_{21} = 0.051942502962449647037182904015976 \\
 \gamma_{16} &= \gamma_{20} = 0.050665090759924496335874344156866 \\
 \gamma_{17} &= \gamma_{19} = 0.049674370639729879054568800279461 \\
 \gamma_{18} &= 0.049317735759594537917680008339338
 \end{aligned} \tag{3.13}$$

In Figures 1 and 2 the cumulative weight plot of the 10-order methods can be seen. We have plotted the pairs (c_i, i) for $i = 1, 2, \dots, s$ being $c_i = \sum_{j=1}^i \gamma_j$.

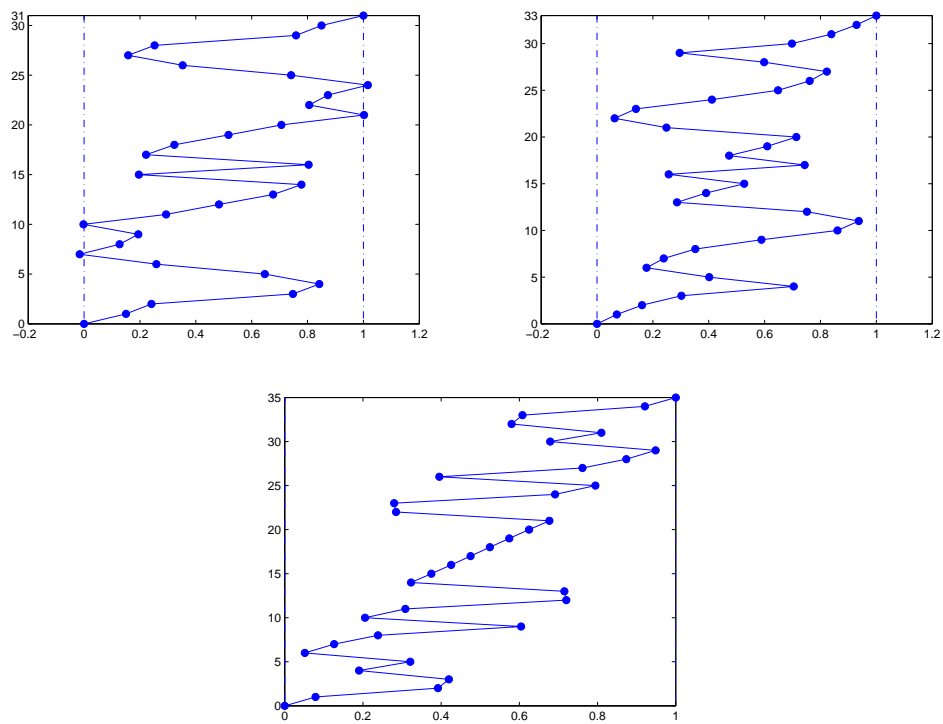


Figure 2: Cumulative weight plot for $s = 31$ (above left), $s = 33$ (above right) and $s = 35$ (below) stages and 10th order methods (Sofroniou and Spaletta).

3.2. Example of resolution: Euler equations

The motion of a rigid body, whose centre of mass is fixed at the origin, is modelled by Euler's equations:

$$\begin{cases} y_1' = \frac{I_2 - I_3}{I_2 I_3} y_2 y_3, \\ y_2' = \frac{I_3 - I_1}{I_3 I_1} y_3 y_1, \\ y_3' = \frac{I_1 - I_2}{I_1 I_2} y_1 y_2 \end{cases} \quad (3.14)$$

The vector $\mathbf{y} = (y_1, y_2, y_3)^T$ represents the angular momentum in the body frame, and I_i for $i = 1, 2, 3$ are the principal moments of inertia. The initial conditions are taken to be $y_1 = \cos(11/10)$, $y_2 = 0$ and $y_3 = \sin(11/10)$. The values of the principal moments are $I_1 = 2$, $I_2 = 1$ and $I_3 = 2/3$. The integration interval is $[0, 200]$. The high precision reference solution at the end of the interval is:

$$\begin{cases} y_1(200) = -0.28324773514861346196610535435048 \\ y_2(200) = 0.50103924378337485218535801654655 \\ y_3(200) = 0.81775937580816814902177599212573 \end{cases} \quad (3.15)$$

The ODE system (3.14) is solved by applying splitting:

$$\frac{d\mathbf{y}}{dt} = \mathbf{f} \quad (3.16)$$

which means that the vector field \mathbf{f} is split into some parts. First, we will consider the case in which it is split into two parts $\mathbf{f} = \mathbf{f}_1 + \mathbf{f}_2$. Let $\phi_{\mathbf{f}_1, h}$ and $\phi_{\mathbf{f}_2, h}$ denote the exact solution (flow). A second order symmetric integration method can be constructed using Strang splitting [28, 36]:

$$\phi_{\mathbf{f}_1, h/2} \circ \phi_{\mathbf{f}_2, h} \circ \phi_{\mathbf{f}_1, h/2} \quad (3.17)$$

Splitting into two vector fields yields methods of the form:

$$\phi_{\mathbf{f}_1, a_{s+1}} \circ \phi_{\mathbf{f}_2, b_s} \circ \phi_{\mathbf{f}_1, a_s} \circ \dots \circ \phi_{\mathbf{f}_2, b_1} \circ \phi_{\mathbf{f}_1, a_1} \quad (3.18)$$

Using the group property of flows, the coefficients for this splitting method are related to the composition coefficients in the following way:

$$\begin{cases} a_1 = \gamma_1/2, & b_1 = \gamma_1 \\ a_2 = (\gamma_1 + \gamma_2)/2, & b_2 = \gamma_2 \\ \vdots & \vdots \\ a_s = (\gamma_{s-1} + \gamma_s)/2, & b_s = \gamma_s \\ a_{s+1} = \gamma_s/2 \end{cases} \quad (3.19)$$

A symmetric generalization of (3.17) to the case in which the vector field is split in $k \geq 3$ parts is given by:

$$\phi_{\mathbf{f}_1,1/2} \circ \dots \circ \phi_{\mathbf{f}_{k-1},1/2} \circ \phi_{\mathbf{f}_k,1/2} \circ \phi_{\mathbf{f}_{k-1},1/2} \circ \dots \circ \phi_{\mathbf{f}_1,1/2} \quad (3.20)$$

The ODE system (3.14) has been split into three components as follows:

$$\begin{aligned} H_1 : \quad y_1' &= 0, & y_2' &= \frac{y_1 y_3}{I_1}, & y_3' &= -\frac{y_1 y_2}{I_1} \\ H_2 : \quad y_1' &= -\frac{y_2 y_3}{I_2}, & y_2' &= 0, & y_3' &= \frac{y_1 y_2}{I_2} \\ H_3 : \quad y_1' &= \frac{y_2 y_3}{I_3}, & y_2' &= -\frac{y_1 y_3}{I_3}, & y_3' &= 0 \end{aligned} \quad (3.21)$$

being their exact solutions $\phi_{\mathbf{f}_1,h}$, $\phi_{\mathbf{f}_2,h}$ and $\phi_{\mathbf{f}_3,h}$:

$$\left\{ \begin{aligned} \phi_{\mathbf{f}_1,h} &= \left(y_{1,0}, y_{2,0} \cos\left(\frac{h \cdot y_{1,0}}{I_1}\right) + y_{3,0} \sin\left(\frac{h \cdot y_{1,0}}{I_1}\right), y_{3,0} \cos\left(\frac{h \cdot y_{1,0}}{I_1}\right) - y_{2,0} \sin\left(\frac{h \cdot y_{1,0}}{I_1}\right) \right) \\ \phi_{\mathbf{f}_2,h} &= \left(y_{1,0} \cos\left(\frac{h \cdot y_{2,0}}{I_2}\right) - y_{3,0} \sin\left(\frac{h \cdot y_{2,0}}{I_2}\right), y_{2,0}, y_{3,0} \cos\left(\frac{h \cdot y_{2,0}}{I_2}\right) + y_{1,0} \sin\left(\frac{h \cdot y_{2,0}}{I_2}\right) \right) \\ \phi_{\mathbf{f}_3,h} &= \left(y_{1,0} \cos\left(\frac{h \cdot y_{3,0}}{I_3}\right) + y_{2,0} \sin\left(\frac{h \cdot y_{3,0}}{I_3}\right), y_{2,0} \cos\left(\frac{h \cdot y_{3,0}}{I_3}\right) - y_{1,0} \sin\left(\frac{h \cdot y_{3,0}}{I_3}\right), y_{3,0} \right) \end{aligned} \right\} \quad (3.22)$$

where $y_{1,0}$, $y_{2,0}$ and $y_{3,0}$ are the initial conditions. Step sizes have been selected from 2^{-i} , $i=0,1/2, \dots, 5$.

In Figure 3 the work-precision comparison at the end of the interval can be seen. In the horizontal axis the number of evaluations (number of steps multiplied by the number of stages) has been represented and in the vertical, the difference between the exact and the calculated solution at the end of the interval. A log-log scale plot has been done, which is a two-dimensional graph of numerical data that uses logarithmic scales on both the horizontal and vertical axes. The Kahan and Li's method's solution is in blue; in red Hairer's method's solution; in black the solution obtained by the Sofroniou's 31 stage method; in green Sofroniou's 33 stage method's solution and in brown the one obtained by the Sofroniou's 35 stage method.

It can be observed that even though the five presented methods are solving the problem (3.14) adequately, the Sofroniou & Spaletta's methods perform better than the rest of the methods. Also the Sofroniou & Spaletta's $s = 31$ stages method performs better than the Kahan & Li's and Hairer, Lubich & Wanner's $s = 33$ stages method. It can also be observed among the Sofroniou & Spaletta's methods that the greater the number of stages the better the obtained accuracy. It seems that the obtained accuracies makes up for the computational cost for the additional stages.

4. Starting points

We have calculated the points $\mathbf{x} = (\gamma_i)_{i=1,\dots,16}$ that satisfy the order conditions (3.3), (3.4), and the first order condition of the expressions (3.5)-(3.7). Let call these five conditions the simplest five order conditions. Take into account that we are solving a system of 5 equations and 16 unknowns. Among the points that satisfy the simplest five order conditions, the ones that locally minimize $\|\gamma\|_2$ are selected. These points have some repeated components, having only 5 different components.

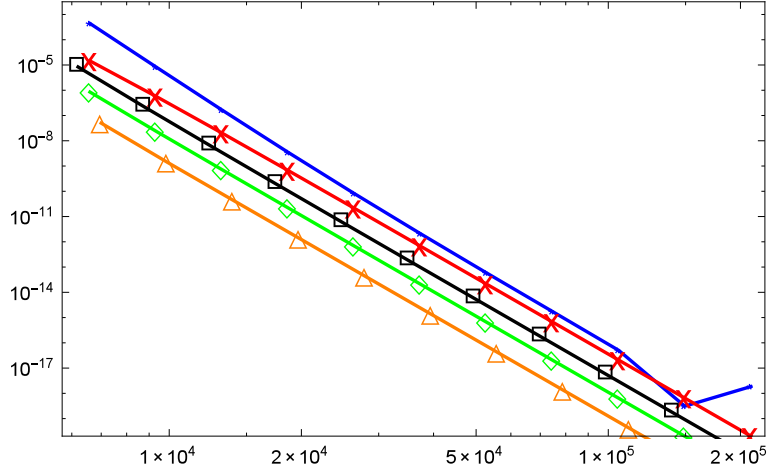


Figure 3: Work-precision comparison at the end of the interval using a log-log scale for the Euler's problem.

Different schemes of sixteen components points having 5 different components can be built. Among all of them, the scheme in which 12 γ_i coefficients are equal, and the rest 4 γ_i coefficients are different is the one that globally minimizes $\|\gamma\|_2$. Let denote this scheme by $(12, 1, 1, 1, 1)$. These points can be calculated by establishing 11 equalities between the 12 equal components and solving the simplest five order conditions' system. Solving this system of 16 equations (11 equalities and 5 order conditions) and 16 unknowns a real solution is obtained. Applying permutations of this real solution, many solutions of the same system can be calculated. Exactly $15!/12! = 2730$ points that satisfy the five simplest order conditions and globally minimize $\|\gamma\|_2$ can be calculated. However, the inconvenient of these points is that they contain few negative coefficients, resulting difficult to find points satisfying the rest of the eleven order conditions around them.

Nevertheless, schemes of sixteen components points having 5 different components such as $(11, 2, 1, 1, 1)$, $(10, 3, 1, 1, 1)$, $(10, 2, 2, 1, 1)$, etc. do not globally minimize $\|\gamma\|_2$, but they can locally minimize $\|\gamma\|_2$ being the value of this minimum sufficiently small. However, again, it seems difficult to find points satisfying the rest of the eleven order conditions around them.

As the solution found by Sofroniou and Spaletta is near of a local minimum that follows the scheme $(9, 4, 1, 1, 1)$, we have decided to chose the points that following the mentioned scheme $(9, 4, 1, 1, 1)$ locally minimize $\|\gamma\|_2$. In this case also a system formed by 16 equations (11 equalities and 5 order conditions) and 16 unknowns is solved and a real solution is obtained. Applying permutations of this real solution, many solutions of the same system can be calculated. Exactly $15!/(9! \cdot 4!) = 150150$ points that satisfy the five simplest order conditions and locally minimize $\|\gamma\|_2$ can be calculated. Among all these 150150 points, the ones having the cummulative weight plot in the interval $[0, 1]$ are 21871 points. Hence, these 21871 points have been selected as starting points.

5. Technique 1

In this section we will describe the first technique used to obtain new symmetric composition methods of basic second order symmetric integrators. As it has been said before we will focus on 10-order and $s = 31$ stages methods. The equalities of the expression (3.2) for 31-stages can be explicitly written as:

$$\begin{aligned}
 \gamma_1 &= \gamma_{31}, & \gamma_9 &= \gamma_{23}, \\
 \gamma_2 &= \gamma_{30}, & \gamma_{10} &= \gamma_{22}, \\
 \gamma_3 &= \gamma_{29}, & \gamma_{11} &= \gamma_{21}, \\
 \gamma_4 &= \gamma_{28}, & \gamma_{12} &= \gamma_{20}, \\
 \gamma_5 &= \gamma_{27}, & \gamma_{13} &= \gamma_{19}, \\
 \gamma_6 &= \gamma_{26}, & \gamma_{14} &= \gamma_{18}, \\
 \gamma_7 &= \gamma_{25}, & \gamma_{15} &= \gamma_{17}, \\
 \gamma_8 &= \gamma_{24}, & \gamma_{16} &
 \end{aligned} \tag{5.1}$$

which means that we have to obtain γ_i for $i = 1, \dots, 16$ satisfying the sixteen order conditions (3.3)-(3.7). Let denote by $\mathbf{x} = (\gamma_i)_{i=1, \dots, 16}$ the unknown solution. As it can be seen, when we consider $s = 31$ stages there are no free parameters.

In order to work in a bounded domain, we will replace the condition (3.3) (the so called consistency condition) by:

$$\sum_{k=1}^s \gamma_k^2 = 18 \tag{5.2}$$

Condition (5.2) means that the points $\mathbf{y} = (\gamma_i)_{i=1, \dots, 31}$ are in the sphere of center $\mathbf{0}$ and radius $\sqrt{18}$. Taking into account the equalities (5.1), the condition of being in the sphere is written as:

$$\sum_{k=1}^{15} 2\gamma_k^2 + \gamma_{16}^2 = 18 \Leftrightarrow \sum_{k=1}^{15} \gamma_k^2 + \frac{\gamma_{16}^2}{2} = 9 \tag{5.3}$$

There is a one-to-one correspondence between the solutions of (3.3)-(3.7) and the solutions of (3.4)-(3.7) and (5.3), satisfying that $\sum \gamma_i \neq 0$. So the system of equations that we will solve is formed by the equations (5.3) and (3.4)-(3.7).

It has to be said that we are not losing generalization when we solve this new system (the one formed by (5.3) and (3.4)-(3.7)) instead of the starting system (3.3)-(3.7). It has to be taken into account that we can pass from the consistency condition (3.3) to the condition of being on the sphere (5.3), and vice versa by doing:

- Moving from the sphere to the consistency condition: If we have a solution $\mathbf{y}_s = (\gamma_i)_{i=1, \dots, 31}$ that verifies conditions (5.3) and (3.4)-(3.7), the point $\mathbf{y}_c = (\tilde{\gamma}_i)_{i=1, \dots, 31}$ given by:

$$\tilde{\gamma}_i = \frac{\gamma_i}{\lambda}, \quad \text{being} \quad \lambda = \sum_{i=1}^{31} \gamma_i \tag{5.4}$$

will satisfy the consistency condition (3.3), as well as the conditions (3.4)-(3.7). This means that the formula (5.4) allows to move from the condition of being on the sphere to the consistency condition. And if \mathbf{y}_s satisfies the order conditions (3.4)-(3.7), the new point \mathbf{y}_c will continue satisfying them.

- Move from the consistency condition to the sphere: In an equivalent way, if the point $\mathbf{z}_c = (\hat{\gamma}_i)_{i=1,\dots,31}$ satisfies the consistency condition (3.3) and the conditions (3.4)-(3.7), we can obtain a point $\mathbf{z}_s = (\bar{\gamma}_i)_{i=1,\dots,31}$ of the sphere that will continue satisfying the order conditions (3.4)-(3.7):

$$\mathbf{z}_s = \frac{(\mathbf{z}_c - \mathbf{c})}{\|\mathbf{z}_c - \mathbf{c}\|} \cdot R + \mathbf{c} \quad (5.5)$$

being \mathbf{c} the center of the sphere and R the radius of the sphere. In this case, $\mathbf{c} = \mathbf{0}$ and $R = \sqrt{18}$. So in this case, the formula (5.5) to obtain a point on the sphere given a point that satisfies the consistency condition is reduced to:

$$\mathbf{z}_s = \frac{\mathbf{z}_c}{\|\mathbf{z}_c\|} \cdot \sqrt{18} \quad (5.6)$$

which means that $\bar{\gamma}_i = \frac{\hat{\gamma}_i}{\sqrt{\sum_{i=1}^s \hat{\gamma}_i^2}} \cdot \sqrt{18}$ for $i = 1, \dots, 31$.

Let denote by $F(\mathbf{x}) = 0$ the system of sixteen equations formed by (5.3) and (3.4)-(3.7) that has to be solved. The aim is to obtain solutions $\mathbf{x} = (\gamma_i)_{i=1,\dots,16}$ of that system. The process that we will follow to find such solutions will be:

- We will be given a starting point $\mathbf{x}_0 = (\gamma_i)_{i=1,\dots,16}$ on the sphere that satisfies the simple order conditions (condition (3.4), and the first equations of (3.5), (3.6) and (3.7)).
- $F(\mathbf{x})$ is partially linearized around $\mathbf{x} = \mathbf{x}_0$.
- New starting points are obtained.
- A local minimization algorithm is applied to the new starting points.
- If after local minimization $\|F(\mathbf{x})\|$ is small enough, then Newton's algorithm is applied to obtain a solution of $F(\mathbf{x}) = 0$.

In Figure 4 the main steps of this process are described.

5.1. Partial linealization

We will call simple order conditions to: the condition of being on the sphere, the condition (3.4), and the first equations of (3.5), (3.6) and (3.7). That is to say:

$$\begin{aligned} \sum_{k=1}^{15} \gamma_k^2 + \frac{\gamma_{16}^2}{2} - 9 = 0, & \quad \sum_{k=1}^s \gamma_k^3 = 0, & \quad \sum_{k=1}^s \gamma_k^5 = 0, \\ \sum_{k=1}^s \gamma_k^7 = 0, & \quad \sum_{k=1}^s \gamma_k^9 = 0 \end{aligned} \quad (5.7)$$

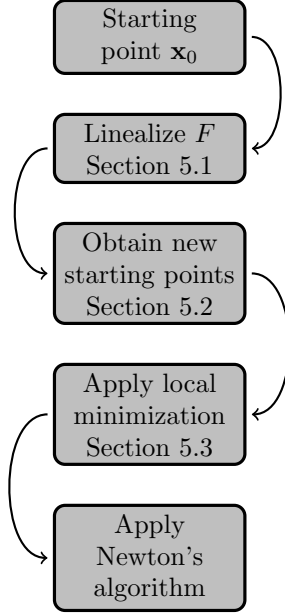


Figure 4: Main process of technique 1.

We are given a starting point $\mathbf{x}_0 = (\gamma_i)_{i=1,\dots,16}$ that satisfies the conditions explained in Section 4. That is to say:

- It verifies the five simple order conditions (5.7).
- It follows the scheme (9, 4, 1, 1, 1).
- It locally minimizes $\|\gamma\|_2$.
- Its cumulative weight plot is in the interval $[0, 1]$.

The function $F(\mathbf{x})$ could be linealized as follows:

$$F(\mathbf{x}) \approx F(\mathbf{x}_0) + F'(\mathbf{x}_0) \cdot (\mathbf{x} - \mathbf{x}_0) \quad (5.8)$$

We will use the singular value decomposition to decompose the jacobian matrix $J_0 = F'(\mathbf{x}_0)$. Let suppose that it can be decomposed as follows:

$$J_0 = P \cdot D \cdot Q^T \quad (5.9)$$

being P and Q orthogonal matrices, and D a diagonal matrix.

We will introduce the following change of variable:

$$\mathbf{x} = \mathbf{x}_0 + Q\mathbf{z} \quad (5.10)$$

Or what is the same as (5.10): $\mathbf{z} = Q^T(\mathbf{x} - \mathbf{x}_0)$.

A new function that depends on \mathbf{z} will be defined:

$$R(\mathbf{z}) = P^T \cdot F(\mathbf{x}_0 + Q\mathbf{z}) \quad (5.11)$$

The derivative of (5.11) is given by:

$$R'(\mathbf{z}) = P^T \cdot F'(\mathbf{x}_0 + Q\mathbf{z}) \cdot Q \quad (5.12)$$

We are interested in \mathbf{x} that makes $F(\mathbf{x}) = 0$. Or what is equivalent, we are interested in finding \mathbf{z} for which $R(\mathbf{z}) = 0$.

From (5.12) the derivative in $\mathbf{z} = 0$ can be calculated. And making use of the decomposition of the jacobian (5.9) and taking into account the orthogonality of the matrices P and Q , we have:

$$R'(0) = P^T \cdot \underbrace{F'(\mathbf{x}_0)}_{P \cdot D \cdot Q^T} \cdot Q = P^T \cdot P \cdot D \cdot Q^T \cdot Q = D \Rightarrow R'(0) = D \quad (5.13)$$

Using the Newton's method we have:

$$R(\mathbf{z}) \approx R(0) + R'(0)(\mathbf{z} - 0) = R(0) + D\mathbf{z} \quad (5.14)$$

And from (5.14), $R(\mathbf{z}) = 0$ can be solved:

$$\mathbf{z} \approx -D^{-1} \cdot R(0) \quad (5.15)$$

being: $R(0) = P^T \cdot F(\mathbf{x}_0)$.

So we can calculate the value of \mathbf{z} in which $R(\mathbf{z}) = 0$ using (5.15). This means that we only have to substitute this value \mathbf{z} in (5.10), and we will have the value of \mathbf{x} in which $F(\mathbf{x}) \approx 0$, provided that the linealization of $F(\mathbf{x})$ around $\mathbf{x} = \mathbf{x}_0$ is a sufficiently good approximation of $F(\mathbf{x})$.

5.2. Obtaining more starting points given one starting point

The second step of the process described in Figure 4 is the obtention of new starting points. Given one starting point \mathbf{x}_0 , the process to obtain new starting points has different parts:

1. Determine the significant part of the linealization following a criteria. The linealization will give "better starting points" than the first one (x_0 , which corresponds to $z = 0$).
2. Set the non-significant part of the linealization following a criteria.
3. The generated point will have the status of starting point if it verifies some conditions.

These steps can be seen in Figure 5.

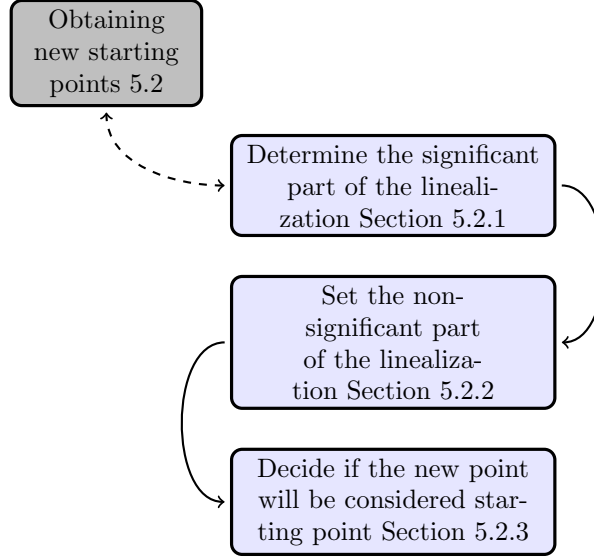


Figure 5: Steps of the process of obtaining starting points.

5.2.1. Determine the significant part of the linealization

In Section 5.1 the function F has been linearized, a new variable \mathbf{z} and a new function $R(\mathbf{z})$ have been defined and the way to obtain $F(\mathbf{x})$ has been explained. What typically happens is that some values of the diagonal matrix D are very small and the non-linear part becomes more significant than the linear part, making the previous linealization useless. In this sense it is necessary to determine the significant part of the linealization, that is to say, the part in which linealization will be applied.

We have a starting point $\mathbf{x}_0 = (\gamma_i)_{i=1,\dots,16}$ and we want to determine the positions in which the linealization will be applied. We calculate the value of the 16 order conditions and the value of the jacobian for this point:

$$F_0 = F(\mathbf{x}_0) \quad (5.16)$$

$$J_0 = J(\mathbf{x}_0) \quad (5.17)$$

being $F_0 = (F_{0,i})_{i=1,\dots,16}$ and $J_0 = (J_{0,i})_{i=1,\dots,16}$ vectors of sixteen components.

Next, the jacobian J_0 is decomposed using the singular value decomposition (5.9), and the change of variable (5.10) is introduced. The value of \mathbf{z}_1 is calculated using (5.15):

$$\mathbf{z}_1 = -D^{-1}R(0) \quad (5.18)$$

obtaining in this way $\mathbf{z}_1 = (z_{1,i})_{i=1,\dots,16}$. The new value \mathbf{x}_1 is calculated using the change of variable (5.10): $\mathbf{x}_1 = \mathbf{x}_0 + Q\mathbf{z}_1$.

All the components of the linealization will be taken into account if the following criteria is

verified:

$$\|F(\mathbf{x}_1)\| < p_1 \cdot \|F(\mathbf{x}_0)\| \quad (5.19)$$

being p_1 a constant that we will establish ($p_1 \in (0, 1)$). Condition (5.19) means that the new value \mathbf{x}_1 satisfies better than the starting point \mathbf{x}_0 the sixteen order conditions. It can be said that \mathbf{x}_1 is a better starting point than \mathbf{x}_0 .

If (5.19) is not verified, not all the linealization will be considered, which means that the new value \mathbf{x}_1 is not better than \mathbf{x}_0 . But we can determine a part in which linealization can be used and which verifies an equivalent condition as (5.19). The part that will be linearized will be determined by following these steps:

- (a) $i = 0$.
- (b) Make $\mathbf{z}_1(16 - i) = 0$. That is to say, $\mathbf{z}_1 = (z_{1,1}, z_{1,2}, \dots, z_{1,15}, 0)$. This means that the number 0 is introduced in the positions $j = 16 - i + 1, \dots, 16$ of the vector \mathbf{z}_1 .
- (c) $i \leftarrow i + 1$.
- (d) Recalculate \mathbf{x}_1 using (5.10): $\mathbf{x}_1 = \mathbf{x}_0 + Q\mathbf{z}_1$.
- (e) Evaluate $F(\mathbf{x}_1)$.
- (f) Comparing norms:

$$\|F(\mathbf{x}_1)_{j=1, \dots, 16-i}\| < p_1 \cdot \|F(\mathbf{x}_0)_{j=1, \dots, 16-i}\| \quad (5.20)$$
- (g) If condition (f) is not satisfied, we return to step (b).

This process has been described in Figure 6.

Following this process the part which will follow the linealization rule is determined and the rest components of \mathbf{z}_1 will be set to zero. That is to say the components $j = 1, \dots, 16 - i$ will follow the linealization and the components $j = 16 - i + 1, \dots, 16$ will be set to zero.

$$\mathbf{z}_{1,lin} = (z_{1,j}), \quad \text{for } j = 1, \dots, 16 - i \quad (5.21)$$

$$\mathbf{z}_{1,zero} = (0)_j, \quad \text{for } j = 16 - i + 1, \dots, 16 \quad (5.22)$$

5.2.2. Set the non-significant part of the linealization

The next step will be to calculate randomly the components of \mathbf{z}_1 that have been set to zero (the components $z_{1,j}$ for $j = 16 - i + 1, \dots, 16$). These components will be chosen randomly in the interval $(-1, 1)$. Let be $\mathbf{z}_{1,random}$ the part that will be completed randomly. Once the components are chosen, the vector $\mathbf{z}_{1,random}$ is resized in the way that verifies:

$$\|\mathbf{z}_{1,random}\| = \|\mathbf{z}_{1,lin}\| \cdot p_2 \quad (5.23)$$

being p_2 a constant that we will establish. The overall vector \mathbf{z}_1 is $\mathbf{z}_1 = [\mathbf{z}_{1,lin}, \mathbf{z}_{1,random}]$, satisfying the condition (5.23). This process is described in the Algorithm 1.

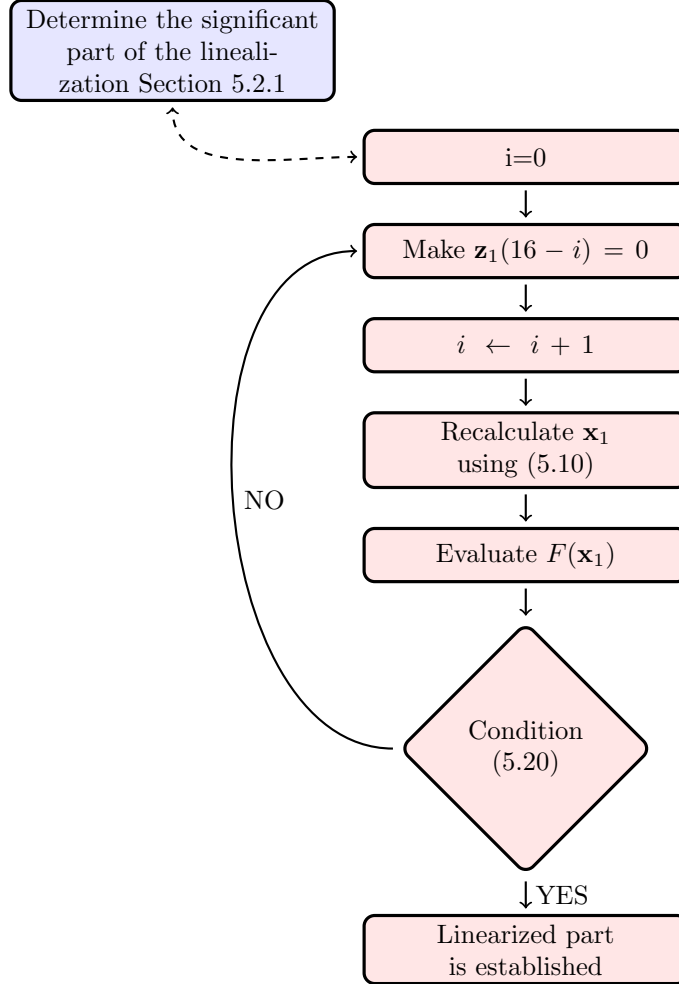


Figure 6: Determination of the significant part of the linearization.

5.2.3. Filtering out starting point candidates

Up to the moment the linearized part has been determined and the part that is not going to be linearized has been chosen as explained in Section 5.2.2. The overall vector $\mathbf{z}_1 = [\mathbf{z}_{1,lin}, \mathbf{z}_{1,random}]$ that has been built in this way will be used to calculate the new starting point $\mathbf{x}_1 = \mathbf{x}_0 + Q\mathbf{z}_1$ only if the following condition is satisfied:

$$\|R(\mathbf{z}_1)\| < p_3 \cdot \|R(0)\| \quad (5.24)$$

being p_3 a constant that we will establish. Only when the condition (5.24) is satisfied will be calculated the new starting point $\mathbf{x}_1 = \mathbf{x}_0 + Q\mathbf{z}_1$. Otherwise, again the $\mathbf{z}_{1,random}$ part will be set as explained in Section 5.2.2, \mathbf{z}_1 will be set to $\mathbf{z}_1 = [\mathbf{z}_{1,lin}, \mathbf{z}_{1,random}]$ and the condition (5.24) will be checked.

Algorithm 1 Algorithm to determine the random part of $z1$.

```

1: procedure LIRANDOM( $z1lin$ ,  $z1zero$ ,  $p_2$ )
2:    $s \leftarrow \text{size}(z1zero)$ 
3:    $s \leftarrow \max(s)$  ▷  $s$  is the number of elements in the vector  $z1zero$ 
4:   for  $i=1:s$  do
5:      $z1zero(i) \leftarrow 2*\text{rand}-1$  ▷ The function “rand” gives a random number of (0,1)
6:   end for
7:   ▷ Make the norms verify the next condition:  $\|z1random\| = \|z1lin\| \cdot p_2$ 
8:    $nlin \leftarrow \text{norm}(z1lin)$ 
9:    $nrand \leftarrow \text{norm}(z1zero)$ 
10:   $z1random \leftarrow z1zero*nlin/nrand*p_2$  ▷ scale  $z1zero$ 
11:   $z1 \leftarrow [z1lin^T \ z1random^T]$  ▷ Concatenate vectors
12:   $z1 \leftarrow z1^T$ 
13: end procedure

```

The overall process to obtain new starting points described in Section 5.2 is provided in Algorithm 2. In this algorithm the variable n_1 indicates the number of starting points that we want to create given a starting point \mathbf{x}_0 .

5.3. Applying local minimization to the new starting points

Given the new starting point \mathbf{x}_1 that has been generated in the previous section, the point that minimizes the function F will be calculated. For this aim, the Matlab local minimization function “lsqnonlin” is applied and we have defined the function that will be minimized:

$$M(\mathbf{x}_1) = \left[H(\mathbf{x}_1, 1), k \cdot \left(\sum_{i=1}^{15} \gamma_i + \frac{\gamma_{16}}{2} - \sum_{i=1}^{15} \tilde{\gamma}_i + \frac{\tilde{\gamma}_{16}}{2} \right) \right] \quad (5.25)$$

being $H(\mathbf{x}_1, 1)$ the value after substituting $t = 1$ in the homotopy function defined by:

$$H(\mathbf{x}, t) = F(\mathbf{x}) - (1 - t) \cdot F(\mathbf{x}_0) \quad (5.26)$$

$\mathbf{x}_1 = (\gamma)_{i=1, \dots, 16}$ the new starting point created following the process, and $\mathbf{x}_0 = (\tilde{\gamma})_{i=1, \dots, 16}$ the first starting point and k a constant that this time has been established as $k = 10^{-5}$. The second part of the expression (5.25) means that we want to obtain points which coefficients measure something similar to the coefficients of \mathbf{x}_0 . The function M has 17 components: the 16 components of $H(\mathbf{x}, t)$ and the additional component will measure the coefficients.

5.4. Some numerical results

Our first goal is to try if we are able to find the 10-order $s = 31$ stages Sofroniou and Spaletta’s solution (3.11) using the mentioned starting points. Among all the 21871 points we have, a point

Algorithm 2 Algorithm to determine new starting points.

```

1: Input:  $x_0, n_1, p_1, p_2, p_3$   $\triangleright n_1$  is the quantity of starting points that we want to create
2:  $x0sig \leftarrow zeros(n_1, 16)$ 
3:  $f0sig \leftarrow zeros(n_1, 16)$ 
4:  $normf0sig \leftarrow zeros(n_1, 1)$ 
5:  $F0 \leftarrow mxrealRest(x_0, 1, zeros(1, 15))$   $\triangleright$  Evaluate the order conditions in  $x_0$  and  $t = 1$ 
6:  $J0 \leftarrow mxrealJacobian(x_0, 1, zeros(1, 15))$   $\triangleright$  Evaluate the Jacobian of the order conditions in  $x_0$ 
   and  $t = 1$ 
7:  $[P, D, Q] \leftarrow$  Singular Value Decomposition of  $J0$ 
8:  $z1 \leftarrow inv(D) * P^T * F0^T$ 
9:  $x1 \leftarrow x0^T + Q * z1$   $\triangleright$  Change of variable
10:  $x1 \leftarrow x1^T$ 
11:  $F1 \leftarrow mxrealRest(x_1, 1, zeros(1, 15))$ 
12:  $R0 \leftarrow P^T \cdot F0$ 
13:  $R1 \leftarrow P^T \cdot F1$ 
14:  $n0 \leftarrow norm(R0)$ 
15:  $n1 \leftarrow norm(R1)$ 
16:  $i \leftarrow 0$ 
17: while  $n1 \geq p_1 * n0$  do  $\triangleright$  Determine the linerized part
18:    $z1(end-i) \leftarrow 0$ 
19:    $i \leftarrow i+1$ 
20:    $x1 \leftarrow x0^T + Q * z1$   $\triangleright$  Recalculate  $x1$ 
21:    $x1 \leftarrow x1^T$ 
22:    $F1 \leftarrow mxrealRest(x_1, 1, zeros(1, 15))$ 
23:    $R1 \leftarrow P^T \cdot F1$ 
24:    $n0 \leftarrow norm(R0(1:end-i))$   $\triangleright$  Recalculate the norm of the possible lin. part
25:    $n1 \leftarrow norm(R1(1:end-i))$   $\triangleright$  Recalculate the norm of the possible lin. part
26: end while  $\triangleright$  After finishing the previous While bucle the linearized part is determined
27:  $Gn0 \leftarrow P^T * F0^T$ 
28:  $gn0 \leftarrow norm(Gn0)$ 
29: for  $j=1:n_1$  do  $\triangleright$  For the creation of each new starting point the following process is followed
30:    $gn1 \leftarrow gn0 * p_3 + 1$ 
31:   while  $gn1 > gn0 * p_3$  do  $\triangleright$  Criteria to be considered starting point
32:      $z1lin \leftarrow z1(1:end-i)$ 
33:      $z1zero \leftarrow z1(end-i+1:end)$ 
34:      $z1 \leftarrow linrandom(z1lin, z1zero, p_2)$   $\triangleright linrandom$  has been explained in Algorithm 1
35:      $x1 \leftarrow x0^T + Q * z1$   $\triangleright$  Recalculate  $x1$ 
36:      $x1 \leftarrow x1^T$ 
37:      $F1 \leftarrow mxrealRest(x_1, 1, zeros(1, 15))$ 
38:      $Gn1 \leftarrow P^T * F1^T$ 
39:      $gn1 \leftarrow norm(Gn1)$ 
40:   end while
41:    $x0sig(j,:) \leftarrow x1$ 
42:    $ff \leftarrow mxrealRest(x_1, 1, zeros(1, 15))$ 
43:    $f0sig(j,:) \leftarrow ff$ 
44:    $normf0sig(j) \leftarrow norm(ff)$ 
45: end for

```

that is quite similar to the solution is selected. The chosen point \mathbf{x}_0 has been the following:

$$\begin{aligned}
\gamma_1 &= \gamma_{31} = 0.127878789499696 \\
\gamma_2 &= \gamma_{30} = 0.127878789499696 \\
\gamma_3 &= \gamma_{29} = 0.356988485581094 \\
\gamma_4 &= \gamma_{28} = 0.127878789499696 \\
\gamma_5 &= \gamma_{27} = -0.202029287967921 \\
\gamma_6 &= \gamma_{26} = -0.202029287967921 \\
\gamma_7 &= \gamma_{25} = -0.202029287967921 \\
\gamma_8 &= \gamma_{24} = 0.127878789499696 \\
\gamma_9 &= \gamma_{23} = 0.127878789499696 \\
\gamma_{10} &= \gamma_{22} = -0.202029287967921 \\
\gamma_{11} &= \gamma_{21} = 0.127878789499696 \\
\gamma_{12} &= \gamma_{20} = 0.127878789499696 \\
\gamma_{13} &= \gamma_{19} = 0.127878789499696 \\
\gamma_{14} &= \gamma_{18} = 0.127878789499696 \\
\gamma_{15} &= \gamma_{17} = -0.420682194566747 \\
&\gamma_{16} = 0.441803510720145
\end{aligned} \tag{5.27}$$

We can obtain a point that satisfies the condition of being on the sphere using (5.6), $\mathbf{x}_{0,s}$:

$$\begin{aligned}
\gamma_1 &= \gamma_{31} = 0.454509202796914 \\
\gamma_2 &= \gamma_{30} = 0.454509202796914 \\
\gamma_3 &= \gamma_{29} = 1.268815200894017 \\
\gamma_4 &= \gamma_{28} = 0.454509202796914 \\
\gamma_5 &= \gamma_{27} = -0.718056301402089 \\
\gamma_6 &= \gamma_{26} = -0.718056301402089 \\
\gamma_7 &= \gamma_{25} = -0.718056301402089 \\
\gamma_8 &= \gamma_{24} = 0.454509202796914 \\
\gamma_9 &= \gamma_{23} = 0.454509202796914 \\
\gamma_{10} &= \gamma_{22} = -0.718056301402089 \\
\gamma_{11} &= \gamma_{21} = 0.454509202796914 \\
\gamma_{12} &= \gamma_{20} = 0.454509202796914 \\
\gamma_{13} &= \gamma_{19} = 0.454509202796914 \\
\gamma_{14} &= \gamma_{18} = 0.454509202796914 \\
\gamma_{15} &= \gamma_{17} = -1.495196581320806 \\
&\gamma_{16} = 1.570266361105709
\end{aligned} \tag{5.28}$$

Using the point $\mathbf{x}_{0,s}$ (5.28), we apply the overall process, obtaining $n_1 = 200$ new starting points and taking $p_1 = p_3 = 0.5$, $p_2 = 1$. With each of this new starting points local minimization has been applied. The best point that we obtain following this process is $\hat{\mathbf{x}}_{best}$ (which is a point that

satisfies the consistency condition):

$$\begin{aligned}
\gamma_1 &= \gamma_{31} = 0.149980166757970 \\
\gamma_2 &= \gamma_{30} = 0.091209376694612 \\
\gamma_3 &= \gamma_{29} = 0.506230734715795 \\
\gamma_4 &= \gamma_{28} = 0.094789495557464 \\
\gamma_5 &= \gamma_{27} = -0.195208621182677 \\
\gamma_6 &= \gamma_{26} = -0.388162197150489 \\
\gamma_7 &= \gamma_{25} = -0.274505111979716 \\
\gamma_8 &= \gamma_{24} = 0.142646518254726 \\
\gamma_9 &= \gamma_{23} = 0.067102617758162 \\
\gamma_{10} &= \gamma_{22} = -0.196431578067715 \\
\gamma_{11} &= \gamma_{21} = 0.296028212910127 \\
\gamma_{12} &= \gamma_{20} = 0.189178035331035 \\
\gamma_{13} &= \gamma_{19} = 0.193946569643248 \\
\gamma_{14} &= \gamma_{18} = 0.101200654564512 \\
\gamma_{15} &= \gamma_{17} = -0.581868670815763 \\
\gamma_{16} &= 0.607727594017418
\end{aligned} \tag{5.29}$$

We have to pass the point $\hat{\mathbf{x}}_{best}$ to the sphere to calculate how this point satisfies the sixteen conditions. After doing this we get: $\|F(\hat{\mathbf{x}}_{best,s})\| = 8.095236171459589e - 09$. Using this point $\hat{\mathbf{x}}_{best,s}$ and applying Newton's algorithm (it can also be done by following a homotopy continuation algorithm), we could improve this result. The improved point on the sphere that has been calculated is $\mathbf{x}_{i,s}$ which is given by:

$$\begin{aligned}
\gamma_1 &= \gamma_{31} = 0.391898821758196 \\
\gamma_2 &= \gamma_{30} = 0.238327708152066 \\
\gamma_3 &= \gamma_{29} = 1.322779725993880 \\
\gamma_4 &= \gamma_{28} = 0.247685054485755 \\
\gamma_5 &= \gamma_{27} = -0.510079508389213 \\
\gamma_6 &= \gamma_{26} = -1.014266851165851 \\
\gamma_7 &= \gamma_{25} = -0.717281648710886 \\
\gamma_8 &= \gamma_{24} = 0.372735260138248 \\
\gamma_9 &= \gamma_{23} = 0.175338547052314 \\
\gamma_{10} &= \gamma_{22} = -0.513275479198167 \\
\gamma_{11} &= \gamma_{21} = 0.773521120431214 \\
\gamma_{12} &= \gamma_{20} = 0.494321437409558 \\
\gamma_{13} &= \gamma_{19} = 0.506782546219677 \\
\gamma_{14} &= \gamma_{18} = 0.264436860646363 \\
\gamma_{15} &= \gamma_{17} = -1.520421491878899 \\
\gamma_{16} &= 1.587990801662441
\end{aligned} \tag{5.30}$$

and obtaining this time $\|F(\mathbf{x}_{i,s})\| = 1.102509095666297e - 12$. And applying the consistency

condition to $\mathbf{x}_{i,s}$ we get the point $\mathbf{x}_{i,c}$ given by:

$$\begin{aligned}
\gamma_1 &= \gamma_{31} = 0.149980700546958 \\
\gamma_2 &= \gamma_{30} = 0.091208635096261 \\
\gamma_3 &= \gamma_{29} = 0.506231248881590 \\
\gamma_4 &= \gamma_{28} = 0.094789715927509 \\
\gamma_5 &= \gamma_{27} = -0.195208757351316 \\
\gamma_6 &= \gamma_{26} = -0.388162567565133 \\
\gamma_7 &= \gamma_{25} = -0.274505556512013 \\
\gamma_8 &= \gamma_{24} = 0.142646755566363 \\
\gamma_9 &= \gamma_{23} = 0.067102518966024 \\
\gamma_{10} &= \gamma_{22} = -0.196431863710003 \\
\gamma_{11} &= \gamma_{21} = 0.296028548924095 \\
\gamma_{12} &= \gamma_{20} = 0.189178102514962 \\
\gamma_{13} &= \gamma_{19} = 0.193947001335706 \\
\gamma_{14} &= \gamma_{18} = 0.101200675807723 \\
\gamma_{15} &= \gamma_{17} = -0.581869267826854 \\
\gamma_{16} &= 0.607728218796252
\end{aligned} \tag{5.31}$$

As it can be observed our point $\mathbf{x}_{i,c}$ is the point of Sofroniou and Spaletta's method (3.11). Hence, up to this moment it seems that if we chose the starting point that is similar to Sofroniou and Spaletta's solution and we follow the process we have designed, we are able to obtain the method (3.11). We could also obtain the same point by creating only 100 new starting points, and also creating only 50. But it has not been possible to obtain this solution in any of the trials performed creating only 5 or 10 new starting points.

5.5. Deciding the starting points that will not follow the process

As it has been said in Section 4, we have 21871 starting points to try with. Since local minimization is computationally expensive, we want to eliminate some of them following a criteria. The process of building better starting points and applying the local minimization will be followed with the starting points that have not been eliminated. The criteria that we will use to eliminate some starting points is the following:

- The first part will be the same as in Algorithm 2. We are given a point \mathbf{x}_0 on the sphere and we determine the part that will be linearized.
- We have explained before the process to obtain \mathbf{z}_1 that satisfies:

$$R(\mathbf{z}_1) = 0 \tag{5.32}$$

And we have found the part that will be linearized. Let denote by $R^{[j]}$ the part that will be linearized:

$$R^{[j]} = \begin{pmatrix} R_1(\mathbf{z}_1) \\ R_2(\mathbf{z}_1) \\ \vdots \\ R_j(\mathbf{z}_1) \end{pmatrix} \tag{5.33}$$

Take into account that \mathbf{z}_1 has two parts $\mathbf{z}_1 = (\mathbf{z}_1^{[j]}, 0)$. That is to say, the coordinates of \mathbf{z}_1 are zero in the components $k = j + 1, \dots, s$. We do some iterations using Newton's method in order to satisfy:

$$R^{[j]}(\mathbf{z}_1^{[j]}, 0) = 0 \quad (5.34)$$

Iterations will be done as follows:

$$\begin{cases} h = -D^{-1} \cdot R(\mathbf{z}_k^{[j]}, 0) \\ \mathbf{z}_{k+1}^{[j]} = \mathbf{z}_k^{[j]} + h^{[j]} \end{cases} \quad (5.35)$$

In each iteration \mathbf{x}_1 will be calculated:

$$\mathbf{x}_1 = \mathbf{x}_0 + Q \begin{pmatrix} \mathbf{z}_1^{[j]} \\ 0 \end{pmatrix} \quad (5.36)$$

In this way the point $\mathbf{x}_1 = (\gamma_i)_{i=1, \dots, 16}$ is calculated which will be considered starting point to follow the process if the following is satisfied:

$$\left| \sum_{i=1}^s \gamma_i \right| \geq \text{value} \quad (5.37)$$

which means that $|\sum_{i=1}^s \gamma_i|$ has not to be very small.

We know that for the starting point that gives the Sofroniou and Spaletta's solution the variable *value* is:

$$\text{value} = 3.36 \quad (5.38)$$

Different intervals for the variable *value* have been chosen and the number of starting points that belong to each interval have been calculated, see Table 5.5.

interval	[0,1)	[1,2)	[2,3)	[3,4)	[4,5)	[5,10)	[10,20)	[20,50)	[50,100)	[100,1000)
points in interval	259	313	553	1250	3367	3142	833	647	384	938
cumulative sums	259	572	1125	2375	5742	8884	9717	10364	10748	11681

Table 3: Number of starting points with $|\sum_{i=1}^s \gamma_i|$ in each interval, and cumulative sums.

It seems reasonable to try the process with the starting points for which $\text{value} \geq 3$. Only around 1125 points out of the 21871 do not satisfy this condition, which means that our beginning list of 21871 nearly is not reduced. Hence, the amount of points to follow the process with is still huge. This process is explained in the Algorithm 3, where we can insert the interval for the variable *value*. That is to say, the points with $\text{value} \in [\text{liminf}, \text{limsup}]$ shown in Table 5.5 are calculated using this algorithm. If we want to use this algorithm to discard the points that will not follow the process, it is sufficient to call this function only with the first three inputs x_0 , p_1 and *liminf*, choosing *liminf* = 3 and to change the condition of the line 37 of the Algorithm 3 as follows:

```

if abs(balio) ≥ liminf then
    aurrera ← 1
end if

```

That is to say, the points satisfying $\text{value} \geq 3$ will follow the process described in Figure 4.

Algorithm 3 Algorithm to discard starting points.

```
1: procedure CLEAN( $x_0, p_1, \text{liminf}, \text{limsup}$ ) ▷  $x_0$  is a starting point in the sphere
2:   F0 ← mxrealRest( $x_0, 1, \text{zeros}(1,15)$ ) ▷ Evaluate order conditions in  $x_0$  and  $t = 1$ 
   (mxrealRest is the homotopy)
3:   J0 ← mxrealJacobian( $x_0, 1, \text{zeros}(1,15)$ )▷ Evaluate the Jacobian of the order conditions in
    $x_0$  and  $t = 1$ 
4:   [P,D,Q] ← Singular Value Decomposition of J0
5:   invD ← inv(D)
6:   z1 ← -invD * PT * F0T
7:   x1 ←  $x_0^T + Q * z1$  ▷ Change of variable
8:   x1 ←  $x_1^T$ 
9:   F1 ← mxrealRest( $x_1, 1, \text{zeros}(1,15)$ )
10:  R0 ← PT · F0
11:  R1 ← PT · F1
12:  n0 ← norm(R0)
13:  n1 ← norm(R1)
14:  i ← 0
15:  while  $n1 \geq p_1 * n0$  do ▷ Determine the linerized part
16:    z1(end-i) ← 0
17:    i ← i+1
18:    x1 ←  $x_0^T + Q * z1$  ▷ Recalculate x1
19:    x1 ←  $x_1^T$ 
20:    F1 ← mxrealRest( $x_1, 1, \text{zeros}(1,15)$ )
21:    R1 ← PT · F1
22:    n0 ← norm(R0(1:end-i)) ▷ Recalculate the norm of the possible lin. part
23:    n1 ← norm(R1(1:end-i)) ▷ Recalculate the norm of the possible lin. part
24:  end while
25: ▷ After finishing the previous While bucle the linearized part is determined and z1 and x1 are
   obtained
26:  z0 ← z1
27:  for k=1:4 do ▷ Newton Raphson iteration, 4 iterations
28:    incrz1 ← -invD * PT * F1T
29:    z1(1:end-i) ← z0(1:end-i) + incrz1(1:end-i)
30:    x1 ←  $x_0^T + Q * z1$ 
31:    x1 ←  $x_1^T$ 
32:    F1 ← mxrealRest( $x_1, 1, \text{zeros}(1,15)$ )
33:    z0 ← z1
34:  end for
35:  balio ← sum(x1)+sum(x1(1:end-1))
36:  aurrera ← 0
37:  if abs(balio) ≥ liminf & abs(balio) < limsup then
38:    aurrera ← 1
39:  end if
40: end procedure
```

5.6. Attempt to improve Algorithm 2

In this section we do an attempt to improve the process described in Section 5.2. Following the process of Section 5.2, we have been able to obtain Sofroniou and Spaletta's solution, but using the same starting point we could not find more adequate solutions, as the solutions that we obtain have big coefficients after applying the consistency condition.

So, the first decision we took was to follow the consistency condition without using the sphere. We have used a scaled version of the consistency condition:

$$2 \cdot \sum_{i=1}^{15} \gamma_i + \gamma_{16} = 6 \quad (5.39)$$

which means that after obtaining one solution, the γ_i coefficients have to be divided by 6. From the expression (5.39), γ_{16} will be solved:

$$\gamma_{16} = 6 - 2 \cdot \sum_{i=1}^{15} \gamma_i \quad (5.40)$$

and it will be substituted in all the order conditions. This means that our new unknown \mathbf{x}_n will have 15 components and we will have also 15 conditions to satisfy (as the scaled consistency condition is included in all of them). After having calculated the first 15 components, γ_{16} is calculated obtaining $(\gamma)_{i=1, \dots, 16}$. Because of this change we have to adapt also some concepts explained in the previous version:

1. The condition to be considered new starting point (5.37) changes. Now the point $\mathbf{x}_1 = (\gamma_i)_{i=1, \dots, 16}$ will be considered starting point to follow the process if the following is satisfied:

$$\sum_{i=1}^s \gamma_i^2 \leq \text{value} \quad (5.41)$$

which means that $\sum_{i=1}^s \gamma_i^2$ has not to be very large.

In this sense, the value that we had before for the starting point that gives the Sofroniou and Spaletta's solution (5.38) also changes:

$$\text{value} = 52.46 \quad (5.42)$$

2. Also the function (5.25) that has to be minimized changes:

$$\begin{cases} \gamma_{16} = 6 - 2 \cdot \sum_{i=1}^{15} \gamma_i \\ \hat{M}(\mathbf{x}_1) = [H(\mathbf{x}_1, 1), k(\gamma_1, \gamma_2, \dots, \gamma_{16})] \end{cases} \quad (5.43)$$

A point with 15 components enters in the function and γ_{16} is calculated. Then, the function \hat{M} that has to be minimized is defined, being $H(\mathbf{x}_1, 1)$ as before the value after substituting $t = 1$ in the homotopy function defined by (5.26) (even though now the homotopy $H(\mathbf{x}, t)$ has 15 components), k a constant that this time has been established also as $k = 10^{-5}$. The second part of the expression (5.43) means that we want to obtain a point with small coefficients. The function \hat{M} has 31 components: the 15 components of $H(\mathbf{x}, t)$ and the additional part with 16 components to assure the coefficients will be small.

Apart from the previous considerations derived of the use of the scaled consistency condition, some new criteria have been introduced in this new process changing the decision to be considered as starting point. The new process will consist in the following steps:

1. Determine the significant part of the linealization following the same process as in Section 5.2.1.
2. Set the non-significant part of the linealization following the same process as in Section 5.2.2. After finishing the first two steps, the linearized part is determined and, $\mathbf{z}_1 = [\mathbf{z}_{1,lin}, \mathbf{z}_{1,random}]$ and \mathbf{x}_1 are calculated. The following steps will consist in the decision to consider the new point \mathbf{x}_1 as starting point.
3. The first condition that \mathbf{z}_1 has to satisfy in order to consider the point \mathbf{x}_1 as new starting point will be similar to something that has been explained in Section 5.5. We have denoted by $R^{[j]}$ the part that has been linearized (5.33). Take into account in this point of the process that the random part of \mathbf{z}_1 has been completed: $\mathbf{z}_1 = [\mathbf{z}_{1,lin}, \mathbf{z}_{1,random}]$. We will do some iterations using Newton's method in order to obtain a new point with a smaller value in the function $R^{[j]}$ than the starting point, maintaining the random part (which means that the Newton's method will affect only the linearized part). Hence, iterations will be done as follows:

$$\begin{cases} h = -D^{-1} \cdot R(\mathbf{z}_k^{[j]}, \mathbf{z}_{1,random}) \\ \mathbf{z}_{1,k+1}^{[j]} = \mathbf{z}_{1,k}^{[j]} + h^{[j]} \end{cases} \quad (5.44)$$

The notation $\mathbf{z}_{1,k}^{[j]}$ means the value of $\mathbf{z}_1^{[j]}$ obtained in the k th iteration using Newton's method. And the new point $\mathbf{z}_{1,k} = [\mathbf{z}_{1,k}^{[j]}, \mathbf{z}_{1,random}]$ will follow the process only if it satisfies this condition:

$$\|R^{[j]}(\mathbf{z}_{1,k})\| \leq p_4 \cdot \|R^{[j]}(\mathbf{z}_{1,0})\| \quad (5.45)$$

being k the number of iterations that Newton's method will do (for example $k = 4$) and p_4 a constant that we will establish.

4. Using the value $\mathbf{z}_{1,k}$ that satisfies the condition (5.45), the point \mathbf{x}_1 will be calculated: $\mathbf{x}_1 = \mathbf{x}_0 + Q\mathbf{z}_{1,k}$. This point $\mathbf{x}_1 = (\gamma_i)_{i=1,\dots,16}$ will have to satisfy the condition (5.41) to be a new starting point, that is to say:

$$\sum_{i=1}^s \gamma_i^2 \leq value$$

One consideration about this has to be done, as this value is different before or after the Newton's iterations for the starting point that gives the Sofroniou and Spaletta's solution:

$$value = \begin{cases} 52.46 & \text{before Newton's 4 iterations} \\ 155.19 & \text{after Newton's 4 iterations} \end{cases} \quad (5.46)$$

5. If the point $\mathbf{x}_1 = (\gamma_i)_{i=1,\dots,16}$ satisfies the condition (5.41), a third condition will be verified. This third condition is the condition (5.24) used in Algorithm 2:

$$\|R(\mathbf{z}_1)\| < p_3 \cdot \|R(0)\|$$

6. The number of trials in which these three conditions will be checked will be set using the parameter m . That is to say, given a starting point x_0 , we will create a better starting point and the trials done with the z random part will be m at maximum.

See Algorithm 4 in which these new criteria are introduced to consider a new point as starting point.

5.6.1. Problems found when finding numerical results

Following the process described in this section it has turned more difficult to obtain results. By choosing the following parameters $p_1 = p_3 = p_4 = 0.5$, $value = 200$, $p_2 = 2.4$ and after creating 1000 new starting points, some results having the norm of the 15 order conditions around $e - 8$ have been obtained. These points have been improved using the homotopy continuation algorithm until this norm was of $e - 11$ order, but we were unable to obtain the Sofroniou and Spaletta's solution. The parameter p_2 has been established taking into account the distance between the starting point and the Sofroniou's solution. As in this version we are considering the first 15 components of the points, this distance has been calculated as follows:

$$d = \sqrt{6 \cdot \mathbf{x}_0(1 : 15) - 6 \cdot \mathbf{x}_s(1 : 15)} = 2.18 \quad (5.47)$$

being $\mathbf{x}_0(1 : 15)$ and $\mathbf{x}_s(1 : 15)$ the first 15 components of the starting point and the Sofroniou and Spaletta's solution. These components have been multiplied by 6, as we are considering the scaled consistency version.

Hence, taking into account the experiments performed with this new version, we can say that the attempt to improve the Algorithm 2 has not succeeded.

6. Technique 2

Up to now we have been following the process described in Section 5 to obtain symmetric composition methods of $s = 31$ stages and 10 order of accuracy. As we have not obtained the expected results we will change the strategy. A symmetric composition method of $s = 31$ stages and 10th order of accuracy must verify the 16 order conditions given by (3.3)- (3.7). We have 21871 starting points that satisfy the simple order conditions and respond to the scheme (9, 4, 1, 1, 1).

We will define a function with 15 conditions and 16 unknowns. The 15 conditions will be equalities between the unknowns or order conditions that the unknowns have to satisfy. The values of the unknowns that satisfy the established 15 conditions define a curve. A different function with a new condition (again, an equality between two unknowns or an order condition) will be also defined, and it will be possible to test if while moving along the 15-condition curve, this new condition is satisfied. Let call *test condition* to this new condition. If one point in the 15-condition curve satisfies the test condition, one of the 15 conditions could be interchanged by this test condition. In this way, a new curve of points satisfying 14 of the starting conditions and the test condition will be obtained. This process is reversible, being possible to return to the original 15-condition curve (it is enough to establish as test condition the condition that has been interchanged). The process to move from some conditions to others has been implemented in C language, and some *MEX* files are used to call them from Matlab.

Algorithm 4 Algorithm to determine new starting points.

```

1: Input:  $x_0, m, p_1, p_2, p_3, p_4, value$ 
2:   ▷ Given a starting point  $x_0$  on the sphere, we will create a better starting point. The trials
   done with the  $z$  random part will be  $m$  at maximum. The parameters  $p_1, p_2, p_3, p_4, value$  are
   the ones that appear in the criteria that will be used.
3:   ▷ Lines 1-28 are the same as in the Algorithm 2, changing only the aspects related to the
   scaled consistency condition
4:  $p \leftarrow 0$ 
5:  $z1lin \leftarrow z1(1:end-i)$ 
6:  $z1zero \leftarrow z1(end-i+1:end)$ 
7: while  $p < m$  do
8:    $z1 \leftarrow \text{linrandom}(z1lin, z1zero, p_2)$                                      ▷ Chose the random part of  $z1$ 
9:    $x1 \leftarrow x0^T + Q * z1$ 
10:   $x1 \leftarrow x1^T$ 
11:   $F1 \leftarrow \text{mxrealRest}(x1, 1, \text{zeros}(1,15))$ 
12:   $Gnini \leftarrow P^T * F1^T$ 
13:   $gnini_j \leftarrow \text{norm}(Gnini(1:end-i))$ 
14:   $z0 \leftarrow z1$ 
15:  for  $k=1:4$  do                                                                 ▷ Newton Raphson iteration, 4 iterations
16:     $\text{incr}z1 \leftarrow -\text{inv}D * P^T * F1^T$ 
17:     $z1(1:end-i) \leftarrow z0(1:end-i) + \text{incr}z1(1:end-i)$ 
18:     $x1 \leftarrow x0^T + Q * z1$ 
19:     $x1 \leftarrow x1^T$ 
20:     $F1 \leftarrow \text{mxrealRest}(x1, 1, \text{zeros}(1,15))$ 
21:     $z0 \leftarrow z1$ 
22:  end for
23:   $Gn1 \leftarrow P^T * F1^T$ 
24:   $gn1 \leftarrow \text{norm}(Gn1)$ 
25:   $gn1_j \leftarrow \text{norm}(Gn1(1:end-i))$ 
26:  if  $gn1_j \leq p_4 * gnini_j$  then
27:     $\text{balio} \leftarrow \text{sum}(x1) + \text{sum}(x1(1:end-1))$ 
28:    if  $\text{abs}(\text{balio}) \leq value$  then
29:      if  $gn1 \leq gn0 * p_3$  then
30:        Accept  $x1$  as starting point and apply local minimization
31:         $p \leftarrow m+1$                                      ▷ It could be also  $p=p+1$  and obtain another starting point
32:      else
33:         $p \leftarrow p+1$ 
34:      end if
35:    else
36:       $p \leftarrow p+1$ 
37:    end if
38:  else
39:     $p \leftarrow p+1$ 
40:  end if
41: end while

```

In this context, we will define a function $F = (f_i)_{i=1,\dots,18}$ of 18 components in the following way:

$$\begin{cases} f_1 = \rho_1 \\ f_i = \lambda_i \rho_i + (1 - \lambda_i) \sum_{j=1}^{16} (\alpha_{i,j} \gamma_j) - \alpha_{i,17}, \quad i = 2, \dots, 15 \\ f_{16} = (1 - \nu) (\beta \cdot (\mathbf{x} - \mathbf{x}_0) - (t - t_0)) + \nu ((1 - t) \beta \cdot (\mathbf{x} - \mathbf{x}_0) + t g(\mathbf{x})) \\ g(\mathbf{x}) = \sum_{i=1}^{15} \mu_i \rho_{i+1} + \sum_{i=1}^{16} (\xi_i \gamma_i) - \xi_{17} \\ f_{18} = -2 \left(\frac{a_0}{R} \right)^2 \end{cases} \quad (6.1)$$

being \mathbf{x}_0 a point that satisfies the simple order conditions and 11 equalities between the γ_i coefficients. The aim is to obtain a new point \mathbf{x} that satisfies the sixteen order conditions. The 17th function of F has been denoted by g ($f_{17} = g$). Before explaining the 18 functions that form the function F , we will explain the components and the parameters that appear in the expression (6.1):

- \mathbf{x} is the unknown of 16 components that has to be calculated: $\mathbf{x} = (\gamma_i)_{i=1,\dots,16}$.
- ρ_1 is the condition of belonging to the sphere of center $\mathbf{0}$ and radius $R = 4$ (we have changed the previous radius of $R = \sqrt{18}$).
- ρ_i is the i th order condition, $i = 2, \dots, 16$.
- λ_i , for $i = 2, \dots, 15$ can take the values 0, 1. In total, there are 14 λ_i parameters.
- μ_i , for $i = 1, \dots, 15$ can take the values 0, 1. In total, there are 15 μ_i parameters.
- $\alpha_{i,j}$, for $i = 2, \dots, 15$ and $j = 1, \dots, 17$ can take the values -1, 0, 1. In total there are $14 \times 17 = 238$ $\alpha_{i,j}$ parameters.
- ξ_i , for $i = 1, \dots, 17$ can take the values -1, 0, 1. In total, there are 17 ξ_i parameters.
- The function f_{18} of the expression (6.1) gives a measure of the coefficients of the new point $\mathbf{x} = (\gamma_i)_{i=1,\dots,16}$, being:

$$a_0 = \frac{2 \sum_{i=1}^{15} \gamma_i + \gamma_{16}}{2} \quad (6.2)$$

This makes a total of 285 parameters (considering also the radius of the sphere as a parameter).

Functions f_i for $i=2, \dots, 15$ and g are used to establish an order condition (ρ_i for $i=2, \dots, 16$) or an equality among the coefficients γ_i . The function g is the one used to establish the *test condition* mentioned before. Only one order condition or one equality between two parameters can be established in each of the functions f_i for $i=2, \dots, 15$ and g . Some observations:

- It can be observed that the parameters λ_i and μ_i are multiplying the order conditions ρ_i . Hence, these parameters will be used to activate the order conditions: if their value is 0 the order conditions will not be activated, and if it is 1, the order condition will be activated.

- It can also be observed that the parameters $\alpha_{i,j}$ and ξ_i will be used to activate the equalities between the components of the solution $\mathbf{x} = (\gamma_i)_{i=1,\dots,16}$. For example, if we want to set the equality $\gamma_2 = \gamma_{12}$ in the equation f_4 , the following values of the parameters have to be taken: first of all the order condition ρ_4 will be deactivated by choosing $\lambda_4 = 0$, $\alpha_{4,2} = 1$, $\alpha_{4,12} = -1$, $\alpha_{4,j} = 0$ for $j = 2, 3, \dots, 11, 13, \dots, 17$. Another option could be by interchanging the values of $\alpha_{4,2}$ and $\alpha_{4,12}$, that is to say: $\alpha_{4,2} = -1$ and $\alpha_{4,12} = 1$ and the rest 0 as before. In the same way, if we want to activate the same equality in the 17th component of F , we can do $\xi_2 = 1$, $\xi_{12} = -1$ and the rest $\xi_i = 0$ (or $\xi_2 = -1$, $\xi_{12} = 1$ and the rest $\xi_i = 0$).

So, the set of parameters λ_i , μ_i , $\alpha_{i,j}$ and ξ_i makes possible to establish order conditions or equalities between components. The first 15 components of F , f_i for $i = 1, \dots, 15$ will be the ones that the point that we have verifies (order conditions or equalities between γ_i). In the 17th component of F , function g , we will specify another condition (order condition or equality between components) that a new point we are looking for has to verify. This means that we can pass from a point that satisfies the conditions specified in f_i for $i = 1, \dots, 15$, to another point that will satisfy also the condition specified in g . We will see some examples in order to clarify this:

- For a point $(\gamma_i)_{i=1,\dots,16}$ that satisfies the 16 order conditions, the values of the parameters will be the following: $R = 4$; $\alpha_{i,j} = 0$ for $i = 2, \dots, 15$ and $j = 1, \dots, 17$; $\lambda_i = 1$ for $i = 2, \dots, 15$; $\mu_i = 0$ for $i = 1, \dots, 14$ and $\mu_{15} = 1$; $\xi_i = 0$ for $i = 1, \dots, 17$.
- For a point $(\gamma_i)_{i=1,\dots,16}$ that satisfies the first 15 order conditions and the equality $\gamma_2 = \gamma_{12}$ the values of the parameters will be the following: $R = 4$; $\alpha_{i,j} = 0$ for $i = 2, \dots, 15$ and $j = 1, \dots, 17$; $\lambda_i = 1$ for $i = 2, \dots, 15$; $\mu_i = 0$ $i = 1, \dots, 15$; $\xi_2 = 1$, $\xi_{12} = -1$ and the rest values of $\xi_i = 0$.

If we have a point that satisfies certain conditions, another point that differs from the previous in one condition (one different order condition or one different equality between γ_i) could be obtained, by changing each time one condition that will be specified in the 17th component of F . This means for example that, having a starting point that satisfies the first 15 order conditions and one equality between γ_i , we can try to obtain a new point that satisfies the overall sixteen order conditions, or viceversa.

The function f_{16} of the expression (6.1) has two parts. The addend multiplied by $(1 - \nu)$ is a moving hiperplane that will be used to move along the curve specified by the first f_i $i = 1, \dots, 15$ functions until a point satisfying g is found. The parameter β is a 16-components vector parallel to the curve we are moving along. The parameter t measures the distance that we have moved along the specified curve. The second addend, which is multiplied by ν means that when $\nu = 1$ and moving from $t = 0$ to $t = 1$ the condition written in the function g will be satisfied.

6.1. The first experiments

6.1.1. Going backwards

In this first experiment we will take the Sofroniou and Spaletta's solution 10-order and $s = 31$ stages method (3.11). This solution (3.11) verifies the 16 order conditions given by (3.3)-(3.7).

Starting from this point, we will obtain its projection in the sphere of radius $R = 4$. That is to say, the consistency condition is changed by the condition of being on the sphere of center $\mathbf{0}$ and $R = 4$. This new point continues verifying the order conditions (3.4)-(3.7). So, taking as starting point this point on the sphere, we will go backwards until we obtain the point given by (5.27) which verifies the simple five order conditions and the scheme (9, 4, 1, 1, 1), that is to say 11 equalities among its γ_i coefficients:

$$\begin{cases} \gamma_1 = \gamma_2 = \gamma_4 = \gamma_8 = \gamma_9 = \gamma_{11} = \gamma_{12} = \gamma_{13} = \gamma_{14} \\ \gamma_5 = \gamma_6 = \gamma_7 = \gamma_{10} \end{cases} \quad (6.3)$$

being γ_3 , γ_{15} and γ_{16} the different coefficients. So, we can say that in $(\gamma_i)_{i=1,\dots,16}$, γ_1 appears nine times following (6.3), γ_5 four times following (6.3), and γ_3 , γ_{15} and γ_{16} appear once.

First of all, it has to be said that starting from Sofroniou and Spaletta's method (3.11), it has been possible to obtain the starting point given by (5.27), which satisfies the simple five order conditions and the equalities given by (6.3).

In Figure 7, we can see the way followed from Sofroniou's method (3.11) to the point (5.27). Some observations about Figure 7:

- The starting point has been denoted by **Sofr. & Spal.** in Figure 7. This point satisfies the sixteen order conditions.
- In the process represented in Figure 7 the point given by (5.27) has been obtained, which satisfies the simple five order conditions and the equalities given by (6.3). In this figure it has been denoted by "Point A0".
- Eleven steps have to be done in order to obtain the point (5.27) denoted by "Point A0" at the bottom of the figure. In each of these steps, one order condition is lost each time and one equality between the coefficients γ_i is gained. It is written in each step which equality in which equation is inserted. For example, in the first step the equality $\gamma_2 = \gamma_4$ is inserted in equation f_{15} , which means that the order condition ρ_{15} is lost. In this first step, 4 points that satisfy the order conditions ρ_1 - ρ_{14} and ρ_{16} (which are written in equations f_1 - f_{14} and f_{16}) and the equality $\gamma_2 = \gamma_4$ are found. The notation used for the points we are obtaining in each step is $p_{i,j}$ being i the number that indicates how many order conditions are satisfied, and j the number of points found in that step following the way and the previous point marked in the scheme (it does not mean that all the points obtained in the previous step have been analysed).
- The simple order conditions are ρ_1 , ρ_2 , ρ_3 , ρ_5 and ρ_8 (which can be activated in the functions f_1 , f_2 , f_3 , f_5 and f_8).
- The branches that are not followed until the end have not been explored.
- The order in which the equalities are set matters. It can happen that in one point of the process one equality does not give any results. However, in a posterior step of the process, it is possible to obtain one result establishing this equality that has failed before. So the failure of an equality in a concrete point of the process does not mean that this possibility will fail later.

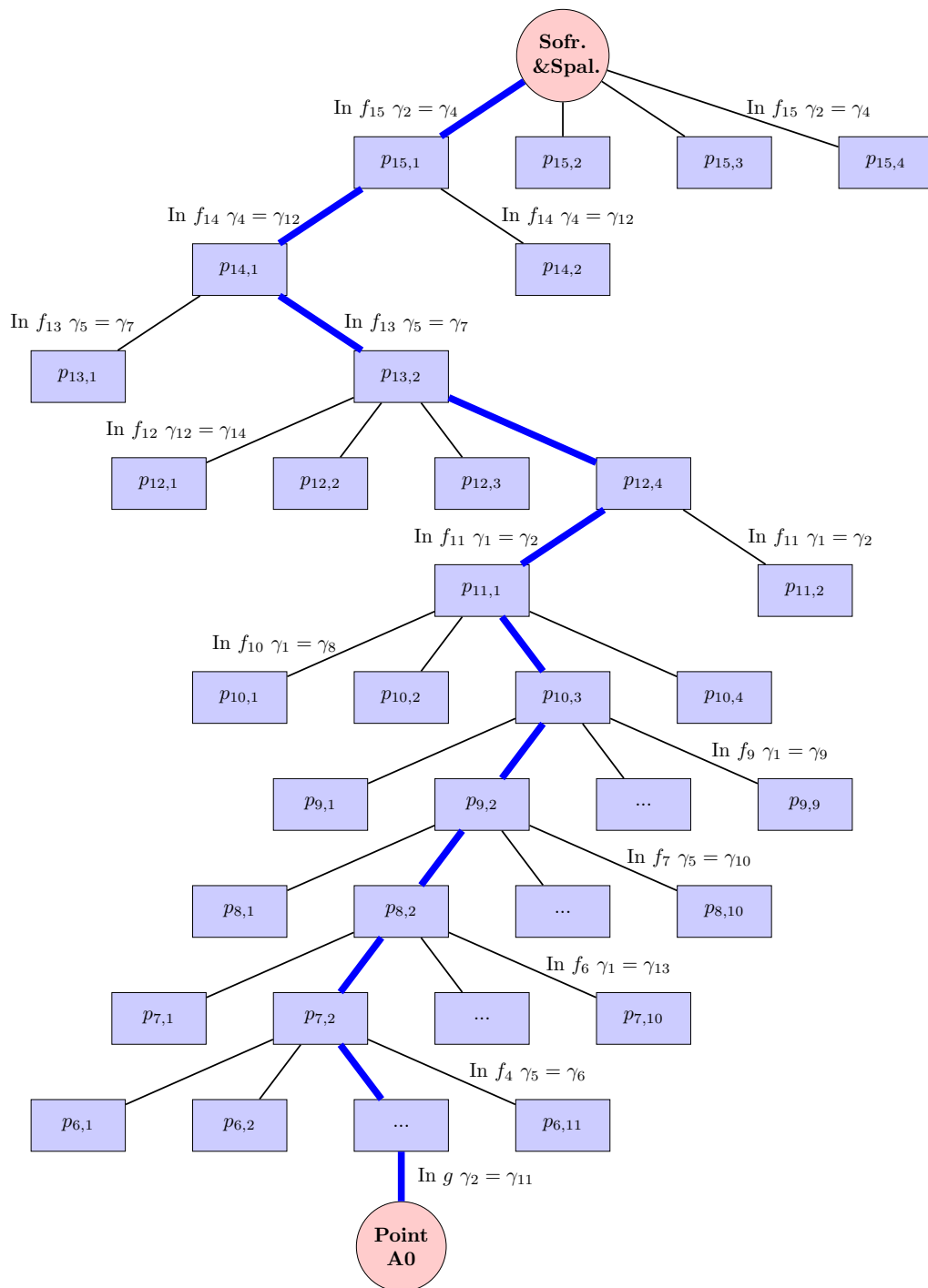


Figure 7: Going backwards from Sofroniou's solution.

6.1.2. Going forwards

In a similar way, the way to go from the starting point (5.27) to the Sofroniou and Spaletta's solution has been followed. The experiments has been developed in the following way:

- This time the starting point is at the bottom of the Figure 7. It is denoted by “Point A0”. This point satisfies the simple 5 order conditions $(\rho_1, \rho_2, \rho_3, \rho_5, \rho_8)$ and 11 equalities between the γ_i coefficients. This equalities have been included in the same way the backwards process has been developed. That is to say:

$$\begin{aligned}
 \text{In } f_{15}, \quad \gamma_2 &= \gamma_4 \\
 \text{In } f_{14}, \quad \gamma_4 &= \gamma_{12} \\
 \text{In } f_{13}, \quad \gamma_5 &= \gamma_7 \\
 \text{In } f_{12}, \quad \gamma_{12} &= \gamma_{14} \\
 \text{In } f_{11}, \quad \gamma_1 &= \gamma_2 \\
 \text{In } f_{10}, \quad \gamma_1 &= \gamma_8 \\
 \text{In } f_9, \quad \gamma_1 &= \gamma_9 \\
 \text{In } f_7, \quad \gamma_5 &= \gamma_{10} \\
 \text{In } f_6, \quad \gamma_1 &= \gamma_{13} \\
 \text{In } f_4, \quad \gamma_5 &= \gamma_6 \\
 \text{In } g, \quad \gamma_2 &= \gamma_{11}
 \end{aligned} \tag{6.4}$$

- We want to go up in the process until we obtain a point that satisfies the sixteen order conditions.
- The process to go up have been done as follows:
 - We are in the “Point A0”. A first step is given activating ρ_4 in g and losing the equality $\gamma_2 = \gamma_{11}$ as a consequence. There are eleven points that satisfy this condition $p_{6,1}, \dots, p_{6,11}$.
 - As ρ_4 is satisfied, this is activated in f_4 , losing the equality $\gamma_5 = \gamma_6$ that has been in f_4 . And we follow the process from one of the points $p_{6,j}$. In the second step ρ_6 is activated in g and losing the equality $\gamma_5 = \gamma_6$ in f_4 . There are ten points that satisfy this condition $p_{7,1}, \dots, p_{7,10}$.
 - And the rest of the steps are similar until the top of the Figure 7 is reached obtaining the point **Sofr. & Spal.**

In Figure 7 the way followed to go up and down has been marked using a thicker blue line.

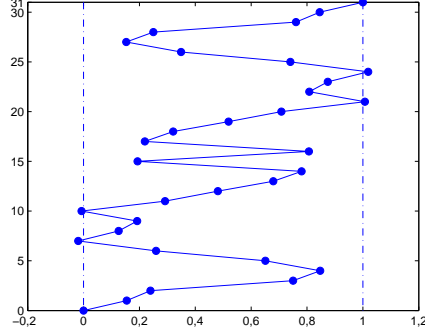


Figure 8: Cumulative weight plot for $s = 31$ stage and 10th order new method.

Following the forwards way and the process described in this second technique, we have been able to find a new point that satisfies the sixteen order conditions, see in Figure 8 its cumulative weight plot. This new point is the following:

$$\begin{aligned}
 \gamma_1 &= \gamma_{31} = 0.154573955942749 \\
 \gamma_2 &= \gamma_{30} = 0.084916229764423 \\
 \gamma_3 &= \gamma_{29} = 0.510725963869653 \\
 \gamma_4 &= \gamma_{28} = 0.096972445176156 \\
 \gamma_5 &= \gamma_{27} = -0.196353863540888 \\
 \gamma_6 &= \gamma_{26} = -0.391377961592734 \\
 \gamma_7 &= \gamma_{25} = -0.278523979360953 \\
 \gamma_8 &= \gamma_{24} = 0.144663174620264 \\
 \gamma_9 &= \gamma_{23} = 0.066283988663858 \\
 \gamma_{10} &= \gamma_{22} = -0.199028217131776 \\
 \gamma_{11} &= \gamma_{21} = 0.299036966780720 \\
 \gamma_{12} &= \gamma_{20} = 0.189133242229514 \\
 \gamma_{13} &= \gamma_{19} = 0.198214273246474 \\
 \gamma_{14} &= \gamma_{18} = 0.101260161817474 \\
 \gamma_{15} &= \gamma_{17} = -0.587096566393321 \\
 \gamma_{16} &= 0.613200371816777
 \end{aligned} \tag{6.5}$$

6.1.3. The algorithms up to now

In this section we will explain the algorithms that we need to do the way down (going backwards) and the way up (forwards):

- An algorithm to change parameters is required. Given a set of parameters $(\lambda_i, \mu_i, \alpha_{i,j}, \xi_i)$ which indicates the conditions (order conditions or equalities) that the present point satisfies, a new set of parameters is obtained. The aim is to obtain a new point that will satisfy

the order conditions and equalities determined in this new set of parameters. When going backwards one order condition will be lost and one equality will be gained. When going forwards the contrary will happen. An algorithm has been designed to change parameters when going backwards and another one to change parameters when going forwards.

- An algorithm to make a step is required. Given a point that satisfies certain conditions specified using the values of the parameters, we obtain a new point that satisfies other conditions specified by a new set of parameters. The same algorithm is used to do the backwards and forwards ways.
- When going forwards, we have a point that satisfies the simple five order conditions and eleven equalities between the coefficients γ_i . In this first experiment we knew in advance the equal elements of this point and their positions, but in general, an algorithm that determines the different values present in the point $\mathbf{x} = (\gamma_i)_{i=1,\dots,16}$ and their positions will be required.
- In the same way when going forwards, we will require an algorithm that will establish the first set of parameters. This algorithm will determine the starting parameters $(\alpha_{i,j}, \xi_i, \mu_i, \lambda_i)$ of the point that satisfies the simple five order conditions and the equalities identified by the previous function.

6.2. Some preliminary analysis before developing the general forwards process

Before developing the general forwards process, which will consist taking each of the 21871 starting points that satisfy the five simple order conditions and following the process described seeing if it is possible to obtain a point that satisfies the sixteen order conditions, the points that have been obtained following the process marked in Figure 7 will be analysed. In this analysis we are interested in three numerical values:

1. The topological distance: This quantity means how many intermediate points separate two points, not how far apart they are. In each of the points, both directions of the present point are followed to find the new points. Following one of the directions, the first point's topological distance will be 1, the second point's topological distance 2, and so on. Following the second direction, the same happens: the topological distance is k for the k th point obtained. Sometimes, the two directions that have to be explored will be joined (the curve will be closed), meaning that we will fall in the starting point after obtaining some points that satisfy the established condition. For example, in a case in which 10 points are obtained and the curve is closed, the topological distance of these points will be $(1, 2, 3, 4, 5, 5, 4, 3, 2, 1)$.
2. A measure of the coefficients: This measure will be defined using the component $f_{18} = -2 \left(\frac{a_0}{R} \right)^2$ defined in (6.2). Observe that it is a negative value.
3. The norm of the value of the sixteen order conditions: These sixteen order conditions can be activated in the functions $f_1 - f_{15}$ and g of the expression (6.1). Let denote the function of the sixteen order conditions as $G(\mathbf{x}) = (f_1, f_2, \dots, f_{15}, g)$. We will be interested in the value of $\|G(\mathbf{x})\|$.

The analysis will be performed with two sets of points:

- The first set will consist in the points obtained in the process described in Figure 7. Considering the process as a forwards process that starts in the point “Point A0”, this means that: eleven points of the first step ($p_{6,1}, \dots, p_{6,11}$) will be analysed; the ten points obtained following one of the $p_{6,j}$ previous points will be analysed ($p_{7,1}, \dots, p_{7,10}$); and so on.
- The second set will consist in considering more points than the ones that have been marked in Figure 7. The branches that have not been followed in this figure will be calculated and many points that we obtain in the process will be analysed. We say many points and not all the points, because the process to obtain all the points of all the branches is really time consuming.

6.2.1. Analysis of the points of the first set

In this section the topological distance, the explained measure of the coefficients and the norm of the sixteen order conditions of the first set of points will be analysed. In Table 4 we can see the topological distance and the measure of coefficients of the first set of points. In this table the following data are written:

- The quantity of points that conform the set in each step is written.
- The maximum value of the measure of the coefficients (as this measure is negative the maximum in absolute value has been considered) and the minimum (minimum in absolute value) of the first set has been written.
- The measure of the coefficients of the point that allows following the process.
- The position of the measure of the coefficients of the point that allows following the process ordered taking from maximum absolute value to the minimum (position 1 corresponds to the point with the greatest absolute value).
- The topological distance of the point that allows following the process.

From Table 4 it can be concluded that the measure of the coefficients of the points that allow following the process is on the interval $[-0.20, -0.13]$. The topological distances of the adequate points varies between 1-5.

A similar table has been created with the norm of the sixteen order conditions of the first set of points, Table 5, but it results difficult to conclude anything from it. The following data can be seen there:

- The quantity of points that conform the set in each step.
- The maximum and the minimum values of $\|G(\mathbf{x})\|$.
- The value of $\|G(\mathbf{x})\|$ of the point that allows following the process.
- The position of $\|G(\mathbf{x})\|$ of the point that allows following the process ordered from the maximum value to the minimum (position 1 corresponds to the point with the greatest $\|G(\mathbf{x})\|$).

Step number	1st step	2nd step	3rd step
Point top. distance	2	3	5
$-2 \left(\frac{a_0}{R}\right)_{\frac{1}{2}}^{max}$	-0.312398460146025	-0.268628439269852	-0.215602343712106
$-2 \left(\frac{a_0}{R}\right)_{\frac{1}{2}}^{min}$	-6.72750783657071e-07	-0.0349144123926289	-0.091318600051002
$-2 \left(\frac{a_0}{R}\right)_{point}$	-0.186254772284937	-0.132013936329637	-0.166988089576315
Point position	4	7	5
Number of points	11	10	10
4th step	5th step	6th step	7th step
1	1	1	1
-0.200597297983226	-0.187123647764713	-0.159487684991583	-0.190499685106902
-0.00192166885238663	-0.109997050134757	-0.135296312995526	-0.127963980986809
-0.200597297983226	-0.168374260797779	-0.159487684991583	-0.137468297031783
1	2	1	3
9	4	2	4
8th step	9th step	10th step	11th step
1	1	1	1
-0.193120955717927	-0.186806493477043	-0.191590667525783	-0.189659525268255
-0.172254272979615	-0.179995355690231	-0.186797385230934	-0.186148238551586
-0.172254272979615	-0.179995355690231	-0.186797385230934	-0.189659525268255
2	2	4	1
2	2	4	2

Table 4: Topological distance and coefficients' measure of the first set.

Given a topological distance for each step, an additional analysis has been developed analysing the points with a smaller topological distance than the given one. In each step if the point that allows to follow the process has topological distance m , the aim has been to study the points that have a topological distance that is $\leq (m + 1)$. We list the results of this analysis step by step, denoting with an asterisk (*) the features of the point that allows to follow the process:

1. In the 1st step points with topological distance 1-3 are analysed, Table 6.
2. In the 2nd step points with topological distance 1-4 are analysed, Table 7.
3. In the 3rd step points with topological distance 1-5 are analysed, Table 8.
4. In the 4th step points with topological distance 1-2 are analysed, Table 9.
5. In the 5th step points with topological distance 1-2 are analysed, Table 10.
6. In the 6th step points with topological distance 1-2 are analysed, Table 11.
7. In the 7th step points with topological distance 1-2 are analysed, Table 12.
8. In the 8th step points with topological distance 1-2 are analysed, Table 13.
9. In the 9th step points with topological distance 1-2 are analysed, Table 14.
10. In the 10th step points with topological distance 1-2 are analysed, Table 15.
11. In the 11th step points with topological distance 1-2 are analysed, Table 16.

Step number	1st step	2nd step	3rd step
$\ G(\mathbf{x})\ _{max}$	212.380137377832	42.1866575302664	0.0362313019152408
$\ G(\mathbf{x})\ _{min}$	1.16423621111419e-05	0.0184911310738061	0.00214997505358903
$\ G(\mathbf{x})\ _{point}$	39.108188219442	0.0184911310738061	0.00214997505358903
Point position	2	10	10
Number of points	11	10	10
4th step	5th step	6th step	7th step
0.021561726236527	0.00864358774698865	0.00524650907498929	0.00885810487642527
5.57793351155797e-06	0.00108206639324003	0.00346675817524766	0.0026928647044555
0.0102278007641977	0.00371588433776787	0.00346675817524766	0.00404818207742273
7	3	2	2
9	4	2	4
8th step	9th step	10th step	11th step
0.00226928972957287	0.00166284205829303	0.000705392545784657	1.71326075912416e-14
0.000795880603936082	0.000702703505191104	0.00010124725974094	8.82441229641858e-15
0.000795880603936082	0.00166284205829303	0.000705392545784657	1.71326075912416e-14
2	1	1	1
2	2	4	2

Table 5: Norm of the sixteen order conditions of the first set.

Topological distance	$-2 \left(\frac{a_0}{R}\right)^2$	$\ G(\mathbf{x})\ $
1	-0.289553090066448	1.164309628723169
2*	-0.186254772284937*	39.108188219441963*
3	-0.00000672750784	0.000011642362111
1	-0.270485839389751	2.123578606560379
2	-0.000181671394244	0.193719054723202
3	-0.00004685166919	1.164967768402042

Table 6: Study of some points of the step 1.

Topological distance	$-2 \left(\frac{a_0}{R}\right)^2$	$\ G(\mathbf{x})\ $
1	-0.162026861492138	33.998529059380139
2	-0.153826367492559	27.317706449428037
3	-0.034914412392629	0.162274012521198
4	-0.268628439269852	0.237681318392343
1	-0.145209911825618	0.096637519613531
2*	-0.132013936329637*	0.018491131073806*
3	-0.206113678134081	28.974712435577434
4	-0.219264114322233	42.186657530266423

Table 7: Study of some points of the step 2.

Topological distance	$-2 \left(\frac{a_0}{R}\right)^2$	$\ G(\mathbf{x})\ $
1	-0.119556120157140	0.018683634539122
2	-0.092510370137795	0.017244738825898
3	-0.091318600051002	0.013302196865789
4	-0.109072997166448	0.010081929456183
5	-0.138610624002485	0.004770155403930
5*	-0.166988089576315*	0.002149975053589*
4	-0.199914383075673	0.022561283653803
3	-0.215602343712106	0.036231301915241
2	-0.196401595811208	0.020686740636044
1	-0.197182410982100	0.022006729485499

Table 8: Study of some points of the step 3.

Topological distance	$-2 \left(\frac{a_0}{R}\right)^2$	$\ G(\mathbf{x})\ $
1*	-0.200597297983226*	0.010227800764198*
2	-0.170964319735531	0.012648105625484
2	-0.110939502156744	0.001159408933126
1	-0.004268019723374	0.000000011144224

Table 9: Study of some points of the step 4.

Topological distance	$-2 \left(\frac{a_0}{R}\right)^2$	$\ G(\mathbf{x})\ $
1*	-0.168374260797779*	0.003715884337768*
2	-0.109997050134757	0.001082066393240
2	-0.161636567146025	0.006017995299712
1	-0.187123647764713	0.008643587746989

Table 10: Study of some points of the step 5.

Topological distance	$-2 \left(\frac{a_0}{R}\right)^2$	$\ G(\mathbf{x})\ $
1*	-0.159487684991583*	0.003466758175248*
1	-0.135296312995526	0.005246509074989

Table 11: Study of some points of the step 6.

Topological distance	$-2 \left(\frac{a_0}{R}\right)^2$	$\ G(\mathbf{x})\ $
1*	-0.137468297031783*	0.004048182077423*
2	-0.127963980986809	0.008858104876425
2	-0.146897375095611	0.002692864704456
1	-0.190499685106902	0.003178873443553

Table 12: Study of some points of the step 7.

Topological distance	$-2 \left(\frac{a_0}{R}\right)^2$	$\ G(\mathbf{x})\ $
1*	-0.172254272979615*	0.000795880603936*
1	-0.193120955717927	0.002269289729573

Table 13: Study of some points of the step 8.

Topological distance	$-2 \left(\frac{a_0}{R}\right)^2$	$\ G(\mathbf{x})\ $
1*	-0.179995355690231*	0.001662842058293*
1	-0.186806493477043	0.000702703505191

Table 14: Study of some points of the step 9.

Topological distance	$-2 \left(\frac{a_0}{R}\right)^2$	$\ G(\mathbf{x})\ $
1	-0.191524556343979	0.000380766760958
2	-0.191590667525783	0.000332854929302
2	-0.190801085135339	0.000101247259741
1*	-0.186797385230934*	0.000705392545785*

Table 15: Study of some points of the step 10.

Topological distance	$-2 \left(\frac{a_0}{R}\right)^2$	$\ G(\mathbf{x})\ $
1	-0.186148238551586	8.824412296418578e-15
1*	-0.189659525268255*	1.713260759124155e-14*

Table 16: Study of some points of the step 11.

6.2.2. Analysis of the points of the second set

In this second analysis more points than in Section 6.2.1 are considered. The analysed points are the following:

- Step 1: Starting from the point “Point A0” 11 points that satisfy 6 order conditions and 10 equalities are obtained. We analyse all these 11 points.
- Step 2: Starting from the 11 points of the step 1, 32 points that satisfy 7 order conditions and 9 equalities are obtained. We analyse all these 32 points.
- Step 3: Starting from the 32 points of the step 2, 132 points that satisfy 8 order conditions and 8 equalities are obtained. We analyse all these 132 points.
- Step 4: Starting from the 132 points of the step 3, 385 points that satisfy 9 order conditions and 7 equalities are obtained. We analyse the first 50 of this set.
- Step 5: Starting from 50 points of the step 4, 257 points that satisfy 10 order conditions and 6 equalities are obtained. We analyse the first 50 of this set.
- Step 6: Starting from 50 points of the step 5, 105 points that satisfy 11 order conditions and 5 equalities are obtained. We analyse the first 50 of this set.
- Step 7: Starting from 50 points of the step 6, 69 points that satisfy 12 order conditions and 4 equalities are obtained. We analyse all these 69 points.
- Step 8: Starting from the 69 points of the step 7, 41 points that satisfy 13 order conditions and 3 equalities are obtained. We analyse all these 41 points.

- Step 9: Starting from the 41 points of the step 8, 66 points that satisfy 14 order conditions and 2 equalities are obtained. We analyse all these 66 points.
- Step 10: Starting from the 66 points of the step 9, 25 points that satisfy 15 order conditions and 1 equality are obtained. We analyse all these 25 points.
- Step 11: Starting from the 25 points of the step 10, 60 points that satisfy 16 order conditions are obtained. We analyse all these 60 points.

In Tables 17 and 18, we can see the measure of the coefficients and the norm of the order conditions of these points. Again, the values of the point that allows following the overall process of Figure 7 have been noted down. This time the topological distance has not been calculated as in steps 5, 6 and 7 we are not considering all the points of the process.

Step number	1st step	2nd step	3rd step
$-2 \left(\frac{a_0}{R}\right)_{2^{max}}^2$	-0.312398460146025	-0.277498808718953	-0.565368924975638
$-2 \left(\frac{a_0}{R}\right)_{2^{min}}^2$	-6.72750783657071e-07	-8.15953250920796e-07	-3.20618670773964e-07
$-2 \left(\frac{a_0}{R}\right)_{point}^2$	-0.186254772284937	-0.132013936329633	-0.166988089576278
Point position	4	16	24
Number of points	11	32	132
4th step	5th step	6th step	7th step
-0.524724254653273	-0.357973232729286	-0.315798269231926	-0.258548452681552
-1.65759397709565e-28	-4.03741553615937e-25	-1.29890849787639e-05	-3.2301340245218e-05
-0.200597297983222	-0.16837426079775	-0.159487684991198	-0.137468297031408
23	47	42	28
50* (385)	50* (257)	50* (105)	69
8th step	9th step	10th step	11th step
-0.193120955717743	-0.186806493477135	-0.191590667526059	-0.189659525265751
-5.42085847786923e-07	-8.91170209750487e-07	-2.73462840023396e-18	-6.84432552978498e-11
-0.172254272979652	-0.179995355690239	-0.18679738523102	-0.189659525265751
2	2	2	1
41	66	25	60

Table 17: Coefficients' measure of the second set.

6.3. The process of going forwards

After the analysis developed in Section 6.2, given a starting point that satisfies the five simple order conditions, the process that we will continue to find the coefficients $(\gamma_i)_{i=1,\dots,16}$ of the new method will follow these criteria:

- In the first step all the points will be considered.

Step number	1st step	2nd step	3rd step
$\ G(\mathbf{x})\ _{max}$	212.380137377832	265.782309260689	8.6315373607896
$\ G(\mathbf{x})\ _{min}$	1.16423621111419e-05	4.54574583717768e-09	7.15194791545681e-13
$\ G(\mathbf{x})\ _{point}$	39.108188219442	0.0184911310738086	0.00214997505358381
Point position	2	26	115
Number of points	11	32	132
4th step	5th step	6th step	7th step
5.47320802605529	0.642489659790803	0.244671395967803	0.0307084279631623
3.77228920781469e-15	2.05947140273216e-12	4.33033458376227e-09	1.06048503834291e-07
0.0102278007641917	0.00371588433773466	0.00346675817524684	0.00404818207743281
191	189	81	51
50* (385)	50* (257)	50* (105)	69
8th step	9th step	10th step	11th step
0.0273533879086008	0.00852574082041072	0.000705392545781703	4.28888611692313e-07
2.13967610544086e-09	5.21842866036111e-09	1.67208590706232e-09	1.14661493610407e-16
0.000795880603934685	0.00166284205827681	0.000705392545781703	3.70772540537407e-14
25	19	1	13
41	66	25	60

Table 18: Norm of the sixteen order conditions of the second set.

- In the subsequent steps (steps 2-11), the points that have an established topological distance will be considered to follow the process. To do this, a vector with topological distances will be established, $(d_2, d_3, \dots, d_{11})$: variable *distop*. In this way, in the step i the points with topological distance less than or equal to d_i will be considered. In the starting steps the topological distance will be wider and then, it will be getting narrower. This criteria has been thought because, it can be seen in Tables 6-16, that in the starting steps the topological distance is greater than in the final ones.
- The norm of the sixteen order conditions will not be used as a criteria in the process. As we can see in Tables 5, 6, 18 that sometimes the norm of the sixteen order conditions of the adequate point is big (it is the case that we see in Table 6) or it is not the smallest one of the set (see Tables 5 and 18).
- It seems reasonable to establish an upper bound and a lower bound for the measure of the coefficients: variables *top* and *bottom*. If we observe Tables 4 and 17, it seems that the measure of the coefficients is on the interval $[-0.20, -0.13]$. This interval could be wider, but it seems reasonable its establishment.
- Finally, even though it cannot be seen in the included tables, some computational experiments show us that when a point with very low coefficients is obtained in the process, it turns difficult to obtain adequate points following the way of that point. Taking into account this, we will also set a lower bound for the measure of the coefficients and when a point with a smaller value than this lower bound is obtained the process will be interrupted: variable *limit*.

Algorithm 5 Algorithm to obtain $(\gamma_i)_{i=1,\dots,16}$ coefficients satisfying 16 order conditions.

```

1: Input:  $\mathbf{x}_0$ , distop, bottom, top, limit
2:  $\mathbf{a}0 \leftarrow \text{sphere}(\mathbf{x}_0)$  ▷ Pass  $\mathbf{x}_0$  to the sphere of center  $\mathbf{0}$  and  $r = 4$ 
3:  $t0 \leftarrow 0$ 
4:  $\text{tend} \leftarrow 16$ 
5:  $\text{beta}0 \leftarrow (1, 0_1, 0_2, \dots, 0_{15})$ 
6:  $\text{equalpositions} \leftarrow \text{findequal}(\mathbf{a}0)$  ▷ Find the different values in  $\mathbf{a}0$  and their positions
7:  $\text{param}0 \leftarrow \text{setinitialparameters}(\text{equalpositions})$  ▷ Set initial parameters:  $\alpha_{0,i,j}, \lambda_{0,i}, \mu_{0,i}, \xi_{0,i}$ 
8:  $\text{condition} \leftarrow 4$  ▷ Order condition that want to satisfy
9:  $\text{param}1 \leftarrow \text{setparameters}(\text{param}0, \text{condition})$  ▷ Set parameters step 1:  $\alpha_{1,i,j}, \lambda_{1,i}, \mu_{1,i}, \xi_{1,i}$ 
10:  $[\text{bek}1\mathbf{r}, \text{bekbeta}1\mathbf{r}] \leftarrow \text{forwards}1(\mathbf{a}0, \text{beta}0, t0, \text{tend}, \text{param}1)$  ▷ All points satisfying  $\text{param}1$ 
11:  $[\text{bek}1, \text{bekbeta}1] \leftarrow \text{cleanrepet}(\text{bek}1\mathbf{r}, \text{bekbeta}1\mathbf{r})$  ▷ Clean the repetitions in  $\text{bek}1\mathbf{r}$ 
12:  $\text{activate} \leftarrow [4, 6, 7, 9, 10, 11, 12, 13, 14, 15, 16]$  ▷ Vector with the rest 11 order conditions
13: for  $k=1:10$  do ▷ Steps 2-11
14:    $\text{param}2 \leftarrow \text{changeforward}(\text{param}1, \text{activate}(k1), \text{activate}(k1+1))$  ▷ New step parameters
15:   if  $\text{size}(\text{bek}1, 2) > 0$  then ▷ If there are elements in  $\text{bek}1$ 
16:      $\mathbf{a}0 \leftarrow \text{bek}1(:,j)$ 
17:      $\text{beta}0 \leftarrow \text{bekbeta}1(:,j)$ 
18:      $\text{bek}3\mathbf{r} \leftarrow []$  ▷ Initialize to save points
19:      $\text{bekbeta}3\mathbf{r} \leftarrow []$  ▷ Initialize to save  $\beta$ -s
20:     for  $j1=1: \text{size}(\text{bek}1,2)$  do
21:        $[\text{bek}2, \text{bekbeta}2] \leftarrow \text{forwards}2(\mathbf{a}0, \text{beta}0, t0, \text{tend}, \text{param}2, \text{distop}(k1), \text{limit})$  ▷
22:       Obtain points satisfying  $\text{distop}(k1)$  and limit
23:        $\text{absf}18 \leftarrow \text{Calculate } |f_{18}| \text{ of all the points of } \text{bek}2$ 
24:        $\text{index} \leftarrow \text{find}(\text{absf}18 < \text{top} \ \& \ \text{absf}18 < \text{bottom})$ 
25:        $\text{bek}3\mathbf{r} \leftarrow [\text{bek}3\mathbf{r} \ \text{bek}2(:,\text{index})]$  ▷ Save elements of  $\text{bek}2$  satisfying  $\text{bottom} < |f_{18}| < \text{top}$ 
26:        $\text{bekbeta}3\mathbf{r} \leftarrow [\text{bekbeta}3\mathbf{r} \ \text{bekbeta}2(:,\text{index})]$  ▷ Save in  $\text{bekbeta}3\mathbf{r}$  the corresponding  $\beta$ 
27:     end for
28:   else
29:     break
30:   end if
31:    $[\text{bek}3, \text{bekbeta}3] \leftarrow \text{cleanrepet}(\text{bek}3\mathbf{r}, \text{bekbeta}3\mathbf{r})$  ▷ Clean the repetitions
32:    $\text{bek}1 \leftarrow \text{bek}3; \text{bekbeta}1 \leftarrow \text{bekbeta}3; \text{param}1 \leftarrow \text{param}2$  ▷ Update parameters
33: end for
34: if  $k1==10 \ \& \ \text{size}(\text{bek}1,2) \geq 1$  then ▷ If the final step has been reached
35:   for  $j=1:\text{size}(\text{bek}1,2)$  do
36:      $\text{consis} \leftarrow \text{consistency}(\text{bek}1(:,j))$  ▷ Pass to consistency condition each point
37:   end for
38: else
39: end if

```

In the Algorithm 5, given a starting point \mathbf{x}_0 that satisfies the five simple order conditions, the process that we will continue to find the coefficients $(\gamma_i)_{i=1,\dots,16}$ of the new method satisfying the sixteen order conditions is described.

6.3.1. Results of the process of going forwards

It has been explained the process that we will follow to go forwards, starting from a point that satisfies the five simple order conditions. Four parameters have to be established: *distop*, *bottom*, *top*, *limit*. Some results and some considerations about the process of going forwards are presented in this section.

- Starting from the starting point \mathbf{x}_0 given by (5.27) and choosing the following values for the parameters: *distop* = [7, 6, 5, 4, 3, 2, 1, 1, 1, 1], *bottom* = 0.1, *top* = 0.3 and *limit* = 0.01.
 - When we establish the equalities among the coefficients of the vector \mathbf{x}_0 as explained in Figure 7, it is possible to obtain the coefficients of Sofroniou and Spaletta’s method (3.11) and the coefficients of our new method (6.5).
 - When we change the way in which the equalities among the coefficients of the vector \mathbf{x}_0 are set, and using the same parameters as before, we cannot reach either the Sofroniou and Spaletta’s solution or our new solution. When we reach the 9th step of the 11 steps that have to be done, we do not have any points so the process is finished. The values of the parameters have to be widened in order to finish the overall process.
 - If the values of the parameters are widened as follows: *distop* = [7, 6, 5, 4, 4, 4, 2, 2, 2, 2], *bottom* = 0.01, *top* = 0.3 and *limit* = 0.01, the 11 steps of the process are done, 25 points are found but even in this case the Sofroniou and Spaletta’s solution or our new solution do not appear. And some of the obtained γ_i coefficients are quite large ($|\gamma_i| \in [1, 3]$).
 - If we widen the parameter related to the topological distance, choosing *distop* = [10, 10, 10, 10, 10, 10, 5, 3, 3, 3], and *bottom* = 0.06, *top* = 0.4 and *limit* = 0.01, we do not have points in the 10th step. Choosing a larger *top* and maintaining the rest of the parameters (that is to say *distop* = [10, 10, 10, 10, 10, 10, 5, 3, 3, 3], *bottom* = 0.06, *top* = 0.5 and *limit* = 0.01) the same happens.
 - Using the following parameters: *distop* = [20, 20, 20, 20, 20, 20, 5, 3, 3, 3], *bottom* = 0.01, *top* = 0.6 and *limit* = 0.001, after the 11 steps 117 points are obtained but most of them have some coefficients verifying $|\gamma_i| \in [1, 3]$. There are only two cases in which all the

coefficients remain on the interval $[-1, 1]$:

$$\begin{array}{rcll}
 \gamma_1 = \gamma_{31} = & 0.216968225174685 & 0.228795449861804 \\
 \gamma_2 = \gamma_{30} = & 0.872929710391992 & 0.851862525878233 \\
 \gamma_3 = \gamma_{29} = & -0.419089368345931 & -0.414041804166289 \\
 \gamma_4 = \gamma_{28} = & -0.388625593493059 & -0.403002032787764 \\
 \gamma_5 = \gamma_{27} = & -0.357731244915905 & -0.329525788276191 \\
 \gamma_6 = \gamma_{26} = & 0.979448960387542 & 0.973077901881892 \\
 \gamma_7 = \gamma_{25} = & -0.626561641226852 & -0.621919440966130 \\
 \gamma_8 = \gamma_{24} = & 0.430047535082709 & 0.433832438014287 \\
 \gamma_9 = \gamma_{23} = & 0.118369840172629 & 0.101029552679953 \\
 \gamma_{10} = \gamma_{22} = & -0.913872092979091 & -0.898389013932081 \\
 \gamma_{11} = \gamma_{21} = & 0.313759643379948 & 0.287842685973578 \\
 \gamma_{12} = \gamma_{20} = & 0.338352126736173 & 0.352976982005111 \\
 \gamma_{13} = \gamma_{19} = & 0.089984942816856 & 0.102208127748936 \\
 \gamma_{14} = \gamma_{18} = & 0.415424629288281 & 0.394084868058467 \\
 \gamma_{15} = \gamma_{17} = & -0.964943625165182 & -0.959969701212588 \\
 & \gamma_{16} = & 0.791075905390409 & 0.802274498477561
 \end{array} \tag{6.6}$$

In Figure 9 the cumulative weight plot of the two methods of the expression (6.6) has been drawn. We can see that both methods do many side-to-side movements (zigzags) and their cumulative weight plots are quite similar to Kahan and Li's $s = 33$ stages and 10 order method (see Figure 1).

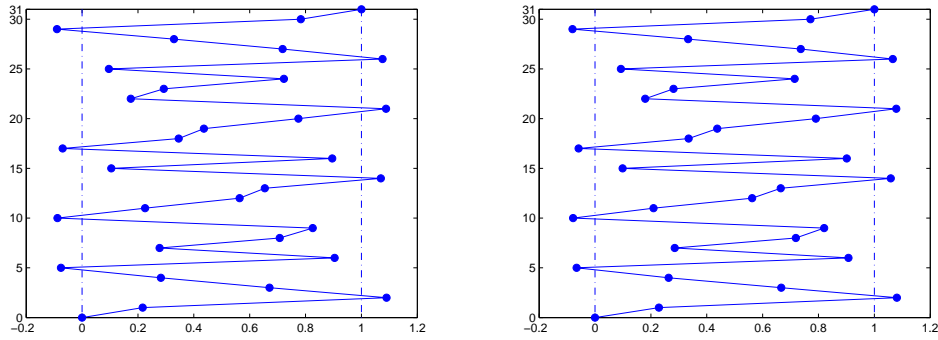


Figure 9: Cumulative weight plot for $s = 31$ stage and 10th order methods: left image, left formula of (6.6) and right image, right formula of (6.6).

- After having experimented with the point that gives the Sofoniou and Spaletta's method, the process described in Algorithm 5 has been carried out with the 21871 starting points. The chosen parameters have been: $distop = [7, 6, 5, 4, 4, 4, 2, 2, 2, 2]$, $bottom = 0.1$, $top = 0.4$ and $limit = 0.01$.

This process is still in execution, having explored up to now 3059 points out of the 21871.

The new point obtained up to this moment is the following:

$$\begin{aligned}
 \gamma_1 &= \gamma_{31} = 0.212278271248785 \\
 \gamma_2 &= \gamma_{30} = 0.632455152658572 \\
 \gamma_3 &= \gamma_{29} = -0.367655814001506 \\
 \gamma_4 &= \gamma_{28} = 0.515991253367719 \\
 \gamma_5 &= \gamma_{27} = 0.020298620699509 \\
 \gamma_6 &= \gamma_{26} = -0.387014967076971 \\
 \gamma_7 &= \gamma_{25} = 0.293430907070892 \\
 \gamma_8 &= \gamma_{24} = -0.010972470912696 \\
 \gamma_9 &= \gamma_{23} = -0.724126279821191 \\
 \gamma_{10} &= \gamma_{22} = 0.190574978132295 \\
 \gamma_{11} &= \gamma_{21} = 0.091802369911264 \\
 \gamma_{12} &= \gamma_{20} = 0.280695074734112 \\
 \gamma_{13} &= \gamma_{19} = 0.256646662172751 \\
 \gamma_{14} &= \gamma_{18} = -0.336392014428401 \\
 \gamma_{15} &= \gamma_{17} = -0.546324360287742 \\
 &\gamma_{16} = 0.756625233065217
 \end{aligned} \tag{6.7}$$

In Figure 10 the cumulative weight plot of the method (6.7) has been drawn.

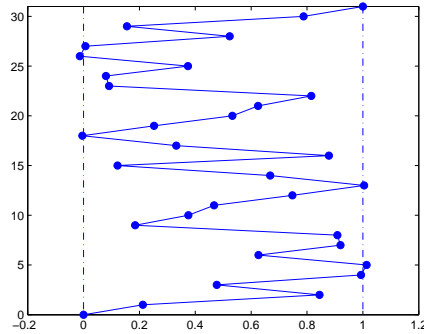


Figure 10: Cumulative weight plot for $s = 31$ stage and 10th order method (6.7).

7. Conclusions and future work

In this work we have built two techniques to obtain the coefficients of $s = 31$ stages (which is the minimal number of stages) and 10 order symmetric composition methods of basic second order symmetric integrators. The second technique has resulted the best of both techniques, allowing to obtain some more results apart from the Sofroniou and Spaletta's solution.

The aim of this work has been the design and the application of these two techniques, which can be used to find the solution of systems of polynomial equations (especially the ones that have to be solved when building high order numerical integrators).

Our next goals are the following:

- To improve our techniques in order to see if we are able to calculate more results.
- To extend the second of the explored techniques to obtain 10 order methods with more than $s = 31$ stages.
- To apply the second of the explored techniques for the construction of efficient 10 order composition methods with processing (different composition methods with processing were obtained by Blanes in [3], but only up to order 8).

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