Runge–Kutta Theory and Constraint Programming*

Julien Alexandre dit Sandretto§
julien.alexandre-dit-sandretto@ensta-paristech.fr

U2IS, ENSTA ParisTech, Université Paris-Saclay,
828 bd des Maréchaux, 91762 Palaiseau cedex France

Abstract

There exist many Runge–Kutta methods (explicit or implicit), more or less adapted to specific problems. Some of them have interesting properties, such as stability for stiff problems or symplectic capability for problems with energy conservation. Defining a new method suitable to a given problem has become a challenge. The size, the complexity and the order do not stop growing. This race to the best method is interesting but an important unsolved problem. Indeed, the coefficients of Runge–Kutta methods are harder and harder to compute, and the result is often expressed in floating-point numbers, which may lead to erroneous integration schemes. Here, we propose to use interval analysis tools to compute Runge–Kutta coefficients. In particular, we use a solver based on guaranteed constraint programming. Moreover, with a global optimization process and a well chosen cost function, we propose a way to define some novel optimal Runge–Kutta methods.

Keywords: Runge–Kutta methods, Differential equations, Validated simulation.
AMS subject classifications: 34A45,65G20,65G40

1 Introduction

Many scientific applications in physical fields such as mechanics, robotics, chemistry or electronics require solving differential equations. This kind of equation appears *e.g.*, when the location is required, but only the velocity and/or the acceleration are available when modelling a system. In the general case, these differential equations cannot be formally integrated, *i.e.*, closed form solutions are not available, and a numerical integration scheme is used to approximate the state of the system. The most

*Submitted: November 30, 2016; Revised: June 7, 2017; Accepted: August 24, 2017).
§Partially funded by the Academic and Research Chair: "Complex Systems Engineering"- Ecole polytechnique ~ THALES ~ FX ~ DGA ~ DASSAULT AVIATION ~ DCNS Research ~ ENSTA ParisTech ~ Telecom ParisTech ~ Fondation ParisTech ~ FDO ENSTA

classical approach is to use a Runge–Kutta scheme – carefully chosen with respect to the problem, desired accuracy, and so on – to simulate the system behaviour.

Historically, the first method for numerical solution of differential equations was proposed by Euler in *Institutiones Calculi Integralis* [7]. His main idea is based on a simple principle: if a particle is located at y_0 at time t_0 and if its velocity at this time is known to be equal to v_0, then at time t_1 the particle will be approximately at position $y_1 = y_0 + (t_1 - t_0)v_0$, under the condition that t_1 is sufficiently close to t_0 (that is, after a very short time), so velocity do not change "too much" over $[t_0, t_1]$. Based on this principle, around 1900 C. Runge and M. W. Kutta developed a family of iterative methods, now called Runge–Kutta methods. While many such methods have been proposed since then, a unified formalism and a deep analysis was first proposed by Butcher in the sixties [4].

Almost from the beginning, after Euler, a race started to obtain new schemes, with better properties or higher order of accuracy. It quickly became a global competition. Recently, an explicit 14^{th} order Runge–Kutta scheme with 35 stages [8] and an implicit 17^{th} order Radau with 9 stages [17] were prposed. From the beginning, methods have been discovered with the help of ingenuity in order to solve the highly complex problem, such as use of polynomials with known zeros (Legendre for Gauss methods or Jacobi for Radau) [10], vanishing of some coefficients [10], or symmetry [8]. All these approaches, based on algebraic manipulations, are reaching their limit, due to the large number of stages. Indeed, to obtain a new method, we need now to solve a high-dimensional under-determined problem with floating-point arithmetic [19]. Even if, as in some, multi-precision arithmetic is used, the result obtained is still not exact. A restriction Runge–Kutta methods which have coefficients represented exactly in the computer can be eventually considered [16]. However, this restriction is really strong, because only few methods can be used, and it is the opposite of our approach.

For this reason, in this paper we introduce application of interval coefficients for Runge–Kutta methods; this could be an interesting research direction for defining new reliable numerical integration methods. We show that the properties of a Runge–Kutta scheme (such as order, stability, symplecticity, etc.) can be preserved with interval coefficients, while they are lost with floating-point numbers. By the use of interval analysis tools [12, 18], and more specifically a constraint programming (CP) solver [21], a general method to build new methods with interval coefficients is presented. Moreover, an optimization procedure allows us, with a well chosen cost function, to define the optimal scheme. The new methods with interval coefficients, obtained with our approach, have properties inclusion properties, meaning that the resulting interval box is guaranteed to contain a scheme that satisfies all the desired properties. They can be either used in a classical numerical integration procedure (but computations have to be done with interval arithmetic), or in a validated integration one [1]. In both cases, the properties of the scheme will be preserved.

In this paper, a recurring reference will be made to the books of Hairer [10], which contains the majority of the results on Runge–Kutta theory.

Outline. We review the classical algorithm of a simulation of an ordinary differential equation with Runge–Kutta methods, as well as a brief introduction to the modern theory of Runge–Kutta methods, in Section 2. In Section 3, we present the interval analysis framework used in this work and the advantages of having Runge–Kutta methods with interval coefficients. We analyze some of the properties of Runge–Kutta methods with and without interval coefficients in Section 4. In Section 5, the constraint satisfaction problem to solve to obtain a new scheme is presented. In Section 6, we

present some experimental results, followed in Section 7 by the application of the new schemes in validated simulation. In Section 8, we summarize the main contributions of the paper.

Notation.

- $\dot{y}$ denotes the time derivative of y, *i.e.*, $\frac{dy}{dt}$.
- a denotes a real value, while $\mathbf{a}$ represents a vector of real values.
- $[a]$ represents an interval value and $[\mathbf{a}]$ represents a vector of interval values (a box).
- The midpoint of an interval $[x]$ is denoted by $\mathrm{m}([x])$.
- The variables y are used for the state variables of the system and t represents time.
- Sets will be represented by calligraphic letter such as $\mathcal{X}$ or $\mathcal{Y}$.
- The real part and the imaginary part of a complex number z will be denoted by $\Re(z)$ and $\Im(z)$ respectively.
- An interval with floating point bounds is written in the short form *e.g.*, $0.123456[7,8]$ to represent the interval $[0.1234567, 0.1234568]$.

2 A Review of Runge–Kutta Methods

Historically, Runge–Kutta methods were used to compute a Taylor series expansion without any derivative computation, which was a difficult problem in the 19^{th} Century. Now, *automatic differentiation* methods [9] can be used to efficiently compute derivatives, but Runge–Kutta methods are more than a simple technique to compute a Taylor series expansion. Mainly, Runge–Kutta methods have strong stability properties (see Section 4 for a more formal definition), which make them suitable for efficiently solving different classes of problems, especially stiff systems. In particular, implicit methods can be algebraically stable, stiffly accurate and symplectic (see Section 4.4). For this reason, the study of the properties of Runge–Kutta methods is highly interesting, and the definition of new techniques to build new Runge–Kutta methods with strong properties is also of interest.

2.1 Numerical Integration with Runge–Kutta Methods

Runge–Kutta methods can solve the *initial value problem* (*IVP*) of non-autonomous *Ordinary Differential Equations* (ODEs) defined by

$$\dot{\mathbf{y}} = \mathbf{f}(t, \mathbf{y}) \quad \text{with} \quad \mathbf{y}(0) = \mathbf{y}_0 \quad \text{and} \quad t \in [0, t_{\text{end}}] \ . \tag{1}$$

The function $\mathbf{f} : \mathbb{R} \times \mathbb{R}^n \to \mathbb{R}^n$ is called the *flow*, $\mathbf{y} \in \mathbb{R}^n$ is called the *vector of state variables*, and $\dot{\mathbf{y}}$ denotes the derivative of $\mathbf{y}$ with respect to time t. We shall always assume at least that $\mathbf{f}$ is globally Lipschitz in $\mathbf{y}$, so Equation (1) admits a unique solution [10] for a given initial condition $\mathbf{y}_0$. Furthermore, for our purpose, we shall assume, as needed, that $\mathbf{f}$ is continuously differentiable. The exact solution of Equation (1) is denoted by $\mathbf{y}(t; \mathbf{y}_0)$.

The goal of a numerical simulation to solve Equation (1) is to compute a sequence of time instants $0 = t_0 < t_1 < \cdots < t_N = t_{\text{end}}$ (not necessarily equidistant) and a

sequence of states $\mathbf{y}_0, \ldots, \mathbf{y}_N$ such that $\forall \ell \in [0, N]$, $\mathbf{y}_\ell \approx \mathbf{y}(t_\ell, \mathbf{y}_{\ell-1})$, obtained with the help of an integration scheme.

A Runge–Kutta method, starting from an initial value $\mathbf{y}_\ell$ at time t_ℓ and a finite time horizon h, the *step-size*, produces an approximation $\mathbf{y}_{\ell+1}$ at time $t_{\ell+1}$, with $t_{\ell+1} - t_\ell = h$, of the solution $\mathbf{y}(t_{\ell+1}; \mathbf{y}_\ell)$. Furthermore, to compute $\mathbf{y}_{\ell+1}$, a Runge–Kutta method computes s evaluations of f at predetermined time instants. The number s is known as the number of *stages* of a Runge–Kutta method. More precisely, a Runge–Kutta method is defined by

$$\mathbf{y}_{\ell+1} = \mathbf{y}_\ell + h \sum_{i=1}^{s} b_i \mathbf{k}_i, \tag{2}$$

with $\mathbf{k}_i$ defined by

$$\mathbf{k}_i = \mathbf{f}\left(t_\ell + c_i h, \mathbf{y}_\ell + h \sum_{j=1}^{s} a_{ij} \mathbf{k}_j\right). \tag{3}$$

The coefficients c_i, a_{ij} and b_i, for $i, j = 1, 2, \cdots, s$, fully characterize the Runge–Kutta methods, and they are usually synthesized in a *Butcher tableau* [4] of the form

$$\begin{array}{c|cccc} c_1 & a_{11} & a_{12} & \ldots & a_{1s} \\ c_2 & a_{21} & a_{22} & \ldots & a_{2s} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ c_s & a_{s1} & a_{s2} & \ldots & a_{ss} \\ \hline & b_1 & b_2 & \ldots & b_s \end{array} \quad \equiv \quad \begin{array}{c|c} \mathbf{c} & \mathbf{A} \\ \hline & \mathbf{b} \end{array} .$$

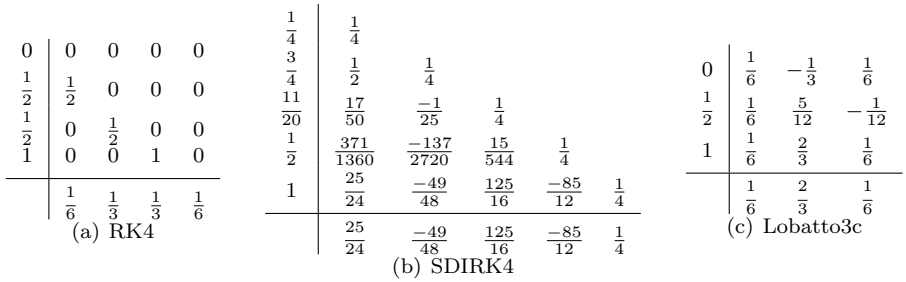
In terms of the form of the matrix $\mathbf{A}$, consisting of the coefficients a_{ij}, a Runge–Kutta method can be

- *explicit*, *e.g.*, as in the classical Runge–Kutta method of order 4 given in Figure 1(a). In other words, the computation of the intermediate $\mathbf{k}_i$ only depends on the previous steps $\mathbf{k}_j$ for $j < i$;
- *diagonally implicit*, *e.g.*, as in the diagonally implicit fourth-order method given in Figure 1(b). In this case, the computation of an intermediate step $\mathbf{k}_i$ involves the value $\mathbf{k}_i$, so non-linear systems in $\mathbf{k}_i$ must be solved. A method is *singly diagonally implicit* if the coefficients on the diagonal are all equal;
- *fully implicit*, *e.g.*, the Runge–Kutta fourth-order method with a Lobatto quadrature formula given in Figure 1(c). In this last case, the computation of intermediate steps involves the solution of a non-linear system of equations in all the values $\mathbf{k}_i$ for $i = 1, 2, \cdots, s$.

The order of a Runge–Kutta method is p if and only if the *local truncation error*, *i.e.*, the distance between the exact solution $\mathbf{y}(t_\ell; \mathbf{y}_{\ell-1})$ and the numerical solution $\mathbf{y}_\ell$ is such that:

$$\mathbf{y}(t_\ell; \mathbf{y}_{\ell-1}) - \mathbf{y}_\ell = \mathcal{O}(h^{p+1}) \ .$$

Some theoretical results have been obtained concerning the relation between the number of stages s and the order p. For the explicit methods, there is no Runge–Kutta method of order p with $s = p$ stages when $p > 4$. For the implicit methods, $p = 2s$ is the largest possible order for a given number of stages, and only Gauss-Legendre methods have this capability [10].



(a) RK4

(b) SDIRK4

(c) Lobatto3c

Figure 1: Different kinds of Runge–Kutta methods

2.2 Butcher's Theory of Runge–Kutta Methods

One of the main ideas of John Butcher in [4] is to express the Taylor expansion of the exact solution of (1) and the Taylor expansion of the numerical solution using the same basis of *elementary differentials* . The elementary differentials are made of sums of partial derivatives of f with respect to the components of $\mathbf{y}$. Another salient idea of John Butcher in [4] is to relate these partial derivatives of order q to a combinatorial problem to enumerate all the trees τ with exactly q nodes. From the structure of a tree τ, one can map a particular partial derivative; see Table 1 for some examples. It follows that one has the three following theorems, used used to express the order condition of Runge–Kutta methods. In theorems 2.1 and 2.2, τ is a rooted tree, $F(\tau)$ is the elementary differential associated with τ, $r(\tau)$ is the order of τ (the number of nodes it contains), $\gamma(\tau)$ is the density, $\alpha(\tau)$ is the number of equivalent trees and $\psi(\tau)$ the elementary weight of τ based on the coefficients c_i, a_{ij} and b_i defining a Runge–Kutta method; see [4] for more details. Theorem 2.1 defines the q-th time derivative of the exact solution expressed with elementary differentials. Theorem 2.2 defines the q-th time derivative of the numerical solution expressed with elementary differentials. Finally, Theorem 2.3 formally defines the order condition of the Runge–Kutta methods.

Theorem 2.1 *The q-th derivative w.r.t. time of the* exact solution *is given by*

$$\mathbf{y}^{(q)} = \sum_{r(\tau)=q} \alpha(\tau) F(\tau)(\mathbf{y}_0) \ .$$

Theorem 2.2 *The q-th derivative w.r.t. time of the* numerical solution *is given by*

$$\mathbf{y}_1^{(q)} = \sum_{r(\tau)=q} \gamma(\tau)\varphi(\tau)\alpha(\tau) F(\tau)(\mathbf{y}_0) \ .$$

Theorem 2.3 (Order condition) *A Runge–Kutta method has order p iff*

$$\varphi(\tau) = \frac{1}{\gamma(\tau)} \quad \forall \tau, r(\tau) \leqslant p \ .$$

These theorems give the necessary and sufficient conditions to define new Runge–Kutta methods. In other words, they define a system of equations, where the unkowns are the coefficients c_i, a_{ij} and b_i, which characterize a Runge–Kutta method. For

Table 1: Rooted trees τ, elementary differentials $F(\tau)$, and their coefficients

$r(\tau)$	Trees	$F(\tau)$	$\alpha(\tau)$	$\gamma(\tau)$	$\varphi(\tau)$
1		$\mathbf{f}$	1	1	$\sum_i b_i$
2		$\mathbf{f}'\mathbf{f}$	1	2	$\sum_{ij} b_i a_{ij}$
3		$\mathbf{f}''(\mathbf{f},\mathbf{f})$	1	3	$\sum_{ijk} b_i a_{ij} a_{ik}$
3		$\mathbf{f}'\mathbf{f}'\mathbf{f}$	1	6	$\sum_{ijk} b_i a_{ij} a_{jk}$
4		$\mathbf{f}'''(\mathbf{f},\mathbf{f},\mathbf{f})$	1	4	$\sum_{ijkl} b_i a_{ij} a_{ik} a_{il}$
4		$\mathbf{f}''(\mathbf{f}'\mathbf{f},\mathbf{f})$	3	8	$\sum_{ijkl} b_i a_{ij} a_{ik} a_{jl}$
4		$\mathbf{f}'\mathbf{f}''(\mathbf{f},\mathbf{f})$	1	12	$\sum_{ijkl} b_i a_{ij} a_{jk} a_{jl}$
4		$\mathbf{f}'\mathbf{f}'\mathbf{f}'\mathbf{f}$	1	24	$\sum_{ijkl} b_i a_{ij} a_{jk} a_{kl}$

example, for the first four orders, and following the order condition, the following constraints on the derivative order have to be solved to create a new Runge–Kutta method

- order 1: $\sum b_i = 1$
- order 2: $\sum b_i a_{ij} = \frac{1}{2}$
- order 3: $\sum c_i b_i a_{ij} = \frac{1}{6}$, $\sum b_i c_i^2 = \frac{1}{3}$
- order 4: $\sum b_i c_i^3 = \frac{1}{4}$, $\sum b_i c_i a_{ij} c_j = \frac{1}{8}$, $\sum b_i a_{ij} c_j^2 = \frac{1}{12}$, $\sum b_i a_{ij} a_{jk} c_k = \frac{1}{24}$

The total number of constraints increases exponentially: 8 for the 4^{th} order, 17 for the 5^{th} order, 37, 85, 200, etc. Note also an additional constraint, saying that the c_i must be increasing, has to be taken into account, and also that c_i are such that

$$c_i = \sum_j a_{ij} \ .$$

These constraints are the smallest set of constraints, known as *Butcher rules*, which have to be validated in order to define new Runge–Kutta methods.

Additionally, other constraints can be added to define particular structure of Runge–Kutta methods [4], as for example, to make it

- Explicit: $a_{ij} = 0, \forall j \geq i$
- Singly diagonal: $a_{1,1} = \cdots = a_{s,s}$
- Diagonal implicit: $a_{ij} = 0, \forall j > i$
- Explicit first line: $a_{11} = \cdots = a_{1s} = 0$
- Stiffly accurate: $a_{si} = b_i, \forall i = 1, \ldots, s$
- Fully implicit: $a_{ij} \neq 0, \forall i, j = 1, \ldots, s$

Note that historically, some simplifications of this set of constraints were used to reduce the complexity of the problem. For example, to obtain a fully implicit scheme

with a method based on Gaussian quadrature (see [5] for more details), the $c_1, \ldots, c_s$ are the zeros of the shifted Legendre polynomial of degree s, given by:

$$\frac{d^s}{dx^s}(x^s(x-1)^s).$$

This approach is called the "Kuntzmann-Butcher methods" and is used to characterize the Gauss-Legendre methods [5]. Another example: by finding the zeros of

$$\frac{d^{s-2}}{dx^{s-2}}(x^{s-1}(x-1)^{s-1}),$$

the Lobatto quadrature formulas are obtained (see Figure 1(c)).

The problems with this approach are obvious. First, the resulting Butcher tableau is guided by the solver and not by the requirements on the properties. Second, a numerical computation in floating-point numbers is needed, and because such computations are not exact, the constraints may not be satisfied.

We propose an interval analysis approach to solve these constraints and hence produce reliable results. More precisely, we follow the *constraint satisfaction problem* approach.

3 Runge–Kutta with Interval Coefficients

As seen before in Section 2.2, the main constraints are the order conditions, also called *Butcher rules*. Two other constraints need to be considered: the sum of a_{ij} is equal to c_i for all the table lines; and the c_i are increasing with respect to i. These constraints have to be fulfilled to obtain a valid Runge–Kutta method, and they can be gathered in a Constraint Satisfaction Problem (CSP).

Definition 3.1 (CSP) *A numerical (or continuous) CSP $(\mathcal{X}, \mathcal{D}, \mathcal{C})$ is defined as follows:*

- $\mathcal{X} = \{x_1, \ldots, x_n\}$ *is a set of variables, also represented by the vector* $\mathbf{x}$.
- $\mathcal{D} = \{[x_1], \ldots, [x_n]\}$ *is a set of domains ($[x_i]$ contains all possible values of x_i).*
- $\mathcal{C} = \{c_1, \ldots, c_m\}$ *is a set of constraints of the form $c_i(\mathbf{x}) \equiv f_i(\mathbf{x}) = 0$ or $c_i(\mathbf{x}) \equiv g_i(\mathbf{x}) \leqslant 0$, with $f_i : \mathbb{R}^n \to \mathbb{R}$, $g_i : \mathbb{R}^n \to \mathbb{R}$ for $1 \leqslant i \leqslant m$. Constraints $\mathcal{C}$ are interpreted as a conjunction of equalities and inequalities.*

An evaluation of the variables is a function from a subset of variables to a set of values in the corresponding subset of domains. An evaluation is *consistent* if no constraint is violated. An evaluation is *complete* if it includes all variables. The *solution* of a CSP is a complete and consistent evaluation.

In the particular case of continuous (or numerical) CSPs, interval based techniques provide generally one or a list of boxes which enclose the solution. The CSP approach is at the same time powerful enough to address complex problems (NP-hard problems with numerical issues, even in critical applications) and simple in the definition of a solving framework [2, 14].

Indeed, the classical algorithm to solve a CSP is the branch-and-prune algorithm, which needs only an evaluation of the constraints and an initial domain for variables. While this algorithm is sufficient for many problems, to solve other problems, some improvements have been achieved, and algorithms based on contractors have emerged

[6]. The branch-and-contract algorithm consists of two main steps: i) the contraction (or filtering) of one variable and the propagation to the others until a fixed point reached, then ii) the bisection of the domain of one variable in order to obtain two problems, easier to solve.

A more detailed description follows.

Contraction A filtering algorithm or contractor is used in a CSP solver to reduce the domain of variables to a fixed point (or a near fixed point), by respecting local consistencies. A contractor Ctc can be defined with the help of constraint programming, analysis or algebra, but it must satisfy three properties:

- $Ctc(\mathcal{D}) \subseteq \mathcal{D}$: contractivity,
- Ctc cannot remove any solution: it is conservative,
- $\mathcal{D}' \subseteq \mathcal{D} \Rightarrow Ctc(\mathcal{D}') \subseteq Ctc(\mathcal{D})$: monotonicity.

There are many contractor operators defined in the literature, most notably:

- (Forward-Backward contractor) By considering only one constraint, this method computes the interval enclosure of a node in the tree of constraint operations with the children domains (the forward evaluation), then refines the enclosure of a node in terms of parents domain (the backward propagation). For example, from the constraint $x + y = z$, this contractor refines initial domains $[x]$, $[y]$ and $[z]$ from a forward evaluation $[z] = [z] \cap ([x] + [y])$, and from two backward evaluations $[x] = [x] \cap ([z] - [y])$ and $[y] = [y] \cap ([z] - [x])$.
- (Newton contractor) This contractor, based on the first order Taylor interval extension: $[f]([\mathbf{x}]) = f(\mathbf{x}^*) + [J_f]([\mathbf{x}])([\mathbf{x}] - \mathbf{x}^*)$ with $\mathbf{x}^* \in [\mathbf{x}]$, has the property: if $0 \in [f]([\mathbf{x}])$, then $[\mathbf{x}]_{k+1} = [\mathbf{x}]_k \cap x^* - [J_f]([\mathbf{x}]_k)^{-1} f(\mathbf{x}^*)$ is a tighter inclusion of the solution of $f(x) = 0$. Some other contractors based on Newton's method, such as the Krawczyk operator [12], have been defined.

Propagation If a variable domain has been reduced, the reduction is propagated to all the constraints involving that variable, allowing the other variable domains to be narrowed. This process is repeated until a fixed point is reached.

Branch-and-Prune A Branch-and-Prune algorithm consists on alternatively branching and pruning to produce two sub-pavings $\mathcal{L}$ and $\mathcal{S}$, with $\mathcal{L}$ the boxes too small to be bisected and $\mathcal{S}$ the solution boxes. We are then sure that all solutions are included in $\mathcal{L} \cup \mathcal{S}$ and that every point in $\mathcal{S}$ is a solution.

Specifically, this algorithm traverses a list of boxes $\mathcal{W}$, initialized $\mathcal{W}$ with the vector $[\mathbf{x}]$ consisting of the elements of $\mathcal{D}$. For each box in $\mathcal{W}$, the following is done: i) Prune: the CSP is evaluated (or contracted) on the current box; if the box is is a solution, it is added to $\mathcal{S}$; otherwise ii) Branch: if the box is large enough, it is bisected and the two boxes resulting are added into $\mathcal{W}$; otherwise the box is added to $\mathcal{L}$.

Example 3.1 *An example of the problems that the previously presented tools can solve is taken from [15]. The CSP is defined as follows:*

- $\mathcal{X} = \{x, y, z, t\}$
- $\mathcal{D} = \{[x] = [0, 1000], [y] = [0, 1000], [z] = [0, 3.1416], [t] = [0, 3.1416]\}$
- $\mathcal{C} = \{xy + t - 2z = 4; x\sin(z) + y\cos(t) = 0; x - y + \cos^2(z) = \sin^2(t); xyz = 2t\}$

We use a Branch-and-Prune algorithm with the Forward-Backward contractor and a propagation algorithm to solve this CSP. The solution ($[1.999, 2.001]$, $[1.999, 2.001]$, $[1.57, 1.571]$, $[3.14159, 3.1416]$*) is obtained with only* 6 *bisections.* ■

3.1 Correctness of CSP Applied to Butcher Rules

By construction, the CSP approach guarantees that the exact solution of the problem, denoted by $(\tilde{a}_{ij}, \tilde{b}_i, \tilde{c}_i)$, is included in the solution provided by the corresponding solver, given by $([a_{ij}], [b_i], [c_i])$. The Butcher rules are then preserved by inclusion through the use of interval coefficients.

Theorem 3.1 *If Runge–Kutta coefficients are given by intervals obtained by a CSP solver on constraints coming from the order condition defined in Theorem 2.3 then they contain at least one solution which satisfies the Butcher rules.*

Proof: Starting from the order condition defined in Theorem 2.3, and given the additional details in [1], if the Runge–Kutta coefficients are given by intervals, such that $\tilde{a}_{ij} \in [a_{ij}], \tilde{b}_i \in [b_i], \tilde{c}_i \in [c_i]$, then $[\varphi(\tau)] \ni \frac{1}{\gamma(\tau)} \quad \forall \tau, r(\tau) \leq p$. In other words, $\mathbf{y}^{(q)} \in [\mathbf{y}_1^{(q)}], \forall q \leq p$, and then the derivatives of the exact solution are included in the numerical ones, and the Taylor series expansion of the exact solution is included (monotonicity of the interval sum) in the Taylor series expansion of the numerical solution obtained from the Runge–Kutta method with interval coefficients. □

Remark 3.1 *If a method is given with interval coefficients such that* $\tilde{a}_{ij} \in [a_{ij}], \tilde{b}_i \in [b_i], \tilde{c}_i \in [c_i]$*, there is an over-estimation of the derivatives* $|\mathbf{y}^{(q)} - [\mathbf{y}_1^{(q)}]|$*. To make this over-approximation as small as possible, the enclosure of the coefficients has to be as sharp as possible.*

3.2 Link with Validated Numerical Integration Methods

To make the Runge–Kutta method validated [1], the challenging question is how to compute a bound on the difference between the true solution and the numerical solution, defined by $\mathbf{y}(t_\ell; \mathbf{y}_{\ell-1}) - \mathbf{y}_\ell$. This distance is associated with the *local truncation error* (LTE) of the numerical method. We showed that LTE can be easily bounded by using the difference between the Taylor series of the exact and the numerical solutions, which is reduced to LTE $= \mathbf{y}^{(p+1)}(t_\ell) - [\mathbf{y}_\ell^{(p+1)}]$, with p the order of the method undere consideration. This difference has to be evaluated on a specific box, obtained with the Picard-Lindelöf operator, but this is outside the scope of this paper, see [1] for more details. For a method with interval coefficients, the LTE is well bounded (even over-approximated), which is not the case for a method with floating-point coefficients. For a validated method, the use of interval coefficients is then a requirement.

4 Stability Properties with Interval Coefficients

Runge–Kutta methods have strong stability properties which are not present for other numerical integration methods such as multi-step methods, *e.g.*, Adams-Moulton methods or BDF methods [10]. It is interesting to understand that these properties, proven in theory, are lost in practice if we use floating-point number coefficients. In this section, we show that the properties of Runge–Kutta methods are preserved with

the use of interval coefficients in the Butcher tableau. The definition of stability can have a very different form depending on the class of problems under consideration.

4.1 Notion of Stability

In [10], the authors explain that when we do not have the analytical solution of a differential problem, we must be content with numerical solutions. As they are obtained for specified initial values, it is important to know the stability behaviour of the solutions for all initial values in the neighbourhood of a certain equilibrium point.

For example, we consider a linear problem $\dot{\mathbf{y}} = \mathbf{A}\mathbf{y}$, with exact solution $\mathbf{y}(t) = \exp(\mathbf{A}t)\mathbf{y}_0$. This solution is analytically stable if all trajectories remain bounded as $t \to \infty$. Theory says that it is the case if and only if the real part of the eigenvalues of $\mathbf{A}$ are strictly negative. If a numerical solution of this problem is computed with the Euler method, the system obtained is:

$$\mathbf{y}(t^* + h) \approx \mathbf{y}(t^*) + \mathbf{A}h\mathbf{y}(t^*) = (\mathbf{I} + \mathbf{A}h)\mathbf{y}(t^*) = \mathbf{F}x(t^*) \ .$$

In the same manner, the explicit Euler method is analytically stable if the discretized system $\mathbf{y}_{k+1} = \mathbf{F}\mathbf{y}_k$ is analytically stable.

Many classes of stability exist, such as A-stability, B-stability, A(α)-stability, Algebraic stability; see [10] for more details. Regarding the linear example above, each stability class is associated with a particular class of problems.

4.2 Linear Stability

We focus on linear stability for explicit methods, which is easier to study, and is enough to justify the use of interval coefficients. For linear stability, the classical approach consists of computing the *stability domain* of the method. The *stability function* of explicit methods is given in [10]:

$$R(z) = 1 + z\sum_j b_j + z^2\sum_{j,k} b_j a_{jk} + z^3\sum_{j,k,l} b_j a_{jk} a_{kl} + \dots \ , \tag{4}$$

which can be written if the Runge–Kutta method is of order p as

$$R(z) = 1 + z + \frac{z^2}{2!} + \frac{z^3}{3!} + \cdots + \frac{z^p}{p!} + \mathcal{O}(z^{p+1}) \ . \tag{5}$$

For example, the stability function for a fourth-order method with four stages, such as the classic RK4 method given in Figure 1(a), is:

$$R(z) = 1 + z + \frac{z^2}{2} + \frac{z^3}{6} + \frac{z^4}{24}. \tag{6}$$

The stability domain is then defined by $S = \{z \in \mathcal{C} : |R(z)| \leqslant 1\}$. This definition of S can be transformed into a constraint on real numbers following an algebraic process on complex numbers, such as

$$S = \{(x, y) : \Re\left(\sqrt{\Re(R(x+iy))^2 + \Im(R(x+iy))^2}\right) \leqslant 1\}.$$

The constraint produced is given in Equation (7).

$$\left(\frac{1}{6}x^3y + \frac{1}{2}x^2y - \frac{1}{6}xy^3 + xy - \frac{1}{6}y^3 + y^2 + \frac{1}{24}x^4 + \frac{1}{6}x^3 - \frac{1}{4}x^2y^2 + \frac{1}{2}x^2 - \frac{1}{2}xy^2 + x + \frac{1}{24}y^4 - \frac{1}{2}y^2 + 1\right)^{\frac{1}{2}} \leqslant 1 \quad (7)$$

The set S is now defined by a constraint on real numbers x, y and can be easily computed by a classical paving method [12]. The result of this method is marked in blue in in Figure 2 for an explicit Runge–Kutta fourth-order method with four stages, such as the classical Runge–Kutta method (RK4).

We can study the influence of the numerical accuracy on the linear stability. If we compute the coefficients (for example 1/6 and 1/24) with low precision (even exaggeratedly in our case), the stability domain is reduced as shown in Figure 2.

First, we consider an error of 1×10^{-8}, which is the classical precision of floating-point numbers for some tools (see Figure 2 on the left). For example, the coefficient equal in theory to 1/6 is encoded by 0.16666667. Then, we consider an error of 0.1 for this example, to see the impact: the stability domain becomes the same as a first order method such as Euler's method. If it seems to be exaggerated, in fact it is not rare to find old implementations of Runge–Kutta with only one decimal digit of accuracy (see Figure 2 on the right).

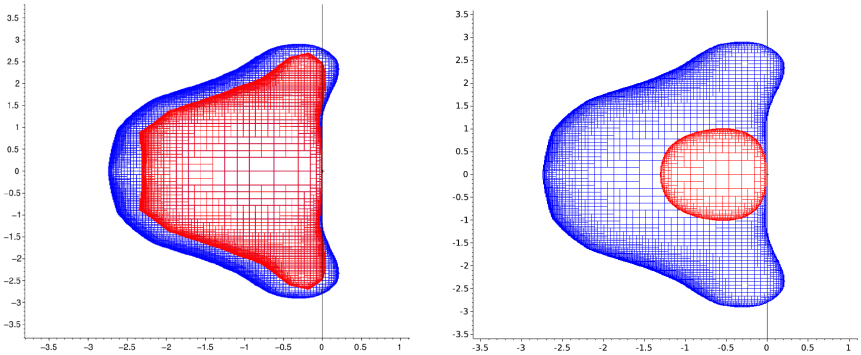


Figure 2: Paving of stability domain for RK4 method with high precision coefficients (blue) and with small error (red) on coefficients (left) and large error on coefficients (right).

4.3 Algebraic Stability

Another interesting stability class for Runge–Kutta methods is algebraic stability, which is useful for stiff problems or to solve algebraic-differential equations. A method is algebraically stable if the coefficients a_{ij} and b_i in the Butcher tableau are such that

$b_i \geq 0, \forall i = 1, \ldots, s:\ \mathbf{M} = (m_{ij}) = (b_i a_{ij} + b_j a_{ji} - b_i b_j)_{i,j=1}^{s}$ is non-negative definite.

The test for non-negative definiteness can be done with constraint programming by solving the eigenvalue problem $\det(\mathbf{M} - \lambda \mathbf{I}) = 0$ and proving that $\lambda > 0$. $\mathbf{I}$ denotes

the identity matrix of dimension $s \times s$. For example, with a three stage Runge–Kutta method, *i.e.*, $s = 3$, the constraint is:

$$(m_{11} - \lambda)((m_{22} - \lambda)(m_{33} - \lambda) - m_{23}m_{32}) - m_{12}(m_{21}(m_{33} - \lambda) - m_{23}m_{13}) + m_{31}(m_{21}m_{32} - (m_{22} - \lambda)m_{31}) = 0. \quad (8)$$

Based on a contractor programming approach [6], the CSP to solve is:

$$\text{Equation (8) has no solution in }]-\infty, 0[\quad \equiv \quad \mathbf{M} \text{ is non-negative definite.}$$

A contractor based on the Forward/Backward algorithm is applied to the initial interval $[-1 \times 10^8, 0]$; if the result obtained is the empty interval, then Equation (8) has no negative solution, and $\mathbf{M}$ is non-negative definite, so the method is algebraically stable.

We apply this method to the three-stage Lobatto IIIC, and the result of contractor is empty, proving there is no negative eigenvalue, hence the matrix $\mathbf{M}$ is non-negative definite and the Lobatto IIIC method is algebraically stable, which is consistent with the theory. Similarly, we apply it to the three-stage Lobatto IIIA, and the contractor finds at least one negative eigenvalue ($-0.048\,112\,5$) so this method is not algebraically stable, which is also consistent with the theory.

Now, if an algebraically stable method is implemented with coefficients in floating-point numbers, this property is lost. Indeed, an error of 1×10^{-9} on a_{ij} is enough to lose the algebraic stability for Lobatto IIIC methods (a negative eigenvalue appears equal to $-1.030\,41 \times 10^{-5}$).

4.4 Symplecticity

Finally, another property of Runge–Kutta methods is tested, the symplecticity. This property is associated with a notion of energy conservation. A numerical solution obtained with a symplectic method preserves an energy quantity, without formally expressing the corresponding law.

Definition 4.1 (Symplectic integration methods) *Hamiltonian systems, given by*

$$\dot{p}_i = -\frac{\partial H}{\partial q_i}(p, q), \quad \dot{q}_i = -\frac{\partial H}{\partial p_i}(p, q), \quad (9)$$

have two remarkable properties: i) the solutions preserve the Hamiltonian $H(p, q)$; ii) the corresponding flow is symplectic, i.e., preserves the differential 2-form $\omega^2 = \sum_{i=1}^{n} dp_i \wedge dq_i$. A numerical method used to solve Equation (9)*, while preserving these properties, is a* **symplectic integration method**.

Definition 4.2 (Symplectic interval methods) *A Runge–Kutta method with interval coefficients $\{[\mathbf{b}], [\mathbf{c}], [\mathbf{A}]\}$, such that a method defined by $\{\mathbf{b}, \mathbf{c}, \mathbf{A}\}$ with $\mathbf{b} \in [\mathbf{b}]$, $\mathbf{c} \in [\mathbf{c}]$, and $\mathbf{A} \in [\mathbf{A}]$ is symplectic, is a* **symplectic interval method**.

A Runge–Kutta method is symplectic if it satisfies the condition $\mathbf{M} = 0$, where

$$\mathbf{M} = (m_{ij}) = (b_i a_{ij} + b_j a_{ji} - b_i b_j)_{i,j=1}^{s}.$$

With interval computation of $\mathbf{M}$, it is possible to verify if $0 \in \mathbf{M}$, which is enough to prove that the method with interval coefficients is symplectic. Indeed, it is sufficient to

prove that a trajectory which preserves a certain energy conservation condition exists inside the numerical solution.

We apply this approach to the three-stage Gauss-Legendre method with coefficients computed with interval arithmetic. The matrix $\mathbf{M}$ contains the zero matrix (see Equation (10)), so this method is symplectic, which is in agreement with the theory.

$$\mathbf{M} = \begin{pmatrix} [-1.3e^{-17}, 1.4e^{-17}] & [-2.7e^{-17}, 2.8e^{-17}] & [-2.7e^{-17}, 1.4e^{-17}] \\ [-2.7e^{-17}, 2.8e^{-17}] & [-2.7e^{-17}, 2.8e^{-17}] & [-1.3e^{-17}, 4.2e^{-17}] \\ [-2.7e^{-17}, 1.4e^{-17}] & [-1.3e^{-17}, 4.2e^{-17}] & [-1.3e^{-17}, 1.4e^{-17}] \end{pmatrix} \tag{10}$$

Now, if we compute only one term of the Gauss-Legendre method with floating-point numbers, for example $a_{1,2} = 2.0/9.0 - \sqrt{15.0}/15.0$, the symplecticity property is lost (see Equation (11)).

$$\mathbf{M} = \begin{pmatrix} [-1.3e^{-17}, 1.4e^{-17}] & [\mathbf{-1.91e^{-09}}, \mathbf{-1.92e^{-09}}] & [-2.7e^{-17}, 1.4e^{-17}] \\ [\mathbf{-1.91e^{-09}}, \mathbf{-1.92e^{-09}}] & [-2.7e^{-17}, 2.8e^{-17}] & [-1.3e^{-17}, 4.2e^{-17}] \\ [-2.7e^{-17}, 1.4e^{-17}] & [-1.3e^{-17}, 4.2e^{-17}] & [-1.3e^{-17}, 1.4e^{-17}] \end{pmatrix} \tag{11}$$

5 A Constraint Optimization Approach to Define New Runge–Kutta Methods

In the previous section, the properties of Runge–Kutta methods with interval coefficients in the Butcher tableau have been studied, and we have shown that these properties are preserved with intervals while they are often lost with floating-point numbers. In this section, an approach based on constraint optimization is presented to obtain optimal Runge–Kutta methods with interval coefficients. The cost function is also discussed, while the solving procedure is presented in Section 6.1.

5.1 Constraints

The constraints to solve to obtain a novel Runge–Kutta method are the ones presented in Section 2.2, and the approach is based on a CSP solver based on contractors and a branching algorithm (see Section 3). The problem under consideration can be under-constrained, and more than one solution can exist (for example, there are countless fully implicit fourth-order methods with three stages). With the interval analysis approach, which is based on set representation, a continuum of coefficients can be obtained. As the coefficients of the Butcher tableau have to be as tight as possible to obtain sharp enclosure of the numerical solution, a continuum (or more than one) of solutions is not serviceable. Indeed, in a set of solutions, or a continuum, it is interesting to find an optimal solution with respect to a given cost.

Note that using the framework of CPS, adding a cost function and hence solving a constraint optimization problem can be done following classical techniques such as those defined in [11].

5.2 Cost function

In the literature, a cost function based on the norm of the local truncation error is sometimes chosen [20].

5.2.1 Minimizing the LTE

There exist many explicit second-order methods with two stages. A general form, shown in Table 2, has been defined. With $\alpha = 1$, this method is Heun's method, while $\alpha = 1/2$ gives the midpoint method (see [4] for details about these methods).

0	0	
α	α	
	1-1/(2α)	1/(2α)

Table 2: General form of ERK with 2 stages and order 2

Ralston has proven that $\alpha = 2/3$ minimizes the sum of square of coefficients of rooted trees in the local truncation error computation [5], which is given by:

$$\min_{\alpha}(-3\alpha/2 + 1)^2 + 1. \tag{12}$$

The resulting Butcher tableau is given in Table 3.

0	0	
2/3	2/3	
	1/4	3/4

Table 3: Ralston method

5.2.2 Maximizing order

Another way to obtain a similar result is to try to attain one order larger than the desired one. For example, if, as Ralston, we try to build an explicit second-order method with two stages but as close as possible to the third order by minimizing:

$$\min_{a_{ij},b_i,c_i} \left(\sum c_i b_i a_{ij} - \frac{1}{6}\right)^2 + \left(\sum b_i c_i^2 - \frac{1}{3}\right)^2 . \tag{13}$$

The same result is obtained (Table 4). This way of optimization is more interesting for us because it reuses the constraint generated by the order condition. It also minimizes the LTE at a given order p, because it tends to a method of order $p + 1$ which has a LTE equal to zero at this order. It is important to note that minimizing the LTE or maximizing the order leads to the same result; the difference is in the construction of the cost function and in the spirit of the approach.

Table 4: Ralston method with interval coefficients

$[-0, 0]$	$[-0, 0]$	
0.6...6[6, 7]	0.6...6[6, 7]	
	$[0.25, 0.25]$	$[0.75, 0.75]$

6 Experiments

Experiments are performed to, first, re-discover Butcher's theory and, second, to find new methods with desired structure.

6.1 Details of Implementation

To implement the approach presented in this paper, two steps need to be performed. The first one is a formal procedure used to generate the CSP, and the second one is applying a CSP solver based on interval analysis.

6.1.1 Definition of the Desired Method and Generation of the CSP

The definition of the desired method consists of the choice of

- Number of stages of the method
- Order of the method
- Structure of the method (singly diagonal, explicit method, diagonally implicit method, explicit first line and/or stiffly accurate method)

Based on this definition and the algorithm defined in [3], a formal procedure generates the constraints associated with the structure and Butcher rules (see Section 2.2), and eventually a cost function (see Section 5.2.2).

6.1.2 Constraint Programming and Global Optimization

Problem solution is done with Ibex, a library for interval computation with a constraint solver and a global optimizer.

This library can address two major problems [22]:

- System solving: A guaranteed enclosure for each solution of a system of (non-linear) equations is calculated.
- Global optimization: A global minimizer of some function under non-linear constraints is calculated with guaranteed bounds on the objective minimum.

Global optimization is performed with an epsilon relaxation, so the solution is optimal but the constraints are satisfied with respect to the relaxation. A second pass with the constraint solver is then needed to find the validated solution inside the inflated optimal solution. The solver provides its result in the form of an interval vector such as $([b_i], [c_i], [a_{ij}])$.

Some experiments are performed in the following. First, the constraint solving part, which allows us to find methods with sufficient constraints to be the unique solution, is tested. Second, the global optimizer is used to find the optimal methods which are under-constrained by order conditions. Both parts are used to find the existing methods and potentially new ones. In the following, just few methods that can be computed are shown. Indeed, numerous methods can be obtained.

6.2 Constraint Solving

The first part of the presented approach is applied. It allows one to solve the constraints defined during the user interface process, without cost function. This option permits

- finding a method if there is only one solution (well-constrained problem),

- knowing if there is no solution available,
- validating the fact that there is a continuum in which an optimum can be found.

To demonstrate the efficiency of this solution part, we apply it with user choices that lead to existing methods and well-known results. After that, we describe some new interesting methods.

6.2.1 Existing Methods

Only One Fourth-Order Method with Two Stages: Gauss-Legendre If we are looking for a fourth-order fully implicit method with two stages, the theory says that only one method exists, the Gauss-Legendre scheme. In the following, we try to obtain the same result with the solution part of our scheme.

The CSP for this method is defined as follows:

$$\mathcal{X} = \{\mathbf{b}, \mathbf{c}, \mathbf{A}\}$$
$$\mathcal{D} = \{[-1,1]^2, [0,1]^2, [-1,1]^4\}$$
$$\mathcal{C} = \left(\begin{array}{r} b_0 + b_1 - 1 = 0 \\ b_0 c_0 + b_1 c_1 - \frac{1}{2} = 0 \\ b_0 (c_0)^2 + b_1 (c_1)^2 - \frac{1}{3} = 0 \\ b_0 a_{00} c_0 + b_0 a_{01} c_1 + b_1 a_{10} c_0 + b_1 a_{11} c_1 - \frac{1}{6} = 0 \\ b_0 (c_0)^3 + b_1 (c_1)^3 - \frac{1}{4} = 0 \\ b_0 c_0 a_{00} c_0 + b_0 c_0 a_{01} c_1 + b_1 c_1 a_{10} c_0 + b_1 c_1 a_{11} c_1 - \frac{1}{8} = 0 \\ b_0 a_{00} (c_0)^2 + b_0 a_{01} (c_1)^2 + b_1 a_{10} (c_0)^2 + b_1 a_{11} (c_1)^2 - \frac{1}{12} = 0 \\ b_0 a_{00} a_{00} c_0 + b_0 a_{00} a_{01} c_1 + b_0 a_{01} a_{10} c_0 + b_0 a_{01} a_{11} c_1 + b_1 a_{10} a_{00} c_0 + \\ b_1 a_{10} a_{01} c_1 + b_1 a_{11} a_{10} c_0 + b_1 a_{11} a_{11} c_1 - \frac{1}{24} = 0 \\ a_{00} + a_{01} - c_0 = 0 \\ a_{10} + a_{11} - c_1 = 0 \\ c_0 < c_1 \end{array}\right)$$

The result from the solver is that there is only one solution, and if this result is written in the Butcher tableau form (Table 5), we see that this method is a numerically guaranteed version of Gauss-Legendre.

Table 5: Guaranteed version of Gauss-Legendre

$0.21132486540[5,6]$	$[0.25, 0.25]$	$-0.038675134594[9,8]$
$0.78867513459[5,6]$	$0.53867513459[5,6]$	$[0.25, 0.25]$
	$[0.5, 0.5]$	$[0.5, 0.5]$

No Fifth-Order Method with Two Stages It is also easy to verify that there is no fifth-order methods with two stages. The CSP generated is too large to be presented here. The solver proves that there is no solution, in less than 0.04 seconds.

Third-Order SDIRK Method with Two Stages The solver is used to obtain a third-order Singly Diagonal Implicit Runge–Kutta (SDIRK) method with two stages. The result obtained is presented in Table 6. This method is known; it is the SDIRK method with $\lambda = 1/2(1 - 1/\sqrt{3})$.

Table 6: Third-order SDIRK method with two stages

$0.21132486540[5,6]$	$0.21132486540[5,6]$	$[0,0]$
$0.78867513459[5,6]$	$0.577350269[19,20]$	$0.21132486540[5,6]$
	$[0.5,0.5]$	$[0.5,0.5]$

6.2.2 Other Methods

Now, it is possible to obtain new methods with the presented approach.

Remark 6.1 *It is hard to be sure that a method is new because there is no database collecting all the methods.*

A Fourth-Order Method with Three Stages, Singly and Stiffly Accurate In theory, this method is promising because it has the capabilities, desirable for stiff problems (and for differential algebraic equations), to simultaneously optimize the Newton's method solution process and to be stiffly accurate (to be more efficient with respect to stiffness). Our approach finds a unique method, unknown to-date, satisfying to these requirements. The result is presented in Table 7.

Table 7: A fourth-order method with three stages, singly and stiffly accurate: S3O4

$0.1610979566[59,62]$	$0.105662432[67,71]$	$0.172855006[54,67]$	$-0.117419482[69,58]$
$0.655889341[44,50]$	$0.482099622[04,10]$	$0.105662432[67,71]$	$0.068127286[68,74]$
$[1,1]$	$0.3885453883[37,75]$	$0.5057921789[56,65]$	$0.105662432[67,71]$
	$0.3885453883[37,75]$	$0.5057921789[56,65]$	$0.105662432[67,71]$

A Fifth-Order Method with Three Stages, Explicit First Line With only 6 non zero coefficients in the intermediate computations, this method could be a good compromise between a fourth-order method with four intermediate computations (fourth-order Gauss-Legendre) and sixth-order with nine intermediate computations (sixth-order Gauss-Legendre). As we know, there is no Runge–Kutta method with the same capabilities as the Gauss-Legendre method, but with fifth order. The result is presented in Table 8.

Table 8: A fifth-order method with three stages, explicit first line: S3O5

$[0,0]$	$[0,0]$	$[0,0]$	$[0,0]$
$0.355051025[64,86]$	$0.152659863[17,33]$	$0.220412414[50,61]$	$-0.0180212520[53,23]$
$0.844948974[23,34]$	$0.087340136[65,87]$	$0.57802125[20,21]$	$0.179587585[44,52]$
	$0.111111111[03,26]$	$0.512485826[00,36]$	$0.376403062[61,80]$

6.3 Global Optimization

When the first part of our solution process provides more than one solution or a continuum of solutions, we are able to define an optimization cost to find the best solution with respect to that cost. We have decided to use a cost which implies that the method tends to a higher order (Section 5.2).

6.3.1 Existing Methods

Ralston We obtain the same result as the one published by Ralston in [20], and described in Section 5.2.2.

Infinitely many Second-Order Methods with Two Stages, Stiffly Accurate and Fully Implicit The theory says that there are infinitely many second-order methods with two stages, stiffly accurate and fully implicit. But there is only one third-order method: radauIIA.

The generated CSP for this method is defined as follows:

$$\mathcal{X} = \{\mathbf{b}, \mathbf{c}, \mathbf{A}\}$$

$$\mathcal{D} = \left\{[-1,1]^2, [0,1]^2, [-1,1]^4\right\}$$

$$\mathcal{C} = \begin{pmatrix} b_0 + b_1 - 1 \leqslant \varepsilon \\ b_0 + b_1 - 1 \geqslant -\varepsilon \\ b_0 c_0 + b_1 c_1 - \dfrac{1}{2} \leqslant \varepsilon \\ b_0 c_0 + b_1 c_1 - \dfrac{1}{2} \geqslant -\varepsilon \\ a_{00} + a_{01} - c_0 = 0 \\ a_{10} + a_{11} - c_1 = 0 \\ c_0 \leqslant c_1 \\ a_{10} - b_0 = 0 \\ a_{11} - b_1 = 0 \end{pmatrix}$$

$$\text{Minimize } \left(b_0 (c_0)^2 + b_1 (c_1)^2 - \frac{1}{3}\right)^2 + \left(b_0 a_{00} c_0 + b_0 a_{01} c_1 + b_1 a_{10} c_0 + b_1 a_{11} c_1 - \frac{1}{6}\right)^2$$

The optimizer find an optimal result in less than 4 seconds; see Figure 9.

The cost of this solution is in $[-\infty, 2.89 \times 10^{-11}]$, which means that 0 is a possible cost, that is to say that a third-order method exists. A second pass with the solver is needed to find the acceptable solution (without relaxation) by fixing some coefficients ($b_1 = 0.75$ and $c_2 = 1$ for example); the well known RadauIIA method is then obtained.

Table 9: Method close to RadauIIA obtained by optimization

0.333333280449	0.416655823215	−0.0833225527662
0.999999998633	0.749999932909	0.250000055725
	0.749999939992	0.250000060009

6.3.2 Other Methods

Now, we are able to obtain new methods with our optimizing procedure.

An Optimal Explicit Third-Order Method with Three Stages There are infinitely many explicit $(3, 3)$-methods, but there is no fourth-order method with three stages. Our optimization process helps us to produce a method as close as possible to fourth order (see Table 10). The corresponding cost is computed to be in $0.00204[35, 49]$. As explained before, this method is not validated due to relaxed optimization. We fix some coefficients (enough to obtain only one solution) by adding the constraints given in Equation 14. After this first step, the solver is used to obtain a guaranteed method, close to the fourth order (see Table 11).

$$\begin{cases} b_1 > 0.195905; \\ b_1 < 0.195906; \\ b_2 > 0.429613; \\ b_2 < 0.429614; \\ b_3 > 0.37448000; \\ b_3 < 0.37448001; \\ c_2 > 0.4659; \\ c_2 < 0.4660; \\ c_3 > 0.8006; \\ c_3 < 0.8007; \\ a_{32} > 0.9552; \\ a_{32} < 0.9553; \\ a_{31} > -0.1546; \\ a_{31} < -0.1545; \end{cases} \tag{14}$$

Table 10: An optimal explicit third-order method with three stages (not validated due to relaxation)

1.81174261766e-08	6.64130952624e-09	9.93482546211e-09	-1.11126730095e-09
0.465904769163	0.465904768843	-1.07174862901e-09	3.94710325991e-09
0.800685593936	-0.154577204301	0.955262788613	9.99497058355e-09
	0.195905959102	0.429613967179	0.37448007372

If we compute the order conditions up to fourth order, we verify that this method is third-order by inclusion, and close to fourth-order. We compute the Euclidean distance between order condition and obtained values. For our optimal method the distance is $0.045221[2775525, 3032049]$ and for Kutta(3,3) [13], which is known to be

Table 11: A guaranteed explicit third-order method with three stages, the closest to fourth-order

[0, 0]	[0, 0]	[0, 0]	[0, 0]
0.4659048[706, 929]	0.4659048[706, 929]	[0, 0]	[0, 0]
0.8006855[74, 83]	−0.154577[20, 17]	0.9552627[48, 86]	[0, 0]
	0.19590[599, 600]	0.42961[399, 400]	0.3744800[0, 1]

one of the best explicit (3,3) method[1], 0.058926. Our method is then closer to fourth order than Kutta(3,3). As far as we know, this method is new.

Table 12: Order conditions up to fourth order

Order	Result of optimal method	Order condition
Order 1	[0.99999998, 1.00000001]	1
Order 2	[0.499999973214, 0.500000020454]	0.5
Order 3	[0.33333330214, 0.333333359677]	0.333333333333
Order 3	[0.166666655637, 0.166666674639]	0.166666666667
Order 4	[0.235675128044, 0.235675188505]	0.25
Order 4	[0.133447581964, 0.133447608305]	0.125
Order 4	[0.0776508066238, 0.0776508191916]	0.0833333333333
Order 4	[0, 0]	0.0416666666667

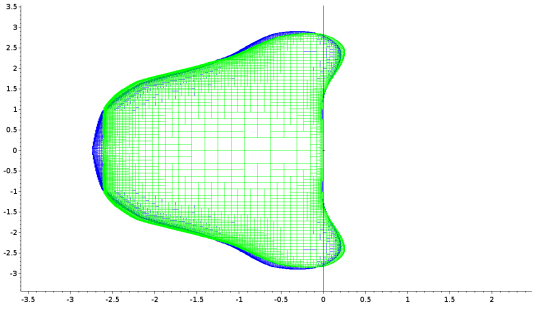


Figure 3: Paving of stability domain for RK4 method with high precision coefficients (blue) and for ERK33 (green).

7 Implementation in the DynIBEX Library

DynIBEX offers a set of validated numerical integration methods based on Runge–Kutta schemes to solve initial value problem of ordinary differential equations and for

[1] "Von den neueren Verfahren halte ich das folgende von Herrn Kutta angegebene für das beste.", C.Runge 1905 [10]

DAE in Hessenberg index 1 form. Even if our approach is applied not only to validated integration but also to classical numerical integration with interval coefficients, the validated integration allows us to obtain a validated enclosure of the final solution of the simulation. This enclosure provides, with its diameter, a guaranteed measure of the performance of the integration scheme. The computation time increases rapidly with respect to the order of the method; because of the LTE, its complexity is $\mathcal{O}(n^{p+1})$, with n the dimension of the problem and p the order. The experimental results provide the sharpest enclosure of the final solution with the lowest possible order.

We implement three new methods: S3O4 (Table 7), S3O5 (Table 8), and ERK33 (Table 11).

7.1 Experiments with S3O4

The test is based on an oil reservoir problem, a stiff problem given by the initial value problem:

$$\dot{\mathbf{y}} = \begin{bmatrix} \dot{y_0} \\ \dot{y_1} \end{bmatrix} = \begin{bmatrix} y_1 \\ y_1^2 - \frac{3}{\epsilon + y_0^2} \end{bmatrix}, \text{ with } y(0) = (10, 0)^T \text{ and } \epsilon = 1 \times 10^{-4} \ . \tag{15}$$

A simulation up to $t = 40s$ is performed. This problem being stiff, the results of the new method S3O4 are compared with the Radau family, specially the RadauIIA of third and fifth order. The results are summarized in Table 13.

Table 13: Results for S3O4

Methods	time	no. steps	norm of diameter of final solution
S3O4	39	1821	5.9×10^{-5}
Radau3	52	7509	2.0×10^{-4}
Radau5	81	954	7.6×10^{-5}

S3O4 is a singly implicit scheme, to optimize the Newton's method solving, and stiffly accurate, to be more efficient with respect to stiff problems. Based on experimental results, S3O4 seems to be as efficient as the fifth-order method RadauIIA, but faster than the third-order method RadauIIA.

7.2 Experiments with S3O5

The test is based on an interval problem, which can quickly explode, given by the initial value problem:

$$\dot{\mathbf{y}} = \begin{bmatrix} \dot{y_0} \\ \dot{y_1} \\ \dot{y_2} \end{bmatrix} = \begin{bmatrix} 1 \\ y_2 \\ \frac{y_1^3}{6} - y_1 + 2\sin(\lambda y_0) \end{bmatrix}, \text{ with } y(0) = (0, 0, 0)^T \text{ and } \lambda \in [2.78, 2.79] \ . \tag{16}$$

A simulation up to $t = 10s$ is performed. Since this problem includes an interval parameter, a comparison with Gauss-Legendre family makes sense, Gauss–Legendre methods have a good contracting property. Thus, we compare to the fourth- and sixth-order Gauss-Legendre methods. Results are summarized in Table 14.

The results show that S305 is more efficient than the sixth-order Gauss-Legendre method and five time faster. Although the fourth-order Gauss-Legendre method is two times faster, the final solution is much wider.

Table 14: Results for S3O5

Methods	time	no. steps	norm of diameter of final solution
S3O5	92	195	5.9
Gauss4	45	544	93.9
Gauss6	570	157	7.0

7.3 Experiments with ERK33

The test is based on the classical Van der Pol problem, which contains a limit circle, and is given by the initial value problem:

$$\dot{\mathbf{y}} = \begin{bmatrix} \dot{y_0} \\ \dot{y_1} \end{bmatrix} = \begin{bmatrix} y_1 \\ \mu(1 - y_0^2)y_1 - y_0 \end{bmatrix}, \text{ with } y(0) = (2, 0)^T \text{ and } \mu = 1 \ . \tag{17}$$

A simulation up to $t = 10s$ is performed. Since this problem contains a limit circle, it can be effectively simulated with an explicit scheme. The two most famous schemes are the explicit Runge–Kutta (RK4), the most used, and Kutta, known to be the optimal explicit third-order scheme. We compare ERK33 with these methods, and present the results in Table 15.

Table 15: Results for ERK33

Methods	time	no. steps	norm of diameter of final solution
ERK33	3.7	647	2.2×10^{-5}
Kutta(3,3)	3.5	663	3.4×10^{-5}
RK4	4.3	280	1.9×10^{-5}

THese results show that ERK33 is equivalent in time consumed but with performance closer to RK4.

7.4 Discussion

After experimentation with the three new Runge–Kutta methods obtained with the constraint programming approach presented in this paper, it is clear that these methods are effective. Moreover, even with coefficients of the Butcher tableau expressed in intervals with a diameter of 1×10^{-10} (for S3O4 described in Table 7 and S3O5 described in Table 8) to 1×10^{-8} (for ERK33 described in Table 11), the final solution is often narrower for the same or higher order methods with exact coefficients. A strong analysis is needed, but it seems that by guaranteeing the properties of the method, the contractivity of the integration schemes is improved.

8 Conclusion

In this paper, a new approach to discovering new Runge–Kutta methods with interval coefficients has been presented. In a first step, we show how interval coefficients can preserve properties such as stability or symplecticity, unlike coefficients expressed in floating-point numbers. We have presented two tools, a CSP solver used to find the unique solution of the Butcher rules, and an optimizer procedure to obtain the best

method with respect to a well chosen cost. This cost will provide a method of order p with a LTE as close as possible to the LTE of a method at order $p+1$. Finally, the methods obtained guarantee that the desired order and properties are obtained. These new methods are then implemented in a validated tool called DynIbex, and some tests on problems well chosen with respect to the required properties are performed. The results lead us to conclude that the approach is valid and efficient in the sense that the new methods provide highly competitive results with respect to existing Runge–Kutta methods.

In future work, we will embed our approach in a high level scheme, based on a branching algorithm to also verify properties such as stability or symplecticity, with the same verification procedures as are presented in this paper.

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