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On the Parametric Instability Caused by Step Size Variation in Runge-Kutta-Nyström Methods*

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Abstract

The parametric instability arising when ordinary differential equations (ODEs) are numerically integrated with Runge-Kutta-Nyström (RKN) methods with varying step sizes is investigated. Perturbation methods are used to quantify the critical step sizes associated with parametric instability. It is shown that there is no parametric instability for linear constant coefficient ODEs integrated with RKN methods that are based on A-stable Runge-Kutta methods, because the solution is nonincreasing in some norm for all positive step sizes, constant or varying.

1 Introduction

In a recent paper [10], Wright showed how instability can arise when linear second-order constant-coefficient ordinary differential equations (ODEs) are numerically integrated with varying step sizes, even when all steps are smaller than the critical step size that ensures stability in constant-step computations. One of his examples was the central difference method applied to the model problem

$$\ddot{x} + x = 0 \tag{1}$$

With constant step size h, the central difference method is known to be stable when $h < 2$. Wright showed how it can become unstable when the step size has small-amplitude oscillation of period 2 about the constant value $h = \sqrt{2}$. The instability manifests itself as oscillation with growing amplitude. Instability also arises if the step size has period-3 oscillation about $h = 1$, and so on to period-6 oscillation about $h \approx 0.518$. He conjectured that instability could arise for arbitrarily small step size. Shortly after Wright's paper was published, Skeel wrote a letter to the editor [8] pointing out that he had already proved Wright's conjecture in a short note published in BIT [7].

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In this work the instability phenomenon is investigated by two approaches: first, stability analysis using contractivity concepts, and second, parametric instability analysis using perturbation methods. Here a brief description of these approaches is given.

In the usual stability analysis of a numerical ODE integration method, the linear ODE system is transformed to diagonal form using a similarity transformation. Because the transformation depends on the the step size, this approach is only useful for methods used with constant step sizes. Contractivity analysis is not based on the diagonalising transformation. The idea is, given an ODE problem whose solution is nonincreasing in some norm, to derive conditions under which the numerical solution will also be nonincreasing. Hairer et al. [2] have used contractivity concepts to derive stability results for a wide class of ODE integration methods with constant step size. The same approach is used here to derive stability results for methods with varying step sizes. It is shown that A-stable methods are stable also with variable step size.

The second line of inquiry is prompted by Wright's observation that

> ... integrating a variable-stiffness system with constant time steps resembles integrating a constant-stiffness system with varying time steps.

It is well known that oscillatory variation of the stiffness parameter in variable-stiffness systems can induce a kind of instability called *parametric resonance* [5]. Wright's remark suggests that the instability he observed is a kind of parametric resonance of the "discrete time system" comprised by the numerical integration method applied to the ODE. Indeed, Wright's stability region diagrams resemble the classic Strutt diagrams used in analysis of parametric resonance.

Although the literature on parametric resonance is vast, there appears to be little on parametric resonance of difference equations. Tanaka and Sato [9] have studied a second order difference equation with periodic coefficients, a kind of discrete Mathieu equation. They compute Strutt diagrams and show how to approximate the stability region boundaries using perturbation methods. This type of analysis is applied here to RKN integrators with periodically varying step size.

2 Runge-Kutta-Nyström methods

In this section a well-known general class of numerical integration methods for second-order ODE initial value problems is presented. Five specific methods from this class are singled out for further study.

The s-stage Runge-Kutta-Nyström (RKN) method for advancing the solution of the second-order velocity-independent ODE

$$\ddot{x} = f(t, x) \tag{2}$$

from $t = t_n$ to $t_{n+1} = t_n + h_n$ is

$$k_i = f(t_n + c_i h_n, x_n + c_i h_n \dot{x}_n + h_n^2 \sum_{j=1}^{s} \bar{a}_{ij} k_j) \quad (1 \le i \le s)$$

$$
\begin{aligned}
x_{n+1} &= x_n + h_n \dot{x}_n + h_n^2 \sum_{i=1}^{s} \bar{b}_i k_i \\
\dot{x}_{n+1} &= \dot{x}_n + h_n \sum_{i=1}^{s} b_i k_i
\end{aligned}
$$

For example, the coefficients for an explicit fourth-order RKN method [3, p.262] are

$$
\begin{array}{c|c} c_i & \bar{a}_{ij} \\ \hline & \bar{b}_i \\ & b_i \end{array} = \begin{array}{c|ccc} 0 & & & \\ 1/2 & 1/8 & & \\ 1 & 0 & 1/2 & \\ \hline & 1/6 & 1/3 & 0 \\ & 1/6 & 4/6 & 1/6 \end{array} \tag{3}
$$

A RKN method is equivalent to a Runge-Kutta method if there exists a coefficient matrix a_{ij} such that

$$
\bar{a}_{ij} = \sum_{k=1}^{s} a_{ik} a_{kj}, \; \bar{b}_i = \sum_{j=1}^{s} b_j a_{ji}
$$

For example, the A-stable third-order 2-stage SDIRK method [3, p.203] corresponds to the RKN method [1]

$$
\begin{array}{c|cc} \alpha & \alpha^2 & \\ 1-\alpha & 2\alpha - 4\alpha^2 & \alpha^2 \\ \hline & (1-\alpha)/2 & \alpha/2 \\ & 1/2 & 1/2 \end{array} \tag{4}
$$

where $\alpha = (3 + \sqrt{3})/6$.

The Newmark method for (2) is a RKN method with two coefficients, β and γ, that appear in the RKN tableau as follows:

$$
\begin{array}{c|cc} 0 & 0 & 0 \\ 1 & (1-2\beta)/2 & \beta \\ \hline & (1-2\beta)/2 & \beta \\ & 1-\gamma & \gamma \end{array}
$$

The central difference method is given by the Newmark parameters

$$
\beta = 0, \; \gamma = \frac{1}{2} \tag{5}
$$

The Newmark method that was shown by Wright to exhibit parametric instability is specified by the parameter values

$$
\beta = \gamma = \frac{1}{2} \tag{6}
$$

The only choice of Newmark parameters that gives a Runge-Kutta method (the trapezoid rule) is

$$
\beta = \frac{1}{4}, \; \gamma = \frac{1}{2} \tag{7}
$$

[1] In [6] it is shown that no R-stable third-order diagonally implicit RKN method can have $-0.547 < c_1 < 1.213$, but this is only for RKN methods satisfying the simplifying condition $c_j^2 = 2\sum_k a_{jk}$.

Applying the RKN method to the linear constant coefficient model problem (1) and eliminating the stage variables gives

$$y_{n+1} = R(h_n)y_n \tag{8}$$

where the state vector y_n is defined as

$$y_n := \begin{bmatrix} x_n \\ \dot{x}_n \end{bmatrix}$$

and the one-step transition (amplification) matrix R is given by

$$R(h_n) = \begin{bmatrix} 1 - h_n^2 \bar{b}^T (I + h_n^2 \bar{A})^{-1} e & h_n - h_n^3 \bar{b}^T (I + h_n^2 \bar{A})^{-1} c \\ -h_n b^T (I + h_n^2 \bar{A})^{-1} e & 1 - h_n^2 b^T (I + h_n^2 \bar{A})^{-1} c \end{bmatrix}$$

with e being a vector of ones. In particular, the transition matrices for the RKN methods presented earlier are as follows.

- The explicit fourth-order RKN method given in Eqn (3):

$$R(h) = \begin{bmatrix} 1 & h \\ -h & 1 \end{bmatrix} + h^2 \begin{bmatrix} -1/2 + h^2/24 & -h/6 \\ h/6 - h^3/96 & -1/2 + h^2/24 \end{bmatrix}$$

- The A-stable third-order 2-stage SDIRK of Eqn (4):

$$\begin{aligned} R(h) &= \begin{bmatrix} 1 & h \\ -h & 1 \end{bmatrix} \\ &+ \frac{h^2}{(1 + h^2\alpha^2)^2} \begin{bmatrix} -(4h^2\alpha^3 - h^2\alpha^2 + 1)/2 & -(h^2\alpha^3 - \alpha + 1)\alpha h \\ (h^2\alpha^3 - \alpha + 1)\alpha h & (4h^2\alpha^3 - h^2\alpha^2 + 1)/2 \end{bmatrix} \end{aligned}$$

- The Newmark method:

$$R(h) = \begin{bmatrix} 1 & h \\ -h & 1 \end{bmatrix} + \frac{h^2}{(1 + h^2\beta)} \begin{bmatrix} -1/2 & -\beta h \\ \gamma h/2 & -\gamma \end{bmatrix}$$

  with, as special cases, the central difference method of Eqn (5):

$$R(h) = \begin{bmatrix} 1 & h \\ -h & 1 \end{bmatrix} + h^2 \begin{bmatrix} -h/2 & 0 \\ h/4 & -1/2 \end{bmatrix}$$

  the Newmark method of Eqn (6):

$$R(h) = \begin{bmatrix} 1 & h \\ -h & 1 \end{bmatrix} + \frac{h^2}{(1 + h^2/2)} \begin{bmatrix} -1/2 & -h/2 \\ h/4 & -1/2 \end{bmatrix}$$

  and the trapezoid method of Eqn (7):

$$R(h) = \begin{bmatrix} 1 & h \\ -h & 1 \end{bmatrix} + \frac{h^2}{(1 + h^2/4)} \begin{bmatrix} -1/2 & -h/4 \\ h/4 & -1/2 \end{bmatrix}$$

3 Contractivity Analysis

The main result of this section is the following theorem, which states that A-stable Runge-Kutta methods such as the trapezoid rule are contractive in a norm that is independent of step size. The same result of course holds for RKN methods derived from A-stable Runge-Kutta methods. Thus, these methods do not exhibit the parametric instability caused by varying step sizes.

Theorem 1 *For any A-stable Runge-Kutta method applied to a stable linear constant-coefficient ODE there exists a symmetric positive definite matrix W, independent of the step size, such that the numerical solution is contractive in the W-weighted euclidean norm, that is, any two numerical solutions $y_n, \bar{y}_n$ satisfy*

$$\|y_{n+1} - \bar{y}_{n+1}\|_W \leq \|y_n - \bar{y}_n\|_W$$

Before looking at the proof of the theorem, a couple of remarks. First, Wright's results for the implicit R-stable Newmark method of Eqn (6) is a counterexample showing that R-stability or implicitness are not sufficient to preclude parametric resonance with varying step size.

Secondly, in his letter to the editor, Skeel [8] mentions that the Newmark method of Eqn (6)

> ... does not satisfactorily deal with variable step size. A method that does is the implicit midpoint method, for which the amplification matrix is an orthogonal matrix. Of course, it has the same practical drawback of implicitness...

The implicit midpoint method has the same transition matrix as the trapezoid rule of Eqn (7). Because the transition matrix is orthogonal, the method is contractive in the euclidean norm. Thus, theorem 1 extends Skeel's remark to cover all RKN methods that are equivalent to A-stable Runge-Kutta methods. However, since A-stable methods are implicit, this result is of limited use to those who want to use explicit methods.

The theorem is proved using three lemmas. The first lemma states that any stable linear constant-coefficient system is contractive in some norm.

Lemma 1 *If A is Hurwitz then there exists a constant symmetric positive definite matrix W such that the solution of the ODE $\dot{y} = Ay$ is contractive in the W-weighted euclidean norm.*

Proof. It suffices to consider the homogeneous problem

$$\dot{y} = Ay$$

Since A is Hurwitz, there exists a symmetric positive definite matrix W that satisfies the Lyapunov equation

$$A^T W + WA = -I$$

Apply the linear transformation $z = W^{1/2} y$ to take the original ODE into

$$\dot{z} = W^{1/2} A W^{-1/2} z$$

The solutions to the ODE are monotonically nonincreasing in the euclidean norm, because

$$\frac{d}{dt}\|z\|^2 = -z^T W^{-1} z \le 0$$

Since $\|z\| = \|y\|_W$, the stated result follows. ■

The s-stage Runge-Kutta method for advancing the solution of the linear constant coefficient ODE

$$\dot{y} = Ay$$

from t_n to $t_{n+1} = t_n + h$ is given by

$$\begin{aligned} g_i &= y_n + h \sum_{j=1}^{s} a_{ij} A g_j \quad (1 \le i \le s) \\ y_{n+1} &= y_n + h \sum_{j=1}^{s} b_j A g_j \end{aligned}$$

Eliminating the stage variables g_i results in

$$y_{n+1} = R(hA) y_n$$

where R is the stability function of the Runge-Kutta method.

A linear transformation $z = Vy$, where V is a constant nonsingular matrix, gives a new ODE

$$\dot{z} = VAV^{-1} z$$

The next result tells us that the result of applying the Runge-Kutta method to the transformed ODE is the same as transforming the numerical results from the original ODE.

Lemma 2 *The following diagram commutes:*

$$\begin{array}{cccccc} & \boxed{y_n} & \xrightarrow{V} & \boxed{z_n} & \\ R(hA) & \downarrow & & \downarrow & R(hVAV^{-1}) \\ & \boxed{y_{n+1}} & \xrightarrow{V} & \boxed{z_{n+1}} & \end{array}$$

Proof. Substitution. ■

Finally, the following result from [4, Corollary 11.3] is needed.

Lemma 3 *If an A-stable Runge-Kutta method is applied to a linear constant-coefficient ODE that is contractive in the euclidean norm, then the numerical solution is contractive in the euclidean norm.*

Combining the three lemmas gives the theorem. Lemma 1 gives the weight W under which the ODE is contractive. $V = W^{1/2}$ is the linear transformation matrix that relates the original variables y to the new variables z that are contractive in the euclidean norm. By lemma 3, numerical sequences z_n computed with A-stable Runge-Kutta methods inherit the contractivity of the ODE, and by lemma 2, this also applies to the original ODE.

4 Stability charts

A necessary and sufficient condition for stable integration of the model problem (1) with constant step size is given by the Schur-Cohn inequalities

$$|\mathrm{trace}(R)| - 1 \leq \det(R) \leq 1 \tag{9}$$

Thus, with constant step sizes the central difference method, Eqn (5), is stable for $0 \leq h \leq 2$, the RKN method of Eqn (3) is stable for $0 \leq h \leq 2(2 + 2^{1/3} - 2^{2/3})^{1/2} \approx 2.59$, and the SDIRK method of Eqn (4), the trapezoid method (Eqn (7)), and the Newmark method of Eqn (6) are stable for all $h \geq 0$, i.e. they are R-stable.

Now consider integration of the model problem (1) with a sequence of step sizes h_n that is periodic with period p. The composition of p steps can be interpreted as a one-step method integrating from $t = t_n$ to $t = t_{n+p} = t_n + h_n + \cdots + h_{n+p-1}$. The application of one step of the composed method gives

$$y_{n+p} = R([h_n, \ldots, h_{n+p-1}])y_n$$

where the transition matrix R of the composed method is given by the matrix product

$$R([h_n, \ldots, h_{n+p-1}]) := R(h_{n+p-1})R(h_{n+p-2}) \cdots R(h_{n+1})R(h_n)$$

This composed transition matrix determines the stability of the linear homogeneous difference equation (8). The stability condition is given by the inequalities (9) applied with the composed transition matrix.

For the periodic step size variation given by

$$h_n = h + \epsilon \cos(2\pi n/p) \tag{10}$$

a stability chart can be made by numerically testing the stability criterion for a large number of specific values of (h, ϵ). Figure 1 shows values giving an unstable composed Nyström method of Equation (3) when the step size period is $p = 6$. Also shown are the corresponding stability charts for the central difference method and the Newmark method of Equation(6).

The instability regions for the central difference and Newmark methods form wedges with their points on the h-axis. Stability charts for other periods p are similar, except that the number of wedges increases with p. The figure resembles a Strutt diagram for the Mathieu equation [5].

The instability regions for the Nyström method are more rounded and, for values of h smaller than the constant-step stability limit, do not reach the h-axis. This figure resembles Strutt diagrams for damped oscillators.

The stability charts for the trapezoid and SDIRK methods are not shown, because they contain no instability points. This is because they are A-stable Runge-Kutta methods, which according to the theorem in section 3 remain stable with varying step size.

5 Perturbation Analysis of Stability Regions

The points on the stability charts where the instability regions intersect the h axis will be called *critical* step sizes. In this section, their values are identified using perturbation analysis.

Substituting the trial solution

$$y_n = y_n^{(0)} + \epsilon y_n^{(1)} + \epsilon^2 y_n^{(2)} + \cdots \tag{11}$$

and the step size (10) into (8) and equating powers of ϵ gives a sequence of coupled difference equations, the first three of which are

$$y_{n+1}^{(0)} = R(h)y_n^{(0)} \tag{12}$$

$$y_{n+1}^{(1)} = R(h)y_n^{(1)} + \cos(2\pi n/p)R'(h)y_n^{(0)} \tag{13}$$

$$y_{n+1}^{(2)} = R(h)y_n^{(2)} + \cos(2\pi n/p)\left(R'(h)y_n^{(1)} + \frac{1}{2}R''(h)y^{(0)}\right)$$

The first equation, Equation (12), is a homogeneous linear constant coefficient difference equation, and is stable provided that the constant component h of the step size is within the stability range for the constant-step method.

The remaining equations are linear constant coefficient difference equations with a harmonic forcing term. If the eigenvalues of R are smaller than one in magnitude (i.e. the method has algorithmic damping), then these equations will all have bounded solutions. For such methods, the "wedges" in the stability chart do not reach the h axis, and the method is stable when the amplitude ϵ of step size oscillation is sufficiently small. This is confirmed by the stability chart (Figure 1) for the Nyström method of Eqn (3), which has algorithmic damping.

Resonance instability may arise in integration methods without algorithmic damping if the forcing frequency matches the natural frequency. It therefore suffices to restrict attention to methods whose transition matrix $R(h)$ has eigenvalues of unit modulus. These eigenvalues can be written as

$$\text{eig}(R(h)) = \exp(\pm i\omega(h)) \tag{14}$$

where ω is a real function of h. For example, the central difference method has

$$\omega(h) = \arctan(h\sqrt{1-h^2/4}, 1-h^2/2) \;\; (0 \le h \le 2)$$

while the Newmark method of Eqn (6) has

$$\omega(h) = \arctan(h\sqrt{1+h^2}) \;\; (0 \le h)$$

For methods satisfying (14), the solution of (12) is a linear combination of trigonometric functions of the form

$$y_n^{(0)} = Y_1 \cos(n\omega) + Y_2 \sin(n\omega) \tag{15}$$

Substituting (15) into (13) gives a forcing function for $y_n^{(1)}$ of the form

$$R'(h)Y_1 \cos(n\omega)\cos(2\pi n/p) + R'(h)Y_2 \sin(n\omega)\cos(2\pi n/p)$$

Resonance occurs when

$$\omega(h) = \frac{\pi}{p} \tag{16}$$

or

$$\omega(h) = \pi - \frac{\pi}{p}$$

p	h^0	h^1
2	$\sqrt{2} \approx 1.4142$	$\pm 1/2$
3	1	$\pm 1/8$
4	$\sqrt{2-\sqrt{2}} \approx 0.7654$	$\pm(2-\sqrt{2})/8 \approx \pm 0.0732$
5	$(\sqrt{5}-1)/2 \approx 0.6180$	$\pm(3-\sqrt{5})/16 \approx \pm 0.0477$
6	$(\sqrt{6}-\sqrt{2})/2 \approx 0.5176$	$\pm(4-\sqrt{12})/16 \approx \pm 0.0335$

Table 1: Smallest critical step size h^0 and wedge width h^1 for period-p oscillation, central difference method

p	h^0	h^1
2	∞	–
3	$\sqrt{2} \approx 1.4142$	$\pm 1/4$
4	$\sqrt{-2+2\sqrt{2}} \approx 0.9102$	$\pm(-1+\sqrt{2})/4 \approx 0.1036$
5	$\sqrt{-4+2\sqrt{5}} \approx 0.6871$	$\pm(-2+\sqrt{5})/4 \approx 0.0590$
6	$\frac{1}{3}\sqrt{-18+12\sqrt{3}} \approx 0.5562$	$\pm(-3+2\sqrt{3})/12 \approx 0.0387$

Table 2: Smallest critical step size h^0 and wedge width h^1 for period-p oscillation, Newmark method

Values of h satisfying these equations are critical step sizes.

The smallest critical step size for period-p step size oscillation is denoted h^0, and is given by the solution of Equation (16). The minimum critical step sizes for various p are listed in Tables 1 and 2. These values agree with those found by Wright [10] by other means.

Any RKN method of order at least 1 has

$$R(h) = \begin{bmatrix} 1 & h \\ -h & 1 \end{bmatrix} + O(h^2)$$

and so

$$\mathrm{eig}(R(h)) = \pm ih + O(h^2)$$

The smallest critical step size for large p is then given by

$$\min h_{\mathrm{crit}} \approx \frac{\pi}{p}$$

Thus, the critical step size can be arbitrarily small. This agrees with Skeel's result [7] for the central difference method.

The method of strained parameters is now used to analyse the shape of the instability region "wedge" near the h-axis. The average step size parameter is assumed to have the form

$$h = h^0 + h^1\epsilon + O(\epsilon^2)$$

where h^0 is a critical step size. The step size then varies according to

$$h_n = h^0 + h^1\epsilon + \epsilon\cos(2\pi n/p) + O(\epsilon^2)$$

Substituting this into the composed transition matrix gives

$$R([h_n, \ldots, h_{n+p-1}]) = R_0 + \epsilon R_1 + O(\epsilon^2)$$

where

$$R_0 := R(h^0)^3$$

and

$$R_1 := (\cos(2\pi 0/p)+h^1)R(h^0)^{p-1}R'(h^0)+\ldots+(\cos(2\pi(p-1)/p)+h^1)R'(h^0)R(h^0)^{p-1}$$

The boundaries of the instability regions are found by solving the stability conditions for the composed transition matrix.

For example, for the central difference method with step size period $p = 3$ we have $h^0 = 1$ and

$$R([h_2, h_1, h_0]) = -I + \frac{\epsilon}{16}\begin{bmatrix} 6 & -64h^1 - 4 \\ 48h^1 - 3 & -6 \end{bmatrix} + O(\epsilon^2)$$

Neglecting terms in ϵ^2, the stability condition (9) is

$$1 \le 1 - \frac{3}{16}\epsilon^2 + 12\,\epsilon^2 (h^1)^2 \le 1$$

which is satisfied when

$$h^1 = \pm\frac{1}{8}$$

The instability region boundary is therefore approximated by

$$h = 1 \pm \frac{1}{8}\epsilon + O(\epsilon^2) \tag{17}$$

Figure 2 shows instability points in the neighbourhood of the critical step size for the central difference method for parametric oscillation of period $p = 3$, and the instability region boundaries predicted by (17). The approximation appears to be correct. Tables 1 and 2 give instability region "wedge" widths for the central difference method and the Newmark method.

6 Conclusions

The following results were presented:

- A-stable Runge-Kutta methods are stable when applied with varying time step to stable linear time invariant ODE systems.
- For numerical ODE integration methods that have numerical damping, there will be no parametric resonance if the step size oscillation amplitude is sufficiently small.
- The critical average step size about which small oscillation may cause parametric resonance in the numerical integration of a simple oscillator can be found using perturbation methods.
- The perturbation analysis indicates that there can be arbitrarily small critical step sizes.
- The method of strained parameters can be used to approximate the shape of the instability region in Strutt diagrams for small amplitude step size oscillation.

Further investigation is needed for the following questions:

- Is A-stability necessary to rule out parametric resonance?
- What about integration of nonlinear ODEs?
- How can a "safe" step size oscillation amplitude be estimated for ODE integration methods that have numerical damping?

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