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Explicit Implementation of Collocation Methods for Stiff Systems with Complex Spectrum [1]

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Abstract: Currently there are two general ways to solve stiff differential equations numerically. The first approach is based on implicit methods and the second uses explicit stabilized Runge–Kutta methods, also known as Chebyshev methods. Implicit methods are great for very stiff problems of not very large dimension, while stabilized explicit methods are efficient for very big systems of not very large stiffness and real spectrum. In this paper we describe methods which are explicit and are capable of solving stiff systems with complex eigenvalues of Jacobi matrix.

Keywords: Stiff problems, explicit methods, collocation methods, iterated Runge-Kutta methods, linear analysis of convergence.

Mathematics Subject Classification: 65L05, 65L06, 65L20

Introduction

Consider an ordinary differential equation (ODE) system

$$y'(x) = f(x, y(x)), \quad y(x_0) = y_0, \quad x \in [x_0, x_0 + h], \quad y : \mathbb{R} \to \mathbb{R}^n, \tag{1}$$

and an s-stage implicit Runge–Kutta (IRK) method given by Butcher matrix $A = \left(a_{ij}\right)_{i,j=1}^{s}$ and vectors $b = (b_1, \ldots, b_s)$, $c = (c_1, \ldots, c_s)$. This method we'll be referred to as the *base method*. By applying it to problem (1) one obtains an approximate solution

$$y_1 = y_0 + h \sum_{i=1}^{s} b_i k_i \approx y(x_0 + h),$$

where the unknown terms k_i, known as "stage derivatives", satisfy a system of algebraic equations which we write in the form

$$k = \mathbf{f}(k), \tag{2}$$

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$k = (k_1, \ldots, k_s)^T \in \mathbb{R}^{ns}$, $\mathbf{f}(k) = (f_1(k), \ldots, f_s(k))^T$, $f_i(k) = f(x_0 + c_i h, y_0 + h\sum_{j=1}^{s} a_{ij}\, k_j)$. An instructive description of standard approach to this system resolving, based on simplified Newton iteration, is given in [6, IV.8]. References to more recent works on further development of this approach can be found in [4]. All these methods exploit different types of Jacobi matrix $\frac{\partial f}{\partial y}(y_0)$ factorization, which is expensive in case of very large n. The way of solving (2) we are going to suggest is a fixed-point-like iteration, resulting in an explicit algorithm which requires only evaluations of f. Initially our approach development was not connected with Runge–Kutta methods, the interested reader can find details in [3].

This paper is organized as follows. The first section is devoted to the theoretical issues: we begin with the derivation of the general form of our method, then perform the analysis of its linear convergence properties. Next follows the comparison of the method we call Euler-Picard iteration with the conventional Picard iteration. Finally the properties of general multistage processes are discussed. The second section contains some reasoning about practical implementation and displays the results of some simple numerical experiments to demonstrate the potentiality of our approach.

1 Generalized Picard iteration

Instead of solving (2) directly we introduce a fictitious variable t and, according to the principle of steadying [2], construct a differential equation such that its steady-state solution coincides with the solution of (2). This differential equation is

$$k'(t) = -k(t) + \mathbf{f}(k(t)) \tag{3}$$

and we shall call it the *embedding equation*. The next step is to select an initial approximation $k^{(0)}$ and trace for the sought steady state of (3) by means of some explicit σ-stage RK method (*auxiliary method*) with fictitious time step τ. This results in an iterative process of the following general form:

$$k^{(l+1)} = \Phi\big(k^{(l)}\big), \quad l = 0, 1, \ldots, N-1, \tag{4a}$$

$$\Phi(k) = k + \tau \sum_{p=1}^{\sigma} \beta_p \big(\mathbf{f}(\mathbf{g}_p(k)) - \mathbf{g}_p(k)\big), \quad \mathbf{g}_p(k) = k + \tau \sum_{q=1}^{p-1} \alpha_{pq} \big(\mathbf{f}(\mathbf{g}_q(k)) - \mathbf{g}_q(k)\big). \tag{4b}$$

Here α_{pq} and β_p are the coefficients of the auxiliary method. If explicit Euler method is used in (4) we obtain

$$k^{(l+1)} = (1-\tau)k^{(l)} + \tau\, \mathbf{f}\big(k^{(l)}\big), \tag{5}$$

which for $\tau = 1$ gives the conventional Picard iteration

$$k^{(l+1)} = \mathbf{f}\big(k^{(l)}\big), \tag{6}$$

or iterated Runge-Kutta method [5]. That's why we call (5) the *Euler-Picard iteration* (EPI) and (4) the *generalized Picard iteration* (GPI). Let us give a short summary of inherent GPI features:
– the resulting method is *explicit* (no matrix factorizations involved);
– the cost is (σs) evaluations of f per iteration;
– the cost can be reduced to $N_f = \sigma$ per iteration if s parallel processors are available.
The justification of the proposed scheme we are going to perform is based on the linear convergence analysis (see [4] and related references).

1.1 Linear convergence analysis

Consider linear test problem

$$y'(x) = \lambda y(x), \quad y(0) = 1, \quad \lambda \in \mathbb{C}. \tag{7}$$

The embedding equation (3) for this problem is

$$k'(t) = (zA - I)k(t) + \lambda e, \tag{8}$$

where $z = \lambda h$, A, as before, is Butcher matrix of the base method, $e = (1, \ldots, 1)^T$. Denote by $\{\mu_j\}_{j=1}^s$ the eigenvalues of A. Consider matrix

$$\Lambda(z) = zA - I \tag{9}$$

and its spectrum $\{\nu_j(z) = z\mu_j - 1\}$. These eigenvalues play important role in linear convergence analysis of GPI (4), and before we proceed it is important to understand that everything we are going to discover for the scalar linear model (7) holds for arbitrary linear ODE system

$$y'(x) = Jy(x), \quad y(0) = y_0, \quad y : \mathbb{R} \to \mathbb{R}^n, \tag{7'}$$

as well. This is due to the fact that for (7') the embedding equation is

$$k'(t) = (hA \otimes J - I)k + e \otimes Jy_0,$$

with eigenvalues of $\Lambda = hA \otimes J - I$ being exactly equal to $\nu_{ij} = h\lambda_i\mu_j - 1$, according to the property of Kronecker product (here $\{\lambda_i\}_{i=1}^n$ is the spectrum of J).

Asymptotic stability analysis. Suppose that the matrix $\Lambda(z)$ (9) is nonsingular, then the sought steady-state solution of (8) is $k^* \equiv -\Lambda(z)^{-1}\lambda e$. For our purposes it is helpful to know whether this solution is asymptotically stable. Thus consider a region $D \subset \mathbb{C}$ such that for all $z \in D$ asymptotic stability criterion holds. More precisely, we introduce

Definition 1. We shall call the the region $D \subset \mathbb{C}$ defined by

$$D = \bigcap_{j=1}^{s} D_j, \quad D_j = \{z \in \mathbb{C} \,:\, \mathrm{Re}(z\mu_j - 1) < 0\}, \tag{10}$$

the *asymptotic stability region* (of linear embedding equation) for given implicit RK method with Butcher matrix A.

Proposition 1. Let A be an $s \times s$ real matrix such that all its eigenvalues $\{\mu_j\}$ have positive real parts. Then

$$D \supset \widetilde{D} = \left\{z \in \mathbb{C} \,:\, |\arg(x_0 - z)| < \alpha\right\}, \tag{11}$$

where $x_0 = (\max_j \mathrm{Re}\,\mu_j)^{-1}$, $\alpha = \pi/2 - |\max_j \arg\mu_j|$, D is asymptotic stability region (10) of RK method corresponding to A.

The proof of this proposition is based on straightforward investigation of the geometric shape of the region (see figure 1).

Hereafter we restrict ourselves to the well-known class of collocation RK methods, namely Gauss (of order $2s$), Radau IIA (of order $2s-1$) and Lobatto IIIA (of order $2s-2$) methods. All these methods are A-stable so their matrices do satisfy the conditions of proposition 1. Corresponding values of α and x_0 are given in table 1. It is interesting that these parameters for Gauss and Lobatto IIIA methods of same order are identical. Note also that for fixed s Lobatto methods have widest D, which is due to the presence of zero eigenvalue.

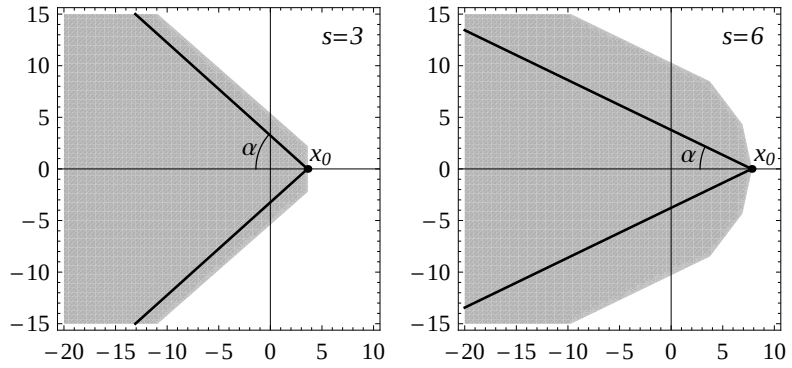

Figure 1: Asymptotic stability regions (gray) and boundaries of their approximations $\widetilde{D}$ for Radau IIA methods.

s	2		3		4		5		6		7	
	α	x_0	α	x_0	α	x_0	α	x_0	α	x_0	α	x_0
Gauss	60°	4	46.3°	4.6	38.4°	6.3	33.1°	7.3	29.2°	8.9	26.4°	9.9
Radau	54.7°	3	41.3°	3.6	33.9°	5.3	29.2°	6.3	25.8°	7.8	23.3°	8.9
Lobatto	90°	2	60°	4	46.3°	4.6	38.4°	6.3	33.1°	7.3	29.2°	8.9

Table 1: Parameters of asymptotic stability regions for collocation RK methods.

Linear convergence criterion. Application of some GPI (4) to the problem (7) gives an iterative process of the form

$$k^{(l+1)} = R\big(\tau\Lambda(z)\big)k^{(l)} + P\big(\tau\Lambda(z)\big)\lambda e, \tag{12}$$

where R is the stability polynomial of the auxiliary method, P is another polynomial depending on this method as well. The following trivial yet important statement in fact is a citation of the well-known result from numerical linear algebra.

Proposition 2. Linear GPI (12) converges iff the spectral radius of $R\big(\tau\Lambda(z)\big)$ is less than 1, or equivalently iff *all eigenvalues of* $\tau\Lambda(z)$ *lie in the stability region of auxiliary RK method*, i.e.

$$\big|R(\tau(z\mu_j - 1))\big| < 1 \quad \forall j = 1, \dots, s.$$

Remark. The global convergence rate (see, e.g., [8, pp. 105-106]) is

$$r(z, \tau) = \max_j |R(\tau(z\mu_j - 1))|. \tag{13}$$

This proposition is the key to the following questions:

(Q1) What auxiliary method should be chosen in (12) in order to achieve fastest convergence?

(Q2) What value of τ should be taken for this purpose?

(Q3) When it is possible to achieve convergence of a GPI with given auxiliary method by means of changing τ?

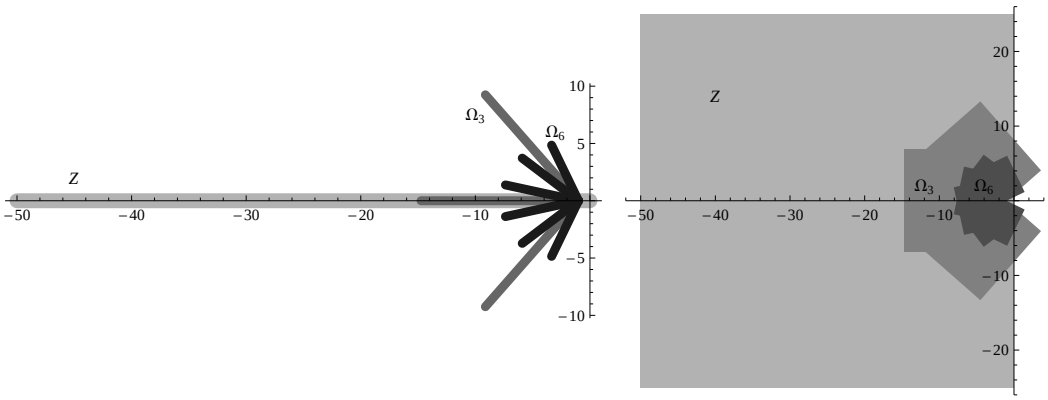

Figure 2: Examples of subsets Ω (14) for Radau IIA methods with s=3 and s=6.

Before answering these questions let's make the reasoning more concrete. Consider a class of linear problems (7) such that $z \in Z \subset \mathbb{C}$ (this generalizes the case of linear ODE system (7′) with $h\lambda_i \in Z$, $i = 1, \ldots, n$). By Ω denote the subset of complex plane where the eigenvalues of corresponding matrices $\Lambda(z)$ (9) are located:

$$\Omega = \bigcup_{j=1}^{s} (\mu_j Z - 1). \tag{14}$$

The examples of subsets Ω corresponding to $Z = (-50, 0)$ and $Z = (-50, 0) + \mathrm{i}(-25, 25)$ for Radau IIA methods are given in figure 2. Finally, let S be the stability region of auxiliary RK method: $S = \{q \in \mathbb{C} : |R(q)| < 1\}$. The answers to the above questions are the following.

(A1) An optimal auxiliary method for given class of problems should have a stability polynomial R such that $|R(q)|$ is minimal possible over $q \in \tau\Omega$.

(A2) The value of τ should be small enough to satisfy $\tau\Omega \subset S$ but large enough to have $|R(q)| \to \min$ for all $q \in \tau\Omega$, since $\min_{q\in\tau\Omega} |R(q)| \to 1$ as $\tau \to 0$.

(A3) For a given auxiliary method it is possible to achieve convergence of corresponding GPI by means of changing τ *only when* S and Ω have compatible shapes, i. e. if $\exists\, \tau > 0$ such that $\tau\Omega \subset S$.

1.2 Euler-Picard iteration versus conventional one

The above results allow us to easily compare EPI method (5) with traditional Picard iteration (6). Recall that both methods are representatives of GPI family (4) and use explicit Euler method as auxiliary one. The difference is that Picard iteration uses fixed fictitious time step size $\tau = 1$. Due to the item (A2) of the above list, this results in severe limitations on the size of region Ω (14):

$$\Omega \subset S_{Euler} = \{q \in \mathbb{C} : |1 + q| < 1\}, \tag{15}$$

and consequently on the step size h. That's why conventional Picard iteration is not appropriate for stiff problems.

On the other hand, Euler-Picard iteration (5) has freedom of choice for the parameter τ, thus admitting much larger values of h. More precisely this is expressed in the following statement and the corollary.

PROPOSITION 3. Consider Euler-Picard iterative process (5) for the linear ODE system (7′):

$$k^{(l+1)} = (1-\tau)k^{(l)} + \tau(hA \otimes J)k^{(l)} + \tau e \otimes Jy_0. \tag{16}$$

Let D be the asymptotic stability region (10) corresponding to the Butcher matrix A. Suppose that spectrum Z of matrix hJ satisfy $Z \subset D$, $i = 1, \ldots, n$. Then there exists $\tau_0 > 0$ such that (16) converges for all positive $\tau < \tau_0$.

Proof. From $Z \subset D$ it follows that $\Omega \subset \mathbb{C}_-$ (see the definitions of D (10) and Ω (14)). Since Ω is bounded it is always possible to select $\tau_0 > 0$ such that subset $\tau\Omega$ fits in circle (15). This implies convergence of (16) due to proposition 2. □

COROLLARY. Let all eigenvalues of matrix J satisfy $|\arg(-\lambda_i)| < \alpha$, where α is the parameter of asymptotic stability region as defined in proposition 1 (see also table 1). Then for any $h > 0$ there exists $\tau_0 > 0$ such that (16) converges for all positive $\tau < \tau_0$.

1.3 Multistage auxiliary methods

As we can see from above, EPI (5) in fact has quite decent properties of convergence on stiff problems. The natural question now is

(Q4) Is there any advantage of using multistage auxiliary methods in GPI (4), when compared to simple σ iterations of EPI (5)?

To answer this question in terms of linear convergence analysis we're going to find weak points of EPI and then try to patch them up by using multistage methods. By $d(\tau\Omega, \partial S)$ denote the distance between $\tau\Omega$ and the boundary of S:

$$d(\tau\Omega, \partial S) = \inf_{\omega \in \Omega, q \in \partial S} |\tau\omega - q|. \tag{17}$$

According to (13), the convergence speed of any GPI can be arbitrary small as $d(\tau\Omega, \partial S) \to 0$. In case of EPI we have $S = S_{Euler}$ (15), so the troubles begin when, in particular,

i) $\exists\, \omega \in \Omega$ such that $\arg\omega \approx \pi/2$, $|\omega| \gg 1$, and

ii) $\exists\, \omega_1, \omega_2 \in \Omega$ such that $|\omega_1|/|\omega_2| \gg 1$.

In both cases we have to take very small values of τ to fit $\tau\Omega$ into S_{Euler} and also inevitably have $d(\tau\Omega, \partial S_{Euler}) \ll 1$. And of course no convergence of EPI can be expected if

iii) $\Omega \not\subset \mathbb{C}_-$.

Now we shall show that in all these three cases it is possible to take advantage of using some special auxiliary methods in (4).

Contour-optimized stability polynomials The basic idea is to construct special stability polynomials in order to minimize the value of $|R(q)|$ over some region of the complex plane. Since we have freedom of selecting the value of τ we are concerned not about the *area* of stability domain, but rather about its *shape*. Another important aspect is that we are not restricted by the order conditions, like in the case of traditional Chebyshev RK methods, and require the auxiliary method to be only of order zero. Thus we are constructing polynomials of the form

$$R_\sigma(q) = 1 + \sum_{j=1}^{\sigma} a_j q^j, \tag{18}$$

such that

$$F(a_1, \ldots, a_\sigma) = \oint_C |R_\sigma(q)|^2 dq \to \min, \tag{19}$$

where C is a closed contour bounding the region of interest. There are several ways of resolving quadratic programming problem (19). In this work we used the straightforward one: after representing R_σ in the trigonometric form we have that the unknown vector $a = (a_1, \ldots, a_\sigma)^T$ is the solution to the linear system

$$Qa = p, \tag{20}$$

where $Q = \left(\oint_C \rho^{i+j} \cos((i-j)\varphi)\, dq\right)_{i,j=1}^{\sigma}$, $p = \left(\oint_C \rho^i \cos i\varphi\, dq\right)_{i=1}^{\sigma}$. The drawback is that condition number of the matrix Q increases quickly with growth of σ. Another, perhaps more stable approach, can be based on the construction of orthogonal polynomial system with respect to the scalar product $(u, v) = \oint_C u(q)\overline{v(q)}dq$.

After resolving (19) we construct corresponding auxiliary explicit RK method by means of simple composition of one- and two-stage methods as described in [7]. It is clear that the choice of C crucially influences the properties of iterative process (4) and ideally should depend on problem (1). The general strategy we suggest is to take the boundary of a unit circle segment:

$$C = C(\theta) = \{\rho\, \mathrm{e}^{\mathrm{i}(\pi-\theta)}\}_{\rho\in[0,1]} \cup \{\mathrm{e}^{\mathrm{i}(\pi+\varphi)}\}_{\varphi\in[-\theta,\theta]} \cup \{\rho\, \mathrm{e}^{\mathrm{i}(\pi+\theta)}\}_{\rho\in[0,1]}. \tag{21}$$

Figure 3 displays the portraits of obtained stability regions and plots of $|R_\sigma(z)|$ along $z \in C(\theta)$, for the cases of $\sigma = 5$ and $\sigma = 20$, $\theta = \frac{\pi}{3}$, $\frac{\pi}{2}$, $\frac{2\pi}{3}$ and $\frac{5\pi}{6}$. Comparing these regions with figure 2 we see that the optimized stability polynomials for smaller angles θ are appropriate for the case of real spectrum of Jacobi matrix. The increasing of θ results in slower general convergence rate but admits convergence for wider range of complex eigenvalues. Note also that for $\theta > \frac{\pi}{2}$ we don't get $|R_\sigma(q)| < 1\ \forall q \in C(\theta)$, so the approach we use may not be optimal. Nevertheless the constructed stability polynomials possess more attractive properties than $R_\sigma(q) = (1+q)^\sigma$ (which is the stability polynomial of σ Euler-Picard iterations (5)).

Let's recall the items i) – iii) from above, where we described the difficult cases for the EPI. Comparing the stability regions from figure 3 with (15) we see that generalized Picard iterations with the constructed auxiliary methods for $\theta = \frac{\pi}{2}$ will perform much better in the case i), since their stability regions cover the segment $[-\mathrm{i}, \mathrm{i}]$ of imaginary axis. Another important fact is that the optimized stability polynomials for $\theta \geqslant \frac{\pi}{2}$ admit convergence in the case iii) (see figures 2 (right) and 3)[3].

As for the item ii), which is the case of very small and very large eigenvalues of Jacobi matrix, this problem is an intrinsic one for all GPI family. It is due to the fact that the general requirement of minimizing the module of stability polynomial falls into contradiction with the natural restriction $R_\sigma(0) = 1$. The only thing we can do in this situation is to construct stability polynomials with fastest possible decay near the zero, i. e. with maximum slope $R'_\sigma(0)$. For σ iterations of EPI we have $\frac{d}{dq}(1+q)^\sigma\Big|_{q=0} = \sigma$. On the other hand, the $C(\pi/3)$-optimized stability polynomial R_{20} has $R'_{20}(0) = 23.0246$. Moreover, it is possible to achieve greater values of the slope using some fixed value for a_1 in (18). So, the answer to the question 4 from above is

(A4) Appropriately constructed multistage auxiliary methods generally have better linear convergence properties than one-stage Euler-Picard iteration.

In terms of contour-optimized stability polynomials which we considered, "appropriately constructed" means that the choice of θ should depend on the distribution of Jacobi matrix eigenvalues. Ideally the solver code should analyze the problem and select θ and τ adaptively on each step.

[3]On the one hand, this looks unnatural because in this case the corresponding embedding equation (8) does not have asymptotic stability property. On the other, we are interested in the convergence of (12) rather than in the approximation of embedding equation solution.

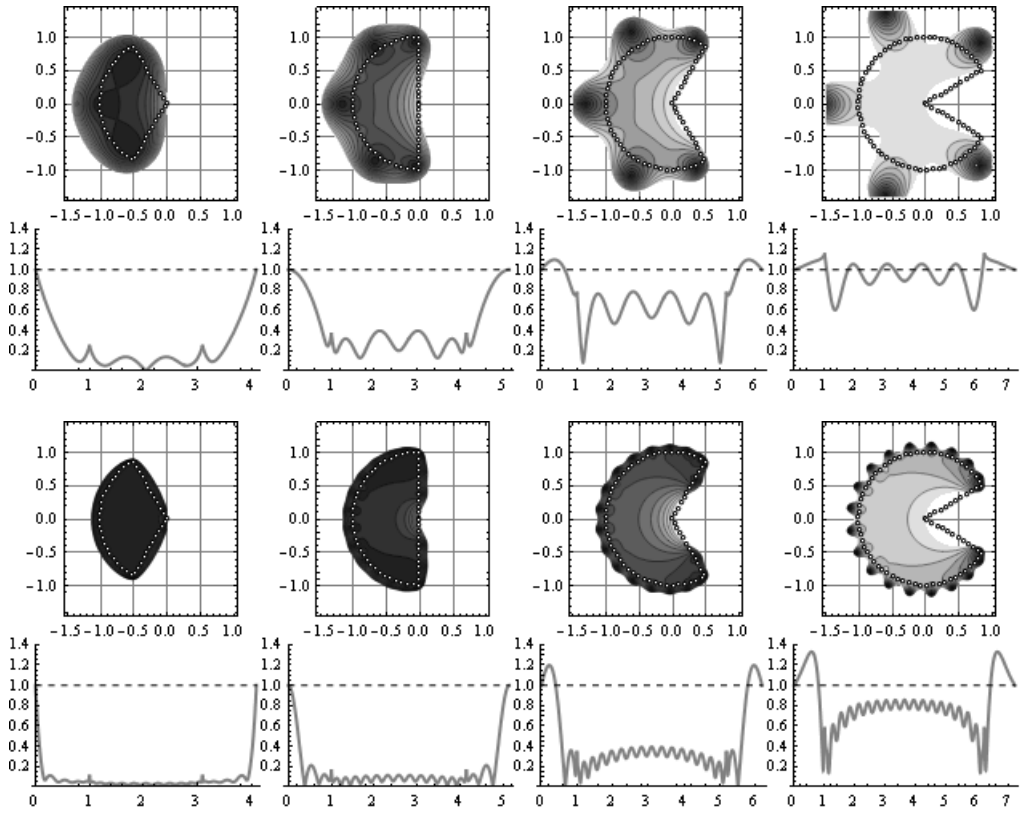

Figure 3: Stability regions of $C(\theta)$-optimized auxiliary methods, $\theta = \frac{\pi}{3}$, $\frac{\pi}{2}$, $\frac{2\pi}{3}$ and $\frac{5\pi}{6}$, s=5 (upper) and s=20.

Currently such an algorithm is one of the subjects for further research. On the other hand, as it is seen from figure 3, $\theta = \frac{\pi}{2}$ is a good universal choice for rather wide class of stiff problems, namely the problems with eigenvalues lying in the corresponding asymptotic stability region of the base RK method (recall definition 1 and figure 1).

2 Numerical examples

Extrapolated initial approximation A very important moment for the implementation of GPI (4) is the sane choice of initial approximations $k^{(0)}$. Since the base methods we choose are collocation ones it is reasonable to exploit the approach which is used in classic codes like RADAU5 [6]. The idea is simple. Collocation methods for problem (1) provide a continuous polynomial approximation $u \approx y$ defined as

$$u(x) = y_0 + h \sum_{i=1}^{s} k_i \int_0^{\frac{x-x_0}{h}} \varphi_i(\xi)\, d\xi, \tag{22}$$

where φ_i are Lagrange basis functions, $\varphi_i(c_j) = \delta_{ij}$. On the intervals where the solution changes slowly the collocation polynomial (22) can give a good approximation not only for $x \in [x_0, x_0 + h]$ but for $x > x_0 + h$ as well. Thus if $u^{(N)}$ is a final approximation to u (22) on the current step of

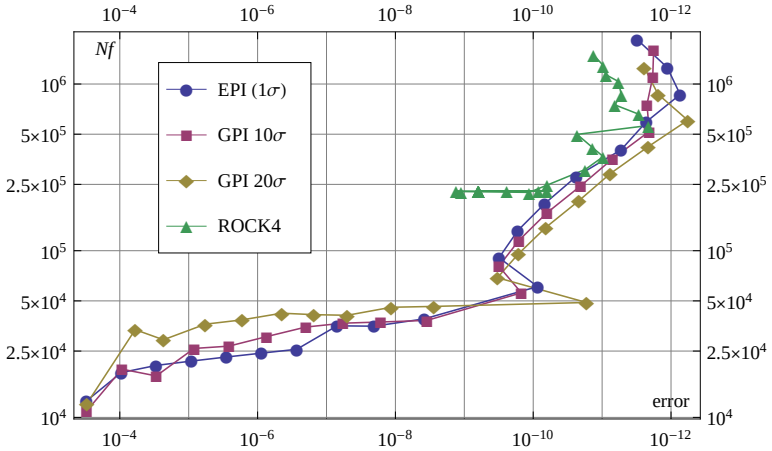

Figure 4: Work-precision diagram for Robertson problem.

length h, then on the next step of length $\hat{h}$ we need an initial collocation polynomial $\hat{u}^{(0)}$, defined by coefficients $\hat{k}_i^{(0)}$, such that $\hat{u}^{(0)}(x) = u^{(N)}(x)\,\forall x$. This results in

$$\hat{k}_i^{(0)} = \sum_{j=1}^{s} k_j^{(N)} \varphi_j(1 + \delta c_i), \quad i = 1, \ldots, s, \tag{23}$$

where $k_j^{(N)}$ are the coefficients corresponding to $u^{(N)}$, $\delta = \hat{h}/h$.

This technique significantly improves the convergence of generalized Picard iterations and is effectively used in the following numerical experiments.

2.1 Robertson problem

Our experimental code is written in *Mathematica* language and does not implement automatic step size and error control yet. The demonstration of the GPI methods potentiality begin with the well-known Robertson problem (see, e. g., [6, p. 11]). To skip the boundary layer we take initial condition $y_0 = \tilde{y}(50000) = (0.03245985, 1.341396 \times 10^{-7}, 0.96754001)^T$, where $\tilde{y}$ is the solution of Robertson problem computed by RADAU5 code with $\tilde{y}(0) = (1, 0, 0)^T$, $atol = rtol = 10^{-15}$. The interval of integration is $[0, 1000]$. The mesh is fixed and imitates "stepsize acceleration": $h_1 = 0.1$, $h_i = \min(1.25\, h_{i-1}, 1.75)$, $i = 2, \ldots, 580$, $h_{581} = 0.874042$ (to get the endpoint equal exactly to 1000).

The stopping criterion in (4) is based on the defect control:

$$||\mathbf{f}(k^{(l)}) - k^{(l)}|| \leqslant \frac{C_0}{h} \times tol, \tag{24}$$

where $C_0 = 0.3$, tol is an accuracy controlling parameter. The presence of h^{-1} is due to the idea that large step sizes require more accurate approximations. The fictitious time step τ should also depend on h and, surely, on the spectral radius of the Jacobi matrix J at y_0, which is equal to $\rho = 9683.49$ in our case. The general formula for τ is

$$\tau = \frac{0.9}{h\,\rho\,\mu_0 + 1}, \tag{25}$$

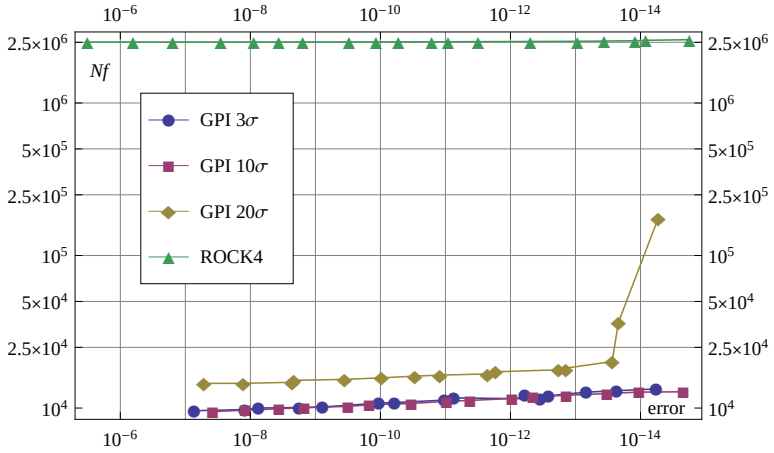

Figure 5: Work-precision diagram for linear problem (26).

where 0.9 is an "insurance factor", $\mu_0 = \max_j |\mathrm{Re}\,\mu_j|$, $\{\mu_j\}$ is, as before, spectrum of Butcher matrix. Since all eigenvalues of J are real we use $C(\pi/3)$-optimized auxiliary methods with $\sigma = 1$, 10 and 20. For $\sigma = 1$ we clearly have slightly tuned Euler-Picard iteration (5). The base method is celebrated Radau IIA method of order 5, $s = 3$.

For comparison we used ROCK4 solver implementing 4th order Chebyshev methods [1] with supplied value of spectral radius equal to 9700. For GPI methods tolerances $tol_i = 10^{-5-\frac{1}{2}i}$, $i = 1, \ldots, 20$, were used, and the fixed grid described above. For ROCK4 we took $atol_i = rtol_i = 10^{-\frac{1}{2}i}$, $i = 1, \ldots, 29$. As an exact solution we used the one obtained by RADAU5 solver with $rtol = atol = 10^{-15}$. Euclidean norms of absolute errors at the endpoint and total numbers of f evaluations N_f are gathered in the diagram (figure 4).

It is necessary to emphasize that these results for GPI methods were obtained in a straightforward way and we expect significant improvement in the presence of step size end error control mechanisms. Nevertheless we see that for medium tolerances our methods perform significantly better than Chebyshev method, while for small tolerances the difference is not so big. It is also interesting that for big tolerances methods with smaller σ are more effective while small tolerances give advantage to the process with greater number of stages. On the other hand all the considered GPIs performed approximately in the same manner, so it is hard to give general recommendations for choosing σ as yet.

2.2 Linear system with complex spectrum

Chebyshev methods are constructed to have extended stability domain along the negative real axis, so it is natural to expect problems with ROCK4 in the case of complex eigenvalues presence. Thus we continue numerical experiment with the simple linear problem

$$y'(x) = \begin{pmatrix} -1000 & 1000 \\ -1000 & -1000 \end{pmatrix} y(x) + \begin{pmatrix} 100 \\ -200 \end{pmatrix}, \quad y(0) = \begin{pmatrix} -100 \\ 200 \end{pmatrix}. \tag{26}$$

The spectrum of the system matrix is $\lambda_{1,2} = -1000 \pm 1000\,\mathrm{i}$. The interval of integration is $[0, 1000]$, so it includes the boundary layer. The mesh for GPI methods is fixed, as before: $h_1 = 0.001$, $h_i = \min(1.5\,h_{i-1}, 10)$, $i = 2, \ldots, 120$, $h_{121} = 7.55652$. The eigenvalues $\lambda_{1,2}$ lie near the border of

asymptotic stability region (10) of the base Radau IIA method (recall figure 1 (left) and table 1), so it is useless to apply Euler-Picard iteration in this case. The natural choice are $C(\pi/2)$-optimized auxiliary methods (see figure 3), we take $\sigma = 3$, 10 and 20. The stopping criterion is (24) with $C_0 = 1$, the value of τ is also determined as before (25). For GPI we take $tol_i = 10^{-3-\frac{1}{2}i}$, $i = 1, \ldots, 14$. For ROCK4 $atol_i = rtol_i = 10^{-5-\frac{1}{2}i}$, $i = 1, \ldots, 19$, the provided spectral radius estimation is 1420. The quite predictable results are displayed in figure 5. The relatively poor behaviour of the 20-stage auxiliary method is probably due to imperfection of accuracy control (24).

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