Chapter 3
Formulation and analysis of a class of direct implicit integration methods for special second-order I.V.P.s in predictor-corrector modes

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Abstract A detailed analysis of different formulations of a class of explicit direct integration methods in predictor-corrector modes for solving special second-order initial-value problems has been carried out (Comput. Phys. Comm. **181** (2010) 1833–1841), showing that the adequate combination of the involved formulas led to an increase in the order of the method. In this paper we consider different formulations of the implicit direct integration methods in predictor-corrector modes. An analysis of the accumulated truncation errors is made and the stability analysis is addressed, including the intervals of stability. Some numerical examples are presented to show the performance of the different formulations. These methods may constitute a reliable alternative to other methods in the literature for solving special second order problems.

Key words: Error analysis, stability analysis, Falkner implicit methods, direct Integration Methods, second-order initial-value problems, predictor-corrector modes

3.1 Introduction

Second-order differential equations appear frequently in the applied sciences. Examples of that are the mass movement under the action of a force, problems of orbital dynamics, or in general, any problem involving Newton's law.

Among the general procedures for direct integration of the so-called *special second-order* initial value problem (I.V.P.)

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$$y''(x) = f(x,y(x)), \quad y(x_0) = y_0, \quad y'(x_0) = y'_0\,, \tag{3.1}$$

the Falkner methods [9] is a class of schemes that may be used for this purpose.

Although it is possible to integrate a second-order I.V.P. by reducing it to a first-order system and applying one of the methods available for such systems, it seems more natural to provide numerical methods in order to integrate the problem directly. The advantage of this procedure lies in the fact that they are able to exploit special information about ODEs, resulting in an increase in efficiency. For instance, it is well-known that Runge-Kutta-Nyström methods for (3.1) involve a real improvement as compared to standard Runge-Kutta methods for a given number of stages ([13], p. 285), although the computational cost remains high because of the number of function evaluations. On the other hand, a linear k-step method for first-order ODEs becomes a $2k$-step method for (3.1), ([13], p. 461), increasing the computational work. In the words of F.T. Krogh [17], "the direct integration of second order systems requires about half the number of function evaluations required for integrating the equivalent first order system".

The explicit Falkner method of k steps consists in a couple of formulas that can be written in the form [5]

$$y_{n+1} = y_n + h y'_n + h^2 \sum_{j=0}^{k-1} \beta_j \bigtriangledown^j f_n\,, \tag{3.2}$$

$$y'_{n+1} = y'_n + h \sum_{j=0}^{k-1} \gamma_j \bigtriangledown^j f_n\,, \tag{3.3}$$

where h is the stepsize, y_n and y'_n are approximations to the values of the solution and its derivative at $x_n = x_0 + nh$, $f_n = f(x_n, y_n)$, and $\bigtriangledown^j f_n$ is the standard notation for the backward differences. The coefficients β_j and γ_j can be obtained using the generating functions

$$G_\beta(t) = \sum_{j=0}^{\infty} \beta_j t^j = \frac{t + (1-t)Log(1-t)}{(1-t)Log^2(1-t)}\,,$$
$$G_\gamma(t) = \sum_{j=0}^{\infty} \gamma_j t^j = \frac{-t}{(1-t)Log(1-t)}\,,$$

which have been obtained similarly as that for the Störmer or Cowell methods (see [14], p. 291).

The implicit Falkner method of k steps consists in two formulas that may be written as [5]

$$y_{n+1} = y_n + hy'_n + h^2 \sum_{j=0}^{k} \beta_j^* \bigtriangledown^j f_{n+1}\,, \tag{3.4}$$

$$y'_{n+1} = y'_n + h \sum_{j=0}^{k} \gamma_j^* \bigtriangledown^j f_{n+1}\,, \tag{3.5}$$

with generating functions for the coefficients given respectively by

$$G_{\beta^*}(t) = \sum_{j=0}^{\infty} \beta_j^* t^j = \frac{t + (1-t)Log(1-t)}{Log^2(1-t)}\,,$$
$$G_{\gamma^*}(t) = \sum_{j=0}^{\infty} \gamma_j^* t^j = \frac{-t}{Log(1-t)}\,.$$

Note that the formulas in (3.3) and (3.5) are respectively the Adams-Bashforth and Adams-Moulton schemes for the problem $(y')' = f(x,y)$, which are used to follow the values of the derivative. All the above formulas are of multistep type, specifically k-step formulas, and so k initial values must be provided in order to proceed with the methods (the Runge-Kutta methods are commonly used to obtain the starting values). In this paper, a rigorous analysis of the errors involved in the formulation of the implicit procedures in predictor-corrector modes (P-C) with fixed step size is made (for a variable step size version of these methods see [30], and for an adapted version of the methods in [23] in case of oscillatory systems see [21] and [20]. A new technique for stepsize changing in case of Adam's method has recently appeared in [2]. Other approaches concerning different formulations of Falkner-type methods have appeared in [24] or [25]).

The implicit formulas in (3.4-3.5) may be used to generate methods for solving the I.V.P. in (3.1). A well-known procedure of this type is the Wilson method [32], which is one of the Newmark family, and is commonly used in molecular dynamics calculations. This method uses the two-step formula in (3.4), given by

$$y_{n+1} = y_n + hy'_n + \frac{h^2}{6}\left(2y''_n + y''_{n+1}\right) \tag{3.6}$$

to obtain the positions, while the formula to update the velocities is the two-step method in (3.5) given by

$$y'_{n+1} = y'_n + \frac{h}{2}\left(y''_n + y''_{n+1}\right). \tag{3.7}$$

Another scheme that uses a Falkner formula is a method due to Gear [11], that consists in the two implicit formulas given by

$$y_{n+1} = y_n + hy'_n + \frac{h^2}{12}\left(y''_{n+1} + 6y''_n - y''_{n-1}\right) \tag{3.8}$$

$$y'_{n+1} = y'_n + \frac{h}{12}\left(5y''_{n+1} + 8y''_n - y''_{n-1}\right), \tag{3.9}$$

where the second formula is the three-step method in (3.5) but the first of these formulas is not the three-step one in (3.4).

The application of any of such procedures to (3.1) results in an implicit system that must be solved at each step, involving a great computational cost, but in practice, an explicit formulation in predictor-corrector mode is frequently used. In this way, the implicit methods in (3.4-3.5) are adequately combined with the explicit ones in (3.2-3.3) so as to avoid having to solve an algebraic system at each step. This P-C formulation may also be used as a starting method, as for example in [6], where the one-step implicit Falkner method in predictor-corrector mode is used to provide the starting values in the application of the De Vogelaere's method. Other examples of such procedures may be found in [1], [12] or [28].

In the last years it seems to be a competition to find the numerical method that performs better in solving different types of problems. This is not the goal of this article; in some cases the proposed methods will do better and in other cases they will perform worst than other specialized methods. But the question is how these general purposed methods can be formulated and why they do work or do not, developing an analysis of the errors involved and the stability characteristics. Anyway, we can say that the methods presented here may constitute a reliable alternative to other methods in the literature for solving special second order problems.

The paper is organized as follows. In the following section different formulations of the explicit and implicit Falkner methods are presented. The analysis of the explicit methods was done in [23] while the analysis of the implicit formulas formulated in P-C mode will be done here. Section 3.3 is devoted to the analysis of the local truncation errors and accumulated truncation errors. Section 3.4 deals with the stability analysis, which results of vital importance in the application of the methods. In Section 3.5 some examples are presented to show the performance of the different formulations. In the final section some conclusions put an end to the article.

3.2 Formulations of Falkner methods in P-C mode

In the application of P-C modes, P indicates the application of the explicit method, in our case the predictor given by the formula in (3.2), and C indicates the application of the implicit method, that is, the corrector given by the formula in (3.4). For the

derivative, we will use P' to indicate the application of the explicit formula in (3.3), and C' to indicate the application of the implicit formula in (3.5). Finally, E refers to the evaluation of the function f in order to use this value either for corrections, or in the next step.

Two different implementations for the explicit methods were considered in [23], and for the implicit methods three implementations will be considered here. They are summarized in what follows.

3.2.1 Explicit methods

3.2.1.1 PP'E mode

The fist formulation of the explicit Falkner method on each step for solving the problem in (3.1) consists in

1. Evaluate y_{n+1} using the formula in (3.2)
2. Evaluate y'_{n+1} using the formula in (3.3)
3. Evaluate $f_{n+1} = f(x_{n+1}, y_{n+1})$

3.2.1.2 PEC' mode

The second formulation of the explicit Falkner method on each step for solving the problem in (3.1) reads

1. Evaluate y_{n+1} using the formula in (3.2)
2. Evaluate $f_{n+1} = f(x_{n+1}, y_{n+1})$
3. Evaluate y'_{n+1} using the formula in (3.5)

which can be accomplished due to the absence of the derivative on the function $f = f(x, y(x))$. Thus, having obtained the value y_{n+1} it is straightforward to obtain f_{n+1} to be used in the formula in (3.5). Note that in this way the "implicit formula" in (3.5) is no longer implicit, resulting in an explicit formulation of the method.

For the PP'E mode the accumulated truncation error is of order $\mathcal{O}(h^k)$ while for the PEC' mode is of order $\mathcal{O}(h^{k+1})$ (for details see [23]). Thus, the second formulation of the explicit Falkner method (PEC' mode) provides a better performance.

3.2.2 Implicit methods

3.2.2.1 P'PECE mode

The first choice for the implementation of the implicit Falkner method is given by

1. Evaluate y'_{n+1} using the formula in (3.3) to obtain ${y'}^P_{n+1}$
2. Evaluate y_{n+1} using the formula in (3.2) to obtain y^P_{n+1}
3. Evaluate $f_{n+1} = f(x_{n+1}, y^P_{n+1})$
4. Evaluate y_{n+1} using the formula in (3.4) to obtain y^C_{n+1}
5. Evaluate $f_{n+1} = f(x_{n+1}, y^C_{n+1})$

3.2.2.2 PEC'CE mode

The second possibility is given by

1. Evaluate y_{n+1} using the formula in (3.2) to obtain y^P_{n+1}
2. Evaluate $f_{n+1} = f(x_{n+1}, y^P_{n+1})$
3. Evaluate y'_{n+1} using the formula in (3.5) to obtain ${y'}^C_{n+1}$
4. Evaluate y_{n+1} using the formula in (3.4) to obtain y^C_{n+1}
5. Evaluate $f_{n+1} = f(x_{n+1}, y^C_{n+1})$

3.2.2.3 PECEC' mode

The last implementation consists in

1. Evaluate y_{n+1} using the formula in (3.2) to obtain y^P_{n+1}
2. Evaluate $f_{n+1} = f(x_{n+1}, y^P_{n+1})$
3. Evaluate y_{n+1} using the formula in (3.4) to obtain y^C_{n+1}
4. Evaluate $f_{n+1} = f(x_{n+1}, y^C_{n+1})$
5. Evaluate y'_{n+1} using the formula in (3.5) to obtain ${y'}^C_{n+1}$

Note that in the above formulations, once we have obtained the final value for y_{n+1} given by y^C_{n+1} we have to evaluate $f_{n+1} = f(x_{n+1}, y^C_{n+1})$, which will be used in the next step. This evaluation is indicated by the last E in the different modes.

Obviously, many more choices could have been considered, taking formulas with different steps and therefore, a different order. Specifically, we have considered a predictor with $k+1$ steps and a corrector with k steps, but we have not obtained any improvements over the methods with k steps in the predictor and the corrector. Or you could have considered further corrections, obtaining methods of the forms $P'P(EC)^nE$, $P(EC'C)^nE$ or $P(EC)^nEC'$. We have done different experiments, and in the latter case the interval of stability varies, resulting in an interval slightly higher, but with so little difference that the computational effort is not worth. We have considered only P-C methods with the same number of steps in all the formulas (as it has been used by Shampine and Gordon [26]), where it is performed only a correction, as is usually done in the Adams methods in P-C mode (see [18]).

3.3 Error analysis

3.3.1 Local truncation errors

Consider the formula resulting after approximating the function f on the exact formula

$$y(x_{n+1}) = y(x_n) + hy'(x_n) + \int_{x_n}^{x_{n+1}} f(x, y(x))(x_{n+1} - x)\, dx \tag{3.10}$$

by the interpolating polynomial on the grid points $x_{n-(k-1)}, \ldots, x_n$, and also consider the formula in (3.2). Using the localization hypothesis that $y(x_j) = y_j$, $j = n-(k-1), \ldots, n$, and following a similar procedure as for the Adams formulas [18] we obtain that the local truncation error for the method in (3.2) is given by

$$\mathfrak{L}_P[y(x_n); h] = y(x_{n+1}) - y^P_{n+1} = h^{k+2} y^{(k+2)}(\xi)\beta_k, \tag{3.11}$$

where ξ is an internal point of the smallest interval containing $x_{n-(k-1)}, \ldots, x_n$.

Similarly, for the formula in (3.3) the local truncation error reads

$$\mathfrak{L}_{P'}[y'(x_n); h] = y'(x_{n+1}) - y'^P_{n+1} = h^{k+1} y^{(k+2)}(\psi)\gamma_k, \tag{3.12}$$

where as before ψ refers to an internal point.

For the formula in (3.4) the local truncation error is given by

$$\mathfrak{L}_C[y(x_n); h] = y(x_{n+1}) - y^C_{n+1} = h^{k+3} y^{(k+3)}(\xi)\beta^*_{k+1}, \tag{3.13}$$

and similarly, for the formula in (3.5) the local truncation error is

$$\mathfrak{L}_{C'}[y'(x_n); h] = y'(x_{n+1}) - y'^C_{n+1} = h^{k+2} y^{(k+3)}(\psi)\gamma^*_{k+1} \tag{3.14}$$

where we have denoted by ξ or ψ the internal points, or if they have to be different, we will use ξ_j or ψ_j, as in the following section.

3.3.2 Accumulated truncation errors for the implicit Falkner method in P-C modes

3.3.2.1 P'PECE mode

Assuming that we have to integrate the problem in (3.1) on the interval $[x_0, x_N]$ and that we know in advance the starting values needed to apply the numerical scheme, we proceed by analyzing the accumulated errors on each successive application of

the method along the grid points on the integration interval. We use a superscript P to indicate the application of the explicit method and a superscript C to indicate the application of the implicit one, regardless of whether the formula is for the solution or for the derivative.

Assuming the localization hypothesis and using the formulas for the local truncation errors in (3.11) and (3.12), for the first step $(n=0)$ we have that the differences between the true values, $y(x_1), y'(x_1)$, and the approximated ones, $y_1^P, y_1'^P$, are given respectively by the local truncation errors, that is,

$$y'(x_1) - y_1'^P = h^{k+1} y^{(k+2)}(\psi_1)\gamma_k, \tag{3.15}$$

$$y(x_1) - y_1^P = h^{k+2} y^{(k+2)}(\xi_1)\beta_k, \tag{3.16}$$

where, for convenience, in the sequel the ξ_j and ψ_j will denote appropriate internal points.

After evaluating $f(x_1, y_1^P)$, using the Mean Value Theorem we can put that

$$f(x_1, y(x_1)) - f_1^P = \frac{\partial f}{\partial y}(x_1, \xi_1)\left(y(x_1) - y_1^P\right)$$

where $f_1^P = f(x_1, y_1^P)$. Assuming the localization hypothesis, we have

$$\begin{aligned} y(x_1) - y_1^C &= y(x_0) + h y'(x_0) + h^2 \sum_{j=0}^{k} \beta_j^* \bigtriangledown^j f(x_1, y(x_1)) \\ &\quad + h^{k+3} y^{(k+3)}(\xi_1)\beta_{k+1}^* - \left(y_0 + h y_0' + h^2 \sum_{j=0}^{k} \beta_j^* \bigtriangledown^j f_1^P \right) \\ &= h^{k+3} y^{(k+3)}(\xi_1)\beta_{k+1}^* + \mathcal{O}(h^{k+4}). \end{aligned} \tag{3.17}$$

After evaluating $f(x_1, y_1^C)$, for the next step $(n=1)$ we have that

$$\begin{aligned} y'(x_2) - y_2'^P &= y'(x_1) + h \sum_{j=0}^{k-1} \gamma_j \bigtriangledown^j f(x_1, y(x_1)) \\ &\quad + h^{k+1} y^{(k+2)}(\psi_2)\gamma_k - \left(y_1'^P + h \sum_{j=0}^{k-1} \gamma_j \bigtriangledown^j f_1^C \right) \end{aligned} \tag{3.18}$$

where we have used the values of the step before, $y_1'^P$ and y_1^C, and have used the notation $f_1^C = f(x_1, y_1^C)$. After some calculations, using the formulas in (3.15) and (3.17), it results that

$$y'(x_2) - y_2'^P = h^{k+1}\gamma_k \left(y^{(k+2)}(\psi_1) + y^{(k+2)}(\psi_2) \right) + \mathcal{O}(h^{k+2}). \tag{3.19}$$

Similarly, for the predictor we have

$$y(x_2) - y_2^P = h^{k+2}\beta_k y^{(k+2)}(\xi_2) + h^{k+2}y^{(k+2)}(\xi_1)\gamma_k + \mathcal{O}(h^{k+3}). \tag{3.20}$$

And finally, for the corrector we get that

$$\begin{aligned} y(x_2) - y_2^C &= y(x_1) + hy'(x_1) + h^2 \sum_{j=0}^{k} \beta_j^* \bigtriangledown^j f(x_1, y(x_1)) \\ &\quad + h^{k+3}y^{(k+3)}(\xi_2)\beta_{k+1}^* - \left(y_1^C + hy_1'^P + h^2 \sum_{j=0}^{k} \beta_j^* \bigtriangledown^j f_2^P \right) \\ &= h^{k+3}\beta_{k+1}^* \left(y^{(k+3)}(\xi_1) + y^{(k+3)}(\xi_2) \right) + h^{k+2}y^{(k+2)}(\psi_1)\gamma_k \\ &\quad + \mathcal{O}(h^{k+4}). \end{aligned} \tag{3.21}$$

Repeating the procedure along the nodes on the integration interval we determine that the accumulated error at the final point x_N is given by

$$\begin{aligned} y(x_N) - y_N^C &= h^{k+2}\gamma_k \sum_{j=1}^{N-1} (N-j)y^{(k+2)}(\psi_j) + h^{k+3}\beta_{k+1}^* \sum_{j=1}^{N} y^{(k+3)}(\xi_j) \\ &\quad + \mathcal{O}(h^{k+4}), \end{aligned} \tag{3.22}$$

and for the derivative we have

$$y'(x_N) - y_N'^P = h^{k+1}\gamma_k \sum_{j=1}^{N} y^{(k+2)}(\psi_j) + \mathcal{O}(h^{k+2}). \tag{3.23}$$

Assuming that the derivatives $y^{(k+2)}(x)$ and $y^{(k+3)}(x)$ are continuous, after using the Mean Value Theorem, the above formulas may be rewritten as follows:

$$\begin{aligned} y(x_N) - y_N^C &= \frac{1}{2} h^k \gamma_k y^{(k+2)}(\psi)(x_N - x_0)(x_N - x_1) \\ &\quad + h^{k+2}\beta_{k+1}^* y^{(k+3)}(\xi)(x_N - x_0) + \mathcal{O}(h^{k+4}) \end{aligned} \tag{3.24}$$

and

$$y'(x_N) - y_N'^P = h^k \gamma_k (x_N - x_0) y^{(k+2)}(\psi) + \mathcal{O}(h^{k+2}). \tag{3.25}$$

3.3.2.2 PEC 'CE mode

In this mode, for the first step ($n = 0$), after the application of the predictor P and the corrector C we have the same results as before, that is,

$$y(x_1) - y_1^P = h^{k+2} y^{(k+2)}(\xi_1)\beta_k\,,$$

and

$$y(x_1) - y_1^C = h^{k+3} y^{(k+3)}(\xi_1)\beta_{k+1}^* + \mathcal{O}(h^{k+4})\,.$$

Now the difference with the mode before results in the application of the corrector C ' to obtain the approximation for the derivative. We have

$$\begin{aligned} y'(x_1) - y_1'^C &= y'(x_0) + h\sum_{j=0}^{k} \gamma_j^* \nabla^j f(x_1, y(x_1)) \\ &\quad + h^{k+2} y^{(k+3)}(\psi_1)\gamma_{k+1}^* - \left(y_0'^C + h\sum_{j=0}^{k} \gamma_j^* \nabla^j f_1^P \right) \\ &= h^{k+2} y^{(k+3)}(\psi_1)\gamma_{k+1}^* + \mathcal{O}(h^{k+3})\,. \end{aligned} \tag{3.26}$$

After the evaluation of $f(x_1, y_1^C)$ and the application of the predictor P to obtain an estimate y_2^P for $y(x_2)$, the application of the corrector C results in

$$\begin{aligned} y(x_2) - y_2^C &= h^{k+3}\beta_{k+1}^* \left(y^{(k+3)}(\xi_1) + y^{(k+3)}(\xi_2) \right) + h^{k+3} y^{(k+3)}(\psi_1)\gamma_{k+1}^* \\ &\quad + \mathcal{O}(h^{k+4})\,, \end{aligned} \tag{3.27}$$

while the application of the corrector C ' produces

$$y'(x_2) - y_2'^C = h^{k+2}\gamma_{k+1}^* \left(y^{(k+3)}(\psi_1) + y^{(k+3)}(\psi_2) \right) + \mathcal{O}(h^{k+3})\,. \tag{3.28}$$

Repeating the procedure along the nodes on the integration interval we obtain that the accumulated error at the final point x_N is given by

$$\begin{aligned} y(x_N) - y_N^C &= h^{k+3}\gamma_{k+1}^* \sum_{j=1}^{N-1} (N-j) y^{k+3)}(\psi_j) + h^{k+3}\beta_{k+1}^* \sum_{j=1}^{N} y^{k+3)}(\xi_j) \\ &\quad + \mathcal{O}(h^{k+4})\,, \end{aligned} \tag{3.29}$$

while for the derivative we have the accumulated error given by

$$y'(x_N) - y_N'^C = h^{k+2}\gamma_{k+1}^* \sum_{j=1}^{N} y^{k+3)}(\psi_j) + \mathcal{O}(h^{k+3})\,. \tag{3.30}$$

Assuming that $y^{(k+3)}(x)$ is continuous, the above formulas for the accumulated errors at the final point x_N may be written as

$$y(x_N) - y_N^C = \frac{1}{2} h^{k+1} \gamma_{k+1}^* y^{(k+3)}(\psi)(x_N - x_0)(x_N - x_1)$$

$$+ h^{k+2} \beta_{k+1}^* y^{(k+3)}(\xi)(x_N - x_0) + \mathcal{O}(h^{k+4}) \tag{3.31}$$

for the solution, and

$$y'(x_N) - y_N'^C = h^{k+1} \gamma_{k+1}^* (x_N - x_0) y^{(k+3)}(\psi) + \mathcal{O}(h^{k+3}) \tag{3.32}$$

for the derivative.

3.3.2.3 PECEC' mode

Now the difference with the mode before results in the application of the corrector C' to obtain the values $y_n'^C$, using $f(x_n, y_n^C)$ instead of $f(x_n, y_n^P)$. The first difference to the previous mode is observed in the first step $(n = 0)$ and results to be

$$y'(x_1) - y_1'^C = y'(x_0) + h \sum_{j=0}^{k} \gamma_j^* \nabla^j f(x_1, y(x_1))$$

$$+ h^{k+2} y^{(k+3)}(\psi_1) \gamma_{k+1}^* - \left(y_0'^{C'} + h \sum_{j=0}^{k} \gamma_j^* \nabla^j f_1^C \right)$$

$$= h^{k+2} y^{(k+3)}(\psi_1) \gamma_{k+1}^* + \mathcal{O}(h^{k+3}). \tag{3.33}$$

Note that the only difference between the formulas in (3.26) and in (3.33) is that f_1^P has been substituted by f_1^C, but this does not change the principal term of the errors. This means that the principal terms in the errors for the final formulas are the same as in the previous mode, and so the formulas in (3.31) and (3.32) remain valid in this mode. This, however, does not mean that the errors are equal, since the remaining terms are different. But since the principal terms are the same the errors will be similar.

For comparison purposes we have included in Table 3.1 the principal terms of the accumulated errors for the different implementations of the explicit and implicit Falkner methods. These terms will be denoted by $PT(y(x_n) - y_N)$ for the solution, and $PT(y'(x_n) - y'_N)$ for the derivative, where the approximated values of the solution and the derivative at the final point are indicated by y_N and y'_N respectively. The formulations of the explicit methods with k steps are named FEABk and $FEAMk$ as in [23], while the implicit method with k steps formulated in P-C modes are named FI[1]k, FI[2]k and FI[3]k corresponding to the P'PECE, PEC'CE and PECEC' modes respectively in the above section.

Remark 1. Note that the above methods may be applied to a system of second-order differential equations of the form

Method	$PT(y(x_n)-y_N)$	$PT(y'(x_n)-y'_N)$
FEABk	$\frac{1}{2}h^k y^{(k+2)}(\psi)(x_N-x_0)(x_N-x_1)\gamma_k$	$h^k y^{(k+2)}(\psi)(x_N-x_0)\gamma_k$
$FEAMk$	$\frac{1}{2}h^{k+1}y^{(k+3)}(\psi)(x_N-x_0)(x_N-x_1)\gamma^*_{k+1}$ $+h^{k+1}y^{(k+2)}(\xi)(x_N-x_0)\beta_k$	$h^{k+1}y^{(k+3)}(\psi)(x_N-x_0)\gamma^*_{k+1}$
FI[1]k	$\frac{1}{2}h^k y^{(k+2)}(\psi)(x_N-x_0)(x_N-x_1)\gamma_k$	$h^k y^{(k+2)}(\psi)(x_N-x_0)\gamma_k$
FI[2]k FI[3]k	$\frac{1}{2}h^{k+1}y^{(k+3)}(\psi)(x_N-x_0)(x_N-x_1)\gamma^*_{k+1}$	$h^{k+1}y^{(k+3)}(\psi)(x_N-x_0)\gamma^*_{k+1}$

Table 3.1 *Principal terms of the accumulated errors for the different implementations of the explicit and implicit Falkner methods.*

$$\begin{cases} \mathbf{y}''(x) = \mathbf{f}(x,\mathbf{y}(x)), \quad x \in [x_0,x_N] \\ \mathbf{y}(x_0) = \mathbf{y}_0 \end{cases}$$

where $\mathbf{y} : \mathbb{R}^m \to \mathbb{R}^m$, and $\mathbf{f} : [x_0,x_N] \times \mathbb{R}^m \to \mathbb{R}^m$, using a componentwise implementation.

3.4 Stability

In the context of ordinary differential equations, the concept of stability refers to what extent a numerical scheme is appropriate for solving an initial-value problem. Roughly speaking, a given method can be said to be stable if small changes in the data result in small changes in the solution obtained.

A procedure commonly used to study stability (zero-stability) consists in writing the difference equations of the method as a one-step recurrence in a space with high dimension and in an adequate norm to bound the finite powers of the resulting matrices. For the different combinations of the implicit method in (3.4) to get the above P-C modes, a similar procedure to that in [23] may be considered to obtain zero-stability. But, the zero stability is only a minimal condition for a numerical method; for second order equations the so-called P-stability is the type of concern together with A-stability.

In order to determine whether a numerical method will produce reasonable results with a given value of $h > 0$, we need a notion of stability that is different from zero-stability. The stability properties are analyzed by using the linear test equation introduced by Lambert and Watson [19]

$$y''(x) = -\mu^2 y(x), \quad \text{with } \mu > 0. \tag{3.34}$$

The application of the above predictor-corrector formulations of the implicit Falkner method to this problem yields the following recursion

$$Y_n = M[i]\, Y_{n-1}\,, \tag{3.35}$$

where Y_n is the $k+1$-vector given by $Y_n = \left(y_{n+1}, y_n, \ldots, y_{n-(k-2)}, h\,y'_{n+1}\right)^T$, and $M[i]\,, i = 1,2,3,$ are $(k+1)\times(k+1)$ matrices whose elements depends on H^2 and the coefficients of the method, where $H = \mu\, h$. The matrices $M[i]$ are called the *stability matrices* and the index i in $M[i]$ is used to denote each implementation according to its appearance in the above section, that is, $i = 1$ stands for the first P-C mode, $i = 2$ for the second P-C mode, and $i = 3$ for the last one.

The entries of each of the stability matrices are given by

$$\begin{aligned}
M[1]_{1\,1} &= 1 + H^2 \sum_{j=0}^{k} \left(j - 1 + H^2 \sum_{s=0}^{k-1} \beta_s \right) \beta_j^* \\
M[1]_{1\,l+1} &= (-1)^l H^2 \sum_{j=0}^{k} \left(\binom{j}{l+1} + H^2 \sum_{s=l}^{k-1} \binom{s}{l} \beta_s \right) \beta_j^*\,, \\
&\qquad l = 1, \ldots, k-1\,. \\
M[1]_{jl} &= \delta_{jl+1}\,, \quad j = 2, \ldots, k \quad l = 1, \ldots, k+1\,. \\
M[1]_{k+1\,l+1} &= (-1)^{l+1} H^2 \sum_{j=l}^{k-1} \binom{j}{l} \gamma_j\,, \quad l = 0, \ldots, k-1\,. \\
M[1]_{k+1\,k+1} &= 1
\end{aligned}$$

where δ_{jl+1} is the Kronecker delta and the notations of type $\binom{j}{l}$ refer to the binomial coefficients.

For the matrices $M[2]$ and $M[3]$ all the entries are the same as for $M[1]$ except for the last row, which for $M[2]$ reads

$$
\begin{aligned}
M[2]_{k+1\,1} &= H^2 \sum_{j=0}^{k} \left(j-1+H^2 \sum_{s=0}^{k-1} \beta_s \right) \gamma_j^* \\
M[2]_{k+1\,l+1} &= (-1)^l H^2 \sum_{j=0}^{k} \left(\binom{j}{l+1} + H^2 \sum_{s=l}^{k-1} \binom{s}{l} \beta_s \right) \gamma_j^* , \\
&\qquad l = 1, \ldots, k-1 . \\
M[2]_{k+1\,k+1} &= 1 - H^2 \sum_{j=0}^{k} \gamma_j^* ,
\end{aligned}
$$

and, similarly, for $M[3]$ the last row results in

$$
\begin{aligned}
M[3]_{k+1\,1} &= H^2 \sum_{j=0}^{k} \left[j-1+H^2 \sum_{s=0}^{k} \left(1-s-H^2 \sum_{t=0}^{k-1} \beta_t \right) \beta_s^* \right] \gamma_j^* \\
M[3]_{k+1\,l+1} &= (-1)^l H^2 \sum_{j=0}^{k} \left[\binom{j}{l+1} - H^2 \sum_{t=0}^{k} \left(\binom{t}{l+1} + H^2 \sum_{s=l}^{k-1} \binom{s}{l} \beta_s \right) \beta_t^* \right] \gamma_j^* , \\
&\qquad l = 1, \ldots, k-1 . \\
M[3]_{k+1\,k+1} &= 1 - H^2 \sum_{j=0}^{k} \left(1 - H^2 \sum_{s=0}^{k} \beta_s^* \right) \gamma_j^* .
\end{aligned}
$$

For example, when $k = 3$ the equation in (3.35) in case of $M[1]$ reads

$$
Y_n = \begin{pmatrix}
\frac{19\left(19H^2-132\right)H^2}{4320} + 1 & \frac{H^2}{10} - \frac{19H^4}{432} & \frac{H^2\left(19H^2-28\right)}{1440} & 1 - \frac{19H^2}{180} \\
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
-\frac{23H^2}{12} & \frac{4H^2}{3} & -\frac{5H^2}{12} & 1
\end{pmatrix} Y_{n-1} ,
$$

while the same equation in case of $M[2]$ results in

$$
Y_n = \begin{pmatrix}
\frac{19\left(19H^2-132\right)H^2}{4320} + 1 & \frac{H^2}{10} - \frac{19H^4}{432} & \frac{H^2\left(19H^2-28\right)}{1440} & 1 - \frac{19H^2}{180} \\
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
\frac{19H^4}{64} - \frac{7H^2}{6} & \frac{5H^2\left(4-3H^2\right)}{96} & \frac{H^2\left(9H^2-8\right)}{192} & 1 - \frac{3H^2}{8}
\end{pmatrix} Y_{n-1} ,
$$

and finally, for the third implementation the matrix $M[3]$ is given by

$$\begin{pmatrix} \frac{19(19H^2-132)H^2}{4320}+1 & \frac{H^2}{10}-\frac{19H^4}{432} & \frac{H^2(19H^2-28)}{1440} & 1-\frac{19H^2}{180} \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ \frac{2508H^4-361H^6-13440H^2}{11520} & \frac{95H^6-216H^4+1200H^2}{5760} & \frac{28H^4-19H^6-160H^2}{3840} & \frac{19H^4-180H^2}{480}+1 \end{pmatrix}$$

The behaviour of the numerical solution will depend on the eigenvalues of the matrices $M[i]$, and the stability properties of the methods will be characterized by the spectral radius, $\rho(M[i])$. According to the terminology introduced by Coleman and Ixaru [7] we have:

- $(0,H_s)$ is an interval of stability for a given method if for all $H \in (0,H_s)$ it is $|r_i| < 1$ where the $r_i, i = 1,\ldots,k+1$ are the eigenvalues of the stability matrix.
- $(0,H_p)$ is an interval of periodicity for a given method if for all $H \in (0,H_p)$ the eigenvalues of the stability matrix, $r_i, i = 1,\ldots,k+1$, satisfy

$$r_1 = e^{i\theta(H)}, \quad r_2 = e^{-i\theta(H)}, \quad |r_i| \leq 1\,,\, i > 2\,,$$

  where $\theta(H)$ is a real function.

In particular, if the interval of stability is $(0,\infty)$ the method is *A-stable*, and if the interval of periodicity is $(0,\infty)$ the method is *P-stable*. Note that A-stability is more restrictive than P-stability, that is, A-stability implies P-stability.

The practical significance of the interval of stability is that, for a given μ in (3.34), there is no explosion of the error in the numerical solution when $0 < h < H_s/\mu$ [7]. The interval of periodicity defines the stepsize which can be used in order for the approximation of the solution of problems with high oscillatory or periodic solution to be of the same order as the algebraic order of the method. When $0 < h < H_p/\mu$ the numerical solution defined by (3.35) is also periodic, as is the exact solution of the test model (3.34) for all non-trivial initial-conditions on y and y'.

A crucial difference between A-stability and P-stability is that for A-stable methods the stability matrix satisfies $(M[i])^n \to 0$ as $n \to \infty$ because $\rho(M[i]) < 1$, but for P-stable methods this fact is not possible because $\rho(M[i]) = 1$, (see [10]). Therefore, A-stable methods alleviate the initial errors whereas for P-stable methods the initial errors do not diminish when the integration progresses in time.
If we let the value μ in (3.34) to be complex, instead of intervals we obtain stability or periodicity regions in the H-complex plane.

The importance of determining the stability characteristics will be shown by considering the Gear's method in (3.8-3.9). This is an implicit method for which we need a predicted value to be formulated in P-C mode. Taking as predictor the two-step explicit Falkner method given by

$$y_{n+1} = y_n + hy'_n + \frac{h^2}{6}\left(4y''_n - y''_{n-1}\right)$$

to obtain y^P_{n+1}, after evaluating $f(x_{n+1}, y^P_{n+1})$ and applying the formula in (3.8) to obtain y^C_{n+1} we can proceed in two ways:

1. we can evaluate $f(x_{n+1}, y^C_{n+1})$ with the best approximation we have for y_{n+1} and then we use the formula in (3.9) to obtain the approximate value y'_{n+1}. We note this formulation as P_2ECEC', where the subindex 2 corresponds to the order of the predictor.
2. or we can use the previous evaluation $f(x_{n+1}, y^P_{n+1})$ in the formula in (3.9) to obtain the approximate value y'_{n+1} . The notation for this formulation results in P_2ECC'.

For the first choice the stability matrix results in

$$\begin{pmatrix} \frac{H^4}{18} - \frac{7H^2}{12} + 1 & -\frac{1}{72}H^2\left(H^2-6\right) & 1 - \frac{H^2}{12} \\ 1 & 0 & 0 \\ \frac{-10H^6+105H^4-468H^2}{432} & \frac{H^2\left(5\left(H^2-6\right)H^2+72\right)}{864} & \frac{5\left(H^2-12\right)H^2+1}{144} \end{pmatrix}$$

for which there are no stability nor periodicity intervals.
In the second case the stability matrix is given by

$$\begin{pmatrix} \frac{H^4}{18} - \frac{7H^2}{12} + 1 & -\frac{1}{72}H^2\left(H^2-6\right) & 1 - \frac{H^2}{12} \\ 1 & 0 & 0 \\ \frac{1}{36}H^2\left(10H^2-39\right) & \frac{1}{72}\left(6H^2-5H^4\right) & 1 - \frac{5H^2}{12} \end{pmatrix}$$

and the stability interval is given by $(0, 1.906123)$. Although at first glance one could intuitively suppose that the first procedure will be the best this is not true. Not only the first procedure requires more computational cost (two evaluations of the function f per step versus one evaluation in the second case) but it also has worst stability properties.

Nevertheless, if we consider as predictor the three-step explicit Falkner method given by

$$y_{n+1} = y_n + hy'_n + \frac{h^2}{24}\left(19y''_n - 10y''_{n-1} + 3y''_{n-2}\right)$$

to obtain y^P_{n+1}, after evaluating $f(x_{n+1}, y^P_{n+1})$ and applying the formula in (3.8) to obtain y^C_{n+1} we can also proceed in two ways:

1. we can evaluate $f(x_{n+1}, y^C_{n+1})$ with the best approximation we have for y_{n+1} and then we use the formula in (3.9) to obtain the approximate value y'_{n+1}. Now the notation for this formulation is P_3ECEC'.
2. or we can use the previous value $f(x_{n+1}, y^P_{n+1})$ in the formula in (3.9) to obtain the approximate value y'_{n+1} . The notation for this formulation is P_3ECC'.

Now in the first case the stability matrix is given by

$$\begin{pmatrix} \frac{19H^4}{288}-\frac{7H^2}{12}+1 & \frac{1}{144}H^2\left(12-5H^2\right) & \frac{H^4}{96} & 1-\frac{H^2}{12} \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ \frac{-95H^6+840H^4-3744H^2}{3456} & \frac{H^2\left(25H^4-60H^2+144\right)}{1728} & -\frac{5H^6}{1152} & \frac{5\left(H^2-12\right)H^2+1}{144} \end{pmatrix}$$

and the stability interval is given by $(0, 0.585417)$. In the second case the stability matrix is given by

$$\begin{pmatrix} \frac{19H^4}{288}-\frac{7H^2}{12}+1 & \frac{1}{144}H^2\left(12-5H^2\right) & \frac{H^4}{96} & 1-\frac{H^2}{12} \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ \frac{1}{288}H^2\left(95H^2-312\right) & \frac{1}{144}H^2\left(12-25H^2\right) & \frac{5H^4}{96} & 1-\frac{5H^2}{12} \end{pmatrix}$$

for which there are no stability nor periodicity intervals. This time the first procedure is the best concerning the stability characteristics.

In Figure 3.1 the stability regions are depicted (left: taking as predictor the two-step explicit Falkner method and using $f(x_{n+1}, y^P_{n+1})$ in the formula in (3.9); right: taking as predictor the three-step explicit Falkner method and using $f(x_{n+1}, y^C_{n+1})$ in the formula in (3.9)).

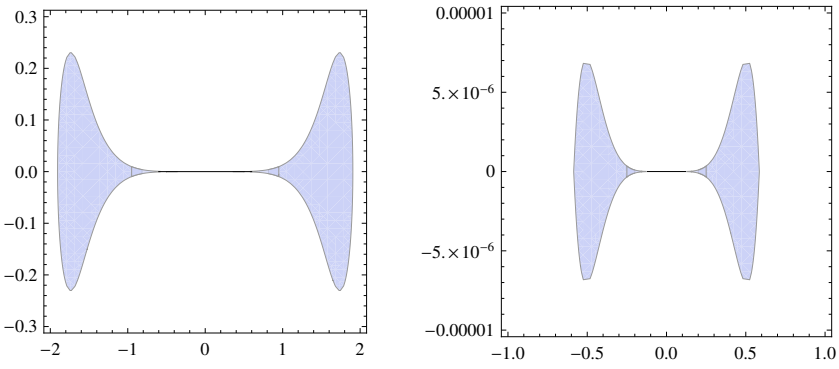

Fig. 3.1 Absolute stability regions for different formulations of Gear's method in P-C mode (left: P_2ECC'; right: P_3ECEC')

These unexpected results show the importance of determining the stability regions in order to obtain appropriate results when applying a numerical method. The numerical results in the following section will confirm this assertion (Tables 3.3 and 3.5 provide a confirmation of the theoretical expectations on the stability of the de-

rived methods).

For the methods presented in the previous sections we have obtained that they are not A-stable nor P-stable up to $k = 14$ (it is also known that there are no A-stable Adams methods for $y' = f(x,y)$). There exists only one interval of periodicity corresponding to the third mode when $k = 1$ being this interval $[0, \sqrt{6}]$. In Table 3.2 the intervals of stability are presented from $k = 1$ up to $k = 14$, where k refers to the number of steps, for the different formulations, named after $FI[1]k$, $FI[2]k$, and $FI[3]k$ respectively, according to the notation used in the above sections.

All these values have been obtained with the help of the Mathematica program. We have considered only the primary stability intervals although for different methods may exist secondary stability intervals, as for the second P-C mode for $k = 2$, for which $[1,2]$ is an interval where $|r_i| < 1, i = 1,2,3$.

k	$FI[1]k$	$FI[2]k$	$FI[3]k$
1	$\varnothing$	$(0,2)$	$\varnothing$
2	$\varnothing$	$\varnothing$	$\varnothing$
3	$(0,0.853006)$	$\varnothing$	$\varnothing$
4	$(0,0.930949)$	$(0,0.534947)$	$(0,1.108998)$
5	$\varnothing$	$(0,0.925569)$	$(0,1.409664)$
6	$\varnothing$	$\varnothing$	$\varnothing$
7	$(0,0.401364)$	$\varnothing$	$\varnothing$
8	$(0,0.285341)$	$(0,0.274630)$	$(0,0.480033)$
9	$\varnothing$	$(0,0.521074)$	$(0,0.821956)$
10	$\varnothing$	$\varnothing$	$\varnothing$
11	$(0,0.100705)$	$\varnothing$	$\varnothing$
12	$(0,0.071103)$	$(0,0.185094)$	$(0,0.300133)$
13	$\varnothing$	$(0,0.362275)$	$(0,0.390144)$
14	$\varnothing$	$\varnothing$	$\varnothing$

Table 3.2 *Intervals of stability for the different formulations of the Falkner implicit method in P-C modes.*

We have included different plots showing the stability intervals. Figure 3.2 shows the absolute value of the eigenvalues of $M[2]$ and $M[3]$ for $k = 1$ versus H, and the resulting stability interval $(0,H_s)$. For the matrix $M[3]$ we have included the interval of periodicity $(0,H_p)$. Figure 3.3 shows the absolute value of the eigenvalues of $M[1]$ and $M[2]$ for $k = 3$ versus H. This time, for the $M[2]$ mode there is no primary stability interval, although a secondary interval of stability exists, $(1.731413, 1.895953)$.

Figure 3.4 shows the absolute value of the eigenvalues of $M[1]$ and $M[3]$ for $k = 5$, showing in case of $M[1]$ a secondary stability interval given by $(0.626085, 0.752697)$. Finally, Figure 3.5 shows two eigenvalues limiting the stability regions in case of

$M[2]$ and $M[3]$ when $k = 9$. We have included as a reference in all the plots the horizontal line at a distance of one unit above the horizontal axis.

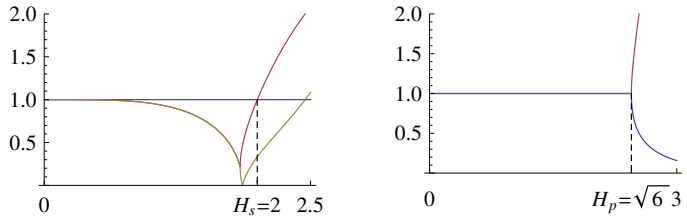

Fig. 3.2 Absolute value of the eigenvalues $|r_i|$, $i = 1,2$ of the stability matrices for the P-C modes: $M[2]$ (left) and $M[3]$ (right) when $k = 1$.

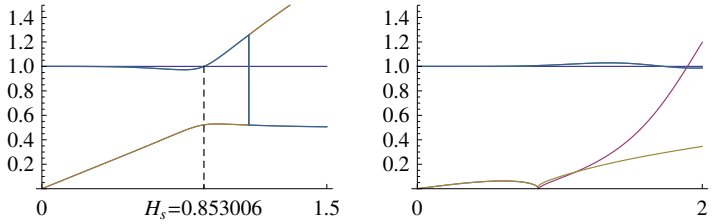

Fig. 3.3 Absolute value of the eigenvalues $|r_i|$, $i = 1,2,3,4$ of the stability matrices for the P-C modes: $M[1]$ (left) and $M[2]$ (right) when $k = 3$.

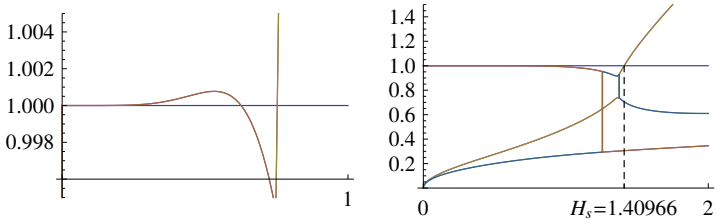

Fig. 3.4 Absolute values of the eigenvalues $|r_i|$, $i = 1,\ldots,6$ of the stability matrices for the P-C modes: $M[1]$ (left) and $M[3]$ (right) when $k = 5$.

In Figure 3.6 appear the stability regions for the methods $FI[i]4$, $i = 1,2,3$.

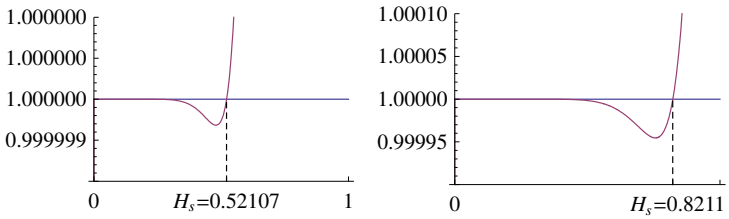

Fig. 3.5 Absolute value of two eigenvalues limiting the stability region for each of the stability matrices for the P-C modes: $M[2]$ (left) and $M[3]$ (right) when $k = 9$.

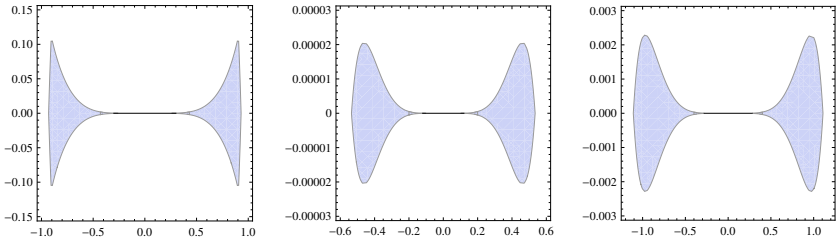

Fig. 3.6 Stability regions for each of the methods $FI[i]4, i = 1,2,3$ (from left to right).

Remark 2. In the application of the P-C modes we may choose to evaluate the final E in order to update the value of f_{n+1} for the next step or not. If we do not make this further evaluation the mode $FI[1]k$ results to be P' PEC instead of P' PECE, but the modes $FI[2]k$ and $FI[3]k$ results to be the same, namely PEC' C, and will be denoted by $\widetilde{FI}[i]k$, $i = 1,2$. We make the observation that the order of the accumulated truncation errors is the same with the evaluation or not of the final E, but the stability characteristics differ markedly in both cases. In fact, if we do not make the last evaluation, the stability regions are smaller. In Figure 3.7 we include a plot with the stability regions for the modes $FI[2]4$ and $\widetilde{FI}[2]4$.

3.5 Numerical examples

In this section we apply to some examples the above formulations in P-C mode to illustrate the performance of the implicit Falkner method. The numerical results obtained with these methods are compared with the results obtained with other numerical methods. The predictor-corrector formulations of the implicit Falkner methods in this paper will be denoted by FI[j]k, where j refers to the implementations 1, 2 or

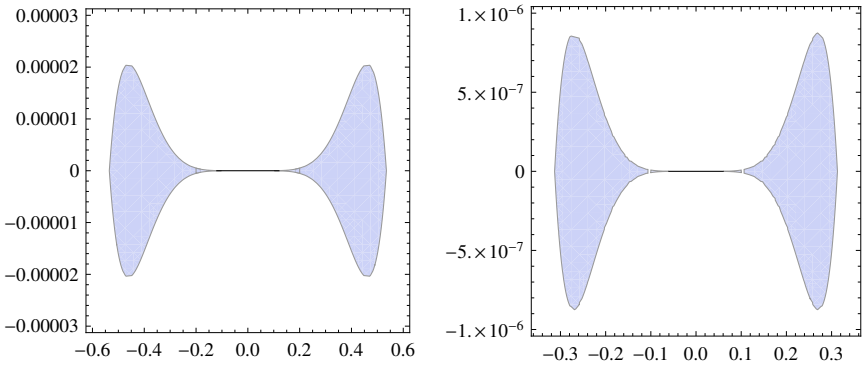

Fig. 3.7 Stability regions for the methods $FI[2]4$ and $\widetilde{FI}[2]4$.

3 in the above sections, and k refers to the number of steps of the method. That is, number 1 refers to the P'PECE mode in the above sections, 2 refers to the PEC'CE mode, and 3 refers to the PECEC' mode.

3.5.1 Example 1.

As a first example we take the classical problem used to test absolute stability, with particular initial values

$$y''(x) = -\mu^2 y(x)\,, \quad y(0) = 0\,, \quad y'(0) = 1 \tag{3.36}$$

whose exact solution is

$$y(x) = \frac{\sin(\mu x)}{\mu}\,.$$

The problem has been integrated on the interval $[0, 5\pi]$ with $\mu = 100$, considering the explicit and implicit implementations, using different values of N and k. Table 3.3 shows the results obtained with $k = 7, 8$ and $N = 3000, 4000$. The values of $h\mu$, the CPU times (in seconds) and the maximum absolute error on the integration interval

$$MaxErr = \max_{j\in 0,\ldots,N} |y(x_j) - y_j|\,,$$

are included.

We observe that the time needed by implicit methods is bigger than for the explicit ones, as expected. Nevertheless, the accuracies obtained by the explicit eight order methods FEAB8 and FEAM8 are not acceptable. Concerning the FEAB7 and FEAM7 methods, for $N = 3000$ the errors are enormous, while for $N = 4000$ they are acceptable. These results are related with the stability intervals (see Table 2 in [23]) since when $N = 4000$ the value $h\mu = 0.3926$ is inside the absolute stability intervals of the methods FEAB7 and FEAM7, and is not in other cases.

In the case of implicit methods there are only two situations in which the value of $h\mu$ is within the ranges of the primary interval of absolute stability: for FI[1]7 and for FI[3]8 when N =4000 (see Table 3.2). Why in some of the other cases the errors seem to behave well? There are two possible reasons, first, there may be a secondary stability interval of the form $[a,b]$ with $a > 0$, where the eigenvalues of the stability matrix are less than unity. Nevertheless, this situation does not occur with the data in Table 3.3 for this example.

On the other hand, it may occur that for some specific data, the eigenvalues of the stability matrix although more than one, are very close to 1. In this situation the errors grow very slowly in each step, indicating that for these values of N the instability does not affect the results yet. This is the case for the data in Table 3.3. For example, for the method FI[2]8 the largest eigenvalues are 1.0000079 when $N = 3000$, and 1.00000024 when $N = 4000$, which justifies the not so bad behavior of the method.

3.5.2 Example 2.

The next example has appeared different times in the literature (see [4], [22]). The problem consists in

$$y''(t) = -w^2 y(t) + (w^2 - 1)\sin(t)\,, \quad y(0) = 1\,, \quad y'(0) = w + 1 \tag{3.37}$$

whose exact solution is

$$y(t) = \cos(wt) + \sin(wt) + \sin(t)\,.$$

This problem has been solved in the interval $[0, 100]$ with the methods $FEAM4$ and $\widetilde{FI}[2]4$ taking $w = 20$. Figure 3.8 shows the efficiency of different methods appeared in the literature, the horizontal axis stands for the number of function evaluations required and the vertical axis stands for the digital logarithm of the maximal global error for the solution. The methods used for comparison are

- RK4: the classical RK method of order four
- RK5: the classical RK method of order five presented in [13]

Method	N steps	$h\mu$	$CPU(s.)$	$MaxErr(y)$
$FEAB7$	3000	0.5235	0.344	3.0150×10^{50}
	4000	0.3926	0.484	3.1289×10^{-3}
$FEAB8$	3000	0.5235	0.391	6.0959×10^{252}
	4000	0.3926	0.547	2.7399×10^{85}
$FEAM7$	3000	0.5235	0.359	3.2187×10^{114}
	4000	0.3926	0.500	2.7601×10^{-4}
$FEAM8$	3000	0.5235	0.422	3.0925×10^{367}
	4000	0.3926	0.547	1.3965×10^{160}
$FI[1]7$	3000	0.5235	0.594	1.9224×10^{185}
	4000	0.3926	0.813	3.2240×10^{-3}
$FI[1]8$	3000	0.5235	0.703	2.3554×10^{387}
	4000	0.3926	0.906	1.8158×10^{259}
$FI[2]7$	3000	0.5235	0.610	5.4653×10^{-4}
	4000	0.3926	0.813	4.9368×10^{-5}
$FI[2]8$	3000	0.5235	0.688	2.4507×10^{-4}
	4000	0.3926	0.921	1.6627×10^{-5}
$FI[3]7$	3000	0.5235	0.610	4.5078×10^{-4}
	4000	0.3926	0.812	4.3100×10^{-5}
$FI[3]8$	3000	0.5235	0.672	1.9418×10^{-4}
	4000	0.3926	0.922	1.4224×10^{-5}

Table 3.3 *Maximum absolute error of the solution for different implementations of the explicit and implicit Falkner methods in P-C mode for solving the problem in (3.36)*

- EFRK4: the four-stage exponentially fitted RK method of order four given in [31]
- SIMOS4: the RK method of order four presented in [27]
- FRK5a: the seven-stage RK method of order five given by (4.17) and (4.20) in [4]
- FRK5b: the seven-stage RK method of order five given by (4.17) and (4.28) in [4]

It is obvious from the graphs that the Falkner methods perform better.

3.5.3 Example 3.

We consider the following nonlinear problem studied by Chawla and Rao in [3]

$$y''(x) + 100y = \sin(y), \quad y(0) = 0, \quad y'(0) = 1 \tag{3.38}$$

For this example, as there is not a known analytical solution, we perform the computation on the interval $[0, 20\pi]$ and measure the absolute error at the final point

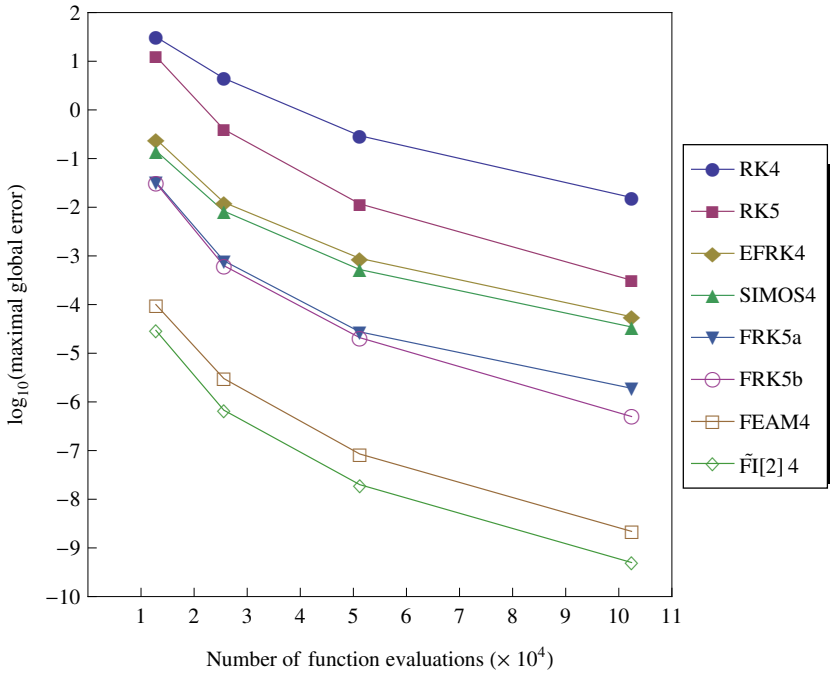

Fig. 3.8 Numerical results for Problem (3.37) with different Runge-Kutta type methods and with the methods $FEAM4$ and $\widetilde{FI}[2]4$

taking the value $y(20\pi) = 0.000392823991$ (see [29]). In Table 3.4 we present the absolute global error at $x = 20\pi$ with the number of function evaluations, F.Ev., for the following methods

- Method 1: the well known Runge-Kutta-Nyström method in [8]
- Method 2: the explicit eighth order method with maximal interval of periodicity in [29]
- Method 3: the sixth order hybrid method of Chawla and Rao in [3]
- Method 4: the P-C eight order method $FI[3]8$ in this paper
- Method 5: the P-C eight order method $\widetilde{FI}[3]8$ in this paper

We note that while the errors are similar with all the methods, the methods $FI[3]8$ and $\widetilde{FI}[3]8$ produce the better performances, being the formulation $\widetilde{FI}[3]8$ which needs the smallest number of function evaluations.

Method	F.Ev.	*MaxErr*
Method 1	14000	3.4×10^{-10}
Method 2	16000	3.2×10^{-10}
Method 3	16000	3.8×10^{-10}
Method 4	12000	1.8×10^{-10}
Method 5	6000	4.1×10^{-10}

Table 3.4 *Data for the problem in (3.38) with different methods*

3.5.4 Example 4.

The next example consists of the mildly stiff problem given by the linear system (see [15], [16])

$$\begin{aligned} &y''(x) = 2498y + 4998z, \quad z''(x) = -2499y - 4999z \\ &y(0) = 0, \quad y'(0) = 1, \quad z(0) = 0, \quad z'(0) = 1 \end{aligned} \tag{3.39}$$

with the exact solution $y = 2\cos x$, $z = -\cos x$.

The eigenvalues of the matrix of the system have modulus $|\lambda_1| = 2500$, and $|\lambda_2| = 1$. We have solved this problem in $[0, 2\pi]$ considering the methods $FEAMk$ and $FI[3]k$ for $k = 5, 6, 7, 8$ taking different number of steps $N = 200, 300, 400$. The results appear in Table 3.5 where we have included the errors measured in the norm $\|\cdot\|_\infty$, and the CPU time needed.

We have considered the methods and number of steps in Table 3.5 for this problem to highlight how important is to choose the method and the stepsize that suit the stability requirements in order to solve the problem properly.

3.5.5 Example 5.

The last example consists in the system that models the motion of two bodies, given by (see [26])

$$\begin{cases} y_1''(t) = \dfrac{-y_1(t)}{r^3} \\ y_2''(t) = \dfrac{-y_2(t)}{r^3} \\ y_1(0) = 1, \quad y_1'(0) = 0, \quad y_2(0) = 0, \quad y_2'(0) = 1, \end{cases} \tag{3.40}$$

Method	N steps	$CPU(s.)$	$MaxErr(y)$	$MaxErr(y')$
$FEAM5$	300	0.125	1.6005×10^{20}	4.4213×10^{21}
	400	0.188	5.2427×10^{-12}	7.1552×10^{-12}
$FI[3]5$	200	0.093	2.5509×10^{4}	1.4710×10^{6}
	300	0.172	5.8347×10^{-12}	7.5593×10^{-12}
$FEAM6$	300	0.125	1.9647×10^{52}	4.8460×10^{53}
	400	0.187	9.3717×10^{20}	3.1892×10^{22}
$FI[3]6$	200	0.109	5.0378×10^{9}	2.3892×10^{11}
	300	0.187	1.8252×10^{-13}	3.4094×10^{-13}
$FEAM7$	300	0.125	3.2773×10^{77}	7.4364×10^{78}
	400	0.187	2.2564×10^{58}	7.1188×10^{59}
$FI[3]7$	200	0.110	2.8934×10^{17}	1.1389×10^{19}
	300	0.203	3.6781×10^{-13}	5.7642×10^{-13}
$FEAM8$	300	0.125	3.3732×10^{97}	7.1745×10^{98}
	400	0.188	3.8269×10^{87}	1.1378×10^{89}
$FI[3]8$	200	0.109	1.0663×10^{26}	1.4867×10^{28}
	300	0.219	1.0280×10^{-13}	1.0943×10^{-12}

Table 3.5 *Maximum absolute error of the solution for different implementations of the explicit and implicit Falkner methods in P-C mode for solving the problem in (3.39)*

with $r = \sqrt{y_1^2 + y_2^2}$, and exact solution

$$y_1(t) = \cos(t), \quad y_2(t) = \sin(t).$$

This problem has been used as a test in a lot of articles presenting methods for solving initial value problems. We have solved the problem in the interval $[0,7]$, as was done in [31], using the methods $FEABk$ and $\widetilde{FI}[2]k$ for $k = 2,\ldots,10$, taking a number of steps $N = 112$ in all cases, which results in a stepsize $h = 0.0625$. The numerical results appear in the Table 3.6.

Finally, in Table 3.7 we show the data with the adapted Runge-Kutta method in [27], the classical Runge-Kutta method and methods $FEAM4$ and $\widetilde{FI}[2]3$. We have calculated at the endpoint of the integration interval the Euclidian norm of the error vector with components defined as the difference between the numerical and the exact solutions. We note that the methods $FEAM4$ and $\widetilde{FI}[2]3$ provide better results, even without considering that the RK methods need more evaluations of the function, and thus more computational effort.

	$FEAMk$:			
k	MaxErr y_1	MaxErr y_2	MaxErr y_1'	MaxErr y_2'
2	1.1651×10^{-3}	1.1781×10^{-3}	1.2740×10^{-3}	8.5695×10^{-3}
3	1.7458×10^{-5}	1.9902×10^{-5}	1.9762×10^{-5}	1.6453×10^{-5}
4	3.9115×10^{-6}	3.9177×10^{-6}	4.2581×10^{-6}	2.8593×10^{-6}
5	5.6869×10^{-8}	7.3229×10^{-8}	7.3142×10^{-8}	5.6222×10^{-8}
6	1.3264×10^{-8}	1.3101×10^{-8}	1.4338×10^{-8}	9.6002×10^{-9}
7	2.3774×10^{-10}	2.9070×10^{-10}	2.9288×10^{-10}	2.1161×10^{-10}
8	4.5591×10^{-11}	4.4313×10^{-11}	4.8903×10^{-11}	3.2613×10^{-11}
9	9.9675×10^{-13}	1.1674×10^{-12}	1.1874×10^{-12}	8.1706×10^{-13}
10	1.5953×10^{-13}	1.5451×10^{-13}	1.7053×10^{-13}	1.1368×10^{-13}
	$\widetilde{FI}[2]k$:			
2	5.3652×10^{-4}	5.4163×10^{-4}	5.8808×10^{-4}	3.9961×10^{-4}
3	3.1679×10^{-6}	1.8396×10^{-6}	2.6416×10^{-6}	1.4614×10^{-6}
4	8.5809×10^{-7}	8.3725×10^{-7}	9.2345×10^{-7}	6.2228×10^{-7}
5	1.4127×10^{-8}	1.0529×10^{-8}	1.3377×10^{-8}	8.3543×10^{-8}
6	1.7960×10^{-9}	1.6812×10^{-9}	1.8923×10^{-9}	1.2603×10^{-9}
7	5.3236×10^{-11}	4.2099×10^{-11}	5.2048×10^{-11}	3.2922×10^{-11}
8	4.1453×10^{-12}	3.6718×10^{-12}	4.2665×10^{-12}	2.7894×10^{-12}
9	1.9606×10^{-13}	1.5978×10^{-13}	1.9451×10^{-13}	1.2401×10^{-13}
10	2.1871×10^{-14}	2.0983×10^{-14}	2.3314×10^{-14}	1.5543×10^{-14}

Table 3.6 *Data for the problem (3.40) with the methods $FEAMk$ and $\widetilde{FI}[2]k$ for $k = 2, \ldots, 10$.*

h	$FEAM4$	$\widetilde{FI}[2]3$	Simos' method	Classical RK method
0.5	0.06	0.08	0.07	0.11
0.25	4.12×10^{-3}	5.54×10^{-3}	8.00×10^{-3}	1.10×10^{-2}
0.125	1.62×10^{-4}	1.80×10^{-4}	6.02×10^{-4}	8.29×10^{-4}
0.0625	5.53×10^{-6}	3.66×10^{-6}	4.05×10^{-5}	5.53×10^{-5}

Table 3.7 *Comparison of the Euclidean norms of the end-point global errors obtained by using Simos' method [27], the classical fourth- order RK method and the methods $FEAM4$ and $\widetilde{FI}[2]3$.*

3.6 Conclusions

Falkner methods are commonly used for solving the special second-order differential initial-value problem, particularly when the values of the derivatives are also needed (particularizations of these methods are the well-known Velocity-Verlet, Beeman's method or Wilson's method). On these approaches two formulas are needed for advancing the solution $y(x)$ and the derivative $y'(x)$. When the formu-

las are implicit, they are usually formulated in predictor-corrector modes.

We have considered three different modes to implement the implicit Falkner formulas and have ma de an analysis of the accumulated truncation errors. Considering the expressions of these errors for the solution and the derivative, we observe that the modes FI[2]k and FI[3]k show the best performance. The resulting errors in this case are both of order $\mathcal{O}(h^{k+1})$. In view of Table 3.1 we note that the errors of the explicit methods $FEAMk$ are also of order $\mathcal{O}(h^{k+1})$. On the other hand, if we do not perform the last evaluation of f with the implicit Falkner method in P-C modes the accumulated errors are also of order $\mathcal{O}(h^{k+1})$, but the stability characteristics are compromised. This fact could suggest that the explicit method $FEAMk$ would be the best choice because explicit methods are in general less time consuming than implicit ones. Nevertheless, the stability is a factor that should be considered (compare different performances in Table 3.5). We can say that if the stability requirements are fulfilled than the $FEAMk$ should be used, but in other situation the $\widetilde{FI}[2]k$ or even the $FI[3]k$ should be used. Some numerical examples are included to make a comparison of the numerical performance of the different implementations, resulting that the proposed methods may be competitive with other methods in the literature. The numerical results agree with the theoretical analysis.

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