**Solving Stiff Systems of Ordinary Differential Equations with Advanced Versions of the Richardson Extrapolation**

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**Abstract**

Different versions of the Richardson Extrapolation can be used together with Implicit Runge-Kutta Methods (**IRKMs)** in the efforts to obtain more accurate results during the numerical solution of stiff systems of Ordinary Differential Equations (**ODEs**). Select an **IRKM**, the order of accuracy of which is . Assume that a -Times Repeated Richardson Extrapolation, a **TRRE**, , where refers to the Classical Richardson Extrapolation (**CRE**) and refers to the Repeated Richardson Extrapolation (**RRE**), is used together with the selected **IRKM**. The order of accuracy of the resulting new numerical method, the combination **IRKM+**, is , which means that the accuracy can be increased substantially when an **IRKM** is applied together with some , but there is a danger that the computational process will become unstable and, therefore, it is also important to preserve the stability during the solution. Two new concepts, practical absolute stability regions and practical A-stability, are introduced. An algorithm, by which it is possible to determine the practical absolute stability regions for **any** combination **IRKM+** when the stability function of the underlying **IRKM** is known is developed. The algorithm can also be used to investigate whether the studied **IRKM+** is practically A-stable. The application of the algorithm is straight-forward. It requires a lot of computations, but that is not a problem when modern computers are used. It is shown that the **practical absolute stability regions** of three well-known particular **IRKMs** combined with different . Moreover, the combinations of two of these particular **IRKMs** with the Classical Richardson Extrapolation lead to practically A-stable methods. Possibilities for generalizing further the results are briefly discussed.

**Key words and phrases:** Ordinary Differential Equations, Implicit Runge-Kutta Methods, Advanced Versions of the Richardson Extrapolation, Accuracy and stability, Practical Absolute Stability Regions, Practical A-stability.

***AMS subject classification*:** 65L05, 65L06, 65L04.

**1. Introduction**

Consider the Initial Value Problem for a system of Ordinary Differential Equations (ODEs):

It is assumed that the system of ODEs defined by **(1)** is stiff, which implies that implicit numerical methods must be used (**[2]**, **[3]**, **[5]**, **[7]**, **[8]**, **[9]**, **[12]**, **[14]**). Approximations of the solution vector:

**, , … , , … ,**

are calculated by applying the selected implicit numerical method on an equidistant grid:

The stepsize used in **(3)** is constant, but some results can be extended for non-equidistant grids.

Runge-Kutta methods are often used in the treatment of **(1)**. These methods were introduced by Heun **[11]**, Kutta **[13]** and Runge **[16]** and are described in many text-books on numerical solution of systems of ODEs (**[2]**, **[3]**, **[7]**, **[8]**, **[9]**, **[10]**, **[14]**, **[17]** and **[18]**). The assumption that **(1)** is stiff implies that **stable** Implicit Runge-Kutta Methods (**IRKMs**) are to be selected and used. If it is desirable to increase the accuracy of the calculated results, then it is appropriate to apply different versions of the Richardson Extrapolation (defined originally in **[15]**, see also **[4]**, **[6]**, **[21]**, **[22]**, **[23]**, **[24]**, **[25]**, **[26]**). However, severe problems related to the preservation of the stability of the computational process based on the use of a combination of an **IRKM** with different versions of the Richardson Extrapolation may arise. It is proved in **[23, p. 133]**, see also **[5]**, that the combination of a numerical method with Richardson Extrapolation might be unstable even if the selected numerical method has very good stability properties (even if it is A-stable). This example shows clearly that it is both necessary and very important to develop a **general algorithm**, which can be easily used to study the stability properties of the combinations of **any IRKM** with a known stability function when it is applied together with different advanced versions of the Richardson Extrapolation. Such an algorithm is presented in **Section 3** and stability regions obtained in the application of this algorithm in connection with three particular **IRKMs** listed in **Section 4** and combined with several versions of the Richardson Extrapolation are discussed in **Section 5**. A family of numerical examples for testing the stability is constructed and used in **Section 6**. Several concluding remarks are given in **Section 7**.

Stability properties of the Classical Richardson Extrapolation and of some lower versions of the Repeated Richardson Extrapolation (One- or Two-Times Repeated Richardson Extrapolation) have been studied in several papers (**[21]** and **[23]-[26]**). The use of more advanced versions of the Richardson Extrapolation, up to Eight-Times Repeated Richardson Extrapolation, for **non-stiff systems** of Ordinary Differential Equations was studied in **[22]**. We shall extend the results presented in **[22]** for the important, from the practical point of view, case when the solved systems of Ordinary Differential Equations are stiff. This fact imposes very often great difficulties with the preservation of the stability during the computations and special methods, which both preserve the stability of the computational process and are sufficiently accurate, have to be developed and used.

**2. Basic properties of the advanced versions of the Richardson Extrapolation**

Several advanced versions of the Richardson Extrapolation were introduced and tested in **[22]** under two major assumptions: **(a)** the system of ODEs **(1)** is non-stiff and **(b)** Explicit Runge-Kutta Methods (**ERKMs**) can successfully be used during the solution process. Some of the main results reported in **[22]** and slightly modified for the purposes of the present paper are briefly discussed in this section. Then these results are applied to study the case where **(1)** is stiff, which implies, as mentioned above, the use of Implicit Runge-Kutta Methods (**IRKMs**). The stability properties of the combinations of **IRKMs** with advanced versions of the Richardson Extrapolation are discussed in the next section.

It is first necessary to describe the calculations that are to be carried out at a given step when an arbitrary **IRKM** is used together with a **q-Times Repeated Richardson Extrapolation (**a **)**.

**Definition 1:** Assume that **(a)** a stable **IRKM** is chosen, **(b)** an integer is fixed and **(c)** a vector is available. Use the selected **IRKM** with stepsizes to perform respectively steps and to calculate auxiliary vectors . The first vector is calculated by performing one step with a stepsize . The second vector is obtained by applying two steps with a stepsize . It is necessary to continue in this way and the last auxiliary vector is obtained by performing steps with a stepsize . The calculations used in the computation of **any** of the auxiliary vectors , are started by . Then the **IRKM+** vector can be calculated by applying the following formula:

**■**

It is assumed in **Definition 1** that the Classical Richardson Extrapolation (**CRE**) is used when while the Repeated Richardson Extrapolation (**RRE**) is used when .

It is necessary to explain how the quantities and can be calculated.

**Calculation of**  It is proved in **[22]** that the values of for can be obtained by applying the following formula:

The calculation of by using **(5)** is a straight-forward but technically difficult task when is large. The computational work can be simplified by applying the recursive formula (**[22]**):

The equalities **(5)** and **(6)** hold **(a)** for an arbitrary **IRKM** and **(b)** for any . It was furthermore **conjectured** in **[22]** that **(5)** and **(6)** are also true when .

**■**

**Calculation of .** Assume that is computed for some by using **(5)** or **(6)**. Then the terms in the expression can successively be calculated as follows. The first term in is obtained by multiplying the first term of by . The second term in is obtained by multiplying the second term of by . This process should be continued in the same manner and the last term in will obtained by multiplying the last term of by .

**■**

The order of accuracy is increased when an **IRKM** is combined with a , .

**Theorem 1:** Let an **IRKM**, the order of accuracy of which is , be used together with some with to solve numerically **(1)**. Then the order of accuracy of the new numerical method, the combination **IRKM+**, will be at least if the right-hand-side of **(1)** is at least times continuously differentiable.

**■**

**Major relationships involving the stability functions of the IRKMs.** Let be the stability function of an **IRKM** (the definition of the stability function of an **IRKM** can be found for example in **[8]**, **[9]** or **[14]**). Assume that the selected **IRKM** is used to solve the following scalar and linear test-problem, proposed originally in **[5]**:

Then the relationships

,

hold, **[14]**, and, therefore, the computational process will be stable for when .

**■**

**Theorem 2:** Consider an **IRKM** with a stability function , . Then the stability function of the combination of this **IRKM** with the -Times Repeated Richardson Extrapolation, the, , can be obtained by using the formula:

**■**

**Calculation of** Assume that is obtained by using either **(5)** or **(6)**. The first term in can be found by multiplying the first term of  by . The second term in  can be found by multiplying the second term of  by . The third term in  can be found by multiplying the third term of  by . Continuing in this way, it is clear that the last term in  can be found by multiplying the last term of  by .

**■**

**Remark 1:** All formulae for and when , can be found in **[22]**.

**■**

**Conjecture 1:** The assertions in **Theorem 1** and **Theorem 2** are true for any non-negative integer .

**■**

It should be mentioned here that the results in this section are simple corollaries of results obtained in **[22]**. These results are needed and will be used in the following sections.

**3. Stability properties of IRKMs applied together with ()**

The second theorem in Section 2, **Theorem 2**, is establishing a relationship between the stability function of an **IRKM** and the stability function of its combination with a when . Unfortunately, this relationship cannot be exploited to draw direct conclusions about the stability of different versions of the Richardson Extrapolation combined with **IRKMs**. Therefore, additional results related to the stability properties of the combinations of **any** **IRKM** with a , are to be derived for . The fact that with can be calculated by using **(9)** when is known plays **a central role** in the construction of the important **Algorithm 1** introduced in the end of this section. The application of this algorithm to study the stability of the three particular **IRKMs** from **Section 4** combined with a  with indicates that the computations will be stable in **extremely** large regions when these methods are applied in the solution of the test-equation ( and ) from **[5]**. Similar results can be established for an arbitrary **IRKM** with a known stability function when this method is combined with any with .

Three parameters, , and , are to be used in the construction of an algorithm for studying the stability properties of the combination of **any** **IRKM** with a , . The domain , in which it is desirable to study the stability, is determined by selecting an appropriate value of parameter (**Definition 2**). A discretization of the specified domain is performed by applying the parameter (**Definition 3**). The third parameter is used in the stability checks (**Definition 4**).

**Definition 2:** If is some positive real number, then  is the square the vertices of which have coordinates .

**■**

**Definition 3:** If is some positive real number and is a positive integer such that , then set contains **all** points with coordinates obtained by using and . The points in set can be considered as grid-points in the domain which are obtained by using a discretization parameter .

**■**

**Definition 4:** Consider some and any **IRKM** with a **known** stability function . Combine this **IRKM** with a -times Repeated Richardson Extrapolation, a , . Use **(9)** to calculate the values of the stability function at all points of , i.e. to calculate the values of for , , , and . The points of the set for which the inequality is satisfied will be called **green points**, while the name **red points** will be used for all points in for which .

**■**

Assume that it is possible to apply **exact arithmetic**. Then the stability check can be used with and the calculations will be stable at the **green points** of . More precisely, the following statement is true:

**Statement 1:** Assume that **exact arithmetic** is used with and that ( and ) is solved with some such that . Then the computations carried out by the combination **IRKM**+ with will be **stable** according to the classical definition from **[5]** when belongs to the set of **green points** in .

**■**

Values of are calculated by using exact arithmetic in **Statement 1** and it is checked whether the requirement is satisfied at the grid-points of . It is desirable however that this inequality holds in the whole when all grid-points of the set are **green** or at the part of which contains only **green points** when there are both **green** and **red** points in . Therefore, it is necessary to assume additionally that the discretization is fine, i.e. that is sufficiently small. Then the computations related to the solution of ( and ) from **[5]** should be expected to be stable in the whole when all points of are **green** or in the part of the domain which contains **the green points** of when there are both **green** and **red** points in this set. This observation allows us to formulate two statements. The first of these statements is useful in the attempts to generalize the classical concept of **A-stability** (the definition of A-stability can be found, for example, in **[14]**), while the second one allows us to generalize the concept of **absolute stability region** (see again **[14]**).

**Statement 2:** Assume that an **IRKM+** with is applied in the solution of the equation ( and ) from **[5]**. If **(A) exact arithmetic** is used with , **(B)** is sufficiently small and **(C)** all points of are **green**, then one should expect that the computations will be **stable** when or, in other words, one should expect that is **a part of the absolute stability region** of the **IRKM+** in the sense of the definition from **[5]**. If the value of is increased keeping fixed and if all points of the increased set are still **green**, then a **larger part** of the **absolute stability region** will be obtained.

**■**

**Statement 3:** Assume that an **IRKM+** with is used in the solution of the equation ( and ) from **[5]**. If **(A)** **exact arithmetic** is used with , **(B)** is sufficiently small and **(C)** there are both **green** and **red** points in , then one should expect the computations to be **stable** in the sub-domain of which contains only the **green points** of , i.e. the sub-domain of which contains only the **green points** of is **a part of the absolute stability region** of the **IRKM+** in the sense of the definition from **[5]**. If is increased keeping fixed then a **larger part** of the **absolute stability region** might be obtained.

**■**

In the above statements it is assumed that **exact arithmetic** is used with . However, exact arithmetic cannot in general be applied when a computer is used in the calculations. The following example shows that the stability check may sometimes cause difficulties when is calculated on computers. More precisely, the rounding errors are creating problems when the value of is very close to . Assume that and that the Backward Euler Formula (see the next section) is used in a combination with the **7TRRE**. Assume furthermore that and that extended machine precision (involving computations with significant digits of the real numbers) is used during the calculations. Then was found for . It is clear that this result may be affected by rounding errors and it is **impossible**, if the computer precision is fixed as above, to answer the question whether is greater than or whether it is less than at the point . If it is necessary to find the answer of this question, then the application of more precise computer arithmetic (using for example significant digits of the real numbers) might give an answer. However, the answer is not very important in this case. The important issue is that  is very close to and one should expect that the results of the computations will not be affected by computational instability even when the exact value of , which we are not able to calculate with the selected extended precision computer arithmetic, is greater than . This example shows clearly that it is worthwhile to introduce a stability check which is more suitable for computers. Such a check can be obtained by replacing the requirement , which causes difficulties when is very close to , with a weaker requirement where . However, the following remark shows that one must be careful.

**Remark 2:** If , then we may have at **some of the green points** of and the classical definition for absolute stability from **[5]** **will not hold** for such points. However, if is **sufficiently small** and if a **finite number of step**s is to be carried out, then the effect of instability will not be observed during the actual computations at any of the **green points** of .

**■**

The above remark shows that it is important to select properly the value of parameter . Many experiments indicate that is giving good results when double precision computer arithmetic (working with sixteen significant digits of the real numbers) is used. This choice is a good compromise. It is not too close to the machine accuracy, which is . On the other hand, is small even if . Other choices could also be made. If, for example, extended machine precision is to be used, then much smaller value of might be selected.

Two concepts, **practical absolute stability regions** and **practical A-stability**, which are important when the stability properties of **IRKMs** combined with some , , are to be investigated, can be introduced now.

**Definition 5 (Practical A-stability):** Assume that an **IRKM+**, , is used to solve the equation ( and ) from **[5]**. If **(A)**  is very large, **(B)**  and are sufficiently small, **(C)** **all** points of are **green** and **(D)** the number of steps is finite, then one should expect that the results will be stable when . The **IRKM+** will be called **practically A-stable** when these conditions are satisfied.

**■**

**Definition 6 (Practical absolute stability regions):** Let an **IRKM+**, , be used to solve the equation ( and ) from **[5]**.If **(A)** and are sufficiently small, **(B)** there are both **green** and **red** points in and **(C)** the number of steps is finite, then the sub-domain of which contains only **green** points of is **a part of the** **practical absolute stability region** (if is increased, but and are kept unchanged, then **the part of the practical absolute stability region** may also be increased). One should expect the computations to be stable when is inside the **practical absolute stability region**.

**■**

**Remark 3:** The comparison of **Definition 5** and **Statement 2** indicates that the classical **A-stability** can be obtained as a boundary case of the **practical A-stability** when . This means that the **practically A-stable** and the **A-stable** methods will have similar properties when is large while both and are small. The comparison of **Definition 6** and **Statement 3** indicates that a part of the classical **absolute stability region** on the domain determined by the choice of parameter can be obtained as a boundary case of the part of the **practical absolute stability region** when . This means that if and are small, then the performance of the numerical methods when is belonging to the practical absolute stability region will be similar to the performance of the numerical methods when is belonging to the absolute stability region.

**■**

**Remark 4:** The regions of **absolute stability** are symmetric with regard to the real axis, **[14]**, and it is sufficient to apply only non-negative values of from when the absolute stability properties of the chosen numerical method are to be investigated. The same is also true if **practical absolute stability regions** and **practical A-stability** are considered, i.e. it is again sufficient to consider only non-negative values of in the stability studies. This fact was exploited in the construction of the square in **Definition 2**.

**■**

**Remark 5:** There is no need to require **bounded approximations** of the solution of () if , i.e. if , because the exact solution of this equation is **unbounded** in this case. It is relevant to introduce the requirement (with some sufficiently small non-negative ) and to study **the practical absolute stability regions** or the **practical A-stability** of the selected **IRKM+** with  **only** when .

**■**

**Remark 6:** The test-equation ( and ) from **[5]** is rather special, but the importance of results derived by using this equation is emphasized in many books and papers; see, for example, **[20, page 37]**. It is of course desirable to obtain more general results. Many attempts to resolve this task and to proof stability results for more general cases, i.e. in connection with more general test-equations, have been carried out (see for example **[2]**, **[3]**, **[8]**, **[9]**, **[12]** and **[14]**). The above definitions and remarks can be modified and applied also for many of these test-equations.

**■**

**Remark 7:** A linear system , ( and ) can be considered instead of . If all eigenvalues () of matrix satisfy the condition and are distinct, then the system can be reduced to **independent** linear and scalar ODEs (see, for example, **[14]**) and the computational process will be stable if holds with a sufficiently small for **all** eigenvalues of matrix , i.e. the relation (where contains only the **green** points of ) must be satisfied for **all** eigenvalues of matrix .

**■**

**Algorithm 1**: Choose an arbitrary **IRKM** with a **known** stability function and select a **large** . Discretize the square with vertices by using a **small** to obtain a set of grid-points **.** Consider some combination **IRKM**+ with and calculate the values of at **all** points of . Use a **small** parameter to determine the **green points** in , i.e. the points for which the inequality is satisfied. If and are **sufficiently small**, then the sub-domain of which contains only **green points** of will be a part of the **practical absolute stability region** of the numerical method based on the selected combination **IRKM**+ with . If furthermore **all** grid-points of set are **green** when the above conditions are satisfied, then the numerical method defined by the combination **IRKM**+ with is **practically A-stable**.

**■**

**Remark 8:** If **exact arithmetic** is used with and with a sufficiently small , then **a part of the absolute stability region**, where the classical definition from **[5]** holds, will be determined when **Algorithm 1** is used.

**■**

**Remark 9:** An example related to the choice of the parameters , and is given in **Section 5**.

**■**

**Remark 10:** All statements from the last two sections are valid for **any** method from the more general class of **one-step methods** for solving systems of ODEs if its stability function is known.

**■**

**4. Selection of three particular Implicit Runge-Kutta Methods**

Three representative **IRKMs** will be presented in this section. The **practical absolute stability regions** of the combinations of these methods with different versions of the Richardson Extrapolation will be studied, by using **Algorithm 1**, in the next section.

**Backward Differentiation Formula:** The Backward Differentiation Formula (well-known also as the Backward Euler Method) is a **One-stage First-order** **IRKM**. The abbreviation **EULERB** will be used. **EULERB** is an L-stable method for solving systems of ODEs (**[2]**, **[3]**, **[9]**, **[10]**, **[12]**, **[14]**, **[19]**, **[20]**) defined by

One system containing algebraic equations must be solved at every step and iterative procedures (normally some versions of the Newton Iterative Method) must be applied when **(1)** is non-linear.

**Two-stage Third-order Diagonally Implicit Runge-Kutta Method (DIRK23 Method):** The second particular method is an A-stable Two-stage Third-order Diagonally Implicit Runge-Kutta Method, a **DIRK23** Method. It is based on the following formulae:

**DIRK** methods were introduced by R. Alexander **[1]** in 1977. The **DIRK23** defined by **(11)** - **(13)** is taken from **[14**]. Only remains unknown in **(13**) when **(12)** is already solved and is found. This means that two systems of algebraic equations, each of them containing equations, have to be solved successively at every step. Iterative procedures (for example, the Newton Iterative Method) must be applied when **(1)** is a non-linear system of ODEs. The coefficients in front of and in the right-hand-sides of **(12)** and **(13)** are the same. Therefore, there is a good chance to solve the second system, **(13)**, by using the factorization obtained during the solution of the system **(12)**.

**Three-stage Fifth-order Fully Implicit Runge-Kutta Method (FIRK35 Method):** A well-known **FIRK35** Method defined by equalities **(14) - (17)** was selected. This method is quoted in many text-books on numerical solution of ODEs, see, for example, **[3]**, **[8]** and **[9]**. Let . Consider some and assume furthermore that andare vectors in. Then the selected **FIRK35** Method is based on the following formulae:

Systems of algebraic equations are to be treated at every step when the above method is used. The Jacobian matrix of the system defined by **(15) - (17)** is a matrix. This causes a substantial increase of the computing work in comparison with the previous two methods where matrices are to be handled. Additional computational problems may arise when the Jacobian matrix of vector from **(1)** has some special property (which often happens in practice). The following example illustrates this fact. If the Jacobian matrix of vector from **(1)** is tridiagonal (which may occur when partial differential equations are semi-discretized, see for example **[19]** and **[20]**), then this feature can very efficiently be exploited when either **EULERB** or **DIRK23** is used. The Jacobian matrix from **(15) – (17)** is not tri-diagonal and this is why **FIRK35** is causing much more computational difficulties than **EULERB** and **DIRK23** when the Jacobian matrix of is tridiagonal.

The **FIRK35** has also some advantages: it is L-stable and very accurate, **[3]**, **[8],** **[9]**.

**Basic properties of EULEB, DIRK23 and FIRK35:** The basic properties of **EULERB**, **DIRK23** and **FIRK35** are described in **Table 1**.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Method** | **Stages** | **Accuracy** | **Stability** | **Stability function** |
| **EULERB** | One | One | L-stable |  |
| **DIRK23** | Two | Three | A-stable |  |
| **FIRK35** | Three | Five | L-stable |  |

**Table 1**

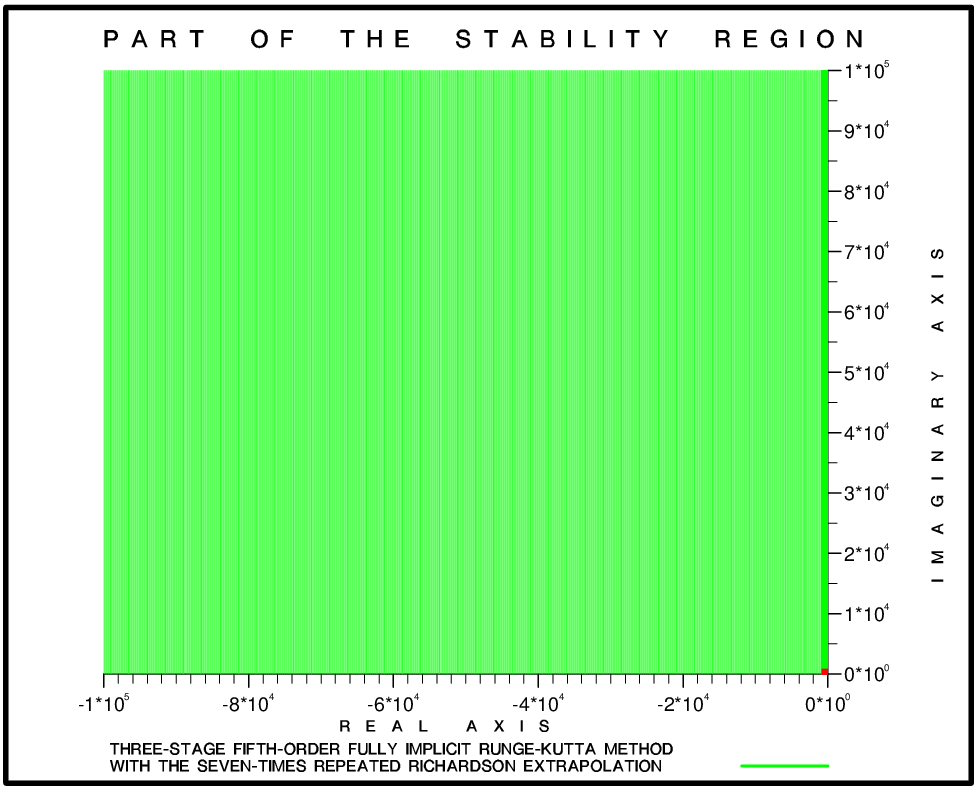
Numbers of stages, orders of accuracy, types of stability and stability functions of the **IRKMs** introduced in this section

**5. Stability of the three special IRKMs combined with**

The combinations of any of the three **IRKMs** from **Section 4** with eight versions of the Richardson Extrapolation obtained with were systematically studied by using **Algorithm 1** with , and . Several experiments with and/or were also carried out. The results from all these investigations show that nearly all of the grid-points of set , obtained after the discretization of the square with vertices by using , excepting quite a few points near to and on the imaginary axis, were **green** for all **27** methods (for the combinations of any of the three **IRKMs** with the nine versions of the Richardson Extrapolation). This means that one should expect the computations to be stable when the test-equation from **[5]** is solved in a large part of the square **excepting some very small areas near to and on the imaginary axis**.

**The part of the practical absolute stability region** for **FIRK35+** is given in **Fig. 1**. The instability intervals on the imaginary axis for the three **IRKMs** applied with eight versions of the  () were determined by using two values of ( and ) and listed in **Table 2**. There are sometimes some small additional areas located very near to the imaginary axis, where the tested versions of the Richardson Extrapolation are unstable too. That is illustrated in **Fig. 2** for the instability region of **FIRK35+** and in **Table 3**, where the intervals of instability near to the imaginary axis are given for when **EULERB** is used together eight versions of the ()**.**

The region shown from **Fig. 2** is the largest instability region of the tested methods, but it is negligibly small in comparison with **the practical absolute stability region** which is presented in **Fig. 1**. A small square with vertices is marked in **red** in **Fig.1**. The rectangle is a very small part (less than **0.01%**) of **the red square** in **Fig. 1**. The instability region shown in **Fig. 2** is located in this rectangle, but it does not fill the whole red rectangle. This fact is illustrating very well the statement that the part of the green square in **Fig. 1**, i.e. the part of the square with vertices , in which the numerical method **FIRK35+** is not stable is negligibly small (it was not possible to show so small instability region in **Fig. 1** and we had to mark in red a much larger area in the efforts to explain better the results). Similar conclusions can be easily derived for all other **26** combinations of the three particular **IRKMs** with ().



**Figure 1**

The green area is a **part of the practical absolute stability region** of **the Three-stage Fifth-order FIRK Method** when it is used together with **the Seven-Times Repeated Richardson Extrapolation**. This plot shows that one should expect that the computations will be stable nearly everywhere in a very large green square whose side is when the test-example from **[5]** is solved. Some problems may arise only in a tiny area near to and on the imaginary axis (see also the results presented in **Table 2**, **Table 3** and **Fig. 2**). A small area in **Fig. 1** is marked in red. Instability may appear in a very small sub-region of the red area which is containing less than **0.01%** of it.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Method** | **EULERB** | | **DIRK23** | | **FIRK35** | |
|  |  |  |  |  |  |
| **CRE** | **No stability problems near to or on the imaginary axis** | | | | [0.2, 0.6] | [0.159, 0.605] |
| **RRE** | [0.1, 0.8] | [0.003, 0.861] | [0.1, 1.0] | [0.037, 1.002] | [0.3, 5.5] | [0.243, 5.501] |
| **2TRRE** | [0.1, 1.7] | [0.023, 1.709] | [0.2, 2.5] | [0.122, 2.518] | [0.4, 12.4] | [0.385, 2.455] |
| **3TRRE** | [0.7, 2.7] | [0.601, 2.748] | [1.0, 5.1] | [0.957, 5.181] | [8.1, 25.2] | [8.089, 25.269] |
| **4TRRE** | [1.3, 4.0] | [1.246, 4.080] | [2.6, 9.8] | [2.510, 9.877] | [1.0, 48.8] | [0.966, 48.859] |
| **5TRRE** | [0.3, 5.7] | [0.268, 5.774] | [5.5, 18.3] | [5.418, 18.373] | [1.6, 91.2] | [1.533, 91.213] |
| **6TRRE** | [0.6, 7.9] | [0.518, 7.901] | [1.7, 45.6] | [1.691, 45.687] | [8.1, 165.1] | [8.045, 165.169] |
| **7TRRE** | [1.0, 10.5] | [0.988, 10.527] | [3.1, 78.4] | [3.019, 78.402] | [3.9, 291.1] | [3.861, 291.138] |

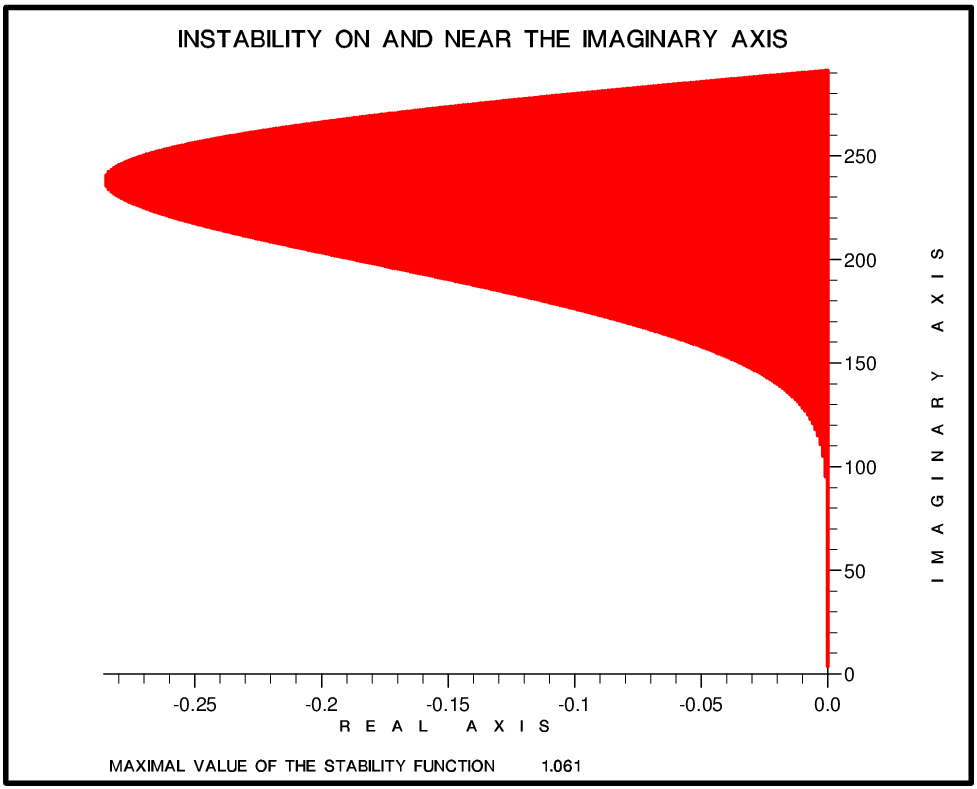
**Table 2**

Instability intervals on the imaginary axis when the three particular **IRKMs** are combined with the Richardson Extrapolation. The **IRKM** () is declared as unstable when . Two values of are used. The instability intervals are becoming slightly larger when is selected. The results from the two tests indicate that the use of is sufficient.Both **EULERB** and **DIRK23** are producing only **green points**, when the check with is used with , i.e. when the Classical Richardson Extrapolation (**CRE**) is used. It should also be noted that some of the methods are unstable not only on the imaginary axis but also in tiny areas near to the imaginary axis, see **Fig. 2** and **Table 3**.

|  |  |  |  |
| --- | --- | --- | --- |
| **Version** |  | **Instability intervals** | **max** |
| **CRE** | **No stability problems near to or on the imaginary axis** | | 1.000000000000000 |
| **RRE** | 0.000 | [0.001, 0.861] | 1.001409700579226 |
| -0.001 | [0.521, 0.774] |
| **2TRRE** | 0.000 | [0.002, 1.709] | 1.002999016157321 |
| -0.001 | [0.869, 1.649] |
| -0.002 | [1.071, 1.566] |
| **3TRRE** | 0.000 | [0.004, 2.748] | 1.002859386184047 |
| -0.001 | [1.542, 2.659] |
| -0.002 | [1.848, 2.532] |
| **4TRRE** | 0.000 | [0.001, 4.080] | 1.002011478645706 |
| -0.001 | [2.634, 3.904] |
| **5TRRE** | 0.000 | [0.001, 5.774] | 1.001134718380822 |
| -0.001 | [4.529, 5.251] |
| **6TRRE** | 0.000 | [0.002, 7.901] | 1.000523089820448 |
| **7TRRE** | 0.000 | [0.001,10.527] | 1.000196510143713 |

**Table 3**

Instability intervals near to and on the imaginary axis when **EULERB** is combined with eight versions of the Richardson Extrapolation. The results are obtained by using and it is clearly seen that the regions of instability are considerably smaller than the region of instability of the **FIRK35+** shown in **Fig. 2**. No instability intervals are detected with the fine accuracy test used in the computations () when the Classical Richardson Extrapolation is used, which indicates that the combination **EULERB+CRE** is practically A-stable.



**Figure 2**

Instability region of**FIRK35+** obtained with . The maximal value of the stability function is **1.061**. Many values of the stability function in the red area are in fact much smaller than **1.061** (but greater than ).

**6. Numerical results**

The following **three-parameters family** was constructed and used systematically in the experiments:

The elements of matrix from **(18)** depend on the parameters , and :

The three components of the exact solution of the problem defined by **(18) – (21)** are given by

**, ,**

The eigenvalues of matrix the elements of which is defined in **(19) - (21)** are:

.

In order to ensure stable computations during the solution of this example, one should require that **all** three points **,**  and are inside the absolute stability region of the chosen numerical method for the selected value of the stepsize. The numerical results indicate that it is enough to require that all eigenvalues are inside **the practical absolute stability region**. The results remain very often stable even if the two points and are outside the practical absolute stability regions, but close to it. That is not a very big surprise because in this case and are greater than but still very close to this number.

It can easily be seen, by studying the formulae representing the exact solution and the eigenvalues of matrix , that the three-parameters family defined by **(18) – (23)** has the following properties:

**(a)** Increasing the absolute value of and keeping the values of and  fixed, leads to an increase of the stability requirements on the negative real axis. That is especially pronounced when and are kept small. If this is so and is large, then it will be enough to require that is inside the absolute stability interval on the negative real axis.

**(b)** Increasing the value of leads to an increase of the oscillations and, thus, to an increase of the accuracy requirements. This is clearly seen by comparing the four plots given in **Fig. 3**. These plots show that the increase of the value of parameter is causing a very significant increase of the number of oscillations and, thus, of the accuracy requirements during the numerical solution. It is becoming more and more difficult to satisfy the accuracy requirements when parameter is increased. However, very large values of will also cause stability problems related to the height of **the practical absolute stability region** (the influence of the complex eigenvalues is becoming more and more significant when is becoming very large).

**(c)** By varying the value of one can move the complex eigenvalues either close to the imaginary axis or long away from it. If it is interesting to study the stability properties of the tested numerical method at the critical points located either near to or even on the imaginary axis, then small values of or even should be selected.

This short analysis shows clearly that it is possible to change systematically the locations of the eigenvalues of matrix in the negative part of the complex plane and to steer in this way both the accuracy requirements and the stability requirements by selecting appropriate values of the three parameters. We are interested in testing the stability of the methods in a small area near to and on the imaginary axis, where difficulties may appear (see the results in the previous section). Therefore, we carried out experiments both with small positive values of and with .

In the tests the values of and are fixed ( and ) and four values (, , and ) are used. The plots of **the first component** of the exact solution when the parameters are selected in this way are shown in **Fig. 3**. It is seen that the number of oscillations is increased very quickly when parameter is becoming larger. The behaviour of the other two components of the solution vector is very similar.

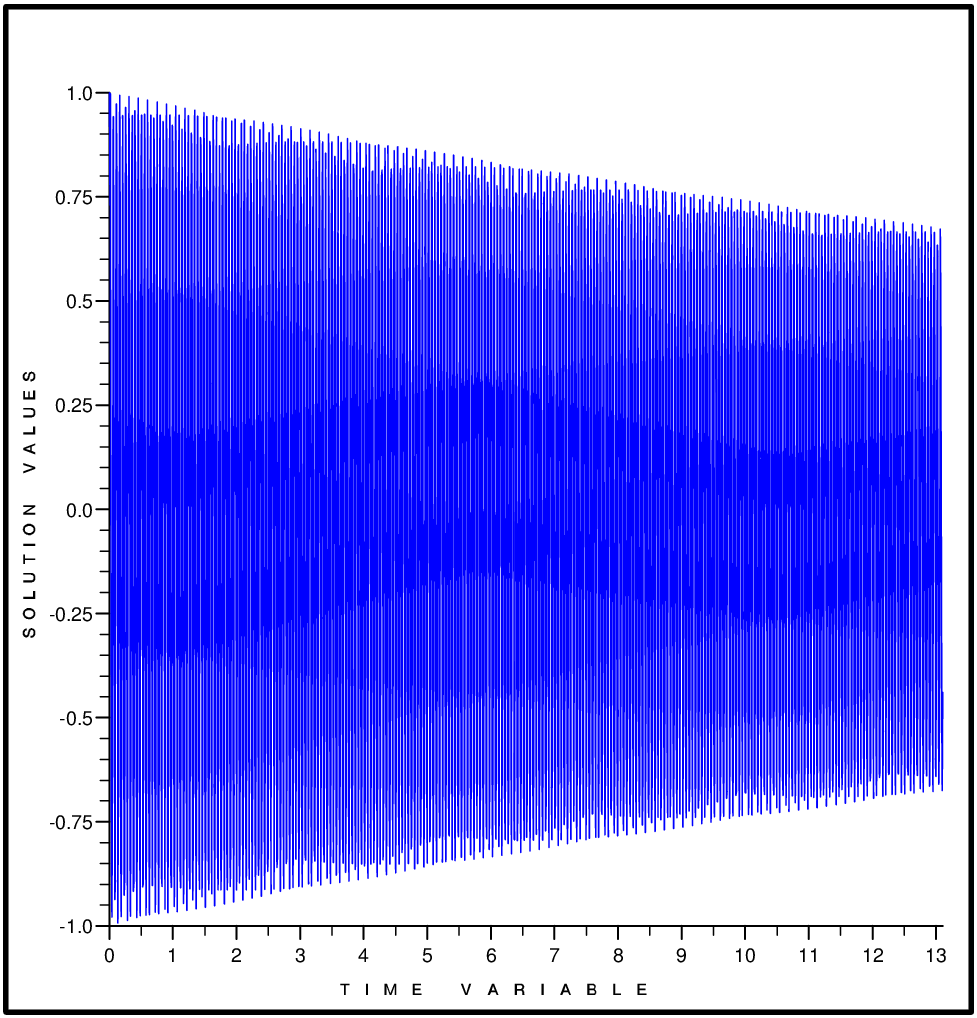
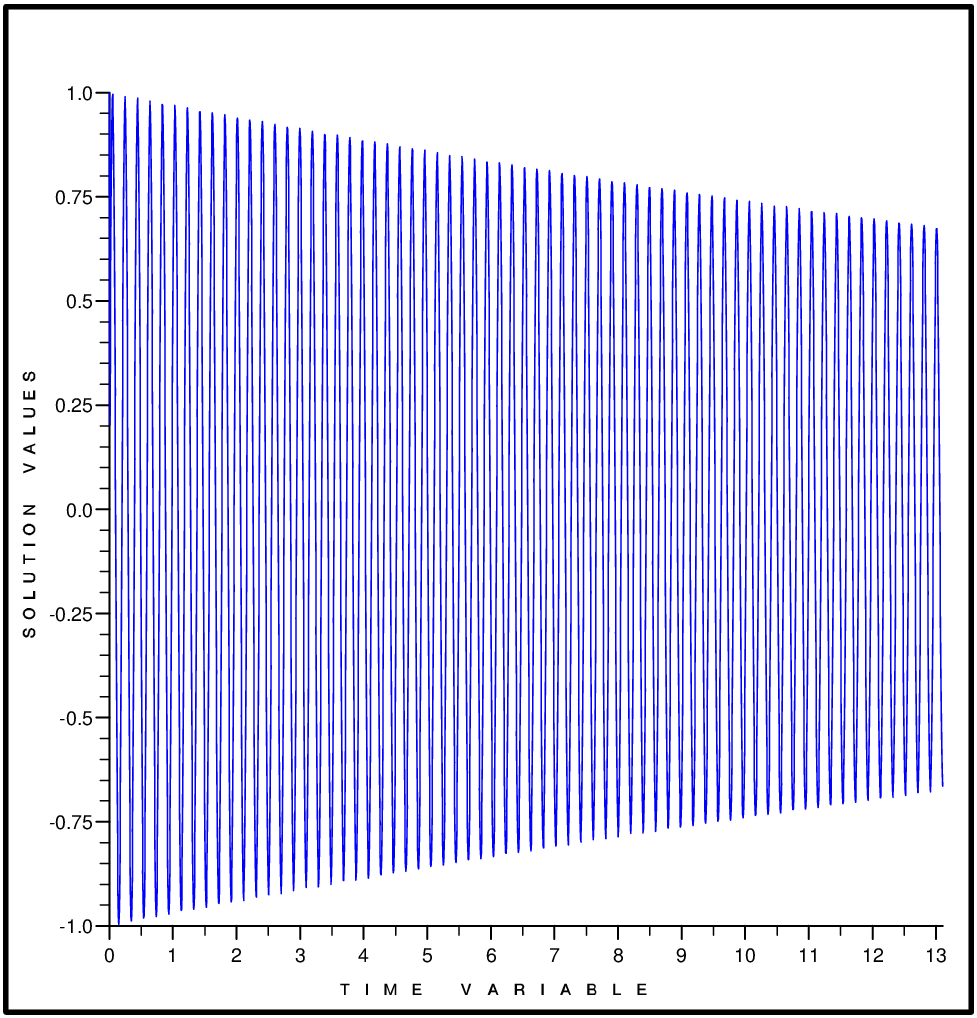
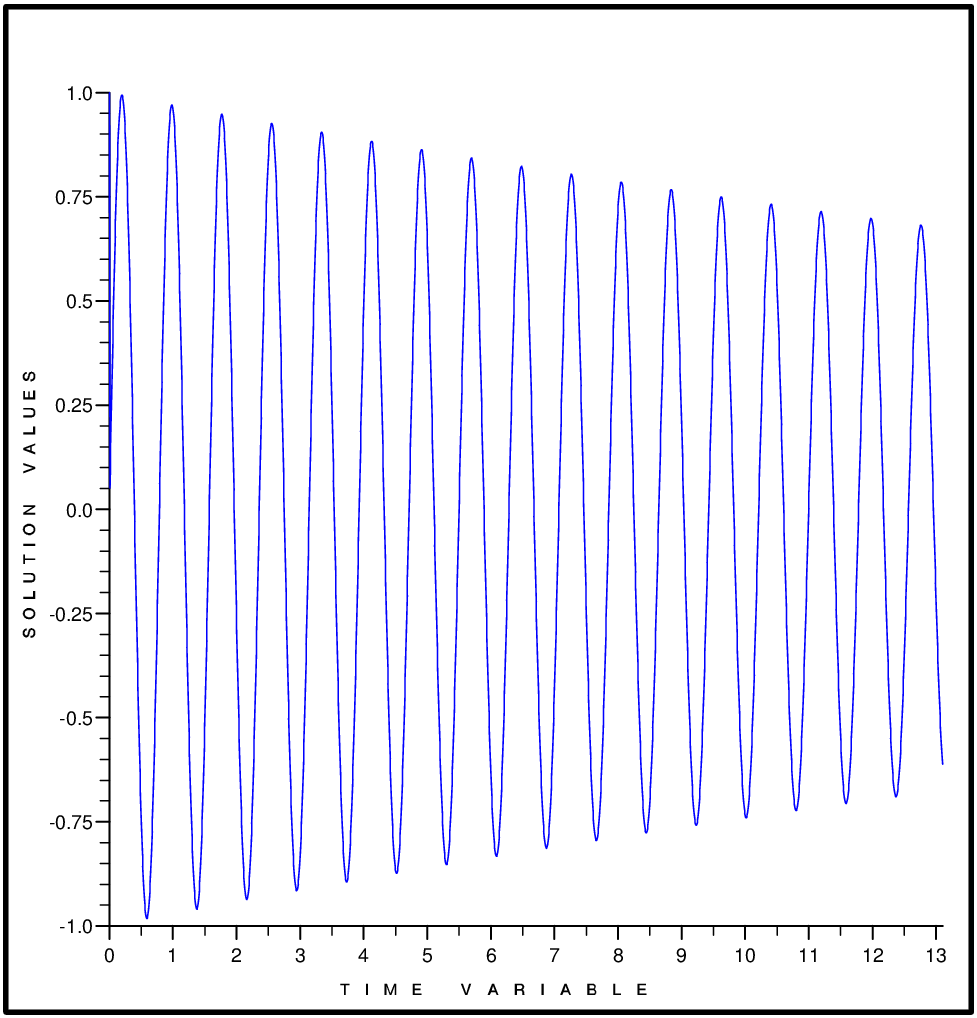
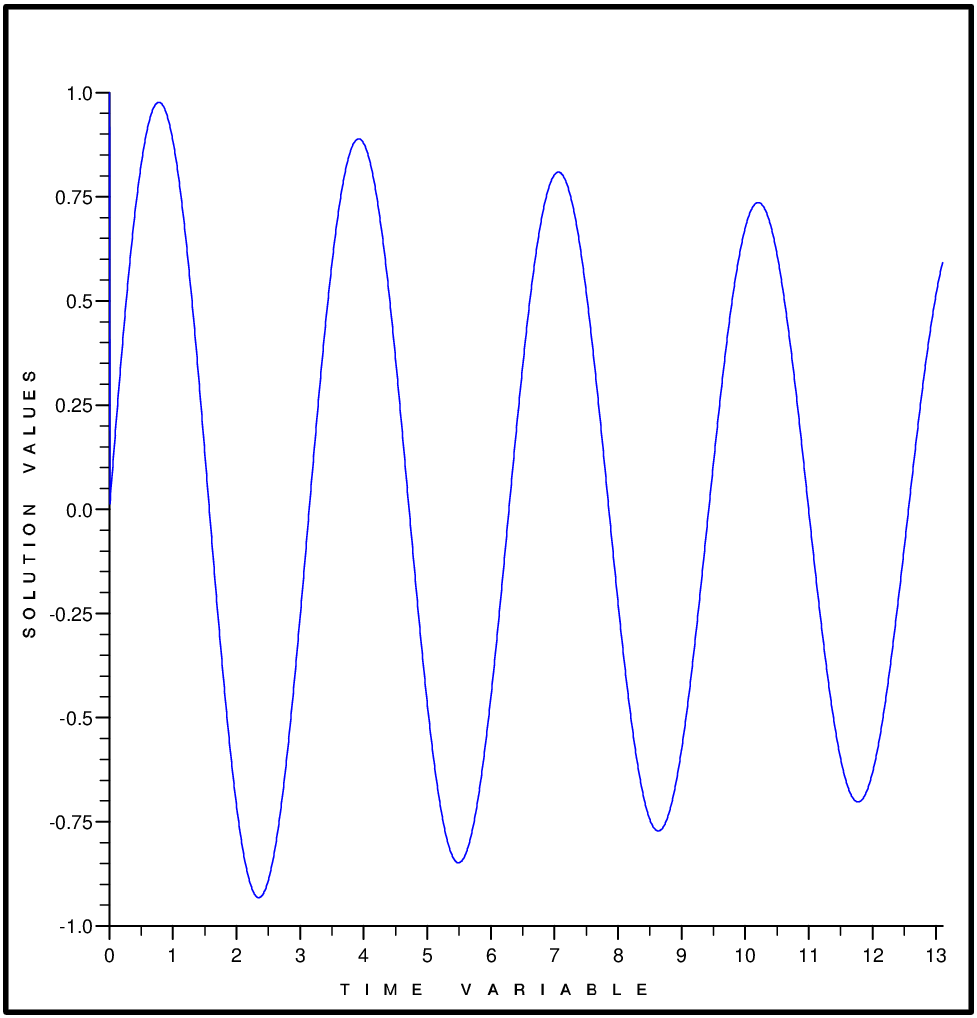
The computations are organized in the following way. The interval was divided into equal sub-intervals. The accuracy of the computed results obtained by the three numerical methods from **Section 4**, when these are applied both directly and in combination with any of the eight versions of the Richardson Extrapolation, was estimated at the end of each sub-interval. Let be the end-point of any of the sub-intervals. The notation , where will be used and is calculated by applying one of the three selected **IRKMs** either directly or in combination with some version of the Richardson Extrapolation. Then the accuracy achieved by the selected numerical method at the point can be evaluated by using the following formula:

The global error is computed by using the values of from **(24)** in the following manner:

The selected three particular **IRKMs** and the combinations **IRKM+**  () were run with four values of ( ) and with **12** different stepsizes We are starting the computations with , halving the stepsize after each successful run, and finishing with in the twelfth run. This means that results from **1296** runs will be compared and discussed.

It must be emphasized here that all results are calculated by selecting **quadruple-precision** (i.e. by applying declarations for the real numbers, which means that the computations are carried out by using about significant digits of the real numbers).

Logarithms of the errors are used in the plots presented in **Fig. 4**, **Fig. 5** and **Fig. 6** when **EULERB**, **DIRK23** and **FIRK35** are used, both directly and in combination with eight versions of the Richardson Extrapolation, in the solution of the test-problem defined by **(18)-(21)**.



**Figure 3**

The first component of the solution of the linear system of ODEs represented by **(18) – (21)** obtained when the values of the first parameter are (the upper left-hand-side plot), (the upper right-hand-side plot), (the lower left-hand-side plot) and (the lower right-hand-side plot). The other two parameters are and **0.03** in all four plots. It is clearly seen that the number of oscillations is increased very substantially and, therefore, the accuracy requirements are increased when parameter is becoming larger.

A requirement to calculate approximations with **at least two correct significant digits** is satisfied when the curves drawn in these three figures are under the dotted line.

**Comments about the results obtained by EULERB:** The requirement for achieving at least two correct significant digits is not satisfied when this method is used directly with . That is true even if the smallest stepsize is used and more than one million steps are carried out. On the other hand, if the advanced versions of the Richardson Extrapolation are used, then the calculated results are often becoming very accurate and the rounding errors are gradually starting to be dominating in spite of the fact that quadruple precision is used.

**Comments about the results obtained by using DIRK23:** The results obtained by using **DIRK23** are in general more accurate than the corresponding results obtained by applying **EULERB**, but if this method is used directly with large stepsizes then the requirement for achieving at least two correct significant digits is again not always satisfied. If advanced versions of the Richardson Extrapolation are used, then the calculated results are often becoming very accurate and the rounding errors are quickly starting to be dominating.

**Comments about the results obtained by using FIRK35:** The results obtained by using this method are more accurate than the corresponding results obtained by applying the other two methods. If **FIRK35** is used directly and if , then the required accuracy (at least two correctly calculated significant digits) is not achieved if the stepsize is large. If the advanced versions of the Richardson Extrapolation are used, then again the calculated results are very often becoming very accurate and the rounding errors are very quickly starting to be dominating.

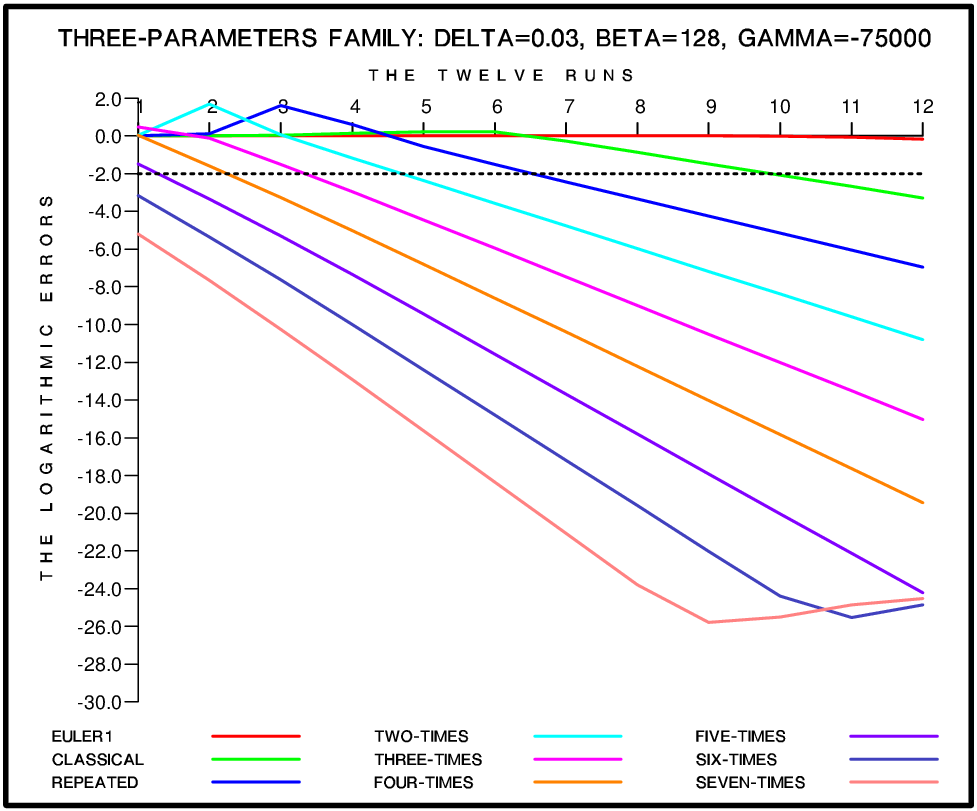
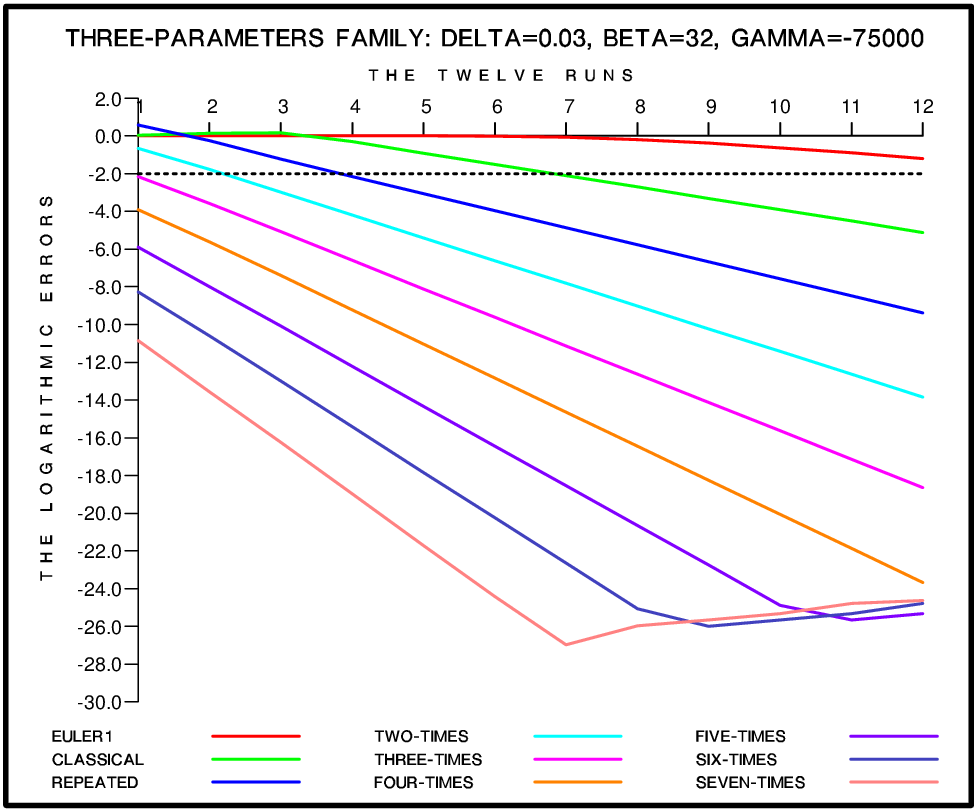
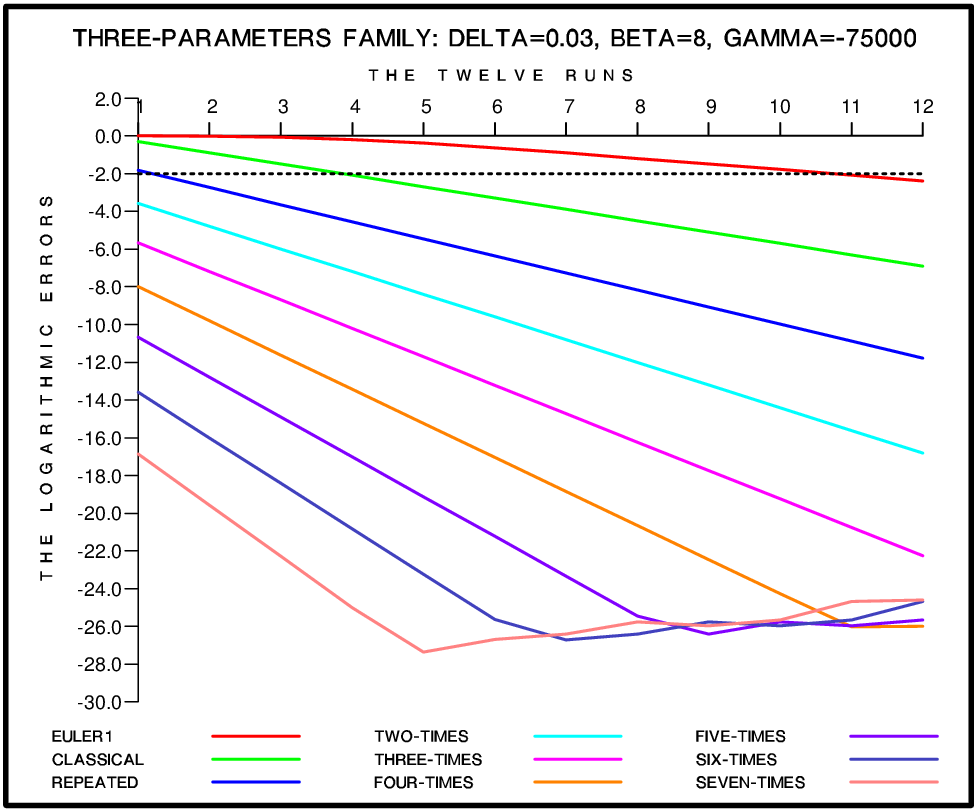
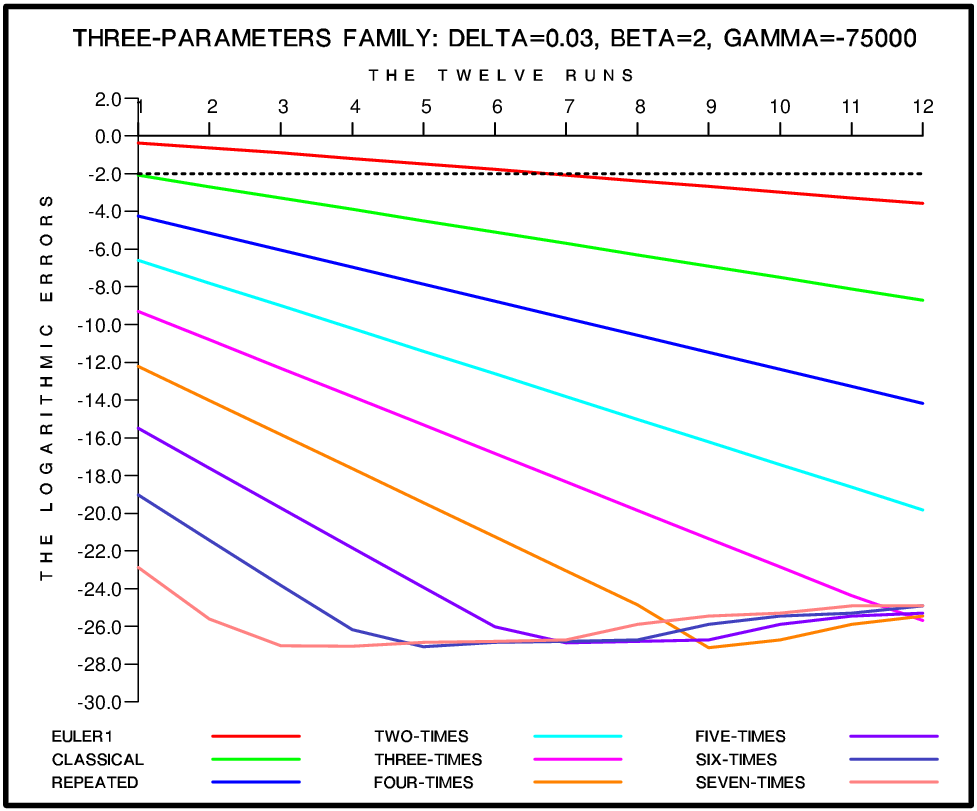
The results in **Fig. 4**, **Fig. 5** and **Fig.6** show clearly that the accuracy of the results is quickly increased both when the stepsize is decreased and when more accurate versions of the Richardson Extrapolation are used. It is also important to know whether the theoretical convergence rates (according to **Theorem 1**) can be achieved. It is seen from **Table 4** that the methods are performing very well and the practically achieved convergence rates are very close to expected rates.

**7. Plans for future research**

Future research can be carried out in different directions. Some examples are listed below.

**Further extension of the stability results:** Two new concepts, practical A-stability and practical absolute stability regions, were introduced in **Section 3**. Stability properties of the combinations of the three particular **IRKMs** from **Section 4** combined with different versions of the Richardson Extrapolation were studied in **Section 5**. It is worthwhile to apply **Algorithm 1** from **Section 3** to some other **IRKMs** and even to some one-step methods when these are combined with any with . It is desirable to find **IRKMs** which produce **practically A-stable methods** for all **IRKM**+ with . It will also be useful to obtain also some extensions to the concepts of **strong A-stability** and **L-stability.**

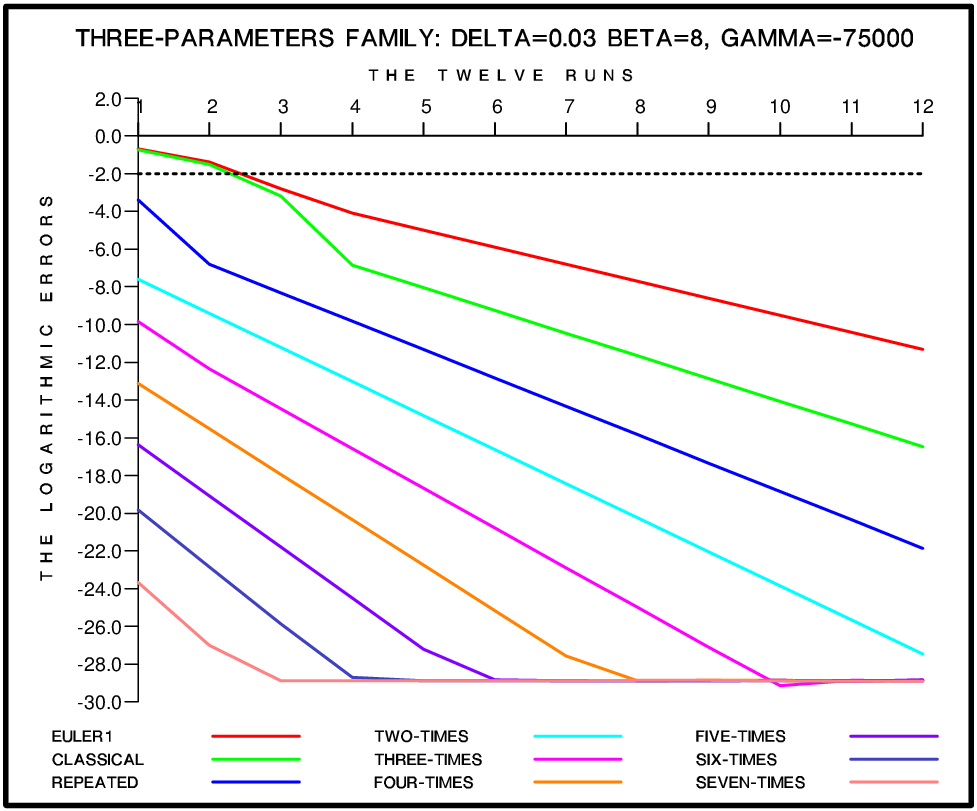
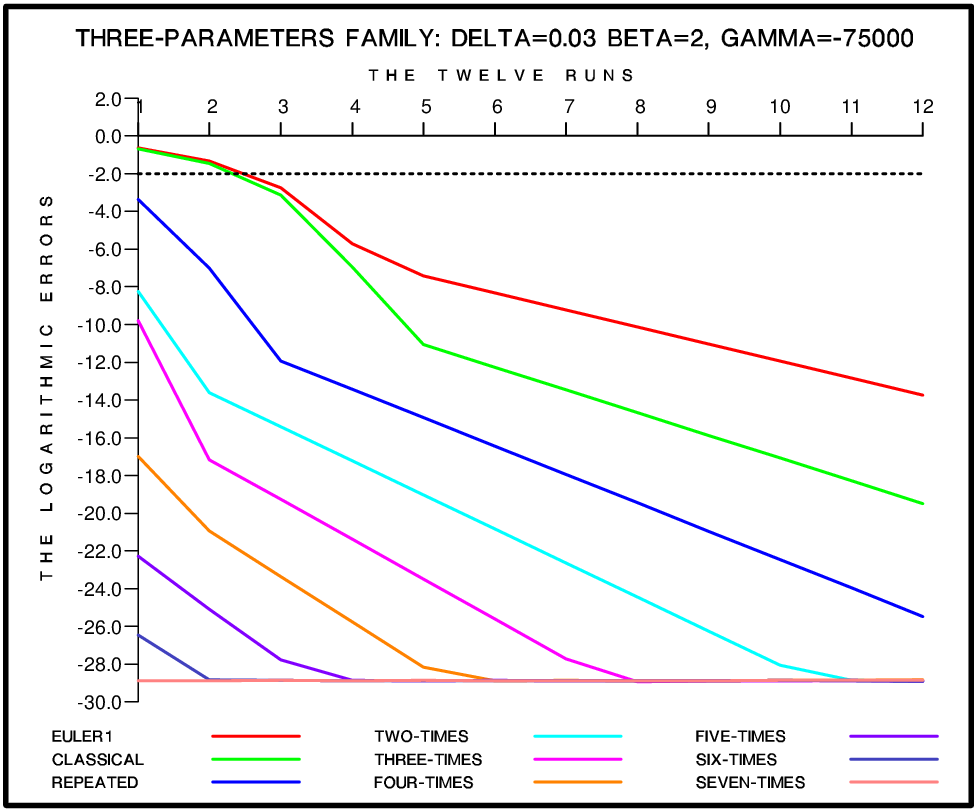
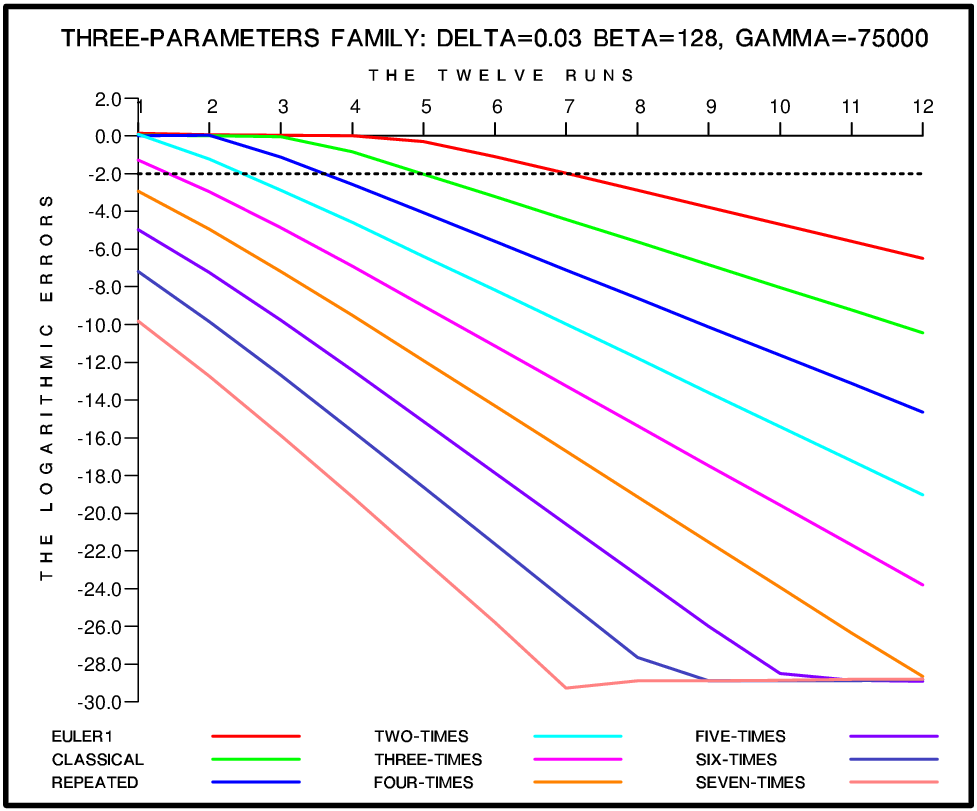
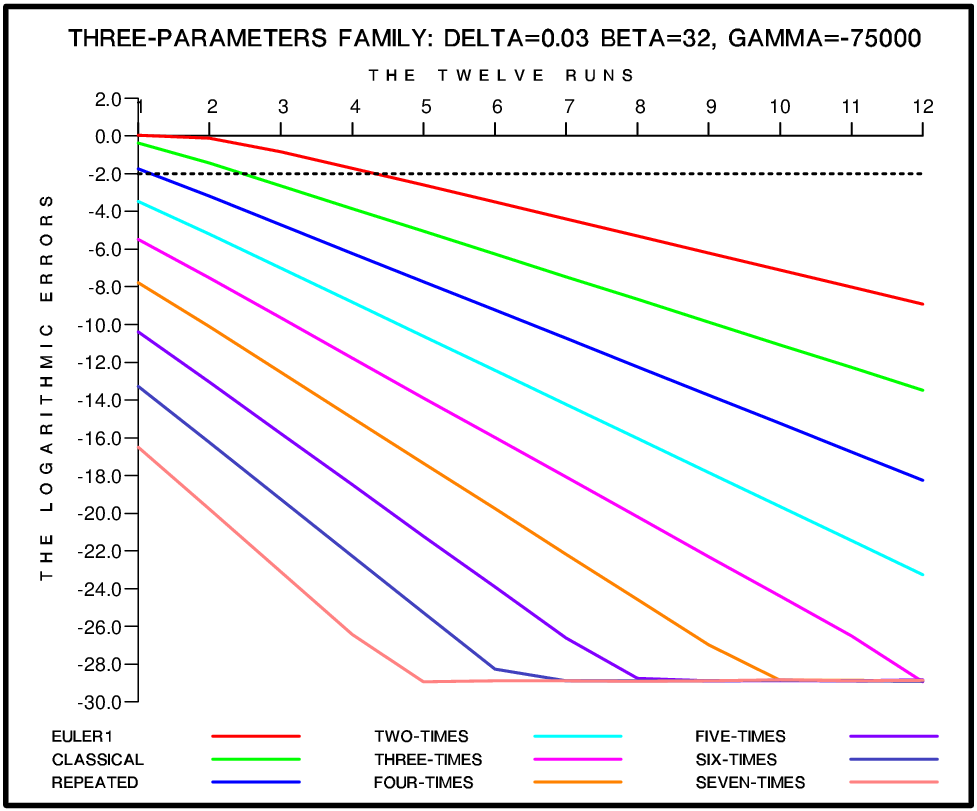
**More numerical tests:** It will be usefulto carry on experiments by using problems arising in large-scale scientific and engineering models. A non-linear atmospheric chemistry scheme from an air pollution model, which is very stiff, ill-conditioned and badly scaled (**[19]**, **[20]**) will also be tested.



**Figure 4**

Logarithmic values of the errors in the solution vector when **EULERB** is used directly and with eight versions of the Richardson Extrapolation. Twelve different stepsizes are used and the errors are evaluated by applying **(24)** and **(25)**. The names **DELTA**, **BETA** and **GAMMA** are used in the plots instead of , and .

**Automatic variation of the stepsize and the versions of the Richardson Extrapolation:** It will be useful to develop a reliable and efficient software, which will allow the users to solve their problems by automatically changing both the stepsize and the used versions of the Richardson Extrapolation according to prescribed requirements. The checks for changing the stepsize and/or the used version of the Richardson Extrapolation are normally related to the required accuracy, but there is always an additional requirement related to the preservation of the stability of the computations. Therefore, it was very important to show that one should expect the computations to remain stable in very large **practical absolute stability regions**, when some well-known **IRKMs** are used together with different versions of the Richardson Extrapolation.

**Figure 5**

Logarithmic values of the errors in the solution vector when **DIRK23** is used directly and with eight versions of the Richardson Extrapolation. Twelve different stepsizes are used and the errors are evaluated by applying **(24)** and **(25)**. The names **DELTA**, **BETA** and **GAMMA** are used in the plots instead of , and .

**References**

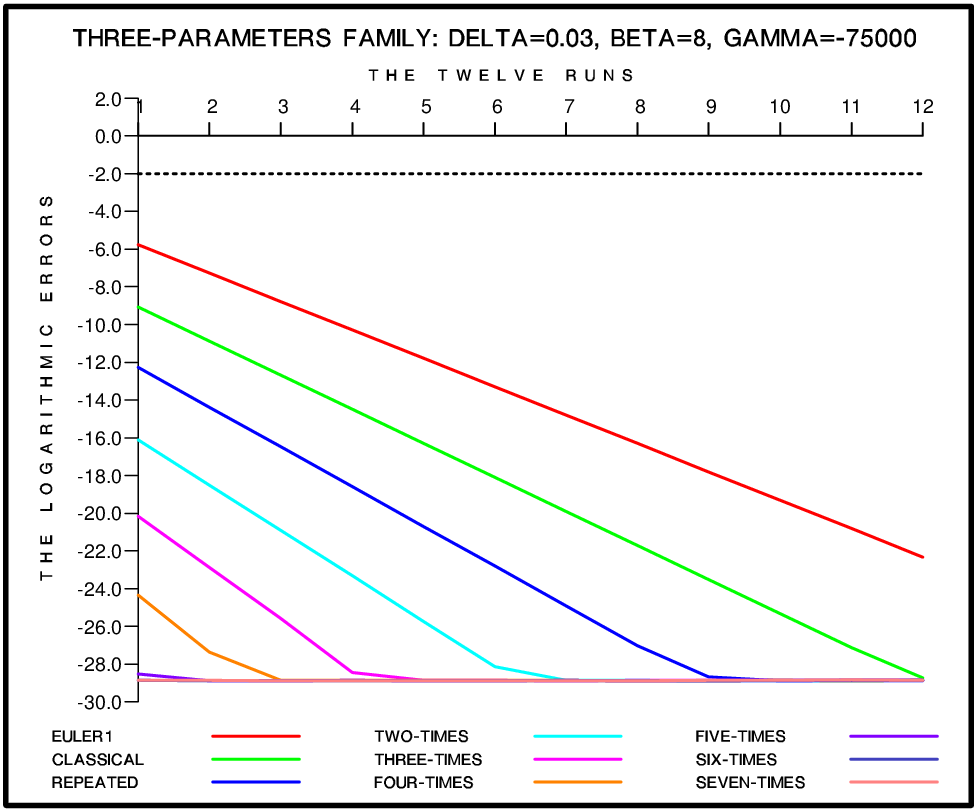
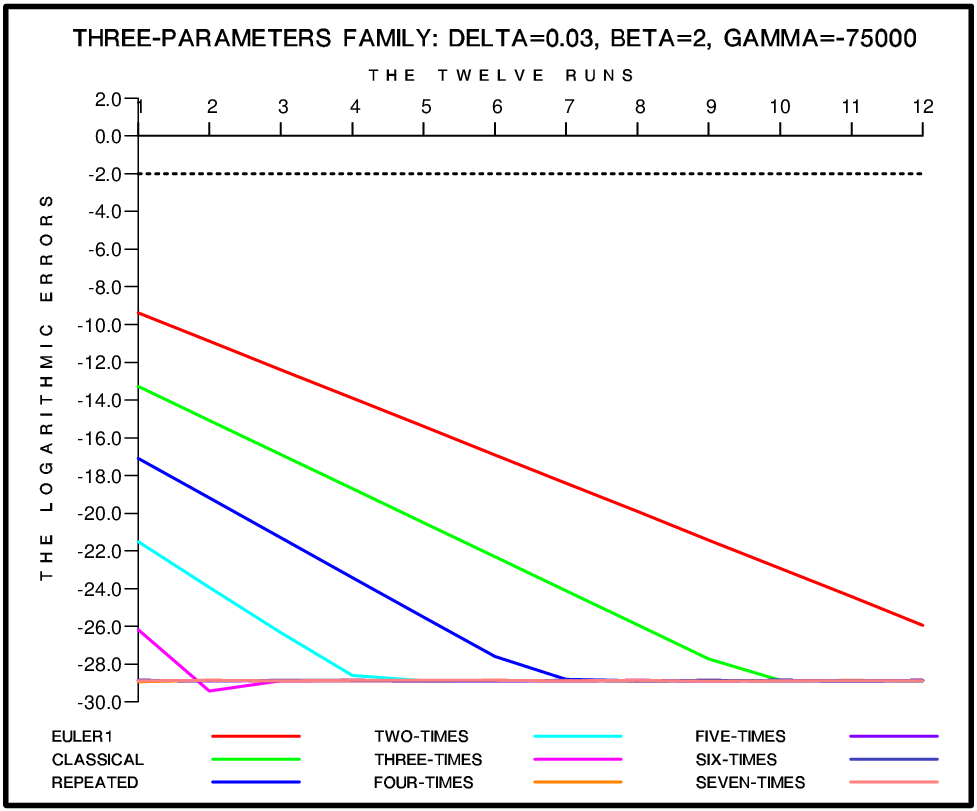
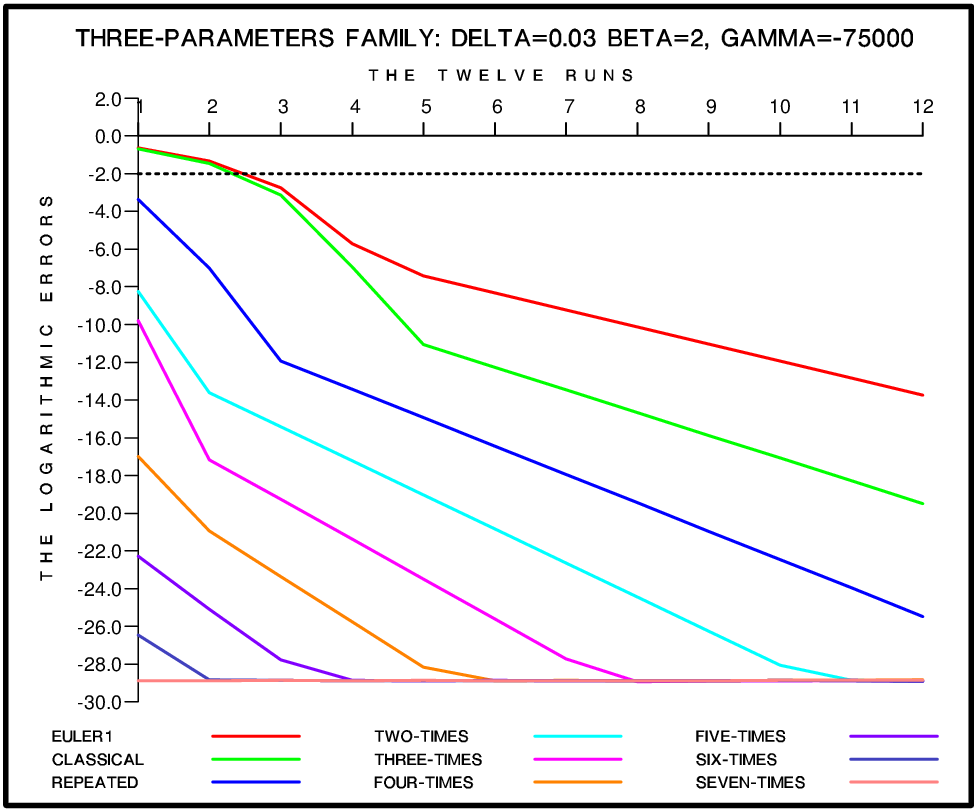
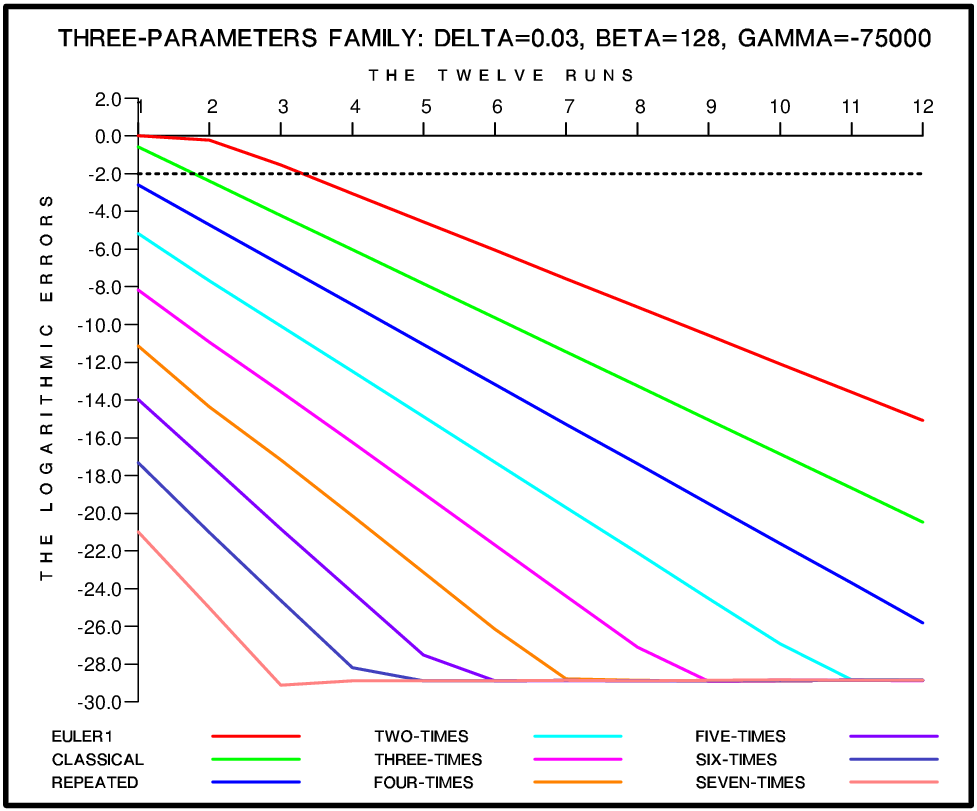
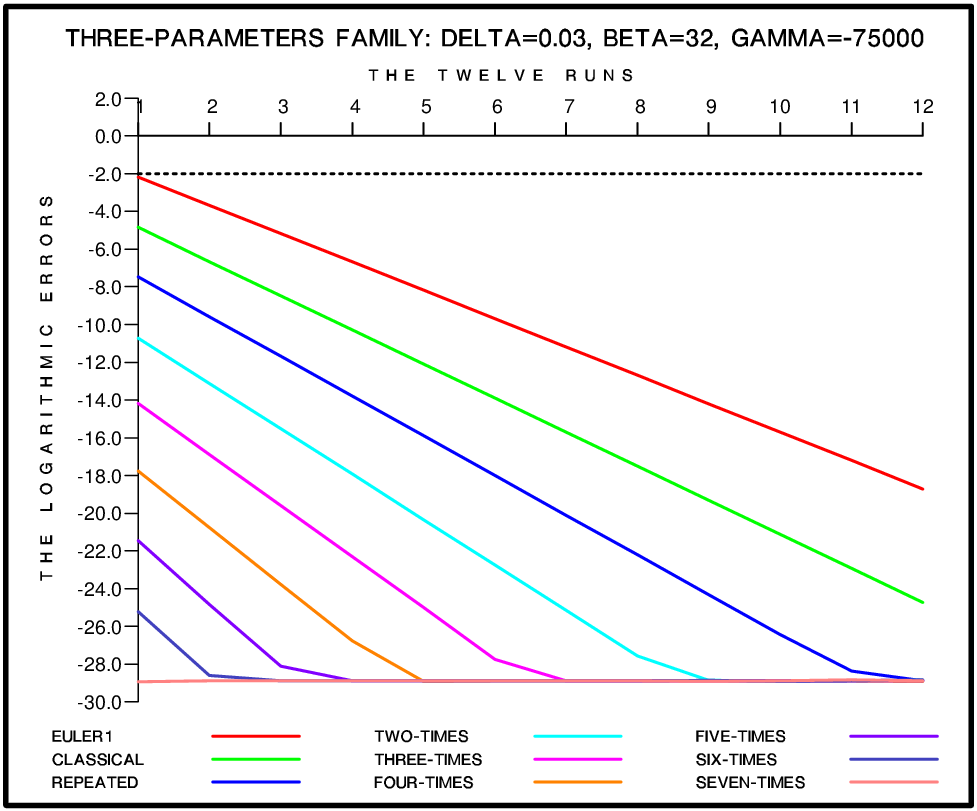
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**Figure 6**

Logarithmic values of the errors in the solution vector when **FIRK35** is used directly and with eight versions of the Richardson Extrapolation. Twelve different stepsizes are used and the errors are evaluated by applying **(24)** and **(25)**. The names **DELTA**, **BETA** and **GAMMA** are used in the plots instead of , and .

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|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Run** | **Steps** | **Stepsize** | **EULERB** | | | **DIRK23** | | **FIRK35** | |
| **Error** | **Rate** | | **Error** | **Rate** | **Error** | **Rate** |
| **1** | 640 | 0.02048 | 1.000E-00 | - | 1.000E-00 | | - | 1.000E-00 | - |
| **2** | 1280 | 0.01024 | 1.000E-00 | 1.00 | 1.000E-00 | | 1.00 | 8.207E-01 | 1.22 |
| **3** | 2560 | 0.00512 | 1.000E-00 | 1.00 | 1.000E-00 | | 1.00 | 5.312E-03 | 154.50 |
| **4** | 5120 | 0.00256 | 1.000E-00 | 1.00 | 1.842E-00 | | 0.54 | 1.019E-05 | 521.30 |
| **5** | 10240 | 0.00128 | 4.087E-00 | 0.24 | 1.409E-01 | | 13.07 | 1.687E-08 | 604.03 |
| **6** | 20480 | 0.00064 | 2.991E-00 | 1.36 | 2.582E-03 | | 54.57 | 2.753E-11 | 612.79 |
| **7** | 40960 | 0.00032 | 6.885E-02 | 33.66 | 3.120E-05 | | 121.79 | 6.649E-14 | 414.05 |
| **8** | 81920 | 0.00016 | 2.480E-03 | 27.76 | 2.760E-07 | | 113.04 | 1.362E-16 | 488.18 |
| **9** | 163840 | 0.00008 | 8.200E-05 | 30.24 | 2.288E-09 | | 120.63 | 2.678E-19 | 508.59 |
| **10** | 327680 | 0.00004 | 2.591E-06 | 31.65 | 1.787E-11 | | 128.04 | 5.223E-22 | 512.73 |
| **11** | 655360 | 0.00002 | 8.033E-08 | 32.25 | 1.388E-13 | | 128.74 | 1.018E-24 | 513.06 |
| **12** | 1310720 | 0.00001 | 2.493E-09 | 32.22 | 1.079E-15 | | 128.64 | 1.992E-27 | 511.04 |

**Table 4**

Results obtained when the **Three-times Repeated Richardson Extrapolation** is used together with the three selected methods (**EULERB**, **DIRK23** and **FIRK35**) in the solution of a test-example obtained by the three-parameter family with , and . The numbers of steps and the stepsizes are given in the second and the third columns of the table. In the remaining six columns the errors and the convergence rates are given (the perfect convergence rates are **32**, **128** and **512** respectively). The three methods are not able to achieve the required accuracy (two correct significant digits) when the stepsize is large (see the grey areas in the table), but the theoretical convergence rates are achieved when the stepsize is sufficiently small.

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