Parallel High-Order Time Integrators

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Declaration

This piece of work is a result of my own work except where it forms an assessment based on group project work. In the case of a group project, the work has been prepared in collaboration with other members of the group. Material from the work of others not involved in the project has been acknowledged and quotations and paraphrases suitably indicated.

Bradley Gadd-Speakman

Thank you to my project advisor Hossein Amini-Kafiabad for the amazing support throughout my final year project and also to my close friends and family.

Abstract

In this project, we investigated and implemented various time integrators with the aim of developing a high-order method for numerically solving first order initial value problems (IVPs) in a parallelisable manner. The method we focused on is revisionist integral deferred correction (RIDC)[4], which consists of a prediction step via a typical time integration method and, once enough predicted values have been calculated, correction steps that then run in parallel to the predictor step. With large enough computation time, RIDC can have an arbitrarily high order of accuracy as it can be shown to be proportional to the total number of prediction and correction steps. The computation time of such a method would normally be large but due to the parallelisable nature of the algorithm we can dedicate one CPU core to each of the prediction and correction steps, thus mitigating the added computational burden of the correction steps in this high-order method.

Contents

Chapter 1

Introduction

Time integration is a fundamental component of numerical methods for solving IVPs described by ODEs or PDEs. Accurate and efficient time integration is crucial for obtaining reliable results in simulations of physical systems and other applications. However, a big issue with most classical time integrators is that they are inherently sequential processes and therefore cannot be parallelised very easily or at all.

This report primarily investigates revisionist integral deferred correction (RIDC) as a high-order time integration method for numerically solving first-order IVPs. RIDC is an adaptation of the integral deferred correction (IDC)[5] method that retains its high accuracy while also allowing the process to be parallelised.

IDC is a predictor-corrector method, which uses an initial time integration technique to 'predict' the approximate values of the solution to an IVP. It then sequentially 'corrects' these prediction values, increasing the order of accuracy of the numerical solution, using an update formula which we derive later in the report. This method is a popular alternative to more classical time integrators but again suffers by not being parallelisable.

RIDC is a modified version of IDC which, following a brief sequential setup phase, can simultaneously calculate correction values at nodes that are staggered in time. This allows it to utilise parallel computing resources effectively, making it ideal for large-scale simulations of IVPs where computational efficiency is critical. Consequently, RIDC offers a significant improvement in computational efficiency compared to IDC due to its parallelisation capabilities.

This report will begin by providing an overview of various classical time integration methods and their properties. Next, we will derive and evaluate IDC. We then move on to describe the modifications made to IDC that have led to RIDC, and explain why RIDC can be parallelised under this new framework. Additionally, we will explore how these methods are used to solve PDEs, which are commonly used to model physical phenomena such as fluid dynamics, heat transfer, and electromagnetism in numerous scientific and engineering applications.

Overall, this report will provide a comprehensive understanding of time integrators, with a particular focus on RIDC and its ability to enable efficient parallelisation for large-scale simulations of IVPs using staggered corrections.

Chapter 2

Time Integration Fundamentals

In this chapter we will discuss the fundamentals of time integration which includes some classical time integrators such as Euler's method and Heun's method. We also cover the concepts of order of accuracy and stability which are properties of a time integrator that we can analyse to determine how well the method performs. More detailed and varied examples of time integrators and their properties can be found in J.C. Butcher's book [2].

Time integrators can be placed into two categories, explicit and implicit methods. Explicit methods calculate the approximate value of the solution at a given point in time using the previously approximated values in time. Implicit methods calculate the approximate value of the solution at a given point in time by solving an equation which involves both this term and previously approximated values in time. This report is solely concerned with explicit time integration methods.

2.1 Classical Time Integrators

To begin our review of classical time integrators, we start with the Euler method, the most basic explicit method. The canonical form of an IVP which we want to solve numerically is,

$$u'(t) = f(u,t), \quad t \in [0,T], \quad u(0) = u_0 \tag{2.1}$$

where $u \in \mathbb{R}^n$, $f : \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}^n$. We will always assume that there exists a unique solution to this IVP and this is precisely what we denote by $u(t)$.

All numerical time integrators begin by discretising the temporal domain into a sufficiently large number of nodes $\{t_n\}_{n\in\mathbb{N}}$. For the entirety of this report, we only consider the most straightforward discretisation of using N equidistant points in time. The constant step-size between these points is given symbolically by h and the time steps are exactly $t_n = nh$.

The formula for the Euler method is derived from equation (2.1) using the first order Taylor series approximation of u expanded about t_n,

$$u(t) = u(t_n) + (t - t_n)f(u(t_n), t_n) + O((t - t_n)^2).$$

After evaluating this equation at time $t = t_{n+1}$, the next time step after t_n, we clearly see that we can get an approximation for the value of u at a new time step using the previous value of u in time. We denote this new approximate value by $\hat{u}_{n+1}$ and the old by $\hat{u}_n$. The forward Euler method is therefore given by,

$$\hat{u}_{n+1} = \hat{u}_n + hf(\hat{u}_n, t_n), \quad \hat{u}_0 = u_0. \tag{2.2}$$

Other examples of explicit methods are Heun's method and the classic Runge-Kutta method (RK4). These methods require more function evaluations and more storage for intermediate values, this means they require more computation time and larger memory requirements. The upside of these methods however is that they have better properties than Euler's method, as will be shown in sections **2.2** and **2.3**.

Heun's method calculates approximate solution values to equation (2.1) using the following formula:

$$\begin{aligned} \tilde{u}_{n+1} &= \hat{u}_n + hf(\hat{u}_n, t_n), \\ \hat{u}_{n+1} &= \hat{u}_n + \frac{h}{2}\Big[f(\hat{u}_n, t_n) + f(\tilde{u}_{n+1}, t_{n+1})\Big]. \end{aligned} \tag{2.3}$$

This method can be interpreted as a combination of Euler's method and the trapezoidal rule, resulting in a new time integration technique with now two unique evaluations of function f required.

The classic Runge-Kutta method is similar to the previous two methods, except now the function f is required to be evaluated four times for each new approximation value. Its formula is given by:

$$\begin{aligned}
k_1 &= f(\hat{u}_n, t_n),\\
k_2 &= f\Big(\hat{u}_n + h\frac{k_1}{2}, t_n + \frac{h}{2}\Big),\\
k_3 &= f\Big(\hat{u}_n + h\frac{k_2}{2}, t_n + \frac{h}{2}\Big),\\
k_4 &= f(\hat{u}_n + hk_3, t_{n+1}),\\
\hat{u}_{n+1} &= \hat{u}_n + \frac{h}{6}\Big[k_1 + 2k_2 + 2k_3 + k_4\Big].
\end{aligned} \tag{2.4}$$

2.2 Order of Accuracy

The first property of time integrators we mention is that of order of accuracy or order of convergence. Before this concept can be understood however, we must know what is meant by the term global error. Global error e_n at time t_n of a numerical integration scheme is defined by $e_n = u_n - \hat{u}_n$. We say a method is convergent to the true solution of an IVP if $\lim_{h\to 0} \max_n |e_n| = 0$. The method will have an order of accuracy p if the absolute global error $|e_n|$ is bound by a constant multiplied by the step-size h to the pth power

$$|e_n| \leq Ch^p. \tag{2.5}$$

Therefore, the order of accuracy is a number which quantifies the rate of convergence to the true solution for any IVP as the step-size is reduced to zero. For this reason it is a pivotal metric in determining how well a time integration method performs, as we ideally want as high an order of accuracy as possible.

You can analytically show that the previously mentioned time integrators: Euler's method, Heun's method and RK4, have orders of accuracy $1, 2$ and 4 respectively. To show proof of these results however is beyond the scope of this project and we instead opt to demonstrate this experimentally. Formal proofs of the orders of accuracy for these methods can be found in [2]. To empirically display these results we use convergence plots. A convergence plot is a graph of $\log(|e_n|)$ against $\log(h)$, the gradient of such a plot we expect to be approximately constant of value p. The intuition behind this is driven directly by inequality (2.5). It is also worth clarifying that all figures included in this report were generated by myself, predominantly using Python's matplotlib package [7].

The IVP we want to solve to obtain the convergence plots is the test equation with its standard initial condition given by

$$u'(t) = \lambda u(t), \quad u_0 = 1 \tag{2.6}$$

where in general we let $\lambda \in \mathbb{C}$. For the case of making convergence plots however, we set $\lambda = 1$ and therefore know that the true solution to this IVP is $u(t) = e^t$.

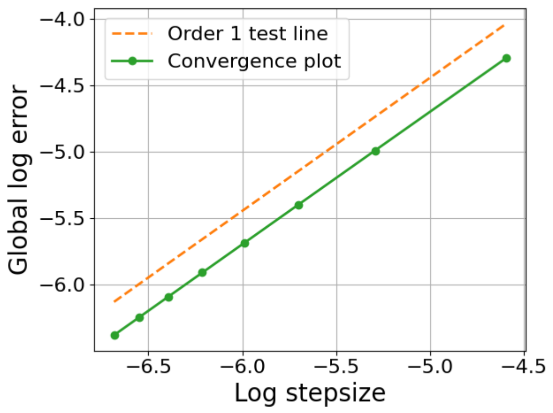
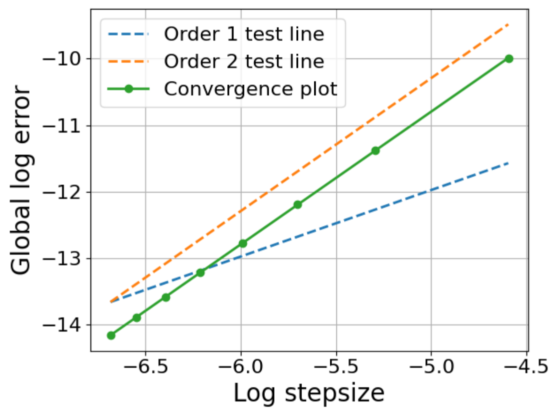


Figure 2.1: Convergence plot for the Euler method. The orange dashed reference line is perfectly straight with a gradient equal to the expected order of the method (in this case one).



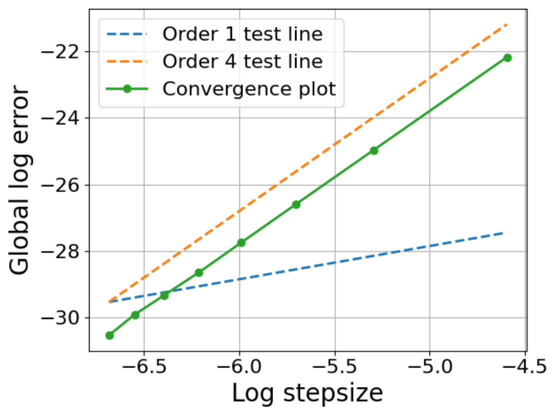


Figure 2.2: (left) The convergence plot for Heun's method. (right) The convergence plot for RK4.

2.3 Stability

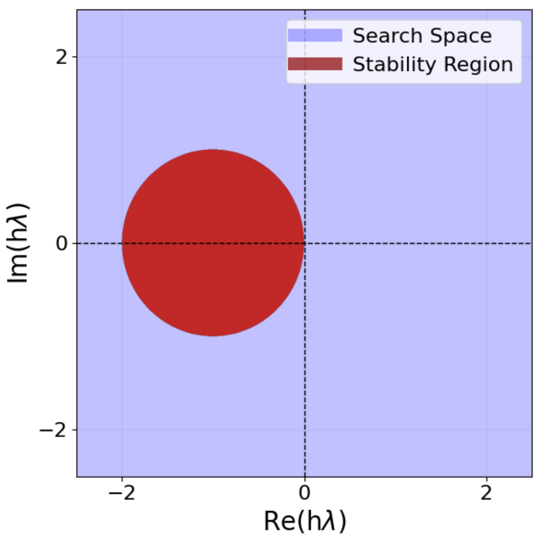
The second property of time integrators we investigate is known as the stability region. We know the solution to the test equation (2.6) is exactly $u(t) = e^{\lambda t}$ and therefore if $\text{Re}(\lambda) < 0$ we have $\lim_{t\to\infty} u(t) = 0$. In this scenario we expect our numerical solution to (2.6) to get smaller in magnitude after a time step of size h. This motivates the following definition of the stability region S:

$$S = \{h\lambda : \text{Re}(\lambda) < 0 \text{ and } |\hat{u}_1| < 1\}. \tag{2.7}$$

The stability regions for all three previously mentioned explicit time integration methods are:

- Euler's Method, $S = \{h\lambda : |1 + h\lambda| < 1\}$.
- Heun's Method, $S = \{h\lambda : \left|1 + h\lambda + \frac{(h\lambda)^2}{2}\right| < 1\}$.
- RK4, $S = \{h\lambda : \left|1 + h\lambda + \frac{(h\lambda)^2}{2} + \frac{(h\lambda)^3}{6} + \frac{(h\lambda)^4}{24}\right| < 1\}$.

As can be found in the book [2] under the stability subsections for these integration techniques.



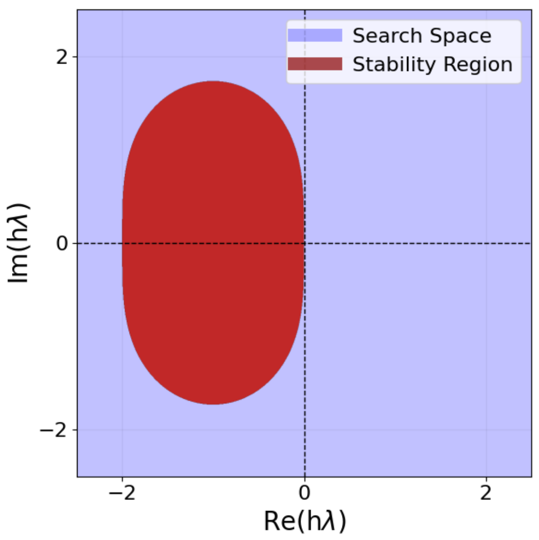


Figure 2.3: (left) The stability plot for Euler's method. (right) The stability plot for Heun's method.

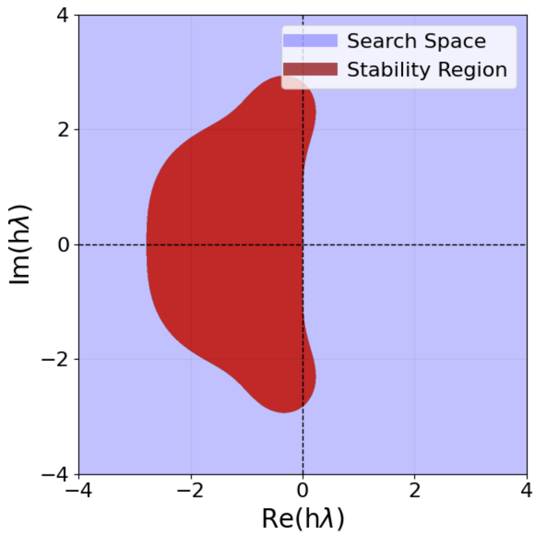


Figure 2.4: Stability plot for RK4.

Stability plots are useful for determining what pairs of values we can choose h and λ to be in order for the approximation to still converge to the true solution. We often want to use a step-size which is as large as possible, while still converging, in order to increase performance and thats why these plots are used. They demonstrate how lenient the methods are relative to one another in the acceptable pairs of values h and λ. From the stability plots, you can clearly see that RK4 has a much larger stability region than Euler or Heun's method.

2.4 Parallelism

All of the methods mentioned, and most time integrators in general, rely on a sequential calculation of new approximate solution values in time using previously calculated values. Time integration is, by its very nature, a sequential process and it is for this reason that it is conceptually difficult to imagine how a technique could possibly performs these calculations in parallel.

As will be shown in **chapter 4** on RIDC, we can get around this sequential limitation by using a method which incorporates multiple tiered corrections to our initial numerical solution values. As we increase the tier of correction, the order of accuracy provided also increases. We can then perform these calculations simultaneously (i.e. in parallel) over these so called correction levels.

Chapter 3

Integral Deferred Correction

The integral deferred correction (IDC) method discretises the time domain slightly differently to the previously seen techniques. IDC first divides the domain into J time intervals of equal size which are then further subdivided into K equidistant nodes in time. There are said to be a total of N nodes across the whole domain. This discretisation scheme is demonstrated below.

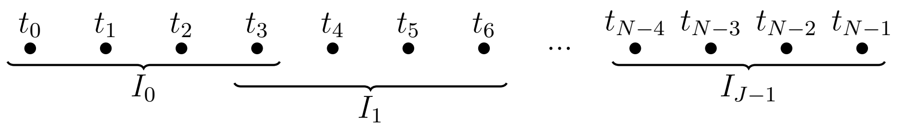


Figure 3.1: Enumeration of the time nodes for the IDC method with $K = 4$ nodes in each time interval.

IDC is a predictor-corrector method which performs iteratively over the time intervals. An initial time integration technique with the order of accuracy P is used to 'predict' the approximate values of the solution to an IVP. It then 'corrects' all these values for each of the M correction levels sequentially. All the predictions and corrections are calculated in the current time interval before moving on to the next. Once the final correction value in the current time interval is calculated, it is dropped down to all lower correction levels to be used as the initial condition for the next time interval.

These corrections are performed using an update formula also of order P derived from the error equation [4],

$$\frac{d\hat{u}^{(m+1)}}{dt} = \left(\int_0^t \hat{f}(\hat{u}^{(m)}, s)ds\right)' + f(\hat{u}^{(m+1)}, t) - f(\hat{u}^{(m)}, t). \qquad (3.1)$$

Where $\hat{u}^{(m)}$ denotes the numerical solution after m corrections, f is the RHS to the canonical form of an IVP (2.1) and h is the step-size. The integral in (3.1) is approximated using a quadrature with integration points given by a subset of the nodes in the current time interval. **If at least $P(M+1)$ points are used to calculate the quadrature then IDC produces a numerical solution which has an order of accuracy of $P(M+1)$[5].** Therefore, for simplicity, the rest of this chapter only considers IDC with $K = P(M+1)$ which results in $N = J(P(M+1)-1)+1$ and $h = \frac{T}{N-1}$.

3.1 Derivation and Overview of IDC

Before we can derive the error equation (3.1) we must first define two metrics, the error and the residual function.

The error function ϵ is given by $\epsilon(t) = u(t) - \hat{u}(t)$. This function quantifies the difference between the true and numerical solution.

The residual function δ is given by $\delta(t) = \hat{u}_0 + \int_0^t f(\hat{u}, s)ds - \hat{u}(t)$. This function quantifies how poorly our numerical solution satisfies the differential equation.

The following steps acquire the error equation:

We start by replacing $u(t)$ in $\epsilon(t)$ with its Picard integral form,

$$\begin{aligned}\epsilon(t) &= \hat{u}_0 + \int_0^t f(u, s)ds - \hat{u}(t) \\ &= \hat{u}_0 + \int_0^t f(\hat{u} + \epsilon, s)ds - \hat{u}(t).\end{aligned}$$

We introduce $\delta(t)$ into $\epsilon(t)$,

$$\epsilon(t) = \delta(t) + \int_0^t f(\hat{u} + \epsilon, s) - f(\hat{u}, s)ds.$$

Now we take the time derivative of both sides,

$$\epsilon'(t) = \delta'(t) + f(\hat{u} + \epsilon, t) - f(\hat{u}, t).$$

The term $\delta'(t)$ is equivalent to,

$$\delta'(t) = \left(\int_0^t f(\hat{u}, s) ds \right)' - \hat{u}'(t).$$

Resulting in,

$$\epsilon'(t) = \left(\int_0^t f(\hat{u}, s) ds \right)' - \hat{u}'(t) + f(\hat{u} + \epsilon, t) - f(\hat{u}, t).$$

We let $\hat{u}(t) = \hat{u}^{(m)}$, $\epsilon(t) = \epsilon^{(m)}$, $\hat{u}^{(m+1)} = \hat{u}^{(m)} + \epsilon^{(m)}$ and, after adding $\hat{u}^{(m)}$ to both sides, we get the error equation,

$$\frac{d\hat{u}^{(m+1)}}{dt} = \left(\int_0^t \hat{f}(\hat{u}^{(m)}, s) ds \right)' + f(\hat{u}^{(m+1)}, t) - f(\hat{u}^{(m)}, t)$$

The function f in the term $\left(\int_0^t f(\hat{u}^{(m)}, s) ds \right)'$ is approximated by an interpolating polynomial from the values of f evaluated using the $P(M+1)$ previous correction level values and time nodes inside the current time interval. To make this clear, the notation for the interpolation of f is given by $\hat{f}$. The error equation can be interpreted more easily after integrating both sides between t_n and t_{n+1},

$$g(\hat{u}^{(m+1)}, t) = f(\hat{u}^{(m+1)}, t) - f(\hat{u}^{(m)}, t),$$

$$\hat{u}_{n+1}^{(m+1)} = \hat{u}_n^{(m+1)} + \overbrace{\int_{t_n}^{t_{n+1}} g(\hat{u}^{(m+1)}, t) dt}^{\text{Order P Integration Method}} + \overbrace{\int_{t_n}^{t_{n+1}} \hat{f}(\hat{u}^{(m)}, t) dt}^{\text{Quadrature}}. \tag{3.2}$$

We now derive update formulae for orders $P = 1, 2$:

Starting with $P = 1$, by Euler's method (2.2) we have,

$$\int_{t_n}^{t_{n+1}} g(\hat{u}^{(m+1)}, t)dt = h\left[f(\hat{u}_n^{(m+1)}, t_n) - f(\hat{u}_n^{(m)}, t_n)\right],$$

Then using (3.2) results in the $P = 1$ update formula

$$\hat{u}_{n+1}^{(m+1)} = \hat{u}_n^{(m+1)} + h\left[f(\hat{u}_n^{(m+1)}, t_n) - f(\hat{u}_n^{(m)}, t_n)\right] + \int_{t_n}^{t_{n+1}} \hat{\hat{f}}(\hat{u}^{(m)}, t)dt. \quad (3.3)$$

For $P = 2$, by Heun's method (2.3) we have,

$$\int_{t_n}^{t_{n+1}} g(\hat{u}^{(m+1)}, t)dt = \frac{h}{2}\left[g(\hat{u}_n^{(m+1)}, t_n) + g(\tilde{u}_{n+1}^{(m+1)}, t_{n+1})\right],$$

$$\tilde{u}_{n+1}^{(m+1)} = \hat{u}_n^{(m+1)} + h\left[f(\hat{u}_n^{(m+1)}, t_n) - f(\hat{u}_n^{(m)}, t_n)\right] + \int_{t_n}^{t_{n+1}} \hat{\hat{f}}(\hat{u}^{(m)}, t)dt.$$

We first find expressions for $g(\hat{u}_n^{(m+1)}, t_n)$ and $g(\tilde{u}_{n+1}^{(m+1)}, t_{n+1})$,

$$g(\hat{u}_n^{(m+1)}, t_n) = f(\hat{u}_n^{(m+1)}, t_n) - f(\hat{u}_n^{(m)}, t_n),$$

$$g(\tilde{u}_{n+1}^{(m+1)}, t_{n+1}) = f(\hat{u}_n^{(m+1)} + hg(\hat{u}_n^{(m+1)}, t_n) + \int_{t_n}^{t_{n+1}} \hat{\hat{f}}(\hat{u}^{(m)}, t)dt, t_{n+1}) - f(\hat{u}_{n+1}^{(m)}, t_{n+1})$$

Then using (3.2) results in the $P = 2$ update formula

$$\hat{u}_{n+1}^{(m+1)} = \hat{u}_n^{(m+1)} + \frac{K_1}{2} + \frac{K_2}{2} + \int_{t_n}^{t_{n+1}} \hat{\hat{f}}(\hat{u}^{(m)}, t)dt, \quad (3.4)$$

where

$$K_1 = h\Big[f(\hat{u}_n^{(m+1)}, t_n) - f(\hat{u}_n^{(m)}, t_n)\Big],$$

$$K_2 = h\Big[f(\hat{u}_n^{(m+1)} + K_1 + \int_{t_n}^{t_{n+1}} \hat{\hat{f}}(\hat{u}^{(m)}, t)dt, t_{n+1}) - f(\hat{u}_{n+1}^{(m)}, t_{n+1})\Big].$$

The quadrature used to approximate the integral in an update formula is given by

$$I_n = \int_{t_n}^{t_{n+1}} \hat{f}(\hat{u}^{(m)}, t)dt \approx \sum_i S_{ni}\hat{f}_i,$$

where the i are the indices for nodes in the current time interval and

$$S_{ni} = \int_{t_n}^{t_{n+1}} \prod_{j\neq i} \frac{t - t_j}{t_i - t_j} dt,$$

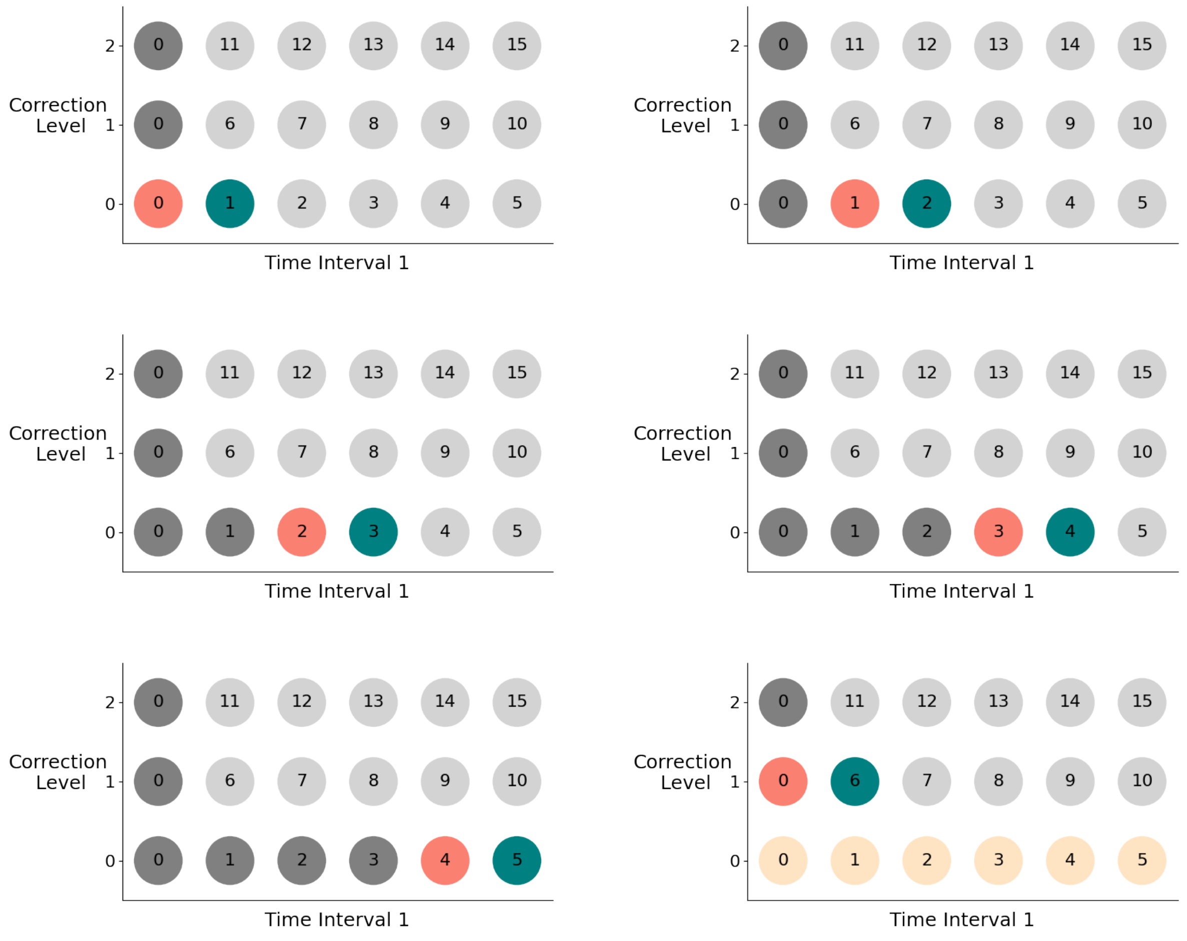
$$\hat{f}_i = f(\hat{u}_i^{(m)}, t_i).$$

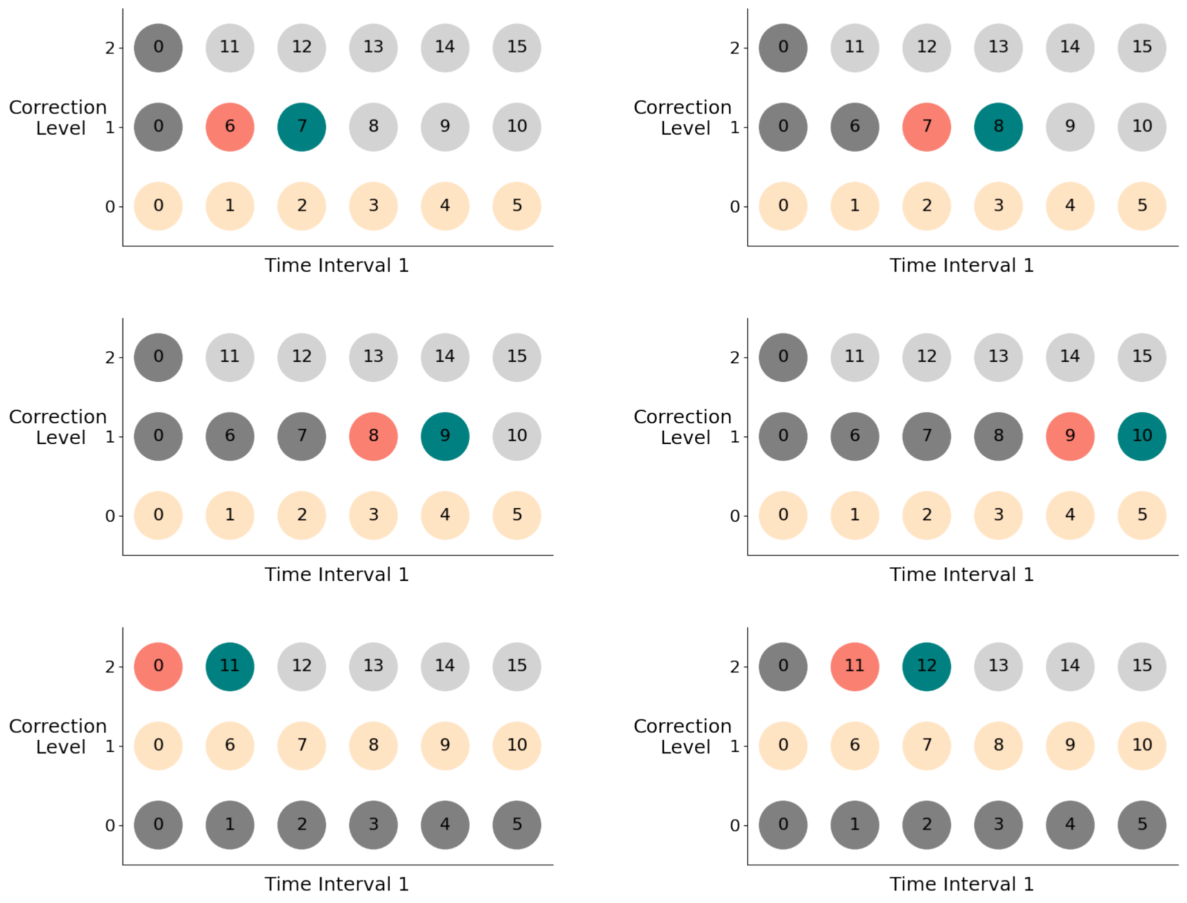
Since we are using equidistant nodes across the whole time domain, the matrix S can be calculated once and never has to be recalculated at any point during the method.

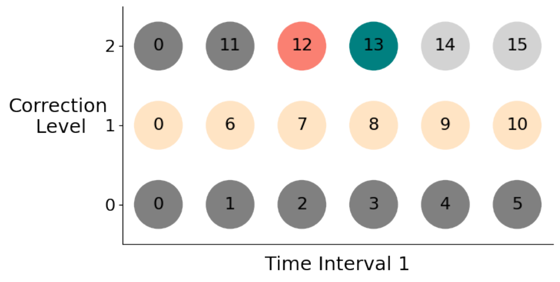
The order of calculation for values in the IDC method can be best visualised using a series of stencil diagrams. Nodes in the stencil diagrams are labelled with a number representing their order of calculation, they are also colour coded as follows:

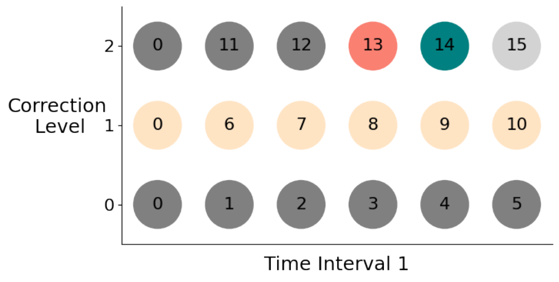
- Darkgray: Node has been calculated.
- Green: Node to be calculated.
- Red: Previous node in time, used to calculate the green node.
- Yellow: Nodes in lower correction level, used to calculate the quadrature in update formulae.

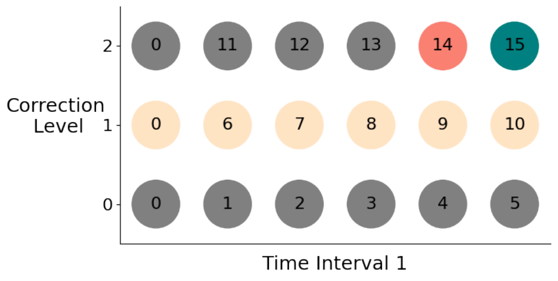
Stencil diagrams for the first time interval of the IDC method with parameters $P = 2$, $M = 2$ are shown below.




Correction Level
Time Interval 1
0
1
2
0
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15







After the 15th node has been calculated, its value is dropped down to the lower corrections and acts as the initial condition for the second time interval. The order of calculated nodes is always the same for every interval.

It is important to note that IDC cannot be parallelised since all of the nodes are still calculated in a sequential manner. In order to make this a parallel algorithm, slight alterations must be made to the method. These changes lead us to RIDC which is covered in **chapter 4**.

3.2 Convergence and Stability of IDC

We now implement IDC, for various values of P and M, to inspect its order of accuracy which is proved in [5] to take the value $P(M+1)$. The IVP we will be trying to solve is

$$u'(t) = 2ut, \quad t \in [0, T], \quad u_0 = 1, \tag{3.5}$$

which has the solution $u(t) = e^{t^2}$.

The code for my implementations of IDC may be found in the appendix.

To obtain the convergence plots for IDC with Euler predictions and corrections i.e. $P = 1$, we used $T = 1$ and gradually decreased the constant step-size by iterating the number of time intervals $J = [16, 18, 20, 22, 24, 26]$.

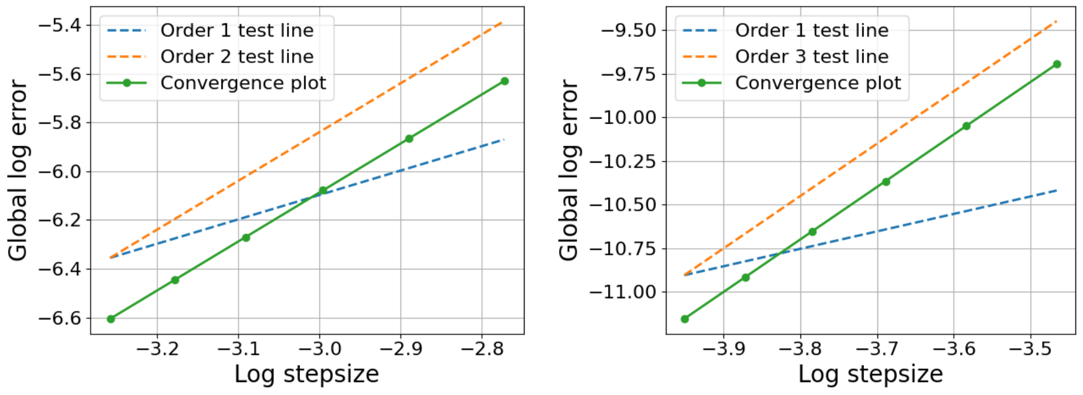


Figure 3.2: (left) IDC with $P = 1$, $M = 1$. (right) IDC with $P = 1$, $M = 2$.

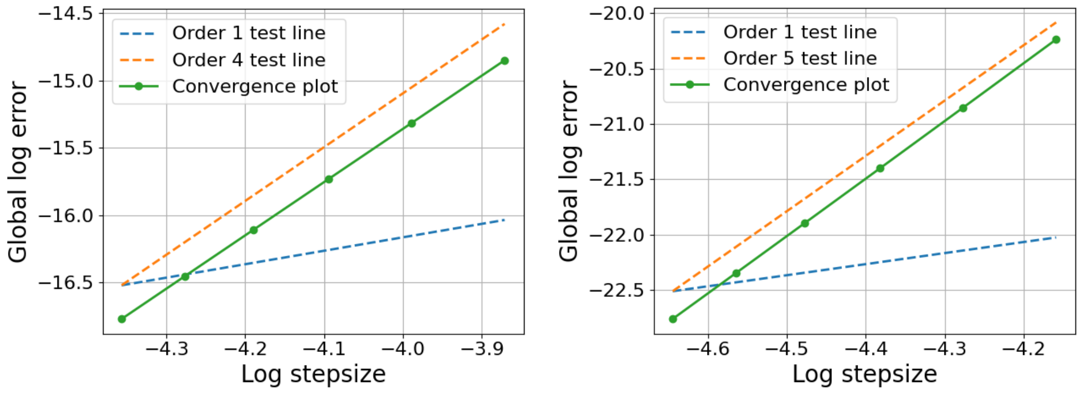


Figure 3.3: (left) IDC with $P = 1$, $M = 3$. (right) IDC with $P = 1$, $M = 4$. The narrowing of the space between the red and green lines at the top right of the right side graph suggests that the step-size is becoming too large for convergence.

To obtain the convergence plots for IDC with Heun predictions and corrections i.e. $P = 2$, we used a larger value $T = 4$ in order to forcefully increase the global error. This is done because otherwise the IDC method with $P = 2$ and $M = 4$ has an order of 10 which often makes global error so small that it reaches the resolution of machine epsilon, introducing huge rounding error in the calculations. The constant step-size was gradually decreased by iterating the number of time intervals $J = [16, 18, 20, 22, 24, 26]$.

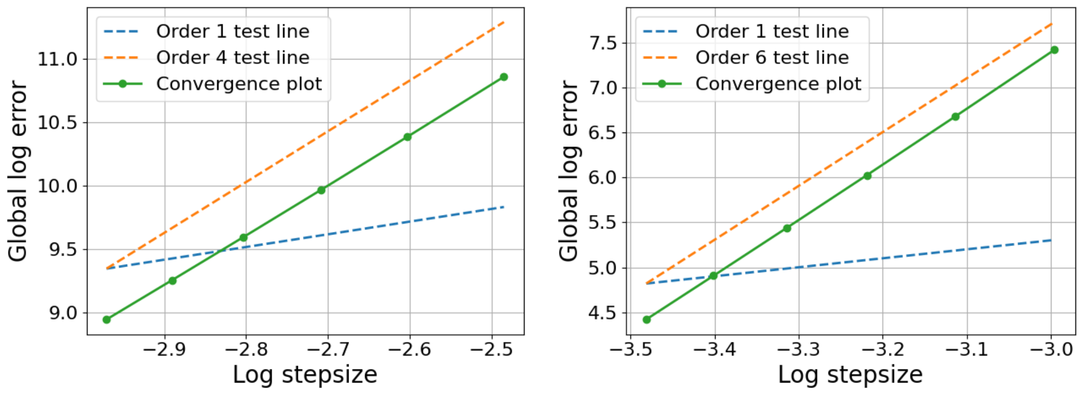


Figure 3.4: (left) IDC with $P = 2$, $M = 1$. (right) IDC with $P = 2$, $M = 2$.

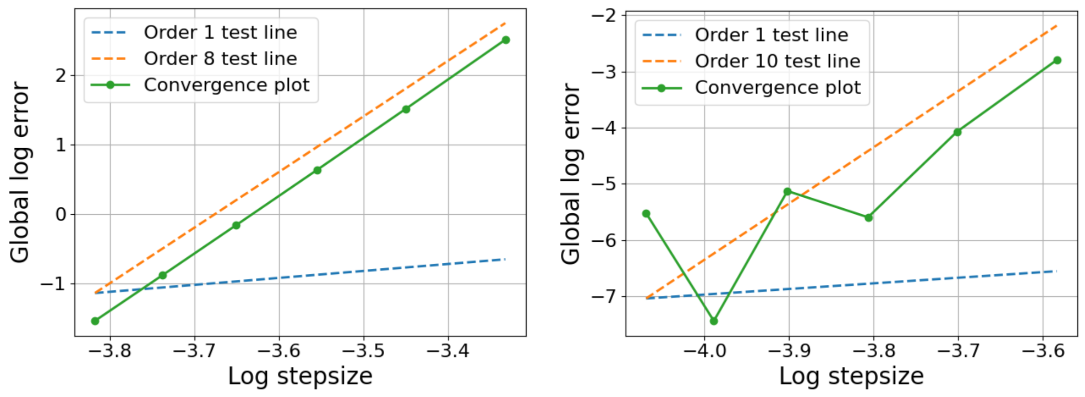


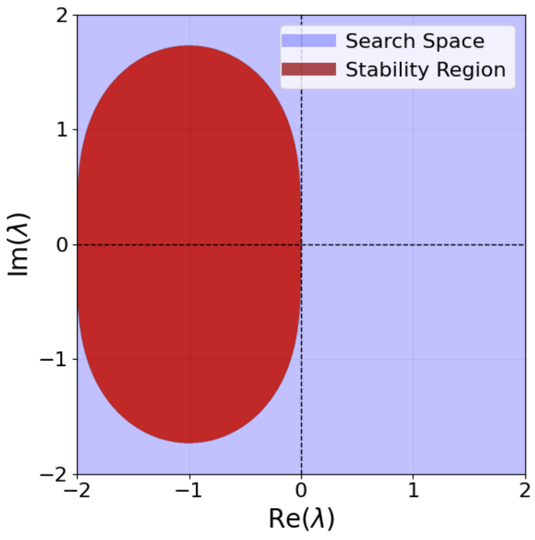
Figure 3.5: (left) IDC with $P = 2$, $M = 3$. (right) IDC with $P = 2$, $M = 4$. The instability at the start of the right side plot is most likely caused by the Runge phenomenon. Runge's phenomenon is the oscillatory inaccuracy of an interpolating polynomial at its boundaries when using high order polynomials and equidistant nodes.

Next we want to obtain stability regions for the IDC method. However, the stability region S given previously by (2.7) cannot be easily plotted for IDC/RIDC. This is because finding all the values $h\lambda$ which gives convergence of the test equation (2.6) is very difficult. So instead we use the following approximation of S:

$$S \approx \{\lambda : |\hat{u}_N| < 1\}, \tag{3.6}$$

where $\hat{u}_N$ is the final value of the numerical solution to (2.6), $J = 1, T = P(M+1) - 1$. We use this value of T since this ensures the step-size is $h = 1$.

The following are stability plots for IDC with $P = 1, 2$:



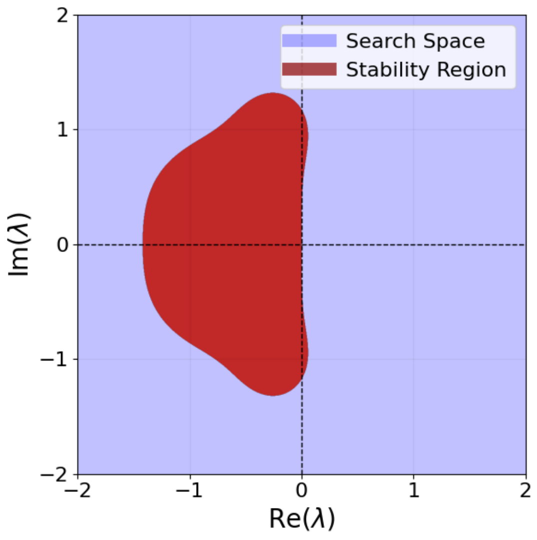
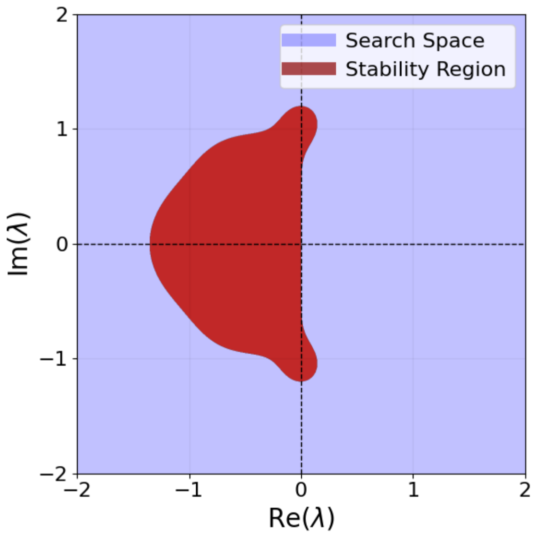


Figure 3.6: (left) $P = 1$, $M = 1$. (right) $P = 1$, $M = 2$.



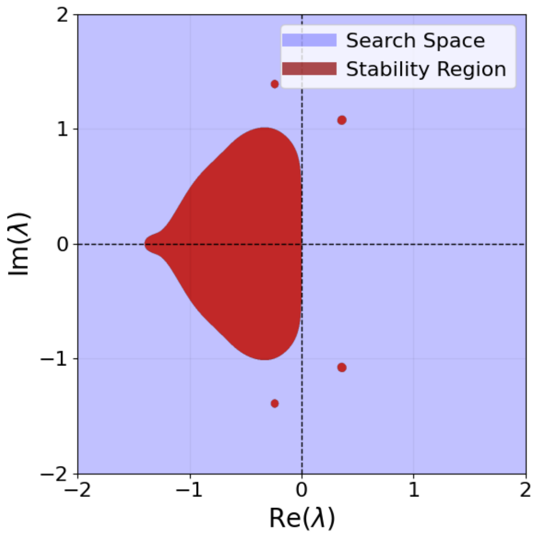


Figure 3.7: (left) $P = 1$, $M = 3$. (right) $P = 1$, $M = 4$.

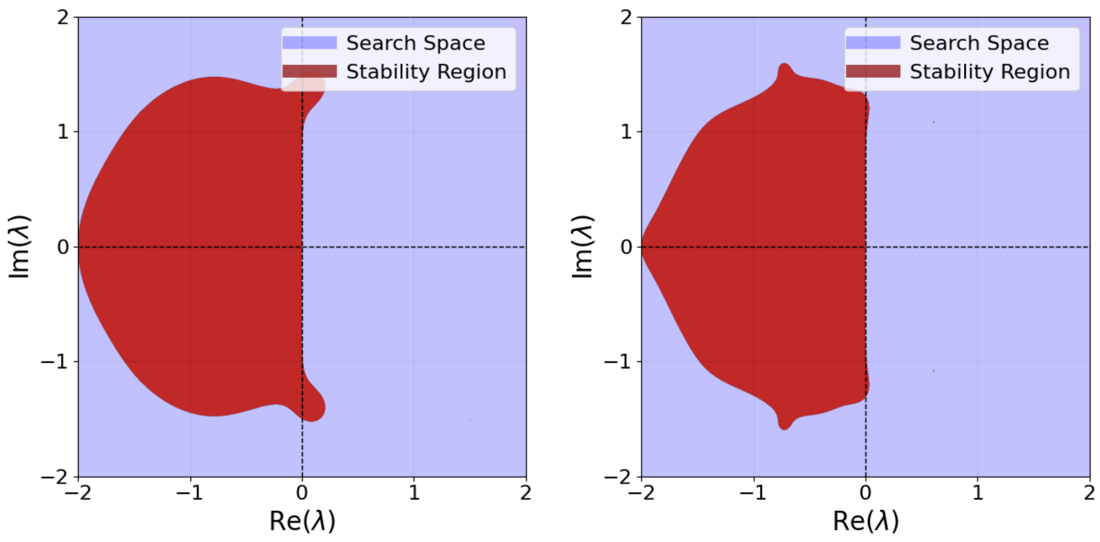


Figure 3.8: (left) $P = 2$, $M = 1$. (right) $P = 2$, $M = 2$.

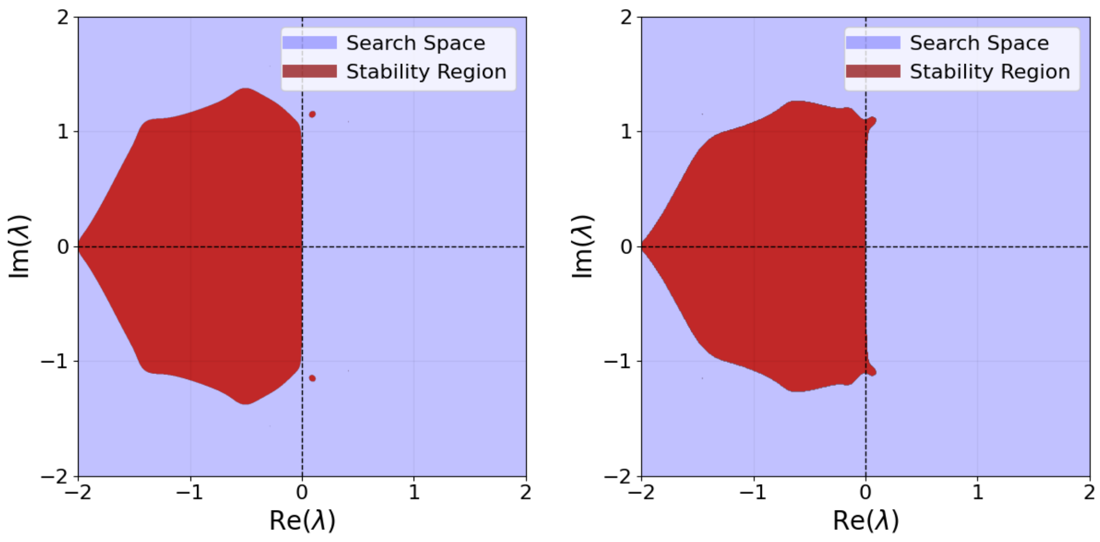


Figure 3.9: (left) $P = 2$, $M = 3$. (right) $P = 2$, $M = 4$.

From the stability plots we determine that higher order IDC methods will typically have better convergence for a wider range of parameters.

Chapter 4

Revisionist Integral Deferred Correction

Revisionist integral deferred correction (RIDC) is an adaptation of the IDC method which, for each time interval, allows the prediction and M correction levels to be calculated in parallel after an initial setup phase which runs sequentially. This theoretically allows for a speedup in computation time up to a factor of $M+1$, with a slight overhead inherent to all parallel algorithms. Each time interval still has K time nodes but the method is most optimal in terms of computation time when K is large. Since $K > P(M+1)$, the quadrature in this stage is no longer fixed to the first $P(M+1)$ nodes and instead advances in time. RIDC still incorporates the same update formulae as IDC and is proven in [4] to have an order of accuracy that is again given by $P(M+1)$.

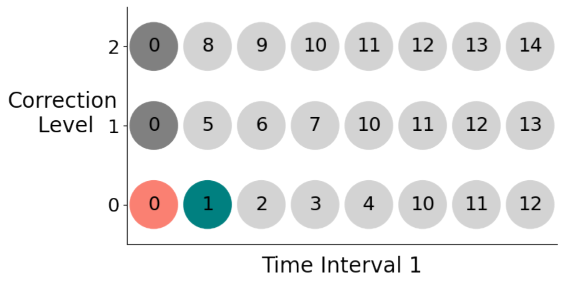
4.1 Overview of RIDC

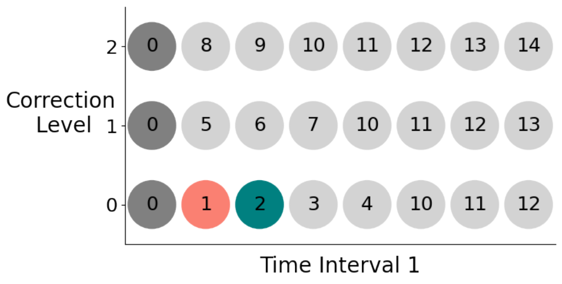
The setup phase has a specific order of calculations which creates a staggered structure of precalculated nodes. The nodes in this first phase are calculated in the following way. We iterate over the correction levels and, for each, only calculate the smallest number of nodes required such that the final level has $P(M+1)$ precomputed nodes.

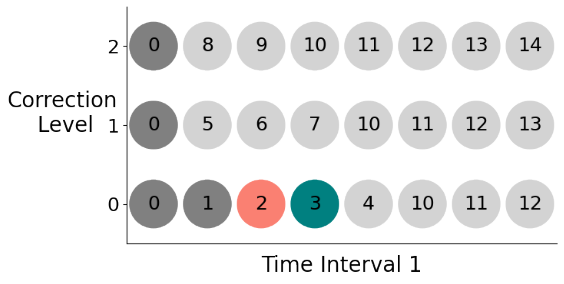
The parallel phase uses an update formula to simultaneously calculate prediction and correction values after the setup phase. This is possible because the staggered node setup means that every correction level contains at least the $P(M+1)$ nodes required for calculating the quadrature in the update formula. **A processor is assigned to each correction level to exclusively calculate values for that particular level. This is why the relative speedup of RIDC over IDC is approximately $\mathbf{M+1}$.**

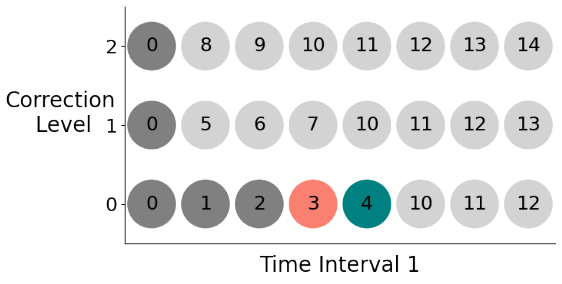
Stencil diagrams for the RIDC method with parameters $P=1, M=2$ and $K=8$ are displayed below:

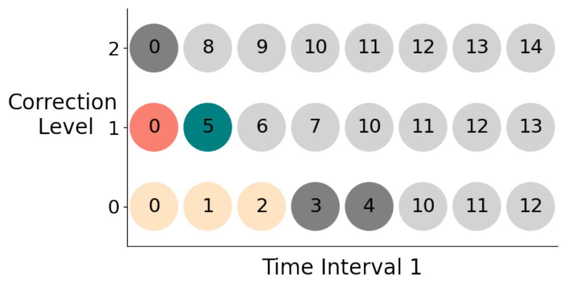
Setup Phase

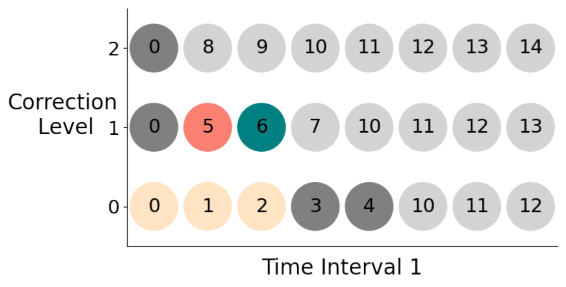


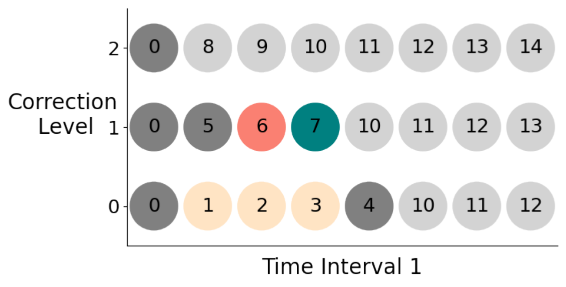


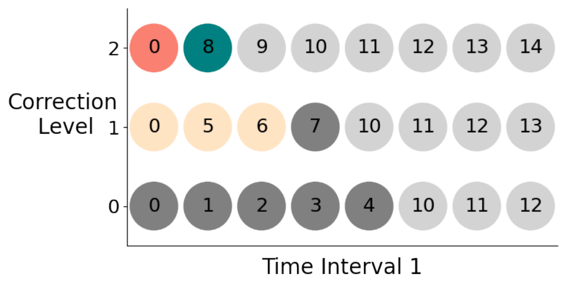


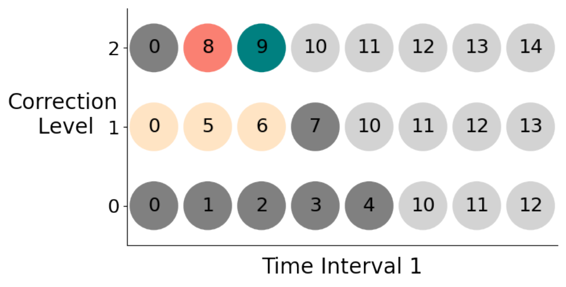



Correction Level
2
1
0
0 8 9 10 11 12 13 14
0 5 6 7 10 11 12 13
0 1 2 3 4 10 11 12
Time Interval 1


Correction Level
2
1
0
0 8 9 10 11 12 13 14
0 5 6 7 10 11 12 13
0 1 2 3 4 10 11 12
Time Interval 1

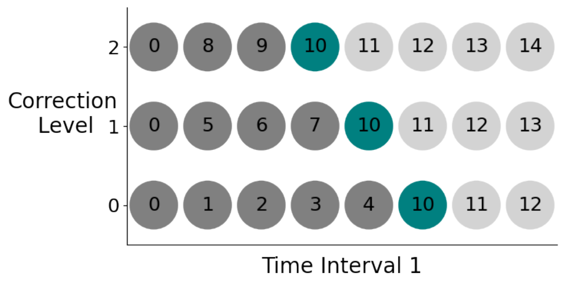

Correction Level
2
1
0
0 8 9 10 11 12 13 14
0 5 6 7 10 11 12 13
0 1 2 3 4 10 11 12
Time Interval 1

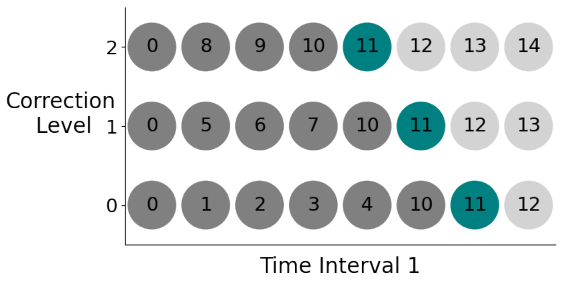

Correction Level
2
1
0
0 8 9 10 11 12 13 14
0 5 6 7 10 11 12 13
0 1 2 3 4 10 11 12
Time Interval 1

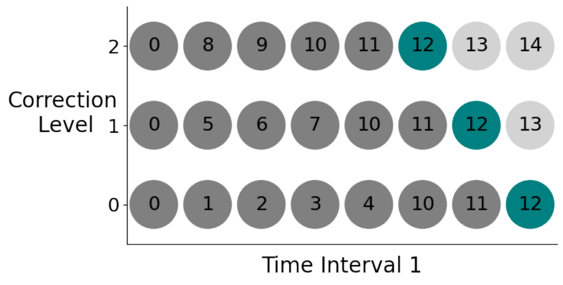

Correction Level
2
1
0
0 8 9 10 11 12 13 14
0 5 6 7 10 11 12 13
0 1 2 3 4 10 11 12
Time Interval 1

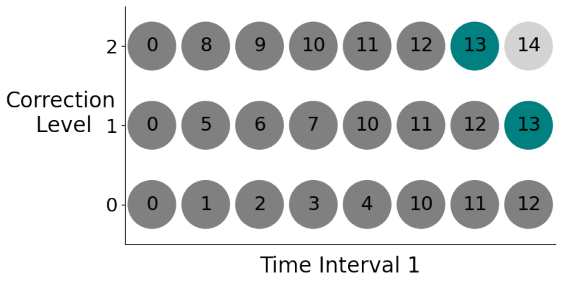
Parallel Phase

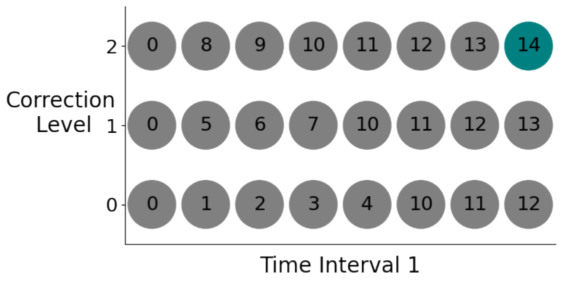
The stencils in the parallel phase don't include the red or yellow node colouring since the previous correction values in time and the quadratures used can overlap. Since there is overlapping of these nodes, this means that RIDC must have some form of memory sharing between the processors running each of the correction levels.











Just like with IDC, once the 14th node has been calculated, its value is dropped down to the lower correction levels to be used as the initial condition for the next time interval.

4.2 Python Code Walkthrough

This subsection provides a detailed walkthrough of my own Python code for a sequential implementation of RIDC, enabling readers to gain a comprehensive understanding of the steps involved in the implementation of the RIDC method with $P = 1$.

Lines 1-31

```python
1  import numpy as np
2  
3  def RIDC_Euler(f:callable, u_0:float, T:float, J:int, K:int, M:int, real:bool=True):
4      """
5      Performs RIDC vector time integration with Euler method predictions and corrections.
6  
7      Args:
8          f: Vector function f(u,t) on RHS of IVP.
9          u_0: Initial condition vector.
10         T: Upper bound on time domain.
11         J: Number of time intervals.
12         K: Number of nodes per interval. (K>>M)
13         M: Number of corrections.
14         real: Set to false if using complex numbers. (optional)
15 
16     Returns:
17         Final correction values for numerical solution across the whole time domain.
18     """
19 
20     # Set default dtype for numpy
21     if real == True:
22         data_type = np.float64
23     else:
24         data_type = np.complex128
25 
26     # Total number of nodes in time domain
27     N = J*(K-1)+1
28     # Get constant step size
29     h = T / (N-1)
30     # Get vector dimension
31     d = len(u_0)
```

1: Numpy is imported. This is the fundamental package for scientific computing in Python, it has features like multidimensional arrays, shape manipulation, linear algebra, etc [6]. It is also the only dependency used in the code.

3: The function 'RIDC_Euler' which will perform the RIDC method on an IVP is defined, along with its input arguments and their types.

4-18: The docstring for 'RIDC_Euler'.

20-31: If complex numbers are desired then the numerical solution will be stored using float64 real and float64 imaginary numbers. Important variables that will be used later are also initialised.

<u>Lines 32-54</u>

```
32
33      # Calculate quadrature weights matrix (uses M+1
    integration points)
34      S = np.zeros(shape=(M, M+1), dtype=data_type)
35      t = np.linspace(0, M*h, num=M+1)
36      for i in range(M+1):
37          coef = np.zeros(shape=(M+1), dtype=data_type)
38          coef[-1] = 1
39          for j in list(range(0, i)) + list(range(i+1, M+1)):
40              coef = np.roll(coef, shift=-1)/(t[i]-t[j]) - coef
    *t[j]/(t[i]-t[j])
41
42          for n in range(M):
43              S[n, i] = (
44                  sum(coef * t[n+1] ** np.arange(M+1, 0, step
    =-1) / np.arange(M+1, 0, step=-1))
45                  -
46                  sum(coef * t[n] ** np.arange(M+1, 0, step=-1)
     / np.arange(M+1, 0, step=-1))
47              )
48
49      # Initialise initial condition
50      u_init = u_0
51
52      # Initialise numerical solution array
53      u_hat = np.zeros(shape=(N, d), dtype=data_type)
54      u_hat[0, :] = u_init
```

33-47: The quadrature weights matrix S is calculated and stored. This only needs to be done once since we are using equidistant nodes, making the polynomial interpolation $\hat{f}$ translationally invariant.

49-50: The variable u_init will hold the initial condition for the current time interval while the process iterates over them. Initially set to the initial condition of the IVP.

52-54: The numerical solution array u_hat is initialised.

Lines 55-80

```
55
56      # Loop over the time intervals
57      for j in range(J):
58          print(f"Time Interval: {j}")
59
60          #
    ------------------------------------------------------------
     #
61          # Setup Phase: Sequentially calculate only the nodes
    necessary
62          # such that the final correction level has P(M+1)
    calculated
63          # nodes.
64
65
66          # Initialise array containing the first 2M-m+1
    vectors for each
67          # pred/corr level, shape: (corr level, time, vec dim)
68          u_first = np.zeros(shape=(M+1, 2*M+1, d), dtype=
    data_type)
69
70          # Get initial condition
71          u_first[:, 0, :] = np.repeat([u_init], M+1, axis=0)
72
73          # First calculate predictions (Euler Method)
74          # Initialise start time
75          t = j*T/J
76          for i in range(2*M):
77              # Get prediction value
78              u_first[0, i+1, :] = u_first[0, i, :] + h*f(
    u_first[0, i, :], t)
79              # Update time value
80              t += h
```

56-58: A for loop over the time intervals since the RIDC method acts sequentially on them.

66-71: Initialisation for the sequential setup phase which occurs at the start of every time interval. The variable u_first is created to contain the first $2M - m + 1$ values for each correction level m.

73-80: The prediction value is calculated using the Euler method.

Lines 81-117

```
81 
82          # Now calculate corrections (Euler Update)
83          for m in range(1, M+1):
84              # Initialise start time
85              t = j*T/J
86              for i in range(2*M-m):
87                  # Get quadrature offset and integration
    points indices
88                  if i >= M:
89                      offset = M-1
90                      int_indices = range(i-(M-1), i+2)
91                  else:
92                      offset = i
93                      int_indices = range(M+1)
94 
95                  # Get quadrature time nodes
96                  quad_nodes = np.linspace(t-offset*h, t+(M-
    offset)*h, num=M+1, dtype=np.float64)
97 
98                  # Get quadrature vector result
99                  f_int = 0
100                 for k in range(M+1):
101                     f_int += (
102                         S[offset, k]
103                         *
104                         f(u_first[m-1, int_indices[k], :],
    quad_nodes[k])
105                     )
106 
107                 # Get correction value
108                 u_first[m, i+1, :] = (
109                     u_first[m, i, :]
110                     +
111                     h*(f(u_first[m, i, :], t) - f(u_first[m
        -1, i, :], t))
112                     +
113                     f_int
114                 )
115 
116                 # Update time value
117                 t += h
```

82-85: A for loop over the correction levels. The initial time value for the current correction level is initialised.

86-93: The indices for the nodes which are used in the quadrature are found and stored by int_indices. The variable offset denotes how many steps to the right of the first quadrature node the previous correction value node is.

95-105: Calculates the time values for each of the nodes in the quadrature. The quadrature value is then computed.

107-117: The correction value is calculated using the $P = 1$ update formula.

<u>Lines 118-140</u>

```
118 
119         # Put the intervals first M+1, final correction
        values
120         # into the solution array
121         u_hat[j*(K-1):j*(K-1)+M+1, :] = u_first[M, :M+1, :]
122 
123         #
        ------------------------------------------------------------
         #
124         # Parallel Phase: Simultaneously (ideally) calculate
        the
125         # new correction values.
126 
127         # Get array for holding the newly calculated values
        in parallel
128         u_new = np.zeros(shape=(M+1, d))
129 
130         # Get array containing the last M+1 values for each
        of the
131         # pred/corr levels, last value is most recent.
132         # shape: (corr level, time, vec dim)
133         u_prev = np.zeros(shape=(M+1, M+1, d))
```

```
134         for m in range(M+1):
135             for i in range(M+1):
136                 u_prev[m, i, :] = u_first[m, i+(M-m), :]
137 
138         # Can now delete the u_first array which is only used
     for setup
139         # to save memory manually
140         del u_first
```

119-121: The first $M+1$ values for the final correction level are stored in the numerical solution matrix.

127-129: A matrix u_new is initialised which can contain all the new values for each correction level which are calculated simultaneously during the parallel phase. Since multiple levels need access to this simultaneously, this variable must be public and shared by all of them.

130-136: A new array u_prev is created which stores the $M+1$ previously calculated values for each correction level. This variable must also be public.

138-140: The u_first variable is deleted to free up memory.

Lines 141-183

```
141 
142         # This is the start of the section which can be
    parallelised
143         # Loop over the time step, we stop if i which
    represents the index
144         # of the current node for the final correction level
    is >= K.
145         for i in range(M, K-1):
146             # Prediction loop
147             if i+M < K-1:
148                 # Get current time
149                 t = j*T/J+(i+M)*h
150                 # Get prediction value
151                 u_corr = u_prev[0, -1, :] + h*f(u_prev[0, -1,
     :], t)
152                 # Add prediction value to new values array
153                 u_new[0, :] = u_corr
154 
155             # Correction loops
156             for m in range(1, M+1):
```

```
157                 if i+M-m < K-1:
158                     # Get time for current loop at current step in algorithm
159                     t = j*T/J+(i+M-m)*h
160
161                     # Get quadrature time nodes
162                     quad_nodes = np.linspace(t-(M-1)*h, t+h, num=M+1)
163
164                     # Get quadrature value
165                     f_int = 0
166                     for k in range(M+1):
167                         f_int += (
168                             S[M-1, k]
169                             *
170                             f(u_prev[m-1, k, :], quad_nodes[k])
171                         )
172
173                     # Get correction value
174                     u_corr = (
175                         u_prev[m, -1, :]
176                         +
177                         h*(f(u_prev[m, -1, :], t) - f(u_prev[m-1, -2, :], t))
178                         +
179                         f_int
180                     )
181
182                     # Add correction value to new values array
183                     u_new[m, :] = u_corr
```

142-144: This is where we would normally begin incorporating multi-threaded parallelism. There are now enough values calculated in each correction level such that the process can run simultaneously over them.

145-183: Much of this is similar to the setup phase, however there are some minor differences. An offset value is no longer necessary and all new values calculated are stored in the u_new array. Once the u_new array is filled for the current time step then the threads are allowed to continue to the next step simultaneously. This prevents a race condition when the u_prev array is updated.

Lines 184-201

```
184
185             # Put the final correction value into the solution array
186             u_hat[j*(K-1)+i+1, :] = u_corr
187
188             # Here we must wait for all threads to arrive at this
189             # point before continuing to update the previous values
190             # array
191             u_prev[:, :-1, :] = u_prev[:, 1:, :]
192             u_prev[:, -1, :] = u_new
193
194         # ------------------------------------------------------------ #
195         # End Phase: Update the initial condition for the next time
196         # interval
197
198         # Drop down final correction value to lower correction levels
199         u_init = u_prev[M, -1, :]
200
201     return u_hat
```

185-186: This puts the final value calculated in the last correction level into the numerical solution array. This would not be feasible under parallelisation since u_corr wouldn't be guaranteed to represent the final correction level.

188-192: If this was a parallelised implementation then we would first have to wait here for all threads to catch up with one another before updating the u_prev array. This is important to do in order to avoid a race condition.

195-199: This is the end phase for the current time interval. The final value in the last correction level is used as the new initial condition for the next time interval.

201: The numerical solution array is returned as the output of the function.

4.3 Validation of RIDC

Although RIDC should have almost identical analytical properties to IDC, it is still important to ensure that the RIDC method has been programmed correctly. We again use convergence plots to check that we obtain the expected order of accuracy, validating our implementation. To obtain the convergence plots, equation (3.5) is again solved with $T = 4$. The RIDC method was initialised with parameters $P = 1$, $K = 100$ and the step size h was gradually decreased by iterating over $J = [1, 2, 3, 4, 5]$.

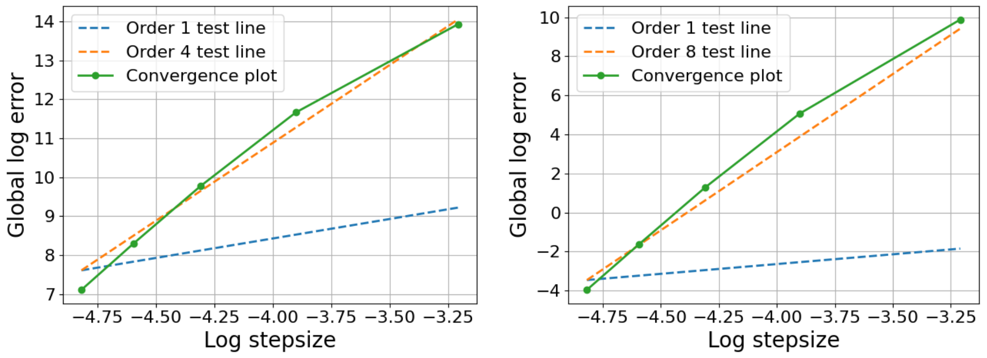


Figure 4.1: (left) RIDC with $P = 1$, $M = 3$, $K = 100$. (right) RIDC with $P = 1$, $M = 7$, $K = 100$. The plots agree with their expected orders of accuracy, 4 and 8 respectively.

We also implemented RIDC on a large 2D n-body problem using a parallelised and sequential version of the code in order to inspect the difference in computation time. A large n-body problem was chosen since the benefit of using parallel RIDC increases as f, the RHS to (2.1), becomes more computationally intensive to evaluate, making the benefit from parallelism as prominent as possible. For this comparison, my own source codes were programmed in Fortran and compiled using the Intel© Fortran Compiler. The parallel implementation uses the OpenMP library [3] to incorporate multi-threaded parallelism over the correction levels.

The 2D n-body problem with $n = 128$ bodies was,

$$x_i''(t) = 0.01 \sum_{j=1,\, j\neq i}^{128} \left(\frac{x_j - x_i}{||x_j - x_i||^3} \mathbb{1}(||x_j - x_i|| > 0.01) \right) - x_i'(t),$$

where $x_i \in \mathbb{R}^2$, $i = 1, 2, ..., 128$, $t \in [0, 1]$ and $\mathbb{1}$ is the indicator function.

This dynamical system is easily put into canonical form, turning this set of 128 second order ODEs into 256 first order IVPs,

$$\begin{cases} u_i'(t) = 0.01 \sum_{j=1,\, j\neq i}^{128} \left(\frac{x_j - x_i}{||x_j - x_i||^3} \mathbb{1}(||x_j - x_i|| > 0.01) \right) - u_i(t), \\ x_i'(t) = u_i(t). \end{cases} \tag{4.1}$$

These 256 vector IVPs of dimension 2 were then flattened into a single vector IVP of dimension 512, which was then solved using the parallel and sequential versions of RIDC, 5 times each. Both of the integrators were setup with the same parameters; $P = 1$, $J = 10$, $K = 1000$, $M = 4$. The results for the total wall-clock time (in seconds) taken for RIDC to complete were as follows:

Version	1	2	3	4	5	Mean
Sequential	350.5472	350.5016	351.3865	350.9930	351.1342	350.9125
Parallel	110.2889	102.8561	100.5951	97.9449	113.5925	105.0555

Based on the mean results from (4.1), I determine that my parallel implementation is a significant improvement on the sequential RIDC method, achieving an average speedup of approximately 3.3 times. However, it is still dissapointing that this value is much below the theoretical maximum speedup of 5 times for this specific setup of RIDC. There are many plausible reasons for why my result is sub-optimal, a list of a few are given below:

- The function f may not be computationally intensive enough to benefit most from parallelism still.
- The value of K could be too low to benefit most from parallelism.
- My application of multi-threaded parallelism is surely sub-optimal.
- All parallel algorithms have inherent initialisation costs of threads/processors.
- CPU time may be a better comparison metric.
- My laptop could have been thermal throttling.

Chapter 5

Partial Differential Equations

Partial Differential Equations (PDEs) are an essential tool for mathematical modeling with broad applications in various fields, including physics, engineering, finance, and biology. PDEs involve multiple variables and their partial derivatives, modeling complex systems that vary continuously in space and time with several interacting variables. As such, finding analytical solutions to PDEs is a difficult task, and numerical methods provide a powerful tool for obtaining approximate solutions.

One common approach to finding numerical solutions of PDEs is to use time integration methods to obtain a sequence of solutions at discrete time points, and then combine these with spatial methods to obtain an approximate solution of the PDE at all points in the domain. The choice of time integration method and spatial discretization method can have a significant impact on the accuracy and efficiency of the numerical solution, and a range of approaches have been developed, including finite difference, finite element, and spectral methods.

The main focus of this chapter is to explore the combination of RIDC with spectral methods as a technique for obtaining numerical solutions to PDEs. By combining these methods, we aim to achieve solutions with both high temporal and spatial order of accuracy within an optimised amount of computation time via parallelism.

5.1 Spectral Methods

Spectral methods are another class of techniques used to numerically solve differential equations, however they are typically used for those which are defined on a spatial domain. They all assume that the solution can be written as a linear combination of a set of predetermined basis functions. We then choose the coefficients which allow the sum to best satisfy the differential equation. The process for which these coefficients are found is what defines a specific spectral method. Spectral methods all have extremely high order of accuracy if the basis functions chosen are suitable to the problem. This is because they interpolate a function globally, rather than locally as in finite element schemes for example.

The general form of a spectral solution $\hat{u}$ to a PDE involving variables in time and space is,

$$\hat{u}(x,t) = \sum_n c_n(t)\psi_n(x), \tag{5.1}$$

where the c_n are time dependent coefficients to be found and the ψ_n are predetermined basis functions.

5.1.1 The Fourier Spectral Method

As an initial example, we will use the spectral method to numerically solve the 1D heat equation, assuming plane wave basis functions. In other words, we are attempting to find the best Fourier series which satisfies the PDE,

$$\begin{gathered}\frac{\partial u}{\partial t} = k^2 \frac{\partial^2 u}{\partial x^2}, \\ u(x+L,t) = u(x,t), \quad u(x,0) = u_0(x), \quad x \in [0,L], \quad t \in [0,T].\end{gathered} \tag{5.2}$$

We begin by substituting (5.1) into (5.2) to obtain,

$$\sum_n c_n'(t)\psi_n(x) = k^2 \sum_n c_n(t)\psi_n''(x).$$

The plane wave basis functions are given by,

$$\psi_n(x) = \tfrac{1}{\sqrt{L}} e^{-i\alpha_n x}, \quad \alpha_n = (-1)^n \lceil \tfrac{n}{2} \rceil \tfrac{2\pi}{L}$$

Resulting in,

$$\sum_n \left(c_n'(t) + \alpha_n^2 c_n(t)\right) \psi_n(x) = 0.$$

We define the inner product by,

$$\langle f, g\rangle = \int_0^L f(x)\overline{g(x)}dx.$$

The plane wave basis functions are orthonormal in this Hilbert space and can therefore be used to find IVPs for the time dependent coefficients c_n,

$$\langle \psi_n, \psi_m\rangle = \begin{cases} 1 & \text{if } n = m \\ 0 & \text{if } n \neq m \end{cases},$$

$$\left\langle \sum_n \left(c_n'(t) + \alpha_n^2 c_n(t)\right) \psi_n, \psi_m \right\rangle = \sum_n \left(c_n'(t) + \alpha_n^2 c_n(t)\right) \langle \psi_n, \psi_m\rangle = 0.$$

The IVPs for finding the c_n are then,

$$c_n'(t) + \alpha_n^2 c_n(t) = 0, \quad c_n(0) = \int_0^L u_0(x)\overline{\psi_n(x)}dx.$$

To make this process an algorithm, only N many basis functions are used in the numerical solution. We then use RIDC to solve for the N coefficient functions. The inner product integral first needs to be calculated to obtain the initial condition values and this is found using a quadrature. In this case, the quadrature we use is the discrete Fourier transform,

$$c_n(0) = \frac{1}{N}\sum_{j=0}^{N-1} u_0(x_j)e^{\frac{2\pi inj}{N}},$$

where the x_j are equidistant nodes in $[0, L]$. We then retrieve N values of the solution (5.1), for each time step, evaluated at the nodes x_j by using the inverse Fourier transform on the coefficients found via RIDC. It is shown in [8] that the Fourier spectral method has an order of accuracy of N if the basis functions used are suitable for the problem being solved.

For our example (5.2), we use $T = 0.2, L = 2\pi, k = 1$ and the initial condition $u_0(x) = 2\sin 3x + \sin 9x - 3\cos 5x$. The joint RIDC, Fourier spectral solution is then acquired by performing the steps above.

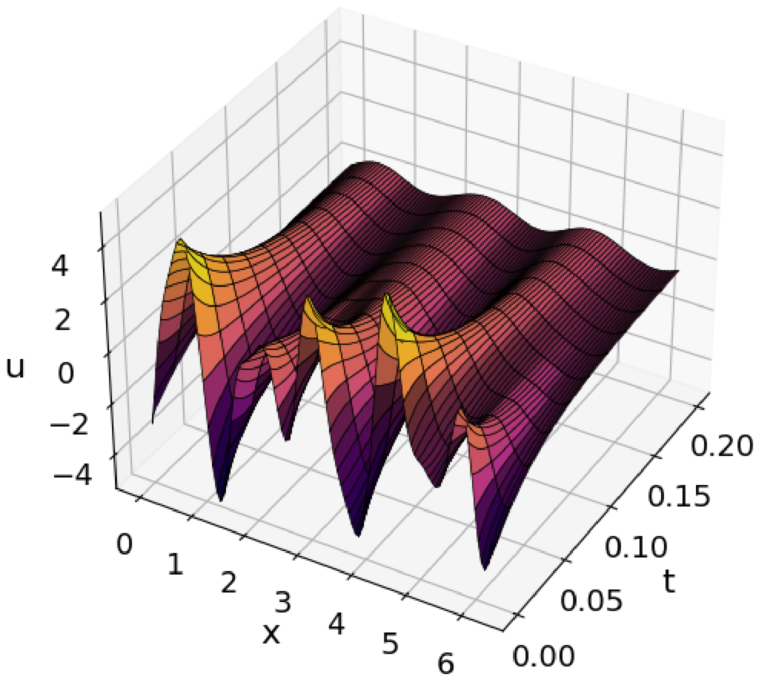


Figure 5.1: The numerical solution to (5.2) using RIDC time integration and the Fourier spectral method. The parameters used for the integration methods are: $N = 100, P = 1, J = 10, K = 1000, M = 3$. We therefore expect this solution to have an order of accuracy in time of 4 and in space of 100.

5.1.2 The Pseudo-Spectral Method

The Fourier spectral method encounters problems when trying to numerically solve more complicated PDEs involving non-linear terms. For example, solution values produced by these non-linear terms can exhibit non-continuous like behaviour, this is a problem for all global interpolation methods. It is also computationally costly to find the coefficients for the product of our numerical solution by another function. This problem can be mitigated via an alteration to the Fourier spectral method known as the pseudo-spectral method.

We want to multiply a numerical solution (5.1) by an arbitrary function $v(x)$. The resulting function is denoted h.

$$h(x) = \hat{u}(x)v(x),$$

$$\hat{u}(x) = \sum_{n=0}^{N} c_n \psi_n(x), \quad h(x) = \sum_{n=0}^{N} \gamma_n \psi_n(x).$$

We need to be able to find the coefficents γ_n in the sum of $h(x)$,

$$\gamma_n = \langle h, \psi_n \rangle = \langle \hat{u}v, \psi_n \rangle,$$

$$\gamma_n = \sum_{m=0}^{N} V_{n,m}\, c_m, \quad V_{n,m} = \langle v\psi_m, \psi_n \rangle.$$

Finding these coefficients requires computational complexity $O(N^2)$ since the matrix vector multiplication is a convolution, this is because V is a Toeplitz matrix. V also needs to be precomputed, adding an extra step to the method.

The pseudo-spectral method assumes that the quadrature, given by the discrete Fourier transform (DFT), used to find $\langle u_0, \psi_n \rangle$ can also be used to approximate $\langle \hat{u}v, \psi_n \rangle$. If we denote the DFT in space by $\mathcal{F}_x$ then we can calculate γ_n using,

$$\gamma_n = \mathcal{F}_x\{\hat{u}(x_i)v(x_i)\}.$$

Therefore, we can remove the need to precompute a matrix and we can also use the fast Fourier transform (FFT) instead of the naive DFT algorithm.

This reduces the computational complexity of finding the γ_n to $O(N \log N)$ [1].

To illustrate the pseudo-spectral method, we try to solve the 2D incompressible vorticity equation with no external forces,

$$\begin{gathered}
\frac{\partial w}{\partial t} = \nu \nabla^2 w - (\mathbf{u} \cdot \nabla) w, \quad -\nabla^2 \mathbf{u} = \nabla \times \mathbf{w}, \\
w(x+L, y+L, t) = w(x,y,t), \quad w(x,y,0) = w_0(x,y), \\
x, y \in [0,L]^2, \quad t \in [0,T].
\end{gathered} \tag{5.3}$$

The steps involved in solving (5.3) with the pseudo-spectral method are as follows:

We apply the FFT to (5.3) and obtain,

$$\begin{aligned}
\frac{\partial \tilde{w}}{\partial t} = & -\mathcal{F}_x\{u_x \mathcal{F}_x^{-1}\{ik_x \tilde{w}\} + u_y \mathcal{F}_x^{-1}\{ik_y \tilde{w}\}\} \\
& -\nu(k_x^2 + k_y^2)\tilde{w}.
\end{aligned}$$

To find the coefficients for the terms in red, which highlight the function multiplication that we want to avoid, we could perform a convolution but instead use the FFT for the previous reasons.

We find that u_x and u_y are sole functions of $\tilde{w}$ using $-\nabla^2 \mathbf{u} = \nabla \times \mathbf{w}$ and noticing,

$$\tilde{u}_x = \frac{k_y}{k_x^2 + k_y^2} i\tilde{w}, \quad \tilde{u}_y = -\frac{k_x}{k_x^2 + k_y^2} i\tilde{w}.$$

Resulting in,

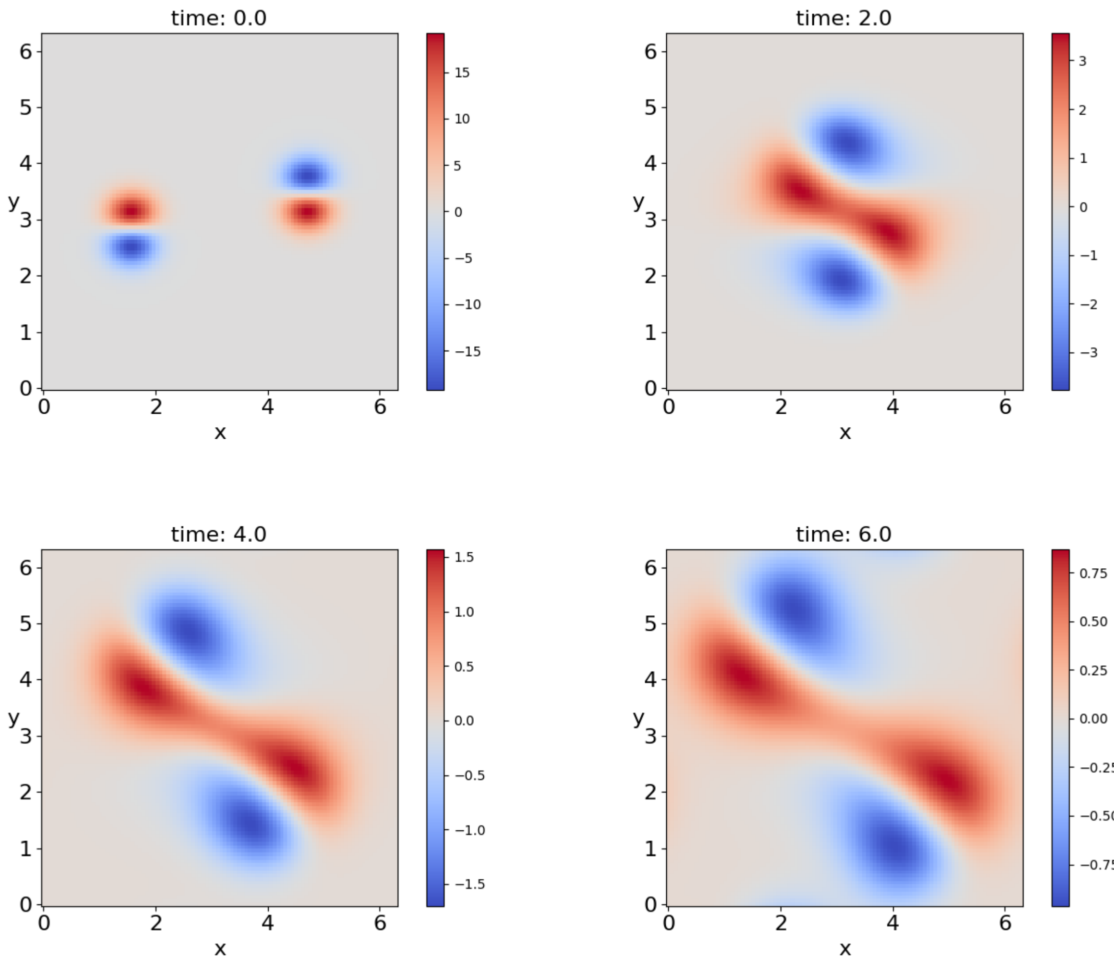
$$\begin{aligned}
\frac{\partial \tilde{w}}{\partial t} = & -\mathcal{F}_x\{\mathcal{F}_x^{-1}\{\tilde{u}_x\}\mathcal{F}_x^{-1}\{ik_x \tilde{w}\} + \mathcal{F}_x^{-1}\{\tilde{u}_y\}\mathcal{F}_x^{-1}\{ik_y \tilde{w}\}\} \\
& -\nu(k_x^2 + k_y^2)\tilde{w}.
\end{aligned} \tag{5.4}$$

Therefore, to find our numerical solution we need to solve for $\tilde{w}$ by using RIDC on (5.4) with the initial condition $\tilde{w}_0 = \mathcal{F}_x\{w_0\}$. We then use the inverse FFT algorithm to obtain our solution values of interest, w from $\tilde{w}$.

For our example to (5.3), we use $T = 10, L = 2\pi, \nu = 0.5$ and the initial condition for the velocity is,

$$\mathbf{u}_0(x, y) = 10(e^{-5((x-0.5\pi)^2+(y-0.9\pi)^2)} - e^{-5((x-1.5\pi)^2+(y-1.1\pi)^2)})\mathbf{e}_x.$$

We find the initial condition for the coefficients using $\tilde{w}_0 = -ik_x\mathcal{F}_x\{\mathbf{u}_0\}$. The joint RIDC, pseudo-spectral solution is then acquired by performing the steps above.



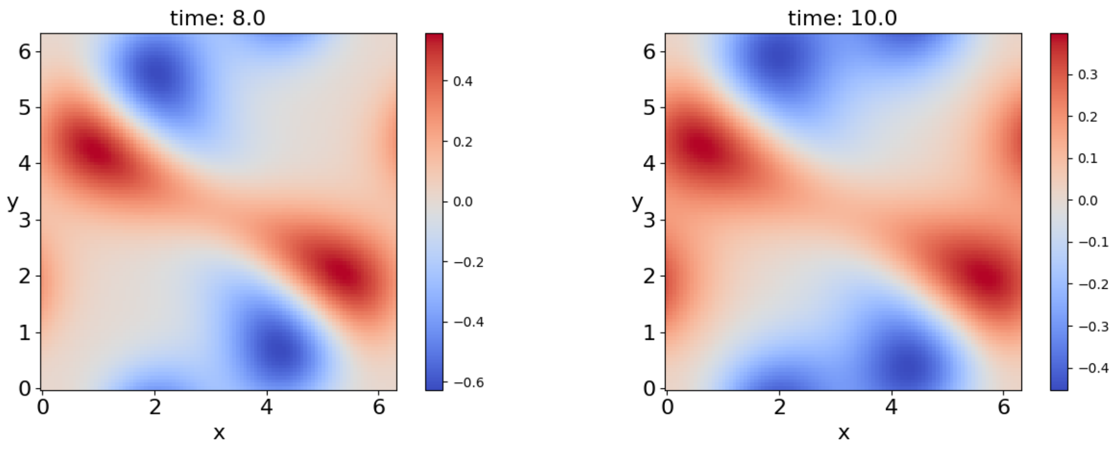


Figure 5.2: The time evolution of the numerical solution to (5.3) using RIDC time integration and the pseudo-spectral method. The parameters used for the integration methods are: $N = 100, P = 1, J = 5, K = 2000, M = 3$. We therefore expect this solution to have an order of accuracy in time of 4 and in space of 100.

Chapter 6

Conclusion

To summarise, this report has provided a detailed discussion on the Revisionist Integral Deferred Correction (RIDC) method as an adaptation to the Integral Deferred Correction (IDC) method, with a focus on its parallel implementation. We began by introducing classical time integrators and their properties, followed by an explanation of the IDC and RIDC methodology.

Through empirical analysis, we have demonstrated that the order of accuracy for both methods is given by P(M+1), where P is the order of the underlying time integration method and M is the number of correction levels. We have also shown that RIDC, when combined with the spectral method, can be used to obtain high order and time-efficient solutions to partial differential equations.

We have also emphasised the advantages of parallelism, particularly when dealing with high order time integrators that involve multiple correction levels. With the parallel implementation of RIDC, adding more correction levels does not necessarily increase the computation time since multiple processors can act simultaneously over the staggered nodes in each correction level. This is made possible through the initial setup phase, which creates a staggered node arrangement in the correction levels.

Overall, this report highlights that the RIDC is a highly efficient and accurate method for time integration. Further research in this area can lead to the development of more accurate and efficient methods for solving complex numerical simulations.

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Appendix A

Fortran Code for Parallel RIDC

```fortran
program RIDCEuler

use omp_lib

implicit none

! Computation time variables
double precision :: start_time, end_time, elapsed_time

! Function input variables
real :: T=1.0
complex :: u_0(1)=[1.0]
integer :: J=10, K=1E7, M=9

! Allocatable function variables
double complex, allocatable :: u_hat(:, :), u_init(:),
    u_first(:, :, :), f_int(:)
double complex, allocatable :: u_new(:, :), u_prev(:, :, :),
    u_corr(:)
double precision, allocatable :: S(:, :), t_nodes(:), coef(:)
    , quad_nodes(:)
integer, allocatable :: powers(:), int_indices(:)

! Function variables
double precision :: h, t_curr
integer :: N, d, offset, thread_id

```

```fortran
! Loop variables
integer :: i_do, j_do, m_do, k_do

! Print max number of threads
call omp_set_num_threads(M+1)
print *, "Num Threads: ", omp_get_max_threads()

! Initialise timer
start_time = omp_get_wtime()

! Body of RIDCEuler
N = J*(K-1)+1
h = T / (N-1)
d = size(u_0)

! ------------------------------------------
! Calculate quadrature weights matrix
allocate(S(M, M+1))
allocate(t_nodes(M+1))
allocate(powers(M+1))

do i_do = 1, M+1
    t_nodes(i_do) = (i_do-1)*h
    powers(i_do) = M+2-i_do
end do

do i_do = 1, M+1
    allocate(coef(M+1))
    coef(1:M) = 0.0
    coef(M+1) = 1.0

    do j_do = 1, M+1
        if (j_do /= i_do) then
            coef = cshift(coef, shift=1) / (t_nodes(i_do)-
  t_nodes(j_do)) &
                  - coef * t_nodes(j_do) / (t_nodes(i_do)-
  t_nodes(j_do))
        end if
    end do

    do j_do = 1, M
        S(j_do, i_do) = sum(coef * t_nodes(j_do+1)**powers /
  powers) &
            - sum(coef * t_nodes(j_do)**powers / powers)
    end do
    deallocate(coef)
```

```fortran
end do

deallocate(t_nodes)
deallocate(powers)

! ------------------------------------------
! Start of RIDC Method

! Initialise initial condition
allocate(u_init(d))
u_init = u_0

! Initialise numerical solution array
allocate(u_hat(N, d))
u_hat(1, :) = u_init

! Loop over the J time intervals
do j_do = 1, J
    print *, "Time Interval:", j_do

    ! ------------------------------------------
    ! Setup Phase: Sequentially compute only the nodes
    ! necessary for each correction level such that the
    ! last has exactly P(M+1) calculated nodes.


    ! Initialise array containing the first 2M-m+1
    ! vectors for each correction level,
    ! shape: (corr_lvl, time, vec_dim)
    allocate(u_first(M+1, 2*M+1, d))
    u_first(:, 1, :) = spread([u_init], dim=1, ncopies=M+1)

    ! Prediction loop (Euler Method)
    ! Initialise start time
    t_curr = (j_do-1)*T/J
    do i_do = 1, 2*M
        ! Get prediction value
        u_first(1, i_do+1, :) = u_first(1, i_do, :) &
            + h*f(u_first(1, i_do, :), t_curr)

        ! Update time value
        t_curr = t_curr + h

    end do

    ! Correction loops (Euler Update)
    do m_do = 2, M+1
        ! Initialise start time
        t_curr = (j_do-1)*T/J
        do i_do = 1, 2*M+1-m_do
            allocate(int_indices(M+1))
            allocate(quad_nodes(M+1))

            ! Get quadrature offset and integration points
            if (i_do >= M+1) then
                offset = M
                do k_do = 1, M+1
                    int_indices(k_do) = k_do+i_do-M
                end do
            else
                offset = i_do
                do k_do = 1, M+1
                    int_indices(k_do) = k_do
                end do
            end if

            ! Get quadrature time nodes
            do k_do = 1, M+1
                quad_nodes(k_do) = t_curr+(k_do-offset)*h
            end do

            allocate(f_int(d))

            ! Get quadrature approximation
            f_int(:) = 0
            do k_do = 1, M+1
                f_int = f_int + S(offset, k_do) &
                    *f(u_first(m_do-1, int_indices(k_do), :), quad_nodes(k_do))
            end do

            deallocate(int_indices)
            deallocate(quad_nodes)

            ! Get correction value
            u_first(m_do, i_do+1, :) = u_first(m_do, i_do, :) &
                + h*(f(u_first(m_do, i_do, :), t_curr) - f(u_first(m_do-1, i_do, :), t_curr)) &
                + f_int

            deallocate(f_int)

            ! Update time value
            t_curr = t_curr + h

        end do
    end do

    ! Put the time intervals first M+1 values for the
    ! final correction level into the solution array
    u_hat((j_do-1)*(K-1)+1:(j_do-1)*(K-1)+M+1, :) = u_first(M+1, 1:M+1, :)

    ! ------------------------------------------
    ! Parallel Phase: Simultaneously calculate the new
    ! correction values.

    ! Initialise array for holding the new values
    allocate(u_new(M+1, d))

    ! Initialise array for holding the M+1 most recent
    ! values calculated for each correction level
    ! shape: (corr lvl, time, vec dim)
    allocate(u_prev(M+1, M+1, d))
    do m_do = 1, M+1
        do i_do = 1, M+1
            u_prev(m_do, i_do, :) = u_first(m_do, i_do+M+1-m_do, :)
        end do
    end do

    deallocate(u_first)
    allocate(u_corr(d))

    ! Loop over the time step, we stop if i which
    ! represents the index of the current node is
    ! >= K+1

    ! This is the section we run in parallel
    !$omp parallel private(i_do, m_do, k_do, t_curr, u_corr, quad_nodes, f_int, thread_id)
    thread_id = omp_get_thread_num()

    do i_do = M+1, K-1
        ! Prediction loop
        if (i_do+M < K .and. thread_id == 0) then
            ! Get current time
            t_curr = (j_do-1)*T/J + (i_do+M-1)*h
            ! Get prediction value
            u_corr = u_prev(1, M+1, :) + h*f(u_prev(1, M+1, :), t_curr)
            ! Add prediction to new values array
            u_new(1, :) = u_corr
        end if

        ! Correction loop
        do m_do = 2, M+1
            if (i_do+M+1-m_do < K .and. thread_id == m_do-1) then
                ! Get current time
                t_curr = (j_do-1)*T/J + (i_do+M-m_do)*h

                ! Get quadrature time nodes
                allocate(quad_nodes(M+1))

                do k_do = 1, M+1
                    quad_nodes(k_do) = t_curr+(k_do-M)*h
                end do

                ! Get quadrature approximation
                allocate(f_int(d))
                f_int(:) = 0
                do k_do = 1, M+1
                    f_int = f_int + S(M, k_do) &
                        *f(u_prev(m_do-1, k_do, :), quad_nodes(k_do))
                end do

                deallocate(quad_nodes)

                ! Get correction value
                u_corr = u_prev(m_do, M+1, :) &
                    + h*(f(u_prev(m_do, M+1, :), t_curr) - f(u_prev(m_do-1, M, :), t_curr)) &
                    + f_int

                deallocate(f_int)

                ! Add correction value to new values array
                u_new(m_do, :) = u_corr

            end if

            if (m_do == M+1 .and. thread_id == M) then
                ! Put the final correction value into solution array
                u_hat((j_do-1)*(K-1)+i_do+1, :) = u_corr
            end if

        end do

        !$omp barrier

        if (thread_id == 0) then
            ! Update the previous values array
            u_prev(:, 1:M, :) = u_prev(:, 2:M+1, :)
            u_prev(:, M+1, :) = u_new
        end if

    end do

    !$omp end parallel


    ! ------------------------------------------------------------
    ! End Phase: Update the initial condition for the next time
    ! interval. Also deallocate arrays

    ! Drop down final correction value to lower correction levels
    u_init = u_prev(M+1, M+1, :)

    deallocate(u_new)
    deallocate(u_prev)
    deallocate(u_corr)

end do

! Get elapsed time
end_time = omp_get_wtime()
elapsed_time = end_time - start_time

print *, "Elapsed Time: ", elapsed_time
read(*, *)

contains
```

```fortran

! RHS of IVP, u'(t)=f(u,t)
function f(u, t)
    implicit none

    double complex, intent (in) :: u(1)
    double precision, intent (in) :: t

    double complex :: f(1)

    f = 2.0*t*u
end function f

end program RIDCEuler
```