Solving Parabolic Equations in 2 and 3 Space Dimensions

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Abstract

In 'Numerical Solution of Parabolic Equations' [18] we have introduced the general theory for finite difference methods for parabolic problems. Inspired by a class of specific problems we shall now extend the theory to address the challenges of some realistic problems. We discuss a number of extensions of the ADI methods to three space dimensions and compare their various merits w.r.t. accuracy and stability in addition to their tendency to produce unwanted oscillations and spikes. Our method of choice is an extension of the SDR-method which will produce smooth solutions. SDR is only first order in time but in the presence of a singularity the meaning of order loses some of its significance. We show that by using extrapolation techniques it is possible to recover and in fact raise the order without losing the smoothness. In order to treat boundary layer problems we use variable steps in space: the exponentially expanding steps. We analyze the stability and accuracy of exponentially expanding steps and show that the global error (in space) is proportional to $(\gamma - 1)^2$ where γ is the expansion factor. With this information we can again use extrapolation techniques to produce accurate solutions with a modest time consumption.

Contents

1 Introduction

A class of electrochemical problems has been modeled in a series of papers ([3, 4, 5, 6, 7, 22]). The problem is that of an electrode embedded in an insulating plane which constitutes the bottom of a large vessel containing a solution of an electroactive substance, initially with a uniform concentration C^* throughout.

At time $T = 0$ an electrochemical reaction starts at the electrode, producing a current $I(T)$, removing the electroactive substance, and subsequently starting a diffusion towards the electrode described by the equation

$$\frac{\partial C}{\partial T} = D(\frac{\partial^2 C}{\partial X^2} + \frac{\partial^2 C}{\partial Y^2} + \frac{\partial^2 C}{\partial Z^2}) \tag{1}$$

where D is the diffusion coefficient. In the first problem the electrode is rectangular with width W in the Y-direction and length L in the X-direction. The Z-direction is perpendicular to the plane of the electrode which is placed with its center at the origin of the coordinate system. The current is computed as

$$I = nFD \int_{-L/2}^{L/2} \int_{-W/2}^{W/2} \frac{\partial C}{\partial Z} |_{Z=0} \; dY dX \tag{2}$$

where n is the number of electrons transferred and F is the Faraday constant.

In the following we shall go deeper into the mathematics and numerics of these problems.

2 Problem 1: a rectangular electrode

We prefer to work with dimensionless variables so we introduce the following normalisations

$$x = \frac{X}{W},\ y = \frac{Y}{W},\ z = \frac{Z}{W},\ l = \frac{L}{W},\ u = \frac{C}{C^*},\ t = \frac{DT}{W^2},$$

and we solve for one quarter of the electrode.

The problem for the rectangular electrode in dimensionless variables is now

$$\begin{array}{lcll}
u_t & = & u_{xx} + u_{yy} + u_{zz}, & t > 0, \qquad x, y, z > 0 \\
u & = & 1, & t = 0 \\
u & = & 1, & x = x_m \text{ or } y = y_m \text{ or } z = z_m \\
u_x & = & 0, & x = 0, \qquad 0 < y < y_m, \qquad 0 < z < z_m \\
u_y & = & 0, & y = 0, \qquad 0 < x < x_m, \qquad 0 < z < z_m \\
u_z & = & 0, & z = 0, \qquad l/2 < x < x_m \text{ or } 1/2 < y < y_m \\
u & = & 0, & z = 0, \qquad 0 < x \leq l/2, \qquad 0 < y \leq 1/2.
\end{array}$$

We solve for $0 \leq x \leq x_m$, $0 \leq y \leq y_m$, $0 \leq z \leq z_m$, where $z_m = 6\sqrt{t_m}$, $y_m = 1/2 + z_m$, $x_m = l/2 + z_m$, and t_m is the maximum time for the simulation process.

The dimensionless current is

$$i \;=\; 4\int_0^{l/2}\int_0^{1/2} u_z|_{z=0}\, dy\, dx \tag{3}$$

and the real-life current is

$$I \;=\; nFDC^*W\, i. \tag{4}$$

This problem poses a number of challenges which we shall deal with one by one in the following:

- Three space dimensions.
- Steep gradients near the boundary of the electrode.
- A singularity at $t = 0$.

3 Problem 2: a circular electrode

If the electrode is a circular disk instead of a rectangle then we can express the diffusion problem in cylindrical coordinates (R, Φ, Z) instead of the usual cartesian coordinates (X, Y, Z) and since $\frac{\partial C}{\partial \Phi} = 0$ the differential equation becomes

$$\frac{\partial C}{\partial T} \;=\; D(\frac{\partial^2 C}{\partial R^2} + \frac{1}{R}\frac{\partial C}{\partial R} + \frac{\partial^2 C}{\partial Z^2}) \tag{5}$$

and the current is

$$I \;=\; 2\pi\, nFD\int_0^A R\frac{\partial C}{\partial Z}\,|_{Z=0}\; dR \tag{6}$$

where A is the radius of the disk in the (R, Φ)-plane which is orthogonal to the Z-axis.

Again we prefer to work with dimensionless variables

$$r = \frac{R}{A},\; z = \frac{Z}{A},\; u = \frac{C}{C^*},\; t = \frac{DT}{A^2},$$

and the problem is now

$$
\begin{array}{lcll}
u_t & = & u_{rr} + \frac{1}{r}u_r + u_{zz}, & t > 0 \qquad r, z > 0 \\
u & = & 1, & t = 0 \\
u & = & 1, & x = r_m \text{ or } \ z = z_m \\
u_z & = & 0, & z = 0, \qquad 1 < r < r_m \\
u & = & 0, & z = 0, \qquad 0 < r \leq 1.
\end{array}
$$

We solve for $0 \leq r \leq r_m$, $0 \leq z \leq z_m$, where $z_m = 6\sqrt{t_m}$, $r_m = 1 + z_m$ and t_m is the maximum time for the simulation process.

The dimensionless current is

$$
i \ = \ \frac{\pi}{2} \int_0^1 r \ u_z|_{z=0} \, dr \tag{7}
$$

and the real-life current is

$$
I \ = \ 4nFDC^*A \ i. \tag{8}
$$

In this problem 2 we only have two space dimensions, but the other two challenges remain. We first deal with the steep gradients.

4 Exponentially expanding steps

When most of the change happens in a small region (a boundary layer) it is tempting to use small steps here and let the step size gradually grow larger further away. One way is the exponentially expanding steps [13, 15] where each step is a factor $\gamma > 1$ larger than the previous step: $h_{j+1} = \gamma h_j$. If the total length is l and the number of steps is N then

$$
l \ = \ h_1 + \gamma h_1 + \gamma^2 h_1 + \cdots + \gamma^{N-1} h_1 \tag{9}
$$

where h_1 is the smallest step size. If l and N are large the latter steps may grow unreasonably, so a modification is to limit the exponential growth to the first M steps, keeping the remaining $N - M$ steps constant:

$$
\begin{aligned}
l \ &= \ h_1 + \gamma h_1 + \cdots + \gamma^{M-1} h_1 + (N - M)\gamma^{M-1} h_1 \\
&= \ h_1 \frac{\gamma^{M-1} - 1}{\gamma - 1} + (N - M + 1)\gamma^{M-1} h_1 \\
&= \ h_1 (\gamma^{M-1}(N - M + \frac{\gamma}{\gamma - 1}) - \frac{1}{\gamma - 1})
\end{aligned} \tag{10}
$$

When γ, l, M, and N are given, h_1 can be determined from (10). $\gamma = 1$ is the limiting case of constant steps. In this case (10) is replaced by $l = Nh_1$. Typical values of γ which usually work well are in the interval $[1.1, 1.2]$ [5].

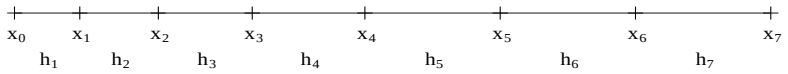

Figure 1: Expanding steps with $M = 5$, $N = 7$, $\gamma = 1.2$

5 The discretizations

We consider three consecutive grid points: x_{j-1}, x_j, and x_{j+1}, and two step sizes $h_j = x_j - x_{j-1}$ and $h_{j+1} = x_{j+1} - x_j$. The function values at these three points are

$$\begin{aligned} u_{j-1} &= u_j - h_j u_x + \frac{1}{2}h_j^2 u_{xx} - \frac{1}{6}h_j^3 u_{xxx} + \frac{1}{24}h_j^4 u_{xxxx} - \cdots \\ u_j &= u_j \\ u_{j+1} &= u_j + h_{j+1} u_x + \frac{1}{2}h_{j+1}^2 u_{xx} + \frac{1}{6}h_{j+1}^3 u_{xxx} + \frac{1}{24}h_{j+1}^4 u_{xxxx} + \cdots \end{aligned} \tag{11}$$

The 3-point discretization of u_{xx} at $x = x_j$ is written as

$$u_{xx} \approx a_j u_{j-1} + b_j u_j + c_j u_{j+1}. \tag{12}$$

Using the first terms on the r.h.s. of (11) we get

$$\begin{aligned} a_j + b_j + c_j &= 0 \\ -a_j h_j + c_j h_{j+1} &= 0 \\ \frac{1}{2}a_j h_j^2 + \frac{1}{2}c_j h_{j+1}^2 &= 1 \end{aligned} \tag{13}$$

$$\tag{14}$$

which gives

$$a_j = \alpha_j h_{j+1}, \;\; c_j = \alpha_j h_j, \;\; b_j = -\alpha_j(h_j + h_{j+1}) \tag{15}$$

with

$$\alpha_j = \frac{2}{h_j h_{j+1}(h_j + h_{j+1})}. \tag{16}$$

The local truncation error is

$$\begin{aligned} u_{xx} - (a_j u_{j-1} + b_j u_j + c_j u_{j+1}) \qquad (17) \\ = \; -\frac{1}{3}(h_{j+1} - h_j)u_{xxx} - \frac{1}{12}\frac{h_{j+1}^3 + h_j^3}{h_{j+1} + h_j}u_{xxxx} - \cdots \\ = \; -\frac{1}{3}(\gamma - 1)h_j u_{xxx} - \frac{1}{12}\frac{\gamma^3 + 1}{\gamma + 1}h_j^2 u_{xxxx} - \cdots \end{aligned}$$

when $h_{j+1} = \gamma h_j$.

When $h_j = h_{j+1}$ the discretization is the well-known second order formula $u_{xx} = \frac{1}{h^2}(u_{j-1} - 2u_j + u_{j+1})$ with local truncation error $-\frac{1}{12}h^2 u_{xxxx}$. When $h_j \neq h_{j+1}$ the approximation is first order in h.

We notice in passing that this discretization can also be written

$$u_{xx} \approx \frac{2}{h_j + h_{j+1}}(\frac{u_{j+1} - u_j}{h_{j+1}} - \frac{u_j - u_{j-1}}{h_j}). \qquad (18)$$

Similarly the discretization of u_x at $x = x_j$ is written as

$$u_x \approx a_j^1 u_{j-1} + b_j^1 u_j + c_j^1 u_{j+1} \qquad (19)$$

where

$$\begin{aligned} a_j^1 + b_j^1 + c_j^1 &= 0 \\ -a_j^1 h_j + c_j^1 h_{j+1} &= 1 \\ \frac{1}{2}a_j^1 h_j^2 + \frac{1}{2}c_j^1 h_{j+1}^2 &= 0 \end{aligned}$$

which gives

$$a_j^1 = -\beta_j h_{j+1}^2, \;\; c_j^1 = \beta_j h_j^2, \;\; b_j^1 = \beta_j(h_{j+1}^2 - h_j^2) \qquad (20)$$

with

$$\beta_j = \frac{1}{h_j h_{j+1}(h_j + h_{j+1})}. \qquad (21)$$

This discretization can also be written

$$u_x \approx \frac{1}{h_j + h_{j+1}}(\frac{h_{j+1}}{h_j}(u_j - u_{j-1}) + \frac{h_j}{h_{j+1}}(u_{j+1} - u_j)). \qquad (22)$$

The local truncation error is

$$u_x - (a_j^1 u_{j-1} + b_j^1 u_j + c_j^1 u_{j+1}) = -\frac{1}{6}h_j h_{j+1} u_{xxx} - \cdots \qquad (23)$$

and is second order in h.

The alternative formulation

$$u_x \approx \frac{1}{2}(\frac{u_{j+1}-u_j}{h_{j+1}}+\frac{u_j-u_{j-1}}{h_j}) \tag{24}$$

has truncation error $\frac{1}{4}(h_j-h_{j+1})u_{xx}$ and is thus first order when $h_{j+1}\neq h_j$.

Sometimes we also need an approximation to u_x at $x=x_{j-1}$ In this case the coefficients are

$$c'_j = -\beta_j h_j^2,\ \ b'_j = \beta_j(h_j+h_{j+1})^2,\ \ a'_j = -b'_j-c'_j \tag{25}$$

and the local truncation error is

$$\frac{1}{6}h_j(h_j+h_{j+1})u_{xxx}-\cdots$$

The first difference $(u_j-u_{j-1})/h_j$ is a first order approximation to u_x anywhere in the interval between x_{j-1} and x_j except at the midpoint where it is second order, the truncation error being

$$u_x(x_j-\alpha h_j)-\frac{u_j-u_{j-1}}{h_j} = (\frac{1}{2}-\alpha)h_j u_{xx}+(\frac{1}{2}\alpha^2-\frac{1}{6})h_j^2 u_{xxx}+\cdots \tag{26}$$

6 The theta method

The discretization of $u_t=u_{xx}$ is written as

$$\begin{aligned}\frac{v_j^{n+1}-v_j^n}{k} &= \theta(a_j v_{j-1}^{n+1}+b_j v_j^{n+1}+c_j v_{j+1}^{n+1}) \\ &\quad +(1-\theta)(a_j v_{j-1}^n+b_j v_j^n+c_j v_{j+1}^n)\end{aligned} \tag{27}$$

or

$$\begin{aligned}v_j^{n+1}-\theta k(a_j v_{j-1}^{n+1}+b_j v_j^{n+1}+c_j v_{j+1}^{n+1}) \\ = v_j^n+(1-\theta)k(a_j v_{j-1}^n+b_j v_j^n+c_j v_{j+1}^n)\end{aligned} \tag{28}$$

where $0\leq\theta\leq 1$, $j=0,1,\ldots,J$, and $n=0,1,\ldots$, k is the step size in time and v_j^n is the approximation to $u(x_j,t_n)$ with $t_n=kn$

If we have Dirichlet boundary conditions we set up these equations at all interior grid points and replace v_0^{n+1} and v_0^n in the first equation and v_J^{n+1} and v_J^n in the last equation by the appropriate boundary values, and we end up with $J-1$ equations to determine the $J-1$ interior values at time step $n+1$.

If we have Neuman conditions ($u_x=0$) we also include the equations for $j=0$ and $j=J$. The fictitious value v_{-1}^{n+1} is by symmetry equal to v_1^{n+1} (because we choose $h_0=h_1$) which we realize by setting $c_0:=c_0+a_0;\ a_0:=0$. Similarly at the right end of the interval we set $a_J:=a_J+c_J;\ c_J:=0$. We have now $J+1$

equations in $J+1$ unknowns.
If $\theta = 0$ we have the explicit method, **EX**, and the system of linear equations is trivial.
If $\theta = 1$ we have the implicit method, **IM**, also known as **BI**.
If $\theta = 0.5$ we have the Crank-Nicolson method, **CN** [8].

7 Stability of IM and CN

The implicit method for $u_t = bu_{xx}$ can be written

$$\frac{v_j^{n+1} - v_j^n}{k} = 2b\{\frac{v_{j-1}^{n+1}}{h_j(h_j + h_{j+1})} - \frac{v_j^{n+1}}{h_j h_{j+1}} + \frac{v_{j+1}^{n+1}}{h_{j+1}(h_j + h_{j+1})}\} \tag{29}$$

and with $h_{j+1} = \gamma h_j$

$$v_j^{n+1} = v_j^n + 2b\frac{k}{h_j^2}(\frac{v_{j-1}^{n+1}}{\gamma + 1} - \frac{v_j^{n+1}}{\gamma} + \frac{v_{j+1}^{n+1}}{\gamma(\gamma+1)}) \tag{30}$$

In the spirit of von Neumann [2, 18] we set $v_j^n = g^n e^{ij\varphi}$ and get

$$\begin{aligned} g &= 1 + 2b\mu(\frac{e^{-i\varphi}}{\gamma+1} - \frac{1}{\gamma} + \frac{e^{i\varphi}}{\gamma(\gamma+1)})g \\ &= 1 + \frac{2b\mu}{\gamma(\gamma+1)}(\gamma(e^{-i\varphi} - 1) + e^{i\varphi} - 1)g \\ &= 1 + \frac{2b\mu}{\gamma(\gamma+1)}(-(\gamma+1)(1 - \cos\varphi) - i(\gamma - 1)\sin\varphi)g \end{aligned}$$

with $\mu = \frac{k}{h_j^2}$, or

$$g_{IM} = \frac{1}{1 + \frac{2b\mu}{\gamma}(1 - \cos\varphi) + i2b\mu\frac{\gamma-1}{\gamma(\gamma+1)}\sin\varphi} \tag{31}$$

In a similar way we get the growth factor for CN:

$$g_{CN} = \frac{1 - \frac{b\mu}{\gamma}(1 - \cos\varphi) - ib\mu\frac{\gamma-1}{\gamma(\gamma+1)}\sin\varphi}{1 + \frac{b\mu}{\gamma}(1 - \cos\varphi) + ib\mu\frac{\gamma-1}{\gamma(\gamma+1)}\sin\varphi}. \tag{32}$$

In both cases $|g| \leq 1$ such that both **IM** and **CN** are unconditionally stable when applied with exponentially expanding steps in space. When $\gamma > 1$ the smaller step sizes tend to be very small (that is the whole idea) and $b\mu$ therefore very large. As a consequence g_{CN} will be very close to -1 and **CN** will respond to sharp changes with oscillations which may take a long time to die out. On the other hand g_{IM} will be very small, and **IM** will produce a very smooth solution. If we combine these methods, such that we take one step with **IM** followed by steps with **CN** we shall have the better of two worlds: The oscillations are damped and the overall method is still second order. We call this combination **IM1** [17, 20].

8 Problem 3

Consider the following problem

$$\begin{aligned} u_t &= u_{xx}, && t > 0, && 0 < x \leq 1, \\ u &= 1, && t = 0, && 0 < x \leq 1, \\ u &= 0, && t > 0, && x = 0, \\ u &= 1, && t > 0, && x = 1. \end{aligned}$$

The true solution is given by:

$$u(t,x) = x + \frac{2}{\pi} \sum_{j=1}^{\infty} \frac{\sin(j\pi x)}{j} e^{-j^2\pi^2 t}. \tag{33}$$

We have solved this test problem with **IM**, **CN**, and **IM1**, using variable steps with $M = 45$, $N = 60$, $\gamma = 1.2$, which yields a smallest step size $h_{min} = 0.0000156$ and a largest step size $h_{max} = 0.0476$. The time step is chosen to be $k = 0.0025$ and we have taken 100000 steps up to $t = 250$. A selection of results is shown in Fig. 2. The step sizes are shown using markings on the x-axis. The computed solution is shown in black when different from the true solution in red. We show only the first 39 x-values corresponding to the interval $[0, 0.1]$.

The first 4 time steps of **CN** are shown illustrating the oscillations (in time) between $+0.999$ and -0.999 in the first x-steps. The oscillations are damped in time but still have an amplitude of 0.795 at $t = 250$ but are now confined to a very small interval near $x = 0$. The first 3 time steps of **IM** are shown above displaying a smooth solution (maybe too smooth), and steps 2–4 of **IM1** show a possibly better solution with no sign of oscillations.

9 Step sizes in practice

Small step sizes result in small discretization errors which is good. But there is a limit. If the step sizes are smaller than 10^{-8} then the coefficients a_j, b_j, and c_j will be of magnitude greater than 10^{16} and we may run into problems with the limited accuracy on common computers. Because of the inevitable rounding errors we may thus encounter situations where algorithms like **CN** do not appear as stable as we expected.

One way to avoid excessively small step sizes is to suggest a minimal step size h_s. With a given γ we then march along with the exponential expansion until we after N steps reach the desired distance l. We shall probably not reach l exactly, but will overshoot slightly. Taking N as our number of steps we then calculate h_1 using (10), knowing that h_1 will be (slightly) smaller than h_s.

We shall use this technique in the x- and y-direction from the edges of the rectangular electrode to the center, or in the r-direction from the edge of the disk electrode to the center. Since this distance is modest there is no need to

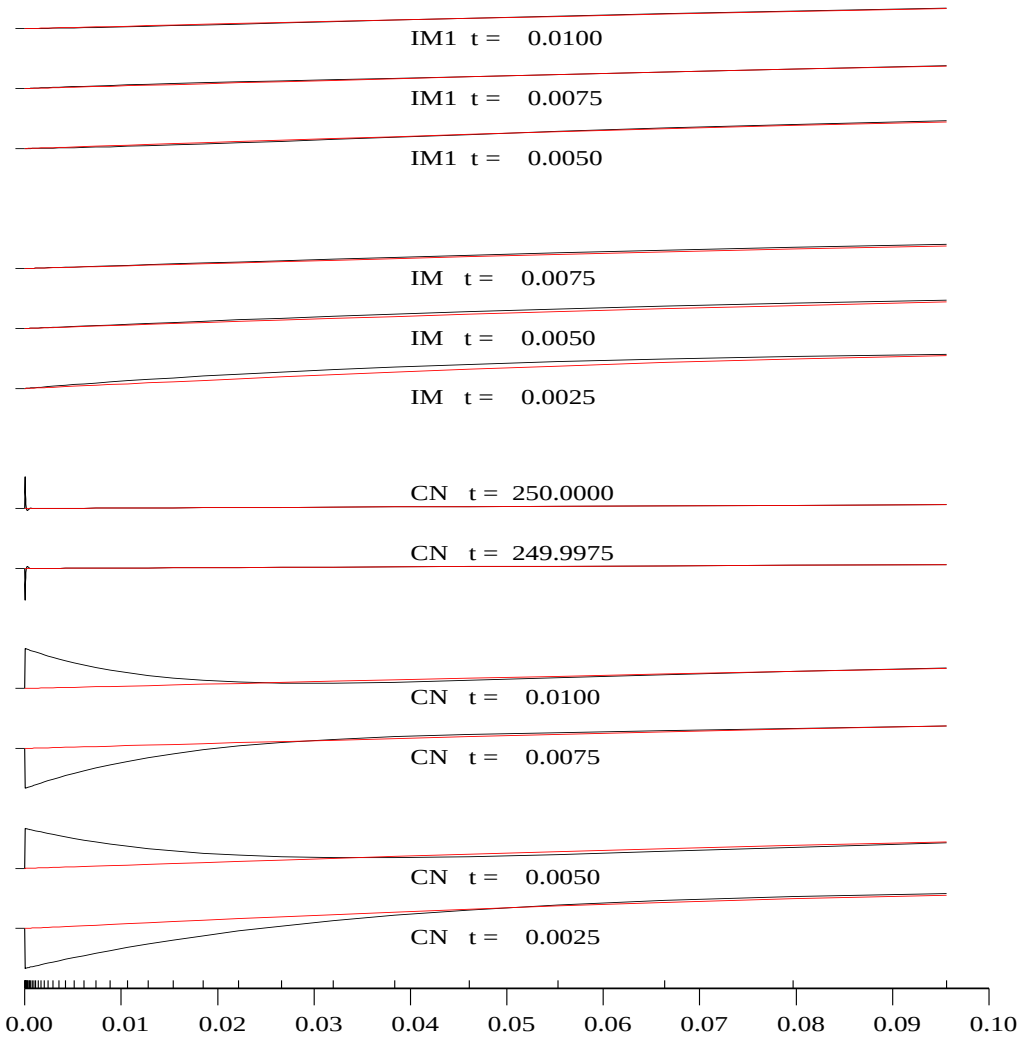

Figure 2: Problem 3 solved with CN, IM and IM1

introduce damping, i.e. we choose $M = N$. In the z-direction we use the same technique on the interval $[0, z_m]$ where z_m is usually chosen as at least $6\sqrt{t_m}$ [12] with t_m being the maximum time for the simulation. There is no need to hit z_m exactly, so instead of adjusting h_s we allow z_m to be slightly bigger. The same set of step sizes can be used in the r-direction or the x- and y-direction outside the electrode. If we use large simulation times, and therefore large values of z_m, the last step sizes become very large, but the concentrations change very little at this distance away from the electrode so we don't use damping here either.

With a given initial step size, h, and distance l we have from formula (9)

$$l \;=\; h(1+\gamma+\gamma^2+\cdots+\gamma^{N-1}) \;=\; h\frac{\gamma^N-1}{\gamma-1} \tag{34}$$

or

$$l(\gamma - 1) \;=\; h(\gamma^N - 1)$$

and after multiplication with $(\gamma + 1)$

$$l(\gamma^2 - 1) \;=\; h(\gamma + 1)((\gamma^2)^{N/2} - 1).$$

If we write $\gamma = 1 + \varepsilon$ then we have $\gamma^2 \approx 1 + 2\varepsilon$ and we see that if we double ε we halve the number of steps. In practice there is a small correction to this because the beginning step size is now $h(\gamma + 1) \approx 2h$ so in principle we should add a number of steps, S, so that $h(\gamma^2)^S \approx h(\gamma + 1)$. This in turn calls for yet another modification of the beginning step size (or of l). S is rather modest, taking the value 12 when $\gamma = 1.03$ and 4 when $\gamma = 1.10$.

We shall return to the practical considerations around variable step sizes, but first we shall look at the implications of the singularity at $t = 0$.

10 The singularity at $t = 0$

In the presence of a singularity the concept of order of a numerical method loses some of its significance. The order is usually defined using (Taylor-)expansions which in turn require higher order derivatives to be bounded in magnitude. The methods may still work and give reasonable results but possibly not with the expected order. To use small step sizes in the beginning is not necessarily a good idea, for it will imply calculations for small t where the concentrations change rapidly and thus possibly imply large errors. Instead we shall use fixed time steps as we are used to.

Practical calculations with **SDR**, [18] (see also section 16), on the disk problem suggest that the error is halved when the (time) step size is reduced by a factor 4 and this leads us to an assumption along the lines of [18], p. 86:

$$v_1 \;=\; u - k^p c - k^r d - \cdots \tag{35}$$

where u is the true solution, v_1 is the computed solution with time step k, p and r are real numbers with $p < r$, and c and d are auxiliary (and unknown) functions.

If we perform a second and third calculation with step sizes $2k$ and $4k$ then we have

$$\begin{aligned} v_2 &= u - (2k)^p c - (2k)^r d - \cdots \\ v_3 &= u - (4k)^p c - (4k)^r d - \cdots \end{aligned}$$

We can then perform two subtractions:

$$\begin{aligned} v_1 - v_2 &= (2^p - 1)k^p c + (2^r - 1)k^r d + \cdots \\ v_2 - v_3 &= (2^p - 1)2^p k^p c + (2^r - 1)2^r k^r d + \cdots \end{aligned}$$

and a division:

$$q \;=\; \frac{v_2 - v_3}{v_1 - v_2} \;=\; 2^p \frac{c + \alpha 2^{r-p} k^{r-p} d + \cdots}{c + \alpha k^{r-p} d + \cdots} \tag{36}$$

with $\alpha = \frac{2^r - 1}{2^p - 1}$.

If the order ratio, q, stabilizes around a certain value, 2^p, this might be an indication that the computed values satisfies an expansion like (35) and that the order of the method can be taken to be p.

As an example we have solved the disk equation in the time interval $[0, 1]$ with $k = 0.00125$ (and $2k$ and $4k$) and with the space discretization in the z-direction defined by $h_s = 0.000015625$, $\gamma = 1.10$, $M_z = N_z = 111$, and $z_m = 6.14$. In the r-direction we use the same step sizes from $r = 1$ out to $r_m = 7.14$. From $r = 1$ down to $r = 0$ we use $\gamma = 1.10$, $M_r = N_r = 92$ and h_s adjusted to 0.00001556. The current is calculated using the trapezoidal rule and the results for the current up to $t = 1.0$ with steps of 0.1 are given in Table 1 in the column marked c-SDR.

Table 1: The disk electrode, discretization in time

time	c-SDR	$v_1 - v_2$	q	w_1	$w_1 - w_2$	q'
0.1	2.1928865	0.0197148	1.223	2.2404822	0.0090910	2.053
0.2	1.8128169	0.0179496	1.340	1.8561511	0.0032146	1.972
0.3	1.6497760	0.0164037	1.369	1.6893780	0.0017925	1.954
0.4	1.5547348	0.0153260	1.382	1.5917351	0.0011975	1.952
0.5	1.4909434	0.0145404	1.389	1.5260469	0.0008822	1.955
0.6	1.4444490	0.0139402	1.394	1.4781037	0.0006912	1.962
0.7	1.4086719	0.0134645	1.397	1.4411781	0.0005648	1.969
0.8	1.3800623	0.0130764	1.399	1.4116315	0.0004757	1.978
0.9	1.3565188	0.0127523	1.401	1.3873056	0.0004101	1.986
1.0	1.3367093	0.0124767	1.402	1.3668308	0.0003598	1.996

The order ratio seems to stabilize around a value near $\sqrt{2} = 1.414$ indicating that p can be taken to be $\frac{1}{2}$.

When a value for p has been established the leading term in the error expansion for v_1 can be eliminated by adding $v_1 - v_2$ divided by $2^p - 1$:

$$w_1 \;=\; v_1 + \frac{v_1 - v_2}{2^p - 1} \;=\; u + \frac{2^r - 2^p}{2^p - 1} k^r d + \cdots \tag{37}$$

This extrapolation process is often associated with the name Richardson who described it in a special case [21]. The process can actually be repeated for v_2 and v_3 (provided we have a fourth calculation with $8k$) and we can now go about estimating r and the next term in the error expansion. This can also be seen in

Table 1 where we give w_1, the difference, and the new order ratio q'. It is seen that the new order ratio (in this example) is very close to 2 indicating that r can be taken to be 1, which is the order we expected from **SDR** in the first place.

11 The discretization error in space

There is also an error component due to the discretization in space and because of the variable step sizes this is more tricky. We can of course repeat the calculations with $h_s = 0.00003125$ and 0.0000625 and give the results in Table 2.

Table 2: The disk electrode, discretization in space

time	c-SDR	$v_1 - v_2$	q	c-extr.
0.1	2.1928865	0.0001204	1.999	2.2496936
0.2	1.8128169	0.0001108	1.999	1.8594766
0.3	1.6497760	0.0001055	1.999	1.6912761
0.4	1.5547348	0.0001020	1.999	1.5930346
0.5	1.4909434	0.0000995	1.999	1.5270286
0.6	1.4444490	0.0000975	1.999	1.4788923
0.7	1.4086719	0.0000959	1.999	1.4418388
0.8	1.3800623	0.0000946	1.999	1.4122018
0.9	1.3565188	0.0000934	1.999	1.3878091
1.0	1.3367093	0.0000925	1.999	1.3672831

The order ratio is very close to 2.0, the method is clearly first order, and the difference $v_1 - v_2$ is a very good estimate of the discretization error. The last column markede c-extr contains the current after elimination of the two k-terms and the h_s-term. But this is not the whole story.

Table 3: The effect of changing h_s.

h_s	0.000062500	0.000031250	0.000015625
hz_{max}	0.588271478	0.573187345	0.558489990
z_m	6.47	6.30	6.14
N_z	97	104	111
hr_{min}	0.000059105	0.000030322	0.000015558
hr_{max}	0.090962823	0.090936656	0.090923234
N_r	78	85	92

As seen in Table 3, changing h_s leaves the larger step sizes, and in fact most step sizes, relatively unchanged. Therefore a large component of the discretization error in space is not detected.

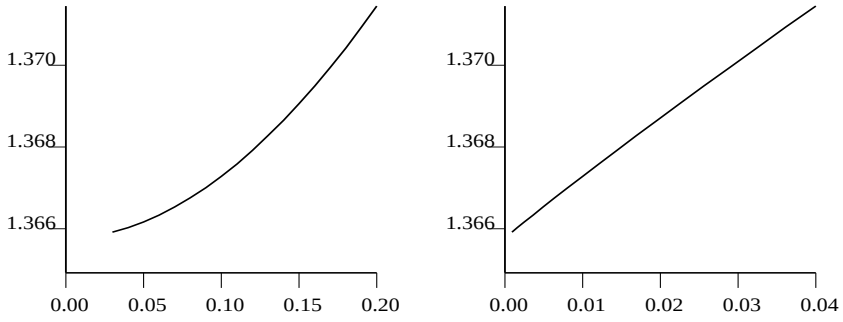

Figure 3: The current as a function of $\gamma - 1$, left, and $(\gamma - 1)^2$, right

Instead we calculate the current up to $t = 1$ with values of γ from 1.03 in steps of 0.01 to 1.20 and keep $k = 0.00125$ and $h_s = 0.000015625$ fixed. In Table 4 we supply values of the (extrapolated) current at $t = 1$ together with the values of N_r and N_z. From equation (17) we know that the local truncation error of the difference approximation in space is proportional to $\gamma - 1$ and it is therefore reasonable to assume that the global error is somehow dependent on $\gamma - 1$. A graph of the current against $\gamma - 1$ (see Fig. 3 left) shows a nice parabola which leads us to draw the current against $(\gamma - 1)^2$ which results in almost a straight line (see Fig. 3 right).

Our hypothesis is now

$$v \;=\; u - b_1(\gamma - 1) - b_2(\gamma - 1)^2 - b_3(\gamma - 1)^3 - \cdots \tag{38}$$

where u is the current at time t, v is the calculated current at time t, and b_1, b_2, and b_3 are functions of t.

Remark. Actually u is the computed current corresponding to $\gamma = 1$, i.e. the solution computed with fixed step size equal to h_s Since h_s is very small and the truncation error for fixed step size is second order, this error will be very small compared to the other error components. □

With the numbers from Table 4 we have 18 linear equations in the unknowns: u, b_1, b_2, ... We intend to solve these equations in the least squares sense. It is not obvious how many parameters, b_1, b_2, ... should be incorporated in (38). The quality of the hypothesis is judged by looking at the differences between the

Table 4: Computed current at $t = 1$ as a function of γ

γ	N_r	N_z	c-extr.
1.03	256	317	1.3659182
1.04	201	246	1.3660272
1.05	166	203	1.3661659
1.06	142	173	1.3663335
1.07	125	151	1.3665296
1.08	111	135	1.3667535
1.09	101	122	1.3670048
1.10	92	111	1.3672831
1.11	85	103	1.3675879
1.12	79	95	1.3679185
1.13	74	89	1.3682749
1.14	70	84	1.3686563
1.15	66	79	1.3690623
1.16	63	75	1.3694927
1.17	60	71	1.3699469
1.18	57	68	1.3704249
1.19	55	65	1.3709258
1.20	52	62	1.3714497
1.00			1.3657681

calculated currents, $v(t)$, and the r.h.s. of (38). These differences will become smaller as we increase the number of parameters and will actually become 0 when the number of parameters match the number of equations. But this is not optimal. The preferred situation is when these differences decay quickly to a certain level and then slowly towards 0. This level determines the quality of our hypothesis.

In this example the maximum differences are 0.0006, 0.00002, and 0.0000006 corresponding to 1, 2, and 3 parameters and $u(1)$ is 1.36577 for $n = 3$ and 1.36570 for $n = 2$. The b-parameters show a greater variation with $b_1 = -0.00041$, $b_2 = -0.15482$, and $b_3 = 0.07416$ for $n = 3$ as opposed to $b_1 = -0.00299$ and $b_2 = -0.12924$ for $n = 2$. With $n = 3$ and $\gamma = 1.10$ this means that the three correction terms are 0.00004, 0.00155, and -0.00007, respectively. The $(\gamma - 1)^2$-term is clearly the dominant one. When $\gamma = 1.30$ the terms are 0.00012, 0.01393, and -0.00200 and it is necessary to include all three terms.

Once we have established the $(\gamma - 1)^2$-behaviour there is less need for calculating with many values of γ and using least squares. If

$$v_1 \;=\; u - b_2(\gamma_1 - 1)^2 \tag{39}$$

Table 5: The disk electrode, discretization in time, $\gamma = 1.10$, large t

time	c-SDR	$v_1 - v_2$	q	w_1	$w_1 - w_2$	q'
100	1.0186413	0.0078445	1.415	1.0375797	-0.0000117	0.359
200	1.0085452	0.0076946	1.415	1.0271216	-0.0000162	0.828
300	1.0040780	0.0076283	1.415	1.0224943	-0.0000181	0.960
400	1.0014171	0.0075888	1.415	1.0197380	-0.0000193	1.025
500	0.9996022	0.0075618	1.415	1.0178580	-0.0000201	1.066
600	0.9982630	0.0075419	1.415	1.0164708	-0.0000207	1.093
700	0.9972226	0.0075265	1.415	1.0153931	-0.0000211	1.114
800	0.9963843	0.0075140	1.415	1.0145247	-0.0000215	1.129
900	0.9956900	0.0075037	1.415	1.0138055	-0.0000218	1.142
1000	0.9951028	0.0074950	1.415	1.0131973	-0.0000220	1.153

and similarly for v_2 and γ_2, then

$$v_1 - v_2 \;=\; b_2((\gamma_2 - 1)^2 - (\gamma_1 - 1)^2) \tag{40}$$

and

$$u \;=\; v_1 + \frac{v_1 - v_2}{(\gamma_2 - 1)^2 - (\gamma_1 - 1)^2}(\gamma_1 - 1)^2. \tag{41}$$

With $\gamma_1 = 1.10$ and $\gamma_2 = 1.15$ we get

$$u = 1.3672831 - 0.0017792/1.25 = 1.3658597$$

and with $\gamma_1 = 1.05$ and $\gamma_2 = 1.10$ we get

$$u = 1.3661659 - 0.0011172/3 = 1.3657935$$

which agree to four decimals with the previously computed value.

We now have several components of the discretization error: a $(p = 1/2)$-term and a $(p = 1)$-term from the discretization in time, a $(p = 1)$-term from changing h_s, and three $(\gamma - 1)$-terms. The order in which we estimate them is not important since they are reasonably independent of each other; but for computational reasons we stick with the above mentioned order and take the γ-terms last. In our example (with $t = 1$ and $\gamma = 1.10$) the larger terms are the $(p = 1/2)$-term (0.0301215) and the $(\gamma - 1)^2$-term (-0.0015482) followed by the two $(p = 1)$-terms from the discretization in time (0.0003598) and space (0.0000925), and the two remaining $(\gamma - 1)$-terms (-0.000041) and (0.0000742).

Remark. We have given the current values and error terms with 7 decimals which is a lot more than can be trusted. There are more error components such

Table 6: The disk electrode, discretization in space, $\gamma = 1.10$, large t

time	c-SDR	$v_1 - v_2$	q	c-extr.
100	1.0186413	0.0000752	1.999	1.0376432
200	1.0085452	0.0000746	1.999	1.0271801
300	1.0040780	0.0000743	1.999	1.0225505
400	1.0014171	0.0000742	1.999	1.0197929
500	0.9996022	0.0000741	1.999	1.0179120
600	0.9982630	0.0000740	1.999	1.0165242
700	0.9972226	0.0000739	1.999	1.0154459
800	0.9963843	0.0000739	1.999	1.0145771
900	0.9956900	0.0000738	1.999	1.0138576
1000	0.9951028	0.0000738	1.999	1.0132491

as the various $\cdots$-terms as well as the error in the final trapezoidal integration which may affect decimals 5, 6, and 7 but these terms are all continuous and do not seriously affect the difference-making which we rely heavily upon in the error estimations. In contrast, rounding would introduce discontinuous errors which might pollute succeeding calculations. Also the numbers should be considered as intermediate results which should undergo a final rounding before being presented to a greater audience. □

12 Computational economy

The above may seem like a complicated and time consuming process, but as we shall show, it is not that expensive and well worth the extra effort. The total error of the computations can be split into various relatively independent parts depending on the time step, k, the initial space step, h_s, and the expansion factor γ. The greater part of computer time is spent on the **SDR**-calculations and is therefore proportional to the number of grid points in time and space. If we were to reduce the discretization error in time (the dominant component) by a factor 2 with **SDR** calculations we would have to reduce the time step, k, by a factor 4, and thus increase computation time by a factor 4. Instead we base our error estimation on extrapolation techniques which imply recomputing with time steps $2k$, $4k$, ... with computation times $1/2$, $1/4$, ... for a total of less than two times the first computation and with a reduction in discretization error (in time) which is a lot more. The results in Table 1 indicate a factor 20 at $t = 0.3$ and a factor 75 at $t = 1.0$. Computation with $2h_s$ and $4h_s$ each cost less that the first computation, but not much less, and it is a good question whether the results merit the extra expense. To estimate the γ-contribution to the discretization

Table 7: Computed current at $t = 1000$ as a function of γ

γ	N_r	N_z	time	c-extr.	steady
1.03	256	450	32334	1.0114893	1.0001414
1.04	201	364	20026	1.0116303	1.0002897
1.05	166	297	13594	1.0118095	1.0004784
1.06	142	252	9640	1.0120259	1.0007062
1.07	125	219	7257	1.0122788	1.0009722
1.08	111	195	5740	1.0125674	1.0012758
1.09	101	175	4639	1.0128910	1.0016163
1.10	92	160	3886	1.0132491	1.0019928
1.11	85	147	3272	1.0136408	1.0024047
1.12	79	136	2797	1.0140656	1.0028513
1.13	74	127	2430	1.0145230	1.0033320
1.14	70	119	2137	1.0150121	1.0038460
1.15	66	112	1897	1.0155326	1.0043929
1.16	63	106	1700	1.0160839	1.0049721
1.17	60	100	1529	1.0166655	1.0055828
1.18	57	96	1389	1.0172769	1.0062249
1.19	55	91	1263	1.0179174	1.0068973
1.20	52	87	1166	1.0185868	1.0075999
1.00					0.9999350

error we must compute with a number of γ. We suggest computing with $\gamma = 1.10$ (0.01) 1.20 which will require less computing time than a single computation with $\gamma = 1.03$ (cf. Tables 4 and 7) and offer more accurate results.

13 The steady state current

As time passes the current diminishes. In Tables 5 and 6 we present the current up to $t = 1000$, calculated with $\gamma = 1.10$ and $z_m = 600$. One difference from Table 1 is that q' in Table 5 has far from settled to near the value 2.0, but since $w_1 - w_2$ is relatively small the implications are not serious.

We repeat the calculations for $\gamma = 1.03$ (0.01) 1.20 and present the results for $t = 1000$ in Table 7 together with values of N_r and N_z and the computation time (in seconds) for each value of γ. Theoretical results indicate that the current will approach a finite value (the steady state current) as time passes and that the convergence will be like $1/\sqrt{t}$ [16]. This can be verified for each value of γ by plotting the current against $1/\sqrt{t}$.

Our hypothesis here is

$$u(t) \;=\; u_s - c_1 t^{-1/2} - c_3 t^{-3/2} - \cdots \tag{42}$$

where u is the current at time t, u_s is the steady state current, and c_1 and c_3 are parameters which depend on γ.

Using least squares we can now calculate the steady state current for each value of γ. These values are given in the last column of Table 7.

Using equation (38) and least squares on the numbers in the last column of Table 7 we find the steady state current to be 0.9999350 together with $b_1 = -0.0006402$, $b_2 = -0.2102762$, and $b_3 = 0.1093653$. With the chosen normalization the steady state current is known to be 1.0000 and our result is seen to have an error of about one unit in the fourth decimal.

Remark: Formula (2) in [16] with our normalization becomes

$$\begin{aligned} u(t) &= 1 + 2\pi^{-3/2} t^{-1/2} + (\frac{1}{9} - \frac{1}{\pi^2}) 4 (\pi t)^{-3/2} \\ &= 1 + 0.35917 t^{-1/2} + 0.0070 t^{-3/2}. \end{aligned} \tag{43}$$

The values for c_1 and c_3 which we calculate for each γ turn out to obey an equation much like (38) and using least squares on these values we arrive at $c_1 = 0.35918$ and $c_3 = 0.0066$. □

It is seen from Tables 4 and 7 that the numbers N_r and N_z increase with small values of γ almost like $(\gamma - 1)^{-1}$ as we saw in Section 9, and the computation time which is proportional to the number of grid points, $(N_r + N_z)N_z$, increases roughly like $(\gamma - 1)^{-2}$. Actually, computations with $\gamma = 1.09$ (0.01) 1.20 will take less time than computation with $\gamma = 1.03$. We therefore recommend the former since this also will give us the opportunity to check the $(\gamma - 1)$-behaviour of the discretization error and to estimate the γ-contribution to the discretization error.

14 Doubling the space step size

The above is a rather complicated method, but there is an alternative technique which can sometimes be used to estimate the discretization error associated with exponentially expanding step sizes.

With a given h_s and γ we can produce a series of step sizes: $h_1 = h_s$, $h_2 = \gamma h_1$, and in general $h_{n+1} = \gamma h_n = \gamma^n h_1$. With these steps we compute a numerical solution v_1 which depends on the beginning step size $h = h_1$ possibly as

$$v_1 \;=\; u - hc - h^2 d - h^3 f - \cdots \tag{44}$$

where u is the true solution and c, d, and f are unknown auxiliary functions.

Table 8: The disk electrode, discretization in space, doubling h.

time	c-SDR	$v_1 - v_2$	q	c-extr.
0.1	2.1928862	-0.0063833	4.035	2.2477009
0.2	1.8128167	-0.0058179	4.117	1.8576593
0.3	1.6497757	-0.0054303	4.188	1.6895778
0.4	1.5547346	-0.0051631	4.236	1.5914182
0.5	1.4909432	-0.0049775	4.266	1.5254692
0.6	1.4444488	-0.0048454	4.288	1.4773737
0.7	1.4086717	-0.0047492	4.304	1.4403499
0.8	1.3800621	-0.0046777	4.316	1.4107353
0.9	1.3565186	-0.0046235	4.325	1.3863596
1.0	1.3367092	-0.0045819	4.332	1.3658468

Doubling the step size will not enable us to reach the same points so instead we define a new series of steps

$$h'_n \;=\; h_{2n-1} + h_{2n} \;=\; \gamma^2 h_{2n-3} + \gamma^2 h_{2n-2} \;=\; \gamma^2 h'_{n-1} \tag{45}$$

This new series of steps will hit every other point from the first calculation and is also exponentially expanding, now with expansion factor γ^2, and beginning step size $h'_1 = h_1 + h_2 = (1+\gamma)h_1$. A second computation with these steps will produce a new solution

$$v_2 \;=\; u - (1+\gamma)hc - (1+\gamma)^2 h^2 d - (1+\gamma)^3 h^3 f - \cdots \tag{46}$$

If the number of steps is divisible by 4 then we can repeat the process with a third series of exponentially expanding steps with beginning step size $h'_1 + h'_2 = (1+\gamma^2)(1+\gamma)h_1$ and expansion factor γ^4. With these steps we can perform a third calculation:

$$\begin{aligned} v_3 \;=\; & u - (1+\gamma^2)(1+\gamma)hc - (1+\gamma^2)^2(1+\gamma)^2 h^2 d \\ & - (1+\gamma^2)^3(1+\gamma)^3 h^3 f - \cdots \end{aligned} \tag{47}$$

We now proceed as in Section 10 with two subtractions and one division:

$$\begin{aligned} v_1 - v_2 \;&=\; \gamma hc + (2+\gamma)\gamma h^2 d + (3+3\gamma+\gamma^2)\gamma h^3 f + \cdots \\ v_2 - v_3 \;&=\; (1+\gamma)\gamma^2 hc + (2+\gamma^2)(1+\gamma)^2\gamma^2 h^2 d \\ &\qquad + (3+3\gamma^2+\gamma^4)(1+\gamma)^3\gamma^2 h^3 f + \cdots \\ q \;&=\; \frac{v_2 - v_3}{v_1 - v_2} \;=\; \frac{(1+\gamma)\gamma c + (2+\gamma^2)(1+\gamma)^2\gamma h d + \cdots}{c + (2+\gamma)hd + \cdots} \end{aligned} \tag{48}$$

Table 9: The disk electrode, discretization in space, doubling h, large t.

time	c-SDR	$v_1 - v_2$	q	c-extr.
100	1.0186412	-0.0053700	4.336	1.0359931
200	1.0085451	-0.0055473	4.327	1.0254786
300	1.0040779	-0.0056401	4.322	1.0208221
400	1.0014170	-0.0057008	4.319	1.0180468
500	0.9996021	-0.0057450	4.317	1.0161530
600	0.9982629	-0.0057792	4.315	1.0147553
700	0.9972225	-0.0058069	4.313	1.0136690
800	0.9963842	-0.0058299	4.312	1.0127934
900	0.9956899	-0.0058496	4.311	1.0120682
1000	0.9951027	-0.0058666	4.310	1.0114548

If $|c| > h|d|$, then the order ratio q will be close to $(1+\gamma)\gamma$ which is slightly larger than 2 when γ is slightly larger than 1. In this case the discretization error is first order and its magnitude can be estimated by $(v_1 - v_2)/\gamma$.

We can modify the computed solution v_1 using this estimate

$$w_1' \;=\; v_1 + \frac{v_1 - v_2}{\gamma} \;=\; u + (1+\gamma)h^2 d + (2 + 3\gamma + \gamma^2)h^3 f + \cdots \qquad (49)$$

and the order of the error is raised from 1 to 2.

If on the other hand c is zero or very small compared to $h|d|$, this is revealed by q being close to $(2+\gamma^2)(1+\gamma)^2\gamma/(2+\gamma)$ which is larger than 4 and for $\gamma = 1.10$ amounts to 5.023.

In Table 8 we show results for t up to 1.0 computed using $\gamma = 1.10$, $k = 0.00125$, $h_s = 0.000015625$. In this case the observed values for q give reason to assume that the error is of order 2. The magnitude of the error is now estimated by $(v_1 - v_2)/((2+\gamma)\gamma)$ and we can perform the correction

$$w_1 \;=\; v_1 + \frac{v_1 - v_2}{(2+\gamma)\gamma} \;=\; u + \frac{(1+\gamma)^2}{2+\gamma} h^3 f + \cdots \qquad (50)$$

which is expected to be third order accurate.

In the last column of Table 8, named 'c-extr.', we have performed this correction together with the two corrections in time, cf. Table 1.

Remark. The values for v_1 in the first column (c-SDR) of Table 8 show deviations of 1-3 units in the seventh decimal place from those in Table 1. This is because the values of N_r and N_z have been increased to be divisible by 8 from 92 and 111 to 96 and 112. All the other numbers in Table 1 are unchanged. □

Remark. We have actually chosen the number of steps to be divisible by 8, so that we can perform a fourth calculation, and in turn have three extrapolated

current values. We then have the possibility to check the new order ratio which turns out to be larger than 8 in this case indicating that the order has been raised from 2 to 3. □

Remark. We should be careful not to choose the expansion factor, γ, too large since the expansion factors in the succeeding calculations are γ^2, γ^4, and γ^8. On the other hand the computing time increases rapidly with smaller γ, cf. Table 7, so a certain balance should be found. □

In Table 9 which is rather similar to Table 8 we now present results for t up to 1000. Again we notice small changes in the seventh decimal (when compared to Table 5) due to the fact that N_r has now been modified from 92 to 96. The object is to compute the steady state current and again we assume that the convergence for $t \to \infty$ is like $1/\sqrt{t}$. We find the steady state current to be 1.0001. A control calculation with $\gamma = 1.05$ gives the value 0.9999, so again we observe an error of about one unit in the fourth decimal place.

Remark. Practical experiments indicate that there is still a small $(\gamma - 1)$-dependence which amounts to a magnitude of 0.0002 at $\gamma = 1.10$ and 0.0014 at $\gamma = 1.20$. This emphasizes the need to keep γ moderately small. □

The above technique for estimating the global error is based on a number of assumptions which we have not been able to justify theoretically. There are, however, a number of built-in checks for the validity of the assumptions and furthermore we have presented two relatively independent methods for estimating the error, and with very similar results, so we feel reasonably confident in these results.

15 Three space dimensions

We consider a linear parabolic equation in three space dimensions:

$$u_t = P_1 u + P_2 u + P_3 u \tag{51}$$

where

$$\begin{aligned} P_1 u &= b_1 u_{xx} - a_1 u_x \\ P_2 u &= b_2 u_{yy} - a_2 u_y \\ P_3 u &= b_3 u_{zz} - a_3 u_z \end{aligned}$$

A term with u can be incorporated in any one of the P_i operators or split between two or three of them, but we do not consider inhomogeneous or mixed derivative terms.

The simplest discretization of (51) is the explicit method (**EX**):

$$\frac{v_{jlm}^{n+1} - v_{jlm}^n}{k} = (P_{1h} + P_{2h} + P_{3h}) v_{jlm}^n \tag{52}$$

or

$$v^{n+1} \;=\; (I + k(P_{1h} + P_{2h} + P_{3h}))v^n \tag{53}$$

where k is the time step, I is the identity, and P_{1h}, P_{2h}, and P_{3h} are discretizations of the differential operators P_1, P_2, and P_3, respectively.

The explicit scheme is consistent and of first order in k and second order in the three space variables.

To investigate the stability properties of **EX** we shall assume constant step sizes and that $a_1 = a_2 = a_3 = 0$ such that

$$P_{1h}v^n_{jlm} \;=\; b_1\,\frac{v^n_{j+1lm} - 2v^n_{jlm} + v^n_{j-1lm}}{h_1^2}$$

and similarly for P_{2h} and P_{3h}. In the spirit of von Neumann [2], [18] p. 25, we set

$$v^n_{jlm} \;=\; g^n e^{ij\varphi_1} e^{il\varphi_2} e^{im\varphi_3} \tag{54}$$

where g is the amplification factor, i the imaginary unit, and j, l, m, and n are the step numbers in the three space dimensions and time, respectively. We then have

$$\begin{aligned} P_{1h}v^n_{jlm} \;&=\; b_1 g^n_{EX}\frac{e^{i(j-1)\varphi_1} - 2e^{ij\varphi_1} + e^{i(j+1)\varphi_1}}{h_1^2} e^{il\varphi_2} e^{im\varphi_3} \\ &=\; -\,4b_1\frac{1}{h_1^2}\sin^2\frac{\varphi_1}{2} v^n_{jlm} \end{aligned}$$

and with $\mu_p = \frac{k}{h_p^2}$ and $x_p = 2b_p\mu_p \sin^2\frac{\varphi_p}{2}$, $p = 1,\, 2,\, 3$:

$$v^{n+1}_{jlm} \;=\; (1 - 2x_1 - 2x_2 - 2x_3)v^n_{jlm} \;=\; g_{EX}v^n_{jlm} \tag{55}$$

Stability requires $-1 \le g_{EX} \le 1$ and therefore $2x_1 + 2x_2 + 2x_3 \le 2$ for all φ and therefore

$$b_1\mu_1 + b_2\mu_2 + b_3\mu_3 \;\le\; \frac{1}{2} \tag{56}$$

This condition puts severe restrictions on the time step, k, and **EX** can therefore not be recommended in practice.

In a similar way we can extend the implicit method, (**IM**) to three dimensions by putting superscripts $n+1$ on the v on the right-hand side of (52) or

$$(I - k(P_{1h} + P_{2h} + P_{3h}))v^{n+1} \;=\; v^n \tag{57}$$

IM is also first order in time. A second order scheme is Crank-Nicolson, (**CN**), where the right-hand side is the average of the two or

$$(I - \frac{1}{2}k(P_{1h} + P_{2h} + P_{3h}))v^{n+1} = (I + \frac{1}{2}k(P_{1h} + P_{2h} + P_{3h}))v^n \tag{58}$$

Analyzing the stability we find the amplification factors

$$g_{IM} = \frac{1}{1 + 2x_1 + 2x_2 + 2x_3} \tag{59}$$

and

$$g_{CN} = \frac{1 - x_1 - x_2 - x_3}{1 + x_1 + x_2 + x_3}. \tag{60}$$

It is easily seen that $0 \leq g_{IM} \leq 1$ and $-1 \leq g_{CN} \leq 1$ so both methods are unconditionally stable. For large values of $b\mu$ g_{IM} will be very small and the solution will be very smooth whereas g_{CN} will be close to -1 and **CN** will be prone to slowly decaying oscillations in time.

Both methods will require the solution of a very large system of equations for each time step and are therefore not economical. We therefore focus attention on ADI methods where each time step is divided into three steps where we solve for each dimension at a time, requiring only to solve tridiagonal systems of equations and therefore have a computing time which is proportional to the number of grid points.

16 A selection of ADI methods

In 1956 Douglas and Rachford presented a method for three space dimensions [11]. This is the traditional Douglas-Rachford method, which we shall call **TDR**, and in our notation it can be written

$$\begin{aligned} (I - kP_{1h})\tilde{v} &= (I + kP_{2h} + kP_{3h})v^n \\ (I - kP_{2h})\tilde{\tilde{v}} &= \tilde{v} - kP_{2h}v^n \\ (I - kP_{3h})v^{n+1} &= \tilde{\tilde{v}} - kP_{3h}v^n \end{aligned} \tag{61}$$

$\tilde{v}$ and $\tilde{\tilde{v}}$ are intermediate values with no particular relation to time step n or $n+1$ or any other time in between. They are merely stepping stones on the way to the solution v^{n+1}. In order to check the connection between v^{n+1} of equation (61) and the result of (57) we apply the three operators to the solution v^{n+1} of (61):

$$\begin{aligned} &(I - kP_{1h})(I - kP_{2h})(I - kP_{3h})v^{n+1} \\ &\quad = (I - kP_{1h})(I - kP_{2h})(\tilde{\tilde{v}} - kP_{3h}v^n) \\ &\quad = (I - kP_{1h})(\tilde{v} - k(P_{2h} + P_{3h} - kP_{2h}P_{3h})v^n) \\ &\quad = (I + k^2(P_{1h}P_{2h} + P_{1h}P_{3h} + P_{2h}P_{3h} - kP_{1h}P_{2h}P_{3h})v^n \end{aligned}$$

or

$$(I - k(P_{1h} + P_{2h} + P_{3h}))v^{n+1} = v^n + k^2(P_{1h}P_{2h} + P_{1h}P_{3h} + P_{2h}P_{3h} - kP_{1h}P_{2h}P_{3h})(v^n - v^{n+1}).$$

Since $(v^n - v^{n+1})$ is $O(k)$ the difference from (57) is $O(k^3)$ which shall be divided by k so we conclude that **TDR** has the same order as **IM** i.e. first order in time.

To study the stability properties we use (54) and similar expressions for $\tilde{g}$ and $\tilde{\tilde{g}}$ leading to

$$\begin{aligned}(1+2x_1)\tilde{g} &= 1 - 2x_2 - 2x_3\\ (1+2x_2)\tilde{\tilde{g}} &= \tilde{g} + 2x_2\\ (1+2x_3)g_{TDR} &= \tilde{\tilde{g}} + 2x_3\end{aligned}$$

$$\begin{aligned}\tilde{g} &= \frac{1 - 2x_2 - 2x_3}{1 + 2x_1}\\ \tilde{\tilde{g}} &= \frac{1 - 2x_2 - 2x_3 + 2x_2(1+2x_1)}{(1+2x_1)(1+2x_2)}\\ g_{TDR} &= \frac{1 - 2x_3 + 4x_1x_2 + 2x_3(1+2x_1)(1+2x_2)}{(1+2x_1)(1+2x_2)(1+2x_3)}\\ &= \frac{1 + 4(x_1x_2 + x_1x_3 + x_2x_3) + 8x_1x_2x_3}{1 + 2(x_1 + x_2 + x_3) + 4(x_1x_2 + x_1x_3 + x_2x_3) + 8x_1x_2x_3}\end{aligned} \quad (62)$$

We observe that $0 \leq g_{TDR} \leq 1$ such that **TDR** is unconditionally stable and has no tendency to produce oscillations in time. But we notice also that if two or three of the x-s are large then g_{TDR} will be close to 1 such that sharp transients in space will only be damped very slowly in time.

In 1961 Brian [1] proposed a slight variation on the theme (**BR**) which in our notation is

$$\begin{aligned}(I - \frac{k}{2}P_{1h})\tilde{v} &= (I + \frac{k}{2}P_{2h} + \frac{k}{2}P_{3h})v^n\\ (I - \frac{k}{2}P_{2h})\tilde{\tilde{v}} &= \tilde{v} - \frac{k}{2}P_{2h}v^n\\ (I - \frac{k}{2}P_{3h})v^{n+1} &= 2\tilde{\tilde{v}} - v^n - \frac{k}{2}P_{3h}v^n\end{aligned} \quad (63)$$

Checking for consistency we apply the three operators to the solution v^{n+1} of (63):

$$\begin{aligned}&(I - \frac{k}{2}P_{1h})(I - \frac{k}{2}P_{2h})(I - \frac{k}{2}P_{3h})v^{n+1}\\ &= (I - \frac{k}{2}P_{1h})(I - \frac{k}{2}P_{2h})(2\tilde{\tilde{v}} - v^n - \frac{k}{2}P_{3h}v^n)\end{aligned}$$

$$
\begin{aligned}
&= (I - \frac{k}{2}P_{1h})(2\tilde{v} - kP_{2h}v^n - (I - \frac{k}{2}P_{2h})(I - \frac{k}{2}P_{3h})v^n) \\
&= (2I + k(P_{2h} + P_{3h}) - (I - \frac{k}{2}P_{1h})(kP_{2h} + I - \frac{k}{2}(P_{2h} + P_{3h}) - \frac{k^2}{4}P_{2h}P_{3h})v^n \\
&= (I + \frac{k}{2}(P_{1h} + P_{2h} + P_{3h}) + \frac{k^2}{4}(P_{1h}P_{2h} + P_{1h}P_{3h} + P_{2h}P_{3h}) - \frac{k^3}{8}P_{1h}P_{2h}P_{3h})v^n
\end{aligned}
$$

or

$$
\begin{aligned}
(I - \frac{k}{2}(P_{1h} + P_{2h} + P_{3h}))v^{n+1} &= (I + \frac{k}{2}(P_{1h} + P_{2h} + P_{3h})v^n \\
&+ \frac{k^2}{4}(P_{1h}P_{2h} + P_{1h}P_{3h} + P_{2h}P_{3h}) - \frac{k^3}{8}P_{1h}P_{2h}P_{3h})(v^n - v^{n+1}).
\end{aligned}
$$

The difference from (58) is $O(k^3)$ so we conclude that **BR**, like **CN**, is second order in time.

For stability we have

$$
\begin{aligned}
(1 + x_1)\tilde{g} &= 1 - x_2 - x_3 \\
(1 + x_2)\tilde{\tilde{g}} &= \tilde{g} + x_2 \\
(1 + x_3)g_{BR} &= 2\tilde{\tilde{g}} - 1 + x_3
\end{aligned}
$$

$$
\begin{aligned}
\tilde{g} &= \frac{1 - x_2 - x_3}{1 + x_1} \\
\tilde{\tilde{g}} &= \frac{1 - x_2 - x_3 + x_2(1 + x_1)}{(1 + x_1)(1 + x_2)} \\
g_{BR} &= \frac{2 - 2x_3 + 2x_1x_2 + (x_3 - 1)(1 + x_1)(1 + x_2)}{(1 + x_1)(1 + x_2)(1 + x_3)} \\
&= \frac{1 - (x_1 + x_2 + x_3) + (x_1x_2 + x_1x_3 + x_2x_3) + x_1x_2x_3}{1 + (x_1 + x_2 + x_3) + (x_1x_2 + x_1x_3 + x_2x_3) + x_1x_2x_3}
\end{aligned} \tag{64}
$$

We observe that $-1 \leq g_{BR} \leq 1$ such that **BR** is unconditionally stable. If one of the three x's is large then $g_{BR} \to -1$ and there is a possibility of slowly damped oscillations in time.

In 1962 Douglas [9] proposed a method, sometimes referred to as Douglas-Gunn (**DG**) [10] which can be written

$$
\begin{aligned}
(I - \frac{1}{2}kP_{1h})\tilde{v} &= (I + \frac{1}{2}kP_{1h} + kP_{2h} + kP_{3h})v^n, \\
(I - \frac{1}{2}kP_{2h})\tilde{\tilde{v}} &= \tilde{v} - \frac{1}{2}kP_{2h}v^n, \\
(I - \frac{1}{2}kP_{3h})v^{n+1} &= \tilde{\tilde{v}} - \frac{1}{2}kP_{3h}v^n.
\end{aligned} \tag{65}
$$

To investigate consistency we consider the solution v^{n+1} from (65) and apply the three operators:

$$\begin{aligned}
&(I-\frac{1}{2}kP_{1h})(I-\frac{1}{2}kP_{2h})(I-\frac{1}{2}kP_{3h})v^{n+1}\\
&\qquad = (I-\frac{1}{2}kP_{1h})(I-\frac{1}{2}kP_{2h})(\tilde{\tilde{v}}-\frac{1}{2}kP_{3h}v^n)\\
&\qquad = (I-\frac{1}{2}kP_{1h})[\tilde{v}-\frac{1}{2}kP_{2h}v^n-\frac{1}{2}k(I-\frac{1}{2}kP_{2h})P_{3h}v^n]\\
&\qquad = [I+\frac{1}{2}kP_{1h}+kP_{2h}+kP_{3h}-\frac{1}{2}k(I-\frac{1}{2}kP_{1h})P_{2h}\\
&\qquad\qquad -\frac{1}{2}k(I-\frac{1}{2}kP_{1h})(I-\frac{1}{2}kP_{2h})P_{3h}]v^n\\
&\qquad = [I+\frac{1}{2}k(P_{1h}+P_{2h}+P_{3h})\\
&\qquad\quad +\frac{1}{4}k^2(P_{1h}P_{2h}+P_{1h}P_{3h}+P_{2h}P_{3h})-\frac{1}{8}k^3P_{1h}P_{2h}P_{3h}]v^n.
\end{aligned}$$

Since the l.h.s. can be expanded to

$$[I-\frac{1}{2}k(P_{1h}+P_{2h}+P_{3h})+\frac{1}{4}k^2(P_{1h}P_{2h}+P_{1h}P_{3h}+P_{2h}P_{3h})-\frac{1}{8}k^3P_{1h}P_{2h}P_{3h}]v^{n+1}$$

we conclude that the solution to (65) satisfies

$$\begin{aligned}
(I-\frac{1}{2}k(P_{1h}+P_{2h}+P_{3h}))v^{n+1} &= (I+\frac{1}{2}k(P_{1h}+P_{2h}+P_{3h}))v^n\\
+\frac{1}{4}k^2(P_{1h}P_{2h}+P_{1h}P_{3h}+P_{2h}P_{3h})(v^n-v^{n+1})&+\frac{1}{8}k^3P_{1h}P_{2h}P_{3h}(v^n-v^{n+1}).
\end{aligned}$$

This is not quite the same as (58) but the difference is only $O(k^3)$, so we conclude that **DG** is also second order in time.

For stability we have

$$\begin{aligned}
(1+x_1)\tilde{g} &= 1-x_1-2x_2-2x_3\\
(1+x_2)\tilde{\tilde{g}} &= \tilde{g}+x_2\\
(1+x_3)g_{DG} &= \tilde{\tilde{g}}+x_3
\end{aligned}$$

$$\begin{aligned}
\tilde{g} &= \frac{1-x_1-2x_2-2x_3}{1+x_1}\\
\tilde{\tilde{g}} &= \frac{1-x_1-2x_2-2x_3+x_2(1+x_1)}{(1+x_1)(1+x_2)}\\
g_{DG} &= \frac{1-x_1-x_2-2x_3+x_1x_2+x_3(1+x_1)(1+x_2)}{(1+x_1)(1+x_2)(1+x_3)}\\
&= \frac{1-(x_1+x_2+x_3)+(x_1x_2+x_1x_3+x_2x_3)+x_1x_2x_3}{1+(x_1+x_2+x_3)+(x_1x_2+x_1x_3+x_2x_3)+x_1x_2x_3} \qquad (66)
\end{aligned}$$

It is easily seen that $-1 \leq g_{DG} \leq 1$ and that g_{DG} will approach -1 when one of the x_p is large and the other two are small. **DG** is therefore absolutely stable but prone to slowly decaying oscillations

Among the simplest ADI methods we find the simplified Douglas-Rachford scheme (**SDR**) [18], [3], [5] which can be written

$$\begin{aligned} (I - kP_{1h})\tilde{v} &= v^n \\ (I - kP_{2h})\tilde{\tilde{v}} &= \tilde{v} \\ (I - kP_{3h})v^{n+1} &= \tilde{\tilde{v}} \end{aligned} \tag{67}$$

Checking for consistency we apply the three operators to the solution v^{n+1} of (67):

$$\begin{aligned} &(I - kP_{1h})(I - kP_{2h})(I - kP_{3h})v^{n+1} \\ &\qquad = \quad (I - kP_{1h})(I - kP_{2h})\tilde{\tilde{v}} \;=\; (I - kP_{1h})\tilde{v} \;=\; v^n \end{aligned}$$

or

$$\begin{aligned} (I - kP_{1h} - kP_{2h} - kP_{3h}) + k^2(P_{1h}P_{2h} + P_{1h}P_{3h} + P_{2h}P_{3h}) & \\ -k^3 P_{1h}P_{2h}P_{3h})v^{n+1} &= v^n. \end{aligned}$$

The difference from (57) is $O(k^2)$ so we conclude that **SDR** is first order in time.

For stability we find that

$$g_{SDR} \;=\; \frac{1}{(1 + 2x_1)(1 + 2x_2)(1 + 2x_3)} \tag{68}$$

such that $0 \leq g_{SDR} \leq 1$, and **SDR** is absolutely stable and will produce a smooth solution.

17 The square electrode

We now consider Problem 1 in the special case where $L = W$, i.e. the electrode is a square. When trying to solve this problem we have a number of ADI methods to choose from. Because of the steep gradients near the electrode boundary, methods which include differences on the right-hand-side are prone to spikes in the concentrations with values less than 0 and greater than 1. Although we have methods to dampen such behaviour it might be preferable to avoid it in the first place. Also we cannot expect full advantage of a second order method because of the singularity at $t = 0$.

One obvious choice is therefore **SDR** supplemented with extrapolation to eliminate the dominating terms in the discretization error [5].

We have a certain freedom in choosing the order of the independent variables we solve with respect to, but since our end result, the current, involves the derivative w.r.t. z it is important that we solve w.r.t. z last.

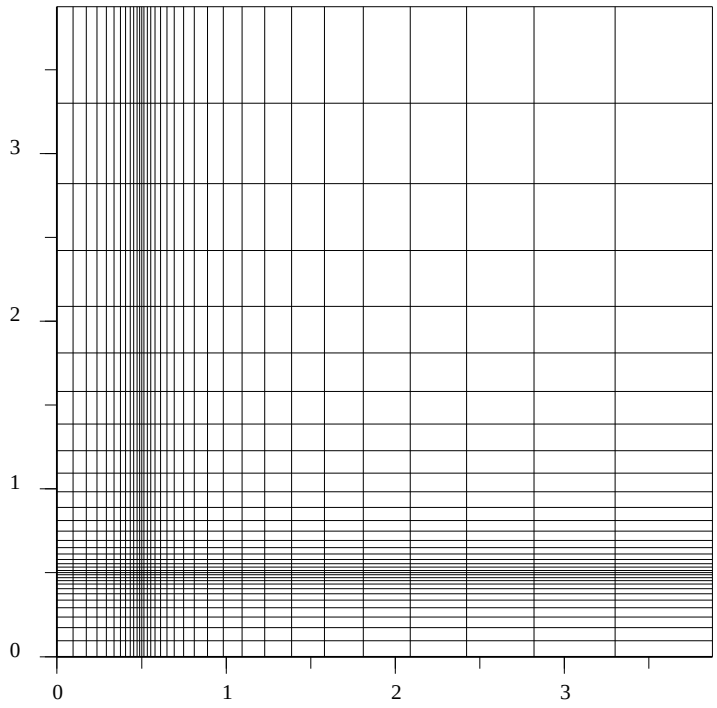

Figure 4: Example of grid in xy-plane with $\gamma = 1.2$, $z_m = 3$, $h_s = 0.015$.

The spatial discretization is copied after that for the disk: with a given γ and h_s we step in the x- and y-direction from the boundary of the electrode and back towards 0, which we shall probably overshoot. This determines the number of grid points inside the electrode, $N_x = N_y$, and the smallest step size is then adjusted (down) such that we hit 0 exactly. In the z-direction we start from 0 with the smallest step size, h_s, and proceed until we have passed z_m. It is not necessary to hit z_m exactly, instead we adjust z_m (upwards) and we have now determined the number, N_z, of grid points in the z-direction. The same step sizes are used in the x- and y-direction from the electrode boundary and out.

In Fig. 4 we show an example of the grid in the xy-plane computed with $\gamma = 1.2$, $z_m = 3$, and $h_s = 0.015$, which gives $N_x = N_y = 12$ and $N_z = 21$.

We see no need to dampen the exponential growth inside the electrode because

Table 10: The square electrode, discretization in time, $\gamma = 1.10$.

time	c-SDR	$v_1 - v_2$	q	w_1	$w_1 - w_2$	q'
0.1	3.7113768	0.0671850	1.319	3.8735757	0.0153771	1.864
0.2	3.2546066	0.0585377	1.359	3.3959290	0.0078051	1.791
0.3	3.0587777	0.0539476	1.370	3.1890188	0.0057508	1.772
0.4	2.9440142	0.0510744	1.375	3.0673188	0.0048068	1.764
0.5	2.8665070	0.0490718	1.378	2.9849769	0.0042625	1.759
0.6	2.8096922	0.0475769	1.380	2.9245529	0.0039061	1.756
0.7	2.7657566	0.0464070	1.382	2.8777929	0.0036530	1.753
0.8	2.7304742	0.0454597	1.383	2.8402236	0.0034629	1.751
0.9	2.7013348	0.0446725	1.383	2.8091838	0.0033141	1.749
1.0	2.6767414	0.0440050	1.384	2.7829789	0.0031940	1.748

of the short distance. Outside the electrode the step sizes might become rather large, especially when t and therefore z_m are large, but the concentration changes little far away from the electrode, so we keep the exponential growth throughout.

In Table 10 which follows the same procedure as Table 1 we give the results for the square electrode for $t = 0.1$ (0.1) 1.0 calculated with $\gamma = 1.10$, $k = 0.00125$, $h_s = 0.0000125$, and $z_m = 60$. As for the disk we find an order ratio which approaches $\sqrt{2}$, albeit slower, and a second order ratio, q', which is close to 2.

In Table 11 we show the results of changing h_s and as with the disk we find a nice first order component of the discretization error. The current value, corrected for the first three error components is shown in the last column (c-extr.) of Table 11. As with the disk there is also another important error component from the discretization in space, a component which we detect by changing γ. In Table 12 we present the results for γ between 1.10 and 1.34. For each γ we supply the values of N_x and N_z together with the computing time (which is roughly proportional to $N_z(N_x + N_z)^2$) and the current at $t = 1$ corrected for the first three error components.

Again we notice the increase in computation time with decreasing γ. Actually a single computation with $\gamma = 1.10$ takes more time than the combined calculation with $\gamma = 1.20$ (0.01) 1.34. In the latter case we have more than sufficient results to test our hypothesis which again is given by equation (38). Using least squares we find $u = 2.7832849$, $b_1 = -0.0053414$, $b_2 = -0.2704971$, and $b_3 = 0.1502102$. The residuals are less than 0.0000056 indicating a reasonable fit.

To summarize: The computed current at $t = 1$ with $\gamma = 1.10$, $h_s = 0.0000125$, $k = 0.00125$ is 2.6767. The main error components are the ($p = 1/2$)-term (0.1062), the $(\gamma-1)^2$-term (-0.0027), and the ($p=1$)-term (0.0032). We have also taken into account the ($p=1$)-term from changing h_s (0.0002), the ($\gamma - 1$)-term

Table 11: The square electrode, discretization in space, $\gamma = 1.10$.

time	c-SDR	$v_1 - v_2$	q	c-extr.
0.1	3.7113768	0.0002472	2.000	3.8892000
0.2	3.2546066	0.0002316	2.000	3.4039658
0.3	3.0587777	0.0002235	2.000	3.1949932
0.4	2.9440142	0.0002184	2.000	3.0723440
0.5	2.8665070	0.0002148	2.000	2.9894541
0.6	2.8096922	0.0002120	2.000	2.9286710
0.7	2.7657566	0.0002098	2.000	2.8816558
0.8	2.7304742	0.0002081	2.000	2.8438945
0.9	2.7013348	0.0002066	2.000	2.8127044
1.0	2.6767414	0.0002053	2.000	2.7863782

Table 12: Computed current at $t = 1$ as a function of γ

γ	N_x	N_z	sec	c-extr.	γ	N_x	N_z	sec	c-extr.
1.10	88	138	2029	2.7863782	1.23	45	68	187	2.7969970
1.11	81	127	1518	2.7869462	1.24	43	65	167	2.7980728
1.12	75	118	1158	2.7875600	1.25	42	63	151	2.7991803
1.13	71	110	914	2.7882180	1.26	41	61	137	2.8003192
1.14	66	103	709	2.7889196	1.27	39	59	120	2.8014888
1.15	63	97	590	2.7896630	1.28	38	58	111	2.8026882
1.16	60	92	486	2.7904473	1.29	37	56	102	2.8039172
1.17	57	87	407	2.7912716	1.30	36	55	93	2.8051741
1.18	54	83	353	2.7921349	1.31	35	53	85	2.8064586
1.19	52	79	302	2.7930357	1.32	35	52	79	2.8077692
1.20	50	76	265	2.7939733	1.33	34	51	72	2.8091069
1.21	48	73	235	2.7949466	1.34	33	49	64	2.8104710
1.22	46	70	206	2.7959553					
1.00				2.7832849					

(-0.0005) and the $(\gamma-1)^3$)-term (0.0002) so our result is 2.7833.

The next error term in the t-discretization is estimated to 0.0008 based on the difference between twice extrapolated values. Altogether we estimate the net effect of the succeeding terms to be less than 0.0010, and the current can be reported as 2.783 ± 0.001 with an error of at most 0.04 %.

Table 13: The square electrode, discretization in space, $\gamma = 1.10$, doubling h

time	c-SDR	$v_1 - v_2$	q	w_1	$w_1 - w_2$	q'
0.10	3.7113768	-0.0234259	3.159	3.6900805	0.0164322	2.464
0.20	3.2546066	-0.0311629	2.812	3.2262767	0.0129281	2.419
0.30	3.0587777	-0.0351254	2.684	3.0268455	0.0108459	2.288
0.40	2.9440142	-0.0375577	2.616	2.9098709	0.0094933	2.101
0.50	2.8665070	-0.0392287	2.573	2.8308445	0.0085408	1.953
0.60	2.8096922	-0.0404627	2.544	2.7729079	0.0078252	1.858
0.70	2.7657566	-0.0414203	2.522	2.7281018	0.0072630	1.801
0.80	2.7304742	-0.0421906	2.505	2.6921191	0.0068075	1.763
0.90	2.7013348	-0.0428273	2.492	2.6624009	0.0064293	1.733
1.00	2.6767414	-0.0433649	2.480	2.6373188	0.0061089	1.702

Table 14: The current for the square electrode at $t = 1.00$ after 2 extrapolations in time and space

γ	c-2ex
1.04	2.7693316
1.05	2.7662841
1.06	2.7633551
1.07	2.7605170
1.08	2.7577449
1.09	2.7550117
1.10	2.7523038
1.00	2.7831500

We now try the alternative technique for estimating the discretization error in space and present the results in Table 13. As before we have used $\gamma = 1.10$, $h_s = 0.0000125$, $k = 0.00125$, and $z_m = 60$. $N_x = 88$ is already divisible by 8 and N_z is adjusted from 138 to 144 but this has no effect on the first 7 decimals of the computed current. The values for q indicate a first order behaviour and we can compute $w_1 = v_1 + (v_1 - v_2)/\gamma$. The new differences are rather large and

the values for q' indicate yet another first order term. One possible explanation is that the assumption (44) is not valid but should be replaced by

$$v_1 \;=\; u - hc - h\log(h)\, g - h^2 d - h^3 f - \cdots \tag{69}$$

where u is the true solution and c, d, f, and g are unknown auxiliary functions.

Computing w_1 will eliminate the first order term and part of the logarithmic term and leave another first order term which then can be eliminated. The result for the current value at $t = 1.0$ is 2.6428723 and including the error components from the time discretization: 2.7523038. This is very different from the value we obtained earlier (2.7832849) and a computation with other values of γ as shown in Table 14 reveals a significant dependence on γ. An extrapolation based on least squares on these numbers and using assumption (38) gives the value 2.7831500 in good agreement with the earlier value.

Remark. Part of the reason for introducing the alternative technique was to avoid the necessity of calculating with several values of γ and extrapolate to $\gamma = 1.00$ using least squares. This worked well for the circular electrode but not at all for the square. Therefore there seems to be no particular reason to use the alternative technique on square (or rectangular) electrodes. □

18 Rectangular electrodes

Table 15: The rectangular electrode, discretization in time ($l = 4,\ \gamma = 1.20$)

time	c-SDR	$v_1 - v_2$	q	w_1	$w_1 - w_2$	q'	diff
0.01	6.9248354	-0.1935813	3.027	6.4574889	6.9248354	4.765	-2.0842485
0.03	4.4245813	0.0143241	-0.956	4.4591627	4.4245813	2.483	-0.0395755
0.10	2.9821748	0.0305745	1.252	3.0559881	2.9821748	1.979	0.0002469
0.30	2.2630602	0.0240504	1.366	2.3211229	2.2630602	1.827	0.0004869
1.00	1.8144437	0.0178070	1.394	1.8574337	1.8144437	1.722	0.0002444
3.00	1.5783227	0.0143098	1.401	1.6128696	1.5783227	1.634	0.0001657
10.00	1.4310156	0.0121019	1.404	1.4602321	1.4310156	1.553	0.0001307

We now consider a rectangular electrode such as defined in Problem 1 and compute the current per unit length, i/l. We follow the same procedure as for the square electrode, the main difference being that $N_x > N_y$ when $l > 1$. In Tables 15 and 16 we give the results for $l = 4$ calculated with $\gamma = 1.20$, $h_s = 0.0000125$, $k = 0.00125$, and $z_m = 60$. We also use the time steps $2k$, $4k$, and $8k$ in order to

Table 16: The rectangular electrode, discretization in space ($l = 4,\ \gamma = 1.20$)

time	c-SDR	$v_1 - v_2$	q	c-extr.
0.01	6.9248354	0.0001802	1.999	7.2113913
0.03	4.4245813	0.0001699	1.999	4.5413056
0.10	2.9821748	0.0001488	1.999	3.0681292
0.30	2.2630602	0.0001288	1.999	2.3240583
1.00	1.8144437	0.0001111	1.999	1.8584246
3.00	1.5783227	0.0001001	1.999	1.6134228
10.00	1.4310156	0.0000927	1.999	1.4606171

compute the error estimates and corrections as described previously. Therefore $t = 0.01$ is the first time when we have results with all four time steps. This is rather close to the singularity at $t = 0$, and we can expect the auxiliary functions c, d, ... (cf. equation (35)) to be rather large, such that we can not be sure that the leading terms in the error series are also the dominant ones. This is witnessed in Table 15 by the fact that the order ratio, q, is far away from $\sqrt{2}$ and also that the next difference, $w_1 - w_2$, is actually larger than the first one. The last column in Table 15 is the difference between the twice extrapolated values and can be taken as an estimate of the error (in time). It is clear from the table that the values for $t = 0.01$ and $t = 0.03$ may have large errors whereas the error in time at $t = 0.1$ is estimated to be less than 0.01 %.

Table 17: The rectangular electrode, discretization in time, small t ($k = 0.0000125$, $l = 4$, $\gamma = 1.20$)

time	c-SDR	$v_1 - v_2$	q	w_1	$w_1 - w_2$	q'	diff
0.0001	60.3609003	-3.1298854	2.554	52.8046885	8.6101886	4.885	-24.8428296
0.0003	34.2691393	-0.4807191	2.225	33.1085808	0.9413397	2.636	-0.5987807
0.0010	19.1379374	-0.0517489	2.426	19.0130046	0.1264221	2.167	-0.0211335
0.0030	11.5493652	0.0031948	-1.540	11.5570780	0.0227821	2.059	-0.0013490
0.0100	6.8921440	0.0082025	1.236	6.9119465	0.0035196	2.082	-0.0002884
0.0300	4.5173851	0.0060142	1.376	4.5319047	0.0005592	2.381	-0.0002128
0.1000	3.0588773	0.0037874	1.415	3.0680208	-0.0000030	-	-0.0001670
0.3000	2.3177354	0.0025416	1.427	2.3238714	-0.0000766	0.236	-0.0001350

In order to get reliable values at smaller times we choose a smaller k. This is no guarantee for more accurate results, since we now have computations at

time values rather close to the singularity at $t = 0$ and therefore prone to large discretization errors. In Table 17 we show results computed with $k = 0.0000125$ and we note that the error in time at $t = 0.003$ is estimated to be less than 0.02 %.

Remark At $t = 0.1$ the difference, $w_1 - w_2$, happens to be very small and the order ratio, q, therefore very large and not representative of the order of the approximation, (cf. [18], section 10.3). □

We now proceed as follows: Compute with $k = 0.00000125$, $2k$, $4k$, and $8k$ from $t = 0$, extrapolate twice (with $p = 1/2$ and 1) in time and record the results for $t \in [0.0003, 0.003[$. We use the smallest step size (in space) $h_1 = 0.0000125$ and use exponential expansion with factor $\gamma = 1.20$. We compute also with $2h_1$ and $4h_1$ and extrapolate (with $p = 1$). This correction is about 0.01 – 0.02 % and is not strictly necessary. We then multiply k by 10, compute again from $t = 0$ and record the results for $t \in [0.003, 0.03[$. There is no distinct advantage in using previous results as initial values since it usually takes a number of steps with the new step size before things settle down and we can trust the various error estimates. We then repeat the process twice, and in the latter case record the results for $t \in [0.3, 100]$.

The next step is to estimate the γ-contribution to the discretization error. We supplement our calculations with $\gamma = 1.20$ and 1.21 with a series of calculations with $\gamma = 1.28, \ldots, 1.34$ and use least squares to compute the current corresponding to $\gamma = 1.00$. The large values of γ are attractive because the computation time is roughly proportional to N^3 and therefore to $(\gamma - 1)^{-3}$. More important, the formula (38) seems to be valid for the whole γ-interval in question as witnessed by the fact that the extrapolated current changes little (at most 0.1 %) when we omit the values for 1.20 and 1.21.

The whole process is then repeated for a selected number of rectangles and the results are presented in Table 18. The results are estimated to be 0.1 % accurate and are rounded accordingly.

Included in Table 18 are also the steady state currents for $t \to \infty$ as computed using the values from $t = 10$, 20, 30, 40, 50, and 100 (and before rounding) using least squares and the assumption (42). Also included in Table 18 are current values for long, thin rectangles ($l \to \infty$). When $l \to \infty$ there is no gradient in the x-direction ($u_x = u_{xx} = 0$) and the problem is reduced to two space dimensions.

19 Comparing a square and a circular electrode

It is interesting to compare the current produced by a square electrode and a circular electrode with the same area.

If the width of the square is W and the radius of the circular disk is A then

$$W^2 \;=\; \pi A^2$$

Table 18: The rectangular electrode, current as a function of l and t

t / l	1	2	4	7	10	∞
0.0003	34.57	34.07	33.82	33.71	33.67	33.57
0.001	19.85	19.34	19.09	18.98	18.94	18.84
0.003	12.32	11.81	11.55	11.44	11.40	11.30
0.01	7.673	7.156	6.898	6.788	6.743	6.642
0.03	5.313	4.785	4.520	4.407	4.362	4.257
0.1	3.885	3.335	3.059	2.941	2.893	2.783
0.3	3.192	2.611	2.316	2.190	2.139	2.022
1	2.783	2.178	1.852	1.710	1.654	1.522
3	2.579	1.961	1.607	1.446	1.381	1.230
10	2.454	1.829	1.455	1.271	1.193	1.009
30	2.390	1.762	1.377	1.178	1.089	0.895
100	2.351	1.720	1.329	1.121	1.024	0.746
∞	2.303	1.670	1.271	1.052	0.944	

If the real time is T and the normalized times are t_{sq} and t_d then we have

$$t_{sq} \;=\; \frac{DT}{W^2}, \quad t_d \;=\; \frac{DT}{A^2} \;=\; t_{sq}\frac{W^2}{A^2} \;=\; \pi\, t_{sq}$$

and using (4) and (8) the ratio of the currents is

$$\frac{I_{sq}}{I_d} \;=\; \frac{nFDC^*W}{4nFDC^*A}\frac{i_{sq}}{i_d} \;=\; \frac{W}{4A}\frac{i_{sq}}{i_d} \;=\; \frac{\sqrt{\pi}}{4}\frac{i_{sq}}{i_d}$$

In Table 19 we present the results for a selection of t_{sq}. The currents for the disk are obtained by linear interpolation between the two nearest values of t_d for which we have information e.g. 0.09 and 0.10 when $t_{sq} = 0.03$

Table 19: Comparing a square and a circular electrode

t_{sq}	i_{sq}	$* \sqrt{\pi}/4$	t_d	i_d	I_{sq}/I_d
0.0003	34.57	15.32	0.000942	15.25	1.005
0.003	12.32	5.459	0.009425	5.370	1.017
0.03	5.313	2.354	0.094248	2.288	1.029
0.3	3.191	1.414	0.942478	1.377	1.027
3	2.579	1.143	9.424778	1.117	1.023
∞	2.303	1.020	∞	1.000	1.020

It is seen that the square produces more current than the disk, but the difference amounts to only 2 - 3 % as reported in [5].

20 Conclusion

We have shown that the Simplified Douglas-Rachford (**SDR**) scheme can be extended to three space dimensions. We have seen that the order in time of **SDR** drops from 1 to 1/2 for the given class of problems because of the singularity at $t = 0$, and that extrapolation can recover and improve the order. We have also seen that the discretization error in space is proportional to $(\gamma - 1)^2$ where γ is the expansion factor of the exponentially expanding space steps, and that we by using extrapolation techniques can correct for this error. We have also seen that we by using a special doubling technique can compensate for this γ-dependence in certain cases.

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