Battery Computing

An MMSC Case Study on Scientific Computing

Candidate Number: 1072462

Abstract

This work shall attempt to

Our Goal: Numerically obtain the solution $\{a(x,T), b(x,T)\}$ of

$$
\begin{cases}
\dfrac{\partial a}{\partial t} = D_a \dfrac{\partial^2 a}{\partial x^2}, & a : \mathbb{R}^+ \times [0,T] \mapsto [0,1],\ T \in \mathbb{R}^+,\ D_a \in \mathbb{R}^+, \quad \text{(1a)} \\
\dfrac{\partial b}{\partial t} = D_b \dfrac{\partial^2 b}{\partial x^2}, & b : \mathbb{R}^+ \times [0,T] \mapsto [0,1],\ D_b \in \mathbb{R}^+, \quad \text{(1b)} \\
a(\infty,t) = 1,\ b(\infty,t) = 0, & \text{boundary conditions } \forall\, t \in [0,T]\,, \quad \text{(1c)} \\
a(x,0) = 1,\ \ b(x,0) = 0, & \text{initial conditions } \forall\, x \in (0,\infty)\,, \quad \text{(1d)} \\
\dfrac{\partial a}{\partial x} + D \dfrac{\partial b}{\partial x} = 0\,, & \quad \text{(1e)}
\end{cases}
$$

and optionally, $a(0,t) = 0$, which corresponds to Chronoamperometry or $\frac{\partial a}{\partial x}\big|_{x=0} = I(t)$ which is set according to a special Linear Sweep Voltammetry method with $I(t)$ given by Equation (4).

The implementation bla bla

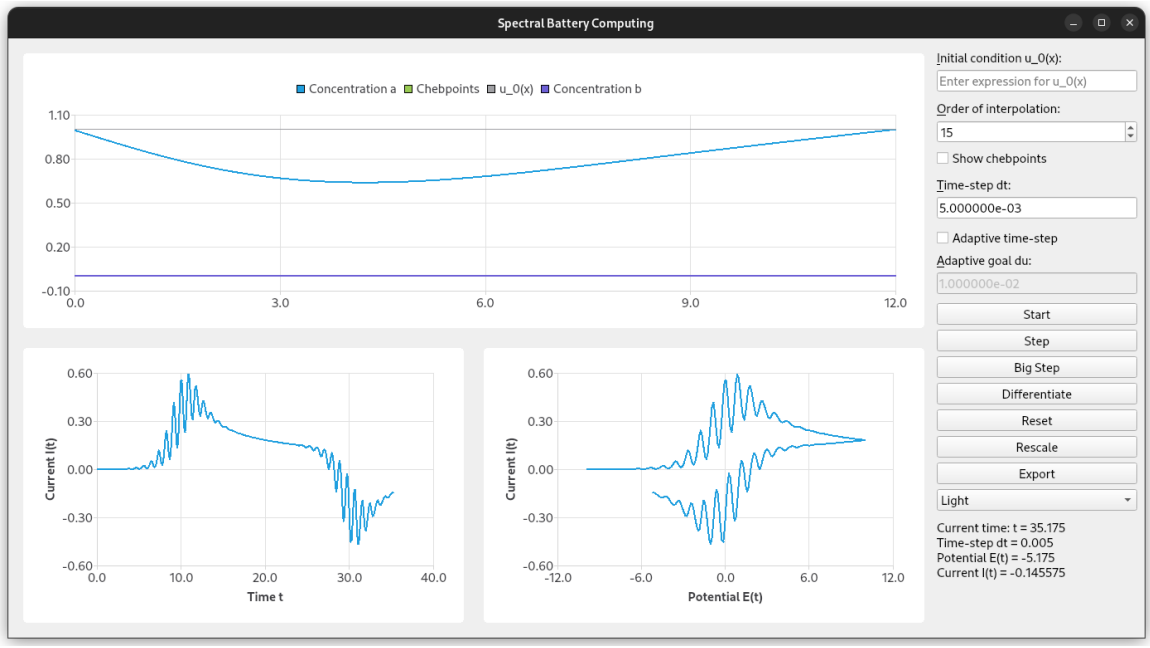

Figure 1: Graphical User Interface

Contents

1 Problem Introduction

Energy storage and its associated challenges are clearly among the most relevant questions, not only for the industrial but also the private sector. Politically, many nations in the world are steering towards greener energy supplies. Renewable energy sources such as wind and sun usually have a fundamental issue however, their availability is subject to an immense amount of fluctuation, which the energy grid must compensate through short- and long-term energy storage.

Long-term solutions include for example pumped-storage hydroelectricity facilities, but these must be complemented with short-term storage approaches such as Lithium-Ion or Lithium-Iron-Phosphate ($LiFePO_4$) batteries. Most modern batteries exploit electrochemical reactions to relate electrical potentials with chemical potentials and their associated difference ($\rightarrow$ voltage) and convert energy accordingly. The oxidation reaction we considere here is

$$A \Rightarrow B + e^{-}?$$

where A and B can be any chemicals and e^{-} is an electron (Gavaghan and Bond 2000).

More bla bla later on.

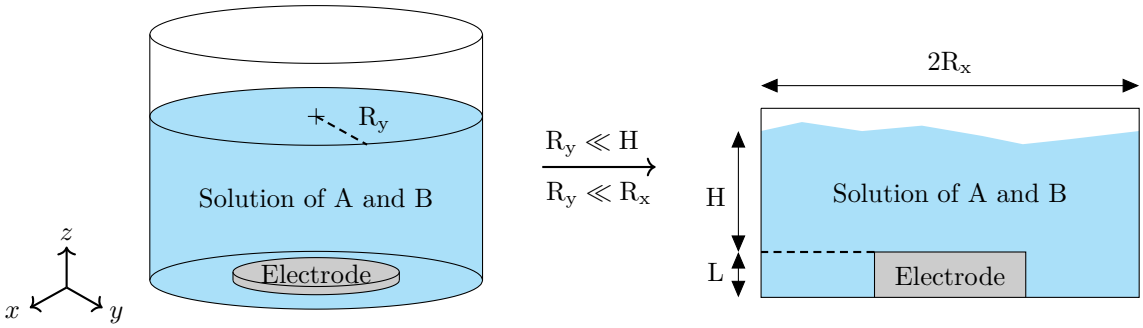

Figure 2: Wohoo.

As stated on Page 1, we consider the following Partial Differential Equation (PDE)s in the concentrations $a, b \in \mathbb{C}^2(\Omega)$

$$\frac{\partial a}{\partial t} = D_a \frac{\partial^2 a}{\partial x^2} \tag{2}$$

$$\frac{\partial b}{\partial t} = D_b \frac{\partial^2 b}{\partial x^2} \tag{3}$$

1.1 Chronoamperometry

1.2 Linear Sweep Voltammetry

$$I(t) = \kappa_0 \left(a\mathrm{e}^{(1-\alpha)(E(t)-E_0)} - b\mathrm{e}^{-\alpha(E(t)-E_0)} \right)_{x=0} \tag{4}$$

1.3 Linear Sweep AC Voltammetry

$$E(t) = E_{dc}(t) + \Delta E \sin(\omega t)\,. \tag{5}$$

2 Mathematical Background

Let $\mathbb{N}$ denote the nonnegative integers, so $0 \in \mathbb{N}$. Similarly, let $\mathbb{R}^+ = [0, \infty)$ denote the nonnegative real numbers.

2.1 Laplace Integral Transform

What is Laplace?

2.1 Definition: Laplace Integral Transform

Given a function $a : \mathbb{R} \mapsto \mathbb{R}$, its Laplace transform $\hat{a} : \mathbb{C} \mapsto \mathbb{C}$ is given by

$$\hat{a}(s) = \mathcal{L}\{a\}(s) = \int_0^\infty a(t)\mathrm{e}^{-st}\,\mathrm{d}t\,.$$

A notation commonly employed in the context of signal processing is $a(t) \circ\!\!-\!\!\bullet\, \hat{a}(s)$ to signify a *transformation pair*, so

$$a(t) \circ\!\!-\!\!\bullet\, \hat{a}(s) \quad \Longleftrightarrow \quad \hat{a}(s) = \mathcal{L}\{t \mapsto a(t)\}(s)\,.$$

In the following, we will mostly consider functions of two variables $a : \mathbb{R} \times \mathbb{R} \mapsto \mathbb{R}$ (the concentration of a chemical being a function of time $t \in \mathbb{R}$ and space $x \in \mathbb{R}$). In these cases, we are only transforming in one variable, namely t, and we will consider x only as a parameter of the transformation pair.

Laplace transforms are especially valuable for physical systems as many of them expose exponentially decaying and/or periodic behaviours which the Laplace transform is well-suited for due to the form of its kernel. Decaying behaviour is captured by the

real component of the argument s, $\mathfrak{Re}(s)$, whereas periodicities are captured by the imaginary part $\mathfrak{Im}(s)$[1].

2.1 Theorem: Laplace Transform of the Derivative

Given a function $a(t)$ and a corresponding Laplace-transform $\hat{a}(s) = \mathcal{L}\{a\}(s)$, the transform of the derivative $a'(t)$ of the original function is given by

$$\mathcal{L}\{a'\}(s) = \mathcal{L}\left\{t \mapsto \frac{\partial a}{\partial t}\right\}(s) = s\hat{a}(s) - a_0\,,$$

where $a_0 := a(t = 0)$.

Proof. Proof for Laplace's differentiation theorem. □

2.2 Theorem: Initial Value

For a function $a \in \mathcal{C}^2(\Omega)$ with corresponding Laplace-transform $\hat{a} = \mathcal{L}\{a\}$,

$$\lim_{s\to\infty} s\hat{a}(s) = \lim_{t\to 0^+} a(t)$$

relates a's *initial value* with the transform evaluated at $s \to \infty$.

2.3 Theorem: Laplace Convolution

For a function $a \in \mathcal{C}^2(\Omega)$ with corresponding Laplace-transform $\hat{a} = \mathcal{L}\{a\}$,

$$\lim_{s\to\infty} s\hat{a}(s) = \lim_{t\to 0^+} a(t)$$

relates a's *initial value* with the transform evaluated at $s \to \infty$.

[1] Consider for comparision the Fourier transform $\mathcal{F}(a)(\omega) := \int_{-\infty}^{\infty} a(t)\mathrm{e}^{\mathrm{i}\omega t}\,\mathrm{d}t$ which captures periodic frequencies, where the kernel automatically follows multiplication along the unit circle due to the imaginary-valued exponent $\mathrm{i}\omega t$ (the argument $\omega \in \mathbb{R}$ is real-valued). Intuitively, the Laplace transform coincides with the Fourier transform if evaluated at $s = \mathrm{i}\omega$.

2.2 Chebyshev Polynomials

2.2 Definition: Chebyshev Polynomial of the First Kind

Chebyshev[2] polynomials $T_k : \mathbb{R} \mapsto \mathbb{R}$ are functions satisfying

$$T_k(x) = T_k(\cos\theta) := \cos(k\theta) = \frac{1}{2}(z^k + z^{-k})$$
$$z := \mathrm{e}^{i\theta}, \quad x := \mathfrak{Re}(z) = \cos(\theta) = \frac{1}{2}(z + z^{-1})$$

for degree $k \in \mathbb{N}$. Then, $T_0(x) = 1$, $T_1(x) = x$, $T_2(x) = 2x^2 - 1$, and so on.

2.3 Definition: Chebyshev Polynomial of the Second Kind

Chebyshev polynomials $U_k : \mathbb{R} \mapsto \mathbb{R}$ are functions satisfying

$$U_k(\cos\theta)\sin\theta := \sin\left((k+1)\theta\right)$$

for degree $k \in \mathbb{N}$. Then, $U_0(x) = 1$, $U_1(x) = 2x$, $U_2(x) = 4x^2 - 1$, and so on.

Note that Chebyhsev polynomials of the first and second kind fulfill the same recurrence relationship, $T_{k+1}(x) = 2xT_k(x) - T_{k-1}(x)$ and $U_{k+1}(x) = 2xU_k(x) - U_{k-1}(x)$. The difference between them arises from the second polynomial respectively which is $T_1(x) = x$ for the first kind and $U_1(x) = 2x = 2T_1(x)$ for the second kind.

Proof of $U_k(-1)$'s value.

3 Finite Differences

Construct $A\boldsymbol{x} = \boldsymbol{b}$.

[2]Named after Pafnuty Lvovich Chebyshev, alternatively transliterated as Tchebycheff, Tchebyshev (French) or Tschebyschow (German).

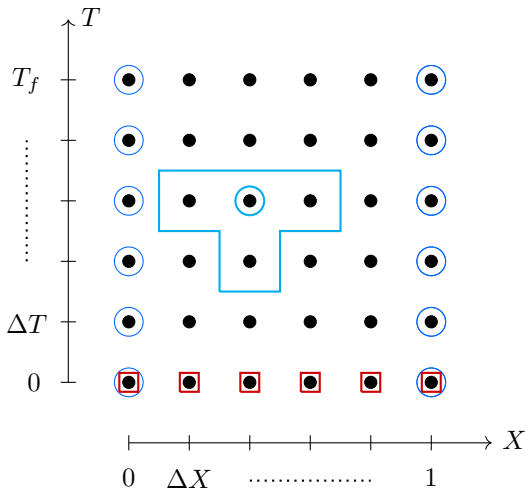

Figure 3: Schematic of the finite different scheme where ... are the nodes specified by initial conditions, and ... are the nodes specified by boundary conditions.

3.1 Results

4 Analytical Approaches

When $D = 1$, $a + b = 1$ because.

4.1 Similarity Solution

Without considering the mass conservation equation $\frac{\partial a}{\partial x} + D\frac{\partial b}{\partial x} = 0$ (Equation (1e)) which couples a with b, the diffusion equations Equation (1a) and Equation (1b) can be solved independently through a similarity solution approach. The idea behind the latter is to turn the PDE into an Ordinary Differential Equation (ODE) by introducing a variable $\eta \in \mathbb{R}$ that depends on both other variables x and t. For a diffusion-type equation, the correct ansatz would be letting

$$a(x,t) = f(\eta), \quad \eta := \frac{x}{\sqrt{t}},$$

with $f : \mathbb{R} \mapsto \mathbb{R}$ and substituting back into Equation (1a) accordingly. Respecting the chain rule on derivatives of f accordingly, we arrive at

$$\frac{\partial a}{\partial t} = -\frac{1}{2}xt^{-\frac{3}{2}}f'(\eta) = D_a\frac{\partial^2 a}{\partial x^2} = D_a t^{-1}f''(\eta)$$

where we multiply both sides by t to arrive at a simple form

$$D_a f''(\eta) + \frac{1}{2}\eta f'(\eta) = 0\,, \tag{6}$$

which can be solved by substituting $h(\eta) := f'(\eta)$ and solving $D_a \frac{\mathrm{d}h}{\mathrm{d}\eta} = \frac{-1}{2}\eta h(\eta)$ by separation of variables:

$$\int \frac{\mathrm{d}h}{h} = \frac{-1}{2D_a}\int \eta \,\mathrm{d}\eta \quad \Rightarrow \quad \ln(h) = -\frac{\eta^2}{4D_a} + \tilde{c_1} \quad \Rightarrow \quad h(\eta) = c_1 \mathrm{e}^{\frac{-1}{4D_a}\eta^2},$$

which in turn may be integrated to get $f(\eta)$ and thereby $a(x,t)$,

$$f(\eta) = c_1 \int \mathrm{e}^{\frac{-1}{4D_a}\eta^2}\mathrm{d}\eta = c_1\sqrt{D_a\pi}\,\mathrm{erf}\left(\frac{\eta}{2\sqrt{D_a}}\right) + c_2\,.$$

Substituting back, we get

$$a(x,t) = c_1\sqrt{D_a\pi}\,\mathrm{erf}\left(\frac{x}{2\sqrt{D_a x}}\right) + c_2\,, \tag{7}$$

$$b(x,t) = c_3\sqrt{D_b\pi}\,\mathrm{erf}\left(\frac{x}{2\sqrt{D_b x}}\right) + c_4\,, \tag{8}$$

where the solution of $b(x,t)$ is obtained by the same procedure.

4.2 Voltammetry Integral Equation

4.2.1 Derivation using the Laplace Transform

As mentioned above, the Laplace Integral Transform is especially useful in the context of differential equations, mostly due to Theorem 2.1. Applying it to our *partial* differential diffusion equation Equation (2) transforms the problem into one of solving an *ordinary* differential equation. Similarly, ODEs could be turned into algebraic equations using a similar approach.

Starting from Equation (2), we Laplace-transform both sides and then apply Theorem 2.1 in time t to arrive at

$$\begin{aligned}
\frac{\partial a}{\partial t} &= D_a \frac{\partial^2 a}{\partial x^2} && \text{Laplace-transform w.r.t. } t \\
\mathcal{L}\left\{t \mapsto \frac{\partial a}{\partial t}\right\} &= D_a \mathcal{L}\left\{t \mapsto \frac{\partial^2 a}{\partial x^2}\right\} && \text{Use Theorem 2.1} \\
s\hat{a}(s) - a_0(x) &= D_a \frac{\partial^2 \hat{a}}{\partial x^2} && \text{Rearrange} \\
\frac{\partial^2 \hat{a}}{\partial x^2} - \frac{s}{D_a}\hat{a} &= -\frac{a_0(x)}{D_a}
\end{aligned}$$

where $\hat{a} := \mathcal{L}\{a\}$ and $a_0(x) := a(x, t=0)$, which is a second-order constant-coefficient Ordinary Differential Equation in space x. Its characteristic polynomial is $\lambda^2 + \frac{s}{D_a} = 0$

which, together with the initial condition $a_0 = 1$ and resulting particular solution $\hat{a}_p(x,s) = \mathcal{L}\{-1\}(s) = \frac{1}{s}$[3], leads us to the general solution

$$\hat{a}(x,s) = c_1 \mathrm{e}^{\sqrt{\frac{s}{D_a}}x} + c_2 \mathrm{e}^{-\sqrt{\frac{s}{D_a}}x} + \frac{1}{sD_a}\,, \quad c_1, c_2 \in \mathbb{R}\,. \tag{9}$$

The constant c_1 then vanishes when applying the initial value theorem (Theorem 2.2)

$$\lim_{s\to\infty} s\hat{a}(s) = \lim_{s\to\infty} \underbrace{c_1 s \mathrm{e}^{\sqrt{\frac{s}{D_a}}x}}_{\to\infty} + \underbrace{c_2 s \mathrm{e}^{-\sqrt{\frac{s}{D_a}}x}}_{\to 0} + 1 \overset{!}{=} \lim_{t\to 0^+} a(t) = 1$$

because $c_1 \neq 0$ would cause its corresponding term to explode. Considering the other boundary condition of linear sweep voltammetry

$$\left.\frac{\partial a}{\partial x}\right|_{x=0} = I(t) \quad \Leftrightarrow \quad \frac{\partial \hat{a}}{\partial x} \overset{!}{=} \hat{I}(s) \quad \Leftrightarrow \quad c_2\sqrt{\frac{s}{D_a}}\mathrm{e}^0 = \hat{I}(s)\,,$$

where $\hat{I}(s) := \mathcal{L}\{I\}(s)$ and we obtain $c_2(s) = \frac{-\hat{I}(s)}{\sqrt{s}}$. So Equation (9) becomes

$$\hat{a}(x,s) = \frac{-\hat{I}(s)}{\sqrt{s}}\mathrm{e}^{-\sqrt{\frac{s}{D_a}}x} + \frac{1}{sD_a}\,, \tag{10}$$

which, evaluated at $x = 0$, becomes $\hat{a}(s,0) = \frac{-\hat{I}(s)}{\sqrt{s}} + \frac{1}{sD_a}$, depending on the Laplace transform of the current $I(t)$.

In principle, this is already a complete result in and of itself, as it provides the full solution on the entire domain in frequency-space [4]. If one obtains the Laplace-transform of the current expression Equation (4) and performs the inverse transform of $\hat{a}$, even just numerically, the linear sweep voltammetry problem is solved in full as a similar procedure leads to the solution of the other concentration b.

4.2.2 At the Boundary

Within the scope of this report, we will consider an integral equation relating current $I(t)$ and the potential $E(t)$ to verify our numerical results. Inverse-transforming Equation (10) at $x = 0$ where our boundary condition is given and using the convolution theorem (Theorem 2.3), we arrive at

$$a(x,t) = -\mathcal{L}^{-1}\left\{s \mapsto \hat{I}(s)\cdot\hat{g}(s)\right\}(t) + \mathcal{L}^{-1}\left\{s \mapsto \frac{1}{sD_a}\right\}(t) = -(I * g)(t) + \frac{1}{D_a}\,,$$

where we introduced $\hat{g}(s) := \frac{1}{\sqrt{s}} = \mathcal{L}\{g\}(s)$ the Laplace transfrom of $g(t) = \frac{1}{\sqrt{\pi t}}$.

[3] $\mathcal{L}\{1\} = \int_0^\infty \mathrm{e}^{-st}\,\mathrm{d}t = \frac{1}{s}\left[\mathrm{e}^{-st}\right]_0^\infty = \frac{-1}{s}$.

[4] Frequency space is a term borrowed from Fourier analysis, where we say that the transformed functions reside in "frequency space". The usage is the same for Laplace's transformation.

Proof. $\mathcal{L}\{t \mapsto \frac{1}{\sqrt{\pi t}}\}(s) = \frac{1}{\sqrt{\pi}} \int_0^\infty t^{-\frac{1}{2}} \mathrm{e}^{-st}\,\mathrm{d}t = \frac{1}{\sqrt{\pi}} \int_0^\infty \cancel{t^{\frac{1}{2}}} \mathrm{e}^{-su^2} \cancel{t^{\frac{1}{2}}}\,\mathrm{d}u = [\mathrm{erf}(\sqrt{s}u)/\sqrt{s}]_0^\infty$ where we used a substitution $u = \sqrt{t}$ to resolve the product in the integrand, resulting in the Gaussian integral and subsequently, the error function $\mathrm{erf}(\sqrt{s}u)$ which satisfies $\mathrm{erf}(0) = 0$ and $\mathrm{erf}(\infty) = 1$ so the full transformation pair is $\frac{1}{\sqrt{\pi t}} \circ\!\!-\!\!\bullet\, \frac{1}{\sqrt{s}}$. □

4.2.3 Simplification when $D = 1$ and $\kappa_0 \gg 1$

When $D = 1$, this results in the following expressions for $a(x = 0, t)$ and $b(x = 0, t)$,

$$a(x = 0, t) = 1 - (I * g)(t) = 1 - \int_0^t \frac{I(\tau)}{\sqrt{\pi(t - \tau)}}\,\mathrm{d}\tau\,, \tag{11}$$

$$b(x = 0, t) = 1 - a(x = 0, t) = \int_0^t \frac{I(\tau)}{\sqrt{\pi(t - \tau)}}\,\mathrm{d}\tau\,, \tag{12}$$

which can be even further simplified when considering $\kappa_0 \gg 1$, where from Equation (4) we have the following relationship of $I(t)$, $E(t)$ and $b_0(t)$

$$\begin{aligned} I(t) &= \kappa_0(1 - b_0)\mathrm{e}^{(1-\alpha)V} - \kappa_0 b_0 \mathrm{e}^{-\alpha V} \\ &= \kappa_0 \left[(1 - b_0)\mathrm{e}^{V} - b_0\right] \mathrm{e}^{-\alpha V} \\ &= \kappa_0 \left[\mathrm{e}^{V} - (1 + \mathrm{e}^{V})b_0\right] \mathrm{e}^{-\alpha V} \end{aligned}$$

where $V(t) := E(t) - E_0(t)$, $a_0 = a(x = 0, t)$ and $b_0 = b(x = 0, t)$. It can be further rearranged and simplified to yield an approximation to b_0,

$$\frac{I(t)}{\kappa_0 \mathrm{e}^{-\alpha V}} = \mathrm{e}^{V} - (1 + \mathrm{e}^{V})b_0 \quad \Leftrightarrow \quad b_0 = \frac{\mathrm{e}^{V} - \frac{I(t)}{\kappa_0 \mathrm{e}^{-\alpha V}}}{1 + \mathrm{e}^{V}} \approx \frac{\mathrm{e}^{V}}{1 + \mathrm{e}^{V}} \quad \text{when } \kappa_0 \gg 1\,,$$

which can be combined with Equation (12) to obtain

$$b_0 = \int_0^t \frac{I(\tau)}{\sqrt{\pi(t - \tau)}}\,\mathrm{d}\tau \approx \frac{1}{1 + \mathrm{e}^{-V}} \quad \Leftrightarrow \quad \int_0^t \frac{I(\tau)}{\sqrt{(t - \tau)}}\,\mathrm{d}\tau \approx \frac{\sqrt{\pi}}{1 + \mathrm{e}^{-(E(t) - E_0)}}\,, \tag{13}$$

which we will use to numerically verify our results.

4.2.4 Numerical Verification

Numerically integrating the left-hand side convolution in Equation (13) using a quadrature rule and comparing it with the right-hand side, from the spectral solver we obtain a relatively close match as can be seen in Figure 4.

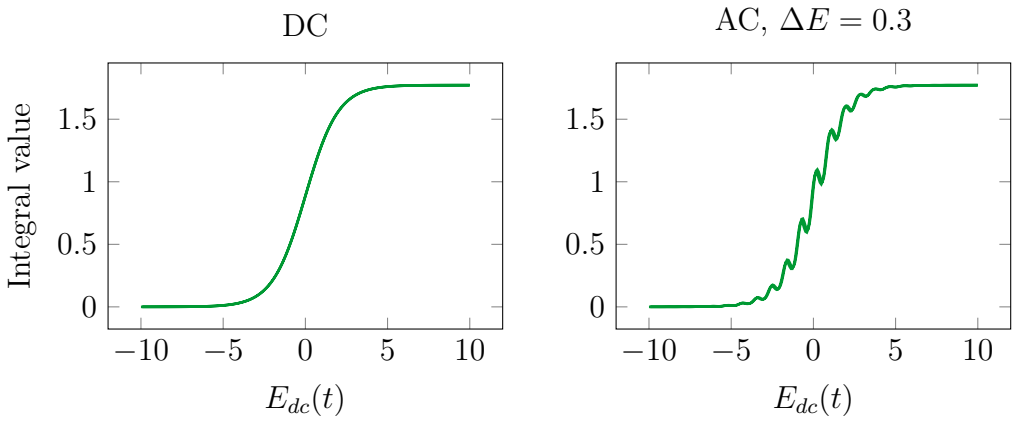

Figure 4: Convolution Integral: Comparing $\int_0^t \frac{I(\tau)}{\sqrt{(t-\tau)}}\,\mathrm{d}\tau$ (in blue) with $\frac{\sqrt{\pi}}{1+\mathrm{e}^{-(E(t)-E_0)}}$ (in green) for the DC and AC case with parameter $\Delta E = 0.3$ over the DC potential $E_{dc}(t)$. $\kappa_0 = 35$ is chosen large and we further have $\alpha = 0.9$, $E_0 = 0$ and $t_{rev} = 20$.

5 Spectral Method

From the definition of Chebyshev polynomials $T_k(x) = \cos(k\theta)$, confer Definition 2.2, we can derive that

$$\frac{\mathrm{d}T_k}{\mathrm{d}x} = \frac{\mathrm{d}T_k}{\mathrm{d}\theta}\frac{\mathrm{d}\theta}{\mathrm{d}x} = \ldots = kU_{k-1}(x)\,,$$

where $U_k : [-1,1] \mapsto \mathbb{R}$ denote the Chebyshev polynomials of the second kind, $U_k(\cos\theta)\sin(\theta) = \sin\left((n+1)\theta\right)$, confer Definition 2.3.

In order to enforce a von-Neumann boundary condition on the left and a Dirichlet boundary condition on the right, we are interested in explicitly setting coefficients a_k such that

$$a_x(-1,t) = \frac{\mathrm{d}a}{\mathrm{d}x}\Big|_{x=-1} = \tilde{l} \quad \text{and} \quad a(1) = r, \quad \text{where} \quad \tilde{l}, r \in \mathbb{R}\,.$$

Using the Chebyshev series ansatz

$$a(x,t) = \sum_{k=0}^{N-1} a_k^{(t)} T_k(x)$$

we have that

$$\frac{\mathrm{d}a}{\mathrm{d}x} = \sum_{k=0}^{N-1} a_k^{(t)} \frac{\mathrm{d}T_k}{\mathrm{d}x}(x)\,,$$

so we are interested in

$$a_x(-1,t) = \frac{\mathrm{d}a}{\mathrm{d}x}\Big|_{x=-1} = \sum_{k=0}^{N-1} a_k^{(t)} \frac{\mathrm{d}T_k}{\mathrm{d}x}\Big|_{x=-1} = \sum_{k=0}^{N-1} a_k^{(t)} kU_{k-1}(-1)\,.$$

Following from TODO (explained on Wikipedia), we know that

$$U_k(-1) = (-1)^k(k+1) \quad \text{and} \quad T_k(1) = 1 \quad \forall k \in \mathbb{N}\,,$$

which turns our conditions into algebraic conditions w.r.t. the coefficients $a_k^{(t)}$,

$$a_x(-1,t) = \frac{\mathrm{d}a}{\mathrm{d}x}\Big|_{x=-1} = \sum_{k=0}^{N-1} a_k^{(t)} k^2 (-1)^{k-1} \stackrel{!}{=} \tilde{l} \quad \text{and} \quad a|_{x=1} = \sum_{k=0}^{N-1} a_k^{(t)} \stackrel{!}{=} r\,.$$

Knowing that the heat equation Forward Euler numerical scheme modifies all but the two highest-degree coefficients in the series, we expand:

$$\begin{aligned} a_x(-1,t) = \sum_{k=0}^{N-1} a_k^{(t)} T_k'(-1) = &\overbrace{-\sum_{k=0}^{N-3} a_k^{(t)} k^2 (-1)^k}^{:=\Sigma_3} - (N-2)^2(-1)^{N-2} a_{N-2} \\ &- (N-1)^2(-1)^{N-1} a_{N-1} = l\,, \\ a(1,t) = \sum_{k=0}^{N-1} a_k^{(t)} T_k(1) = &\underbrace{\sum_{k=0}^{N-3} a_k^{(t)}}_{:=\Sigma_2} + a_{N-2} + a_{N-1} = r\,, \end{aligned}$$

5.1 Enforcing Boundary Conditions

Von Neumann on the left

5.2 Stability and Implicit Euler

5.3 Implementation

The solver was implemented in C++, using TschebFun and is based on the HeatFun numerical integrator.

5.4 Results

Chronoamperometry (step potential),

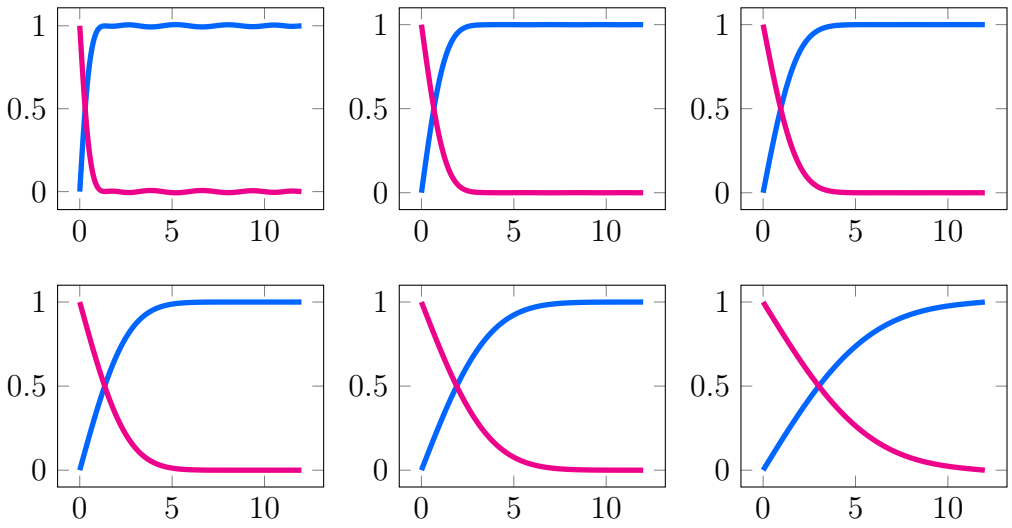

Figure 5: Chronoamperometry

DC Linear Sweep Voltammetry, AC Linear Sweep Voltammetry

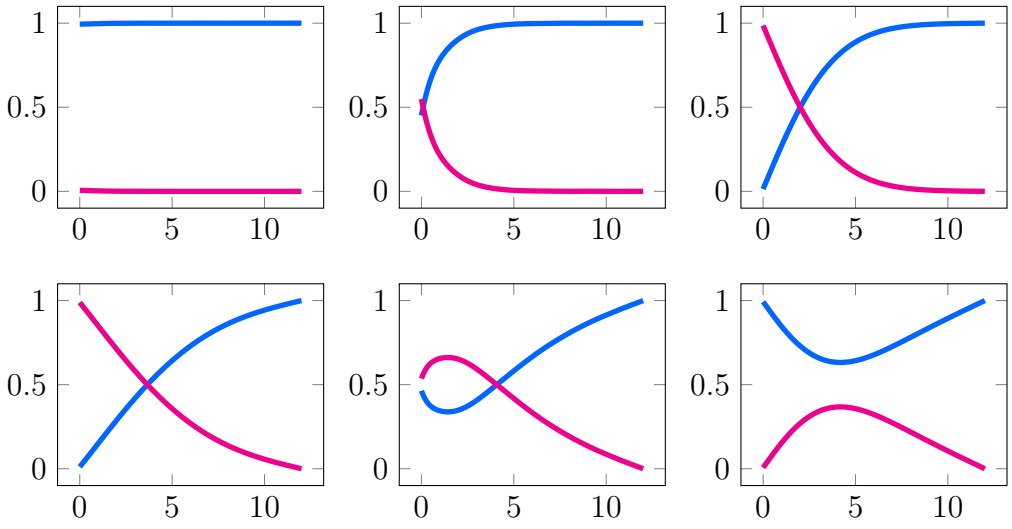

Figure 6: AC Voltammetry

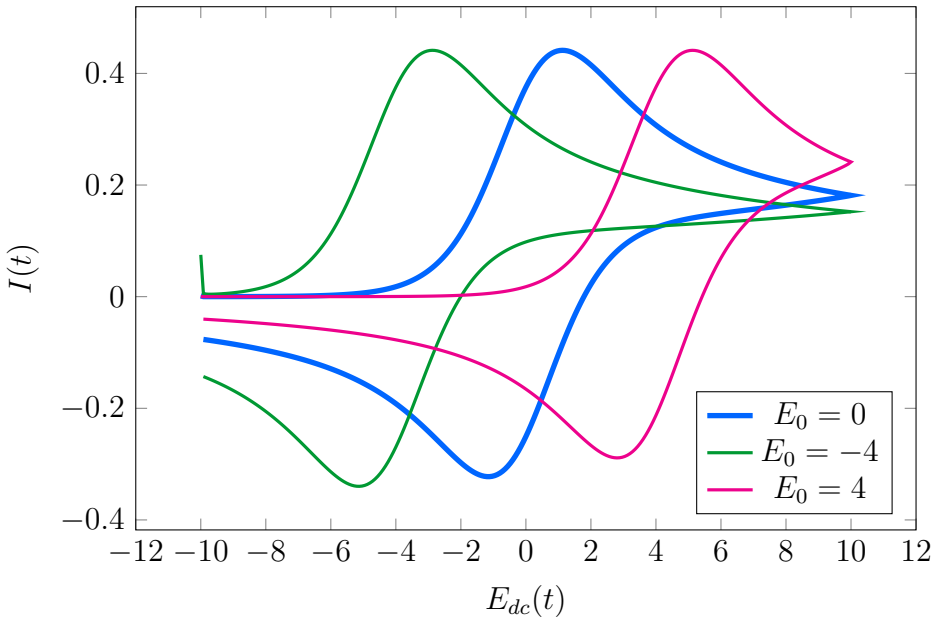

Figure 7: Voltammetry Current $I(t)$ vs. the DC Potential $E_{dc}(t)$

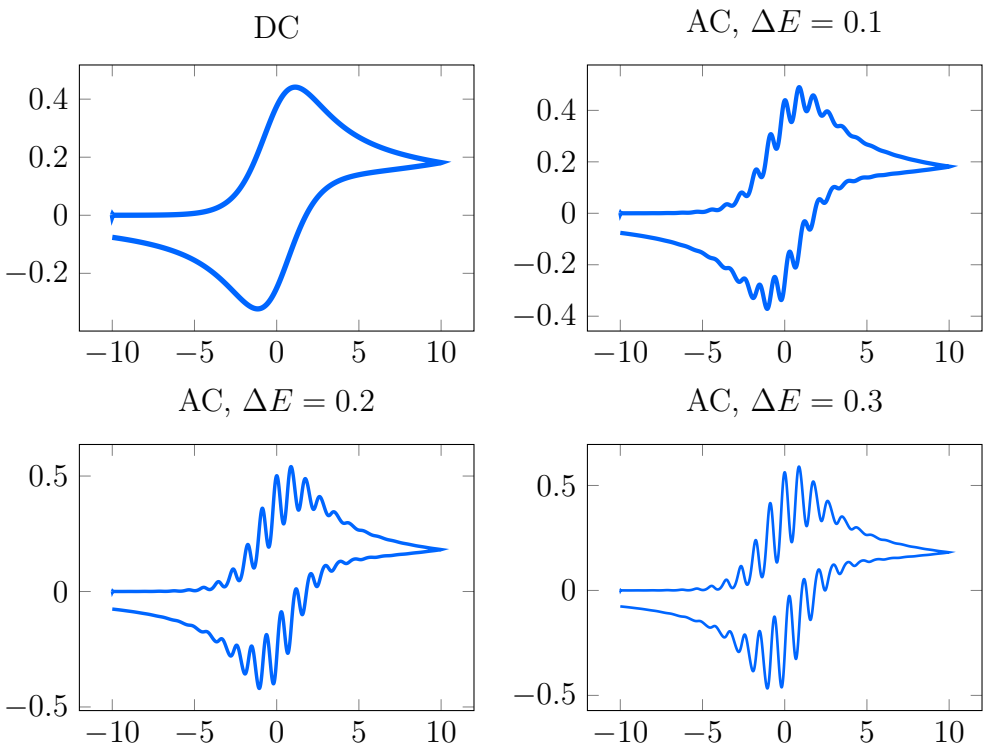

Figure 8: Voltammetry Current $I(t)$ vs. the DC Potential $E_{dc}(t)$

5.5 Convergence behaviour

6 Conclusion

Table 1: Runtime Comparison

References

Gavaghan, D. J. and A. M. Bond (Jan. 2000). 'A complete numerical simulation of the techniques of alternating current linear sweep and cyclic voltammetry: analysis of a reversible process by conventional and fast Fourier transform methods'. In: *J. Electroanal. Chem.* 480.1, pp. 133–149. ISSN: 1572-6657. DOI: 10.1016/S0022-0728(99)00476-3.

Acronyms

ODE	Ordinary Differential Equation	7
PDE	Partial Differential Equation	3

A Implementation

The results above were obtained using implementations of the numerical methods described. Three (independent) solvers are available, in MATLAB and in Python and the spectral solver (cf. the folder named `SpectralSolver`) which is written in C++. All code is available on GitHub, in the MrP01/BatteryComputing repository.