

Battery Computing

An MMSC Case Study on **SCIENTIFIC COMPUTING**

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Abstract

This work shall attempt to

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

$$\begin{cases} \frac{\partial a}{\partial t} = D_a \frac{\partial^2 a}{\partial x^2}, & a : \mathbb{R}^+ \times [0, T] \mapsto [0, 1], T \in \mathbb{R}^+, D_a \in \mathbb{R}^+, \\ \frac{\partial b}{\partial t} = D_b \frac{\partial^2 b}{\partial x^2}, & b : \mathbb{R}^+ \times [0, T] \mapsto [0, 1], D_b \in \mathbb{R}^+, \\ a(\infty, t) = 1, b(\infty, t) = 0 & \forall t \in [0, T] \\ a(x, 0) = 1, b(x, 0) = 0 & \forall x \in (0, \infty) \\ a(0, t) = 0, \frac{\partial a}{\partial x} + D \frac{\partial b}{\partial x} = 0 \end{cases}$$

The implementation bla bla

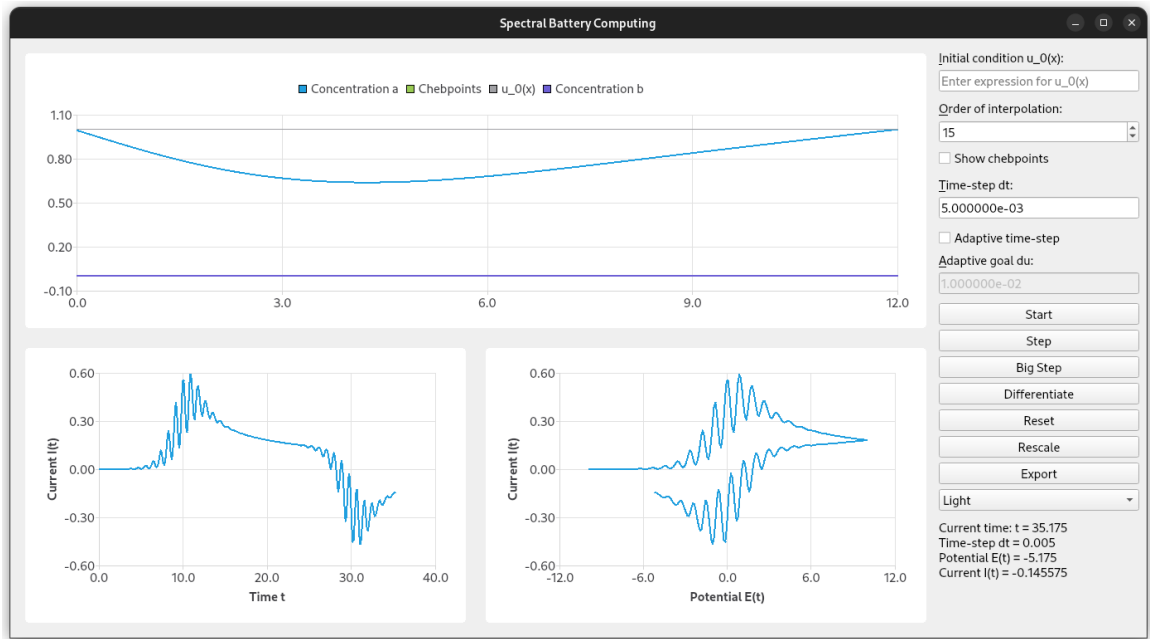


Figure 1: Graphical User Interface

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1 Problem Introduction

Clearly, batteries relevant.

Figure

Figure 2: Wohoo

1.1 Chronoamperometry

1.2 DC Voltammetry

1.3 AC Voltammetry

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. Figure 2.

2.1 Laplace Integral Transform

What is Laplace?

Proof for Laplace's differentiation theorem.

2.2 Chebyshev Polynomials

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

3 Finite Differences

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

3.1 Results

4 Analytical Approaches

4.1 Similarity Solution

4.2 Integral Equation

4.2.1 Derivation

4.2.2 Numerical Solution

5 Spectral Method

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

$$\frac{dT_k}{dx} = \frac{dT_k}{d\theta} \frac{d\theta}{dx} = \dots = kU_{k-1}(x),$$

where $U_k : [-1, 1] \mapsto \mathbb{R}$ denote the Chebyshev polynomials of the second kind, which in turn are defined by

$$U_k(\cos \theta) \sin(\theta) = \sin((n+1)\theta).$$

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

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

Using the Chebyshev series ansatz

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

we have that

$$\frac{da}{dx} = \sum_{k=0}^{N-1} a_k^{(t)} \frac{dT_k}{dx}(x),$$

so we are interested in

$$a_x(-1, t) = \left. \frac{da}{dx} \right|_{x=-1} = \sum_{k=0}^{N-1} a_k^{(t)} \left. \frac{dT_k}{dx} \right|_{x=-1} = \sum_{k=0}^{N-1} a_k^{(t)} k U_{k-1}(-1).$$

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 $a_k^{(t)}$,

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

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

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

5.1 Enforcing Boundary Conditions

Von Neumann on the left

5.2 Implicit Euler

5.3 Implementation

The solver was implemented in C++.

5.4 Results

Chronoamperometry, DC Voltammetry, AC Voltammetry

6 Conclusion