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

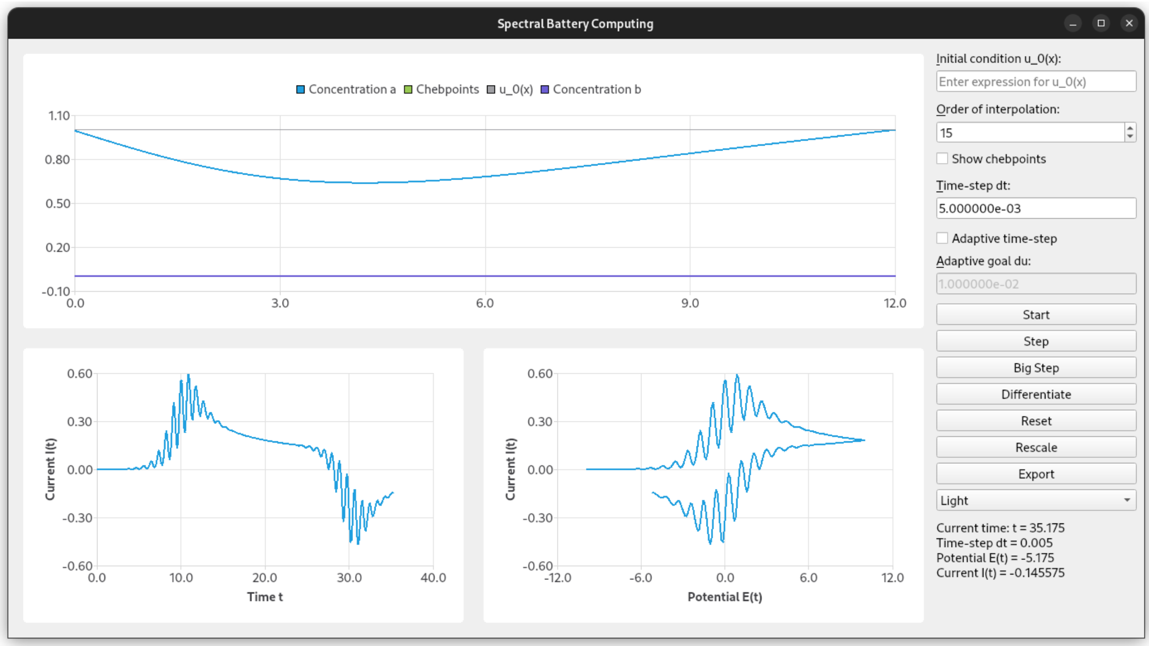

Figure 1: Graphical User Interface

Figure

Figure 2: Wohoo

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.

From the definition of Chebyshev polynomials $T_k(x) = \cos(k\theta)$, 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, which in turn are defined by

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

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

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

Using the Chebyshev series ansatz

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

we have that

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

so we are interested in

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

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 $a_k^{(t)}$,

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

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

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