Modeling with partial differential equations

Part 3

Icahn School of Medicine at Mount Sinai

SBCNY

Outline: Part 3

Practical issues in solving PDEs

Converting derivatives into discrete form

Explicit versus implicit solutions

The 1-D cable equation

$$C_m \frac{\partial V}{\partial t} = \frac{a}{2\rho_i} \frac{\partial^2 V}{\partial x^2} - I_{ion}$$

How would we actually solve this in practice?

Solving PDEs

$$C_m \frac{\partial V}{\partial t} = \frac{a}{2\rho_i} \frac{\partial^2 V}{\partial x^2} - I_{ion}$$

First step: **convert each derivative to discrete form**

$$\left.\frac{\partial V}{\partial t}\right|_j^t \approx \frac{V_j^{t+\Delta t} - V_j^t}{\Delta t}$$

$$\left.\frac{\partial^2 V}{\partial x^2}\right|_j \approx \frac{V_{j+1} - 2V_j + V_{j-1}}{\Delta x^2}$$

Next: **when do we evaluate the spatial derivative?**

Explicit versus Implicit Solutions

$$C_m \frac{\partial V}{\partial t} = \frac{a}{2\rho_i} \frac{\partial^2 V}{\partial x^2} - I_{ion}$$

Explicit solutions

Solve for each future value of V based on current values of variables

$$C_m \frac{V_j^{t+\Delta t} - V_j^t}{\Delta t} = \frac{a}{2\rho_i} \frac{V_{j+1}^t - 2V_j^t + V_{j-1}^t}{\Delta x^2} - I_{ion}^t$$

Implicit solutions

Solve for future values of V based on future values of variables

$$C_m \frac{V_j^{t+\Delta t} - V_j^t}{\Delta t} = \frac{a}{2\rho_i} \frac{V_{j+1}^{t+\Delta t} - 2V_j^{t+\Delta t} + V_{j-1}^{t+\Delta t}}{\Delta x^2} - I_{ion}^{t+\Delta t}$$

Explicit versus Implicit Solutions

Explicit solutions are simple to implement

Rearrange so that future is on LHS, present on RHS

$$V_j^{t+\Delta t} = V_j^t + \Delta t \frac{a}{2\rho_i C_m}\left[\frac{V_{j+1}^t - 2V_j^t + V_{j-1}^t}{\Delta x^2} - I_{ion}^t\right]$$

plus similar equations for $V_{j+1}^{t+\Delta t}$, $V_{j-1}^{t+\Delta t}$ **, etc.**

This just converts the PDE into large system of ODEs

Advantage: simple
Disadvantage: for stability $\Delta t \sim \Delta x^2$, must be very small

Explicit solutions of PDEs can take a very long time to run.

Explicit versus Implicit Solutions

Implicit solutions are conceptually more difficult

$$C_m \frac{V_j^{t+\Delta t} - V_j^t}{\Delta t} = \frac{a}{2\rho_i} \frac{V_{j+1}^{t+\Delta t} - 2V_j^{t+\Delta t} + V_{j-1}^{t+\Delta t}}{\Delta x^2} - I_{ion}^{t+\Delta t}$$

Computing $I_{ion}^{t+\Delta t}$ requires knowing $m^{t+\Delta t}$, $h^{t+\Delta t}$, $n^{t+\Delta t}$.

In practice, reaction treated explicitly, diffusion implicitly.

$$C_m \frac{V_j^{t+\Delta t} - V_j^t}{\Delta t} = \frac{a}{2\rho_i} \frac{V_{j+1}^{t+\Delta t} - 2V_j^{t+\Delta t} + V_{j-1}^{t+\Delta t}}{\Delta x^2} - I_{ion}^{t}$$

Even with this simplification, the equation still has 3 unknowns!

$$-\frac{a}{2\rho_i \Delta x^2} V_{j+1}^{t+\Delta t} + \left[\frac{a}{\rho_i \Delta x^2} + \frac{C_m}{\Delta t}\right] V_j^{t+\Delta t} - \frac{a}{2\rho_i \Delta x^2} V_{j-1}^{t+\Delta t} = \frac{C_m}{\Delta t} V_j^t - I_{ion}^t$$

Must solve for the three unknowns simultaneously.
This requires inverting a matrix.

Implicit Solution of HH Equations

$$\begin{bmatrix} \ddots & & \ddots & & & \\ \frac{-a}{2\rho_i \Delta x^2} & \left(\frac{a}{\rho_i \Delta x^2} + \frac{C_m}{\Delta t}\right) & \frac{-a}{2\rho_i \Delta x^2} & & \\ & \frac{-a}{2\rho_i \Delta x^2} & \left(\frac{a}{\rho_i \Delta x^2} + \frac{C_m}{\Delta t}\right) & \frac{-a}{2\rho_i \Delta x^2} & \\ & & \frac{-a}{2\rho_i \Delta x^2} & \left(\frac{a}{\rho_i \Delta x^2} + \frac{C_m}{\Delta t}\right) & \frac{-a}{2\rho_i \Delta x^2} \\ & & & \ddots & \ddots \end{bmatrix} \cdot \begin{bmatrix} \vdots \\ V_{j-1}^{t+\Delta t} \\ V_j^{t+\Delta t} \\ V_{j+1}^{t+\Delta t} \\ \vdots \end{bmatrix} = \frac{C_m}{\Delta t} \begin{bmatrix} \vdots \\ V_{j-1}^{t} \\ V_j^{t} \\ V_{j+1}^{t} \\ \vdots \end{bmatrix} - \begin{bmatrix} \vdots \\ I_{ion\,j-1}^{\;t} \\ I_{ion\,j}^{\;t} \\ I_{ion\,j+1}^{\;t} \\ \vdots \end{bmatrix}$$

This is a matrix equation Ax = b

x = A^{-1}b

Thus, implicit solutions involve inverting a matrix, which can be a complicated procedure

Summary

Solving PDEs, like solving ODEs, requires converting derivatives into discrete form.

If spatial derivatives are evaluated at the current time, this implies an ***explicit*** solution of the PDE; if these are evaluated at a future time, this implies an ***implicit*** solution of the PDE.

Explicit solutions are conceptually easy but can be slow to run; ***implicit*** solutions can be faster but more challenging to implement.