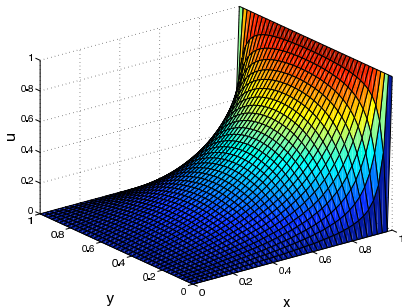


ODEs & PDEs in Mathematical Biology
& Numerical Methods to Solve Them

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PDEs in Math Biology

- ▶ Wave equation (*hyperbolic PDE*)
- ▶ Diffusion or heat equation (*parabolic PDE*)
- ▶ Laplace's & Poisson's equations (*elliptic PDEs*)
 - ▶ for electrostatic potential
- ▶ Cable equation (*parabolic diffusion PDE with source terms*)
 - ▶ models electrical impulses along axons & dendrites
 - ▶ *active cable is coupled to ODEs describing channel activation*
- ▶ Advection-diffusion equation (*parabolic PDE*)
 - ▶ models fluid transport of ions (coupled to Poisson's equation)
 - ▶ or of bacteria & nutrients, etc.

Derivatives & Notation

Second-order accurate central difference approx. to first derivative

$$\left(\frac{df}{dx}\right)_i \approx \frac{f_{i+1} - f_{i-1}}{2\Delta x}$$

Second-order accurate central difference approx. to second derivative

$$\left(\frac{d^2f}{dx^2}\right)_i \approx \frac{f_{i+1} - 2f_i + f_{i-1}}{\Delta x^2}$$

First-order accurate one-sided difference approx. to first derivative

$$\frac{du}{dt} \approx \frac{u_{n+1} - u_n}{\Delta t}$$

Taylor Series

To verify formulas, use Taylor series

$$f_{i\pm 1} = f(x_i \pm \Delta x) = f_i \pm \Delta x f'_i + \frac{\Delta x^2}{2!} f''_i \pm \frac{\Delta x^3}{3!} f'''_i + \dots$$

Then

$$\frac{f_{i+1} - f_{i-1}}{2\Delta x} = f'_i + \frac{\Delta x^2}{6} f'''_i + \dots$$

ODE (IVP) Methods on One Page!

For $du/dt = f(u)$: $du/dt \approx (u_{n+1} - u_n)/\Delta t = f(u)$

$$u_{n+1} = u_n + \Delta t f(u_n) \quad (\text{Forward Euler})$$

FE is explicit, stable if Δt is small, & first-order accurate.

$$u_{n+1} = u_n + \Delta t f(u_{n+1}) \quad (\text{Backward Euler})$$

BE is implicit, A-stable & L-stable, & first-order accurate.

$$u_{n+1} = u_n + \frac{\Delta t}{2} (f(u_n) + f(u_{n+1})) \quad (\text{TR})$$

TR is implicit, A-stable but not L-stable, & second-order accurate.

First-Order Wave (Advection) Equation

$$\frac{\partial u}{\partial t} + c \frac{\partial u}{\partial x} = 0, \quad u(x, t = 0) = u_0(x)$$

Solution is

$$u(x, t) = u_0(x - ct)$$

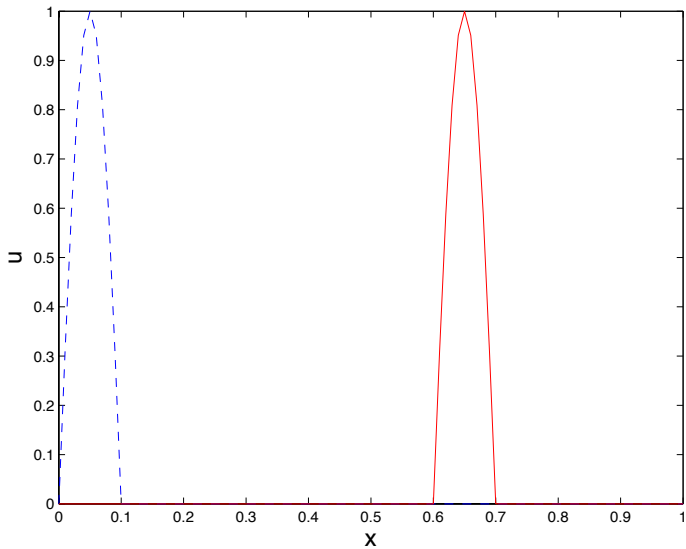
Numerical method: *upwind*

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = -c \frac{u_i^n - u_{i-1}^n}{\Delta x}$$

$$u_i^{n+1} = u_i^n - c \frac{\Delta t}{\Delta x} (u_i^n - u_{i-1}^n)$$

First-order accurate & stable for $\Delta t \leq \frac{\Delta x}{c}$ (CFL condition)

Wave Equation



Diffusion Equation

$$\frac{\partial u}{\partial t} = D \frac{\partial^2 u}{\partial x^2}, \quad u(x, t = 0) = u_0(x), \quad u(x = -1, t) = 0 = u(x = 1, t)$$

Numerical method: *backward Euler*

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = D \frac{u_{i+1}^{n+1} - 2u_i^{n+1} + u_{i-1}^{n+1}}{\Delta x^2}$$

$$u_i^{n+1} = u_i^n + D \frac{\Delta t}{\Delta x^2} \left(u_{i+1}^{n+1} - 2u_i^{n+1} + u_{i-1}^{n+1} \right)$$

L-stable & first-order accurate

In matrix form with $u = [u_2, u_3, \dots, u_N]^t$ & $u_1 = 0 = u_{N+1}$,

$$u^{n+1} = u^n + \frac{D\Delta t}{\Delta x^2} Au^{n+1}$$

$$\left(I - \frac{D\Delta t}{\Delta x^2} A \right) u^{n+1} = u^n$$

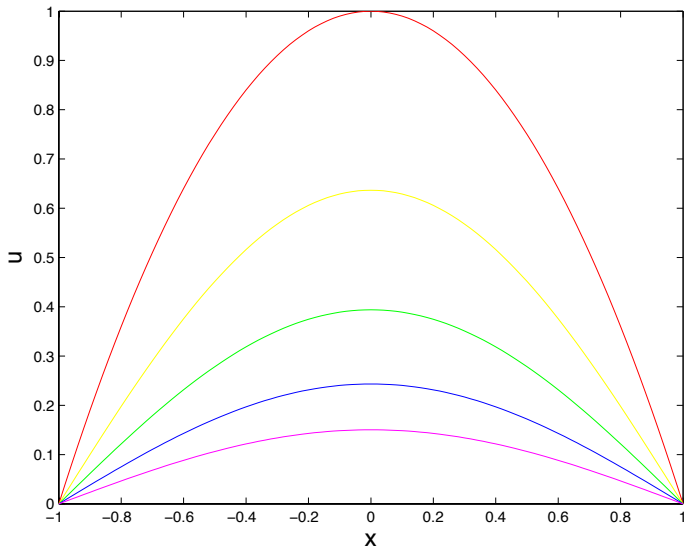
Diffusion Equation

$$\left(I - \frac{D\Delta t}{\Delta x^2} A \right) u^{n+1} = u^n$$

where (for $N = 10$)

$$A = \begin{bmatrix} -2 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & -2 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & -2 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & -2 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -2 \end{bmatrix}$$

Diffusion Equation



Poisson's Equation & Laplace's Equation

Poisson equation

$$\nabla^2 u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = -\rho(x, y)$$

Laplace equation

$$\nabla^2 u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0$$

Numerical method: *second-order accurate central differences & Gauss-Seidel iteration*

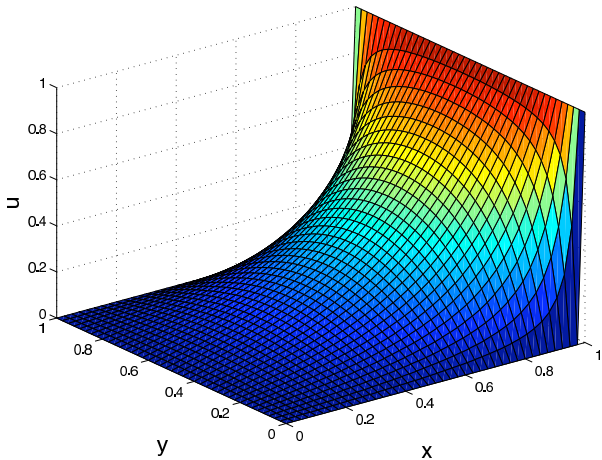
Define residual (set $\Delta x = \Delta y = h$)

$$r_{ij} = (u_{i+1,j} + u_{i-1,j} + u_{i,j+1} + u_{i,j-1} - 4u_{ij}) / h^2 \rightarrow 0$$

Jacobi iteration

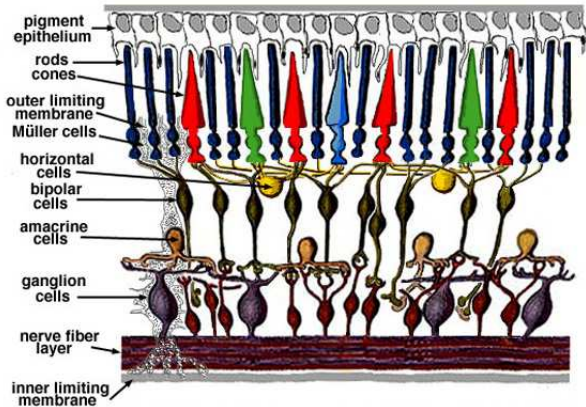
$$u_{ij}^{(k+1)} = \frac{1}{4} \left(u_{i+1,j}^{(k)} + u_{i-1,j}^{(k)} + u_{i,j+1}^{(k)} + u_{i,j-1}^{(k)} \right) = u_{ij}^{(k)} + \frac{h^2}{4} r_{ij}^{(k)}$$

Laplace's Equation



Reaction-Diffusion Modeling and the Retina

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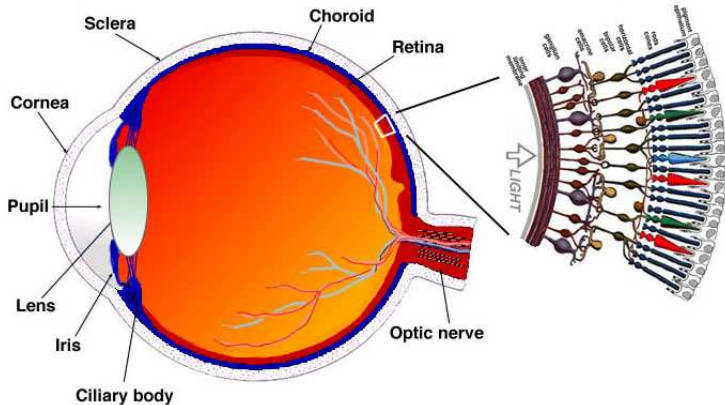


Fig. 1.1. A drawing of a section through the human eye with a schematic enlargement of the retina.

<http://webvision.med.utah.edu/>

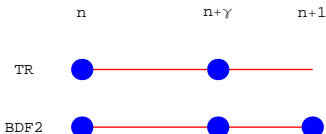
I. TRBDF2 Numerical Method

$$\frac{du}{dt} = f(u, t), \quad \gamma = 2 - \sqrt{2}$$

$$u^{n+\gamma} - \gamma \frac{\Delta t_n}{2} f^{n+\gamma} = u^n + \gamma \frac{\Delta t_n}{2} f^n \quad (\mathbf{TR})$$

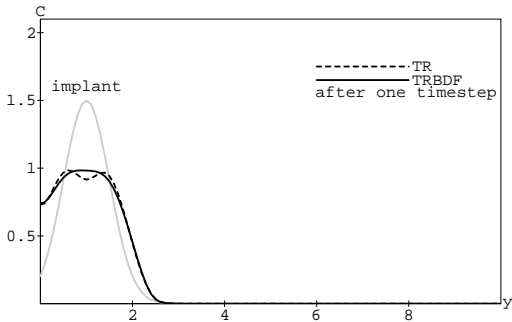
$$u^{n+1} - \frac{1-\gamma}{2-\gamma} \Delta t_n f^{n+1} = \frac{1}{\gamma(2-\gamma)} u^{n+\gamma} - \frac{(1-\gamma)^2}{\gamma(2-\gamma)} u^n \quad (\mathbf{BDF2})$$

Use Newton's method if $f(u)$ is nonlinear



Advantages of TRBDF2

- ▶ One-step (composite) method
- ▶ Second-order accurate & L-stable
- ▶ Easy to adjust Δt dynamically



II. Continuum Model for a 2D Horizontal Cell Sheet

$$\tau_m \frac{\partial V_c}{\partial t} = -(V_c - V_{Lc}) - (V_c - V_{Cl}) G_{Cl} R_m + I_{app} R_m$$

$$\tau_m \frac{\partial V_h}{\partial t} = \lambda^2 \left(\frac{\partial^2 V_h}{\partial x^2} + \frac{\partial^2 V_h}{\partial y^2} \right) - (V_h - V_{Lh}) + \bar{n} R_S \frac{(U_h - V_h)}{R_{ss}} + I_{ext} R_m$$

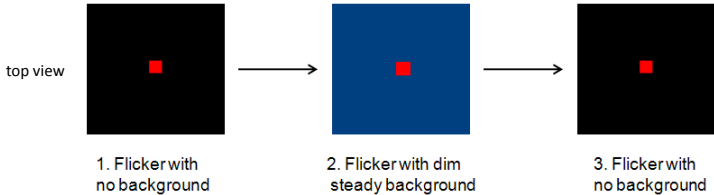
$$\tau_m \frac{\partial U_h}{\partial t} = -(U_h - V_{Lh}) - \frac{R_m}{A_{sh}} \frac{(U_h - V_h)}{R_{ss}} - k_6 R_m [GL] U_h$$

$$\tau_2 \frac{\partial [S]}{\partial t} = k_2 \left(U_h - \frac{58 \ln([S]/[S_I])}{n_i \ln 10} \right)$$

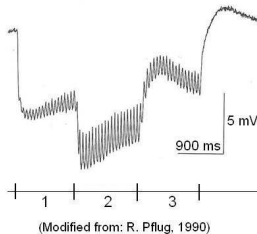
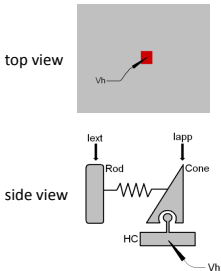
$$\tau_0 \frac{\partial [Ca]}{\partial t} = \frac{A}{2} \left(\frac{1 + \tanh(a(V_c - \alpha U_h + 20))}{k_{Oca}[S] + 1} \right) - [Ca]$$

$$\tau_5 \frac{\partial [GL]}{\partial t} = k_4 [Ca] - k_5 [GL] (E_{Na} - U_h)$$

1-2. Introduction: the Background-induced Flicker Enhancement (BIFE) Effect



➤ The red small-spot flicker is cone-selective, while the dim blue steady background is rod-selective.



➤ The increase in the amplitude of flicker response observed during the background illumination is the enhancement effect.

➤ Additional characteristics: sag, post-inhibitory rebound (PIR), and phase advance.

➤ Percent Enhancement E is defined as: $E = 100[(F_{\text{bkgd}}/F_{\text{dark}})-1]$

2D model, 16 Hz, percent enhancement E = 92.1%

