Solutions and Behavior of Lattice Differential Equations

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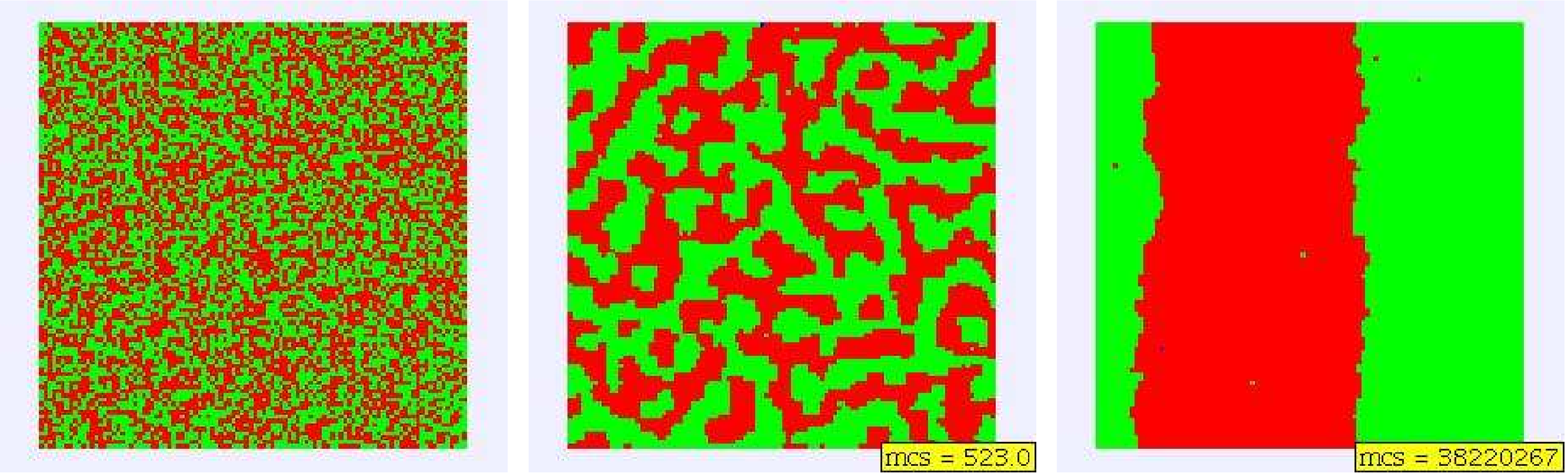
Numerical reproduction of spinodal decomposition

Erik Van Vleck & Tony Humphries

Spinodal Decomposition



(a) (b) (c)

(a) Initial condition: well-mixed metals form a molten alloy

(b) Short time: phase separation, characteristic length scale

(c) Long time: metals are separated, decomposition is complete

Special thanks to David Landy and Linli Wang for the images which were posted on http://www.personal.psu.edu/dal233/project3.html

Cahn-Hilliard Equation

$$u_t = -\Delta(\epsilon^2 \Delta u + f(u)), \qquad f(u) = u - u^3$$

$u \in [-1, 1]$ represents concentrations of one metallic component.

$f'(m) > 0 \Rightarrow m \in (-1/\sqrt{3}, 1/\sqrt{3})$ and m is unstable.

Almost all orbits starting close to m exit a neighborhood of that point close to a strongly unstable invariant subspace.

These orbits

- behave similarly to orbits of $\quad v_t = -\Delta(\epsilon^2 \Delta v + f'(m)v)$
- exhibit characteristic pattern formation

Lattice Differential Equations

$$\frac{d^2u}{dx^2} \approx \frac{u(x+h) - 2u(x) + u(x-h)}{h^2}$$

$$\frac{d^2u}{dx^2} \approx \frac{1}{h^2} \begin{bmatrix} \ddots & \ddots & \ddots & & & & \\ & 1 & -2 & 1 & & & \\ & & 1 & -2 & 1 & & \\ & & & 1 & -2 & 1 & \\ & & & & \ddots & \ddots & \ddots \end{bmatrix} \begin{bmatrix} \vdots \\ u_{-1} \\ u_0 \\ u_1 \\ \vdots \end{bmatrix}$$

We call this matrix Δ_h.

It is an approximation of the Laplacian operator $\Delta = \frac{d^2}{dx^2}$.

Linear Analysis

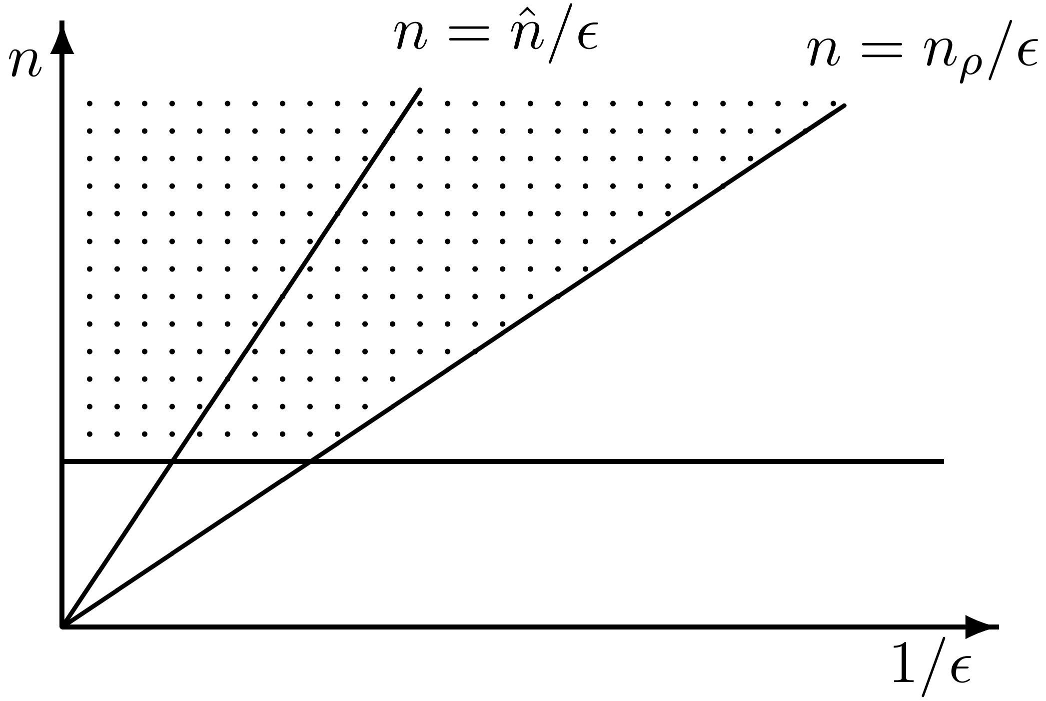
Define $A_\epsilon = -\Delta(\epsilon^2\Delta + f'(m))$

$\kappa_j = j^2\pi^2$ are eigenvalues of $-\Delta,$ μ_j are eigenvalues of $-\Delta_h$

So, eigenvalues of A_ϵ are $\lambda_j = \kappa_j(f'(m) - \epsilon^2\kappa_j)$ which are positive when $0 < \kappa_j < f'(m)/\epsilon^2$

For $0 < \rho \ll 1$, and $\mu_j < (2f'(m))/\epsilon^2$ for some $j \in [0, \ldots, n]$ there exists a $n_\rho > 0$ such that for all $n \geq n_\rho/\epsilon$

$$|\frac{\mu_j}{\kappa_j} - 1| < \rho \qquad \text{for} \qquad |\mu_j - \kappa_j| < \frac{3f'(m)\rho}{\epsilon^2}$$



Spinodal decomposition occurs in the shaded region.

Numerical reproduction of conservation laws

Sebastian Reich

Hamiltonian Partial Differential Equations

According to Bridges (1997), these equations can be written

$$\mathbf{K}z_t + \mathbf{L}z_x = \nabla_z S(z)$$

- $\mathbf{K}$ and $\mathbf{L}$ are skew-symmetric matrices
- $z = z(x, t)$ is the vector of state variables
- S is smooth

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Energy and momentum conservation laws are derived directly from this equation

Conservation Laws

$$\mathbf{K} z_t + \mathbf{L} z_x = \nabla_z S(z)$$

- Take the inner product of the equation with z_t to get the Energy Conservation law

$$E_t + F_x = 0$$

for $E = S(z) + (z_x^T \mathbf{L} z)/2$ and $F = (z^T \mathbf{L} z_t)/2$

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- Take the inner product of the equation with z_x to get the Momentum Conservation Law

$$G_x + I_t = 0$$

for $G = S(z) + (z_t^T \mathbf{K} z)/2$ and $I = (z^T \mathbf{K} z_x)/2$

Spatial Discretizations

- Implicit midpoint scheme in space gives

$$\mathbf{K}z_t^{n+1/2} + \mathbf{L}\frac{z^{n+1} - z^n}{h} = \nabla S(z^{n+1/2})$$

with

$$z^{n+1/2} = \frac{1}{2}\left(z^{n+1} + z^n\right)$$

- Symplectic Euler in space gives

$$\mathbf{K}z_t^n + \mathbf{L}_+\frac{z^{n+1} - z^n}{h} + \mathbf{L}_-\frac{z^n - z^{n-1}}{h} = \nabla S(z^n)$$

with

$$\mathbf{L} = \mathbf{L}_+ + \mathbf{L}_-, \qquad \mathbf{L}_+^T = -\mathbf{L}_-$$

Energy Conservation

Energy conservation laws satisfied exactly by lattice equations

- Implicit Midpoint $E_t^{n+1/2} + \frac{F^{n+1}-F^n}{h} = 0$ for

$$E^{n+1/2} = S(z^{n+1/2}) - \frac{1}{2}\left(\frac{z^{n+1}-z^n}{h}\right)^T \mathbf{L} z^{n+1/2}$$

$$F^n = \frac{1}{2}(z^n)^T \mathbf{L} z_t^n$$

- Symplectic Euler $E_t^n + \frac{F^{n+1}-F^n}{h} = 0$ for

$$E^n = S(z^n) - \left(\frac{z^n - z^{n-1}}{h}\right)^T \mathbf{L}_+ z^n \qquad F^n = (z^n)^T \mathbf{L}_- z_t^{n-1}$$

Modified Equations Represent the Lattice Equation

Taylor series implies

$$\frac{z(x_{n+1}) - z(x_n)}{h} = z_x\left(x_{n+1/2}\right) + \frac{h^2}{2^2 2!} z_{xxx}\left(x_{n+1/2}\right) + \dots$$

along with similar expansions gives the modified equation

$$\mathbf{K} z_t + \mathbf{L}\left(z_x - \frac{h^2}{3 \cdot 2^2} z_{xxx} + \dots\right) = \nabla_z S(z),$$

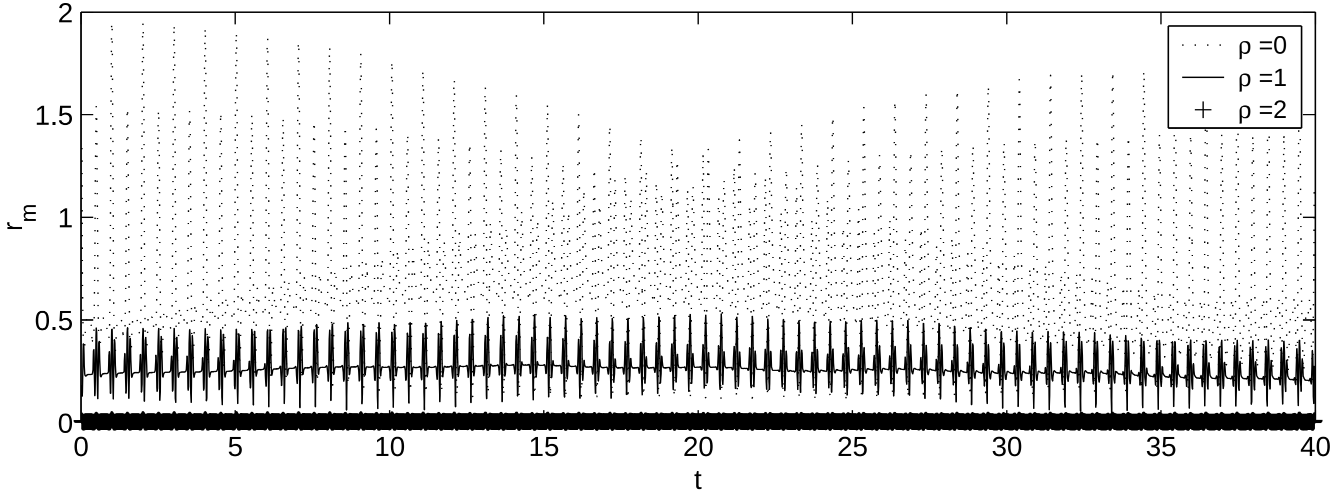
which can be rewritten

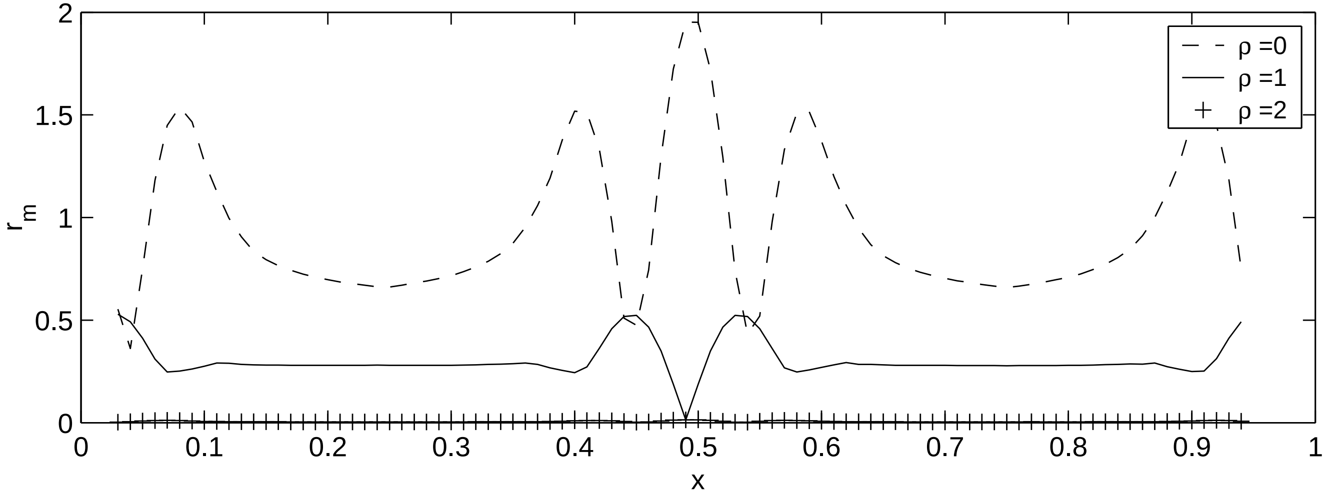
$$\tilde{\mathbf{K}} \tilde{z}_t + \tilde{\mathbf{L}} \tilde{z}_x = \nabla_{\tilde{z}} \tilde{S}(\tilde{z}).$$

This equation satisfies a momentum conservation law.

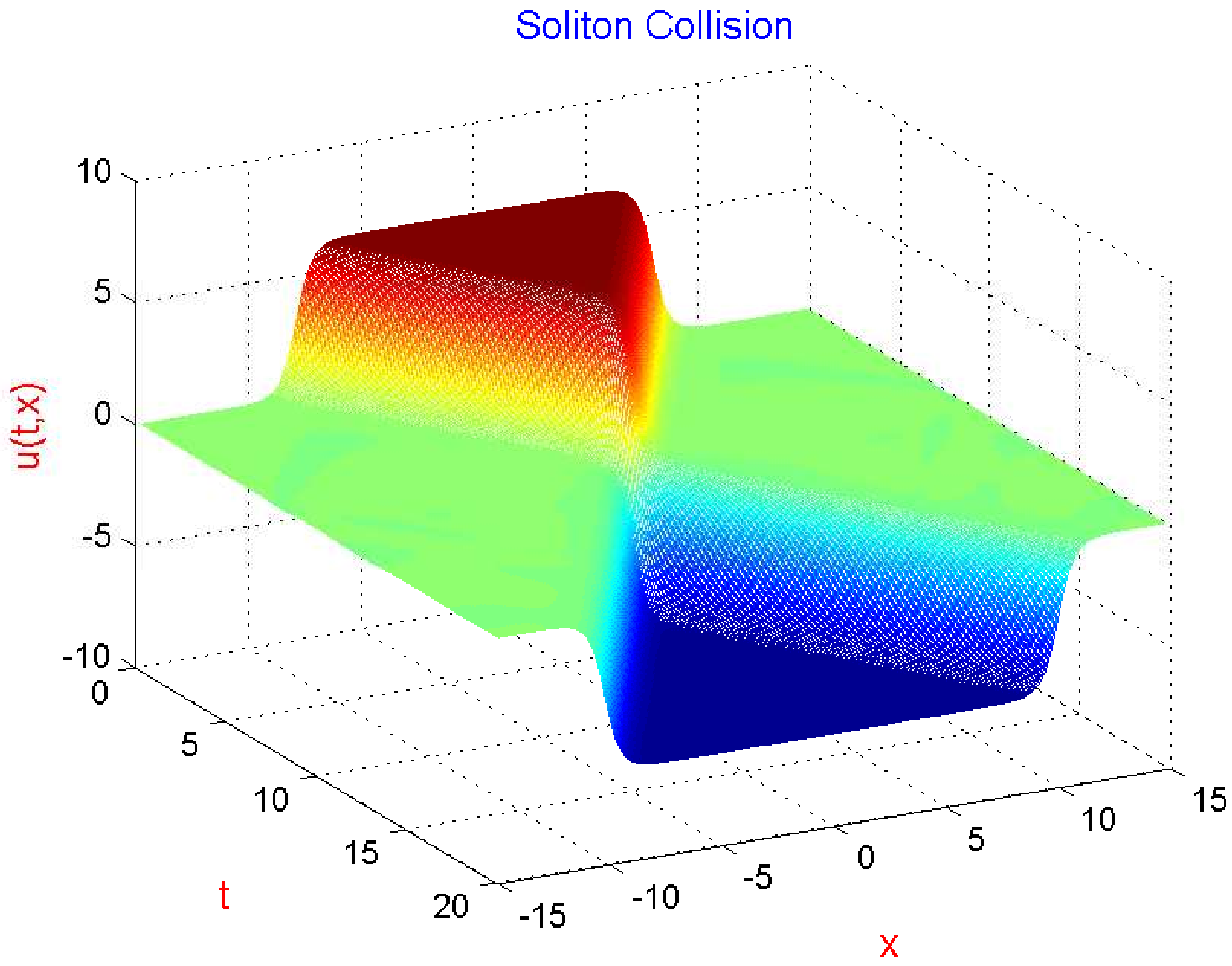
Residual in Momentum Conservation Law

$h = \Delta t = 0.01$

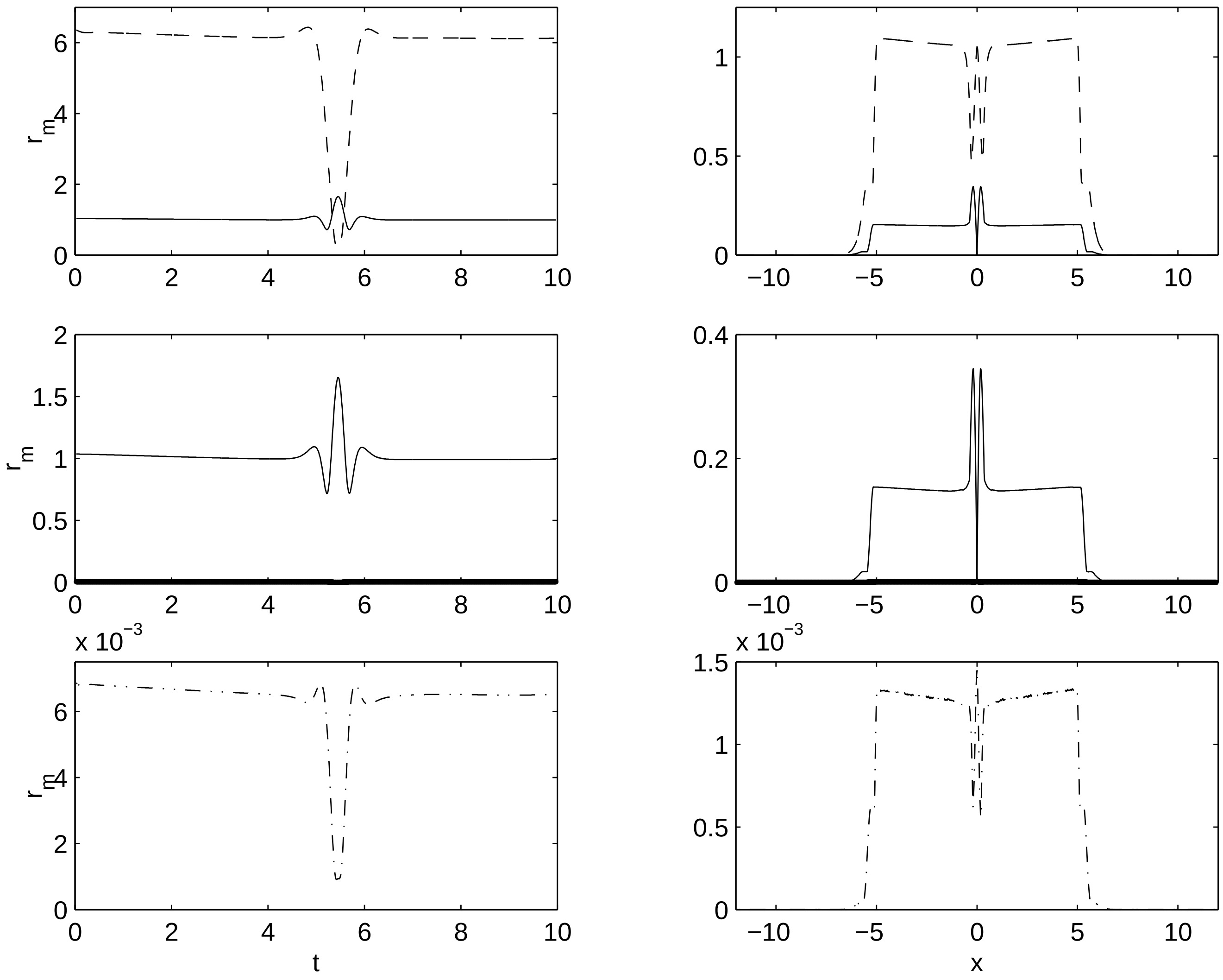




A Soliton Collision



Residual in Momentum Conservation Law for a soliton collision, $h = 0.02$, $\Delta t = 0.01$

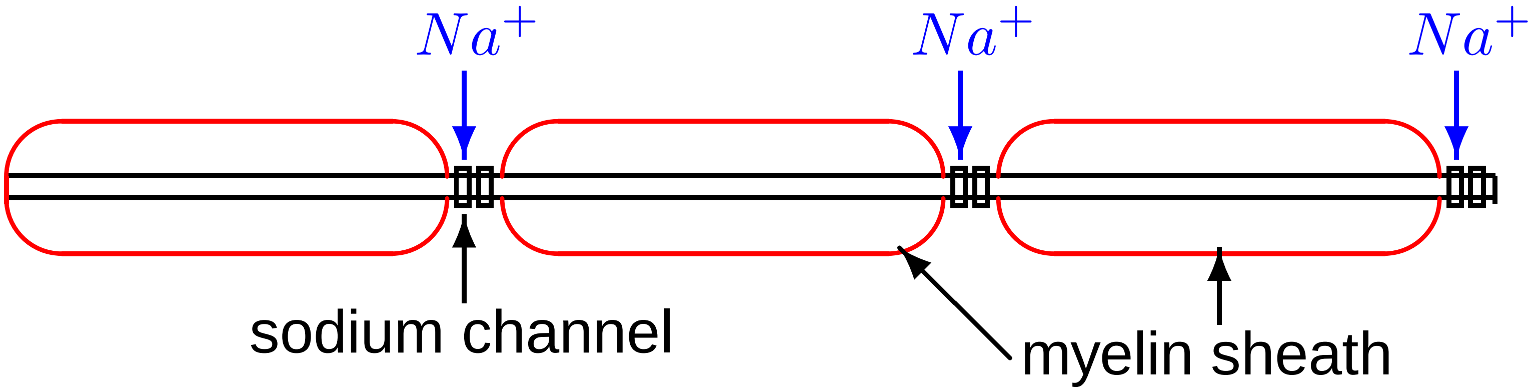


3.

Derivation of exact solutions for an LDE

Tony Humphries & Erik Van Vleck

Our Nervous System



The nervous cells live inside the “Hot Dog Buns” which are called myelin sheath.

The inrush of sodium (Na^+) at the sodium channels causes the electric impulse to jump to the next cell.

Multiple Sclerosis causes the destruction of myelin, which helps carry electrical signals.

Bistable Equation with Inhomogeneous Diffusion

$$\dot{u}_j = \alpha_j(u_{j+1} - u_j) - \alpha_{j-1}(u_j - u_{j-1}) - f(u_j)$$

with

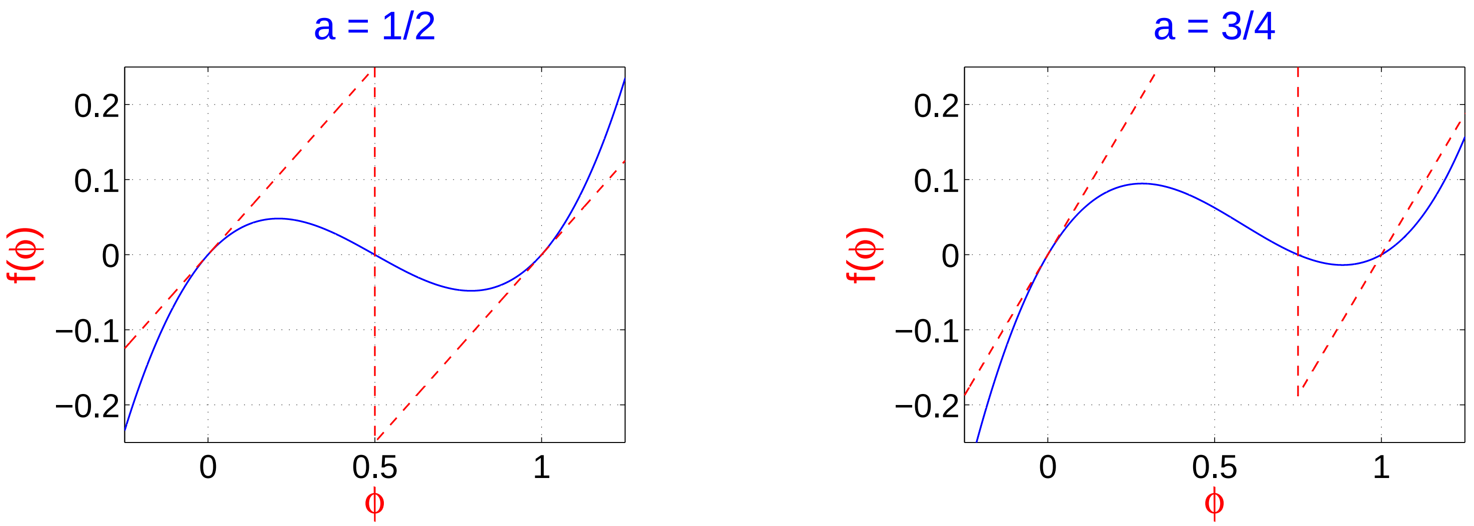
$$\alpha_j = \begin{cases} \alpha_j & -m \leq j \leq n \\ \alpha & j < -m \text{ or } j > n \end{cases}$$

$m, n \in \{0\} \cup \mathbb{N}$

The nonlinearity is the derivative of a double-well potential,

typically $f(u) = u(u-a)(u-1)$ with $a \in (0,1)$.

McKean’s Caricature of the Cubic



Solid blue line: $f(u) = u(u-a)(u-1)$

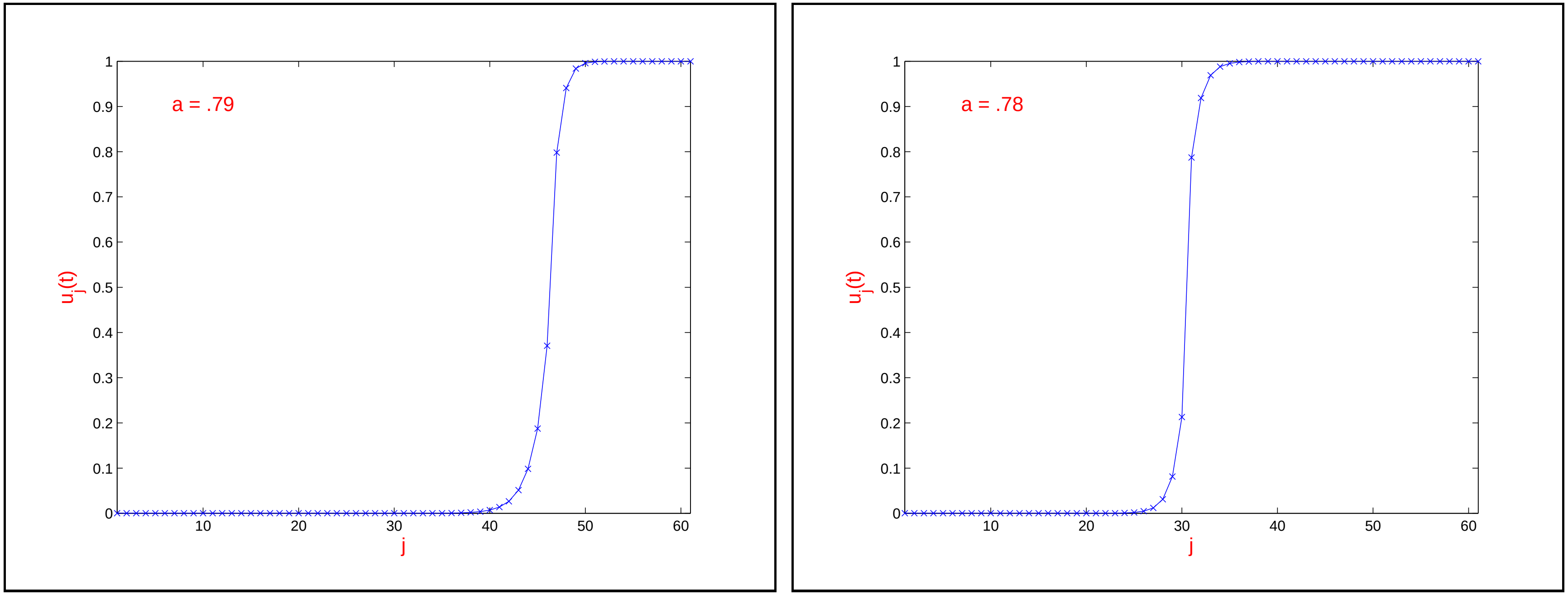
Dashed red line:

$$f(u) = u - h(u-a) \qquad\qquad h(x) = \begin{cases} 1 & x > 0 \\ [0,1] & x = 0 \\ 0 & x < 0 \end{cases}$$

Numerical Simulations
for the Evolution Equation

For the case of a single defect

$$\alpha_j = \begin{cases} 0.6 & j = 30 \\ 1 & j \neq 30 \end{cases}$$



A slightly slower wave is stopped by the defect.

Steady State Solutions

Definition: The range of a values that yield standing waves is called the *interval of propagation failure*.

Standing waves are solutions of $\dot{u}_j = 0$ or equivalently

$$\alpha_j(u_{j+1} - u_j) - \alpha_{j-1}(u_j - u_{j-1}) = f(u_j)$$

$$\lim_{j\to\infty} u_j = 1 \qquad \lim_{j\to-\infty} u_j = 0$$

where $f(u_j) = u_j - h(u_j - a)$.

Note: Solutions are not translationally invariant.

Families of Standing Waves

Define $\xi^* \in \mathbb{R}$ a parameter that determines the position of the wave relative to the defect region.

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We seek solutions that satisfy

$$u_j < a \quad \text{for} \quad j < \xi^* \qquad \text{and} \qquad u_j > a \quad \text{for} \quad j > \xi^*.$$

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We seek solutions that satisfy

$$u_j < a \quad \text{for} \quad j < \xi^* \qquad \text{and} \qquad u_j > a \quad \text{for} \quad j > \xi^*.$$

$$\Longrightarrow \qquad f(u_j) = u_j - h(u_j - a) = u_j - h(j - \xi^*)$$

Derivation of Solutions

We use Jacobi operator theory (Teschl 2000) to solve the difference equation

$$\alpha_j(u_{j+1} - u_j) - \alpha_{j-1}(u_j - u_{j-1}) - u_j = -h_j$$

for

$$h_j = \begin{cases} \text{1} & j > j^* \\ h_{j^*} & j = j^* \\ \text{0} & j < j^* \end{cases}$$

where

$$h_{j^*} = \begin{cases} \text{[0,1]} & \xi^* = j^* \\ \text{0} & j^* < \xi^* < j^* + 1 \end{cases}$$

Standing Wave Solutions

General Solution = Homogeneous Solution + Particular Solution

$$u_j = u_{j^*}\rho_j + u_{j^*+1}\sigma_j + \begin{cases} -\sum_{k=j^*+1}^{j} \frac{h_k}{\alpha_k}\sigma_{j-k} & j > j^* \\ 0 & j = j^* \\ \frac{h_{j^*}}{\alpha_{j^*}}\sigma_{j-j^*} & j < j^* \end{cases}$$

ρ_j and σ_j are fundamental solutions and may be constructed recursively using

$$\alpha_j(u_{j+1} - u_j) - \alpha_{j-1}(u_j - u_{j-1}) - u_j = 0$$

with

$$\rho_{j^*} = 1, \quad \rho_{j^*+1} = 0, \quad \sigma_{j^*} = 0, \quad \sigma_{j^*+1} = 1.$$

The particular solution can be found in Teschl (2000).

Interval of Propagation Failure

Theorem (Humphries, Moore, Van Vleck 2010)

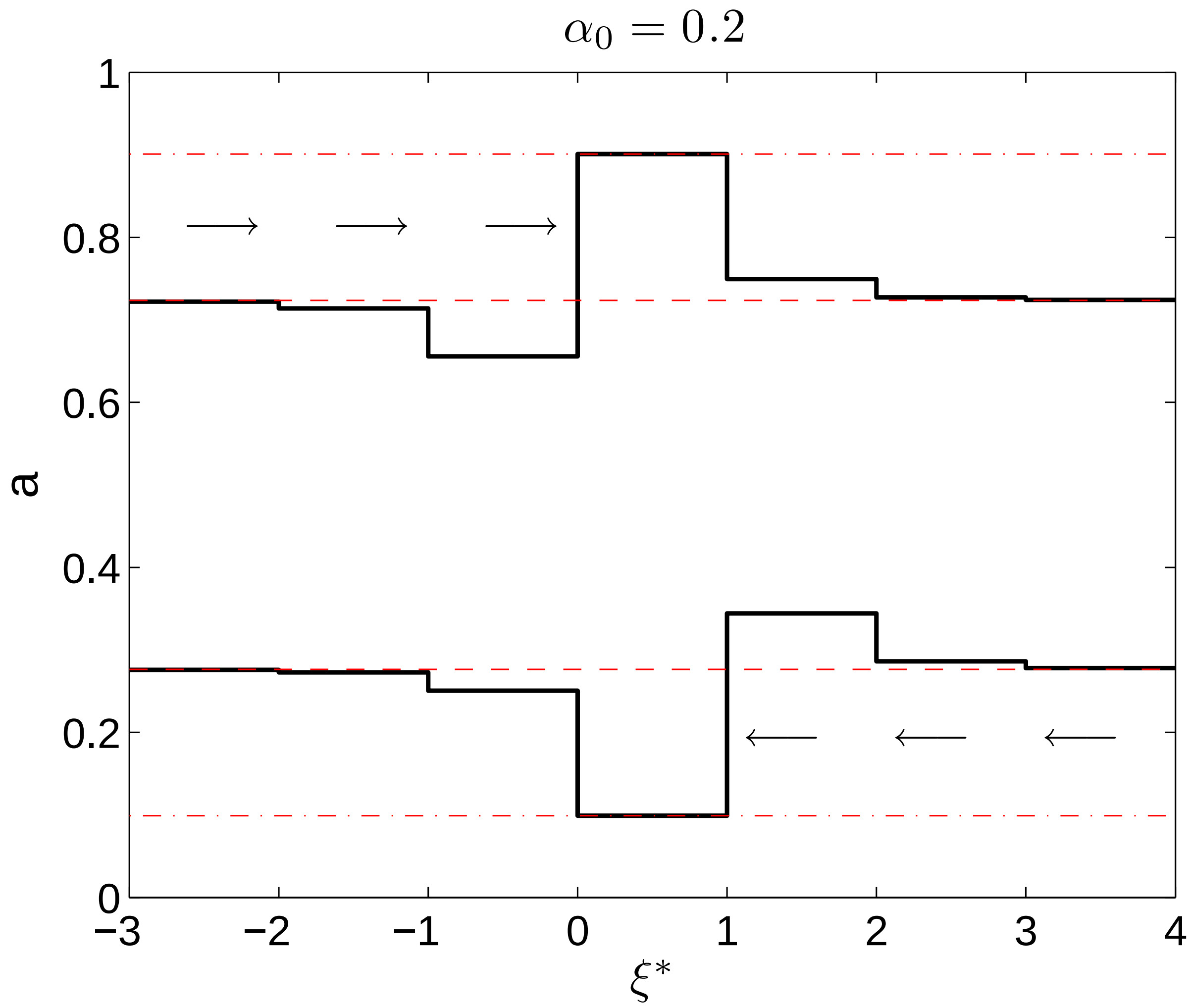
If a yields a traveling wave for $\alpha_0 = \alpha$, then

- Either $a \in (0, 1/(\lambda+2))$ or $a \in ((\lambda+1)/(\lambda+2), 1)$ with $\lambda = (1+\sqrt{1+4\alpha})/2\alpha$
- There are no corresponding standing waves for $\alpha_0 < \alpha$ and $\xi^* \notin (0,1)$, nor for $\alpha_0 > \alpha$ and $\xi^* \in (0,1)$.
- There exist standing waves for $\alpha_0 < \alpha$ and $\xi^* \in (0,1)$, and for $\alpha_0 > \alpha$ and $\xi^* \notin (0,1)$, provided

$$a \in \left[\frac{\alpha_0/\alpha}{\lambda + 2(\alpha_0/\alpha)}, \frac{\lambda + \alpha_0/\alpha}{\lambda + 2(\alpha_0/\alpha)}\right].$$

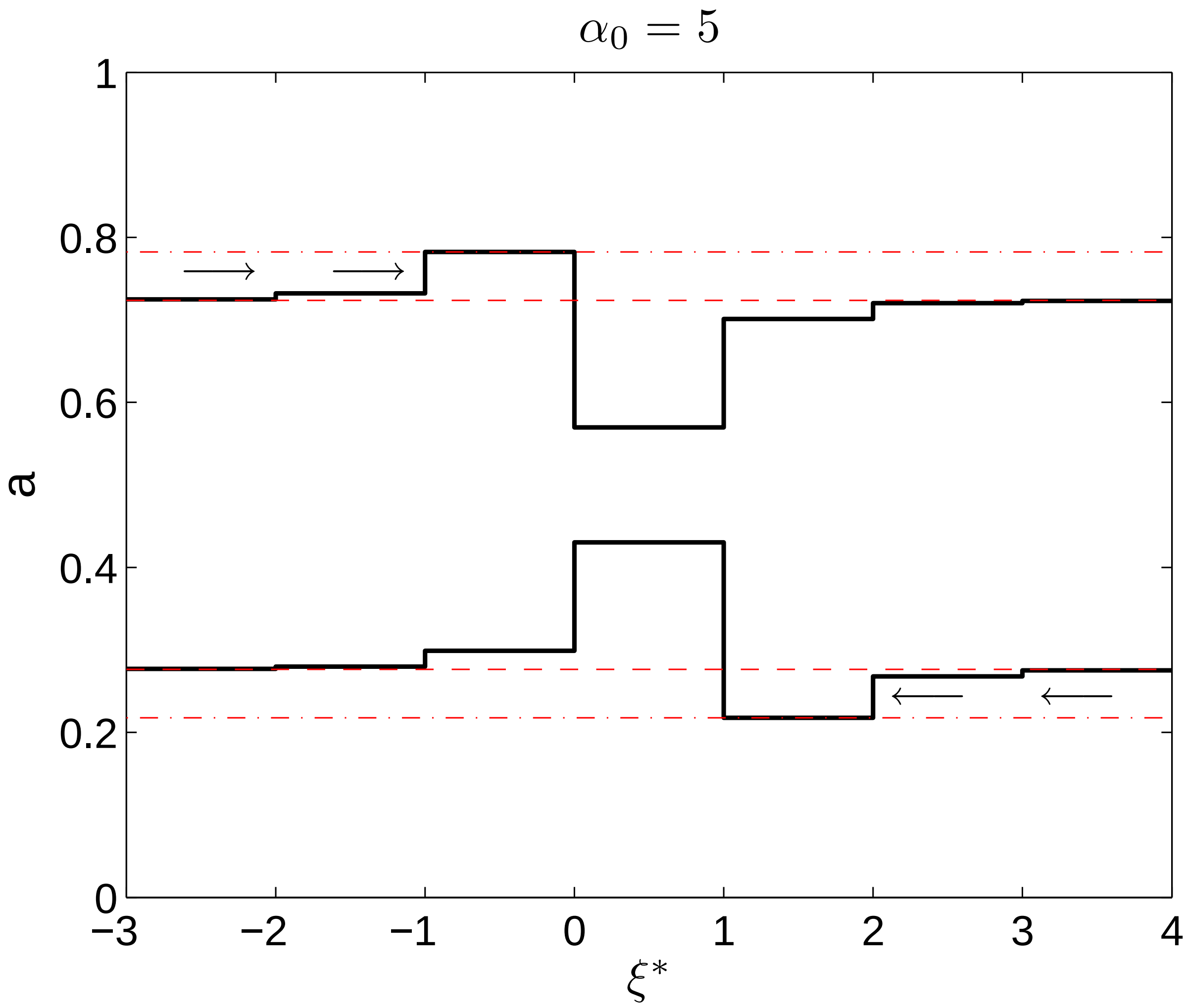
Interval of Propagation Failure

$\alpha = 1$



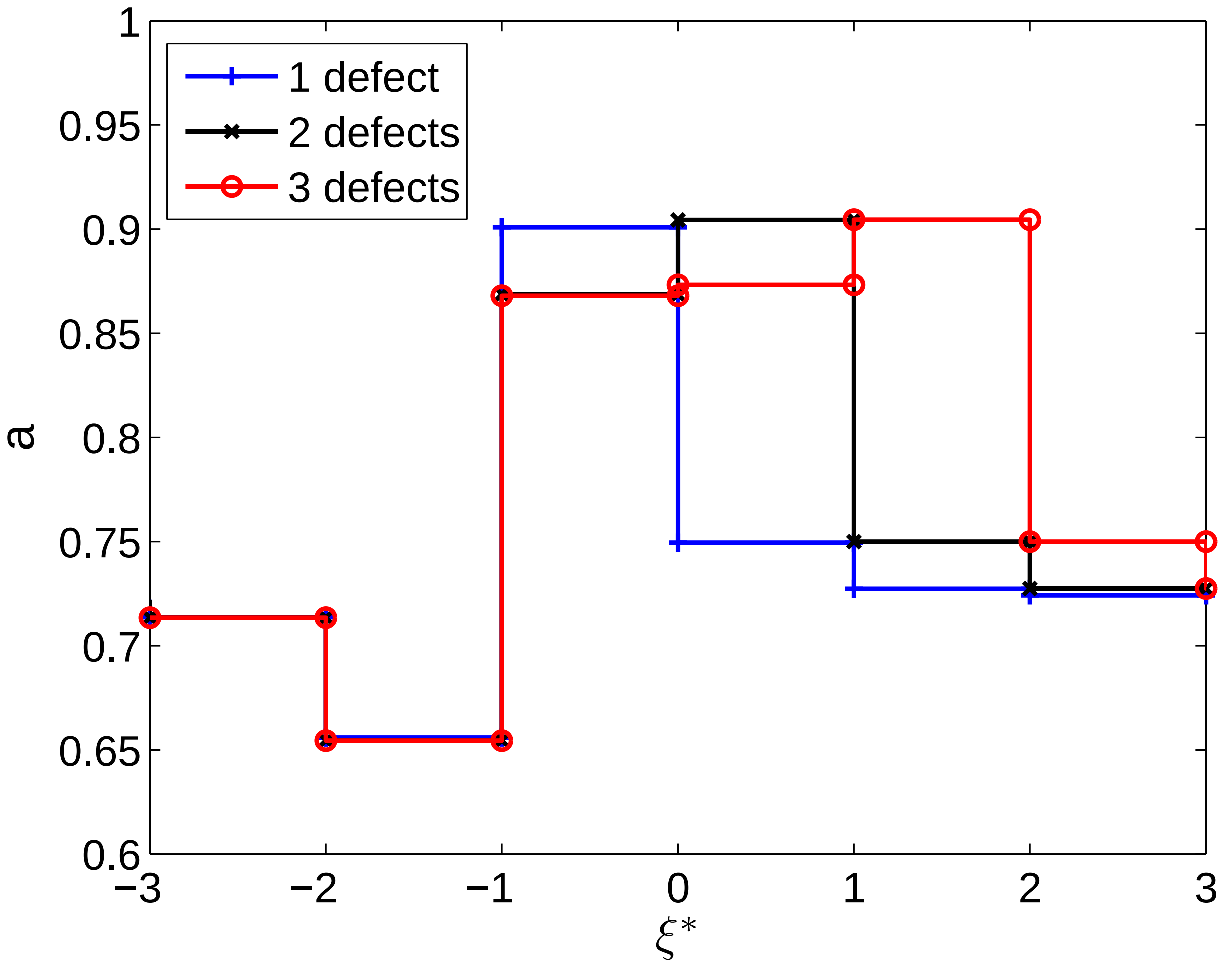
Interval of Propagation Failure

$\alpha = 1$



Interval of Propagation Failure

$\alpha = 1, \alpha_{defect} = 0.2$



Non-zero Wave Speed Solutions

We make a ‘traveling wave’ ansatz

$$u_j(t) = \varphi(\xi_j; \xi^*) \qquad \xi_j = \begin{cases} j - c_j(t), & j \in R \\ j - ct, & j \notin R \end{cases}$$

and define

$$\begin{aligned} R &= \{j \in \mathbb{Z} : c_j(t) \neq ct\}, \\ S &= \overline{R} = \{j \in \mathbb{Z} : j \in R, j+1 \in R, \ or \ j-1 \in R\}, \\ T &= \{j \in \mathbb{Z} : \alpha_j \neq \alpha\}. \end{aligned}$$

$$\begin{aligned} -c_j'\varphi'(\xi_j) &= \alpha_j(\varphi(\xi_{j+1}) - \varphi(\xi_j)) + \alpha_{j-1}(\varphi(\xi_{j-1}) - \varphi(\xi_j)) \\ &\quad -\varphi(\xi_j) + h(\xi_j - \xi^*) \end{aligned}$$

Non-Zero Wave Speed Solution: Part 1

$$\varphi(\xi;\xi^*) = \psi(\xi;\xi^*) + \chi(\xi;\xi^*),$$

where

$$\psi(\xi;\xi^*) = \frac{1}{2}+\frac{1}{\pi}\int_0^\infty \frac{A(s)\sin(s(\xi-\xi^*))}{s\left(A(s)^2+c^2s^2\right)}ds+\frac{c}{\pi}\int_0^\infty \frac{\cos(s(\xi-\xi^*))}{A(s)^2+c^2s^2}ds$$

for

$$A(s) = 1 + 2\alpha(1-\cos(s)),$$

ψ is the solution to the equation with $\alpha_j = \alpha,\ \forall\, j \in \mathbb{Z}$.

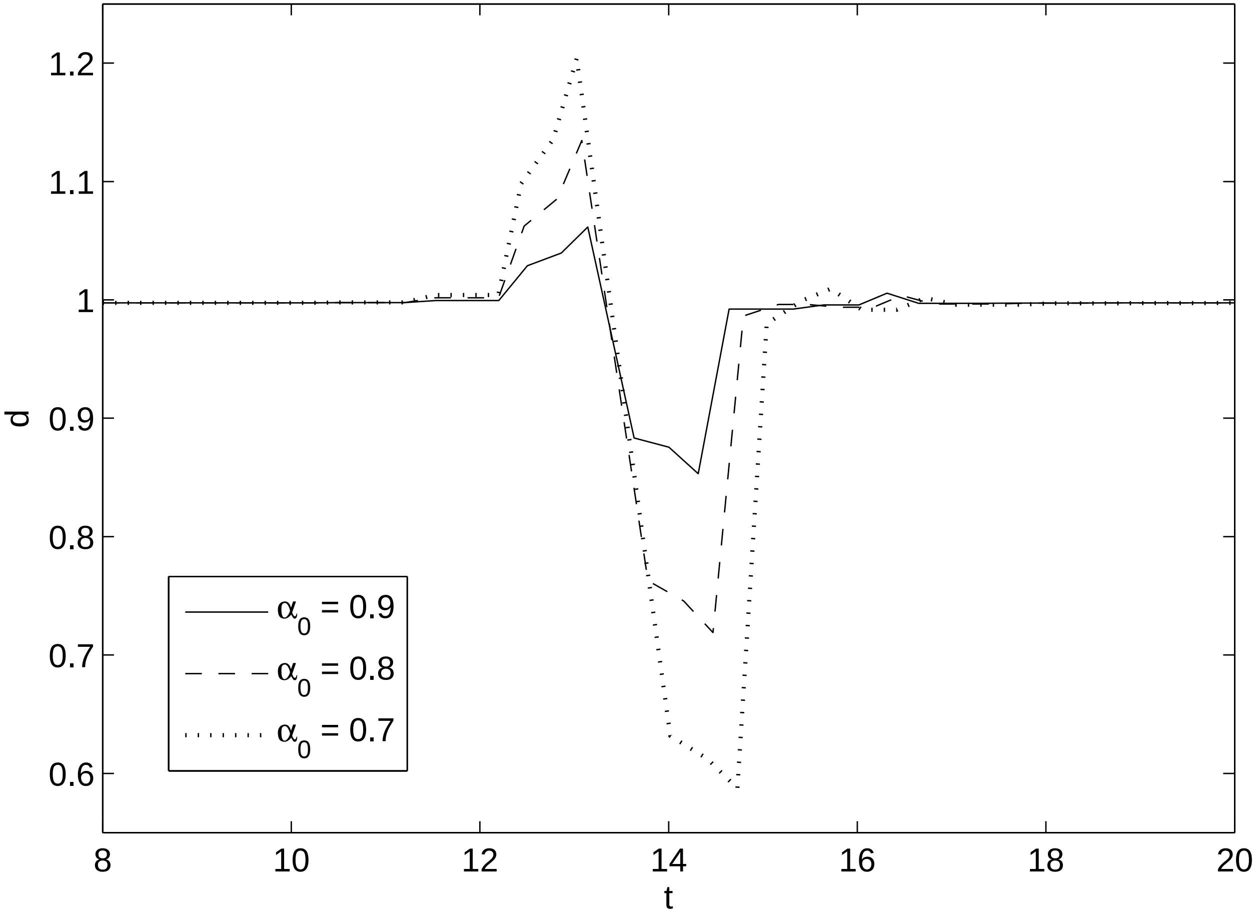
Non-Zero Wave Speed Solution: Part 2

$$\begin{aligned}\chi(\xi;\xi^*) &= \sum_{j\in R} b_j F_j(\xi) B_j(\xi^*) + \alpha \sum_{j\in S} F_j(\xi) C_j(\xi^*) \\ &\quad + \sum_{j\in T} \gamma_j \left(F_j(\xi) - F_{j+1}(\xi)\right) D_j(\xi^*)\end{aligned}$$

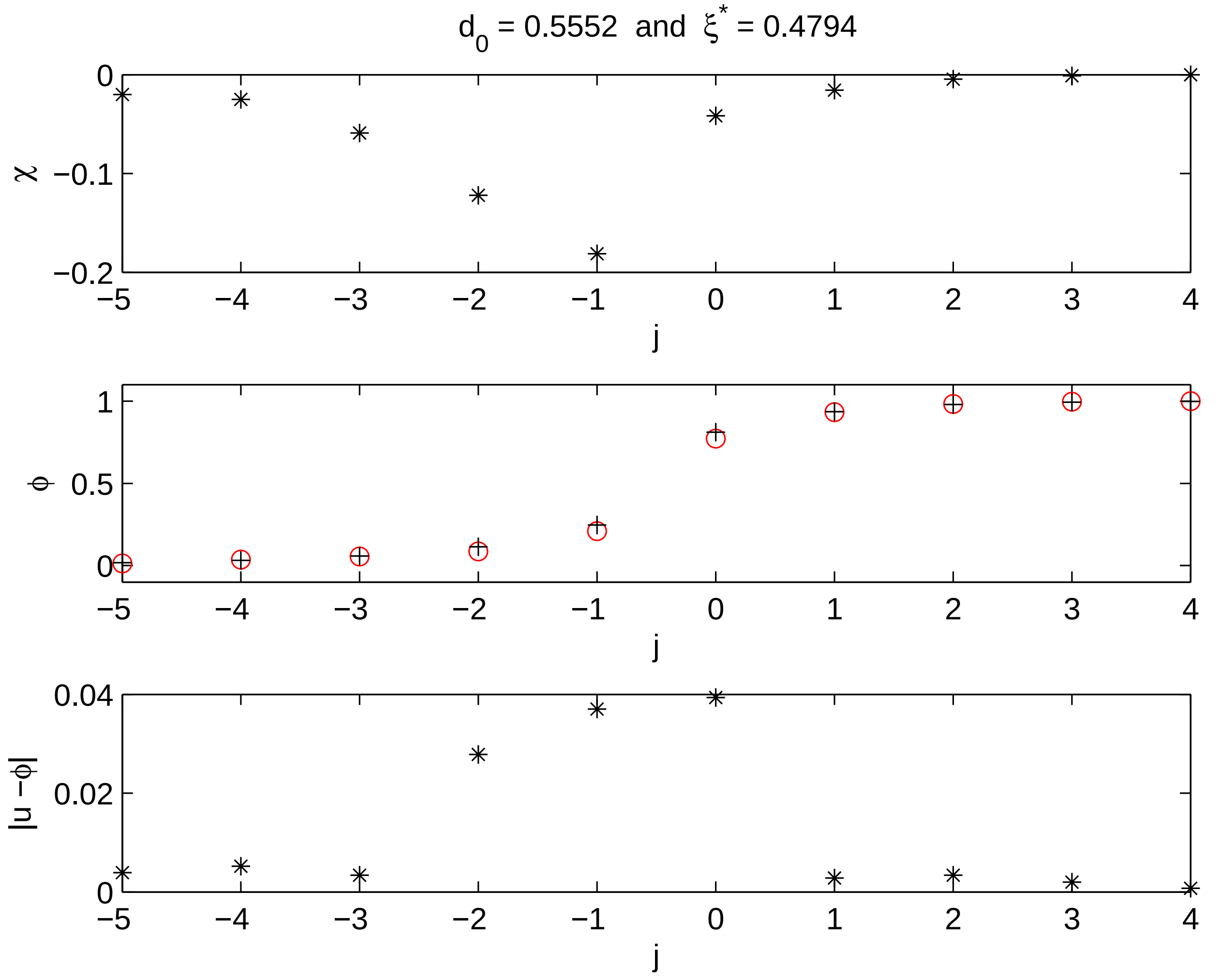
$$F_j(\xi) = \frac{1}{\pi}\int_0^\infty \frac{A(s)\cos(s(\xi-\xi_j)) - cs\sin(s(\xi-\xi_j))}{A(s)^2 + c^2 s^2} ds.$$

$$\begin{aligned}B_j(\xi^*) &= \alpha_j \left(\varphi(\xi_{j+1};\xi^*) - \varphi(\xi_j;\xi^*)\right) + \alpha_{j-1}\left(\varphi(\xi_{j-1};\xi^*) - \varphi(\xi_j;\xi^*)\right) \\ &\quad -\varphi(\xi_j;\xi^*) + h(\xi_j - \xi^*). \\ C_j(\xi^*) &= \varphi(\xi_{j+1};\xi^*) - \varphi(\xi_j+1;\xi^*) + \varphi(\xi_{j-1};\xi^*) - \varphi(\xi_j - 1;\xi^*), \\ D_j(\xi^*) &= \varphi(\xi_{j+1};\xi^*) - \varphi(\xi_j;\xi^*),\end{aligned}$$

Approximation of Wave Speeds



Computation of Traveling Front



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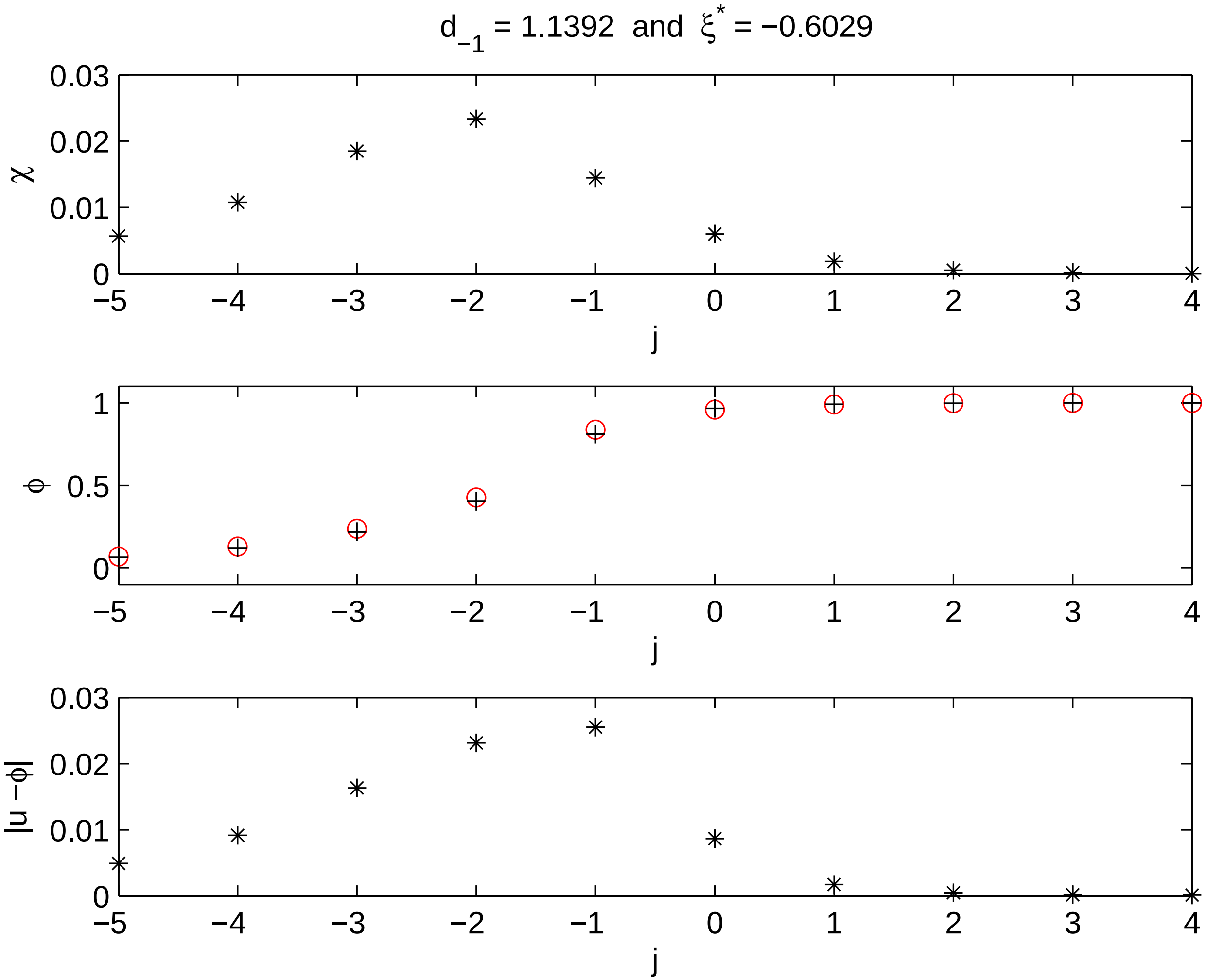

Conclusions

- Go to seminars. It could change your life.
- LDEs are the coolest.