Discretization Schemes vs Travelling Waves for Reaction-Diffusion Systems

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Patterns

PDE \quad u_t = F(u, \nabla u, \Delta u)
Desertification

vegetation patch size ~ power law

[Kéfi et al; Nature (2007)]
Nerve Conduction

Signal ‘hopping’

Myelene coating

Nerve fibre
Reaction-diffusion PDE

\[ u_t = \Delta u - G'(u) \]
Reaction-diffusion PDE

\[ u_t = \Delta u - G'(u) \]

\[ G(u) \]

Two competing rest states

\[ u = 0 \]
\[ u = 1 \]
Reaction-diffusion PDE

\[ u_t = \Delta u - G'(u) \quad \text{PDE} \]

Structure: Invasion wave \( u(t, x) = \Phi(x + ct) \)

\[ c\Phi'(\xi) = \Phi''(\xi) - G'(\Phi(\xi)) \quad \text{ODE} \]

[Fife+McLeod; 1970s]
Reaction-diffusion - continuous space

Speed

$G(u)$

$u = 0$

$u = 1$

wins!

(In)balance

time  space
Reaction-diffusion - continuous space

Speed

one wins!

zero wins!

(In)balance

standoff!

G(u)

u = 0

u = 1

G(u)

u = 0

u = 1

G(u)

u = 0

u = 1

G(u)

u = 0

u = 1

time

space
Continuous vs Discrete Space

\[ c\Phi'(\xi) = \Phi''(\xi) - G'(\Phi(\xi)) \quad \text{ODE} \]

\[ c\Phi'(\xi) = \Phi(\xi + 1) + \Phi(\xi - 1) - 2\Phi(\xi) - G'(\Phi(\xi)) \quad \text{MFDE} \]

Translational symmetry broken
Reaction-diffusion - discrete space

Speed

one wins!

waves pinned!

(In)balance

zero wins!

time  space
Propagating Failure

At $c = 0$, planar recurrence relation for pair $\left( \Phi(j), \Phi(j + 1) \right)$.

Typical at balance:

Heteroclinic for recursion relation $\leftrightarrow$ standing wave for LDE.
Propagation Failure

Edge of pinning region:

\[ W^u(0,0) \text{ (1,1)} \]

\[ W^s(1,1) \]

(0,0)

[Keener, Hoffman, Mallet-Paret, Van Vleck, Elmer, Scheel, ...]
For concreteness, will use quartic potential; i.e.

\[-G''(u) = -G''(u; a) = g_{\text{cub}}(u; a) = u(1 - u)(u - a)\]
Discrete Nagumo LDE - Propagation failure

Wave profiles:

\[ \phi(\xi) \]

- ■ a = 0.05
- ● a = 0.15
- △ a = 0.25
- ▼ a = 0.35
- ● a = 0.45
- ◇ a = 0.46
- × a = 0.50

Zero speed
Propagation Failure - Discrete map

Special multi-site discretizations:

Continuous family of standing waves instead of just two flavours.

\[ \mathcal{W}^u(0,0) = \mathcal{W}^s(1,1) \]
Thm. [H., Sandstede, Pelinovsky] No pinning for LDE

\[ \frac{d}{dt} u_j = u_{j-1} + u_{j+1} - 2u_j + (u_j - a) \left( u_{j-1}(1-u_{j+1}) + u_{j+1}(1-u_{j-1}) \right) \]
**Propagation Failure**

**Thm.** [H., Sandstede, Pelinovsky] Do have pinning for LDE

\[
\frac{d}{dt} u_j = u_{j-1} + u_{j+1} - 2u_j + 4u_j(1 - u_j)(u_{j-1} + u_{j+1} - 2a) \\
-5(a - \frac{1}{2}) \sin(2\pi u_j)(\frac{6}{5} + \frac{8}{5}u).
\]
Continuum regime

Rescale grid: $\mathbb{Z} \mapsto h\mathbb{Z}$.

\[
\begin{array}{cccccccc}
\cdots & \bullet & \cdots & \bullet & \cdots & \bullet & \cdots & \bullet & \cdots \\
& u_{-3h(t)} & u_{-2h(t)} & u_{-h(t)} & u_0(t) & u_h(t) & u_{2h(t)} & u_{3h(t)} & \\
\end{array}
\]

Rescale LDE:

\[
\frac{d}{dt} u_{jh}(t) = \frac{1}{h^2} \left[ u_{(j+1)h}(t) + u_{(j-1)h}(t) - 2u_{jh}(t) \right] - G''(u_{jh}(t))
\]

Travelling wave $u_{jh}(t) = \Phi(jh + ct)$ must satisfy

\[
c\Phi'(\xi) = [\Delta_h \Phi](\xi) - G''(\Phi(\xi))
\]

with

\[
[\Delta_h \Phi](\xi) = \frac{1}{h^2} \left[ \Phi(\xi + h) + \Phi(\xi - h) - 2\Phi(\xi) \right]
\]
Lifting waves

Recall

\[ [\Delta_h \Phi] = \frac{1}{h^2} [\Phi(\xi + h) + \Phi(\xi - h) - 2\Phi(\xi)] \]

Goal: bifurcate off PDE waves

\[ c_0 \phi_0'(\xi) = \phi_0''(\xi) - G'(\phi(\xi)) \]

to get LDE waves

\[ c\Phi'(\xi) = [\Delta_h \Phi](\xi) - G''(\Phi(\xi)) \]

for \( 0 < h \ll 1 \).

[Bates, Chen, Chmaj (2003)]: 'spectral convergence'.
The perturbation

Bifurcation problem

\[ \Phi(\xi) = \phi_0(\xi) + v(\xi), \quad c = c_0 + \tilde{c} \]

where \((c_0, \phi_0)\) is PDE wave.

The perturbation is singular, in the sense that one must solve

\[ L_h v = O(v^2 + h + \tilde{c}), \]

with \(L_h : H^1 \rightarrow L^2\) given by

\[ [L_h v](\xi) = -c_0 v'(\xi) + [\Delta_h v](\xi) - G''(\phi_0(\xi))v(\xi). \]

Compare with PDE operator \(L_0 : H^2 \rightarrow L^2\)

\[ [L_0 v](\xi) = -c_0 v'(\xi) + v''(\xi) - G''(\phi_0(\xi))v(\xi). \]

Note: operators act on different spaces.
Spectral Convergence

Recall

\[ \mathcal{L}_h v(\xi) = -c_0 v'(\xi) + \Delta_h v(\xi) - G'''(\phi_0(\xi)) v(\xi). \]

Want to show: \( \mathcal{L}_h - 1 \) invertible for \( 0 < h \ll 1 \).

- Assume \((\mathcal{L}_h - 1) v_h = w_h \) with \( \|v_h\|_{H^1} = 1 \).

- Goal: show \( \|w_h\|_{L^2} \gtrsim 0 \) as \( h \downarrow 0 \).

- Take weak limits:
  \[ v_h \rightharpoonup v_0 \in H^1, \quad w_h \rightharpoonup w_0 \in L^2 \]

- Observe: \([\mathcal{L}_0 - 1] v_0 = w_0 \) so
  \[ v_0 = [\mathcal{L}_0 - 1]^{-1} w_0 \]

- Danger: \( v_0 \) and \( w_0 \) could be zero.
• For compact $K \subset \mathbb{R}$, we have (after subsq) strong convergence

$$v_h \to v_0 \in L^2(K)$$

Can we exclude $v_0 = 0$? **Danger:**

$$v_h = h \sin(\xi/h), \quad v_h' = \cos(\xi/h)$$

Notice:

$$\|v_h\|_{L^2([−\pi; \pi])} = h\sqrt{\pi}$$

while

$$\|v_h'\|_{L^2([−\pi; \pi])} = \sqrt{\pi}$$

So: $\|v_h\|_{L^2(K)} \sim O(h)$ while $\|v_h\|_{H^1(K)} \sim O(1)$
Weak Limits

\[
\begin{align*}
\psi_h & \quad \psi_h' \\
\pi & \quad -\pi & \quad \pi & \quad -\pi
\end{align*}
\]

\(h = 1\)

\[
\begin{align*}
\psi_h & \quad \psi_h' \\
\pi & \quad -\pi & \quad \pi & \quad -\pi
\end{align*}
\]

\(h = \frac{1}{4}\)
Weak Limits

\[ \|v_h\|_2 = O(h) \]

\[ \|v'_h\|_2 = O(1) \]
Compact Interval

Pick $K$ large so that $G'' > \eta$ outside $K$:
Spectral convergence [Bates, Chen, Chmaj (2003)]

\[ \langle \Delta_h v_h, v_h' \rangle = 0 \]

\[ \| v'_h \|_{L^2} \leq C \left( \| v_h \|_{L^2} + \| w_h \|_{L^2} \right) \]

\[ \langle \Delta_h v_h, v_h \rangle \leq 0 \text{ & bistability} \]

\[ \| v_h \|_{L^2(K)}^2 \geq \epsilon \| v_h \|_{L^2(\mathbb{R})}^2 - C \| w_h \|_{L^2(\mathbb{R})}^2 \]

\[ \| w_h \|_{L^2} \rightarrow 0 \quad \rightarrow \quad \| v'_h \|_{L^2} \text{ under control} \quad \rightarrow \quad \| v_h \|_{L^2} \geq 0 \]

\[ \| w_0 \|_{L^2} = 0 \]

\[ \| v_h \|_{L^2(K)} \geq 0 \]

strong convergence

\[ \| v_0 \|_{L^2(K)} \geq 0 \]
Neural Fields

Complex (discrete) topology

Long range interactions

[Bressloff (2012)]

Search for effective eqns
Infinite-Range FitzHugh-Nagumo LDE

Discrete FitzHugh-Nagumo

\[ \begin{align*}
\dot{u}_{jh} &= \frac{1}{h^2} \sum_{k > 0} \alpha_k [u(j+k)h + u(j-k)h - 2u_{jh}] - G'(u_{jh}) - w_{jh} \\
\dot{w}_{jh} &= \rho [u_{jh} - \gamma w_{jh}] 
\end{align*} \]

- Coefficients \( \alpha_k \) decay sufficiently fast
- Not necessarily positive
- Spectral conditions ensure Laplace-like properties

Infinite-range discretization of FHN PDE

\[ \begin{align*}
\dot{u} &= u_{xx} - G'(u) - w \\
\dot{w} &= \rho [u - \gamma w] 
\end{align*} \]

Goal: transfer existence and stability of PDE waves to LDE (for \( 0 < h \ll 1 \))
Infinite-Range FitzHugh-Nagumo LDE

Discrete FitzHugh-Nagumo

\[
\begin{align*}
\dot{u}_{jh} &= \frac{1}{h^2} \sum_{k>0} \alpha_k \left[ u_{j+k}h + u_{j-k}h - 2u_{jh} \right] - G'(u_{jh}) - w_{jh} \\
\dot{w}_{jh} &= \rho \left[ u_{jh} - \gamma w_{jh} \right]
\end{align*}
\]

When \( \alpha_k = 0 \) for \( k > 1 \): Lin’s method [Sandstede + H.].
Wave Equation

LDE travelling wave equation:

\[
\begin{align*}
c \bar{u}'(\xi) &= \left[ \Delta_{h;\inf} \bar{u}(\xi) - G'(\bar{u}(\xi)) \right] - \bar{w}(\xi) \\
c \bar{w}'(\xi) &= \rho \left[ \bar{u}(\xi) - \gamma \bar{w}(\xi) \right]
\end{align*}
\]

with

\[
\Delta_{h;\inf} \Phi(\xi) = \frac{1}{h^2} \sum_{k>0} \left[ \Phi(\xi + kh) + \Phi(\xi - kh) - 2\Phi(\xi) \right]
\]

PDE waves:

\[
\begin{align*}
c_0 \bar{u}'_0 &= u''_0 - G'(\bar{u}_0) - \bar{w}_0 \\
c_0 \bar{w}'_0 &= \rho \left[ \bar{u}_0 - \gamma \bar{w}_0 \right]
\end{align*}
\]

**Assumption:** PDE waves exist and spectrally stable.
Results

Recall travelling wave MFDE

\[
\begin{align*}
c\bar{u}'(\xi) &= \left[\Delta_{h;\inf \bar{u}}(\xi) - G'(\bar{u}(\xi)) - \bar{w}(\xi)\right] \\
c\bar{w}'(\xi) &= \rho[\bar{u}(\xi) - \gamma \bar{w}(\xi)]
\end{align*}
\]

**Thm.** [H. and W. Schouten 2017] Suppose \(\sum k^2 \alpha_k < \infty\). For every \(0 < h \ll 1\) there is a travelling pulse solution which converges to \((c_0, \bar{u}_0, \bar{w}_0)\) as \(h \downarrow 0\).

**Thm.** [H. and W. Schouten 2017] Suppose

\[
\sum e^{\nu k} \alpha_k < \infty
\]

for some \(\nu > 0\). Then the travelling pulses above are **nonlinearly stable**.

**Remark:** Existence of pulses obtained earlier by [Scheel and Faye] without restriction on \(h\), but with exponential decay on \(\alpha_k\).
Linear operators

Proofs hinge on understanding transition from PDE operator $L_0 : H^2 \times H^1 \to L^2 \times L^2$:

\[
L_0 = \begin{pmatrix}
-c_0 \frac{d}{d\xi} + \frac{d^2}{d\xi^2} - G'''(u_0) & 1 \\
\rho & -c_0 \frac{d}{d\xi} - \gamma \rho
\end{pmatrix}
\]

to LDE operator $L_h : H^1 \times H^1 \to L^2 \times L^2$:

\[
L_h = \begin{pmatrix}
-c_0 \frac{d}{d\xi} + \Delta_h - G'''(u_0) & 1 \\
\rho & -c_0 \frac{d}{d\xi} - \gamma \rho
\end{pmatrix}.
\]

As before: operators act on different spaces

- 'Spectral convergence' can be extended
- Cross-terms needs to be kept under control
- Very useful: slow system is linear
Spectral Stability

Periodicity: $\lambda \mapsto \lambda + 2h^{-1} \pi i c_h$

Need to understand $\mathcal{L}_h - \lambda$ uniformly in $\lambda$ as $h \downarrow 0$
Spectral Stability

Periodicity: \( \lambda \mapsto \lambda + 2h^{-1} \pi i c_h \)

\[ R_1 : \text{delicate} \]
\[ R_2 : \text{standard} \]
\[ R_3 : \text{Fourier transform} \]
\[ R_4 : \text{Modified 'Bates'} \]
Near $\lambda = 0$ - Beyond 'Bates'

PDE: $\mathcal{L}_0$ is Fredholm with index zero; simple eigenvalue $\lambda = 0$.

In particular, given $f = (f_1, f_2) \in L^2 \times L^2$, there exist $(v, w) \in H^2 \times H^1$ and $\gamma \in \mathbb{R}$ for which

$$\mathcal{L}_0(v, w) = f + \gamma (\bar{u}_0', \bar{w}_0')$$

with orthogonality condition

$$\langle (\bar{u}_0', \bar{w}_0'), (v, w) \rangle_{L^2 \times L^2} = 0.$$

Thm. [H., Schouten] For all $0 < h \ll 1$ and all $f = (f_1, f_2) \in L^2 \times L^2$ there are $(v, w) = (v_h, w_h)(f) \in H^1 \times H^1$ and $\gamma = \gamma_h(f) \in \mathbb{R}$ so that

$$\mathcal{L}_h(v, w) = f + \gamma (\bar{u}_0', \bar{w}_0')$$

with same orthogonality condition as above.
Full discretization

\[ \dot{u}_j = u_{j+1} + u_{j-1} - 2u_j - G'(u_j) \]

\[ \frac{1}{\Delta t}[u_j(t) - u_j(t - \Delta t)] = u_{j+1}(t) + u_{j-1}(t) - 2u_j(t) - G'(u_j(t)) \]

BDF-1 (Backward-Euler)

\[ \frac{3}{2\Delta t}[u_j(t) - \frac{4}{3}u_j(t - \Delta t) + \frac{1}{3}u_j(t - 2\Delta t)] = u_{j+1}(t) + u_{j-1}(t) - 2u_j(t) - G'(u_j(t)) \]

BDF-2

BDF-6
Full discretization

Travelling waves under BDF-k must solve:

\[ c[D_{k,c,\Delta t}\Phi](\zeta) = \Phi(\zeta + 1) + \Phi(\zeta - 1) - 2\Phi(\zeta) - G'(\Phi(\zeta)) \]

BDF-1:

\[ [D_{1,c,\Delta t}\Phi](\zeta) = \frac{1}{c\Delta t} \left[ \Phi(\zeta) - \Phi(\zeta - c\Delta t) \right] \]

BDF-2:

\[ [D_{2,c,\Delta t}\Phi](\zeta) = \frac{3}{2c\Delta t} \left[ \Phi(\zeta) - \frac{4}{3}\Phi(\zeta - c\Delta t) + \frac{1}{3}\Phi(\zeta - 2c\Delta t) \right] \]

For smooth functions \( \Phi \):

\[ [D_{k,c,\Delta t}\Phi](\zeta) - \Phi'(\zeta) \sim (\Delta t)^k \left\| \Phi^{(k+1)} \right\|_{\infty}. \]
**Full discretization**

Travelling waves under BDF-k must solve:

\[ c[D_{k,c,\Delta t}\Phi](\zeta) = \Phi(\zeta + 1) + \Phi(\zeta - 1) - 2\Phi(\zeta) - G'(\Phi(\zeta)) \]

Write \((\Phi_*, c_*)\) for spatially discrete wave (assume \(c_* > 0\)).

**Thm. [H. and Van Vleck 2015]** Fix integer \(P \geq 1\). For all small

\[ \epsilon \in \frac{P}{\mathbb{N}_{>0}} \]

there exists a **family** of travelling waves \((\Phi, c)\) near \((\Phi_*, c_*)\) for BDF-k with timestep \(\Delta t = \frac{\epsilon}{c}\).

**Observation** The wavespeed loses its uniqueness. (We have a proof for BDF-1 in anti-continuum regime).
Reaction-diffusion - discrete time + space

Speed

one wins!

(In)balance

pinning!
Bifurcation

Bifurcate from spatially discrete wave $\Phi_*$ by writing

$$\Phi(\zeta) = \Phi_*(\vartheta + \zeta) + v(\zeta).$$

Pair $(c, \Phi)$ must solve fully discrete travelling wave system

$$c[D_{k,c,\Delta t}\Phi](\zeta) = \Phi(\zeta + 1) + \Phi(\zeta - 1) - 2\Phi(\zeta) - G'(\Phi(\zeta);a).$$

Write $\mathbb{Z}_{c,\Delta t}$ for domain of $\zeta$. For $c\Delta t = \frac{p}{q}$ we have $\mathbb{Z}_{c,\Delta t} = q^{-1}\mathbb{Z}$. Otherwise dense.
Singular perturbation

Fix $\vartheta = 0$ and concentrate on bifurcation problem

$$\Phi(\zeta) = \Phi_*(\zeta) + v(\zeta), \quad c = c_* + \bar{c}$$

where $(c_*, \Phi_*)$ is **spatially discrete** wave.

The perturbation is singular, in the sense that one must solve

$$L_{k,c,\Delta t}v = O(v^2 + c\Delta t + \bar{c}),$$

with $L_{k,c,\Delta t} : \ell^2(\mathbb{Z}_M; \mathbb{R}) \to \ell^2(\mathbb{Z}_M; \mathbb{R})$ given by

$$[L_{k,c,\Delta t}v](\zeta) = -c_* D_{k,c,\Delta t}v + v(\zeta + 1) + v(\zeta - 1) - 2v(\zeta) + g'(\Phi_*(\zeta))v(\zeta).$$

Want to exploit spatially-discrete linearization $L_* : H^1(\mathbb{R}; \mathbb{R}) \to L^2(\mathbb{R}; \mathbb{R})$

$$[L_*v](\xi) = -c_* v'(\xi) + v(\xi + 1) + v(\xi - 1) - 2v(\xi) + g'(\Phi_*(\xi))v(\xi).$$

Note: operators act on different spaces.
Spectral convergence

- Proof based on adaptation of 'spectral convergence' technique [Bates, Chen, Chmaj].

- Step A: Assuming \((\mathcal{L}_{k,c_j, (\Delta t)_j} - \delta)v_j \rightarrow 0\), use interpolation to pass to a weak limit \(V \in H^1\).

- Step B: recover 'missing' information on \(V\) by exploiting bistable structure.
Step A: Weak Convergence

Need to build an $H^1$-function from sequence

Here $c\Delta t = \frac{2}{3}$ so $\zeta \in \mathbb{Z}_{c,\Delta t} = \frac{1}{3}\mathbb{Z}$.

Cannot directly do interpolation in a controlled fashion.
After splitting; can interpolate. Size of derivative controlled by $D_{k,c,\Delta t} v$. 
Adaptive Grid

\[ \Phi(h\mathbb{Z}) \]

Fixed Grid

Adaptive Grid

\[ \Phi(x_j \in \mathbb{Z}) \]

\[ x_j \in \mathbb{Z} \]
Adaptive Grid

Lattice system:

\[
\dot{u}_j = \left( \frac{u_{j+1} - u_{j-1}}{x_{j+1} - x_{j-1}} \right) \dot{x}_j \\
+ \frac{2}{x_{j+1} - x_{j-1}} \left[ \frac{u_{j-1} - u_j}{x_j - x_{j-1}} + \frac{u_{j+1} - u_j}{x_{j+1} - x_j} \right] - G'(u_j; a).
\]

Starting point: instant equidistribution of arclength:

\[
h^2 = (x_{j+1} - x_j)^2 + (u_{j+1} - u_j)^2 \quad \text{for all } j \in \mathbb{Z}
\]

Boundary condition:

\[
x_j \rightarrow jh \quad \text{as } j \rightarrow -\infty
\]

(only local movement of grid-points)
\[
\dot{u}_j = \left( \frac{u_{j+1} - u_{j-1}}{x_{j+1} - x_{j-1}} \right) \dot{x}_j + \frac{2}{x_{j+1} - x_{j-1}} \left[ \frac{u_{j-1} - u_j}{x_j - x_{j-1}} + \frac{u_{j+1} - u_j}{x_{j+1} - x_j} \right] - G'(u_j; a).
\]

Ansatz: \( u_j(t) = \Phi(x_j(t) + ct) = \Phi(\xi) \).

Implicitly define grid distance in terms of wave-coordinate \( \xi \):

\[
x_{j+1}(t) - x_j(t) = h_+[\xi; \Phi], \quad x_j(t) - x_{j-1}(t) = h_-[\xi; \Phi]
\]
Adaptive Grid

Travelling wave equation is state-dependent MFDE with infinite shifts.

Example: diffusive term $\Phi''$ becomes:

$$
\frac{2}{h_+[\xi; \Phi] + h_-[\xi; \Phi]} \left[ \frac{\Phi(\xi + h_+[\xi; \Phi]) - \Phi(\xi)}{h_+[\xi; \Phi]} - \frac{\Phi(\xi - h_-[\xi; \Phi]) - \Phi(\xi)}{h_-[\xi; \Phi]} \right]
$$

**Thm.** [H., Van Vleck and Huang, 2017]: For $0 < h \ll 1$ the adaptive scheme has travelling waves.

**Observation:** Pinning region is significantly smaller with adaptive grids.
Outlook

- Transfer of stability properties?
- Wavespeed (non)-uniqueness hidden in exponentially small terms
- Can we handle fast (but non-instantaneous) grid movement:
  \[ \tau \dot{x}_j = \sqrt{(x_{j+1} - x_j)^2 + (u_{j+1} - u_j)^2} - \sqrt{(x_{j-1} - x_j)^2 + (u_{j-1} - u_j)^2}, \]
- Other structural perturbations: di-atomic lattices