Modulated Travelling Waves in Discrete Reaction Diffusion Systems

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Discrete Reaction-Diffusion Systems

We consider the prototype reaction diffusion system

\[ \partial_t y(x, t) = \gamma \partial_{xx} y(x, t) + [L_D y](x, t) + f(y(x, t)) \]

with discrete Laplacian

\[ [L_D y](x, t) = y(x + 1, t) + y(x - 1, t) - 2y(x, t). \]

- When \( \gamma = 0 \), we have a pure lattice system
- For \( \gamma > 0 \), we have a partially discrete reaction-diffusion system
- Useful for models with local and nonlocal interactions
- Allows study of transition continuous \( \rightarrow \) discrete (Van Vleck, Elmer, H., Verduyn Lunel).
Wave trains

We are interested in wave train solutions (periodic travelling waves). Ansatz

\[ y(x, t) = u(\omega t - kx) \]

leads to second order MFDE \( F(u, \omega, k) = 0 \) with

\[ F(u, \omega, k) := -\gamma k^2 u''(\zeta) + \omega u'(\zeta) - [u(\xi - k) + u(\xi + k) - 2u(\xi)] - f(u(\zeta)) \]

We require periodicity \( u(\zeta) = u(\zeta + 2\pi) \).

Under generic assumptions, if \( F(u_0, \omega_0, k_0) = 0 \), then can construct 1-parameter family of wave-train solutions

\[ y(x, t) = u(\omega_{n1}(k)t - kx; k) \text{ for } k \approx k_0 \]

phase velocity \( c_p = \frac{\omega}{k} \)

\[ \text{group velocity } c_g = \frac{d\omega}{dk} \]
Linear stability

To consider the linear stability of the wave train, insert Floquet Ansatz

\[ y(x, t) = u(\zeta; k_0) + e^{\lambda t} e^{-\nu \zeta / k_0} w(\zeta), \]

with \( \zeta = \omega_0 t - k_0 x \). Ignoring higher order terms, we must have

\[ \mathcal{L}_{st}(\nu) w = \lambda w, \]

with (for \( \gamma = 0 \))

\[ \mathcal{L}_{st}(\nu) w = [\nu c_p - \omega_0 D] w + [e^{\nu} w(\cdot - k_0) + e^{-\nu} w(\cdot + k_0) - 2w] + Df(u(\cdot; k_0)) w. \]

We find a set of curves \( \nu \rightarrow \lambda_j(\nu) \) that are analytic except at intersection points.
Linear dispersion relation

Note that $L_{st}u'(\cdot; k_0) = 0$. If the eigenvalue $\lambda = 0$ is simple, we find a curve

$$\nu \mapsto \lambda_{\text{lin}}(\nu)$$

that is analytic for $\nu \approx 0$, with

$$\lambda_{\text{lin}}(0) = 0, \quad \lambda'_{\text{lin}}(0) = c_p - c_g$$

Spectral stability hypothesis ($d > 0$):

$$\lambda_{\text{lin}}(i\gamma) = i(c_p - c_g)\gamma - d\gamma^2 + \mathcal{O}(\gamma^3)$$
PDE Reaction-Diffusion Systems

Step back for a moment and consider the PDE

\[ y_t = y_{xx} + f(y), \]

again with the 1-parameter family of wave-trains \( u(\omega_{n1}(k)t - kx; k). \)

Consider the formal Ansatz

\[ y(x, t) = u(kx - \omega t + \phi(X, T); k + \epsilon \phi_X(X, T)) \]

where \( X = \epsilon(x - c_g t), \quad T = \epsilon^2 t/2 \quad \text{and} \quad \epsilon \ll 1 \)

Wavenumber \( q = \phi_X \) formally satisfies the viscous Burgers equation:

\[ \frac{\partial q}{\partial T} = \lambda''(0) \frac{\partial^2 q}{\partial X^2} - \omega''_{n1}(k) (q^2)_X \]

[Howard and Koppel, 1977]
Predictions from the Burgers equation

- Issue 1: Validity of Burgers equation over natural time scale $[0, \epsilon^{-2}]$: [Doelman, Sandstede, Scheel, Schneider]

- Issue 2: Predictions from Burger equation

Lax shocks of Burgers equation $\rightarrow$ Weak defects:

(convex dispersion relation: $\omega''_{nl}(k) > 0$)
Verifying the existence of the lax shock

The shock that we seek is a modulated travelling wave. Write as

\[ y(x, t) = u_*(x - c_* t, \omega_* t) \]

where \( u_* \) is \( 2\pi \) periodic in the second variable.

Asymptotics

\[ u_*(x - c_* t, \omega_* t) \to u(\omega_\pm t - k_\pm x; k_\pm) \text{ as } x - c_* t \to \pm \infty \]

Space-time plot for \( \omega_* t \in [0, 2\pi] \):

Since \( c^-_g > c_* > c^+_g \), transport occurs towards defect \( \to \) sink.
Construction of lax shock in continuous setting

Introduce new variables \( v(\xi, \tau) = u_*(\xi, \tau) \) and \( w(\xi, \tau) = \partial_\xi u_*(\xi, \tau) \), with \( \xi = x - c_* t \) and \( \tau = \omega_* t \).

In the continuous case, we find

\[
\partial_\xi \begin{pmatrix} v \\ w \end{pmatrix} = \begin{pmatrix} w \\ -\gamma^{-1}[c_* w - \omega_* \partial_\tau v + f(v)] \end{pmatrix}
\]

Following the spatial-dynamics approach due to [Kirchgässner], [Mielke], view as an ODE on the space \( H^2_{per}([0, 2\pi]) \times H^1_{per}([0, 2\pi]) \).

Fix \( k_0 \) and write

\[
\begin{align*}
c_* &= c_g(k_0) = \omega'_{nl}(k_0) \\
\omega_* &= \omega_{nl}(k_0) - k_0 \omega'_{nl}(k_0) + \bar{\omega}
\end{align*}
\]

For small \( \bar{\omega} \) with appropriate sign, there exist:

- Wave numbers \( k_\pm(\bar{\omega}) \) with \( k_\pm(\bar{\omega}) \to k_0 \) as \( \bar{\omega} \to 0 \).
- Periodic solutions \( v_\pm(\xi) = u(-k_\pm \xi + \cdot; k_\pm) \) (with accompanying \( w_\pm \))
Construction of lax shock in continuous setting

For $\bar{\omega} = 0$, we have the $\xi$-periodic solution

\[
\begin{align*}
v_0(\xi)(\tau) &= u(-k_0\xi + \tau; k_0) \\
w_0(\xi)(\tau) &= -k_0 u'(-k_0\xi + \tau; k_0)
\end{align*}
\]

Idea: construct center manifold around $(v_0, w_0, \bar{\omega} = 0)$ that captures all solutions that remain orbitally close to $(v_0, w_0)$, for small $\bar{\omega}$.

Crucial ingredient: change of variables $\sigma = \tau - k_0\xi$ into temporal comoving frame yields

\[
\partial_\xi \begin{pmatrix} v \\ w \end{pmatrix} = k_0 \partial_\sigma \begin{pmatrix} v \\ w \end{pmatrix} + \begin{pmatrix} w \\ -\gamma^{-1}[c_* w - \partial_\sigma v + f(v)] \end{pmatrix}
\]

This change of variables turns periodic solution $(v_0, w_0)$ into a ring of equilibria.

Orbitally close in original frame $\leftrightarrow$ close to equilibria-ring in temporal comoving frame
**Temporal Comoving Frame**

Recall temporal-comoving frame

\[
\partial_\xi \begin{pmatrix} v \\ w \end{pmatrix} = k_0 \partial_\sigma \begin{pmatrix} v \\ w \end{pmatrix} + \left( -\gamma^{-1}[c_* w - \omega_* \partial_\sigma v + f(v)] \right)
\]

Center space around equilibrium \( u_0 = (v_0, w_0) \) is **two** dimensional by our choice \( c_* = c_g \). Spanned by

\[
u_0' = (u'(\cdot; k_0), -k_0 u''(\cdot; k_0)), \quad u_1 = (-\partial_k u(\cdot; k_0), k_0 \partial_k u'(\cdot; k_0) + u'(\cdot; k_0))\]

Formally insert Ansatz

\[
(v, w) = u_0(\cdot - \theta) - \kappa u_1(\cdot - \theta) + O(\theta^2 + \kappa^2)
\]

and derive ODE

\[
\begin{align*}
\partial_\xi \theta &= \kappa + O(|\bar{\omega}| + |\kappa|^2) \\
\partial_\xi \kappa &= 2\chi''(0)^{-1}(\frac{1}{2} \omega''(k_0) \kappa^2 - \bar{\omega}) + O(|\bar{\omega}|^2 + |\bar{\omega} \kappa| + |\kappa|^3)
\end{align*}
\]

Read off heteroclinic connections.
Heteroclinic connections

Recall

$$\partial_\xi \begin{pmatrix} v \\ w \end{pmatrix} = k_0 \partial_\sigma \begin{pmatrix} v \\ w \end{pmatrix} + \left( -\gamma^{-1}[c_*w - \omega_* \partial_\sigma v + f(v)] \right)$$

No general global center manifold result for such mixed hyperbolic - elliptic systems.

To get CM, need to exploit CM result by [Mielke] for original equation

$$\partial_\xi \begin{pmatrix} v \\ w \end{pmatrix} = \left( -\gamma^{-1}[c_*w - \omega_* \partial_\tau v + f(v)] \right)$$

Result states that solutions that are orbitally close to \((v_0, w_0)\) can be captured.
Discrete Case

In discrete setting, the equation to solve becomes

$$
\partial_\xi \begin{pmatrix} v \\
 w \end{pmatrix} = \begin{pmatrix}
-\gamma^{-1} [c_* w - \omega_* \partial_\tau v + [v(\cdot + 1) + v(\cdot - 1) - 2v] + f(v)] \\
 w
\end{pmatrix}
$$

This is a functional differential equation of mixed type (MFDE) posed on the space $H^2_{per}([0, 2\pi]) \times H^1_{per}([0, 2\pi])$.

- The center manifold result developed by Mielke no longer works for MFDEs
- The situation was partially remedied in [Hupkes, Verduyn Lunel, 2008], where center manifolds are constructed around periodic solutions to MFDEs
- However, orbital closeness is still an unresolved issue.
- In addition, results only for MFDEs posed on $\mathbb{C}^n$, not general Hilbert spaces
Discrete Case

For simplicity, we choose to work directly in temporal comoving frame and solve

$$\partial_\xi \begin{pmatrix} v \\ w \end{pmatrix} = k_0 \partial_\sigma \begin{pmatrix} v \\ w \end{pmatrix} + \begin{pmatrix} w \\ -\gamma^{-1}[c_* w - \omega_* \partial_\sigma v + f(v)] \end{pmatrix} + \begin{pmatrix} 0 \\ [v(\cdot + 1)(\cdot - k_0) + v(\cdot - 1)(\cdot + k_0) - 2v] \end{pmatrix}$$

posed on the space $H^2_{per}([0, 2\pi]) \times H^1_{per}([0, 2\pi])$.

Goal is to construct global center manifold near ring of equilibria

$$\left( u(\vartheta + \cdot; k_0), -k_0 u'(\vartheta + \cdot; k_0) \right)$$

parametrized by $\vartheta \in [0, 2\pi]$.

Most important issues:

- The $\partial_\sigma$ derivatives prevent use of bootstrapping methods to get regularity of solutions.
- The Hilbert space setting prevents explicit construction of characteristic equations.
Finite dimensional example

For simplicity, let us consider the planar ODE

\[ y' = f(y) \]

- Write \( \rho(\vartheta) \) for rotation with angle \( \vartheta \).
- Suppose \( f : \mathbb{R}^2 \to \mathbb{R}^2 \) invariant, i.e. \( \rho(-\vartheta)f(\rho(\vartheta)v) = f(v) \) for \( v \in \mathbb{R}^2 \).
- Suppose \( f(\overline{y}) = 0 \) for \( \overline{y} \neq 0 \).

Change of variables

\[ y(\xi) = \rho(\theta(\xi))[\overline{y} + u(\xi)] \]

with normalization condition

\[ \langle D\rho(0)\overline{y}, u(\xi) \rangle = 0. \]
Finite dimensional example - continued

Recall \( y' = f(y) \) with

\[
y(\xi) = \rho(\theta(\xi))[\overline{y} + u(\xi)], \quad \langle D\rho(0)\overline{y}, u(\xi) \rangle = 0.
\]

Differentiation yields

\[
u'(\xi) = -\theta'(\xi)D\rho(0)[\overline{y} + u(\xi)] + f(\overline{y} + u(\xi))
\]

\[
\theta'(\xi) = [\langle D\rho(0)\overline{y}, D\rho(0)\overline{y} \rangle + \langle D\rho(0)\overline{y}, D\rho(0)u(\xi) \rangle]^{-1}\langle D\rho(0)\overline{y}, f(\overline{y} + u(\xi)) \rangle.
\]

Variable \( \theta \) can hence be eliminated from equation for \( u \), allowing use of standard CM theory.

However, turning to our setting \( y'(\xi) = f(y(\xi), y(\xi - 1), y(\xi + 1)) \), we find:

- Symmetry \( \rho \) acts as translation \( \longrightarrow \) the term \( D\rho(0)u(\xi) \) becomes unbounded.
- Equation for \( \theta \) no longer decouples.
Global center manifold

To resolve the unboundedness issue, need to use Ansatz

\[ y(\xi) = \rho(\theta(\xi))\bar{y} + u(\xi). \]

We need to obtain CM for the coupled system

\[
\begin{align*}
    u'(\xi) &= -\theta'(\xi)D\rho(\theta(\xi))\bar{y} + f(\theta, u) \\
    \theta'(\xi) &= [\langle D\rho(0)\bar{y}, D\rho(0)\bar{y} \rangle + \langle D\rho(\theta(\xi))\bar{y}, u(\xi) \rangle]^{-1}\langle D\rho(\theta(\xi))\bar{y}, f(\theta, u) \rangle
\end{align*}
\]

in which \( u \) is small, but without bound on \( \theta \).

\[ f(\theta, u) = f(\rho(\theta(\xi))\bar{y} + u(\xi), \rho(\theta(\xi - 1))\bar{y} + u(\xi - 1), \rho(\theta(\xi + 1))\bar{y} + u(\xi + 1)). \]

Notice that linearization of equation for \( u' \) includes dependence on \( \theta(\xi), \theta(\xi \pm 1) \).

Key idea: For small \( u \), the variable \( \theta \) is \textit{slowly varying}. Linearized equation for \( u \) thus has slowly varying coefficients, allowing us to solve for prescribed \( \theta \).
Close connection with singularly perturbed systems

\[
\begin{align*}
\theta' &= \epsilon g_s(\theta, u, \epsilon) \\
u' &= g_f(\theta, u, \epsilon),
\end{align*}
\]

that admit a manifold \( \tilde{u}(\vartheta) \) of equilibria

\[ g_f(\vartheta, \tilde{u}(\vartheta), 0) = 0. \]

Key question: persistence of invariant manifold as slow flow is turned on (\( \epsilon > 0 \)).

- Fenichel (1970s): in absence of extra center directions (normal hyperbolicity), manifold persists

- Large literature on persistence of center manifolds for general normally-hyperbolic invariant sets

- Some results on situations where normal-hyperbolicity fails [Chow, Liu, Yi]
Analytic techniques

- Almost all results rely on geometric Hadamard graph transform techniques
- Need analytic setup for generalization to infinite dimensions
- [Sakamoto, 1990] Analytic proof of first Fenichel theorem by fixed point argument. Idea:
  - For prescribed slowly modulated function $\theta$, construct solution operator $\mathcal{K}(\theta)$ to solve linearized system for $u$.
  - Solve fixed point system

$$u = \mathcal{K}(\theta[u])G(u),$$

in appropriate weighted function space, where $G$ contains nonlinear terms.

Unfortunately, normal-hyperbolicity is essential.
Construction of global CM

Crucial idea, inspired by technique in [Yi]: use two fixed point arguments in succession.

Equation to solve: \(( E \) denotes extension from center space to solutions to homogeneous linear system)

\[
    u = E(\theta[u])\Pi_{ct}u(0) + \mathcal{K}(\theta[u])G(u)
\]  

(1)

- Assume that CM has the form \( h : (\kappa, \theta) \rightarrow H \)
- Plug in Ansatz

\[
    u = \rho(\theta)\bar{y} + \kappa\rho(\theta)u_1 + h(\kappa, \theta)
\]

and using center projections and fixed point argument, determine evolution for the center variables \((\kappa, \theta)\). Evolution depends only on \(\kappa(0), \theta(0), h\).

- Pick arbitrary \(\kappa(0)\) and \(\theta(0)\), determine \(\kappa(\xi)\) and \(\theta(\xi)\) from this and compute right hand side of (1).
- Evaluating at zero and equating with left hand side of (1) yields fixed point equation for CM function \( h\).
Main Result

Theorem 1 (H., Sandstede, JDDE, to appear). Consider the partially discrete system

$$\partial_t y(x, t) = \gamma \partial_{xx} y(x, t) + [L_D y](x, t) + f(y(x, t))$$

with $\gamma > 0$. Suppose that $\omega''_{nl}(k_0) \neq 0$ and $\lambda''_{lin} > 0$. Suppose furthermore that some technical conditions hold for the lattice.

Then for $k_1 \approx k_0$, there exists $k_2 \approx k_0$ and a modulated travelling wave that connects the wavetrain at $k_-$ to the wave train at $k_+$, in which $k_- = k_1$ and $k_+ = k_2$ if $\omega''_{nl}(k_0) < 0$ and vice versa if $\omega''_{nl}(k_0) > 0$.

- The technical conditions on the lattice are absent in the continuous case.
- They arise due to the fact that the $\theta$ equation is an MFDE.
- Equation is scalar, but many eigenfunctions can in principle appear.
- To make sure flow on CM depends only on $\theta(0)$ and $\kappa(0)$, need to ensure that there are no resonances.
- In the limit $\gamma \to 0$ one cannot avoid these resonances.
Technical conditions on the lattice

Characteristic equation (for $c_\ast = c_g$) is given by

$$\mathcal{L}_{\text{ch}}(z)v = [-\mathcal{L}_{\text{st}}(z) + z(c_p - c_g)]v$$

Associated operator

$T(z) : H^2_{\text{per}}([0, 2\pi]) \times H^1_{\text{per}}([0, 2\pi]) \rightarrow H^1_{\text{per}}([0, 2\pi]) \times H^0_{\text{per}}([0, 2\pi])$ given by

$$T(z) \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = \begin{pmatrix} \frac{1}{\gamma}c_g - k_0D & 0 \\ -(z + \frac{1}{\gamma}c_g - k_0D) & 1 \end{pmatrix} \begin{pmatrix} -\gamma z + \gamma k_0D & \gamma \\ \mathcal{L}_{\text{ch}}(z) & 0 \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \end{pmatrix},$$

- We have $\langle u'_0, T'(0)u'_0 \rangle \neq 0$ and $\langle u'_0, T(i\kappa)u'_0 \rangle \neq 0$ for $\kappa \in \mathbb{R} \setminus \{0\}$. [The MFDE for normalization $\theta$ is well-defined after fixing $\theta(0)$]

- We have $\Delta(i\kappa) \neq 0$ for $\kappa \in \mathbb{R} \setminus \{0\}$ and $\Delta''(0) \neq 0$, for

$$\Delta(z) = -\gamma z \| u_1 \|^2_{H^1 \times H^0} \langle u'_0, T(z)u'_0 \rangle - \langle u_1, T'(0)u'_0 \rangle \langle u'_0, T(z)u'_0 \rangle$$

$$+ \langle u'_0, T'(0)u'_0 \rangle \langle u'_0, T(z)u'_0 \rangle,$$

[Evolution on center manifold defined after fixing $\kappa(0)$ and $\theta(0)$].
The limit $\gamma \to 0$.

To get a further idea what goes wrong in $\gamma \to 0$ limit, study the characteristic equation (for $\gamma = 0$)

$$
\mathcal{L}_{\text{ch}}(z)v = [-\mathcal{L}_{\text{st}}(z) + z(c_p - c_g)]v
= [zc_g - (\omega_* + k_0 c_g)D]v + [e^z v(\cdot - k_0) + e^{-z} v(\cdot + k_0) - 2v]
+ D f(u(\cdot; k_0))v.
$$

Consider $\ell \in \mathbb{Z}$ and $\Delta k \in \mathbb{Z}$, and

$$
\tilde{v} = \exp[i\Delta k \cdot]v
\tilde{z} = z + ik_0 \Delta k + 2\pi \ell
$$

We get

$$
\exp[-i\Delta k \cdot] \mathcal{L}_{\text{ch}}(\tilde{z}) \tilde{v} = \mathcal{L}_{\text{ch}}(z)v + i(2\pi c_g \ell - \omega_* \Delta k)v
$$

If $\pi c_g$ and $\omega_*$ are not rationally related, there is no hope of getting a uniform bound on $\mathcal{L}_{\text{ch}}(z)$ in vertical strips if $\mathcal{L}_{\text{ch}}(z_0)$ has eigenvalue with $\Re \lambda = \Re z_0$. 