Numerical computation of coherent structures in spatially-extended systems

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Example of coherent structures

Problem setting

- Coherent structures: solutions to nonlinear evolution equations with a particular spatial and temporal structure

- Problem setting: compute special solutions to an Initial-Boundary-Value problem

Evolution equations $\partial_t u(x,t) = \mathcal{F}(u;p)(x,t), \qquad (x,t) \in \Omega \times (0,T]$

Boundary conditions $\mathcal{B}(u;p)(x,t) = 0, \qquad (x,t) \in \partial\Omega \times (0,T]$

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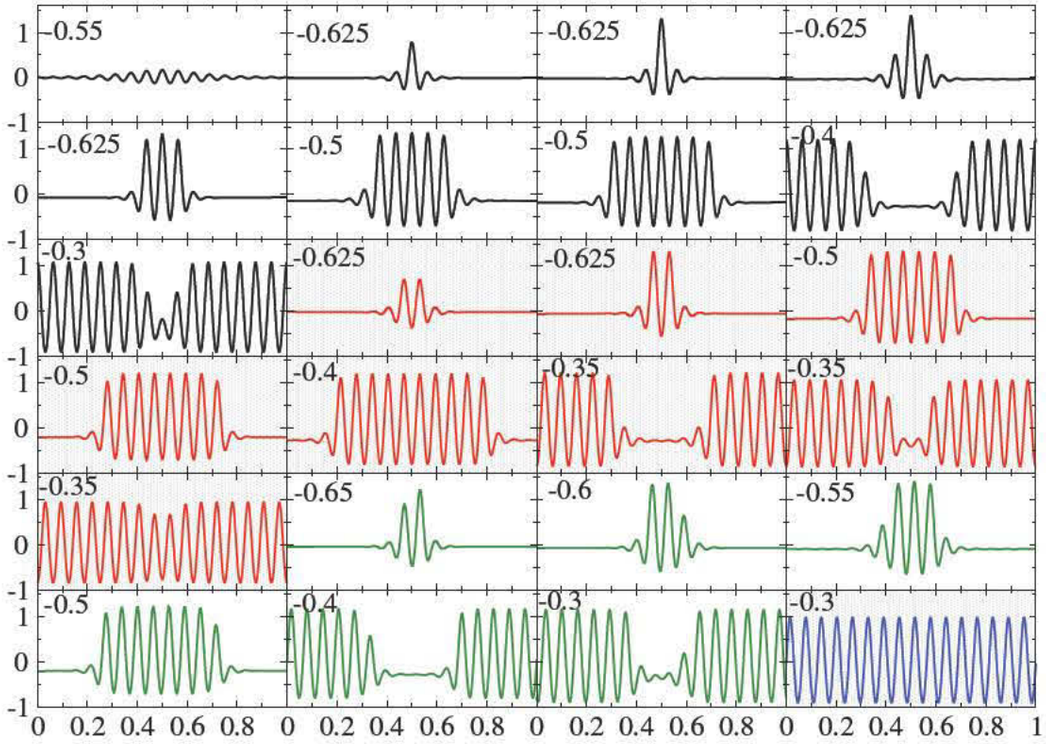
  - DIY - version of the day [see Codes]

Localised steady states

Steady states (Swift-Hohenberg Eq.)



[Thiele, Archer, Robbins, Gomez, Knobloch]

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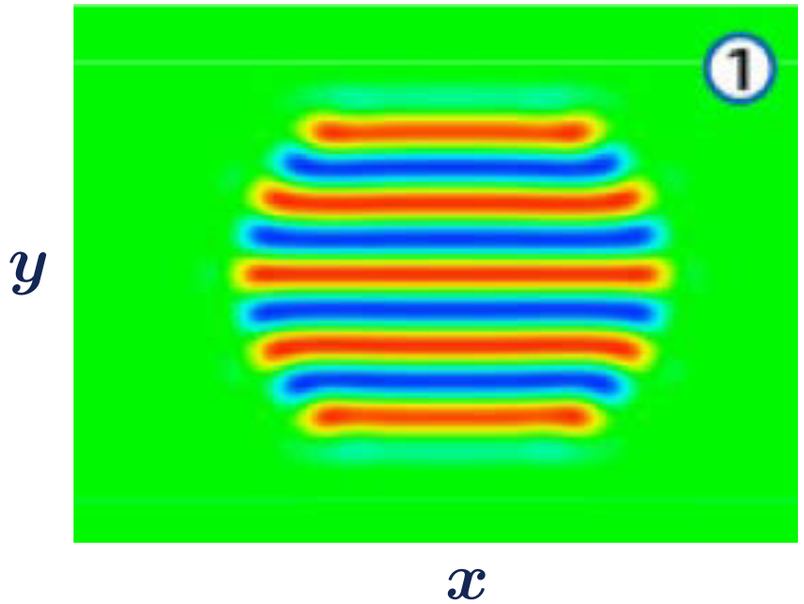

[A., Burke, Lloyd,
Sandstede, Knobloch]

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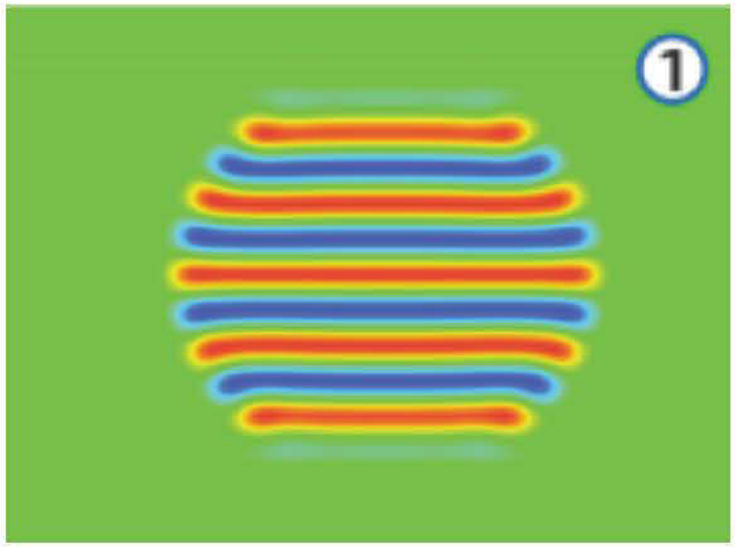
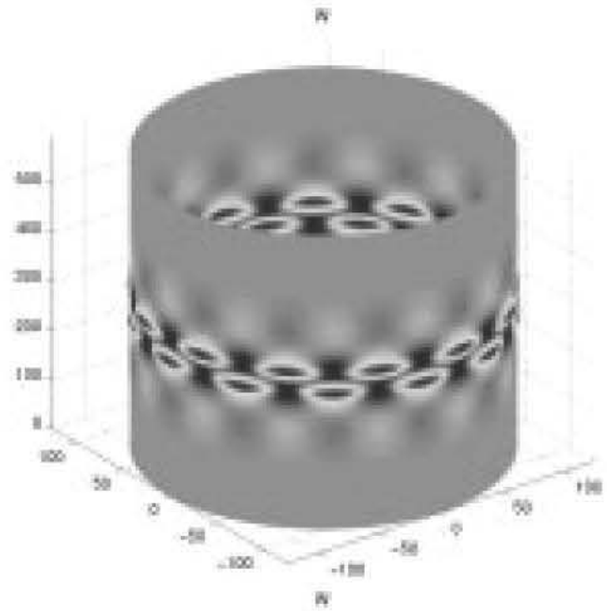


[A., Burke, Lloyd, Sandstede, Knobloch]

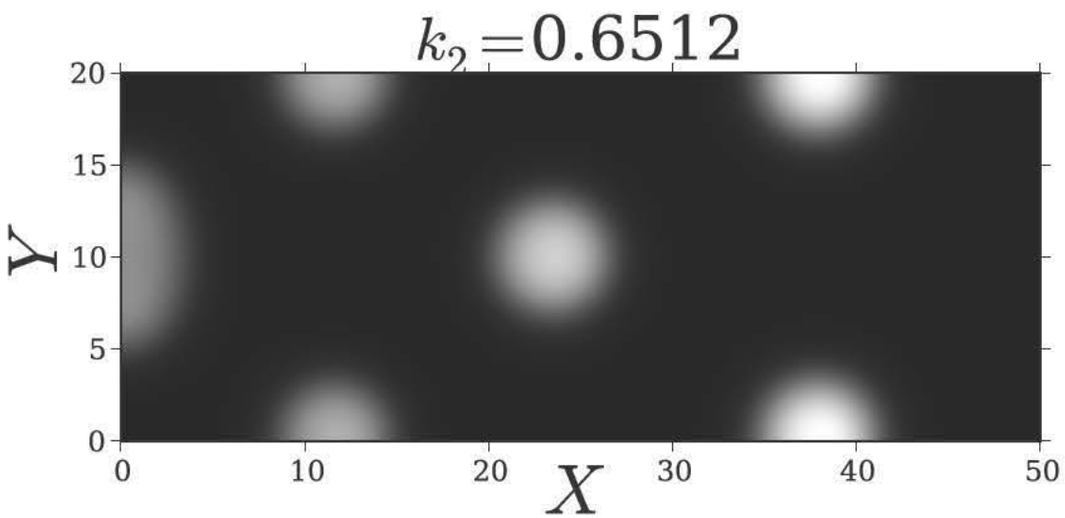
Localised steady state (von Kármán Eq.)



[Champneys, Hunt, Lord]

Steady states

Stationary pattern
(Reaction-Diffusion-Advection system)



[Brena-Medina, A., Champneys, Ward]

Steady states

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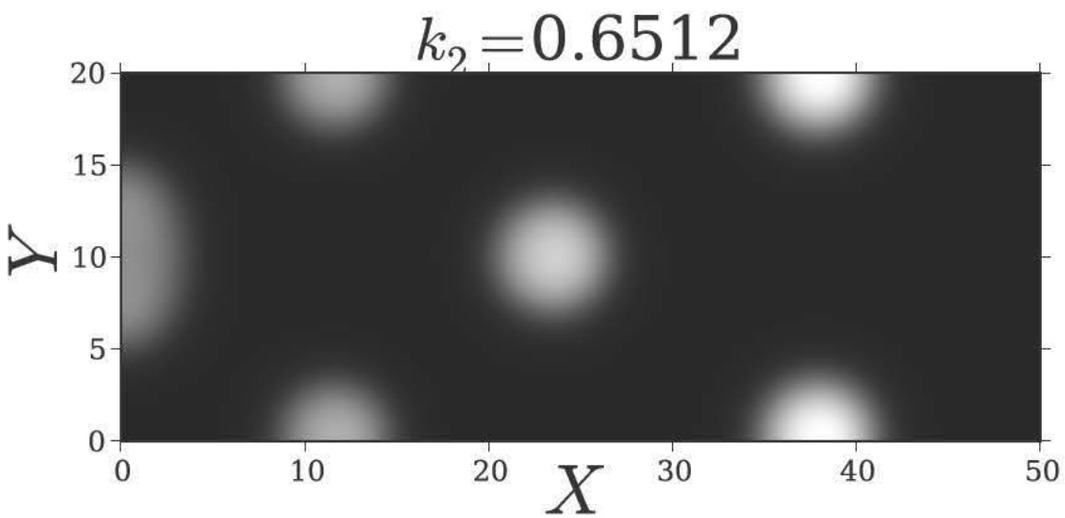
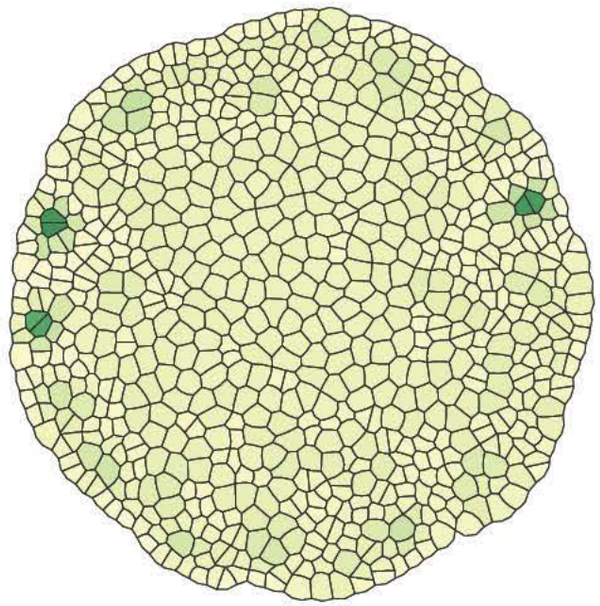


[Brena-Medina, A., Champneys, Ward]

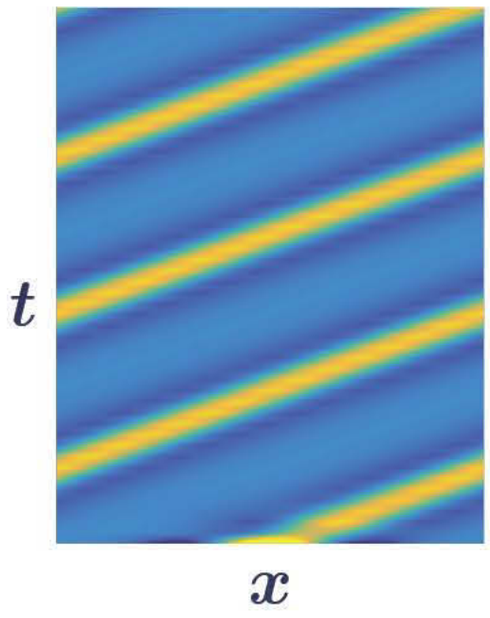
Localised auxin spots (plant root section)



[Draelants, A., Vanroose]

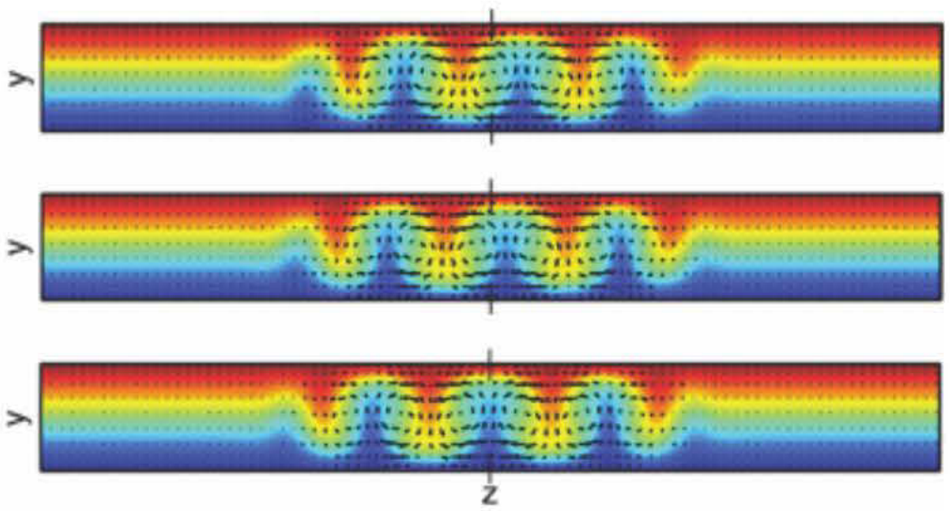
Travelling waves

Travelling wave (Neural Markov-chain)



[A., Wedgwood]

Travelling wave (Navier-Stokes)



[Schneider, Gibson, Burke]

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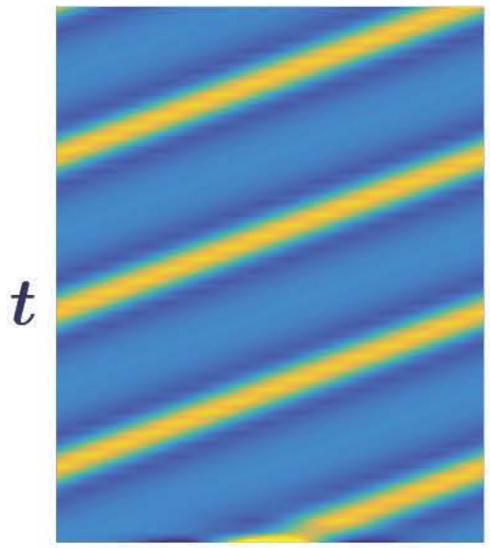

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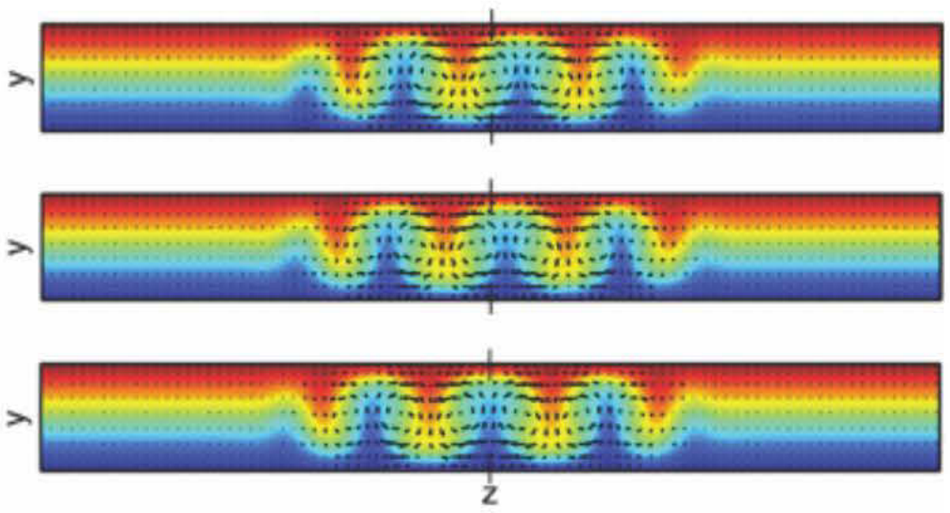
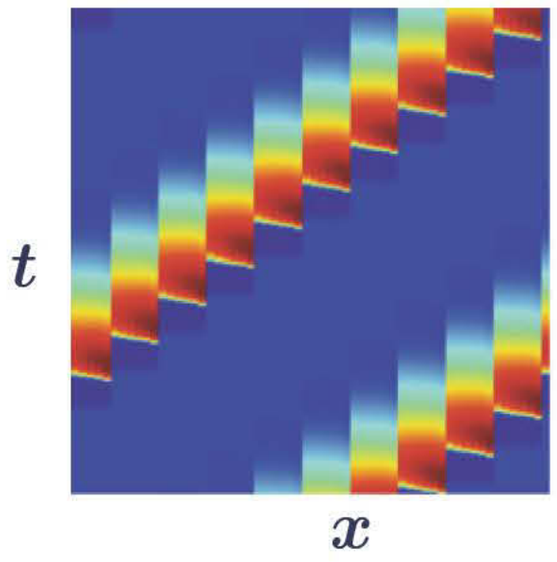


[Schneider, Gibson, Burke]

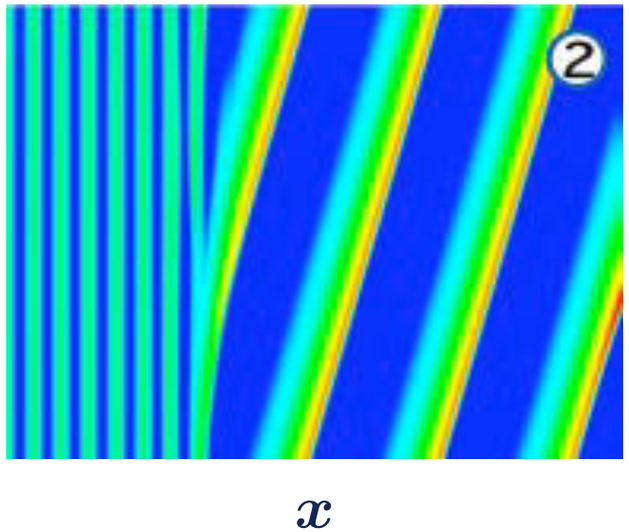
Lurching wave (Neural field model)



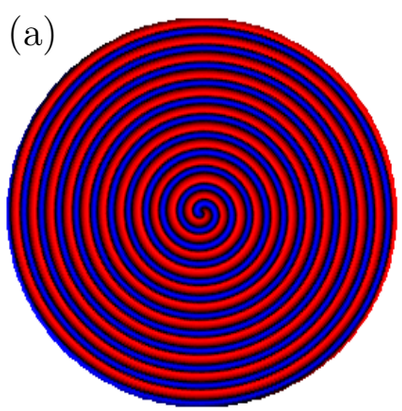
[Wasylenko, Cisternas, Laing, Kevrekidis]

Other examples of coherent structures

Defect/spiral waves
(Reaction-diffusion system)



[A.]



[Wheeler, Barkley]

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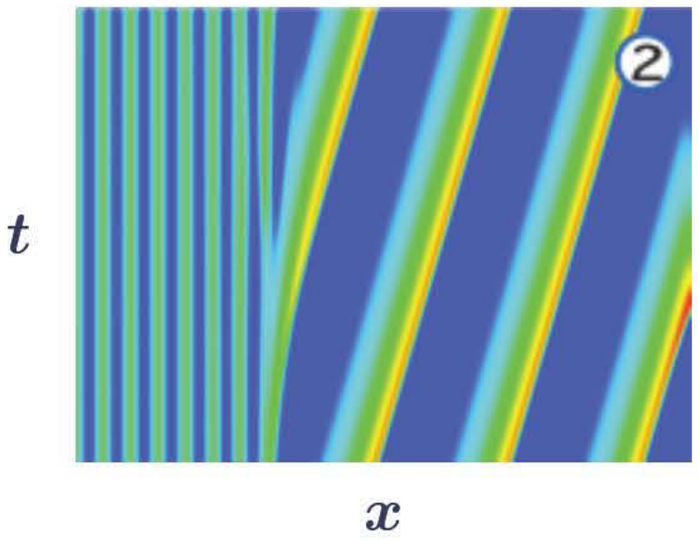
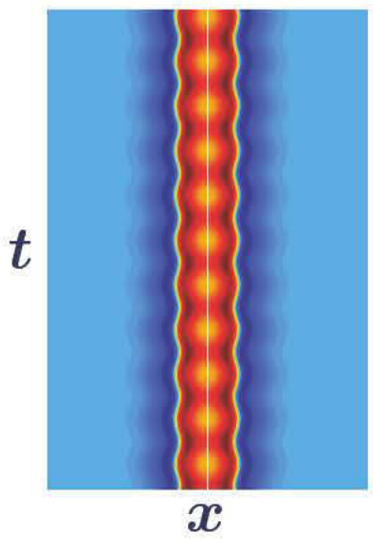


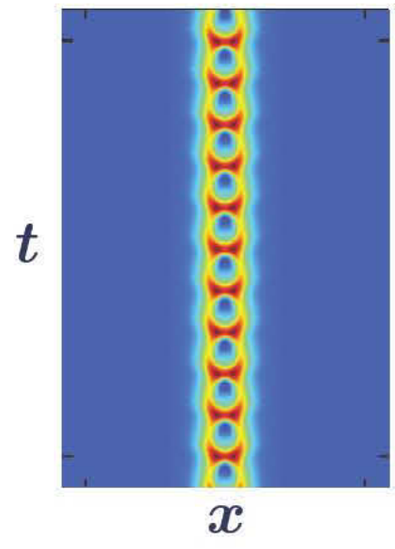
[A.]

Oscillon (Neural field)

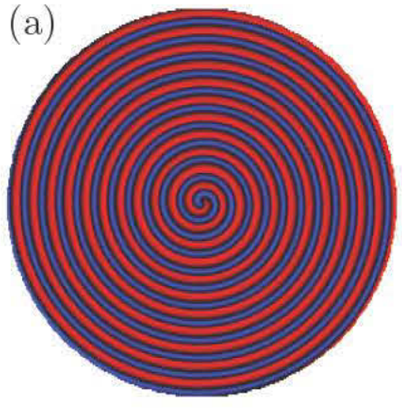


[Coombes, Schmidt, A.]

Oscillons (Complex Ginzburg-Landau Eq.)



[Burke, Yochelis, Knobloch]



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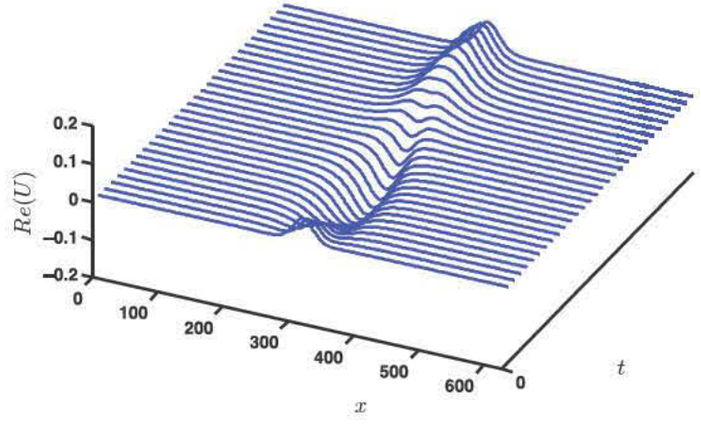

[Alnahdi, Niesen, Rucklidge]

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Time stepping

Example of time stepping

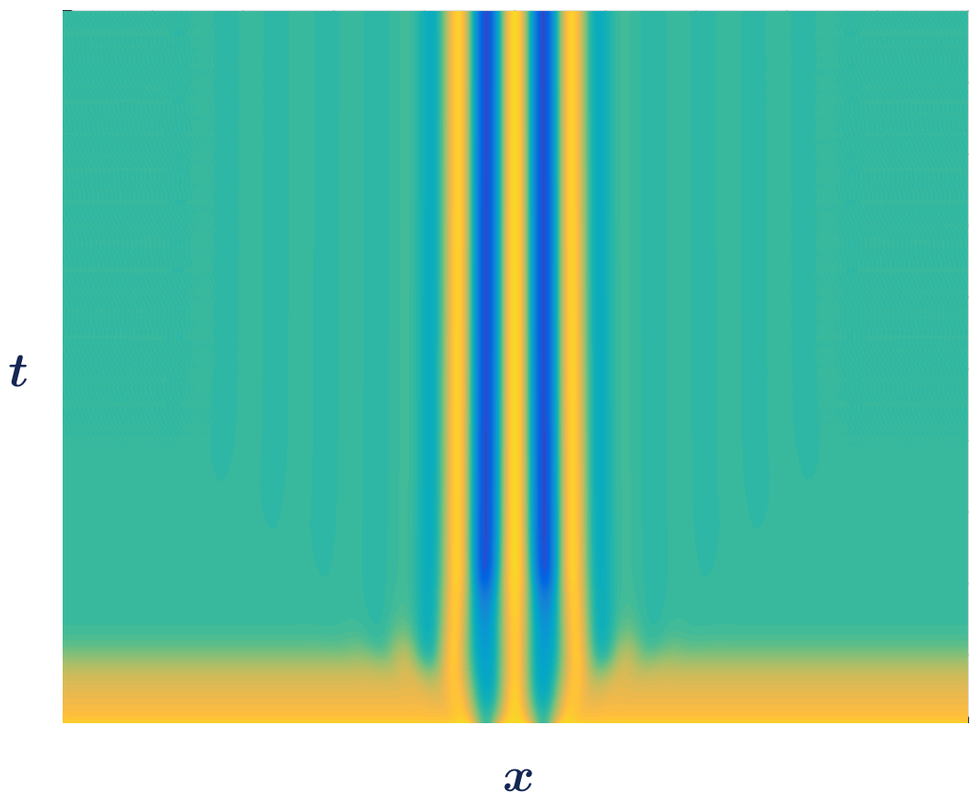
- 1D spatial domain $\Omega = [-L, L) \in \mathbb{R}$

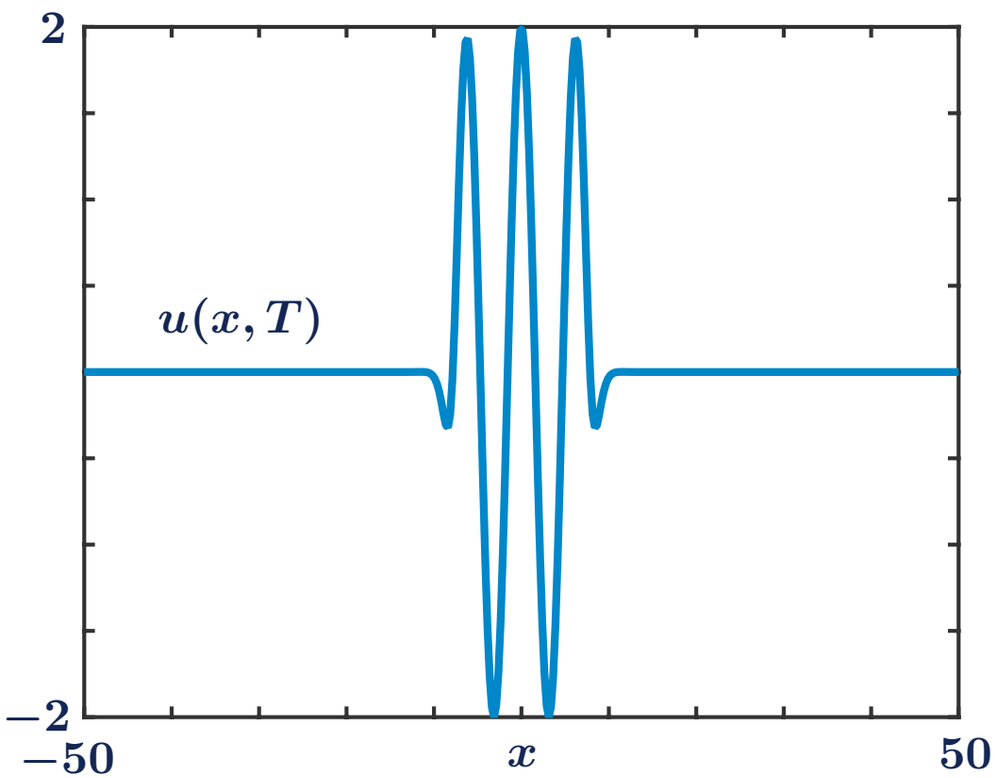
- Swift-Hohenberg equation with cubic-quintic nonlinearity

  $\partial_t u = -(1 + \partial_x^2)^2 u - \mu u + \nu u^3 - u^5$

- Periodic boundary conditions

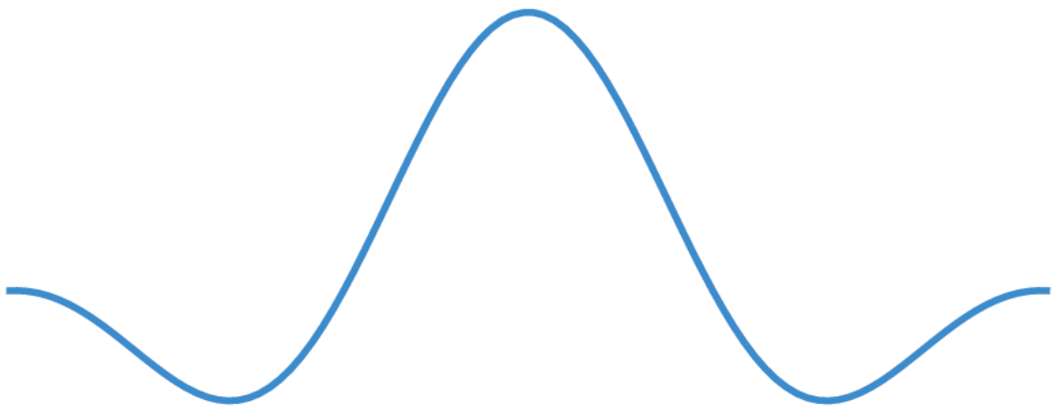
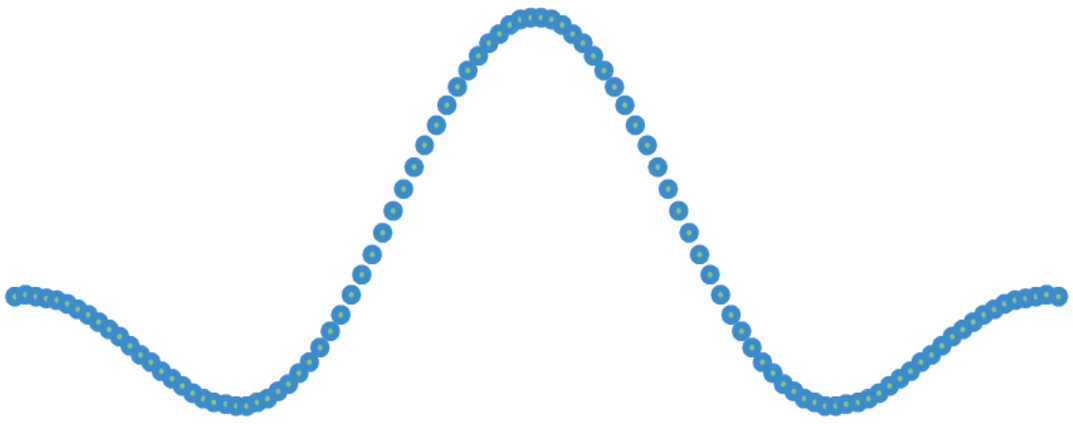
- Localised initial condition $u(x, 0) = 2 + \cos(x)[\tanh(x + 8) - \tanh(x - 8)]$





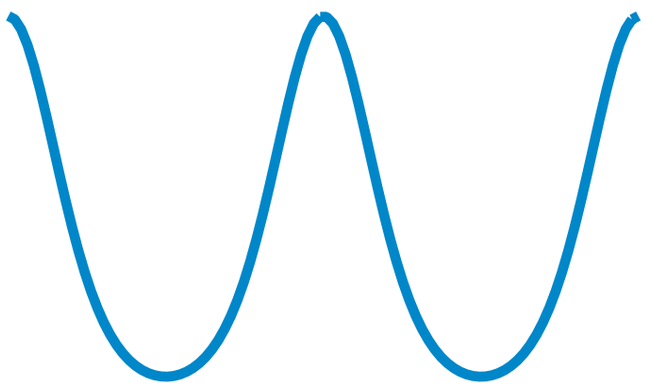
Method of lines

- A possible strategy is to use the method of lines
  1. Discretise spatial coordinate in the PDE
  2. Time step the resulting ODE

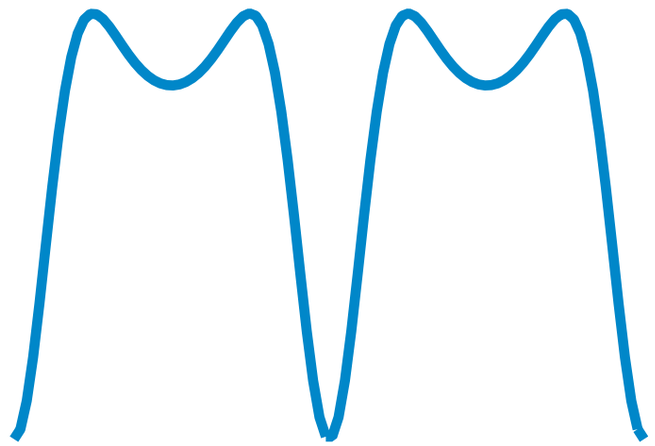
Continuum		Discrete
		
$u(x,t)$	State	$U(t), U_i(t) \approx u(x_i,t)$
$\mathcal{F}(u)$	Nonlinear operator	$F(U), F_i(U) \approx \mathcal{F}(u)(x_i)$
$\partial_t u = \mathcal{F}(u)$	Evolution equation	$\dot{U} = F(U)$

Approximation of derivatives [Trefethen]

- Differential operator $\partial_{xx} : u(x) \mapsto v(x) = u''(x)$



$$u \mapsto \partial_{xx} u$$

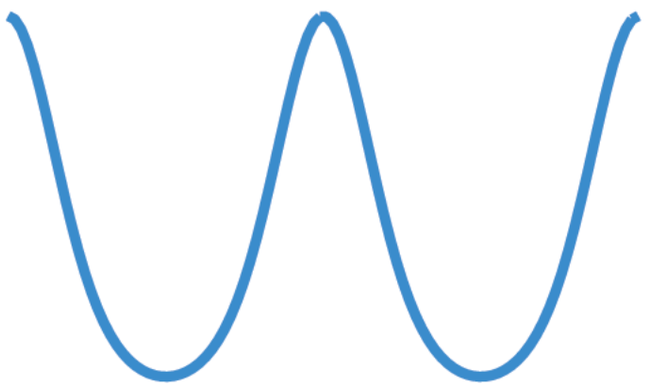


$$u(x) = \exp\left(\cos\frac{4\pi x}{L}\right)$$

$$\partial_{xx} u(x) = \frac{16\pi^2}{L^2} e^{\cos\frac{4\pi x}{L}} \left[\sin^2\frac{4\pi x}{L} - \cos\frac{4\pi x}{L}\right]$$

Approximation of derivatives [Trefethen]

- **Differential operator** $\partial_{xx} : u(x) \mapsto v(x) = u''(x)$



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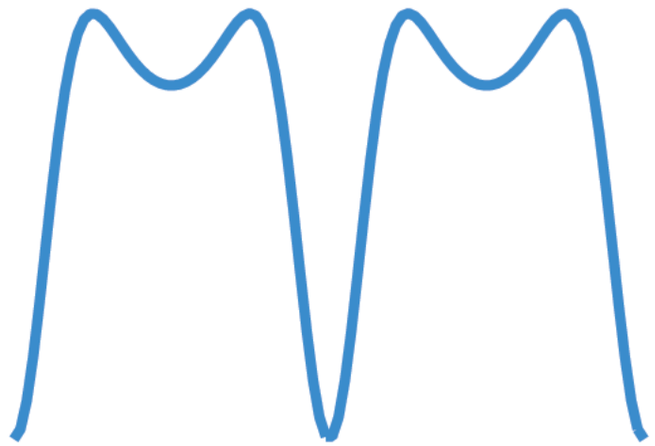

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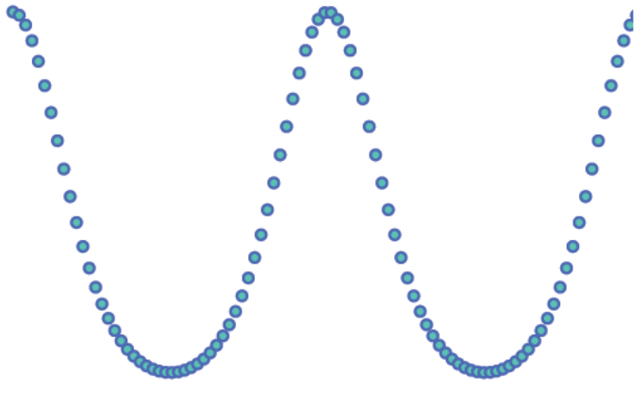
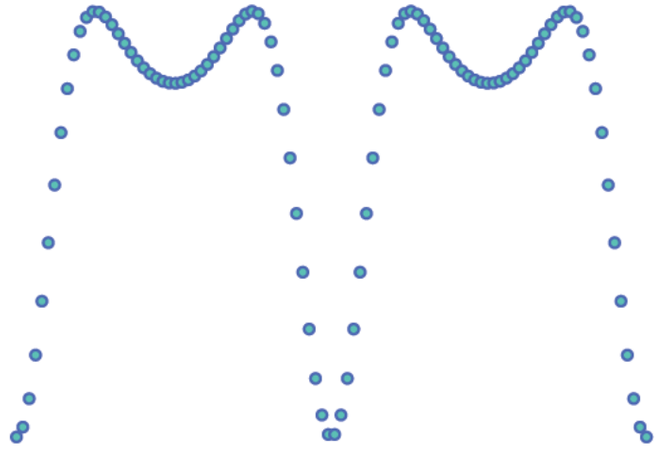
- **Differentiation matrix** $D_{xx} : U \mapsto V, \quad V_i = \dfrac{U_{i+1} - 2U_i + U_{i-1}}{h_x^2} \approx u''(x_i)$



$$U \mapsto D_{xx} U$$



Discretising the Swift-Hohenberg operator

- Swift-Hohenberg equation with cubic-quintic nonlinearity

$$\partial_t u = \mathcal{F}(u) \qquad \mathcal{F}(u) = -(1+\partial_x^2)^2 u - \mu u + \nu u^3 - u^5$$

- Discretised Swift-Hohenberg equation with cubic-quintic nonlinearity

$$\dot{U} = F(U) \qquad F(U) = -(I_n + D_{xx})^2 U - \mu U + \nu U^{\odot 3} - U^{\odot 5}$$

- Note the Hadamard product/power symbol (component-wise product/power)

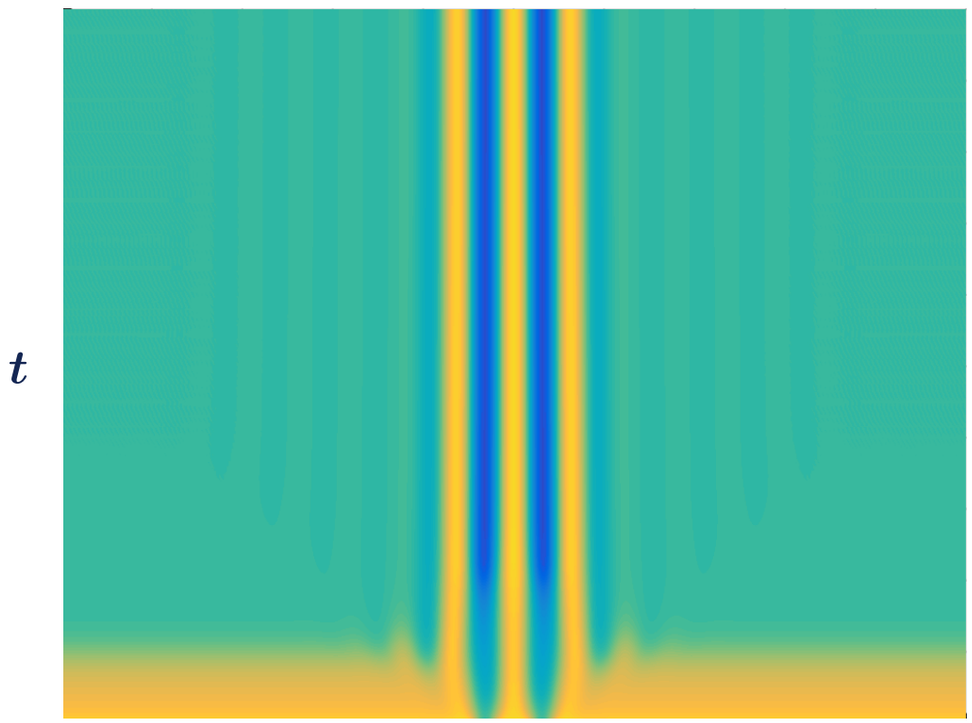
  Product between vectors $(U \odot V)_i = U_i V_i$

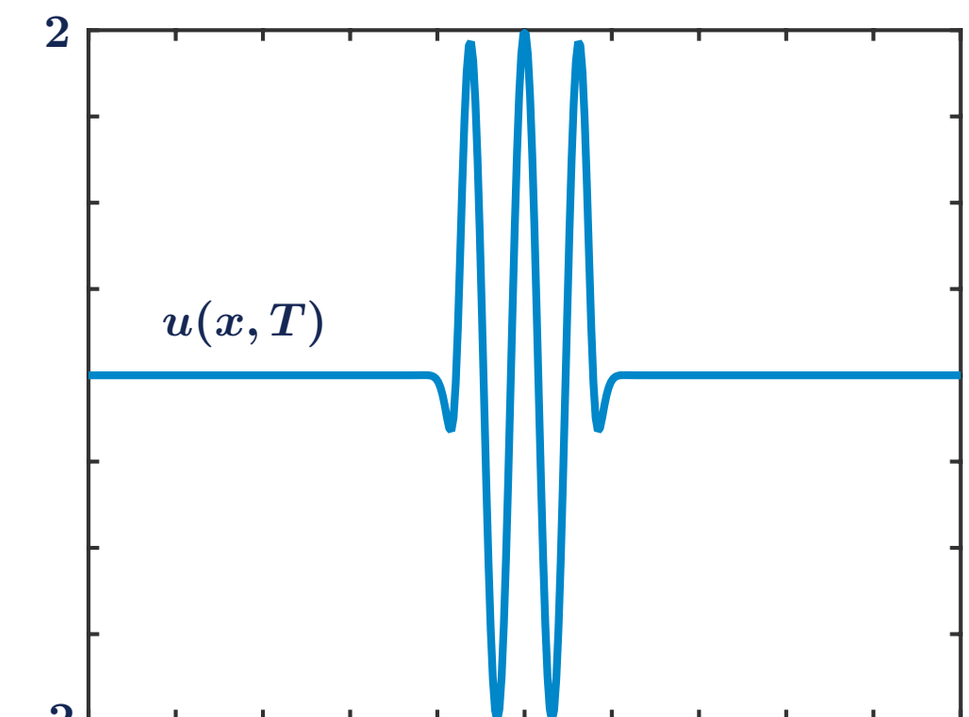
  Power of a vector $(U^{\odot 3})_i = (U \odot U \odot U)_i = U_i^3$

- The similarity between $\mathcal{F}(u)$ and $F(U)$ is striking (and useful in practice)!

Comments on time stepping

See Codes





- Discretised Swift-Hohenberg equation with cubic-quintic nonlinearity

$$\dot{U} = F(U) \qquad F(U) = -(I_n + D_{xx})^2 U - \mu U + \nu U^{\odot 3} - U^{\odot 5}$$

- I used standard stiff ODE integrators, but other choices are available/advisable
  1. Semi-implicit time-steppers
  2. Splitting methods
  3. Exponential time steppers
  4. Other problem-dependent time steppers (symplectic integrators, etc.)

Numerical continuation

Numerical continuation - introduction

- We want to study how steady states of $\partial_t u = \mathcal{F}(u; p)$ depend upon parameters

- In principle, we could change p and perform a new simulation. However
  1. There may be long transients before a new steady state is reached
  2. Only *stable* steady states are observable with time simulations
  3. For fixed p there may coexisting steady states, and which one is found depends on the initial condition

- Main idea behind numerical continuation:
  1. Start from (u_0, p_0) such that $\mathcal{F}(u_0, p_0) = 0$
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  4. Solutions are collected into branches with possibly different symmetry properties
  5. Can be applied to periodic orbits, travelling waves, spiral waves

Continuation of steady states in ODEs

See Codes

- **Evolution equation**

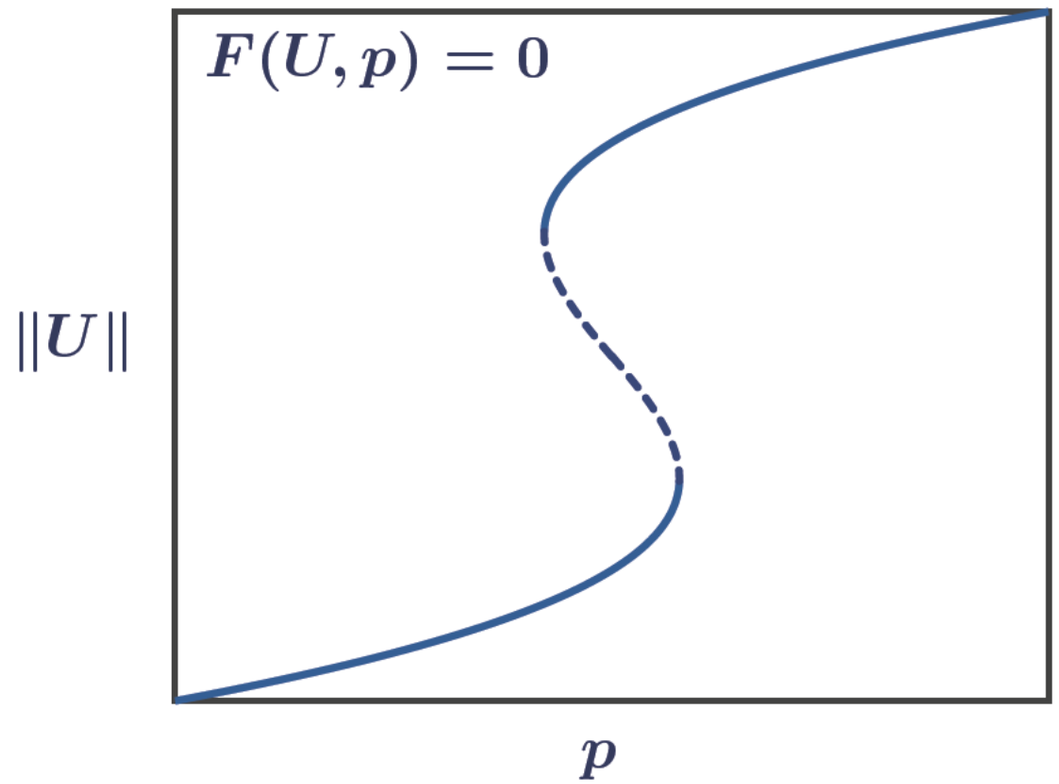
$$\dot{U} = F(U; p)$$

- **Branch of steady states**

$$F(U(s), p(s)) = 0$$

- **Stability of a steady state** (U_*, p_*)

$$D_U F(U_*, p_*)\tilde{U} = \lambda \tilde{U}$$



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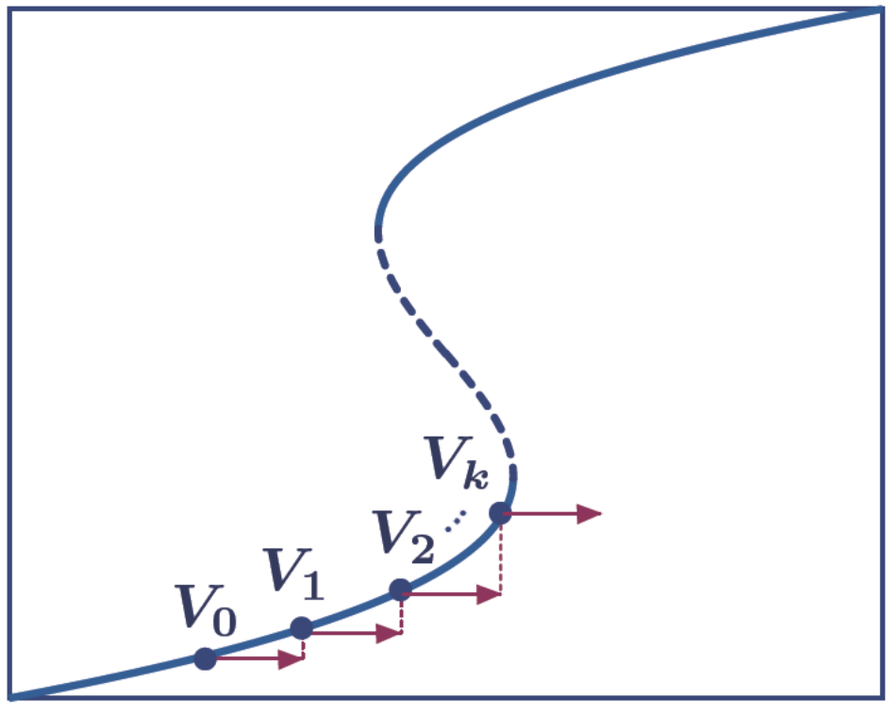

- **Assume knowledge of** $V_0 = (U_0, p_0) \in \mathbb{R}^{n+1}$ **such that** $F(U_0, p_0) = 0$

1. Fix h
2. For each $k > 0$ find (U, p) such that

$$\begin{aligned} F(U, p) &= 0 \\ p - p^{k-1} - h &= 0 \end{aligned} \qquad \text{or} \qquad G(V; p^{k-1}, h) = 0$$

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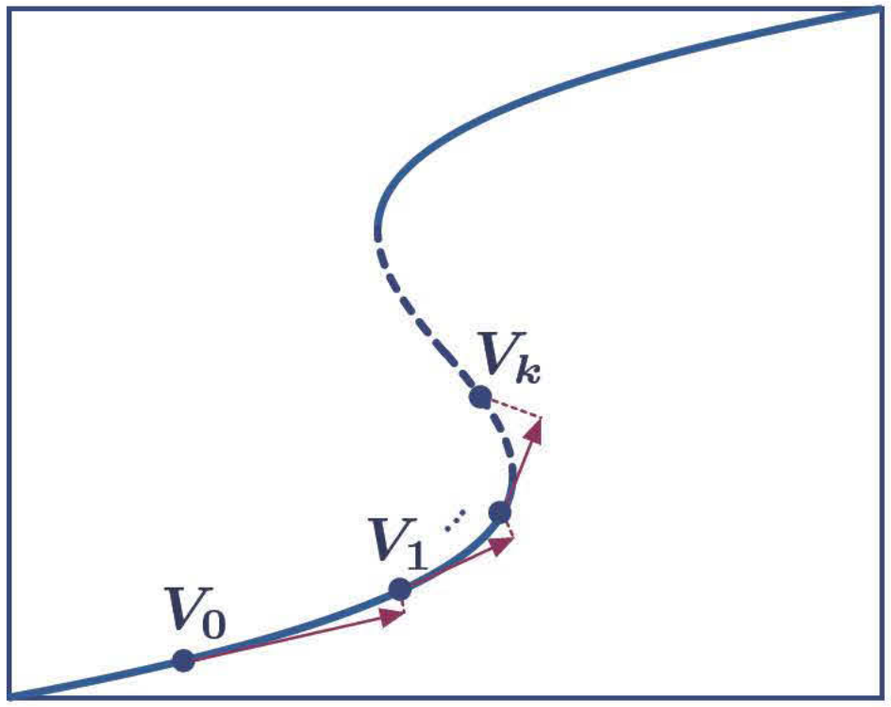

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  2. For each $k > 0$
     A. Predict along the tangent $\tilde{V}_k = V_k + hT_k$
     B. Correct in the normal direction: find V such that

$$\begin{aligned} F(V) &= 0 \\ \langle V - \tilde{V}_k, hV_k \rangle &= 0 \end{aligned} \qquad \text{or} \qquad G(V; V_k, \tilde{V}_k, h) = 0$$

Newton's method

- At each continuation step, we solve the problem $G(V) = 0$
- Newton's method with initial guess V_0 : repeat until convergence
  1. Solve $D_V G(V_l)\tilde{V}_l = -G(V_l)$ for $\tilde{V}_l$
  2. Compute $V_{l+1} = V_l + \tilde{V}_l$
- At each continuation step we need to solve *several* linear problems
- In any continuation package, the functions $G(V)$, $D_V G(V)$ are constructed automatically from $F(U,p)$, $D_U F(U,p)$, $D_p F(U,p)$, which are provided by the user
- For PDEs, most computational time is spent in function evaluations and solutions of large linear problems

Application to the Swift-Hohenberg operator

- Fix μ, ν. Find u such that

$$-(1+\partial_x^2)^2 u - \mu u + \nu u^3 - u^5 = 0$$
$$u(L,t) - u(-L,t) = 0$$

or

$$\mathcal{F}(u) = 0$$
$$\mathcal{B}(u) = 0$$

Application to the Swift-Hohenberg operator

- Swift-Hohenberg operator and its Fréchet Derivative at u

$$\mathcal{F}(u) = -(1+\partial_x^2)^2 u - \mu u + \nu u^3 - u^5$$

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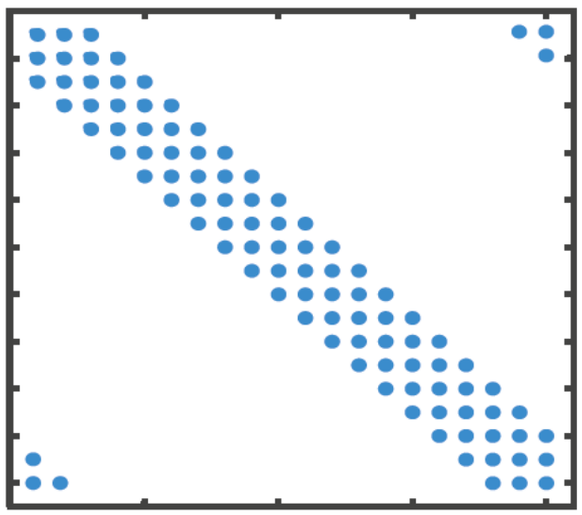
- Sparsity pattern example $n = 20$

$$D_U F(U) =$$



$$-(I_n + D_{xx})^2$$

Fixed!

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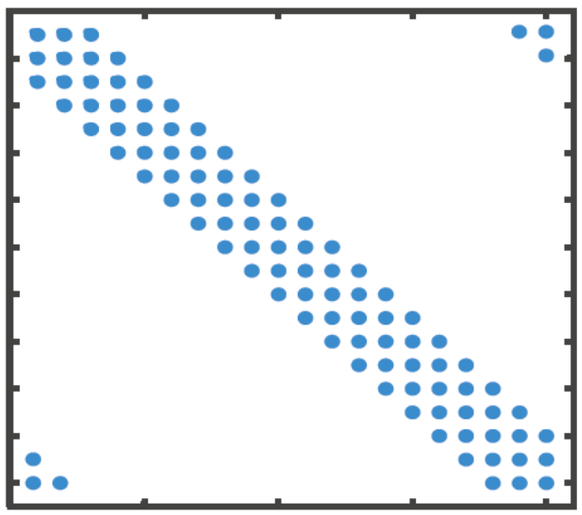
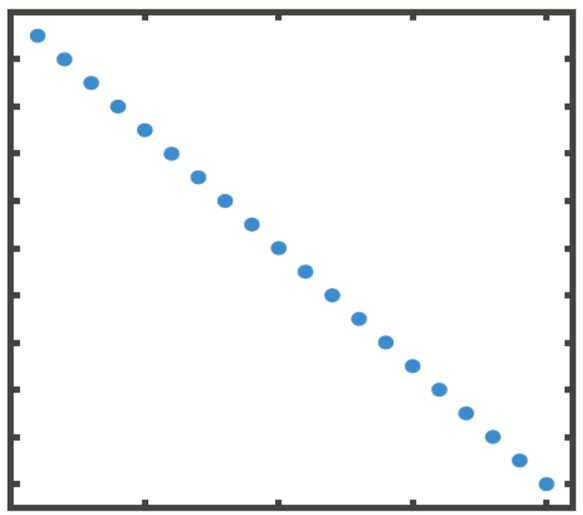


$$+$$



$-(I_n + D_{xx})^2$

Fixed!

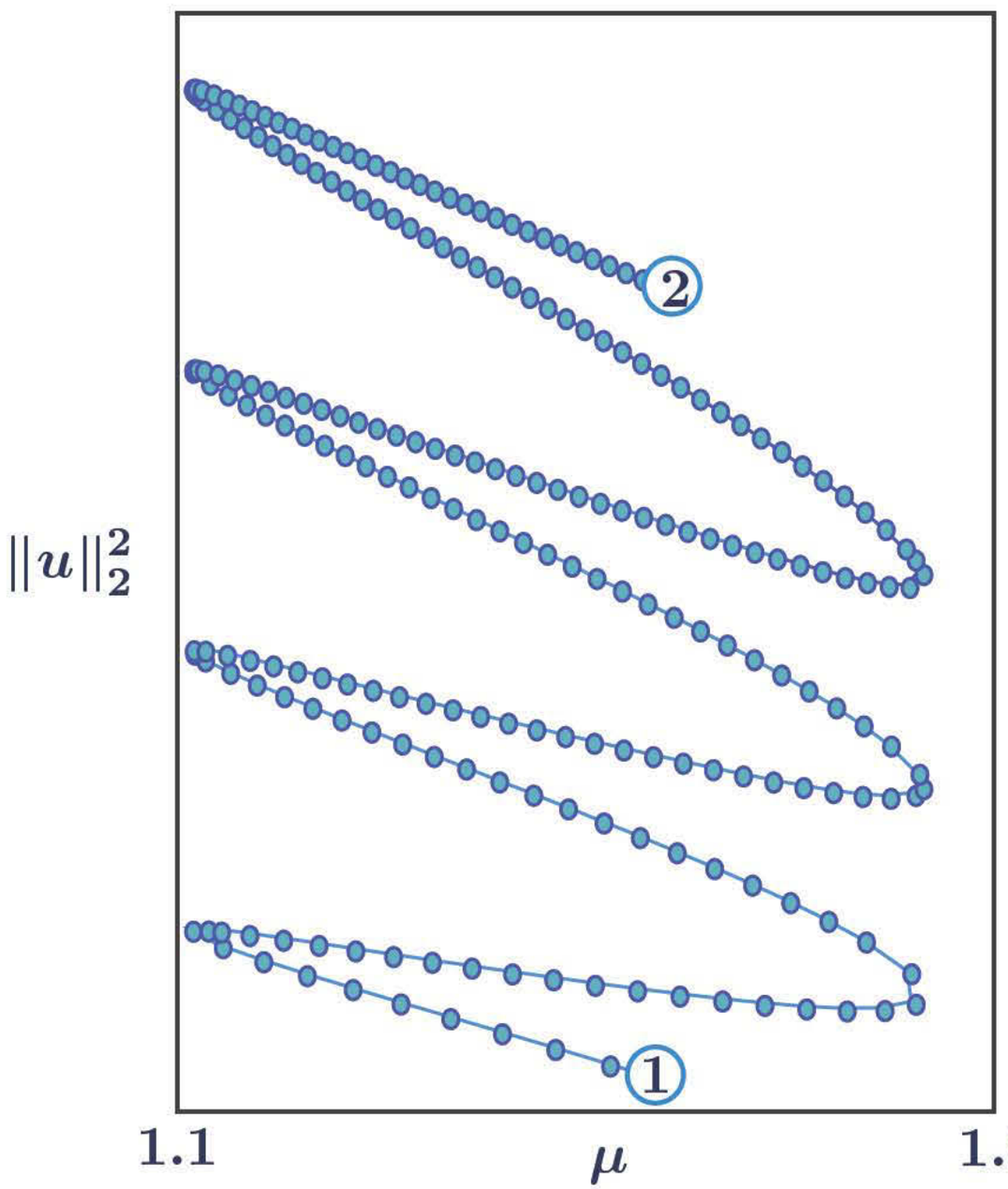
$-\mu I_n + \mathrm{diag}(3U^{\odot 2} - 5U^{\odot 4})$

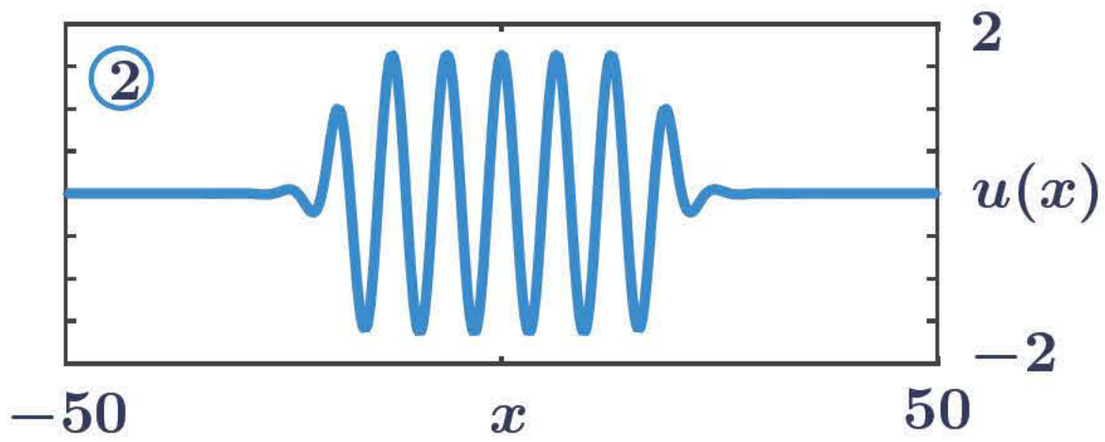
Variable

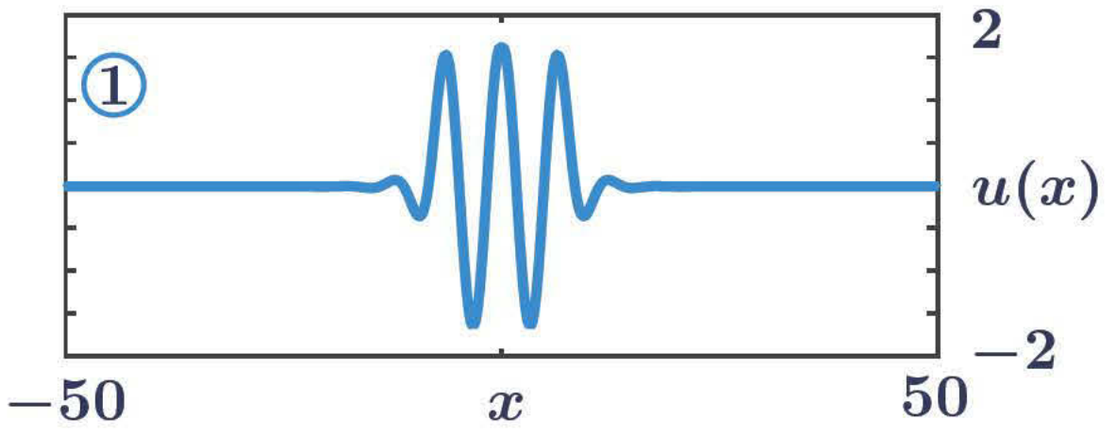
Example of numerical continuation

See Codes

$$\Omega = (-50, 50),\ \nu = 3,\ n = 400$$







Linear stability

Linear stability of steady states

- Equilibrium u_* of the evolution equation

$$\partial_t u = \mathcal{F}(u), \qquad \mathcal{F}(u_*) = 0$$

- Study the evolution of *small* perturbations to u_*

$$u(x,t) = u_*(x) + \varepsilon \tilde{u}(x,t), \qquad 0 < \varepsilon \ll 1, \quad \|\tilde{u}\| = \mathcal{O}(1)$$

- At $\mathcal{O}(\varepsilon)$, the perturbations evolve according to

$$\partial_t \tilde{u} = \partial_u \mathcal{F}(u_*)\tilde{u} := \mathcal{L}(u_*)\tilde{u}$$

- The ansatz $\tilde{u}(x,t) = e^{\lambda t}\psi(x)$ leads to the eigenvalue problem

$$\lambda \psi = \mathcal{L}(u_*)\psi$$

- The state u_* is linearly stable if $\mathrm{Spec}\left[\mathcal{L}(u_*)\right]$ is contained in the left half of the complex plane

Numerical calculations

See Codes

- Continuum problem

$$\lambda\psi = \mathcal{L}(u_*)\psi \qquad \mathcal{L}(u_*) = -(1+\partial_x^2)^2 - \mu + 3\nu u_*^2 - 5u_*^4$$

- Discrete problem

$$\lambda\Psi = L(U_*)\Psi \qquad L(U) = -(I_n + D_{xx})^2 - \mu I_n + \mathrm{diag}(3U^{\odot 2} - 5U^{\odot 4})$$

A function which computes L has already been used in the Newton iterations!

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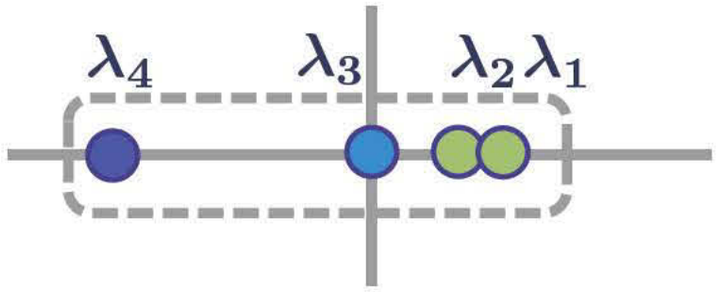
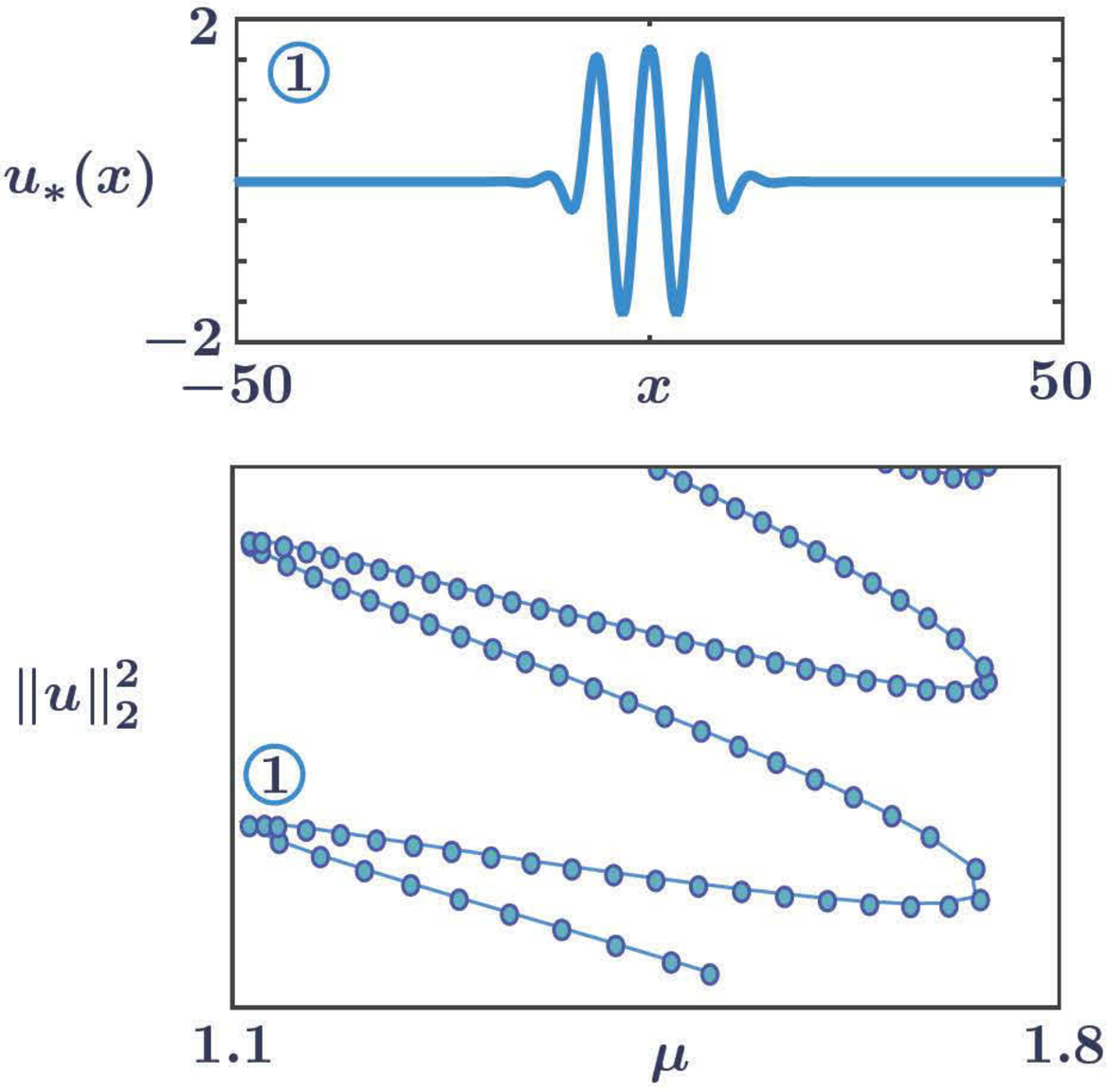
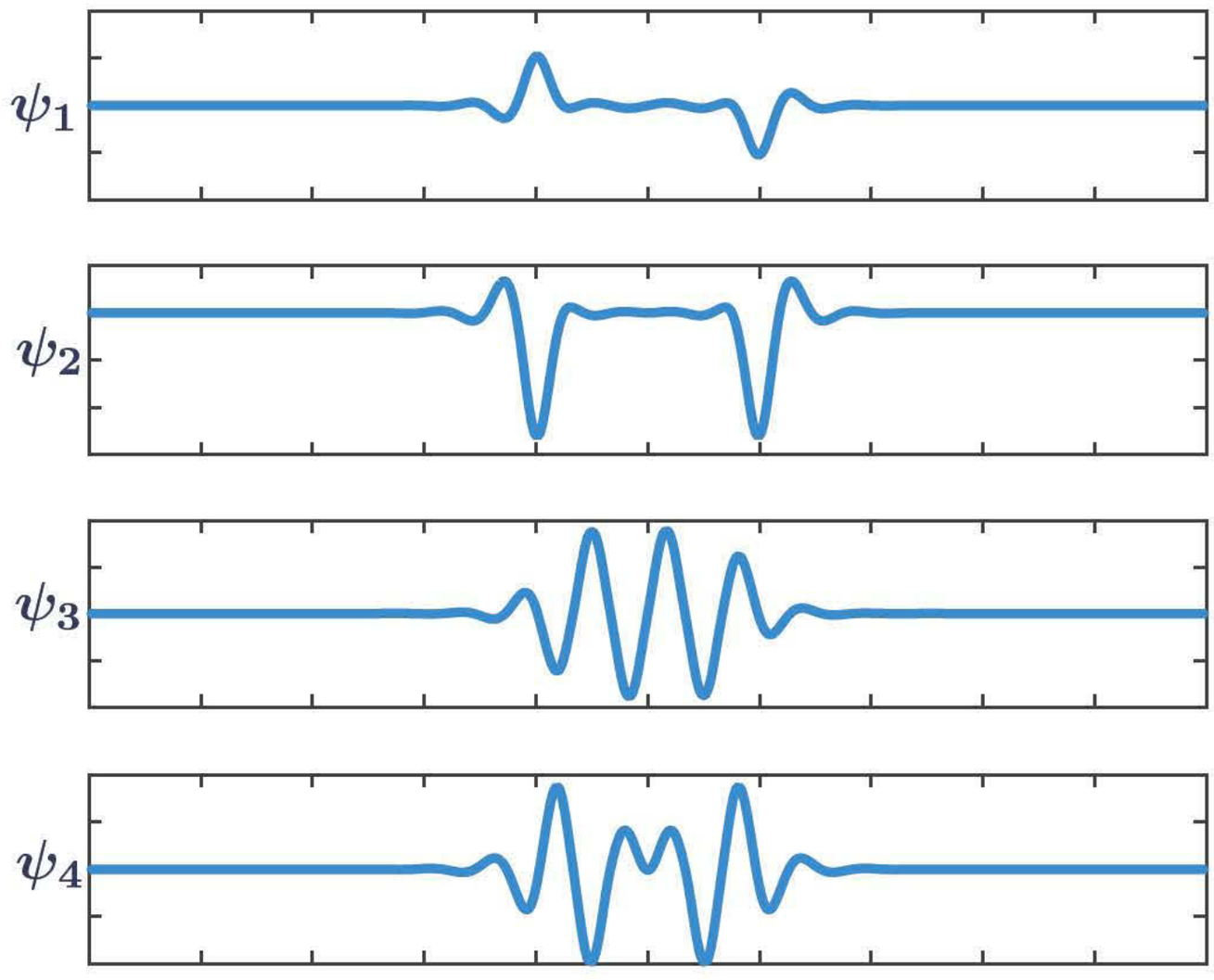
- Computations of eigenvalues
  1. Can be done on-the-fly, during continuation
  2. May be performed as a post-processing step

Results for a profile close to a saddle-node







Translation invariance

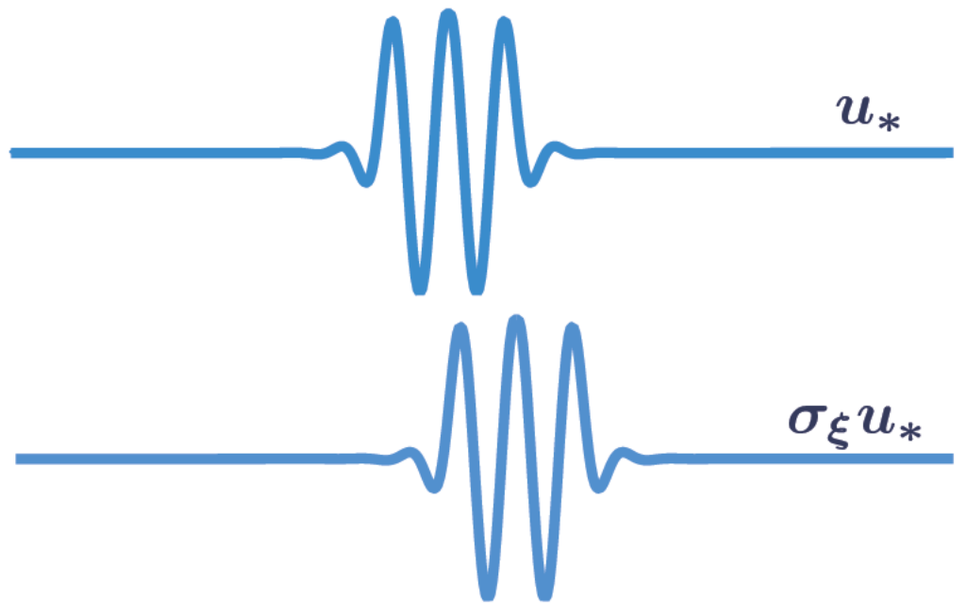
Translation invariance

- SH equation with periodic boundary conditions

$$\partial_t u = \mathcal{F}(u)$$

- Consider spatial translations via the action

$$\sigma_\xi : v(\cdot) \mapsto v(\cdot + \xi), \quad \xi \in \mathbb{R}$$



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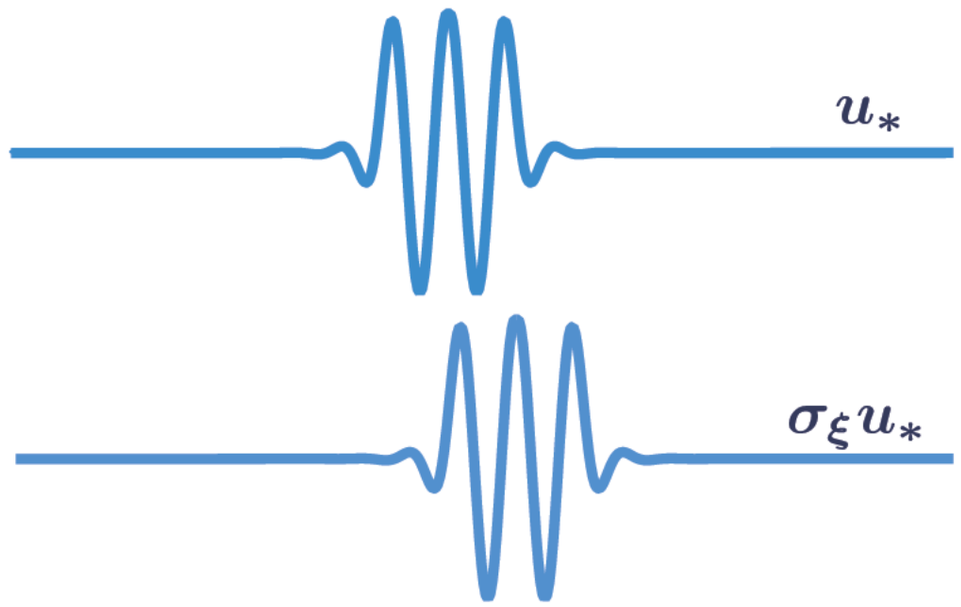

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$$\sigma_\xi : v(\cdot) \mapsto v(\cdot + \xi), \quad \xi \in \mathbb{R}$$

- The SH operator is equivariant under this action, that is, $\sigma_\xi \mathcal{F}(u) = \mathcal{F}(\sigma_\xi u)$

$$\begin{aligned}
\sigma_\xi \mathcal{F}(u) &= \sigma_\xi \big[-(1+\partial_x^2)^2 u - \mu u + \nu u^3 - u^5 \big] \\
&= -(1+\partial_x^2)^2 \sigma_\xi u - \mu \sigma_\xi u + \nu (\sigma_\xi u)^3 - (\sigma_\xi u)^5 \\
&= \mathcal{F}(\sigma_\xi u)
\end{aligned}$$

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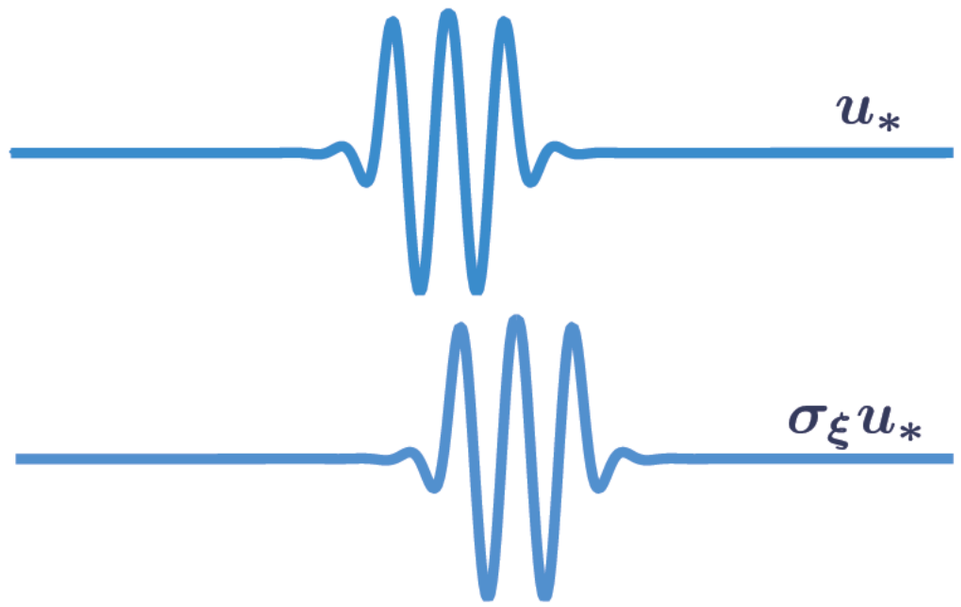

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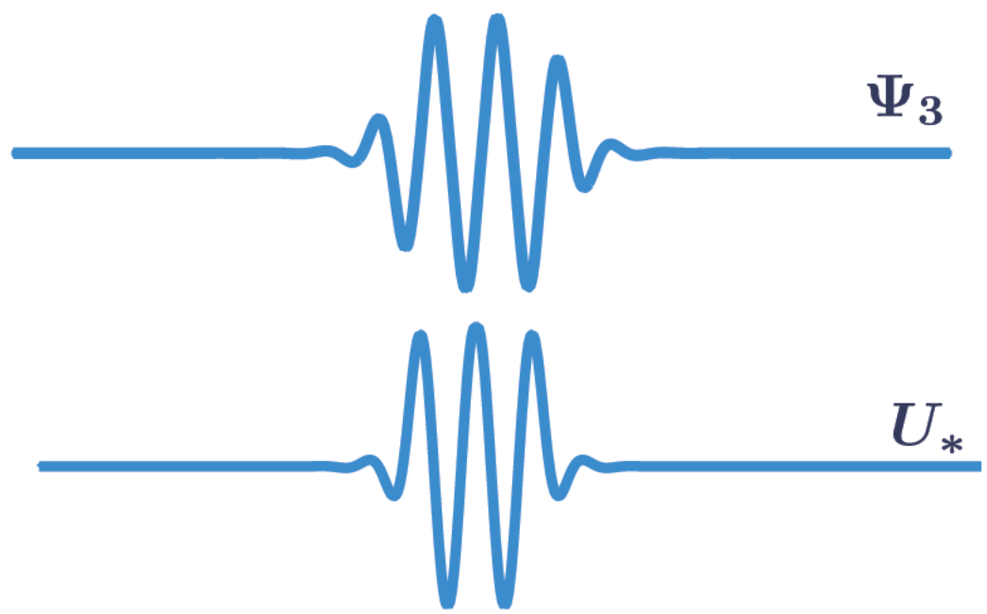
- Consequences of translation invariance:
  1. If $u_*(x)$ is a steady state, so is an arbitrary translation $u_*(x+\xi)$
  2. The operator $\partial_u \mathcal{F}(u_*)$ has an eigenvalue 0 corresponding to eigenfunction $\partial_x u_*$

Numerical considerations

- Our differentiation matrices impose periodicity
- We expect an eigenvalue $\lambda \approx 0$ with eigenvector $\Psi \approx D_x U_*$

$\lambda_3 \approx 7 \times 10^{-11}$



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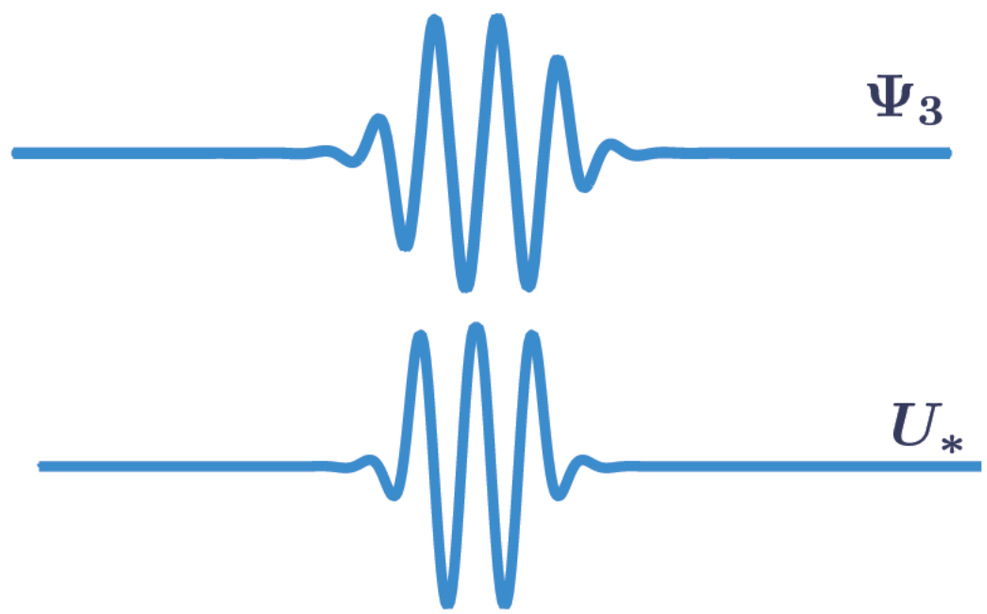

Numerical considerations

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- We expect an eigenvalue $\lambda \approx 0$ with eigenvector $\Psi \approx D_x U_*$
- This means $D_U F(U_*)$ is nearly singular.
- The solution U_* is not a regular zero of F

This is a disaster for Newton's iterates!

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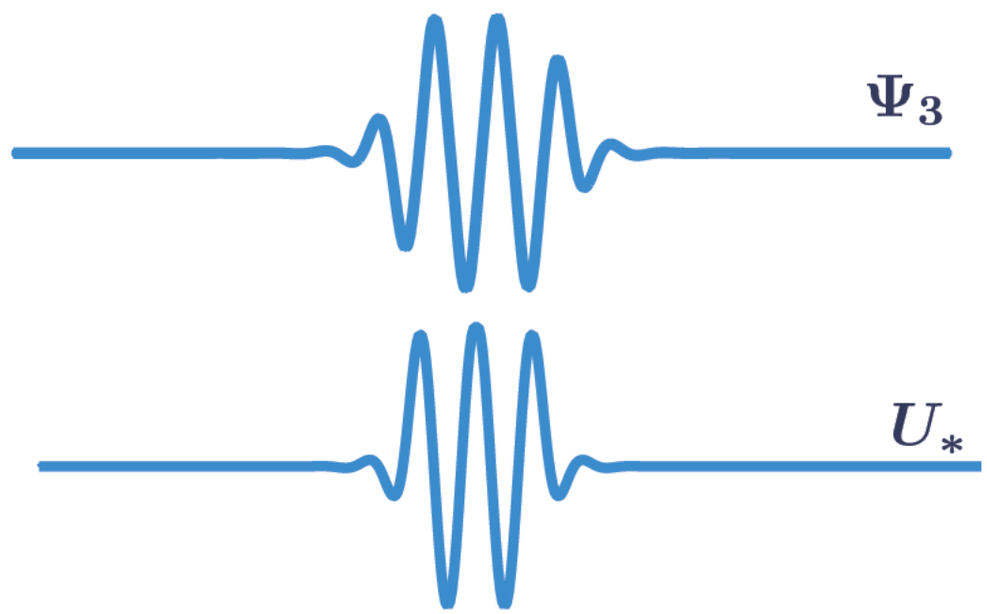

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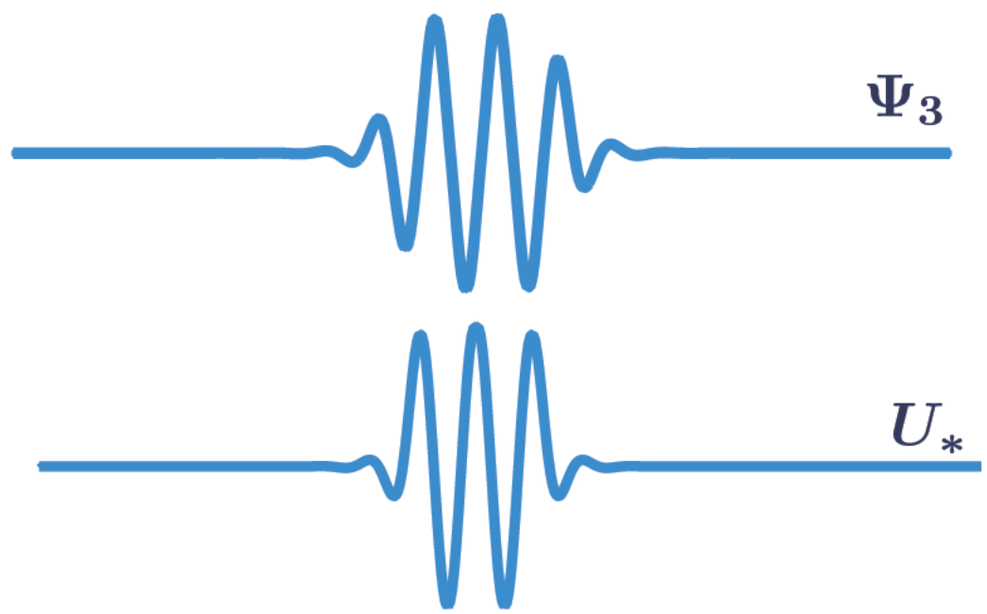

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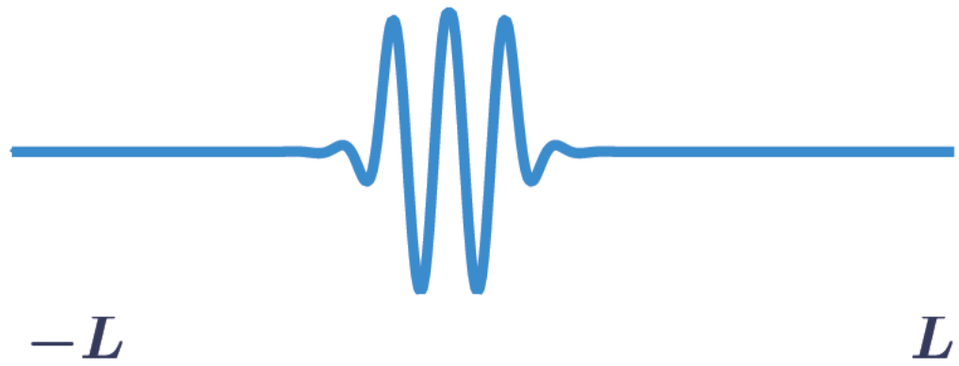
This is a disaster for Newton's iterates!

- Possible remedies:
  1. Remove invariance via boundary conditions
  2. Regularise the problem via a phase condition

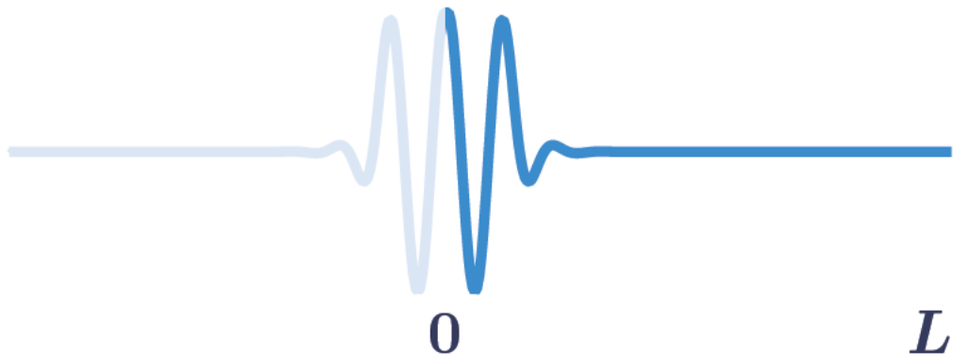
Regularisation via boundary conditions

See Codes



Regularisation via boundary conditions

See Codes



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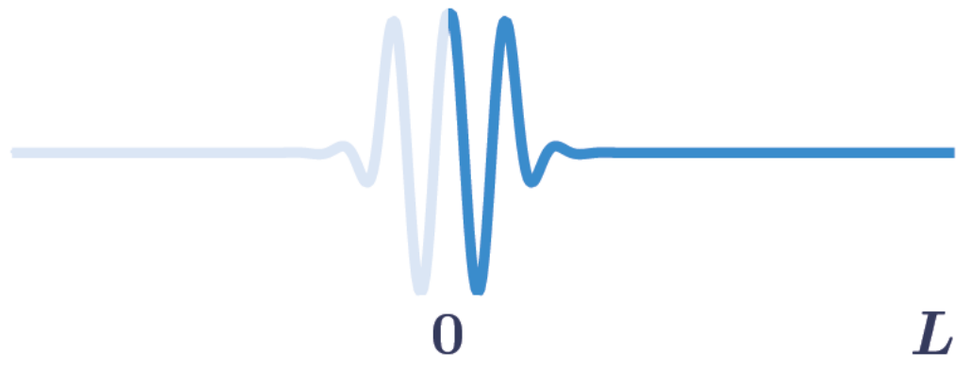

- Pose the problem on half-domain with Neumann boundary conditions

$$-(1+\partial_x^2)^2 u - \mu u + u^3 - u^5 = 0 \qquad x \in (0, L)$$

$$\partial_x u = 0, \quad \partial_x^3 u = 0 \qquad x = 0, L$$

Regularisation via boundary conditions

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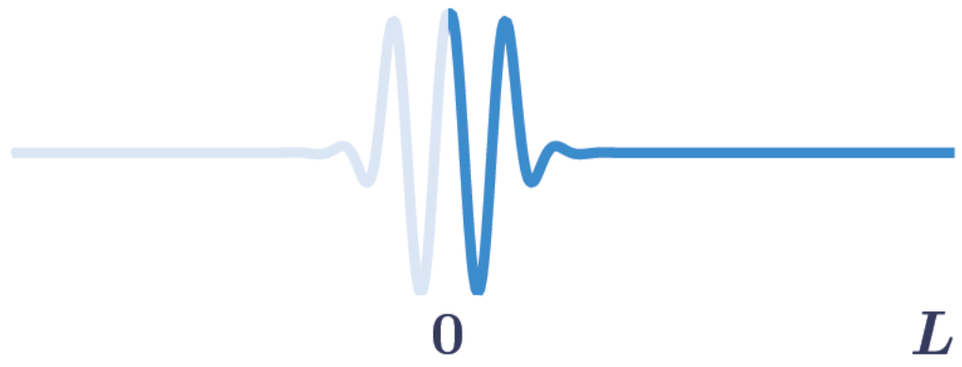

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  1. Only a change in differentiation matrix is required
  2. The same accuracy is obtained with half the number of grid points

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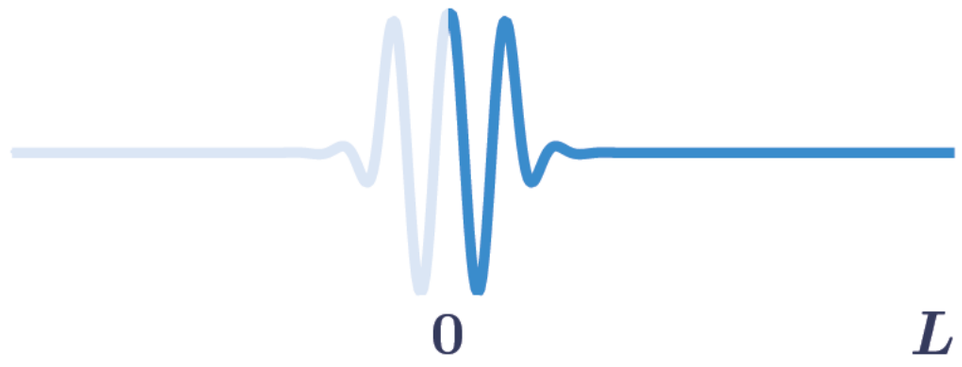

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- Advantages:
  1. Only a change in differentiation matrix is required
  2. The same accuracy is obtained with half the number of grid points

- Disadvantages:
  1. Only *even* solutions to the original BVP are computed
  2. Stability calculations require some amendments

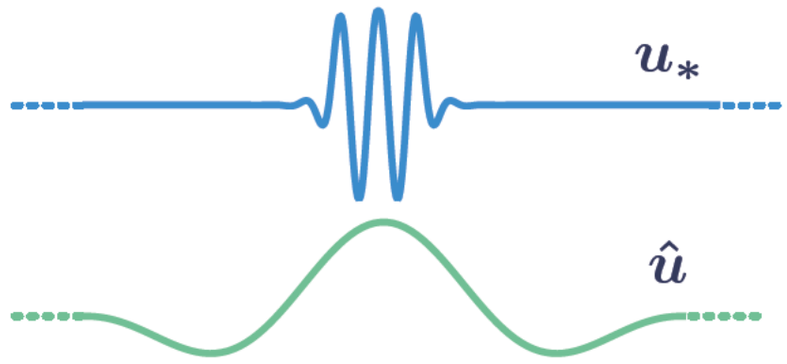
Regularisation via phase conditions

- Solve for (u, c) the following BVP with periodic boundary conditions

$$-(1+\partial_x^2)^2 u - \mu u + u^3 - u^5 + c\partial_x u = 0, \qquad x \in [-L, L)$$
$$\mathcal{B}_{\text{per}}(u) = 0$$
$$\varphi(u, \hat{u}) = 0$$

- Where
  1. The original BVP has been perturbed by a term $c\partial_x u$
  2. The solution $\hat{u}$ is a reference/template solution
  3. The last equation is a phase condition

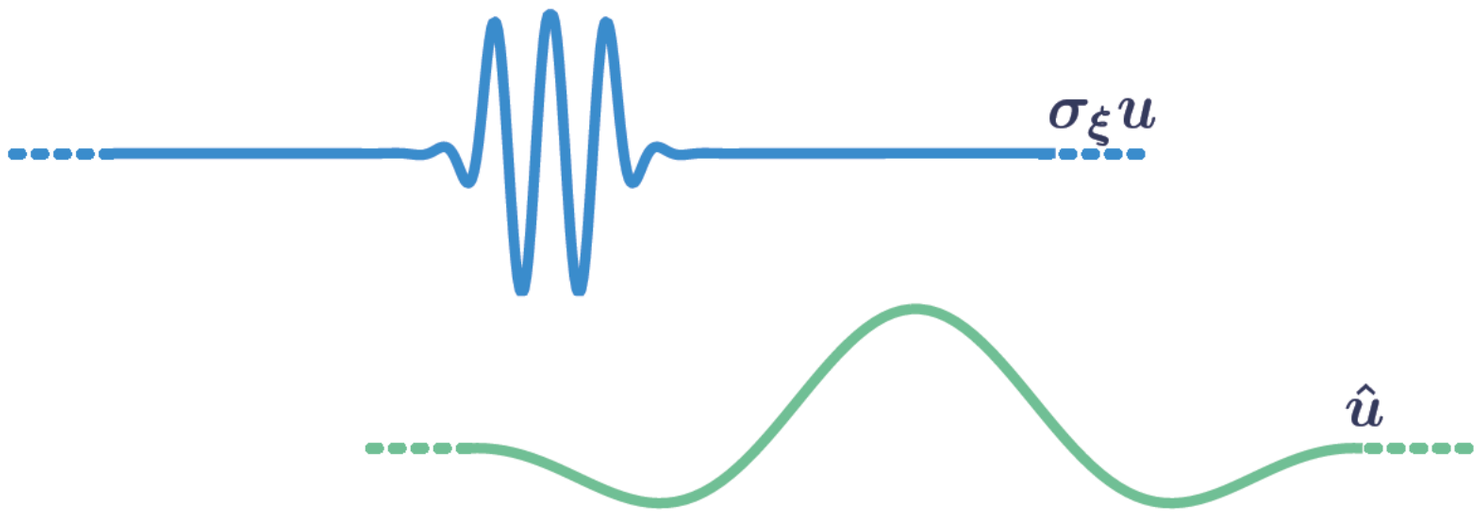
$$\varphi(u, \hat{u}) = \int_{-L}^{L} \partial_x \hat{u}(x)\big(u(x) - \hat{u}(x)\big)\, dx$$



- Things to note:
  1. $(u_*, 0)$ is a regular solution to the BVP above (Bordering Lemma)
  2. The phase condition tries to minimise the L_2-distance to the template solution

Phase condition

See Codes

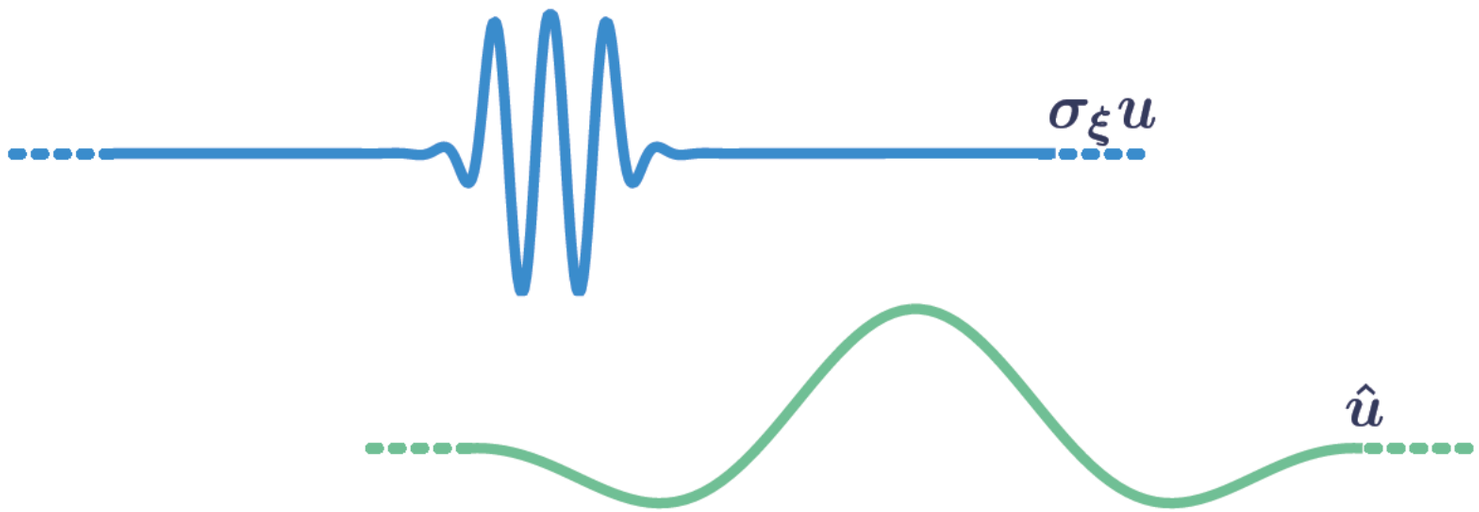


- Distance between shifted solution and reference function

$$\mathcal{D}(u,\xi) = \int_{-L}^{L} |u(x-\xi) - \hat{u}(x)|^2 \, dx = \|\sigma_\xi u - \hat{u}\|_{L_2}^2$$

Phase condition

See Codes



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- Differentiating w.r.t. ξ we obtain a necessary condition for a local minimum

$$\int_{-L}^{L} \partial_x \hat{u}(x) \big(u(x-\xi) - \hat{u}(x)\big) \, dx = 0$$

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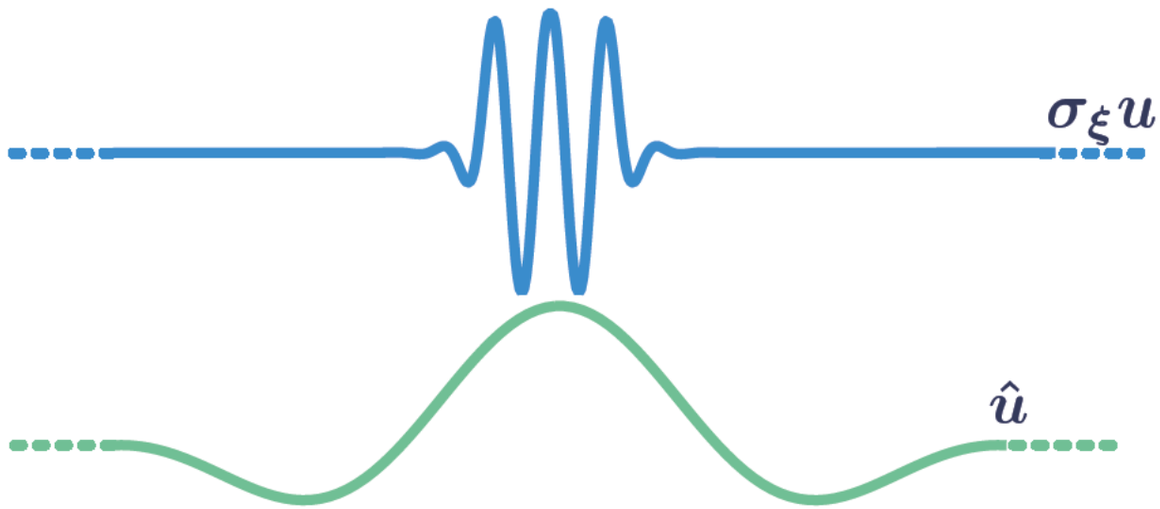
See Codes



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- The phase condition $\varphi(u,\hat{u}) = 0$ selects a solution for which the above equation holds at $\xi = 0$

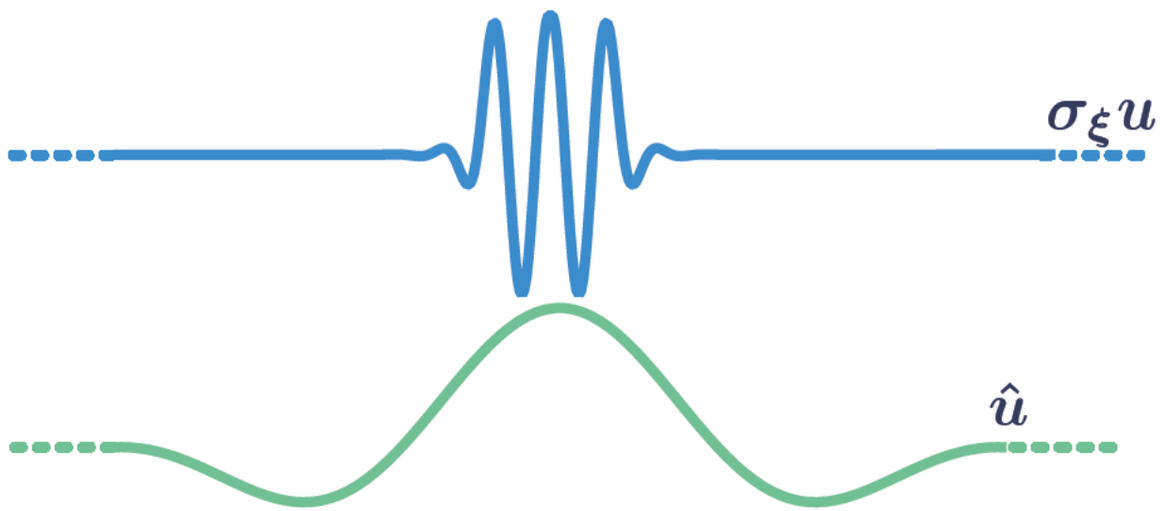
Phase condition

See Codes

[Doedel]

[Beyn, Thümmler]

[Champneys, Sandstede]



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- Phase conditions (and borderings) can be constructed for more general symmetries

Neural fields: PDE and integral form

Integral Neural Field Model

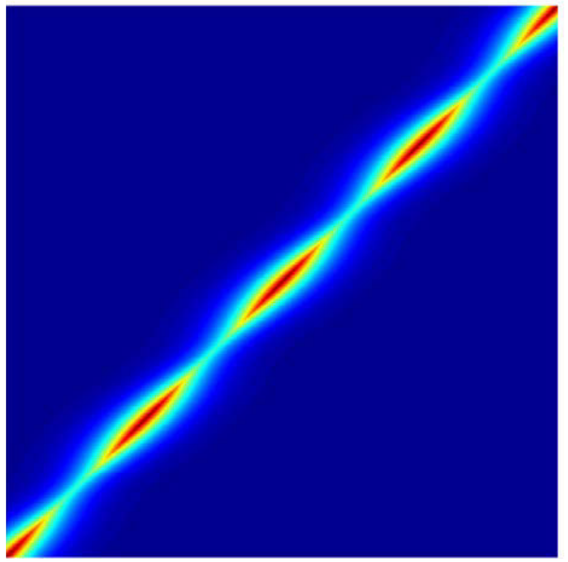
- **Wilson-Cowan-Amari neural field equation**

$$\partial_t u(x,t) = -u(x,t) + \int_{-\infty}^{\infty} W(x,y) f(u(y,t))\,\mathrm{d}y, \quad x \in \mathbb{R}$$

- **Heterogeneous connectivity function**

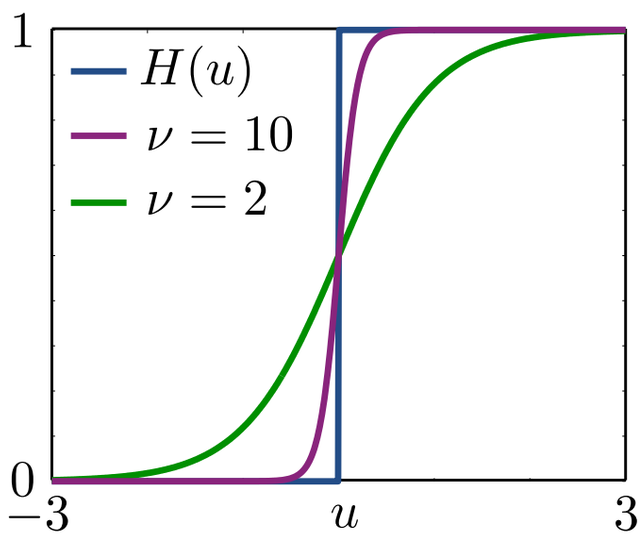
$$\begin{aligned} W(x,y;a,\varepsilon) &= w(|x-y|)A(y;a,\varepsilon) \\ &= \frac{1}{2} e^{-|x-y|}\big(1 + a\cos(y/\varepsilon)\big), \end{aligned}$$

$W(x,y)$



- **Firing rate function**

$$f(u;h,\nu) = \frac{1}{1+\exp(-\nu(u-h))}$$



[A. & Schmidt, Bressloff, Schmidt et al, Coombes & Laing]

PDE method [Laing]

- Fourier transform

$$\partial_t \hat{u}(\xi,t) = -\hat{u}(\xi,t) + \hat{w}(\xi)\widehat{\big(Af(u)\big)}(\xi,t),$$

where $\hat{w}(\xi) = P(\xi)/Q(\xi)$

- Inverse Fourier transform

$$\mathcal{L}_Q\left[\partial_t u + u\right] = \mathcal{L}_P\left[A(x)f(u;h,\nu)\right]$$

- For our choice of the kernel:

Evolution equation $$(1-\partial_x^2)\partial_t u = (\partial_x^2 - 1)u + A(x)f(u)$$

Steady states $$0 = (\partial_x^2 - 1)u + A(x)f(u)$$

Stability $$\lambda(1-\partial_x^2)\psi = \left[\partial_x^2 - 1 + A(x)f'(u)\right]\psi$$

PDE discretisation

See Codes

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- Form the matrix $M = I_n - D_{xx}$

  Time step using mass matrix $$M\dot{U} = -MU + A \odot f(U)$$

  Steady states continuation $$0 = -MU + A \odot f(U)$$

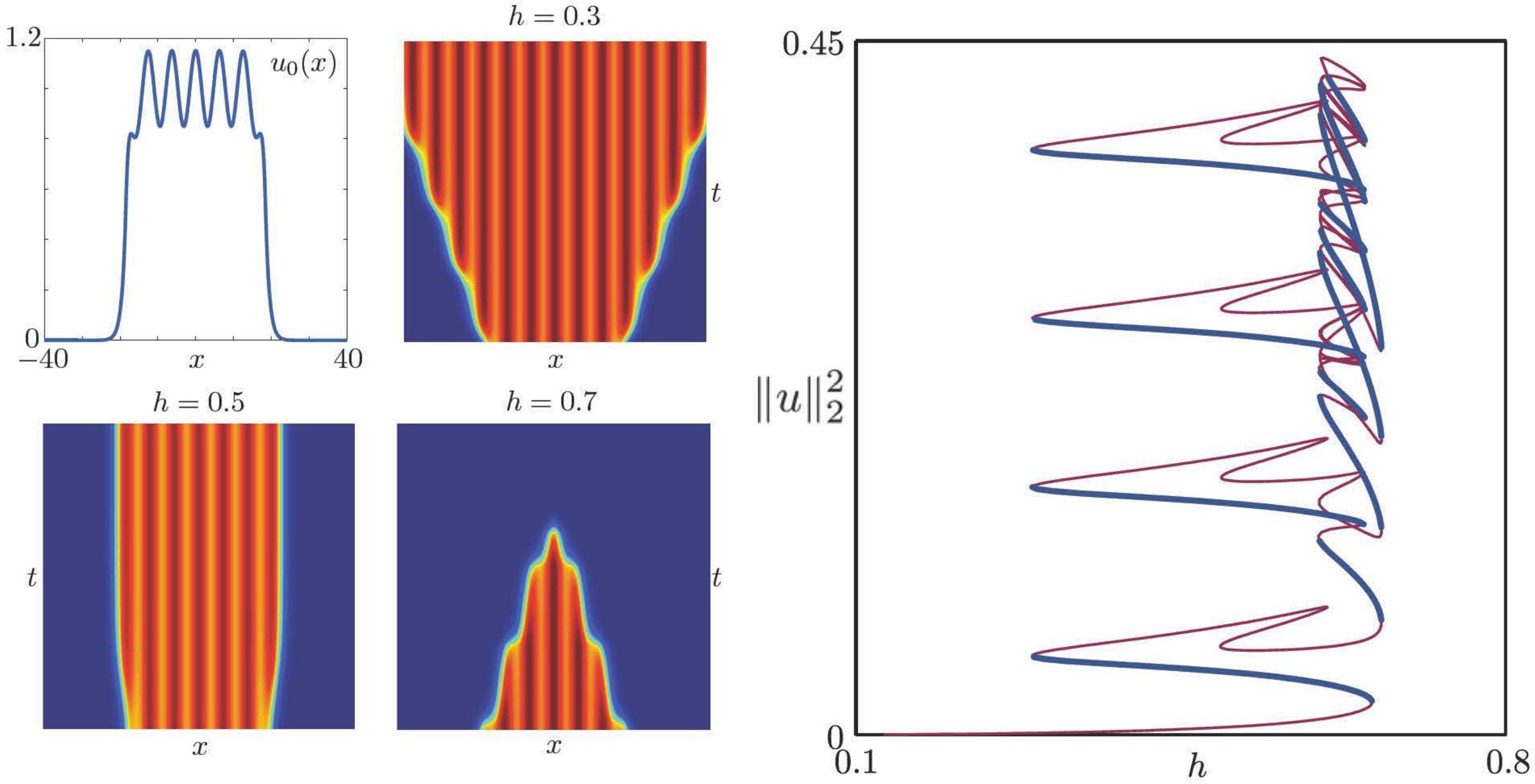
  Steady states stability $$\lambda M\Psi = \left[-M + \mathrm{diag}(A \odot f'(U))\right]\Psi$$

- This fits into the framework used for the SH equation!

- Read on for continuation of neural field models in integral form.

Numerical computations

See Codes

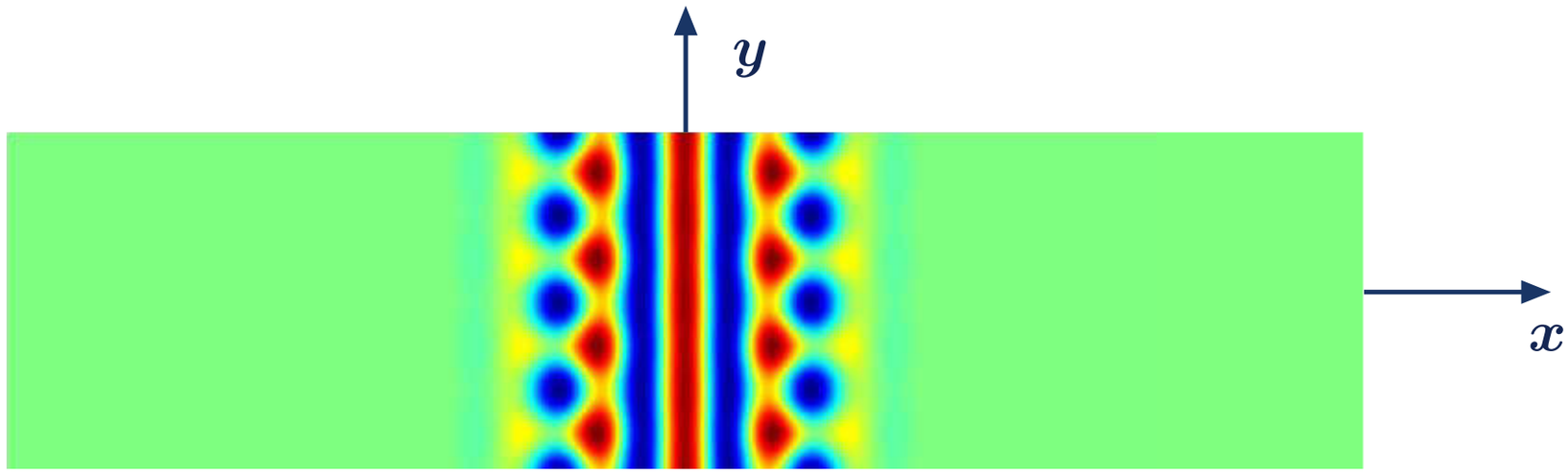


[A. & Schmidt]

From 1D to 2D

Swift-Hohenberg on a plane

See Codes



- Swift-Hohenberg equation posed on a 2D domain

$$\partial u_t = -(1+\Delta)^2 u - \mu u + \nu u^3 - u^5, \qquad (x,y) \in \mathbb{R} \times \mathbb{R}/2L_y\mathbb{Z}$$

- We would like to obtain a discrete form of this type

$$\dot{U} = -(I+L)^2 U - \mu U + \nu U^{\odot 3} - U^{\odot 5}$$

- The matrix L is the *differentiation matrix* for the Laplacian
  1. It can be computed elegantly for tensor grids
  2. Different discretisations (or discretisation methods!) are allowed for x and y

Building the Laplacian for differentiation matrices

- Consider a grid of $N_x \times N_y$ nodes, and pose $u(x_i, y_j) \approx U_{i,j}$

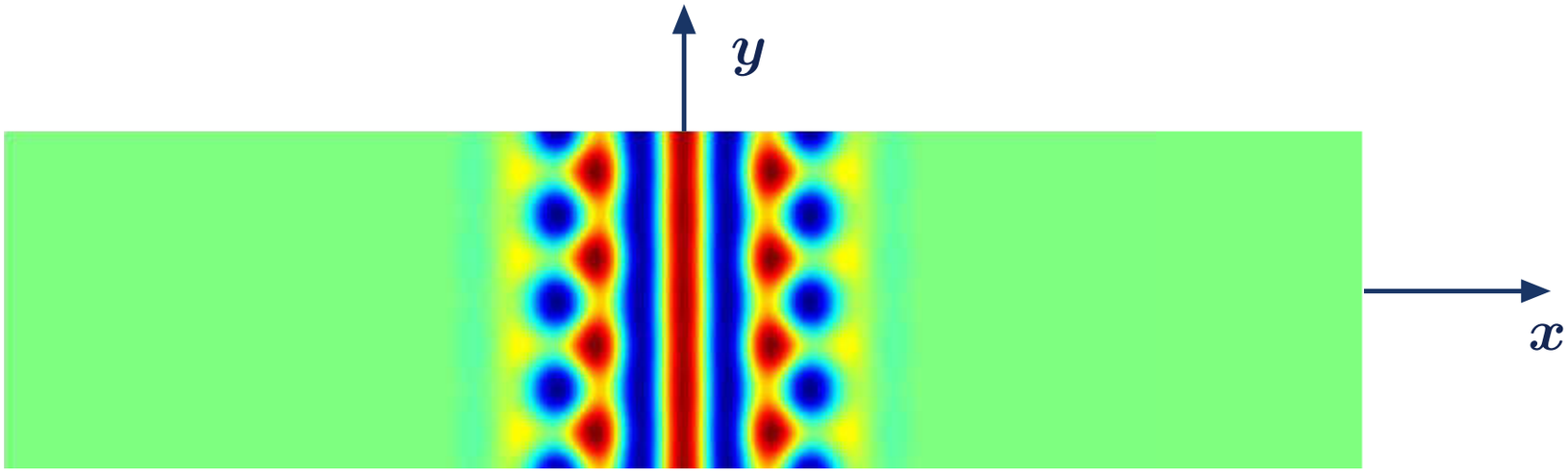
- If the component of the unknown vector $U \in \mathbb{R}^{N_x N_y \times 1}$ are in lexicographic order, the discrete Laplacian can be computed using the Kronecker product $\otimes$

$$L = D_{xx} \otimes I_y + I_x \otimes D_{yy}$$

- Where $D_{xx}, I_x \in \mathbb{R}^{N_x \times N_x}$ and $D_{yy}, I_y \in \mathbb{R}^{N_y \times N_y}$ are calculated independently

- The framework seen in 1D is easy to adapt to the 2D case

Notes on 2D calculations



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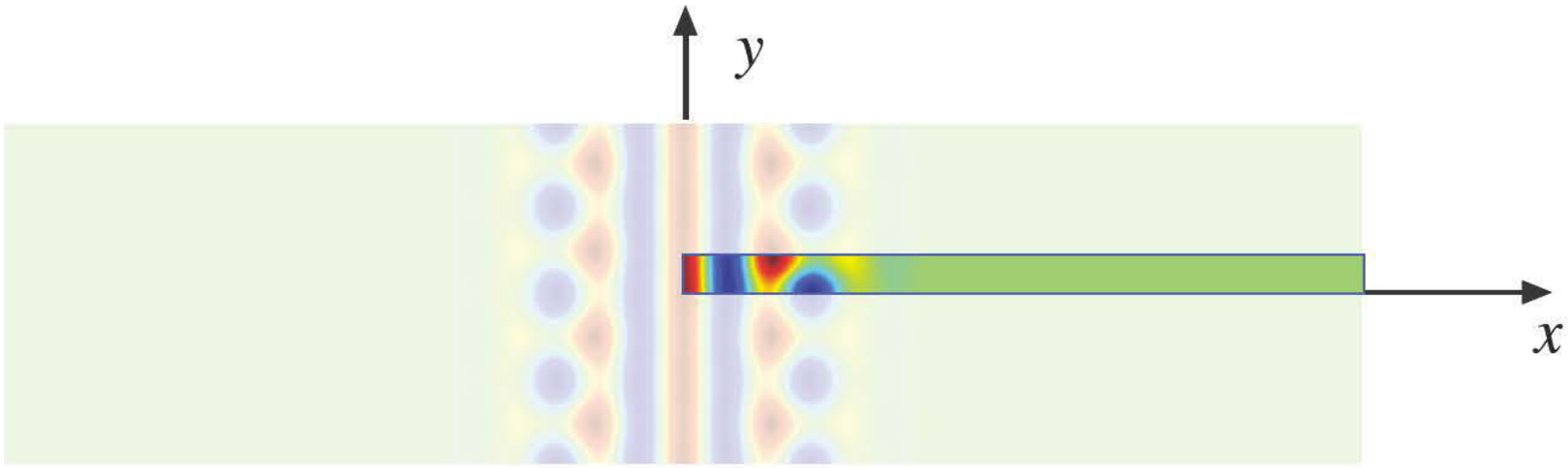

- Use symmetries whenever possible

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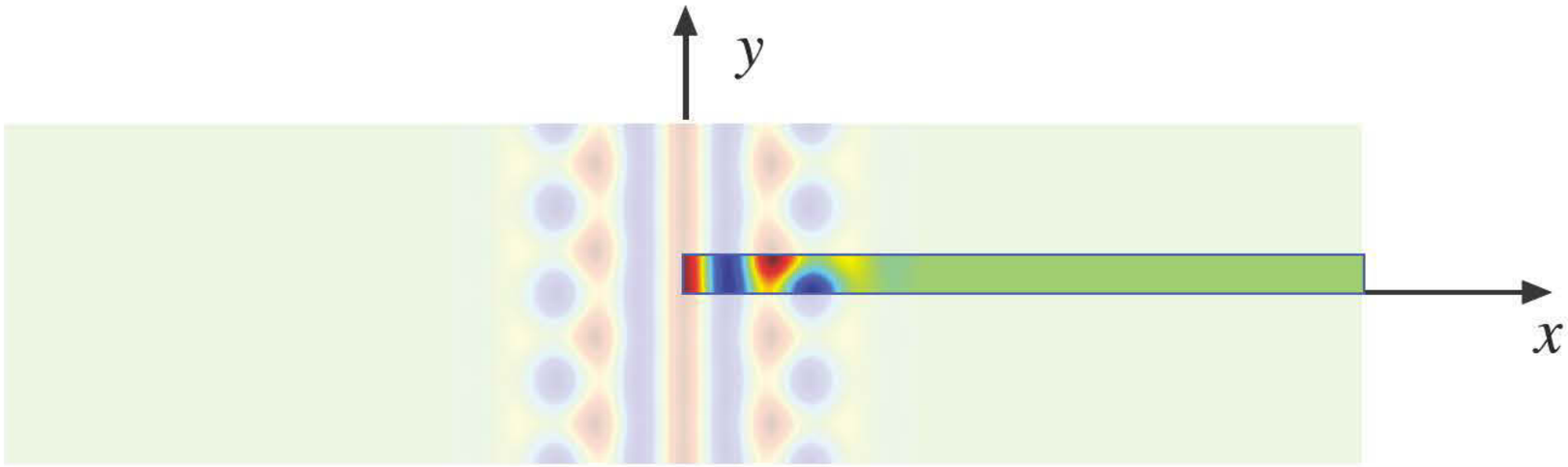
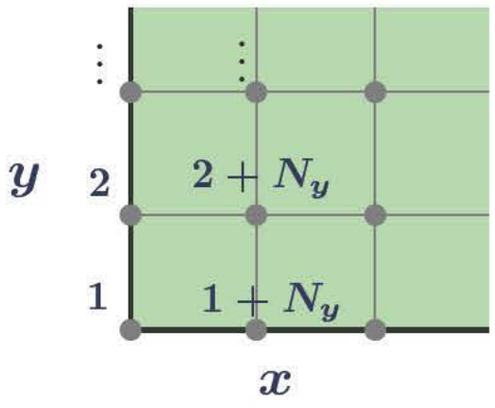


- Use symmetries whenever possible
- Ordering may affect the sparsity pattern/matrix bandwidth



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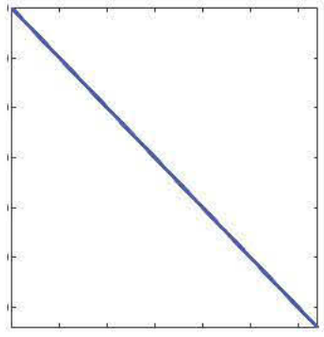

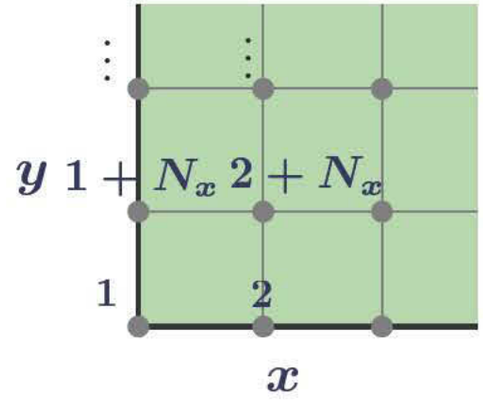

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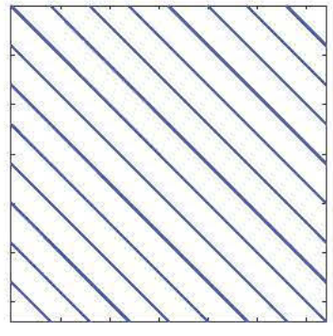


Notes on 2D calculations

- Linear algebra routines could be a bottleneck. Sometimes we need to
  1. Use of efficient solvers for bordered systems
  2. Use of Matrix-Free methods (Krylov methods)
  3. Use preconditioners for iterative linear systems

- Finite Element methods may be more efficient:
  1. Allow a greater flexibility in allocating nodes
  2. Mesh adaptation is possible
  3. The tensor-product trick will not work in general

Spatio-temporal structures

Coherent structures

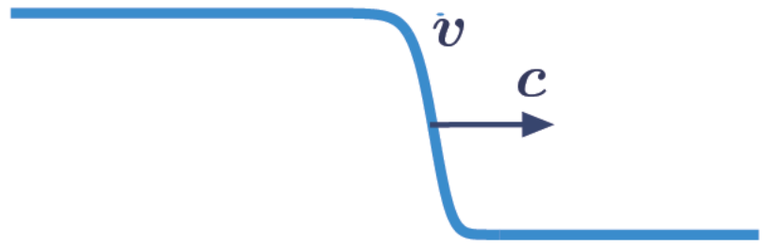
- *Coherent structures*: solutions to nonlinear evolution equations with a special spatio-temporal structure
  1. Travelling waves and solitons
  2. Spiral waves in 2D
  3. Breathers
  4. Oscillons

- Strategy to compute coherent structures
  1. Prescribe a defining system of equations (a well-posed BVP, often symmetries require phase conditions)
  2. Setup an eigenvalue problem for linear stability
  3. Use the methods seen in the past sections

Travelling wave continuation

- We derive the defining problem for TW of

$$\partial_t u = \mathcal{F}(u)$$
$$0 = \mathcal{B}(u)$$



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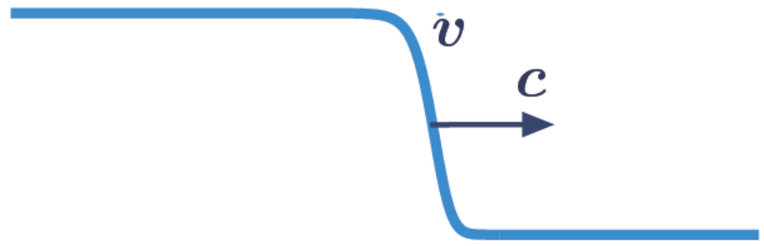

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$$u(x,t) = v(x - ct)$$

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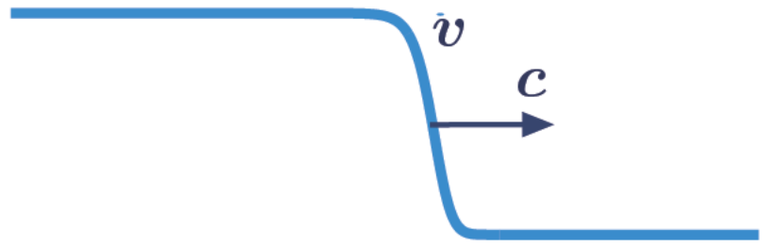

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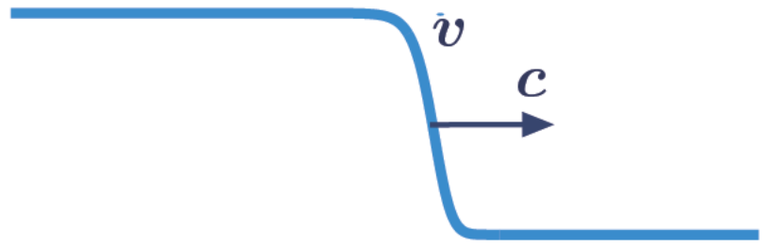


- Travelling waves are special solutions to the evolution equation above

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

- Need to determine the *profile* v and the *wave speed* c

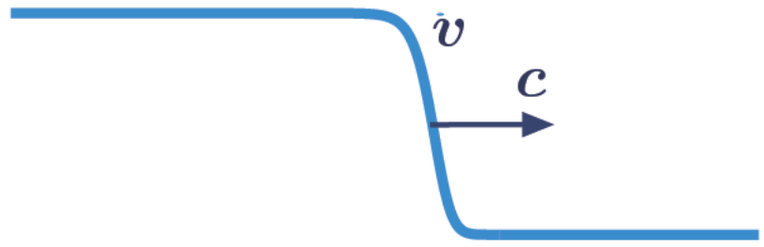
- Let $z = x - ct$ and substitute the TW ansatz in the evolution equation

$$c\partial_z v(z) + \mathcal{F}(v)(z) = 0$$

Travelling wave continuation

- We derive the defining problem for TW of

$$\partial_t u = \mathcal{F}(u)$$
$$0 = \mathcal{B}(u)$$



- Travelling waves are special solutions to the evolution equation above

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

- Need to determine the *profile* v and the *wave speed* c

- Let $z = x - ct$ and substitute the TW ansatz in the evolution equation

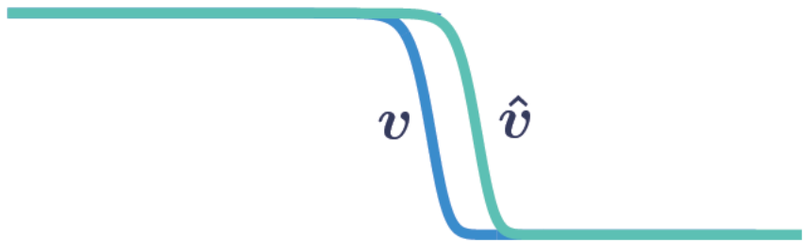
$$c\partial_z v(z) + \mathcal{F}(v)(z) = 0$$

- This is not a valid defining system!
  1. We need one extra equation to determine c
  2. The linearised operator has a 0 eigenvalue, with eigenfunction $\partial_z v$

Travelling waves - defining system

- Defining system: find (v, c) such that

$$c\partial_z v + \mathcal{F}(v) = 0$$
$$\mathcal{B}(v) = 0$$
$$\varphi(v, \hat{v}) = 0$$



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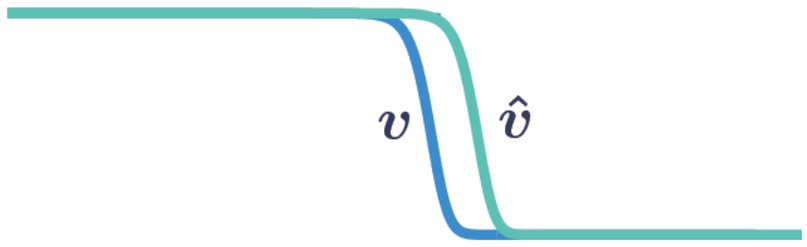

- Stability of a travelling wave (v_*, c_*)

$$u(x,t) = v_*(x - ct) + \varepsilon\tilde{v}(x - ct, t), \qquad 0 < \varepsilon \ll 1, \quad \|\tilde{v}\| = \mathcal{O}(1)$$

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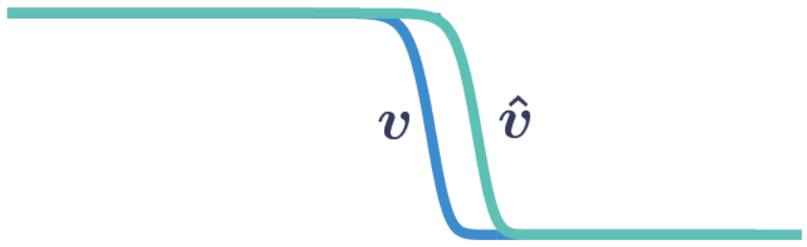

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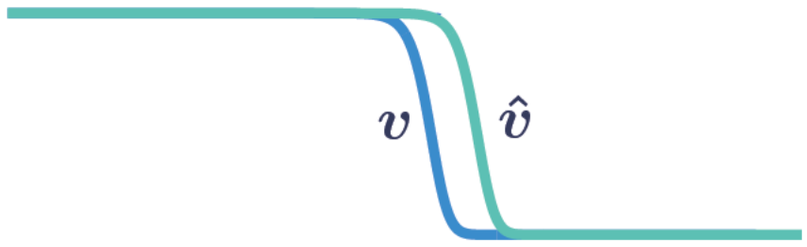

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- The travelling wave is linearly stable if $\mathrm{Spec}\left[\mathcal{L}(v_*, c_*)\right] \setminus \{0\}$ is contained in the left half of the complex plane

Travelling waves in a neural field

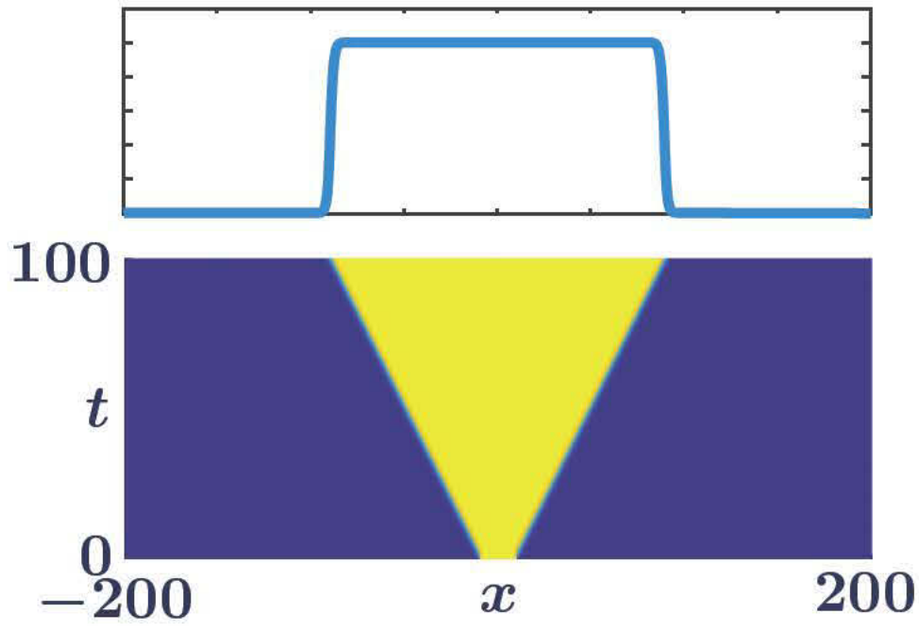
See Codes

- **Neural field example** $x \in \mathbb{R}$

$$\partial_u(x,t) = -u(x,t) + \int_{\mathbb{R}} w(x-y) S(u(y,t))\, dy,$$

- **Synaptic kernel and firing-rate function**

$$w(x) = \frac{1}{2} e^{-|x|}, \qquad S(u) = \frac{1}{1+e^{-\beta(u-h)}}$$



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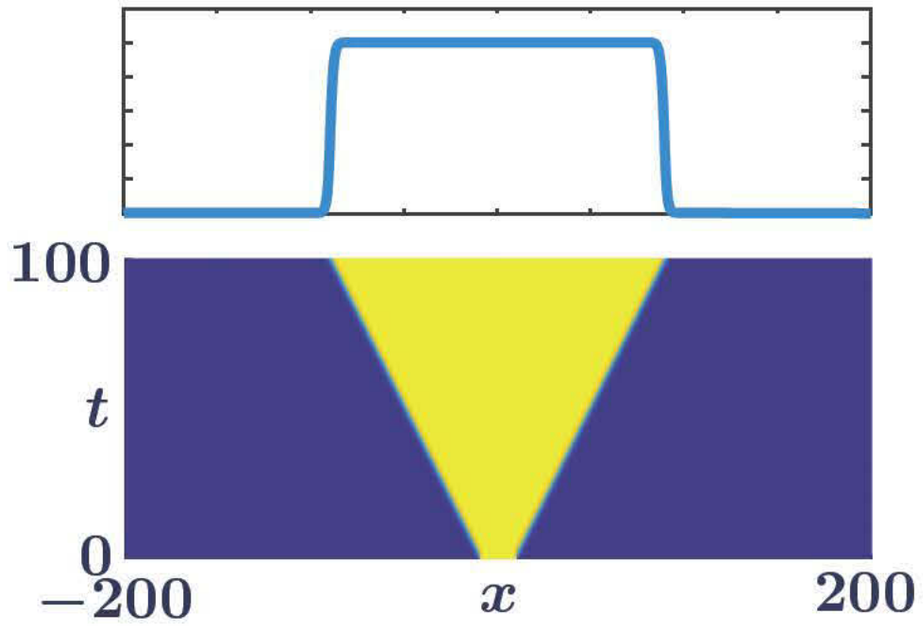

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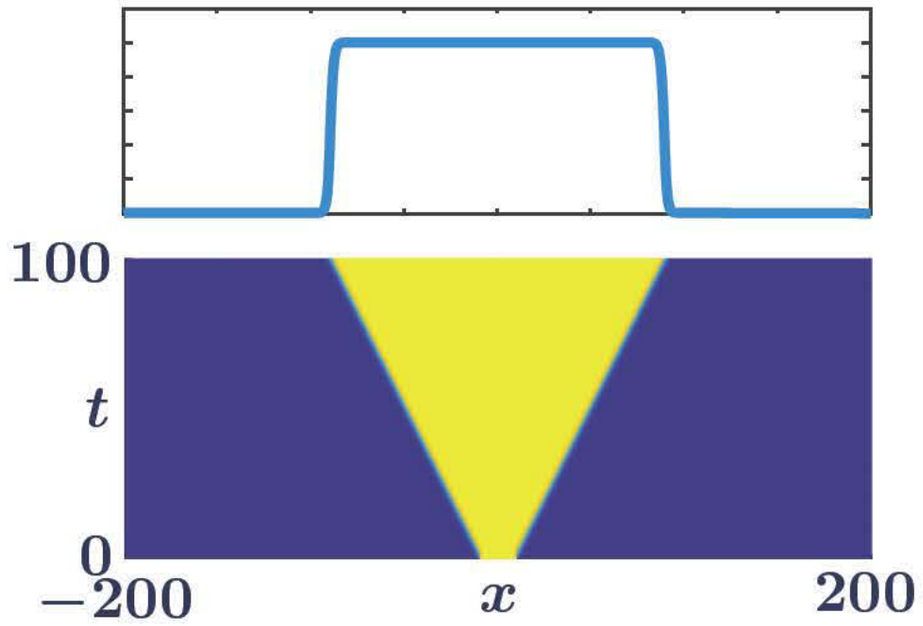

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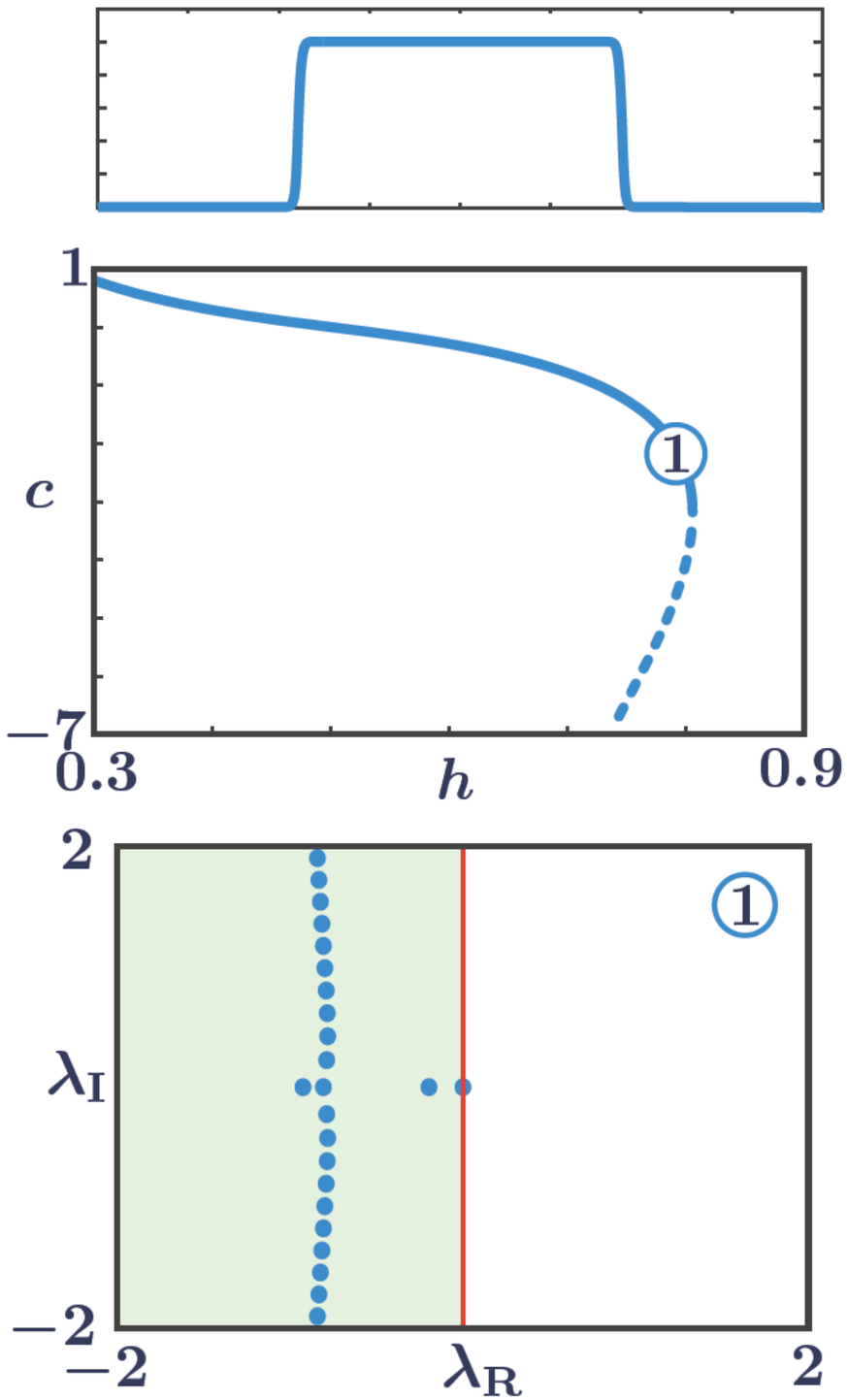

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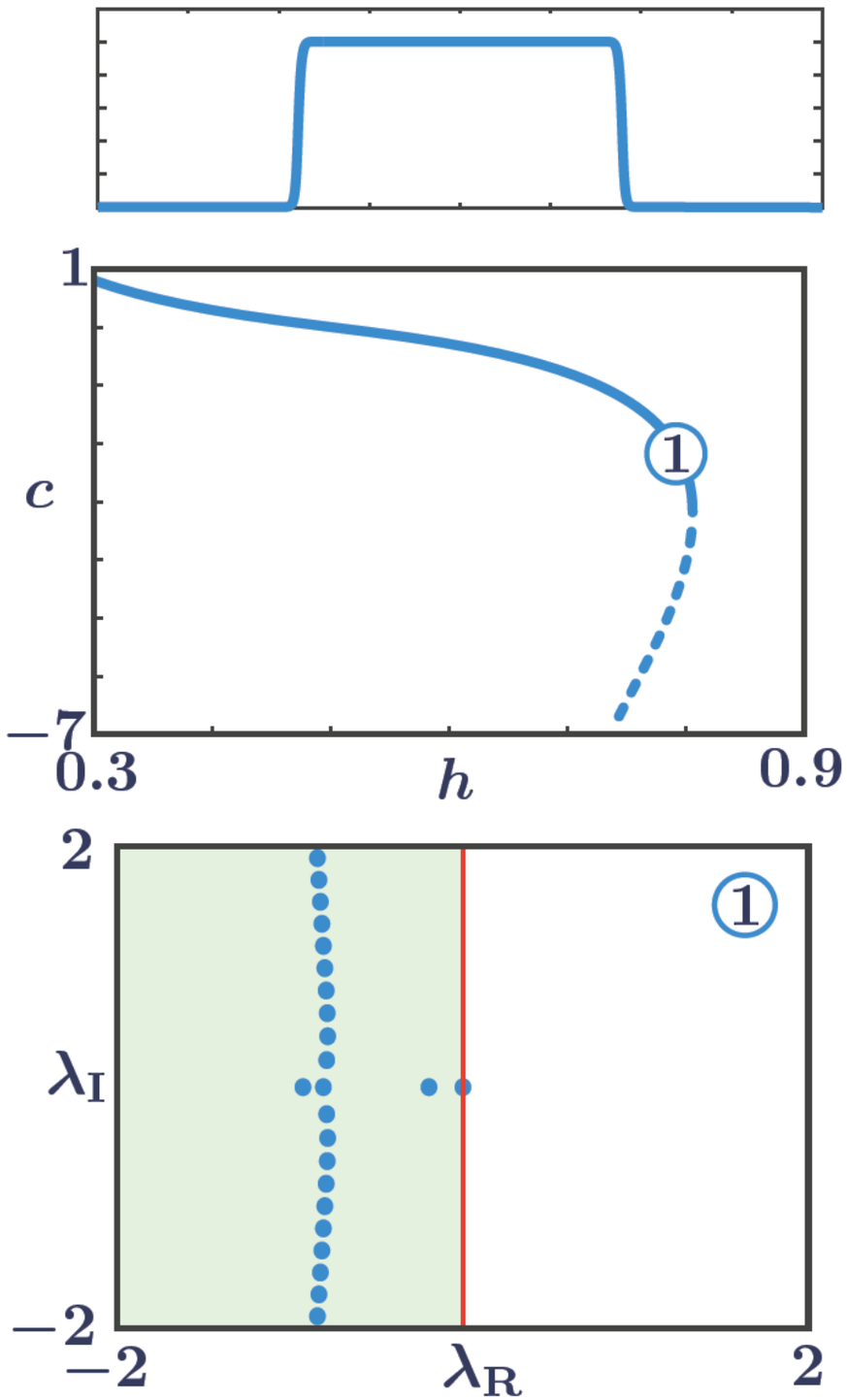

- **Convolution integrals can be evaluated efficiently using FFTs. See the NewtonGMRES code in the heterogeneous example [Rankin, A., Faye, Lloyd]**

See Codes

Conclusions

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- The steps above can also wrap around a *numerical time stepper*

$$\dot{U} = F(U; p), \qquad \Phi_T : U(t) \mapsto U(t + T)$$

[Keller] [Lust] [Tuckermann, Barkley] [Cvitanovich et al.] [Sanchez-Umbria]

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