Dynamics Reading Group

Initiation of excitation fronts

Burhan Bezekci

advised by

Professor Vadim Biktashev

College of Engineering, Mathematics and Physical Sciences

UNIVERSITY OF EXETER

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Reaction diffusion system

One-dimensional reaction-diffusion system:

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2} + f(u), \quad (x,t) \in [0,+\infty) \times [0,+\infty) \qquad (1)$$

$$u(x,0) = U_r + U_{stim}(x), \qquad (2)$$

$$Du_x(0,t) = -I_{stim}(t) \qquad (3)$$

- $u \in \mathbb{R}^d$ – d-component reagents field,
- U_r – resting state, D – diagonal diffusion coefficients
- $U_{stim}(x)$ – initial perturbation, i.e., $U_{stim}(x) = U_{stim} H(x, X_{stim})$, H– shape of initial perturbation,
- $f(u)$ – kinetics specifying the local dynamics,

For some chosen I.C. and B.C, the solution of the system as $t \to \infty$:

- "decay" – solution s.t. $\max_x u(x,t) \to U_r$
- "initiation" – solution s.t. $\max_x |u - U(x - ct - \Delta)| \to 0$ where $U(x - ct - \Delta)$– the propagation wave solution, $c \neq 0$ – wave propagation speed, Δ –arbitrary constant defining the parameter of the family.

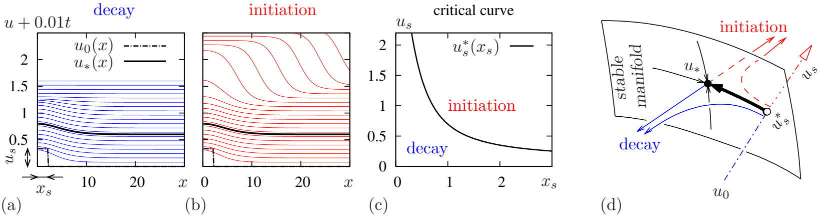


Figure : Initiation of excitation in ZFK equation[1]

Formulation

Only one of $U_{stim}(x)$ and $I_{stim}(t)$ is taken as nonzero:

- Stimulation by voltage: $I_{stim}(t) = 0$, $U_{stim}(x) = U_{stim}X(x) = U_{stim}\Theta\left(x_s - x\right)e$
- Stimulation by current : $U_{stim}(x) = 0$, $I_{stim}(t) = I_{stim}T(t) = I_{stim}\Theta\left(t_s - t\right)e$

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2} + f\left(u\right) + h\left(x,t\right), \left(x,t\right) \in \mathbb{R}\times\mathbb{R}_+ \tag{4}$$

$$u\left(x,0\right) = U_r + u_s(x), \quad h(x,t) = 2I_{stim}\Theta\left(t_s - t\right)\delta(x)$$

$$u_s(-x) = u_s(x) = \begin{cases} U_{stim}X(x) & : x \geq 0 \\ U_{stim}X(-x) & : x < 0 \end{cases}$$

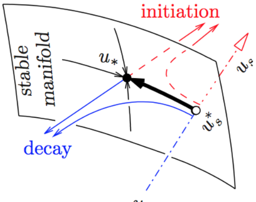
Critical nucleus

Critical nucleus– time independent, unstable- nontrivial stationary solution of

$$D\frac{\partial^2 u_{cr}}{\partial x^2} + f\left(u_{cr}\right) = 0 \quad (5)$$

The importance of the critical nucleus:

- It is a unique solution.
- Its linearized spectrum has only one unstable eigenvalue(others stable) and hence its stable manifold has codimension one.
- It represent a threshold, the minimum stimulus needed to perform an action potential, for propagation.



(d)

Linear approximation of the stable manifold

We linearize our nonlinear equation around the critical nucleus $u_{cr}(x)$ by setting $u(x,t) = u_{cr}(x) + v(x,t)$
where $v(x,t)$ is a perturbation satisfying $|v| < 1$. Linearized problem:

$$\partial_t v = \mathcal{L}v + h, \quad \mathcal{L} = D\frac{\partial^2}{\partial x^2} + F(x), \quad F(x) = \frac{\partial f}{\partial u}|_{u=u_{cr}(x)}$$

$$v(x,0) = u_r + u_s(x) - u_{cr}(x)$$

Eigenfunctions of $\mathcal{L}$ are determined via: $\mathcal{L}V_j(x) = \lambda_j V_j(x)$.
General solution in the generalized Fourier series:

$$v(x,t) = \sum_j a_j(t) V_j(x)$$

such that a_j's satify : $\frac{\mathrm{d}a_j}{dt} = \lambda_j a_j + h_j(t)$ where

- $h_j(t) = \langle W_j(x) \, | h(x,t) \rangle$, $\quad a_j(0) = \langle W_j(x) \, | v(x,0) \rangle$
- Scalar product– $\quad \langle u(x) \, | v(x) \rangle = \int_{-\infty}^{\infty} u(x)^\top v(x) \, \mathrm{d}x$
- W_j– eigenfunctions of the adjoint operator, $\mathcal{L}^+ W_j = \lambda_j W_j$, for scalar models $\mathcal{L}^+ = \mathcal{L}$.
- Eigenfunction normalized – $\quad \langle W_j \, | V_k \rangle = \delta_{j,k}$

Equivalent form: $a_j(t) = e^{\lambda_j t} \left(a_j(0) + \int_0^t h_j(\tau) \, e^{-\lambda_j \tau} \mathrm{d}\tau \right)$ which implies $a_1(0) + \int_0^{t_s} h_1(\tau) \, e^{-\lambda_1 \tau} \mathrm{d}\tau = 0$

Hence, we have

$$\langle W_1(x)\,|u_s(x)\rangle + \int_0^{t_s} e^{-\lambda_1\tau}\,\langle W_1(x)\,|h(x,\tau)\rangle\,\mathrm{d}\tau = \langle W_1(x)\,|u_{cr}(x) - u_r\,\rangle$$

Strength-extent curve: For $t_s = 0$, e fixed vector, and $u_s(x) = U_s X(x) = U_s \Theta(x_s - x)\,\Theta(x_s + x)\,e$, we have:

$$U_s = \frac{\int_0^\infty W_1(x)^\top\left(u_{cr}(x) - u_r\right)\,\mathrm{d}x}{\int_0^{x_s} W_1(x)^\top e\,\mathrm{d}x}$$

Strength-duration curve: For $u_s = 0$ and $h(x) = h(x,t) = 2I_s\Theta(t_s - t)\,\delta(x)e$, we have

$$I_s = \frac{I_{rh}}{1 - \exp(-\lambda_1 t_s)}, \quad I_{rh} = \frac{\lambda_1 \int_0^\infty W_1(x)^\top\left(u_{cr}(x) - u_r\right)\mathrm{d}x}{W_1(0)^\top e}$$

Quadratic approximations

For simplicity, we write RDS in the following Einstein's summation convention form (Greek letter-component of the RDS):

$$\frac{\partial u^\alpha}{\partial t} = D^{\alpha\beta}\frac{\partial^2 u^\beta}{\partial x^2} + f^\alpha\left(u^\beta\right)$$

- Transformation– $u^\alpha(x,t) = u^\alpha_{cr}(x) + v^\alpha(x,t)$,
- $u^\alpha_{cr}(x)$– stationary sol. : $D^{\alpha\beta}\frac{\partial^2 u^\beta_{cr}}{\partial x^2} + f^\alpha(u_{cr}) = 0$
- RDS – $\dot{v}^\alpha = D^{\alpha\beta}v^\beta_{xx} + f^\alpha_{,\beta}(u_{cr})\,v^\beta + \frac{1}{2}f^\alpha_{,\beta\gamma}(u_{cr})\,v^\beta v^\gamma + \cdots$
- Eigenfunctions normalized– $\langle W_j \,|\, V_k\rangle = \delta_{j,k}$

Seek solution in the generalized Fourier series form:

$$v^{\alpha}(x,t) = \sum_j a_j(t) V_j^{\alpha}(x)$$

- Fourier coefficients– $a_j(t) = \langle W_j(x) \,|v(x,t)\rangle = \int_{-\infty}^{\infty} \overline{W_j^{\alpha}(x)} v^{\alpha}(x,t)\,\mathrm{d}x,$
- Time differentiation of a_j : $\dot{a}_j = \lambda_j a_j + \sum_{m,n} B^j_{m,n} a_m a_n$ where $B^j_{m,n} = B^j_{n,m} = \frac{1}{2}\int_{-\infty}^{\infty} W_j^{\alpha}(x) f^{\alpha}_{,\beta\gamma}(u_{cr}(x))\, V_m^{\beta}(x) V_n^{\gamma}(x)\mathrm{d}x$
- Initial values of Fourier coefficients – $A_j = a_j(0) = \int_{-\infty}^{\infty} \overline{W_j^{\alpha}(x)} v^{\alpha}(x,0)\mathrm{d}x$
- Nonlinear ode results in– $a_j(t) = e^{\lambda_j t}\left(A_j + \int_0^t e^{-\lambda_j \tau} \sum_{m,n} B^j_{m,n} a_m(\tau)\, a_n(\tau)\,\mathrm{d}\tau\right)$

Direct iteration method to solve the system:

$$a_j^{(i+1)}(t) = e^{\lambda_j t}\left(A_j + \int_0^t e^{-\lambda_j \tau} \sum_{m,n} B^j_{m,n} a_m^{(i)}(\tau)\, a_n^{(i)}(\tau)\, \mathrm{d}\tau\right) \quad (6)$$

- Taking $a_j^{(0)} = 0$, first iteration– $a_j^{(1)} = A_j e^{\lambda_j t} \Rightarrow A_1 = 0$, $A_j \in \mathbb{R}$, $j \neq 1$
  which corresponds to the linear approximation.
- Second iteration :

$$a_j^{(2)} = e^{\lambda_j t}\left(A_j + \sum_{m,n\neq 1} \frac{B^j_{m,n} A_m A_n}{\lambda_j - \lambda_m - \lambda_n}\right) - \sum_{m,n\neq 1} \frac{B_{m,n} A_m A_n}{\lambda_j - \lambda_m - \lambda_n} e^{(\lambda_m + \lambda_n)t}$$

$a_1^{(2)}(t) \to 0$ gives a quadratic equation in terms of u_s

$$A_1 = -\sum_{m,n\neq 1} \frac{B_{m,n} A_m A_n}{\lambda_1 - \lambda_m - \lambda_n}$$

Zeldovich-Frank Kamenetsky equation

One component ZFK equation has:

- the kinetics– $f(u) = u(u-\theta)(1-u)$
- initial condition – $u(x,0) = u_s\Theta(x_s - x)$
- Boundary condition– $u_x(0,t) = -I_s\Theta(t_s - t)$
- Critical nuclues solution–

$$u_*(x) = \frac{3\theta\sqrt{2}}{(1+\theta)\sqrt{2} + \cosh\left(x\sqrt{\theta}\right)\sqrt{2 - 5\theta + 2\theta^2}}$$

- Linearization near crit.nuc.
  $v_t = \mathcal{L}v, \quad \text{where} \quad \mathcal{L} = \frac{\partial^2}{\mathrm{d}x^2} + \left[\frac{\partial f}{\partial u}\right]_{u=u_*(x)}$
- Eigenfunction– $v(x,t) = \sum_{j=1}^{\infty} a_j e^{\lambda_j t}\phi_j(x), \quad a_1 \neq 0$
  as $t \to \infty \Rightarrow v(x,t) \approx a_1 e^{\lambda_1 t}\phi_1(x) \Rightarrow \phi_1(x) \approx \frac{v(x,t)}{v(0,t)}$.
- Eigenvalue– $\lambda_1 = \frac{\ln(v(0,t)) - \ln(a_1)}{t}$, least square method can be used to get rid of a_1.

Analytical expressions

Strength-extent curve

- Linear– $u_s\left(x_s\right)=\dfrac{\int_0^{\infty}\phi_1(x)u_*(x)\mathrm{d}x}{\int_0^{x_s}\phi_1(x)\mathrm{d}x}$
- Quadratic(First two eigenpair only)– $A_1=-\dfrac{B_{22}A_2^2}{\lambda_1-2\lambda_2}$, where
- $B_{22}=\dfrac{\int_{-L}^{L}\phi_1(x)\phi_2^2(x)f''(u(x))|_{u=u_*}\mathrm{d}x}{2\|\phi_1\|\|\phi_2\|^2}$,
- $A_1=\dfrac{\int_{-L}^{L}(u(x,0)-u_*(x))\phi_1(x)\mathrm{d}x}{\|\phi_1\|}$, $A_2=\dfrac{\int_{-L}^{L}(u(x,0)-u_*(x))\phi_2(x)\mathrm{d}x}{\|\phi_2\|}$
- Employing these gives – $\mathcal{N}_1u_s^2+\mathcal{N}_2u_s+\mathcal{N}_3=0$ where

$$\mathcal{N}_1=\frac{2\left(\int_0^L\phi_1(x)\phi_2^2(x)f''(u(x))|_{u=u_*}\mathrm{d}x\right)\left(\int_0^{x_s}\phi_2(x)\mathrm{d}x\right)^2}{(\lambda_1-2\lambda_2)\|\phi_2\|^4},$$

$$\mathcal{N}_2=\int_0^{x_s}\phi_1(x)\mathrm{d}x-\frac{4\left(\int_0^{x_s}\phi_2(x)\mathrm{d}x\right)\left(\int_0^L u_*(x)\phi_2(x)\mathrm{d}x\right)\left(\int_0^L\phi_1(x)\phi_2^2(x)f''(u(x))|_{u=u_*}\mathrm{d}x\right)}{(\lambda_1-2\lambda_2)\|\phi_2\|^4}$$

$$\mathcal{N}_3=\frac{2\left(\int_0^L u_*(x)\phi_2(x)\mathrm{d}x\right)^2\left(\int_0^L\phi_1(x)\phi_2^2(x)f''(u(x))|_{u=u_*}\mathrm{d}x\right)}{(\lambda_1-2\lambda_2)\|\phi_2\|^4}-\int_0^L u_*(x)\phi_1(x)\mathrm{d}x$$

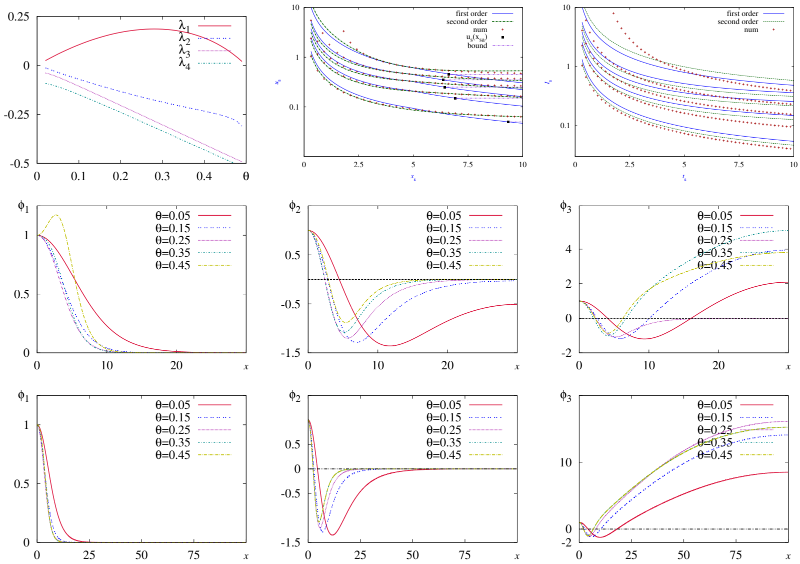
Strength-duration curve

- Linear– $I_s(t_s) = \frac{I_{rh}}{1-e^{-t_s/\tau}}$, $I_{rh} = \frac{\lambda_1 \int_0^\infty \phi_1(x) u_*(x) \mathrm{d}x}{\phi_1(0)}$, $\tau = (\lambda_1)^{-1}$
- Quadratic(First two eigenpair only)– $\mathcal{N}_4 I_s^2 + \mathcal{N}_5 I_s + \mathcal{N}_6 = 0$, where
- $\mathcal{N}_4 = 4B_{22}^1 \left\{ \frac{\phi_2(0)}{\lambda_2} \left(\frac{e^{(2\lambda_2-\lambda_1)t_s}-1}{2\lambda_2-\lambda_1} - 2\frac{e^{(\lambda_2-\lambda_1)t_s}-1}{\lambda_2-\lambda_1} - \frac{e^{-\lambda_1 t_s}-1}{\lambda_1} \right) - \frac{e^{(2\lambda_2-\lambda_1)t_s}}{2\lambda_2-\lambda_1} \left(\frac{\phi_2(0)\left(e^{-\lambda_2 t_s}-1\right)}{\lambda_2} \right)^2 \right\}$,
- $\mathcal{N}_5 = 4B_{22}^1 A_2 \phi_2(0) \left\{ \frac{e^{(2\lambda_2-\lambda_1)t_s}\left(e^{-\lambda_2 t_s}-1\right)}{\lambda_2(2\lambda_2-\lambda_1)} - \frac{e^{(\lambda_2-\lambda_1)t_s}-1}{\lambda_2(\lambda_2-\lambda_1)} + \frac{e^{(2\lambda_2-\lambda_1)t_s}-1}{\lambda_2(2\lambda_2-\lambda_1)} \right\} - \frac{2\phi_1(0)\left(e^{-\lambda_1 t_s}-1\right)}{\lambda_1}$,
- $\mathcal{N}_6 = -\frac{B_{22}^1 A_2^2}{2\lambda_2-\lambda_1} + A_1$,
- $A_j = -\frac{\int_{-L}^{L} u_*(x)\phi_j(x)\mathrm{d}x}{\|\phi_j\|}$, for $j = 1, 2$.

Numerical methods

- Discretization formula for the ZFK equation–
  $U_i^{j+1} = U_i^j + \frac{\Delta t}{(\Delta x)^2}\left(U_{i-1}^j - 2U_i^j + U_{i+1}^j\right) + \Delta t \cdot U_i^j\left(1 - U_i^j\right)\left(U_i^j - \theta\right),$
- Numerical solution of $v_t = \mathcal{L}v$– $v^{j+1} = Tv^j$,
  $T = \left(\frac{\Delta t}{(\Delta x)^2} T_1 + 1 + \Delta t \left[\frac{\partial f}{\partial u}\right]_{u=u_*(x)}\right)$, $T_1 = tridiag(1, -2, 1)$
- Eigenfunctions (Gram-Schmidt)– For some chosen orthonormal basis $\{x_1, \cdots, x_n\}$ we use FDM to get $x_1^{j+1} = Tx_1^j, \cdots x_n^{j+1} = Tx_n^j$ and hence
  $\phi_1 = x_1, \cdots, \phi_n = x_n - \langle x_n | x_1 \rangle x_1 - \cdots - \langle x_n | x_{n-1} \rangle x_{n-1}$
- Trapezoidal rule to calculate integrals–
  $I_1(0, L) = \int_0^L \phi_1(x) u_*(x) \mathrm{d}x =$
  $\frac{\Delta x_1}{2}\left[\phi_1(0)u_*(0) + \phi_1(L)u_*(L) + 2\sum_{k=1}^{N-1} \phi_1(k\Delta x_1)\, u_*(k\Delta x_1)\right]$

Results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λ2
λ3
λ4
θ
first order
second order
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us(xsa)
bound
xs
us
ts
ls
ϕ1
ϕ2
ϕ3
θ=0.05
θ=0.15
θ=0.25
θ=0.35
θ=0.45
x

McKean model has

- the kinetics– $f(u) = -u + \Theta(u-a)$
- Critical nucleus–
  $u_0(x) = \begin{cases} 1-(1-a)\frac{\cosh(x)}{\cosh(x_*)}, & x < x_*, \\ a\exp(x_* - x), & x_* < x, \end{cases}$, where
  $x_* = \frac{1}{2}\ln\left(\frac{1}{1-2a}\right)$
- Linearization about crit. nuc. $v_t = v_{xx} + \left(-1 + \frac{\delta(x-x_*)}{a}\right) v$
- Solution in the form $v(x,t) = e^{\lambda t}\phi(x) \Rightarrow \mathcal{L}\phi = \lambda\phi$,
  $\mathcal{L} = \frac{\mathrm{d}^2}{\mathrm{d}x^2} - 1 + \frac{1}{a}\delta(x-x_*)$
- Eigenfunction –
  $\phi_1(x) = \begin{cases} \cosh(kx), & x < x_*, \\ \cosh(kx_*)\,e^{k(x_*-x)}, & x_* < x, \end{cases}$,
- Eigenvalue– $\lambda = \left[\frac{1}{2a} + \frac{W_0\left(\frac{1}{2a}\ln\left(\frac{1}{1-2a}\right)\left(\frac{1}{1-2a}\right)^{-1/2a}\right)}{\ln\left(\frac{1}{1-2a}\right)}\right]^2 - 1.$

  where W_0 is the Lambert W function satisfying
  $z = W_0(z)e^{W_0(z)}$.

Numerical methods

- Finite difference discretization formula for the McKean model–
$U_i^{j+1} = U_i^j + \frac{\Delta t}{(\Delta x)^2}\left(U_{i-1}^j - 2U_i^j + U_{i+1}^j\right) + \Delta t \cdot \left(-U_i^j + \Theta\left(U_i^j - a\right)\right)$,
- Finite element method– $A\frac{\mathrm{d}\hat{u}}{\mathrm{d}t} + \left(A + B - \frac{1}{a}C\right)\hat{u} = 0$ where

$$\Phi_j(x_i) = \begin{cases} (x - x_{i-1})/h, & x \in [x_{i-1}, x_i] \\ (x_{i+1} - x)/h, & x \in [x_i, x_{i+1}] \\ 0, & \text{otherwise} \end{cases}$$

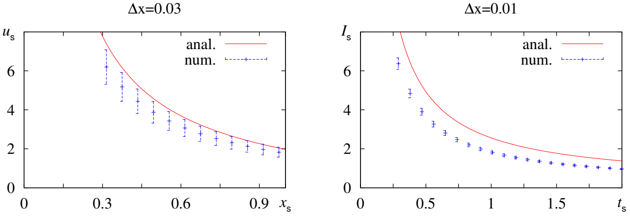
$$A = [a_{i,j}] = \int_0^L \Phi_i(x)\Phi_j(x)\mathrm{d}x = tridiag(\Delta x/6, 2\Delta x/3, \Delta x/6),$$

$$B = [b_{i,j}] = \int_0^L \Phi_i'(x)\Phi_j'(x)\mathrm{d}x = tridiag(-1/\Delta x, 2/\Delta x, -1/\Delta x)$$

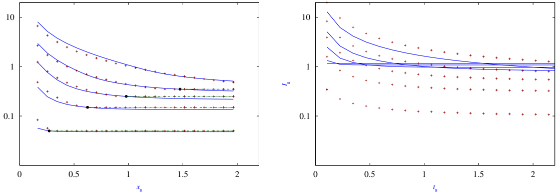
$$C = [c_{i,j}] = \int_0^L \delta(x - x_*)\Phi_i(x)\Phi_j(x)\mathrm{d}x = \Phi_i(x_*)\Phi_j(x_*)$$

Linearized approximation results

Finite difference: frozen solution phenomenon



Finite element: preventing discontunuity caused by Heaviside f.



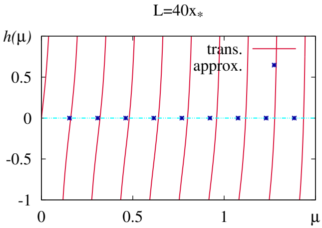
Quadratic approximation results

We proceed as follows:

- Finding the general form of left eigenfunctions $(\lambda = -1 - \mu^2)$

$$\phi_\mu(x) = \begin{cases} -a\mu\cos(\mu x), & x < x_*, \\ -[a\mu + \sin(\mu x_*)\cos(\mu x_*)]\cos(\mu x) + \cos^2(\mu x_*)\sin(\mu x), & x_* < x, \end{cases}$$

- Obtaining transcendental equation via boundary, contunuity, matching conditions
  $h(\mu) := \tan(\mu L) - \tan(\mu x_*) - \frac{a\mu}{\cos^2(\mu x_*)} = 0.$
- Finding eigenvalues from the transcendental equation and employing them into quadratic approximation expression
- How to choose the parameter L? When $\mu \to 0$ and $L \to \infty$ we have $\mu \sim L^{-1}$ such that $\mu L = \mathcal{O}(1)$, $\mu x_* \to 0$, $\cos(\mu x_*) \approx 1$, $\sin(\mu x_*) \approx \mu x_*$. Hence our transcendental equation reduces to $\tan(\eta) = \frac{a+x_*}{L}\eta$ where $\eta = \mu L$. For any positive integer n we define $\eta_* = n\pi + \epsilon_n$ for $|\epsilon_n| \ll 1$. Thus, we have $\mu = \frac{\eta_*}{L} = \frac{n\pi}{L}\left(1 + \frac{a+x_*}{L}\right) \approx \frac{n\pi}{L}$.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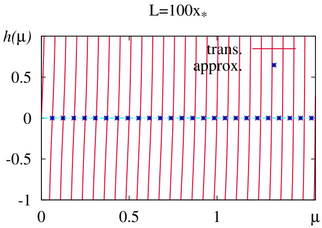
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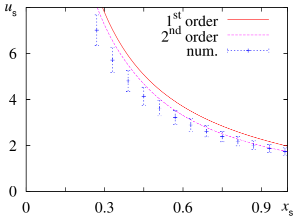
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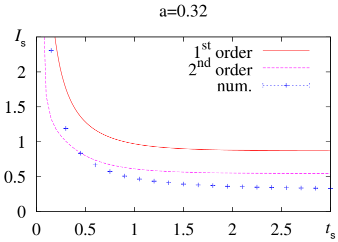
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1.5
1
0.5
0
0
0.5
1
1.5
2
2.5
ts

Idris, I., and V. N. Biktashev.
Analytical approach to initiation of propagating fronts.
Physical review letters, 244101,2008.

G. Flores.
The stable manifold of the standing wave of the Nagumo equation.
J. Differential Equations, 80:306–314, 1989.

H. P. McKean.
Nagumo's equation.
Adv. Math., 4(3):209-223, 1970.