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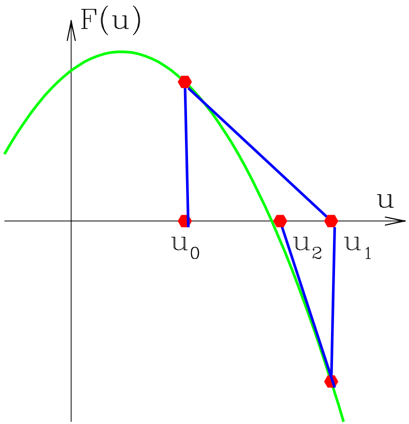
Numerical Methods for Differential Equations in Physics

Time stepping: $\partial_t U = LU + N(U)$

Steady state solving: $0 = LU + N(U)$

$$0 = F(U)$$

Newton's method



$$0 = F(U - u) \approx F(U) - DF(U)u$$

$$\begin{cases} DF(U)u = F(U) \\ U \leftarrow U - u \end{cases}$$

Newton's Method converges quadratically

$$U_{n+1} = U_n - \frac{F(U_n)}{F'(U_n)}$$

$$F(\overline{U}) = 0 = F(U_n) + F'(U_n)(\overline{U} - U_n) + \tfrac{1}{2}F''(U_n)(\overline{U} - U_n)^2 + \ldots$$

$$0 = \frac{F(U_n)}{F'(U_n)} + \frac{F'(U_n)}{F'(U_n)}(\overline{U} - U_n) + \frac{1}{2}\frac{F''(U_n)}{F'(U_n)}(\overline{U} - U_n)^2 + \ldots$$

$$0 = \frac{F(U_n)}{F'(U_n)} + (\overline{U} - U_n) + \frac{1}{2}\frac{F''(U_n)}{F'(U_n)}(\overline{U} - U_n)^2 + \ldots$$

$$0 = -U_{n+1} + \overline{U} + \frac{1}{2}\frac{F''(U_n)}{F'(U_n)}(\overline{U} - U_n)^2 + \ldots$$

$$U_{n+1} - \overline{U} = \frac{1}{2}\frac{F''(U_n)}{F'(U_n)}(\overline{U} - U_n)^2 + \ldots$$

$$\epsilon_{n+1} = \frac{1}{2}\frac{F''(U_n)}{F'(U_n)}\epsilon^2 + \ldots$$

Typical sequence: $\epsilon = 10^{-1}, 10^{-2}, 10^{-4}, 10^{-8}, 10^{-16}$

Much faster than timestepping:

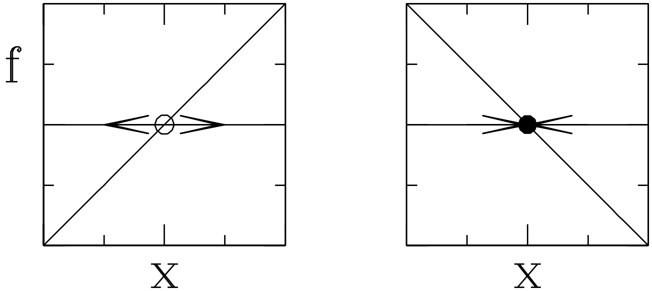
$$U(t) = \overline{U} + ce^{-\lambda t}$$
$$U(t_n) - \overline{U} = ce^{-\lambda t_n}$$
$$U(t_{n+1}) - \overline{U} = ce^{-\lambda(t_n+\Delta t)} = e^{-\lambda \Delta t}(U(t_n) - \overline{U}))$$

Linear convergence: $\epsilon_{n+1} \sim c\epsilon_n$.

In addition to converging faster than timestepping, Newton's method can converge to unstable states.

Fixed points and linear stability. $\dot{x} = f(x)$

unstable **stable**



$0 = f(\bar{x})$ **Fixed point $\bar{x}$**

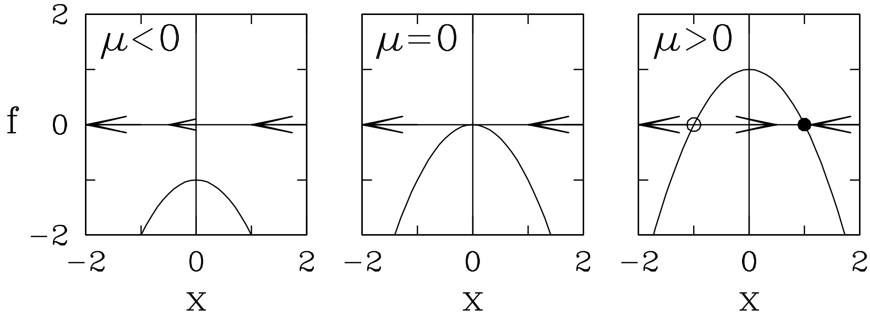
Linear stability of $\bar{x}$

$$\frac{d}{dt}(\bar{x} + \epsilon(t)) = f(\bar{x} + \epsilon)$$

$$\dot{\epsilon} = f(\bar{x}) + f'(\bar{x})\epsilon + \frac{1}{2}f''(\bar{x})\epsilon^2 + \cdots \approx f'(\bar{x})\epsilon$$

$$\epsilon(t) = e^{tf'(\bar{x})}\epsilon(0) \begin{cases} \text{increases if } f'(\bar{x}) > 0 \\ \text{decreases if } f'(\bar{x}) < 0 \end{cases}$$

Saddle-node Bifurcations



$$\dot{x} = f(x) = \mu - x^2$$

Fixed points:

$$\bar{x}_\pm = \pm\sqrt{\mu} \quad \textbf{for } \mu > 0$$

Stability:

$$f'(\bar{x}_\pm) = -2\bar{x}_\pm = -2(\pm\sqrt{\mu}) = \mp 2\sqrt{\mu}$$

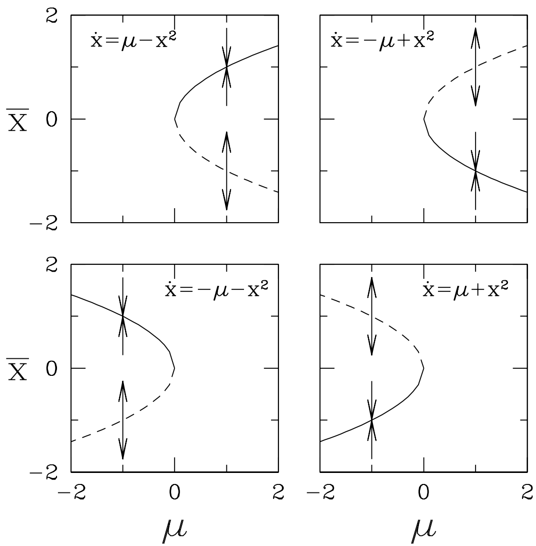
$$f'(\bar{x}_+) = f'(\sqrt{\mu}) = -2\sqrt{\mu} < 0 \implies \bar{x}_+ \textbf{ stable}$$

$$f'(\bar{x}_-) = f'(-\sqrt{\mu}) = 2\sqrt{\mu} > 0 \implies \bar{x}_- \textbf{ unstable}$$

$$
\begin{aligned}
f(x,\mu) &= c_{00} + c_{10}x + c_{01}\mu + c_{20}x^2 + \dots \\
&= \pm\tilde{\mu} \pm \tilde{x}^2
\end{aligned}
$$

general quadratic polynomial

four cases, depending on signs of c's



Newton's method finds steady states independently of their stability
Where might saddle-node bifurcations occur?

Swift-Hohenberg equation

$$\partial_t u = \mu u - \left(q_c^2 + \Delta\right)^2 u - u^3$$

Derived by J. Swift and P.C. Hohenberg (Phys. Rev. A 15, 319 (1977)) to describe pattern formation in convection

For $u \ll 1$,

$$\partial_t u = \mu u - \left(q_c^2 + \Delta\right)^2 u$$

$$u \sim \exp(ikx + \sigma t)$$

$$\sigma u = \mu u - \left(q_c^2 - k^2\right)^2 u \Longrightarrow \sigma = \mu, k = q_c$$

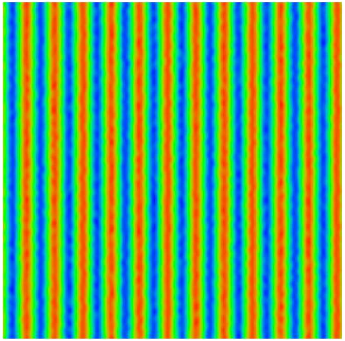
Add quadratic term to obtain hexagons

$$\partial_t u = \mu u - \left(q_c^2 + \Delta\right)^2 u + g_1 u^2 - u^3$$

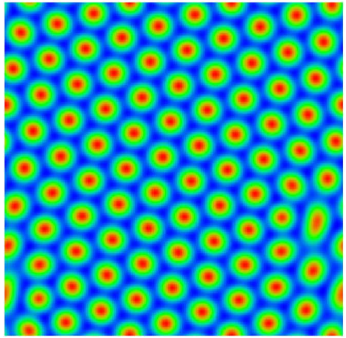
Include q_c and $q_c' = 1$ to obtain quasipatterns

$$\partial_t u = \mu u - \left(q_c^2 + \Delta\right)^2 (1 + \Delta)^2 u + g_1 u^2 - u^3$$

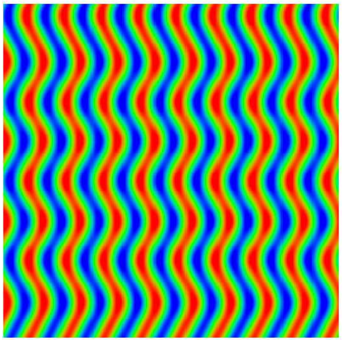
2D Patterns produced by Swift-Hohenberg equation



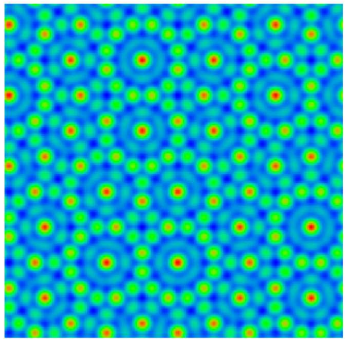
Stripes



Hexagons

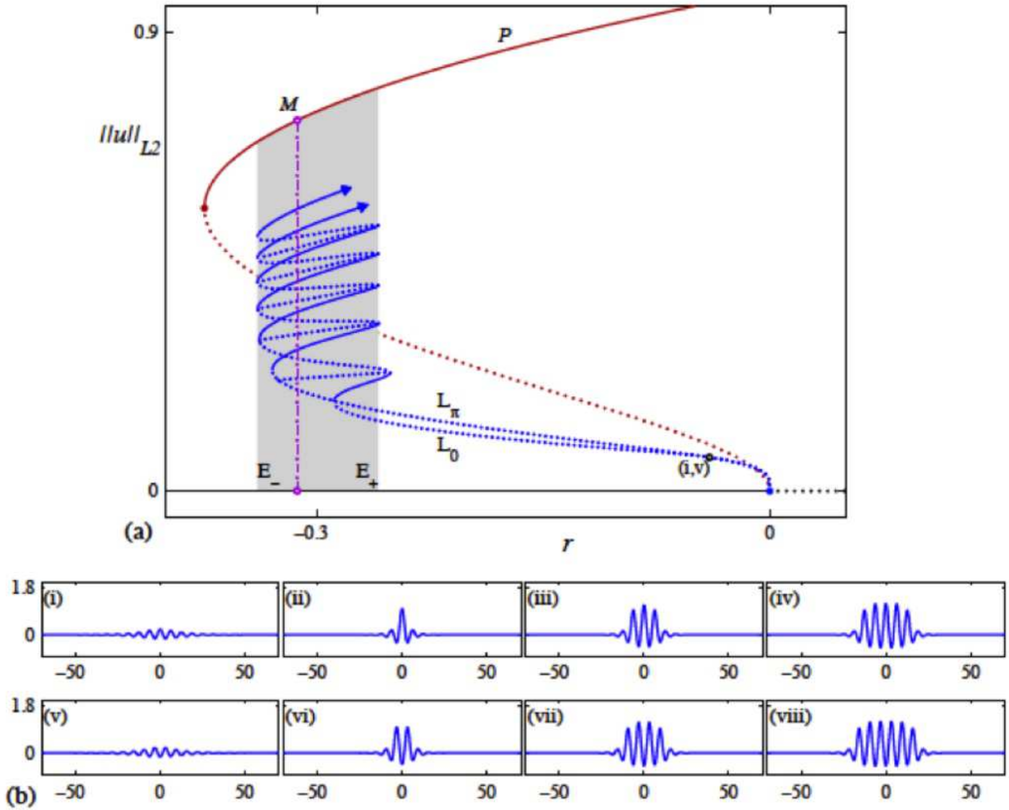


Zigzag instability

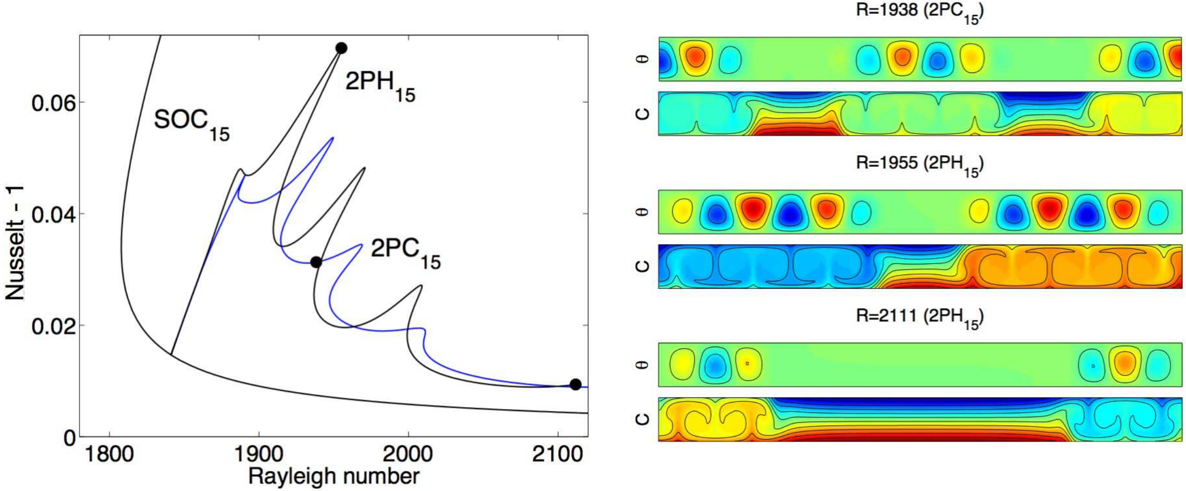


Quasicrystals

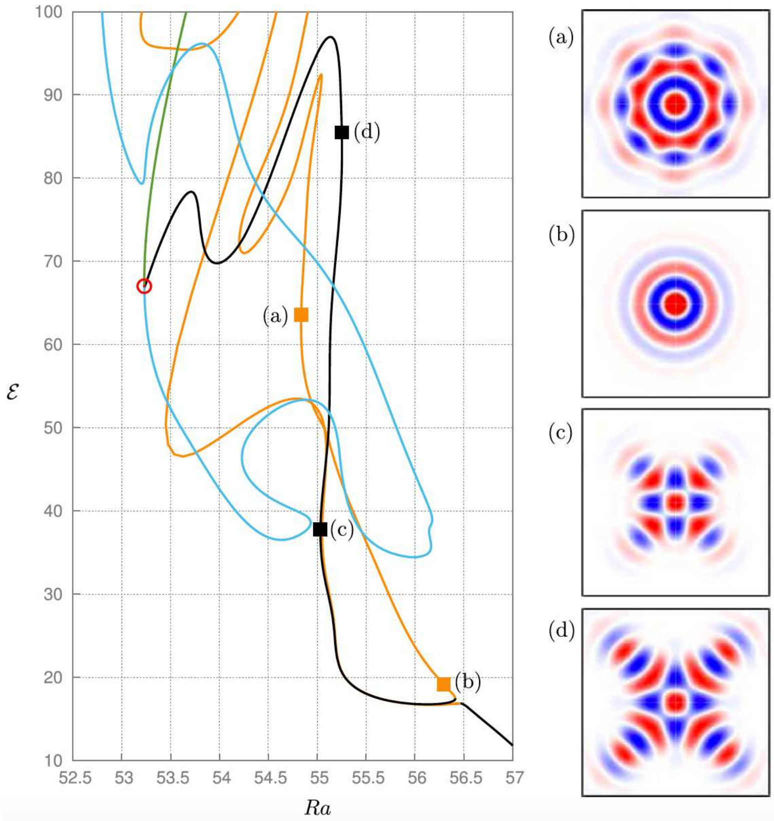
Snaking in 1D Swift-Hohenberg Equation



Thermosolutal Convection: Patterns with 1D snaking



Thermosolutal Convection: Patterns with 2D snaking



Newton's method: example

Swift-Hohenberg equation:

$$\partial_t U = F(U) = \mu U - \left(q_c^2 + \Delta\right)^2 U - U^3$$

Equation for steady state:

$$0 = F(U) = \mu U - \left(q_c^2 + \Delta\right)^2 U - U^3$$

Loop: calculate and compare with ϵ:

$$||F(U)|| \equiv ||\mu U - \left(q_c^2 + \Delta\right)^2 U - U^3|| < \epsilon \text{ ?}$$

If $||F(U)|| \not< \epsilon$, then U not solution, so try $U - u$:

$$\begin{aligned} 0 &= \mu(U-u) - \left(q_c^2 + \Delta\right)^2 (U-u) - (U-u)^3 \\ &= \mu U - \left(q_c^2 + \Delta\right)^2 U - U^3 - \left(\mu u - \left(q_c^2 + \Delta\right)^2 u - 3U^2 u - 3U u^2 - u^3\right) \end{aligned}$$

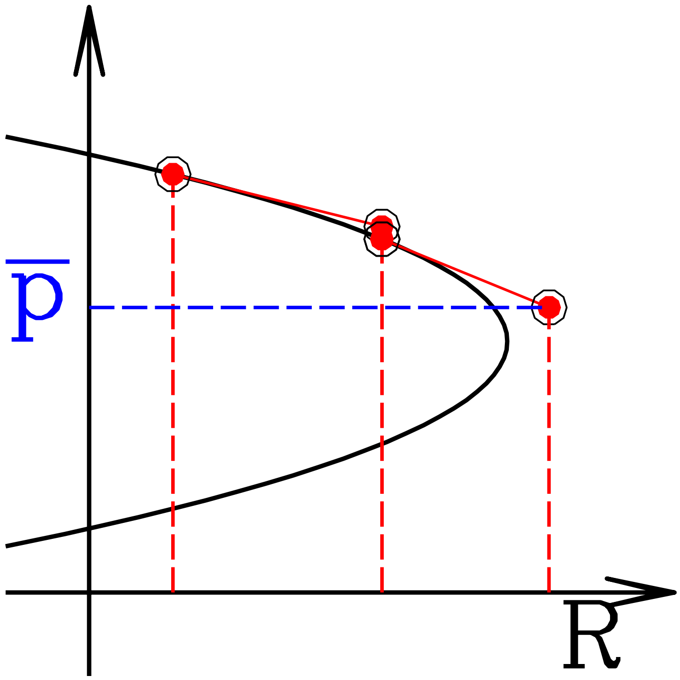
Newton step: truncate at first order in u and solve for $u(x)$:

$$\mu u - \left(q_c^2 + \Delta\right)^2 u - 3U^2 u = \mu U - \left(q_c^2 + \Delta\right)^2 U - U^3$$

Then replace and try again:

$$U \leftarrow U - u$$

Continuation: going around saddle-nodes



Goal:

$$0 = RN(U) + LU$$

$$0 = p(U,R) - \bar{p} \quad \text{where} \quad \left\{ \begin{array}{l} U_i \text{ some component} \\ R \end{array} \right\}$$

Newton step:

(U, R) not solution, so try $(U - u, R - r)$

$$\begin{aligned} 0 &= (R-r)N(U-u) + L(U-u) \\ &= RN(U) + LU - RN_U u - rN(U) - Lu + O(r,u)^2 \end{aligned}$$

$$0 = p(U-u, R-r) - \bar{p} = \left\{ \begin{array}{c} U_i - \bar{p} - u_i \\ R - \bar{p} - r \end{array} \right\}$$

$$\underbrace{\left[\begin{array}{c|c} RN_U + L & N(U) \\ \hline 0\ 0 \ldots 0\ 1\ 0 \ldots 0 & 1 \end{array}\right]}_{or} \begin{bmatrix} u \\ r \end{bmatrix} = \begin{bmatrix} RN(U) + LU \\ \left\{ \begin{array}{c} U_i - \bar{p} \\ R - \bar{p} \end{array} \right\} \end{bmatrix}$$

If $p(U, R) = R$ (i.e. set Reynolds number), then set $R = \bar{p}$, $r = 0$ and get previous case:

$$[RN_U + L]\,[u] = [RN(U) + LU]$$

If $p(U, R) = U_i$, then must solve extended system for (u, r).

$$\left[\begin{array}{c|c} (RN_u + L) & N(U) \\ \hline 0\ 0 \ldots 0\ 1\ 0 \ldots 0 & 0 \end{array}\right] \begin{bmatrix} u \\ r \end{bmatrix} = \begin{bmatrix} (RN(U) + LU) \\ U_i - \bar{p} \end{bmatrix}$$

$$\left.\begin{array}{l} \textbf{Set } u_i = U_i - \bar{p} \\ \textbf{Calculate } (RN_U + L)u \\ \textbf{Add } N(U)r \end{array}\right\}$$

It may be sufficient to extrapolate quadratically.

Far from saddle-node bifurcation, U is considered to be a function of R. To get an initial guess for U at a new R, extrapolate.

Zeroth order extrapolation:

$$U(R^{(2)})_{\text{initial guess}} = U(R^{(1)})$$

Linear extrapolation:

$$U(R^{(2)})_{\text{initial guess}} = U(R^{(1)}) + (U(R^{(1)}) - U(R^{(0)}))\frac{R^{(2)} - R^{(1)}}{R^{(1)} - R^{(0)}}$$

Quadratic extrapolation:

Fit quadratic polynomials through $U(R^{(0)})$, $U(R^{(1)})$, $U(R^{(2)})$ as functions of R and evaluate polynomial at new value $R^{(3)}$.

Close to saddle-node bifurcation, choose distinguished value U_i and consider U_j, $j \neq i$ and R to be quadratic functions of U_i.

Set new value of U_i, and evaluate new estimate of U_j and R
Now, ΔR can change sign and can go around saddle-node.

Reaction-Diffusion Equations

$$\partial_t u_i = \underbrace{f_i(u_1, u_2, \ldots)}_{\text{reaction}} + \underbrace{D_i \Delta u_i}_{\text{diffusion}}$$

Reactions f_i couple <u>different</u> species u_i at <u>same</u> location

Diffusivity D_i couples <u>same</u> species u_i at <u>different</u> locations

Describe oscillating chemical reactions, such as famous Belousov-Zhabotinskii reaction, discovered by two Soviet scientists in 1950s-1960s.

Also describe phenomena in

–biology (population biology, epidemiology, neurosciences)

–social sciences (economics, demography)

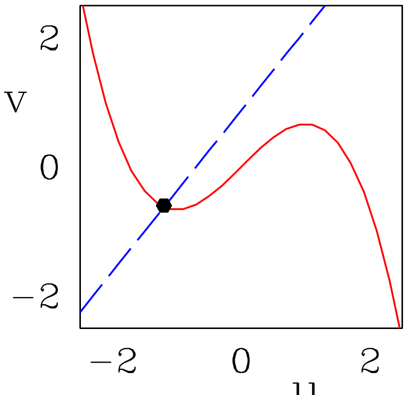
–physics

Two species

$$\partial_t u = f(u,v) + D_u \Delta u$$
$$\partial_t v = g(u,v) + D_v \Delta v$$

FitzHugh-Nagumo model

$$f(u,v) = u - u^3/3 - v + I$$
$$g(u,v) = 0.08\,(u + 0.7 - 0.8\,v)$$

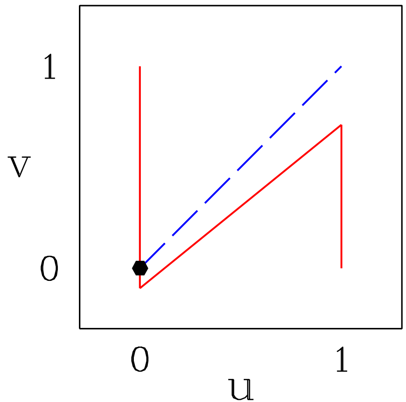


Spatially homogeneous

$$\partial_t u = f(u,v)$$
$$\partial_t v = g(u,v)$$

Barkley model

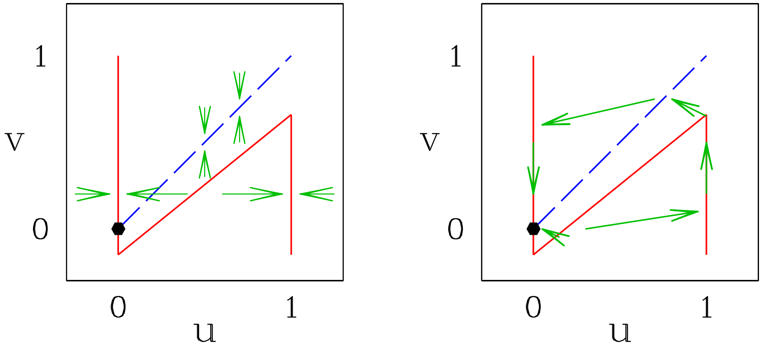
$$f(u,v) = \frac{1}{\epsilon}\,u(1-u)\left(u - \frac{v+b}{a}\right)$$
$$g(u,v) = u - v$$



u-nullclines $f(u,v) = 0$, v-nullclines $g(u,v) = 0$, • steady states

stable if eigenvalues of $\begin{pmatrix} f_u & f_v \\ g_u & g_v \end{pmatrix}$ **have negative real parts**

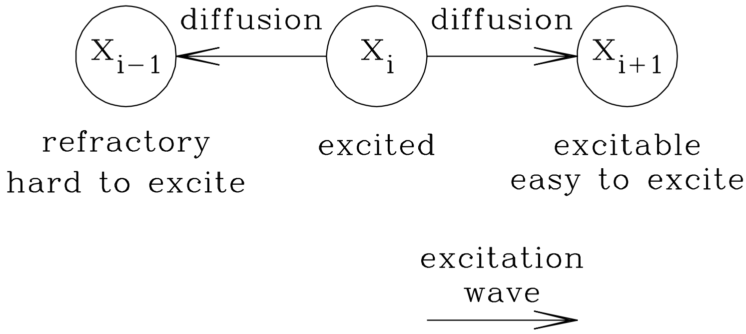
$$f(u,v) = \frac{1}{\epsilon}\, u(1-u)\left(u - \frac{v+b}{a}\right) \qquad g(u,v) = u - v$$



$\partial_t u = f = 0$	**separates**	$\longleftarrow$	**and**	$\longrightarrow$	$O(\epsilon^{-1})$
$\partial_t v = g = 0$	**separates**	$\uparrow$	**and**	$\downarrow$	$O(1)$

$u = 1$		**excited phase**
$u = 0$	$v \sim 1$	**refractory phase**
$u = 0$	$v \ll 1$	**excitable phase**
$u = (v+b)/a$		**excitation threshold**

Waves in Excitable Medium



Spatial variation + diffusion + excitability $\Longrightarrow$ propagating waves

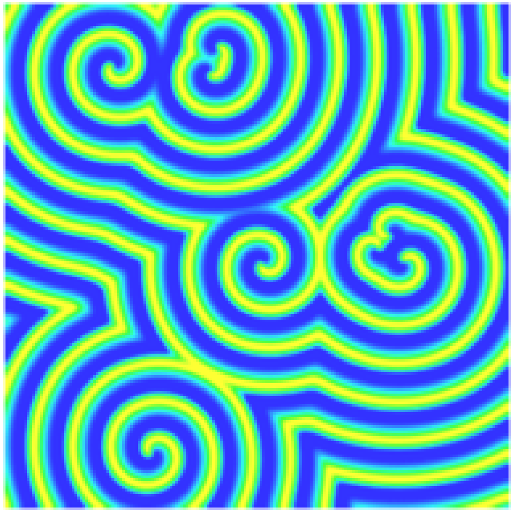
Excitable media in physiology:

–neurons

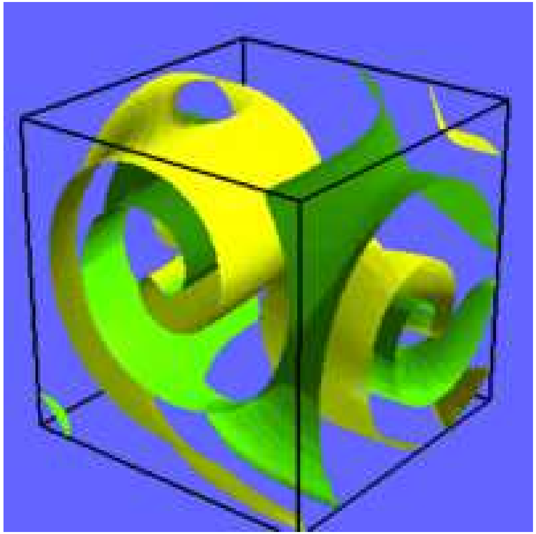
–cardiac tissue (the heart)

Pacemaker periodically emits electrical signals, propagated to rest of heart

Simulations from *Barkley model*, Scholarpedia



Spiral waves in 2D



Spiral waves in 3D

Traveling waves: $U(x - Ct, y, z)$

$$\text{Goal}: \begin{cases} 0 = C\partial_x U + N(U) + LU \\ 0 = p(U) - \bar{p} \end{cases}$$

Newton step:

(U, C) **not solution, so try** $(U - u, C - c)$

$$\begin{aligned} 0 &= (C - c)\partial_x(U - u) + N(U - u) + L(U - u) \\ &= C\partial_x U + N(U) + LU - C\partial_x u - c\partial_x U - N_U u - Lu \\ 0 &= p(U - u, R - r) - \bar{p} = \begin{Bmatrix} U_i - \bar{p} - u_i \\ R - \bar{p} - r \end{Bmatrix} \end{aligned}$$

$$\left[\begin{array}{c|c} C\partial_x + N_U + L & \partial_x U \\ \hline 0\,0\ldots0\,1\,0\ldots0 & 0 \end{array}\right] \begin{bmatrix} u \\ c \end{bmatrix} = \begin{bmatrix} C\partial_x U + N(U) + LU \\ U_i - \bar{p} \end{bmatrix}$$

Navier-Stokes Equations

$$\begin{aligned}
\partial_t \boldsymbol{U} &= -(\boldsymbol{U}\cdot\boldsymbol{\nabla})\boldsymbol{U} - \boldsymbol{\nabla} \boldsymbol{P} &+ \boldsymbol{\nu \Delta U} \\
&= -(\boldsymbol{I} - \boldsymbol{\nabla\nabla}^{-2}\boldsymbol{\nabla}\cdot)(\boldsymbol{U}\cdot\boldsymbol{\nabla})\boldsymbol{U} &+ \boldsymbol{\nu \Delta U} \\
&= \boldsymbol{N}(\boldsymbol{U}) &+ \boldsymbol{L}\,\boldsymbol{U}
\end{aligned}$$

$$\begin{aligned}
\boldsymbol{N_U u} &\equiv -(\boldsymbol{U}\cdot\boldsymbol{\nabla})\boldsymbol{u} - (\boldsymbol{u}\cdot\boldsymbol{\nabla})\boldsymbol{U} \\
\boldsymbol{A_U u} &= \boldsymbol{N_U u} + \boldsymbol{L u}
\end{aligned}$$

Must solve

$$\boldsymbol{L u} + \boldsymbol{N_U u} = \boldsymbol{L U} + \boldsymbol{N}(\boldsymbol{U})$$