Computing turbulent processes in physics, chemistry & biology

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http://www.ucalgary.ca/complexity/

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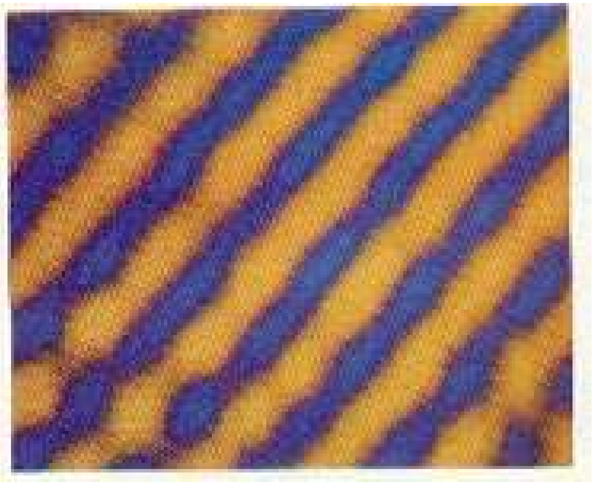
I. Spontaneous pattern formation in reaction-diffusion media



Reaction-diffusion media (mass action kinetics)

$$\partial_t \vec{c}(\vec{r}) = \vec{R}(\vec{c}(\vec{r})) + D\nabla^2 \vec{c}(\vec{r})$$

$$A_1 + X_1 \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} 2X_1 \qquad X_1 + X_2 \underset{k_{-2}}{\overset{k_2}{\rightleftharpoons}} 2X_2 \qquad A_5 + X_2 \underset{k_{-3}}{\overset{k_3}{\rightleftharpoons}} A_2$$

$$X_1 + X_3 \underset{k_{-4}}{\overset{k_4}{\rightleftharpoons}} A_3 \qquad A_4 + X_3 \underset{k_{-5}}{\overset{k_5}{\rightleftharpoons}} 2X_3 \, .$$

$$\frac{\mathrm{d}c_1}{\mathrm{d}t} = k_1 c_{A_1} c_1 - k_{-1} c_1^2 - k_2 c_1 c_2 + k_{-2} c_2^2 - k_4 c_1 c_3 + k_{-4}$$

$$\frac{\mathrm{d}c_2}{\mathrm{d}t} = k_2 c_1 c_2 - k_{-2} c_2^2 - k_3 c_{A_5} c_2 + k_{-3} c_{A_2}$$

$$\frac{\mathrm{d}c_3}{\mathrm{d}t} = -k_4 c_1 c_3 + k_{-4} c_{A_3} + k_5 c_{A_4} c_3 - k_{-5} c_3^2 \, .$$

$A_1, \ldots, A_5$ pool chemical of fixed concentration; model constructed phenomenologically

II. Non-equilibrium dynamics: (Bio-)Chemical oscillations

Example: Peroxidase-oxidase reaction

Destruction of bacteria by white blood cells (metabolic process):

$$2\text{NADH} + \text{O}_2 + 2\text{H}^+ \xrightarrow{\text{Per}} 2\text{NAD}^+ + 2\text{H}_2\text{O}$$

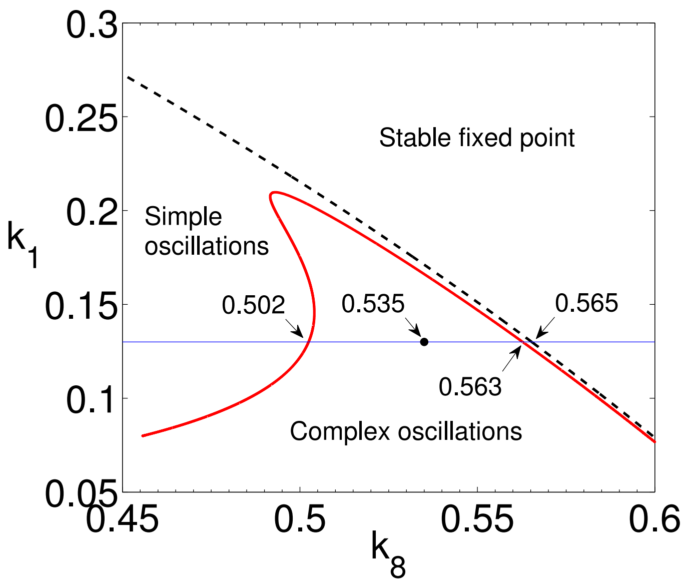
NADH: nicotinamide adenine dinucleotide

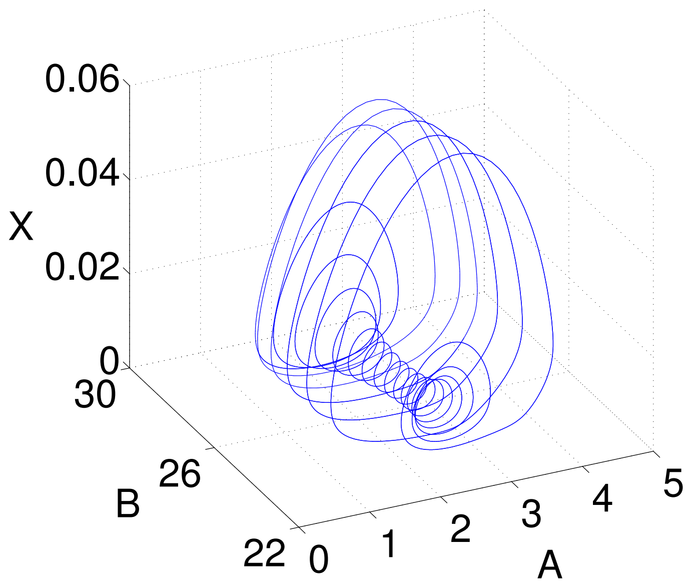
reaction catalyzed by enzyme (horseradish peroxidase), its concentration acts as the control parameter

oscillations and more complex dynamics

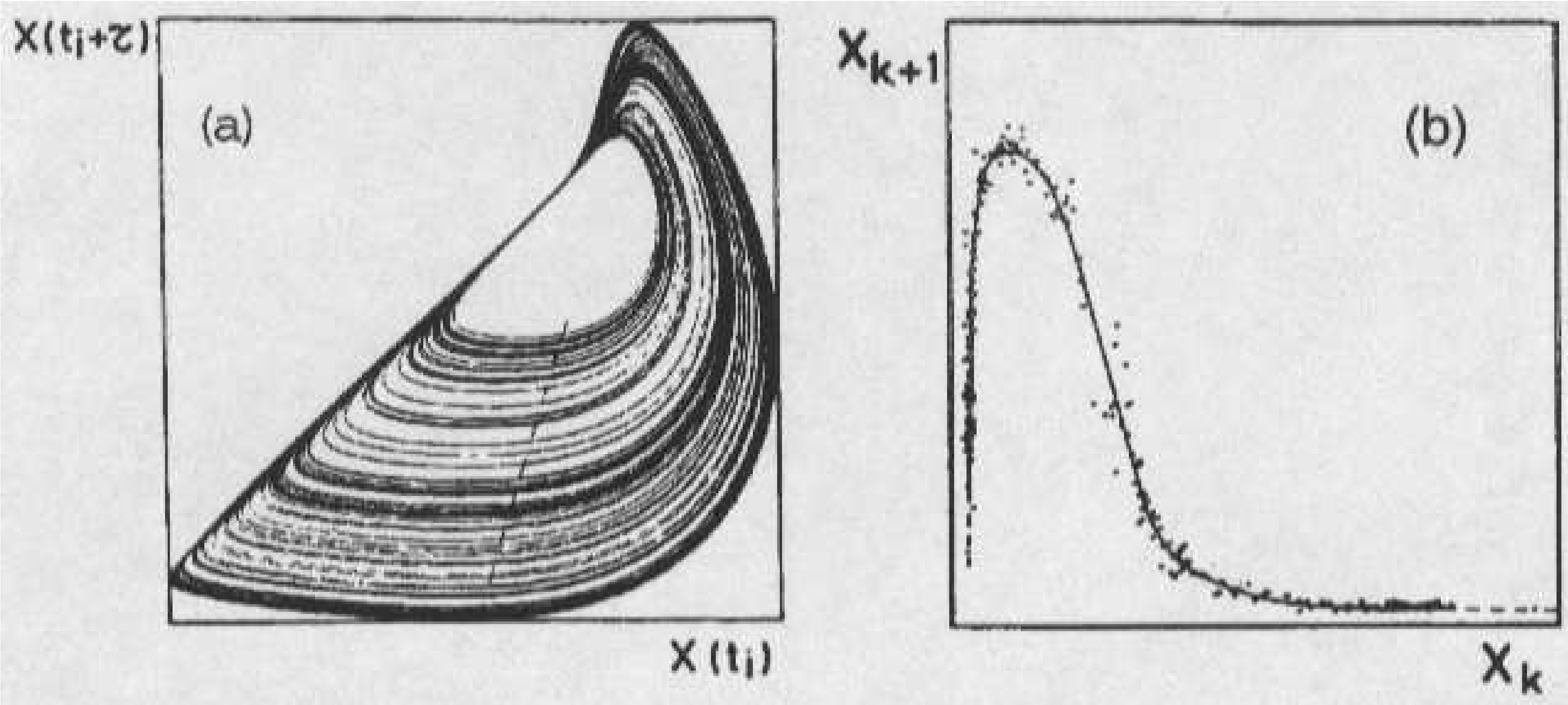
Simple model of peroxidase-oxidase reaction (Steinmetz *et al.* ’91)

$$\begin{aligned}
\dot{A} &= k_7 - k_1 ABX - k_3 ABY - k_9 A \\
\dot{B} &= k_8 - k_1 ABX - k_3 ABY \\
\dot{X} &= k_6 + k_1 ABX + 2k_3 ABY - 2k_2 X^2 - k_4 X \\
\dot{Y} &= 2k_2 X^2 - k_3 ABY - k_5 Y
\end{aligned}$$



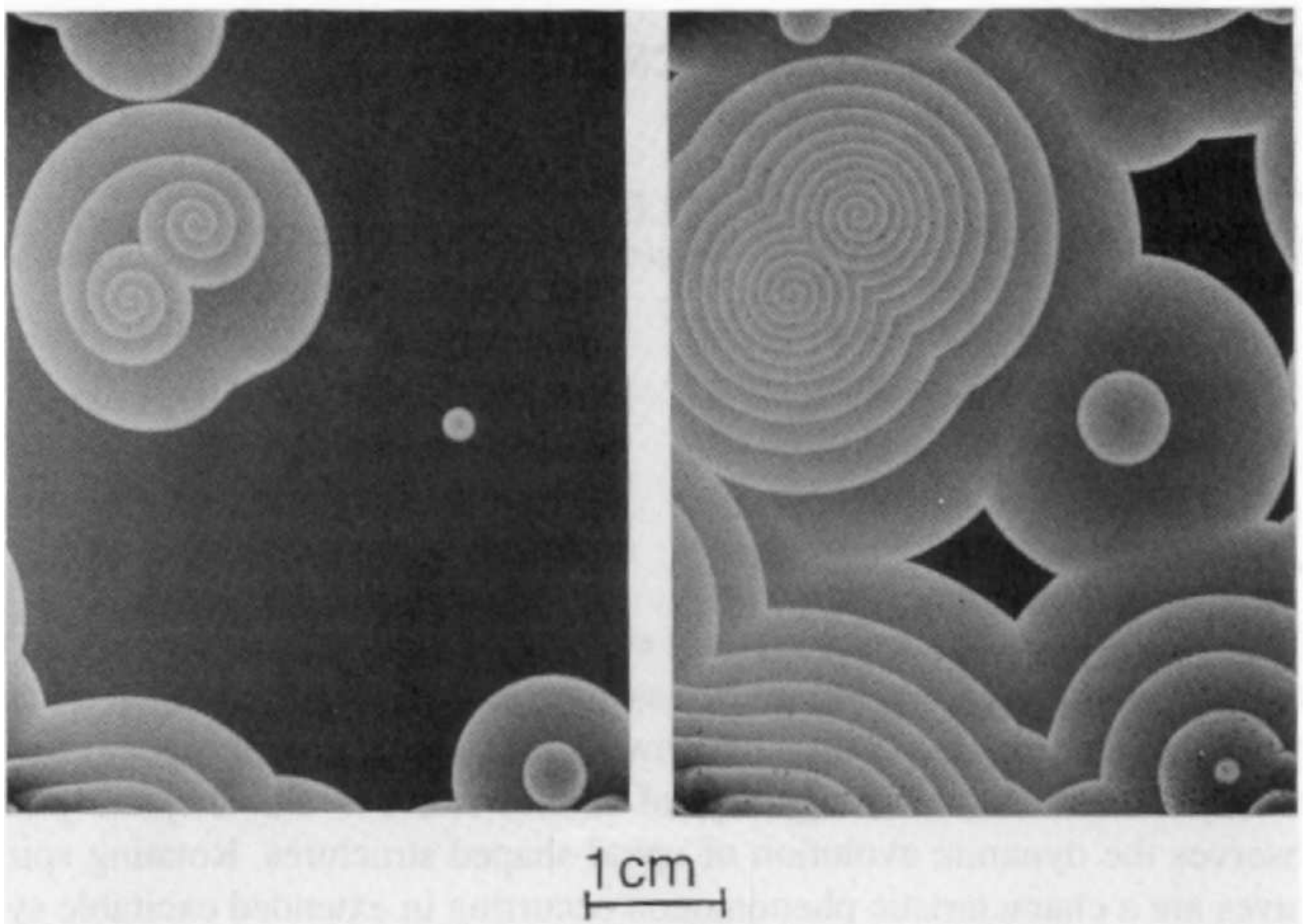


Chemical chaos in Belousov-Zhabotinsky reaction (Roux *et al.* '81)



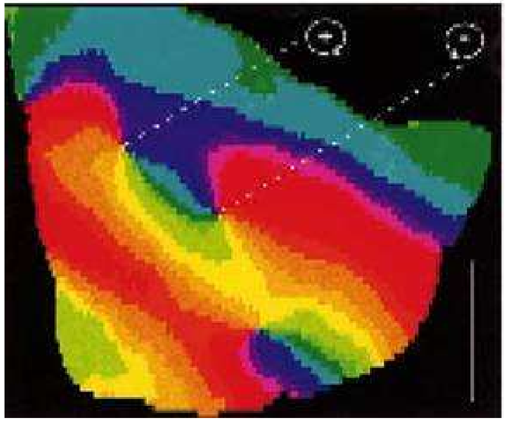
III. Nonlinear wave patterns: Spiral waves

Spiral waves in 2d media (Scott '91)

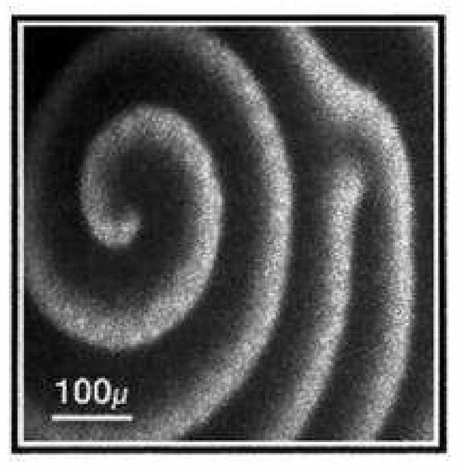


Examples

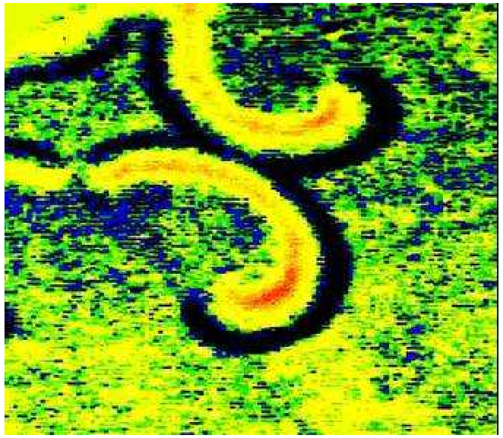
CO oxidation



heart tissue

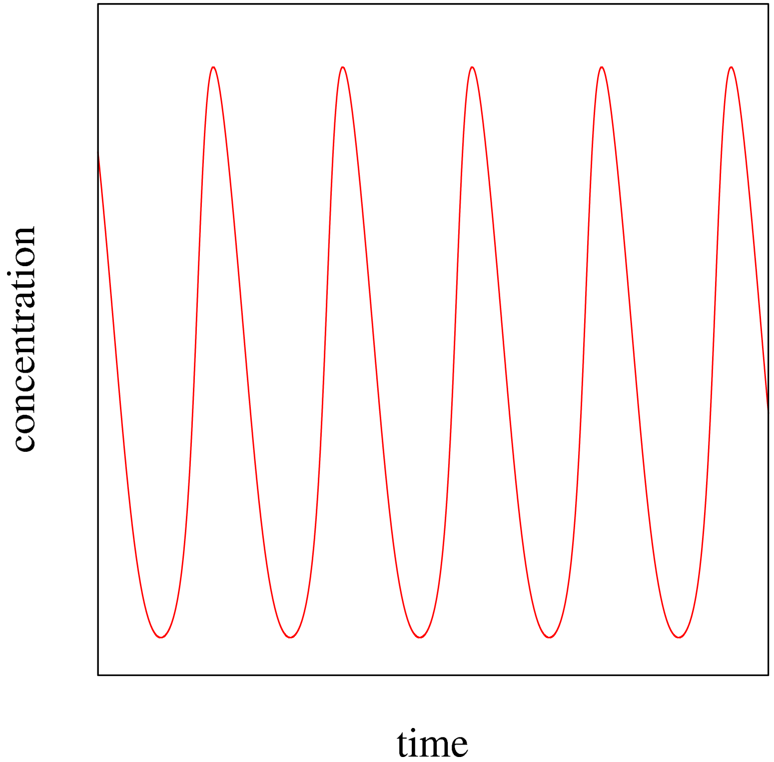


calcium waves in frog eggs



glycolysis in yeast

Topological definition of spirals



Periodic signal in 2d phase space (e.g., excitable or oscillatory media):
phase description ϕ with $\frac{d\phi}{dt} = \omega_0$

Phase locking:
$|\phi_1(t) - \phi_2(t)| < const$

$$I_t = \frac{1}{2\pi} \oint \nabla\phi(\mathbf{r}, t) \cdot d\mathbf{l}$$ (index, topological charge)

Topological theorem for spirals

$$\Sigma_A I_t = 0$$

Implications:

☞ In the bulk, single-armed spirals are created and annihilated pairwise with opposite index I

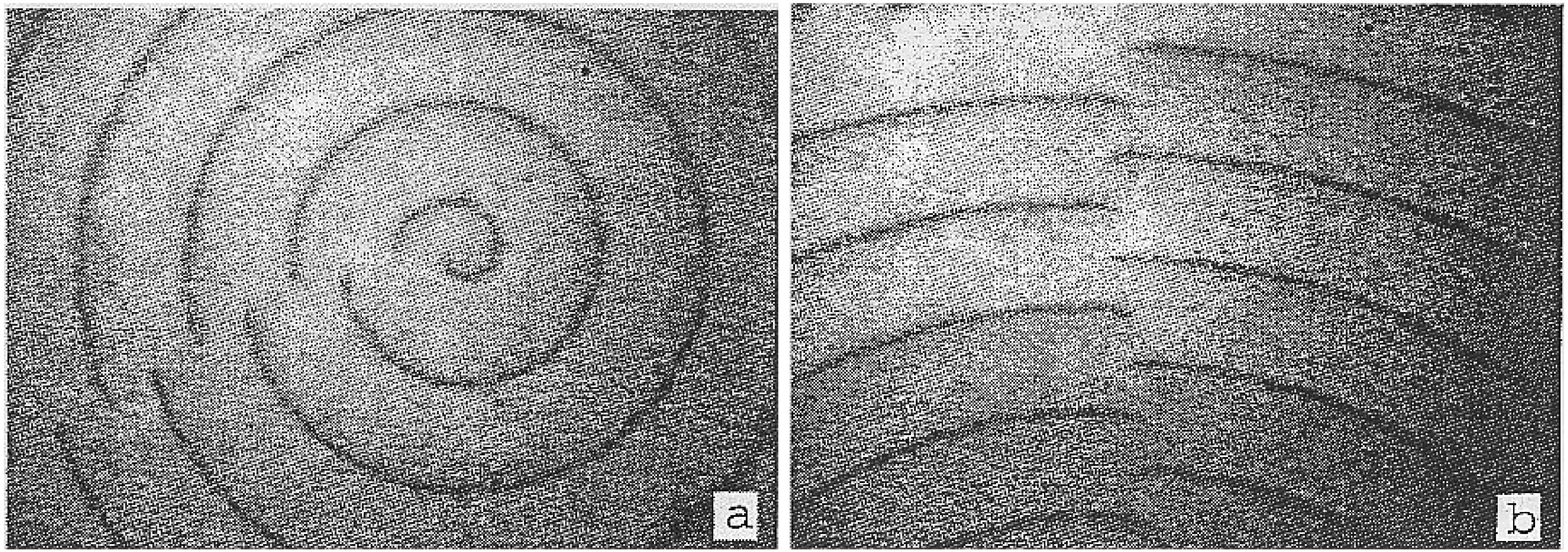
☞ Single spirals can be created and annihilated at the boundaries

For oscillatory media (Hagan '82):

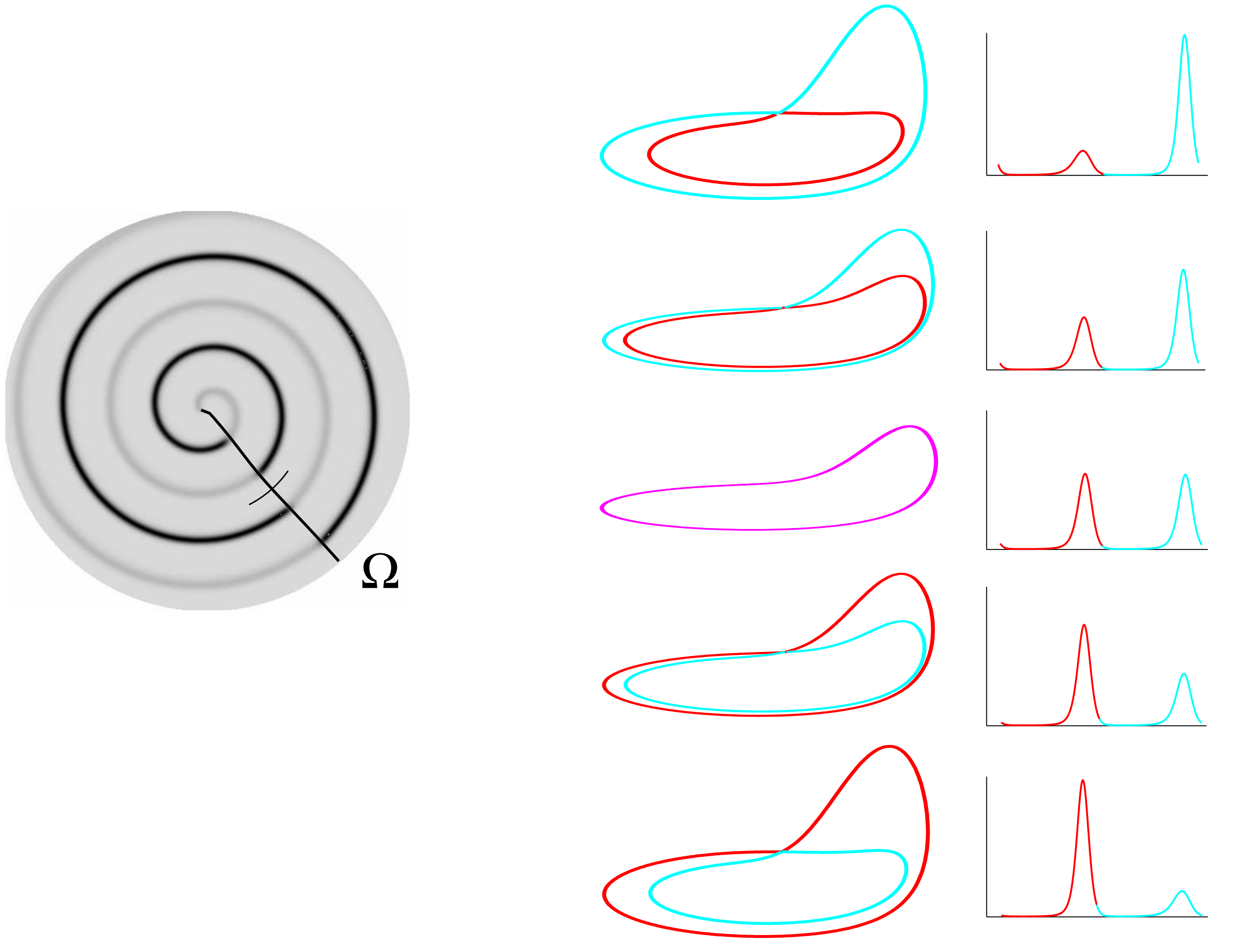
$$I_t = \pm 1$$

IV. Spirals in complex-oscillatory media

“Broken” spirals (Yoneyama *et al.* ’95)



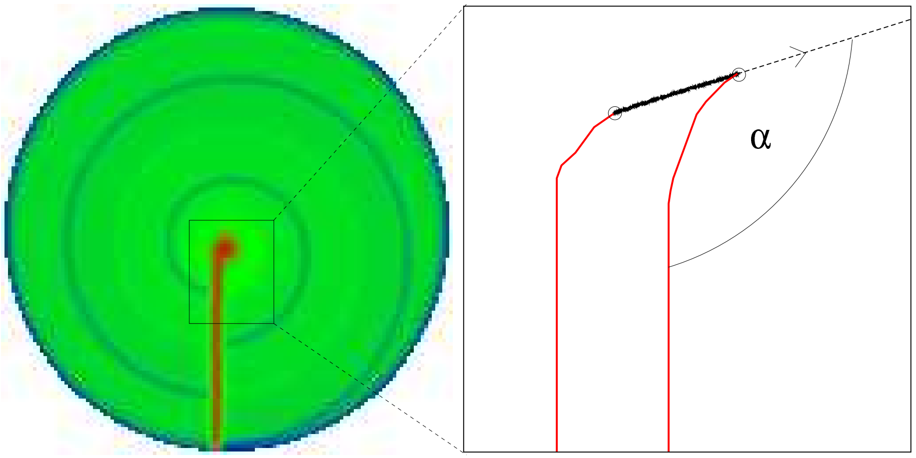
Period-2 media: Synchronization defect line (Goryachev *et al.* ’00)

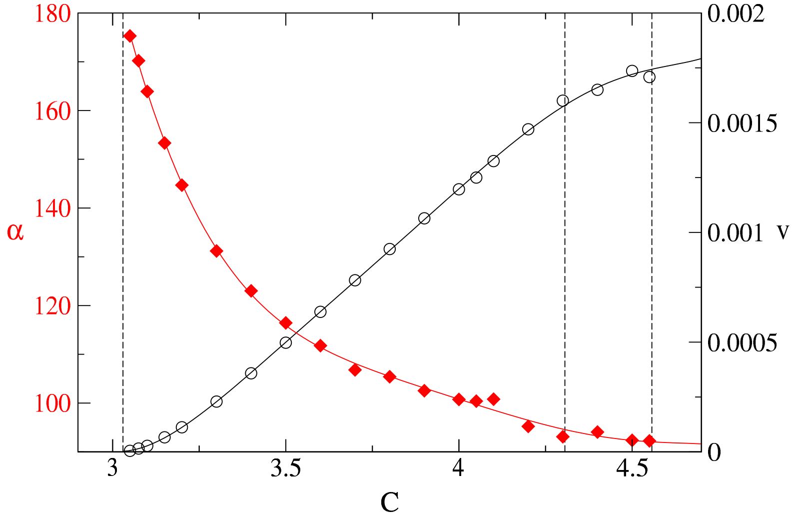


Rössler model (Davidsen *et al.* '04)

$$\partial_t \mathbf{c}(\mathbf{r},t) = \mathbf{R}[\mathbf{c}(\mathbf{r},t)] + D\nabla^2 \mathbf{c}(\mathbf{r},t),$$

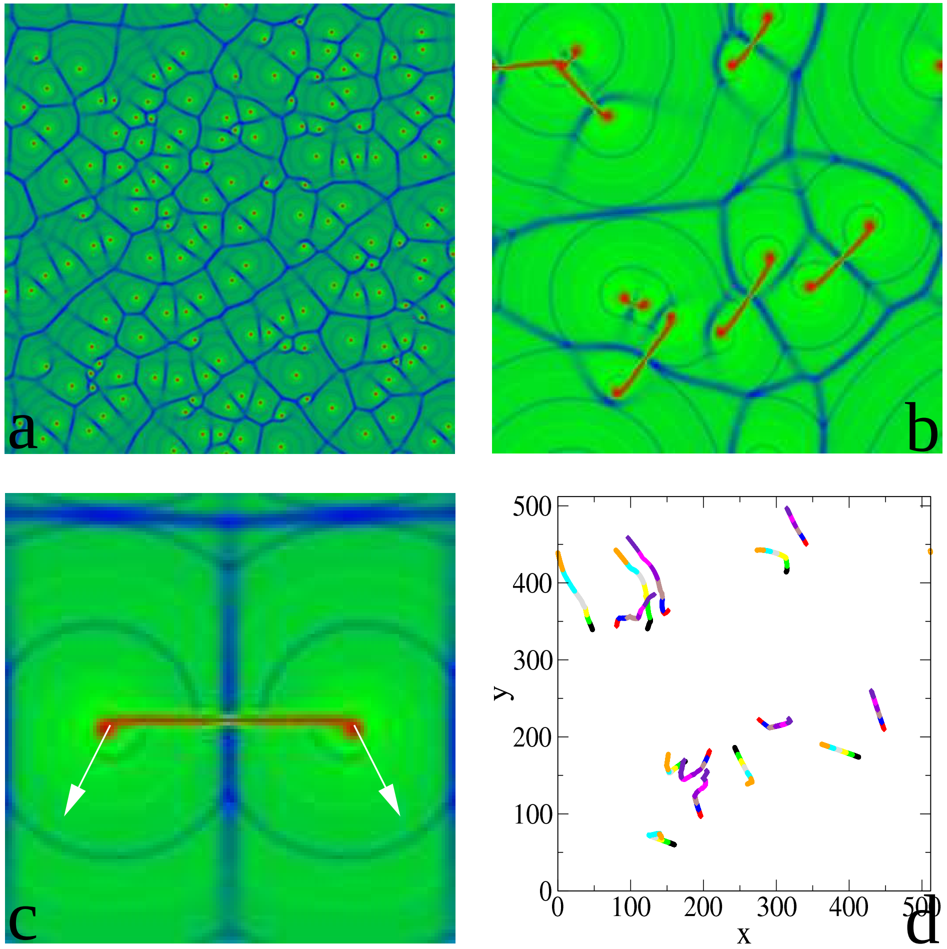
$R_x = -c_y - c_z$, $R_y = c_x + 0.2c_y$, $R_z = c_x c_z - Cc_z + 0.2$ with $C \in [2.0, 6.0]$





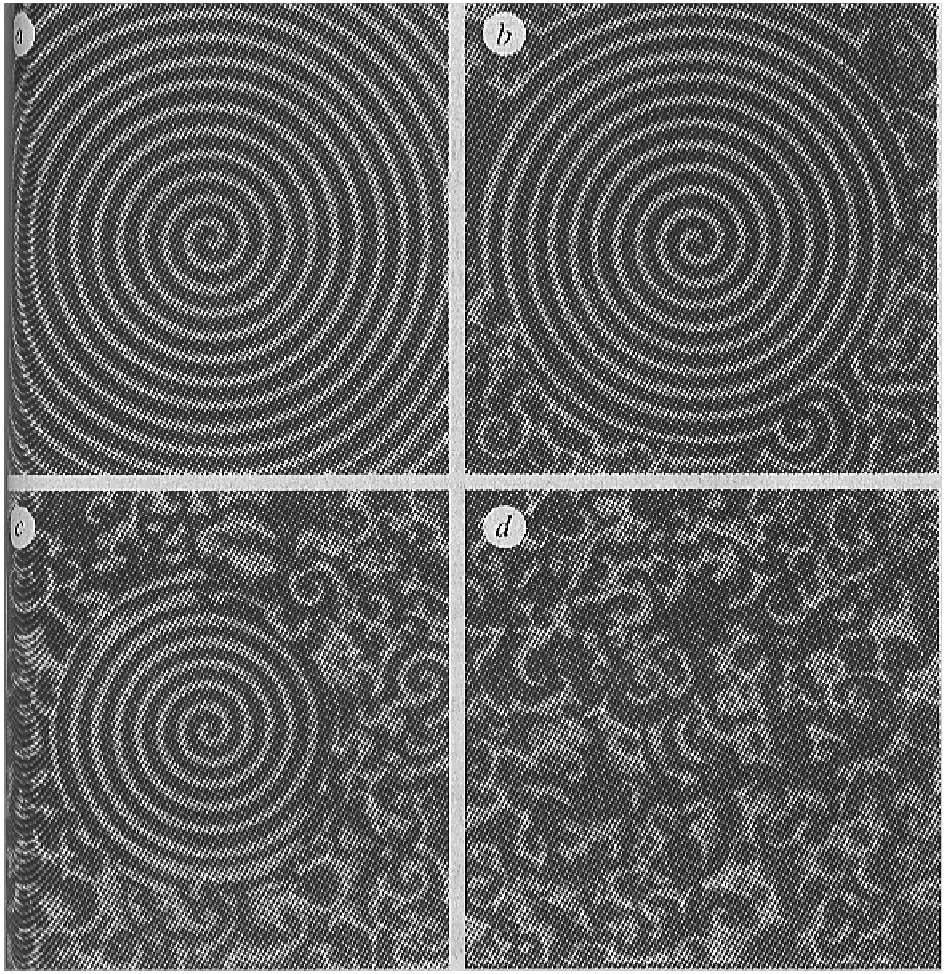
$v \propto (C - C_2)^\gamma$ with $C_2 \approx 3.03$, $\gamma \approx 1.5$

Multi-spiral pattern: Novel vortex liquid



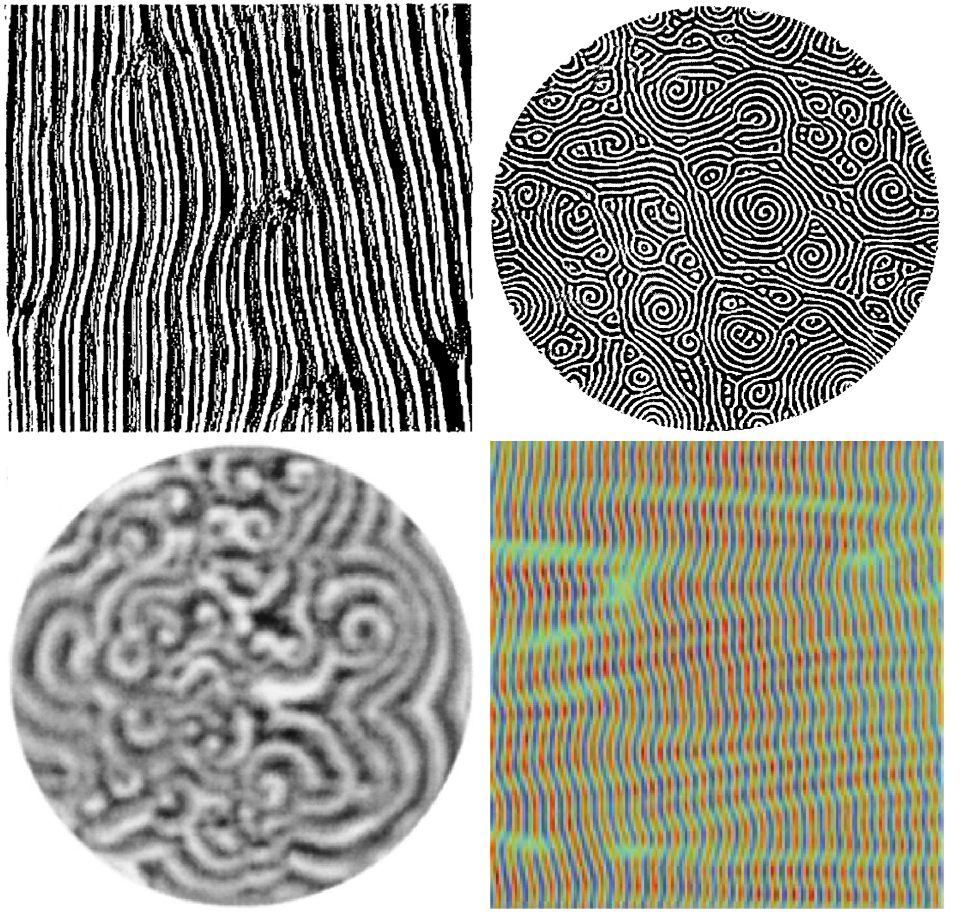
(a): P1 regime ($C = 2.5$, $L = 1024$). (b,c): P2 regime ($C = 3.5$, $L = 512$). (d): Trajectories of spiral cores leading to the configuration shown in (b).

V. Defect-mediated turbulence



spiral break-up induced by change in control parameter

Examples

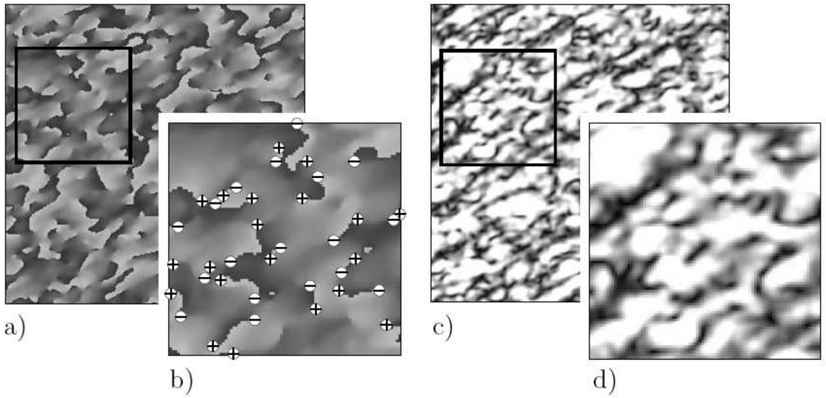


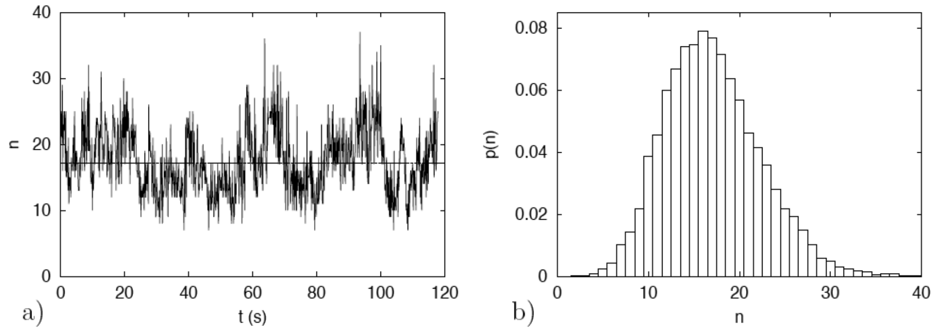
taken from Rehberg *et al.* ’89, Morris *et al.* ’93, Ouyang *et al.* ’00, Daniels *et al.* ’02

$$\partial_t A = A + (1 + i\alpha)\nabla^2 A - (1 + i\beta)|A|^2 A \qquad \text{(Complex Ginzburg Landau)}$$

Definition

defects are created and annihilated to give a statistically stationary number of defects pairs in the system (caused by far-field or core instabilities, for example (Bär *et al.* ’04))





experimental results for CO oxidation on Pt (110) (Beta *et al.* ’06)

Reduced description: Markov model (Gil *et al.* '90)

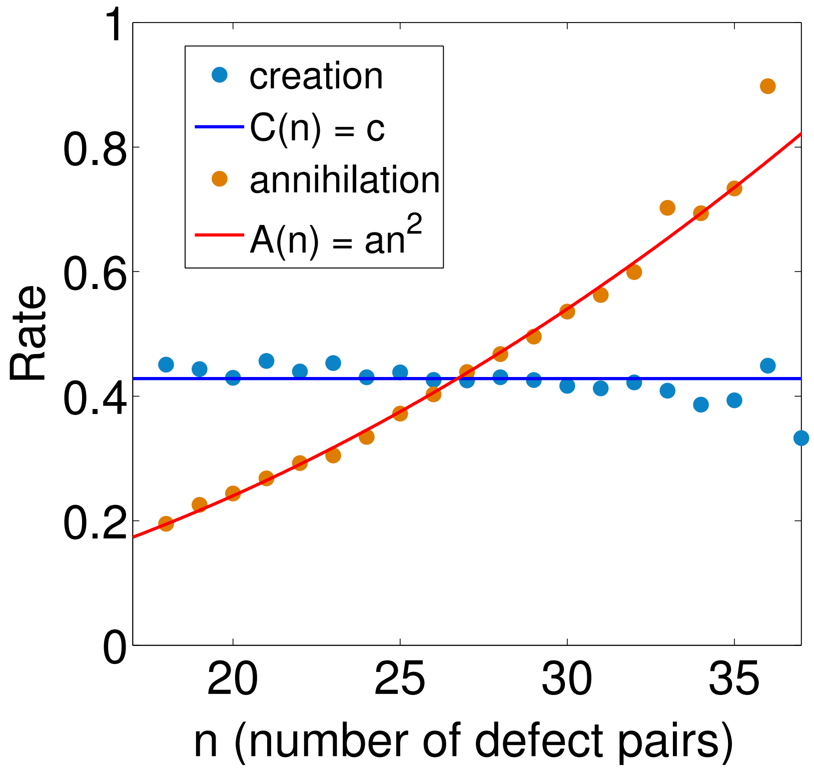
Assumptions:

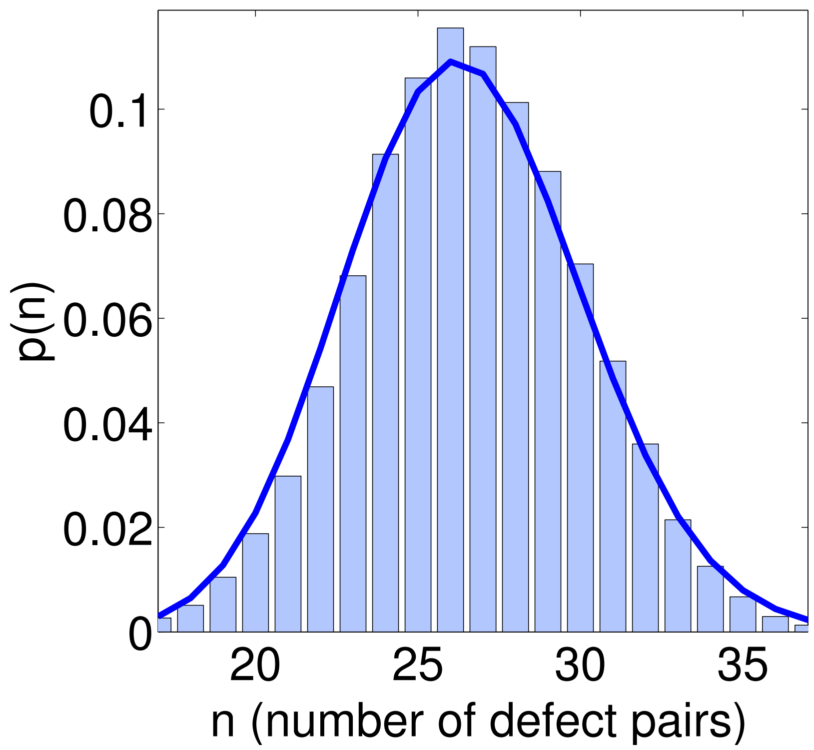
- ☞ Defect pairs are statistically independent entities
- ☞ Creation rate: $c(n) = c = \mathrm{const}$
- ☞ Annihilation rate: $a(n) = an^2$

Predictions:

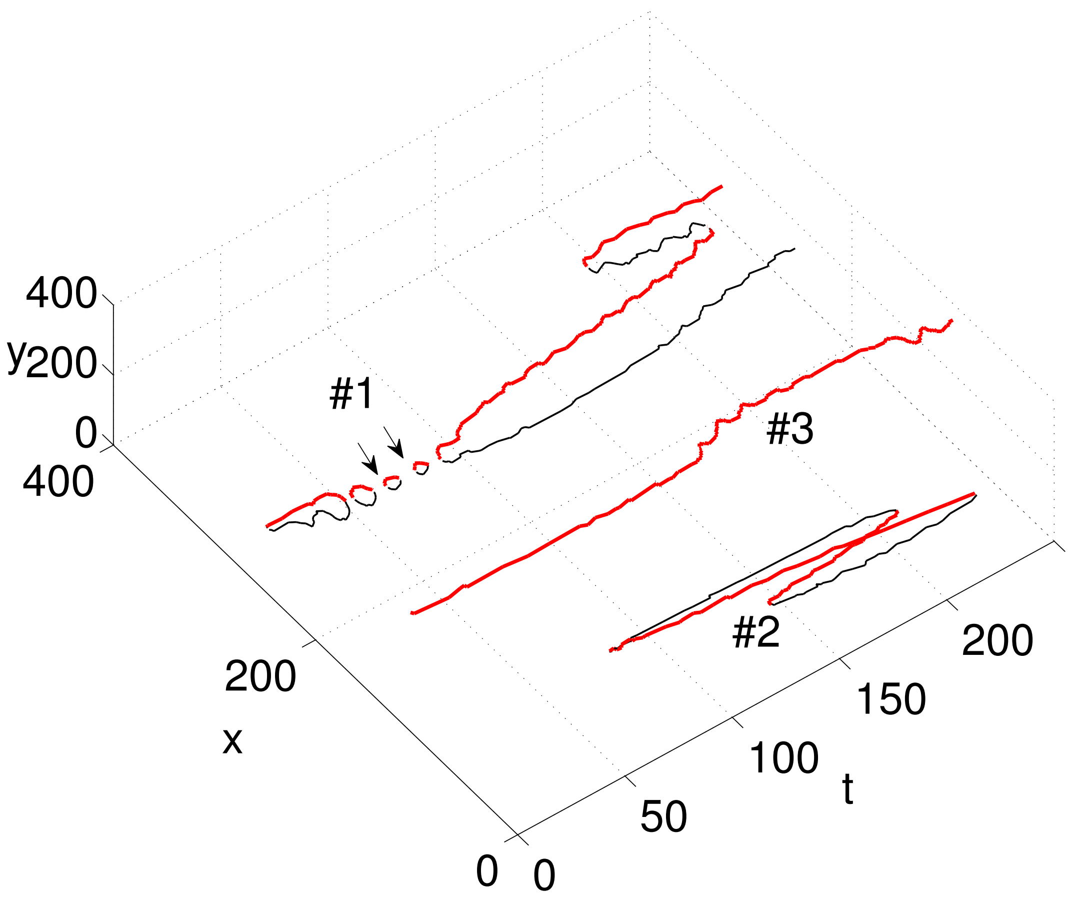
- ☞ $\frac{dp(n,t)}{dt} = c(n-1)p(n-1,t) + a(n+1)p(n+1,t) - [a(n)+c(n)]p(n,t)$
- ☞ $p(n) = [c(n-1)/a(n)]p(n-1)$
- ☞ $p(n) \propto (c/a)^n/(n!)^2$
- ☞ modifications apply if boundary effects, strong correlations and/or induced nucleation have to be taken into account

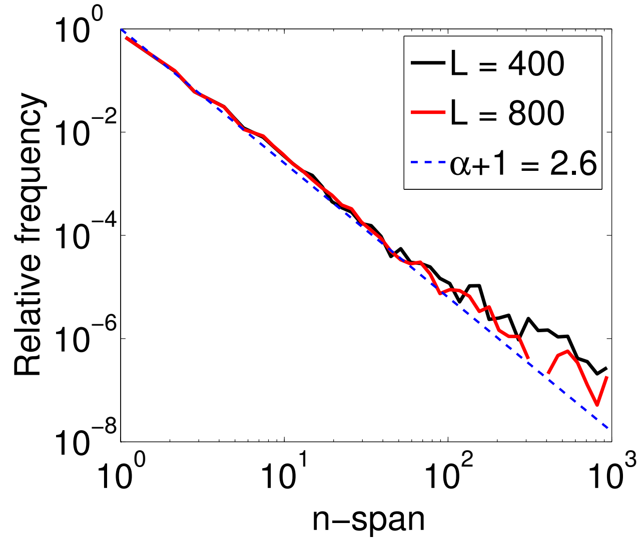
Simple model of peroxidase-oxidase reaction (St-Yves *et al.* ’10)

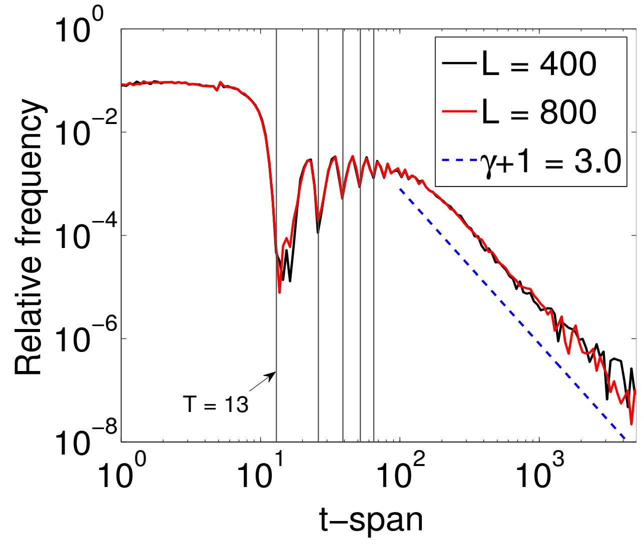




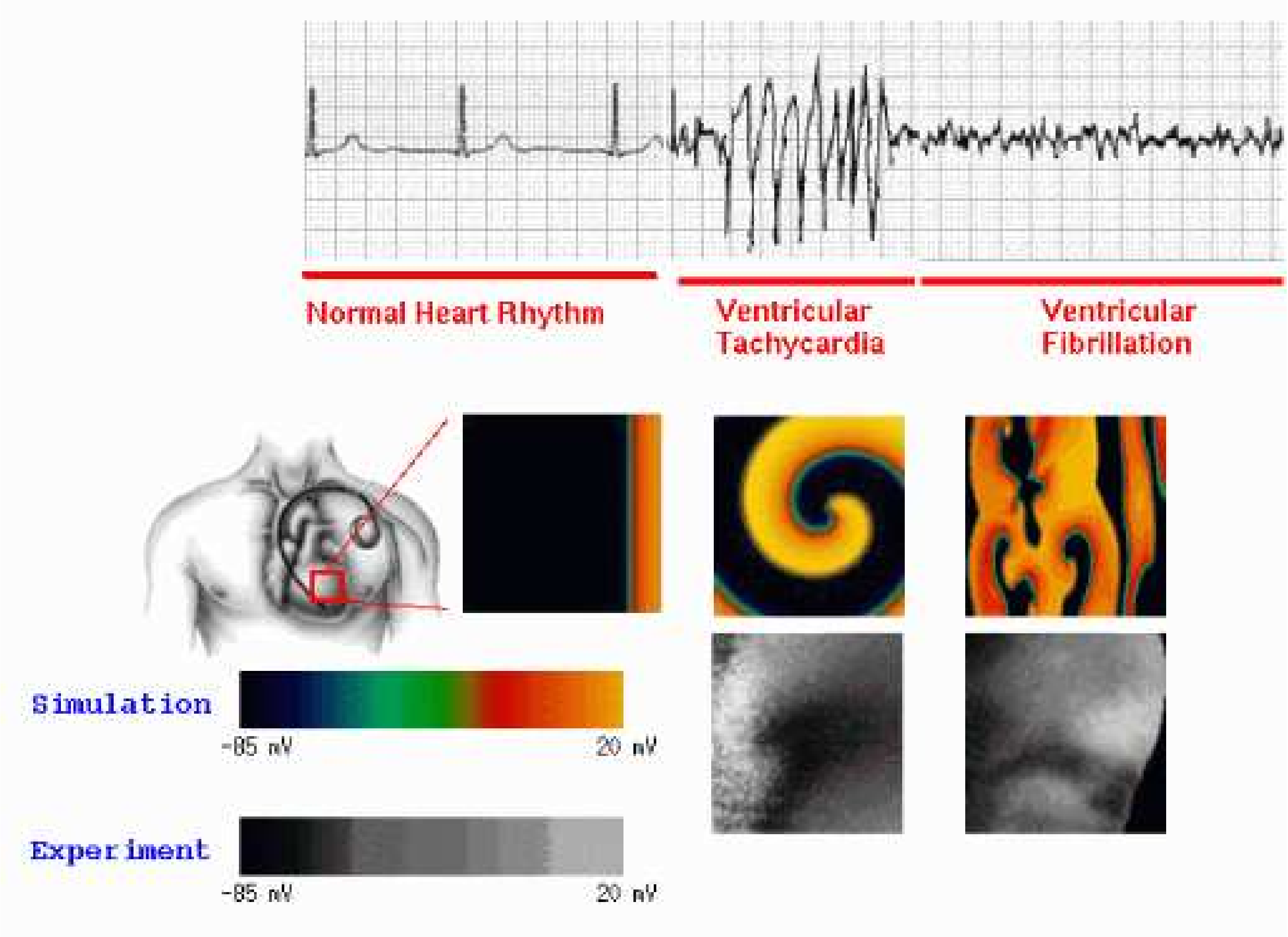
Loops of defect trajectories



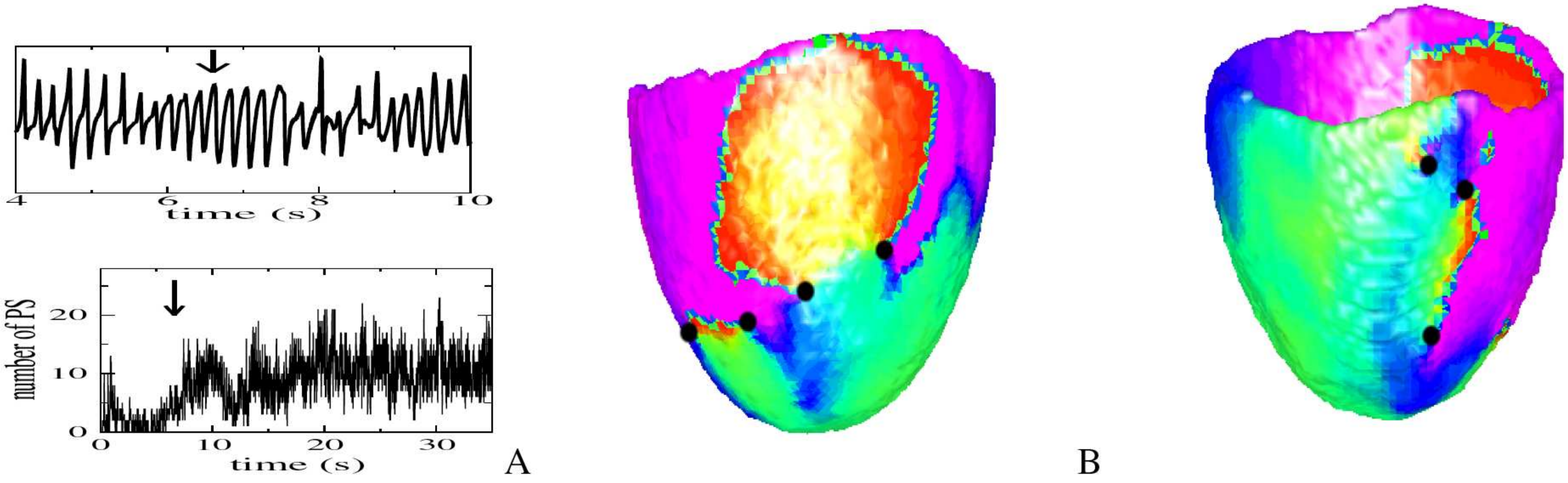




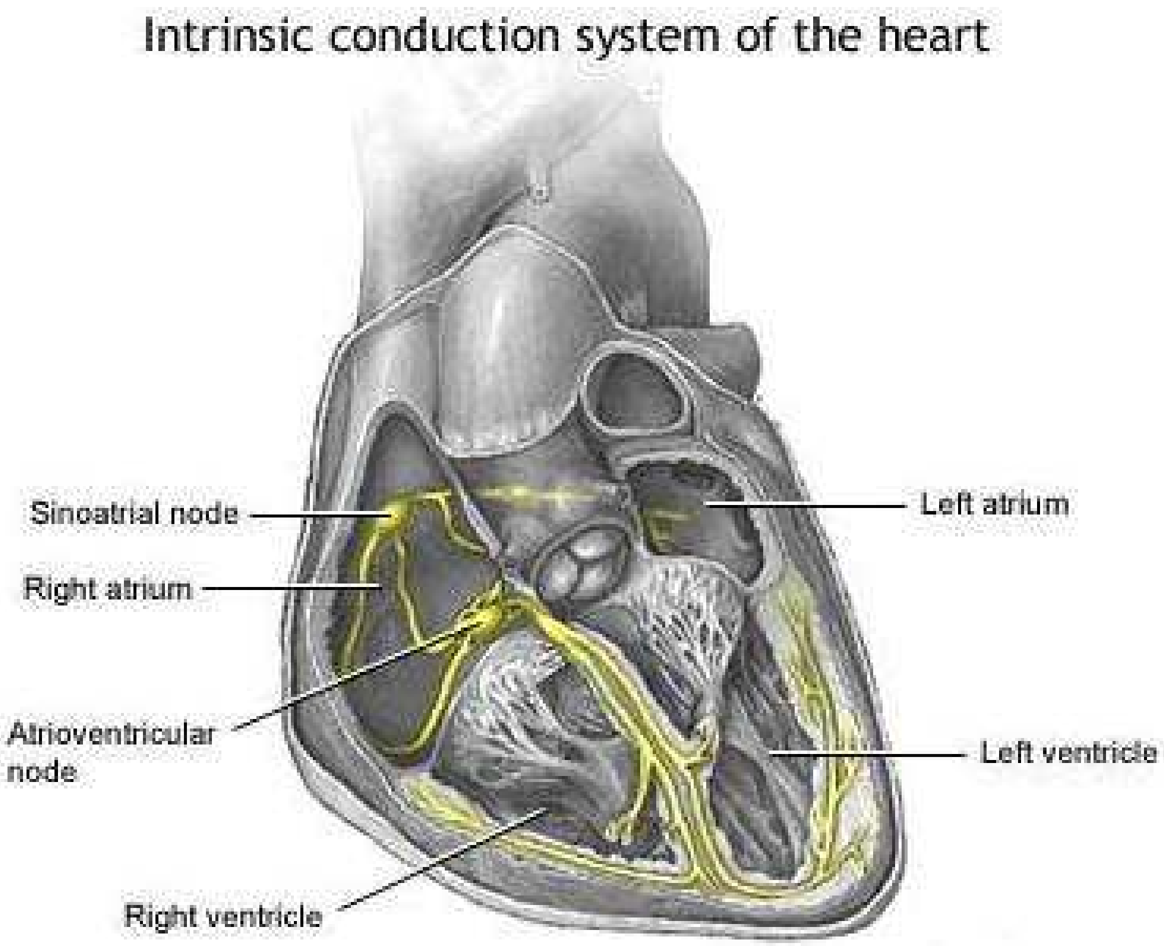
Cardiac arrhythmia: Ventricular fibrillation (Fenton *et al.* ’02)



In-vivo episode of human VF (ten Tusscher *et al.* ’09)

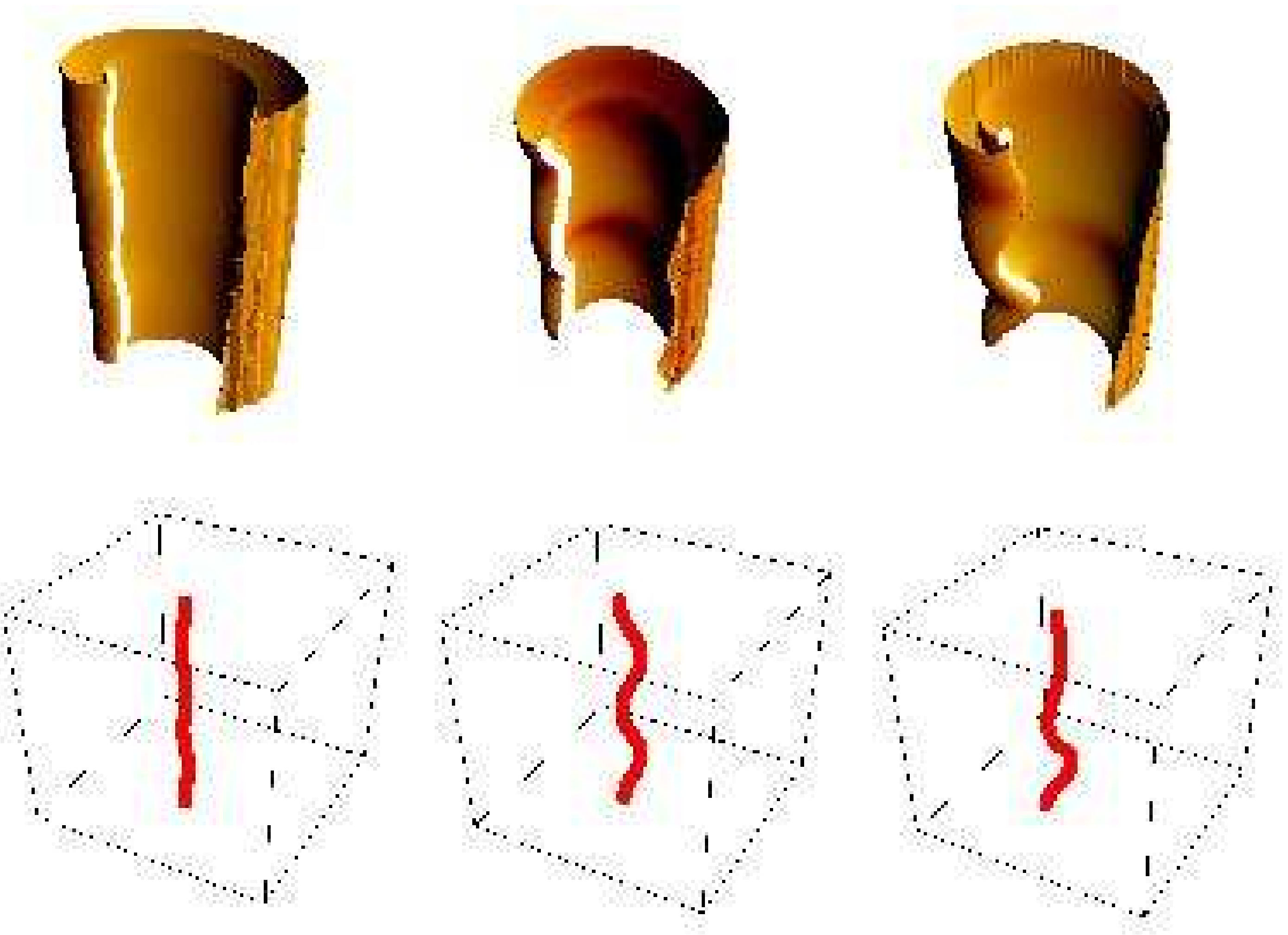


Geometry of the heart

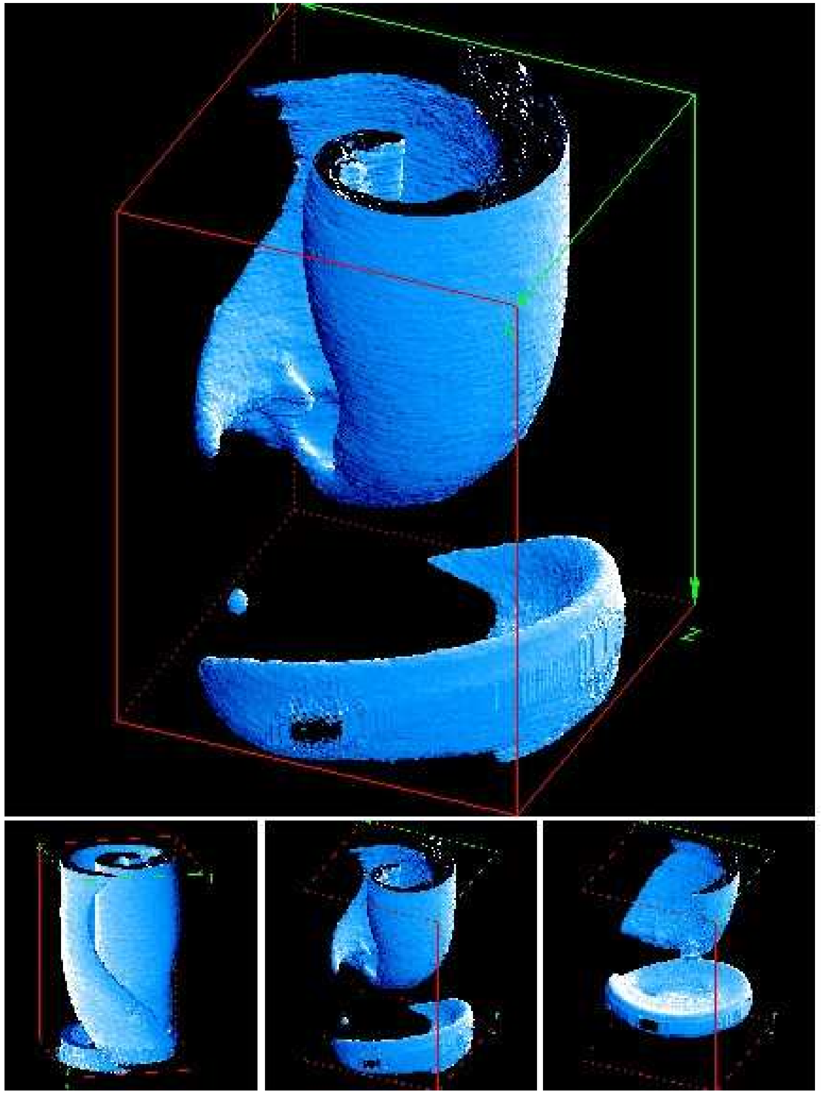


thin atria (2d) vs thick ventricles (3d)

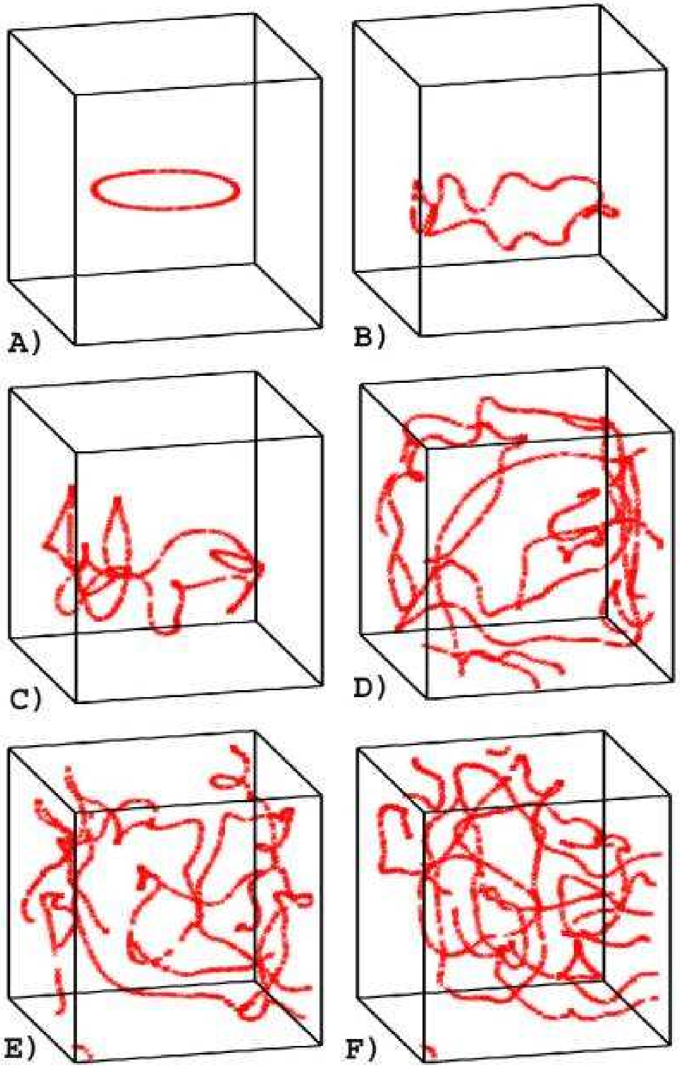
VI. Scroll waves & filaments

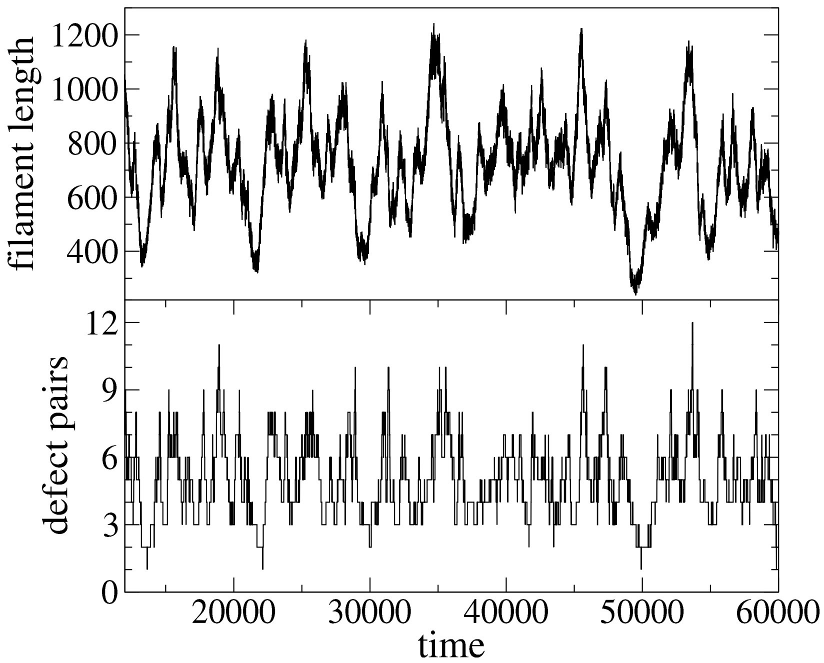


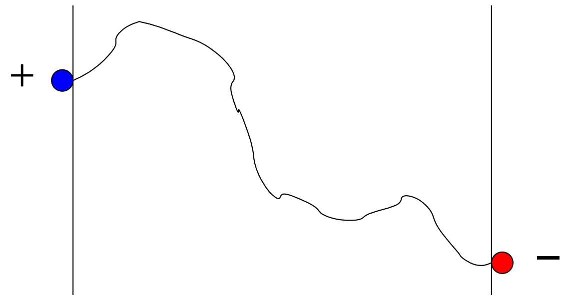
Scroll wave break-up (Luengviriya *et al.* '08)



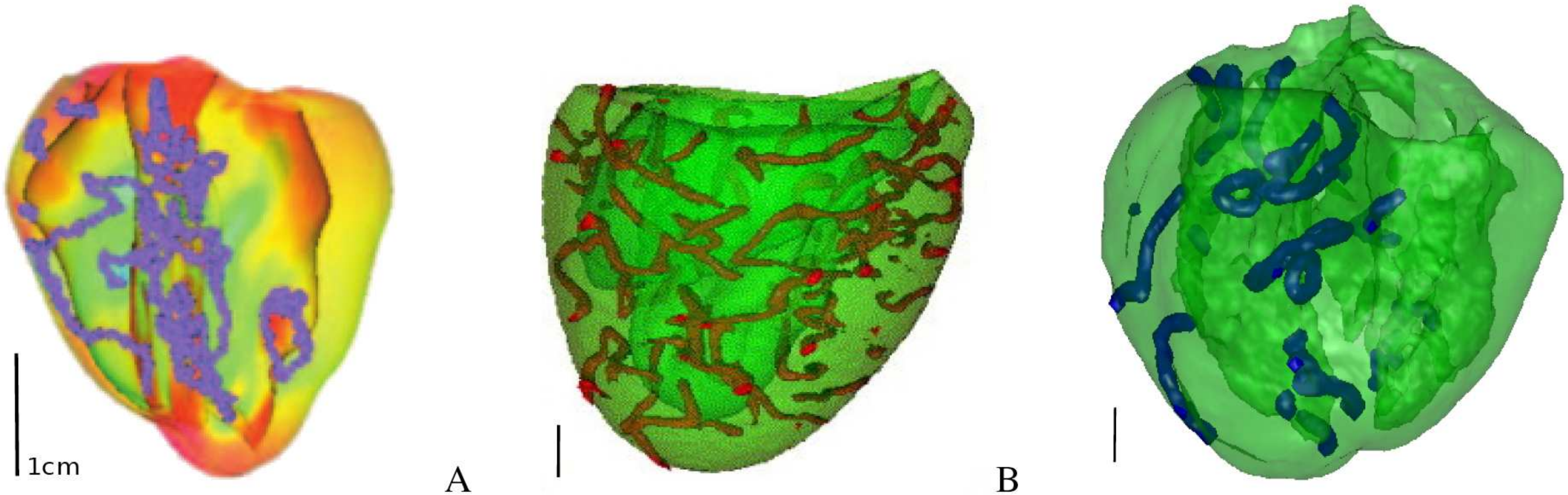
Negative line tension instability (Winfree '94; Alonso *et al.* '03)





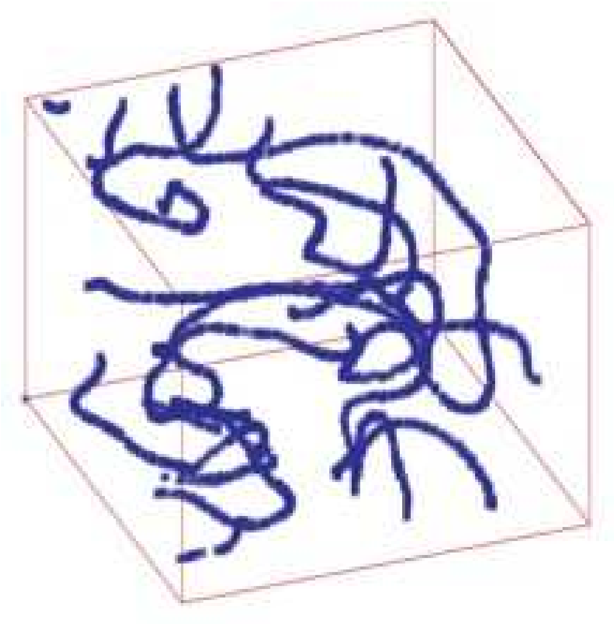


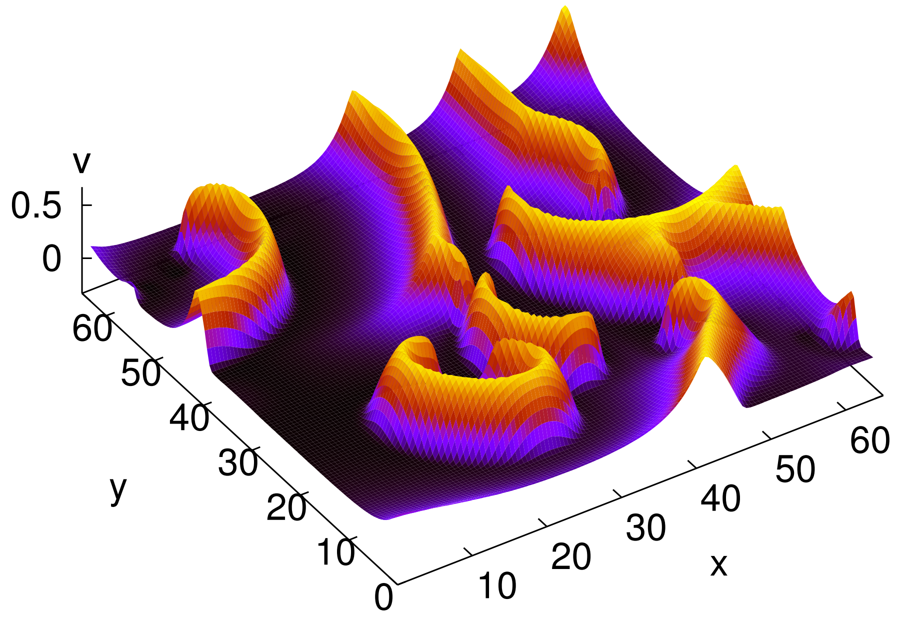
Scroll wave dynamics in cardiac tissue (ten Tusscher *et al.* ’09)



in cardiac tissue models of realistic heart geometries, nature of filament turbulence depends on size and action potential duration

VII. Filament-induced surface spiral turbulence (Davidsen ’08)



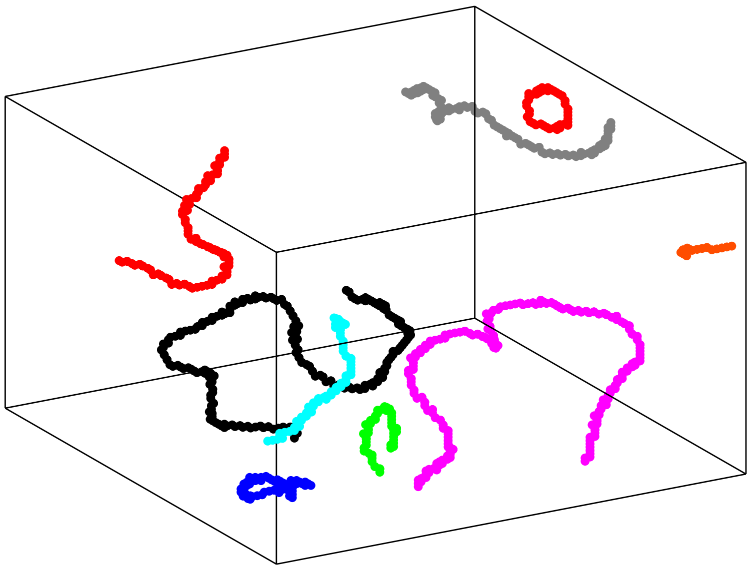


Is it possible to distinguish between the negative line tension instability and 2D spiral breakup mechanisms if observations are constrained to the turbulent dynamics of spiral waves on the surface?

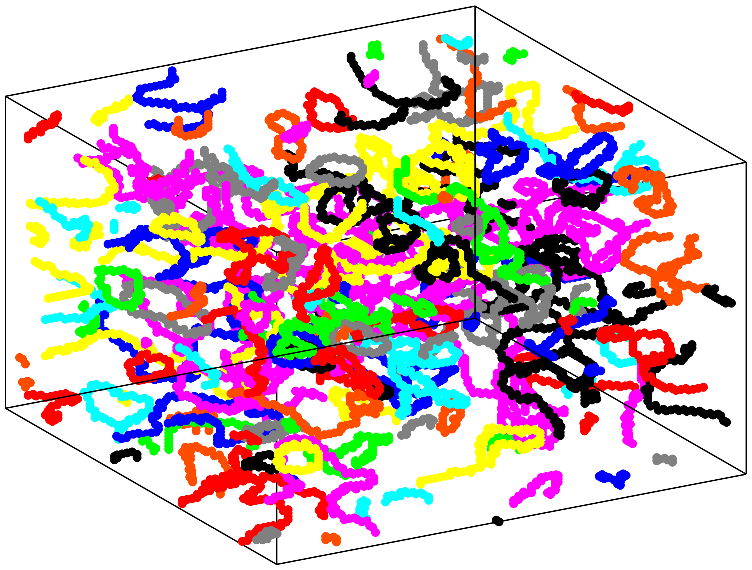
Filament turbulence: Complex Ginzburg-Landau (Reid *et al.* ’10)

$$\partial_t A = A + (1+ib)\nabla^2 A - (1+ic)|A|^2 A$$

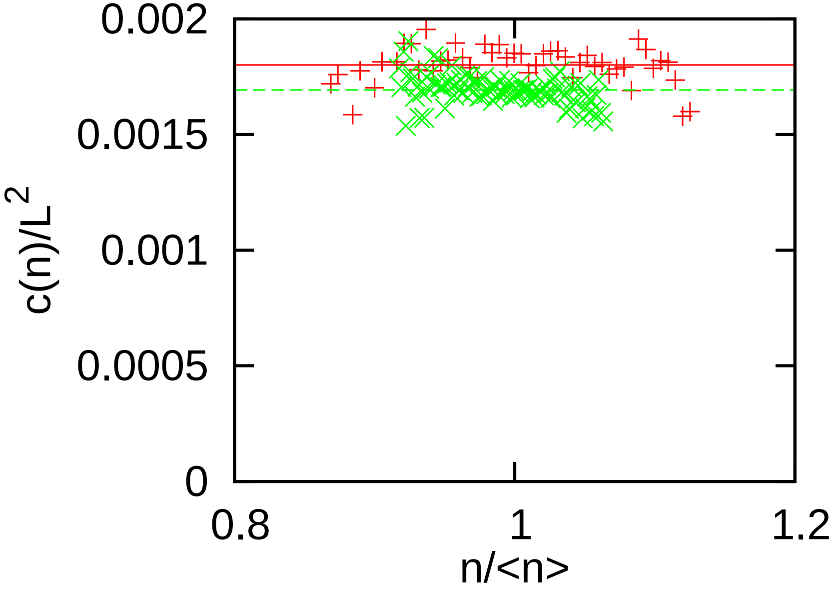
NLT regime: $b = 5$, $c = 0$

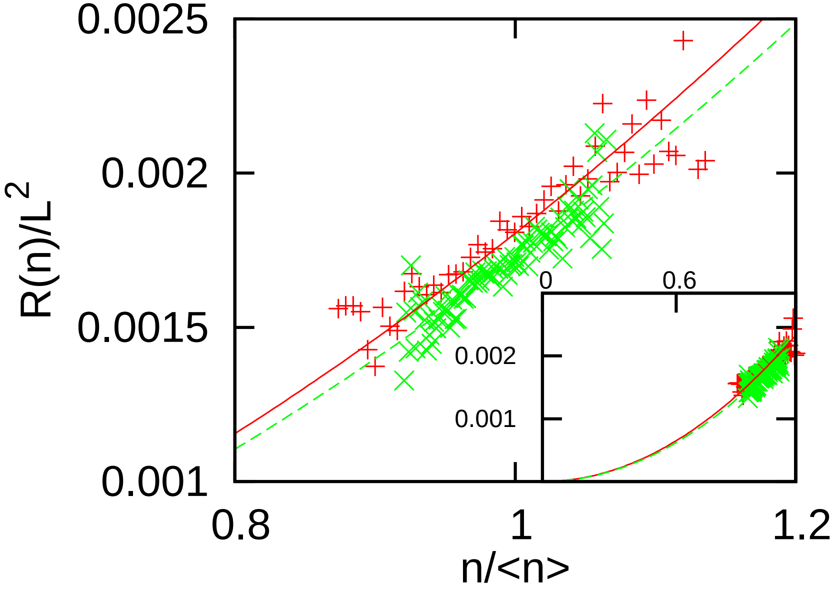


AT regime: $b = 1$, $c = -1.5$



CGLE: Amplitude turbulence regime

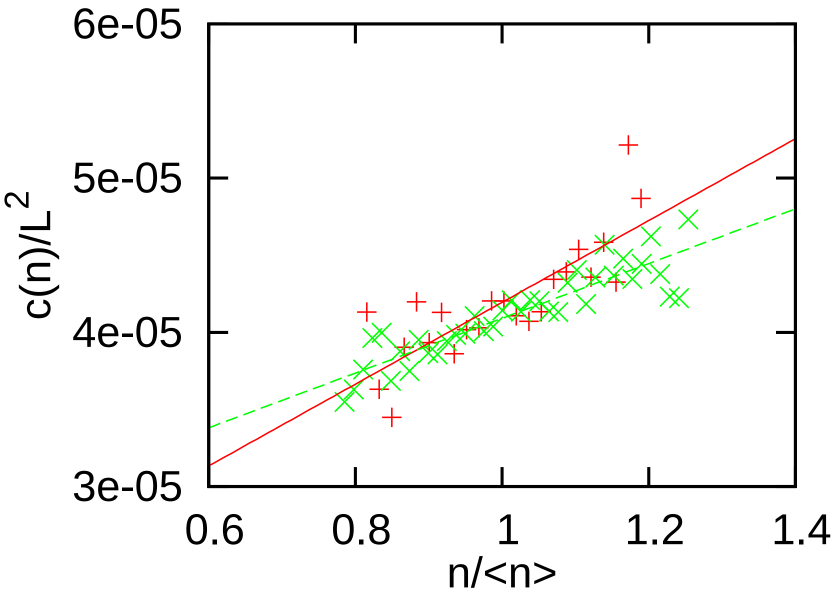


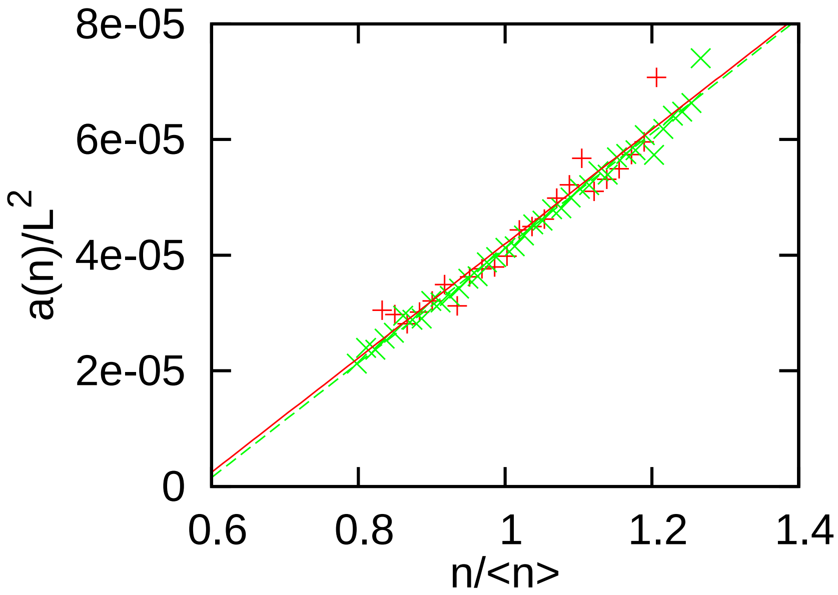


$$c(n) = \beta_1$$

$$a(n) = \alpha_3 n^2$$

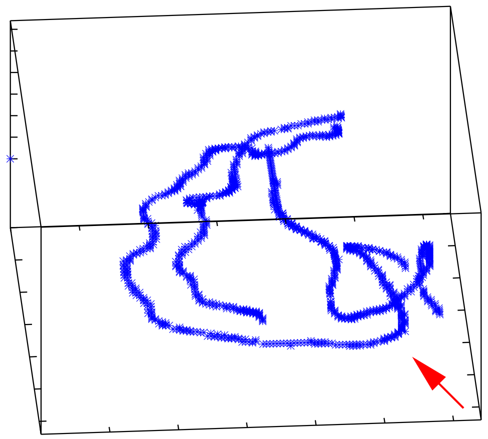
CGLE: Negative line tension regime



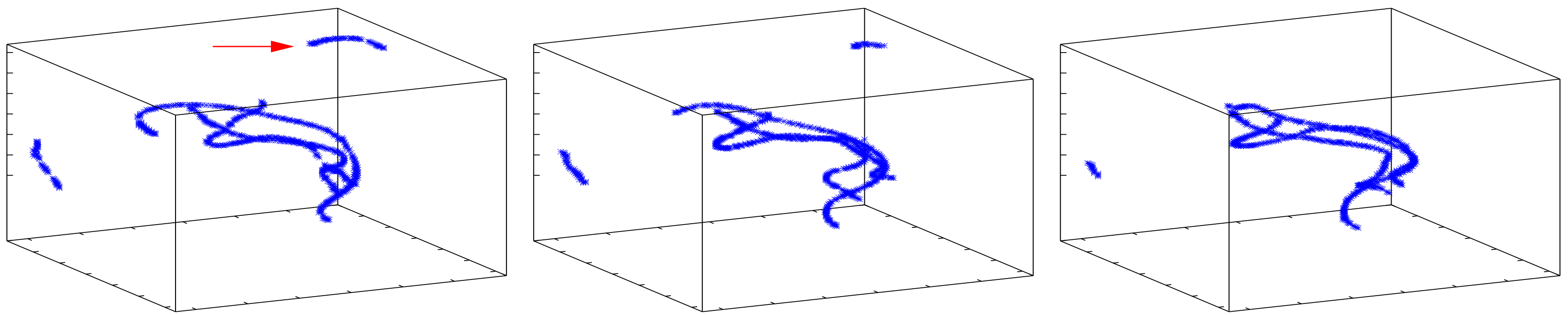


$$c(n) = \beta_1 + \beta_2 n \qquad a(n) = \alpha_1 + \alpha_2 n$$

Creation of filaments



Annihilation of filaments



VIII. Summary & Outlook

☞ *pattern formation is an exciting and highly-interdisciplinary field*

☞ *chemical systems are prime examples for chaotic and turbulent dynamics*

☞ *topological defects (spirals, synchronization defect lines, filaments) allow a reduced description of complex spatiotemporal dynamics and their behavior characterizes the underlying instabilities/bifurcations*

☞ *surface dynamics can tell it all*

☞ *important applications include cardiac arrhythmia and ventricular fibrillation*

Thanks!

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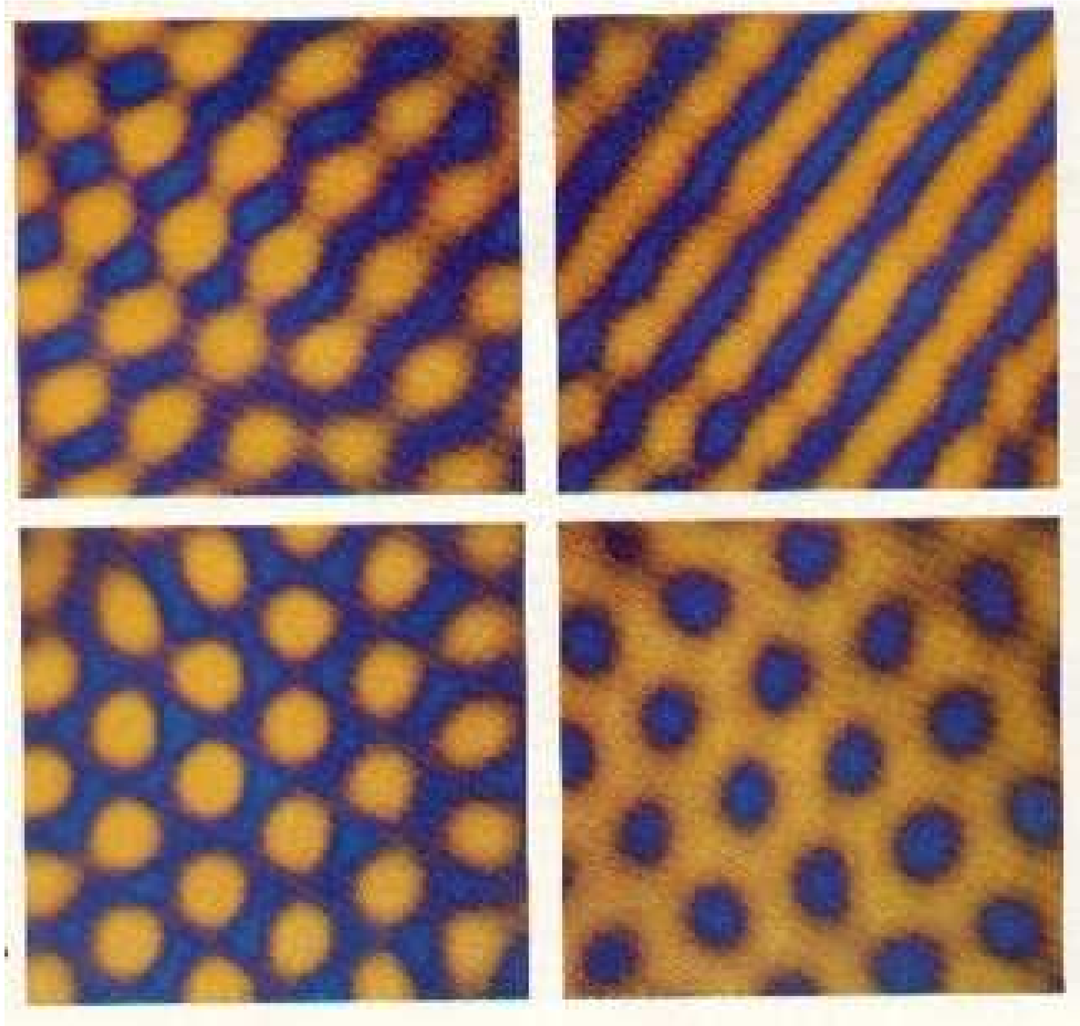
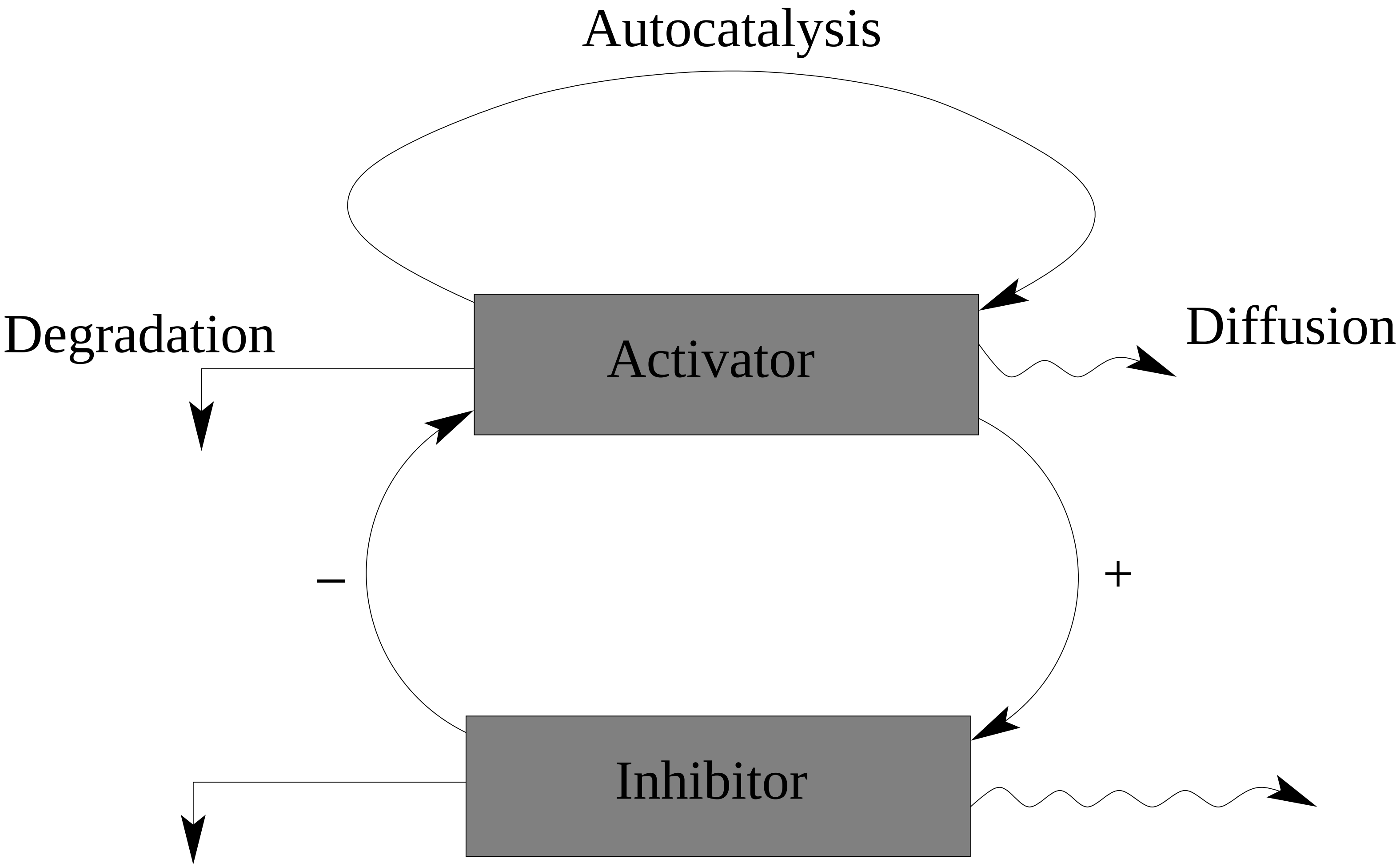
http://www.ucalgary.ca/complexity/

J. Chem. Phys. 133, 044909; Phys. Rev. Lett. 101, 208302;
Phys. Rev. Lett. 93, 018305; Phys. Rev. Lett. 91, 058303

“Stationary” chemical patterns: CIMA reaction (Ouyang *et al.* ’91)



Turing patterns: Activator-inhibitor scheme (Gierer & Meinhardt ’72)



local self-enhancement & long-range inhibition ($D_a \ll D_h$)

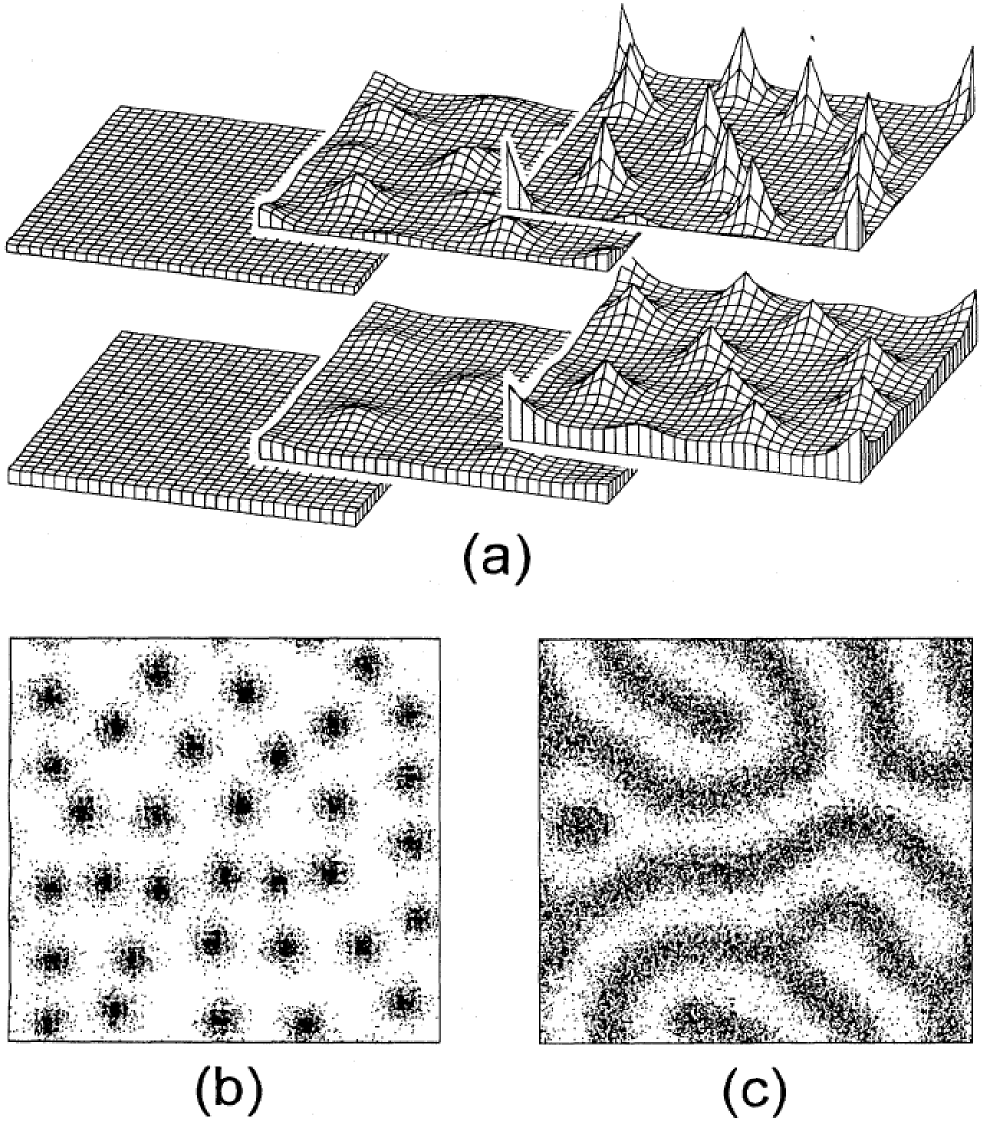
Gierer-Meinhardt model

$$\frac{\partial a}{\partial t} = D_a \nabla^2 a + \rho_a \frac{a^2}{(1+\kappa_a a^2)h} - \mu_a a + \sigma_a$$

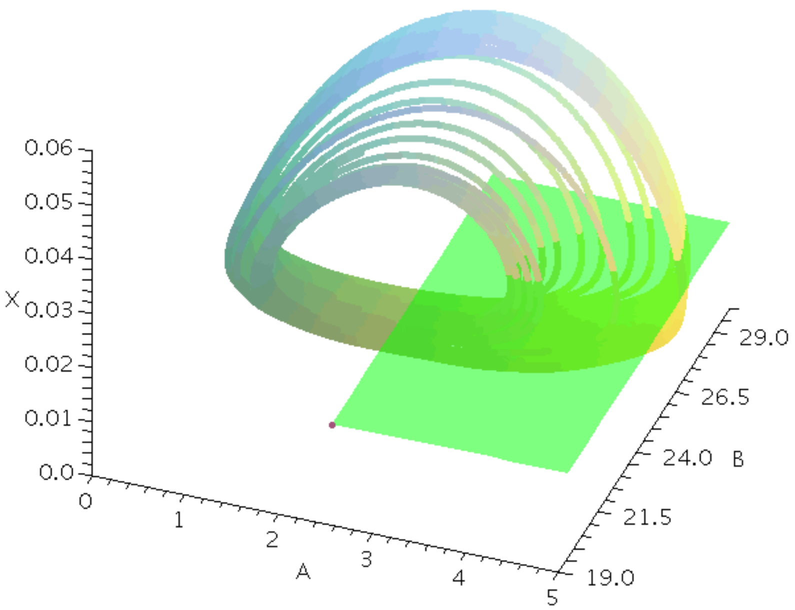
$$\frac{\partial h}{\partial t} = D_h \nabla^2 h + \rho_h a^2 - \mu_h h + \sigma_h$$

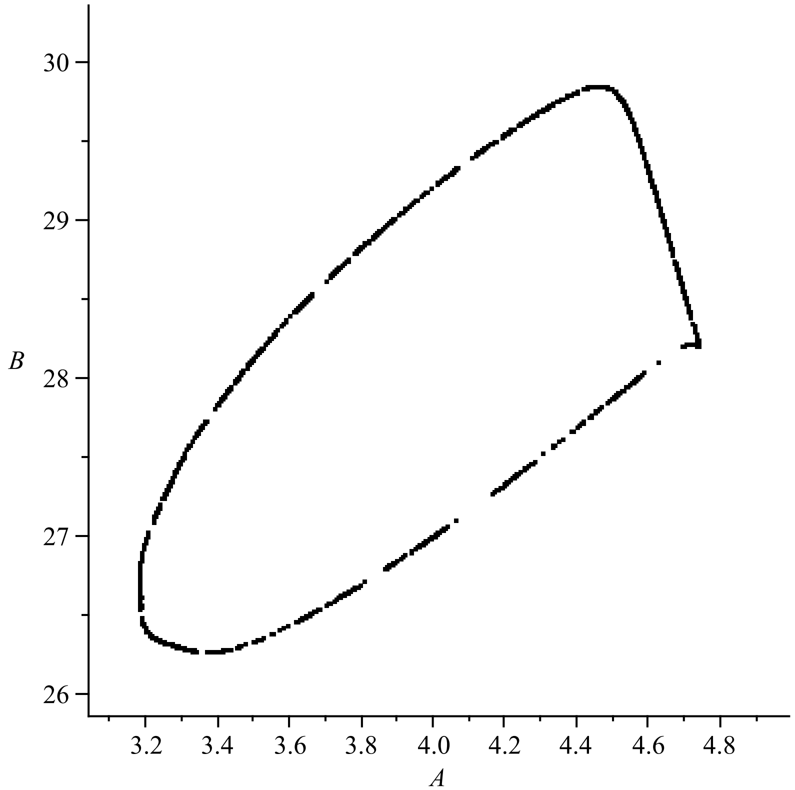
Turing patterns: $D_a \ll D_h$ and $\mu_h > \mu_a$

Turing patterns in the Gierer-Meinhardt model



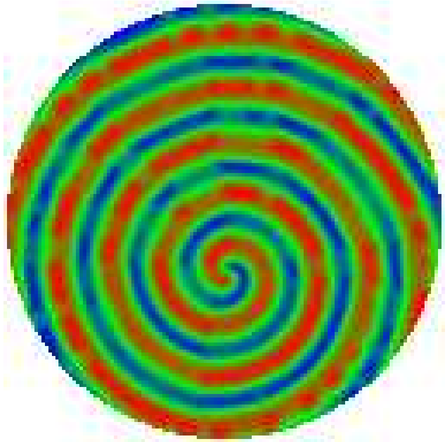
Quasiperiodicity: Torus attractor (St-Yves *et al.* '10)

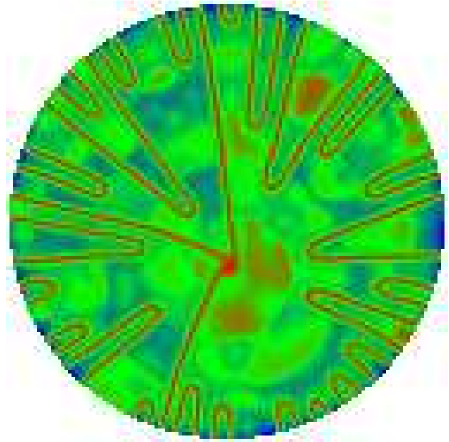


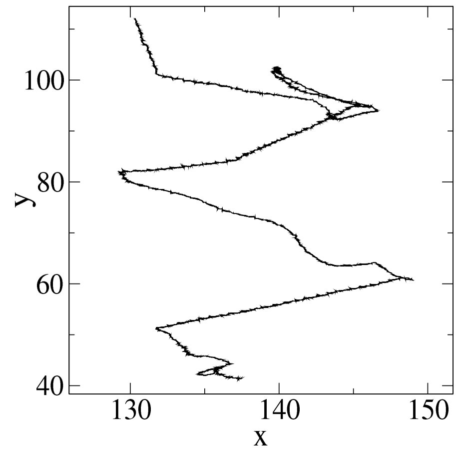


Turbulent synchronization defect lines

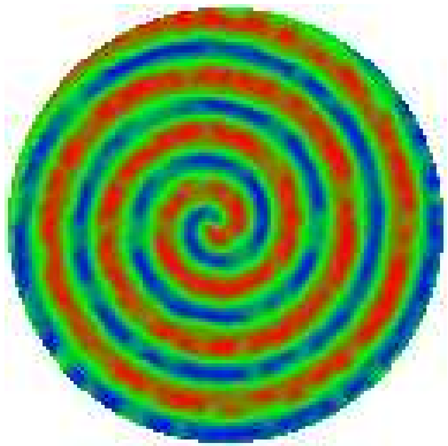
C=4.6

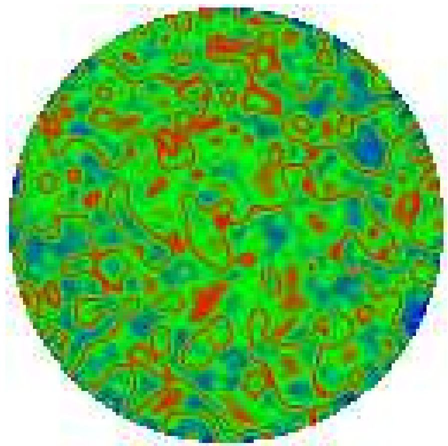


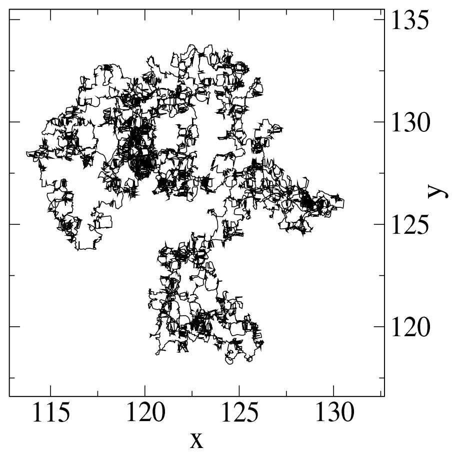




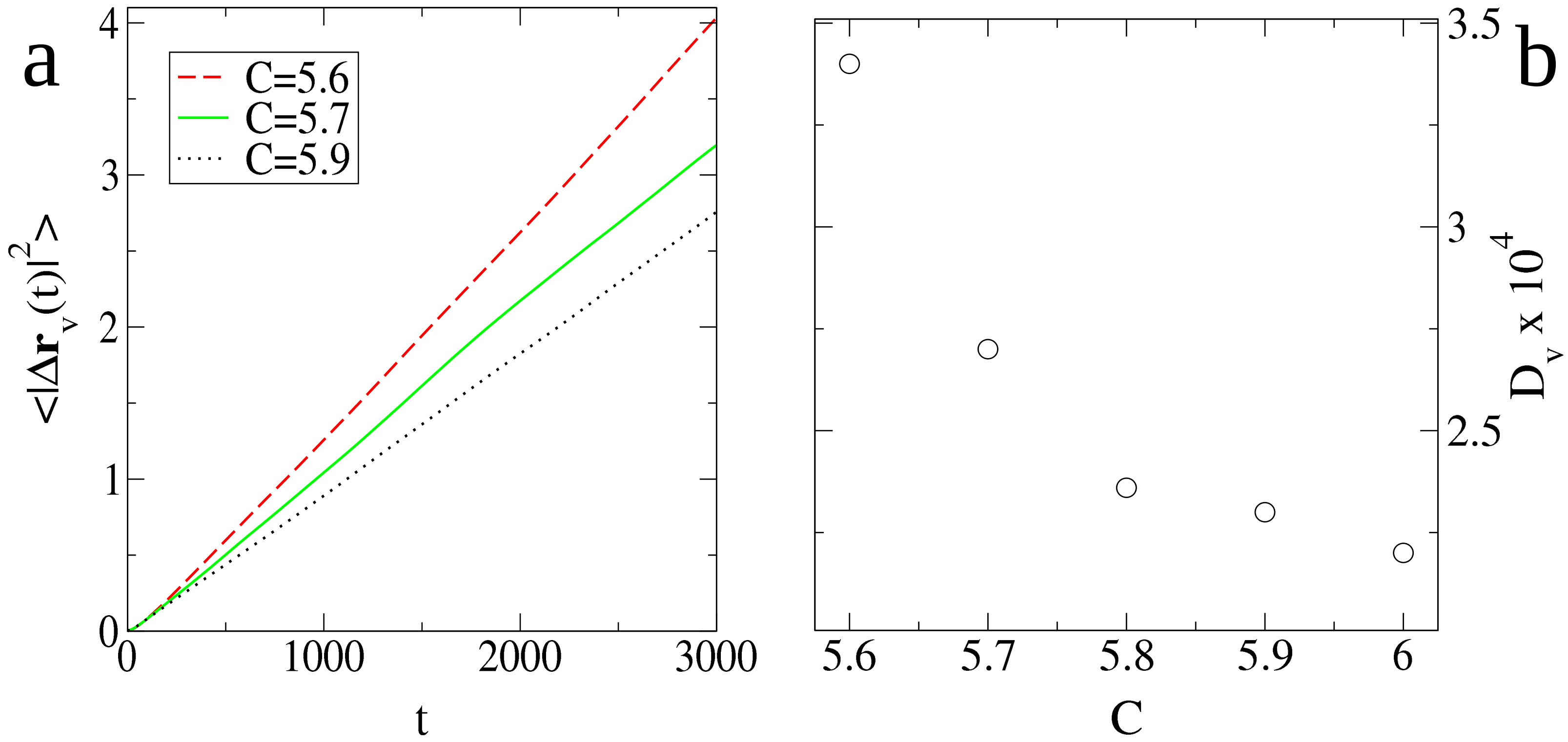
C=5.8







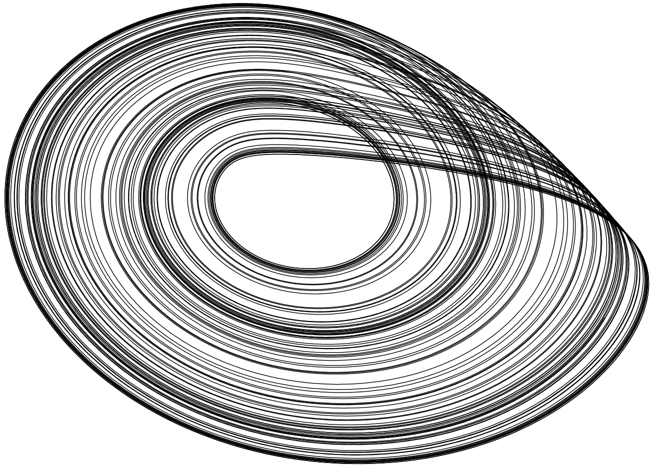
Diffusive motion of spiral cores

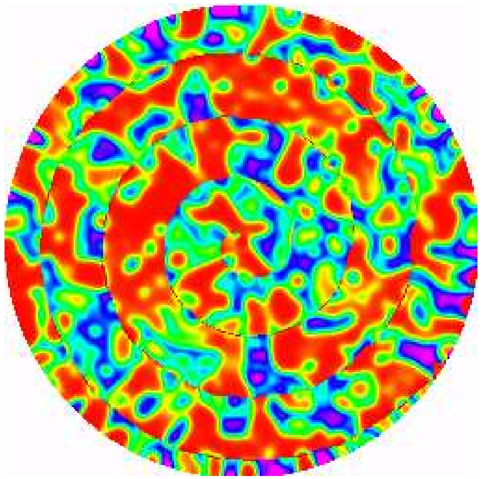


(a): Mean squared displacement $\langle|\Delta\mathbf{r}(t)|^2\rangle = \langle|\mathbf{r_v}(t) - \mathbf{r_v}(0)|^2\rangle$ for different values of C in the turbulent regime. Here, $\mathbf{r_v}(t)$ is the position of the core at time t. (b): The core diffusion coefficient D_v — defined by $\langle|\Delta\mathbf{r_v}(t)|^2\rangle = 4D_v t$ — as a function of C.

Chaotic media

Definition. *A* *chaotic oscillator* *is a chaotic dynamical system with the property that a well-defined phase variable (monotonically growing quantity on the attractor) exists. Two non-identical chaotic oscillators are said to be* *phase synchronized* *if their phases are locked but their "amplitudes" are not ($\neq$ complete synchronization).*



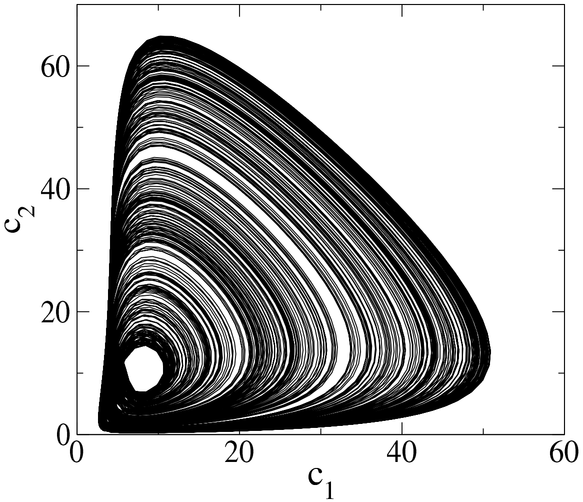


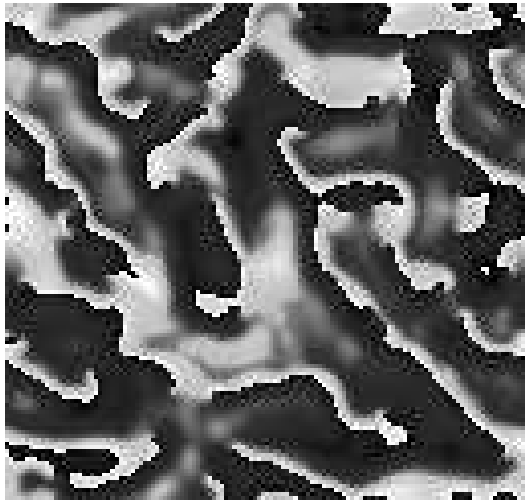
$$\tan\phi(\mathbf{r},t) = \frac{x_2(\mathbf{r},t)}{x_1(\mathbf{r},t)}$$

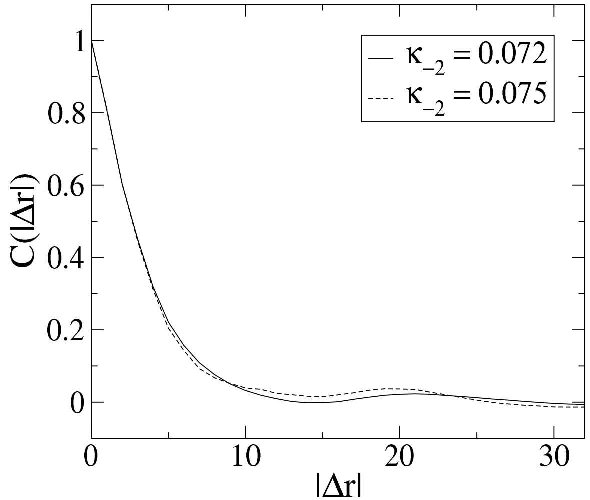
Chemical model: Willamowski-Rössler (WR)

$$\partial_t \mathbf{c}(\mathbf{r},t) = \mathbf{R}[\mathbf{c}(\mathbf{r},t)] + D\nabla^2 \mathbf{c}(\mathbf{r},t),$$

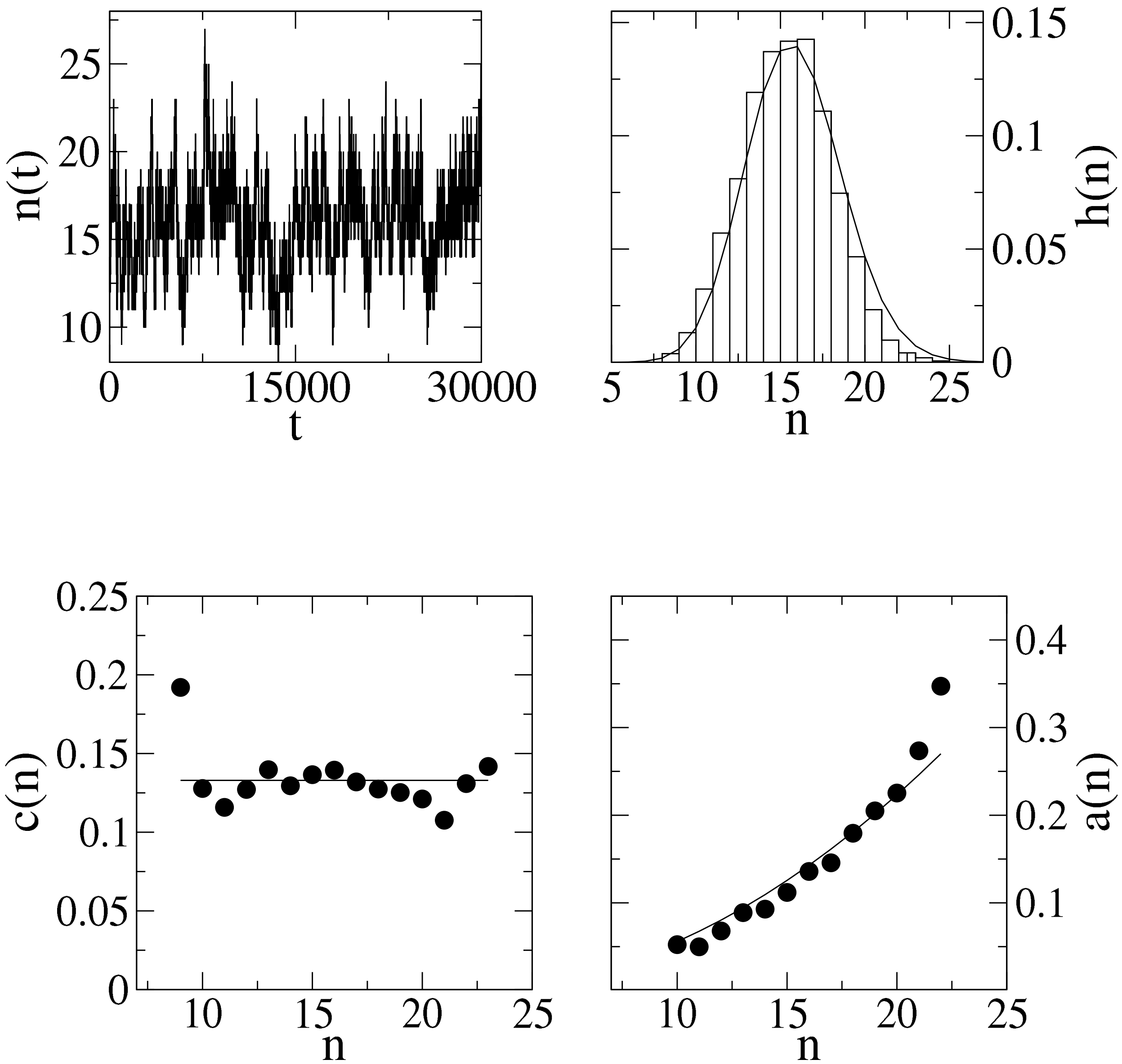
$R_1 = 31.2c_1 - 0.2c_1^2 - 1.45c_1c_2 + \kappa_{-2}c_2^2 - 1.02c_1c_3 + 0.01,$
$R_2 = 1.45c_1c_2 - \kappa_{-2}c_2^2 - 10.8c_2 + 0.12$ and $R_3 = -1.02c_1c_3 + 0.01 + 16.5c_3 - 0.5c_3^2$.



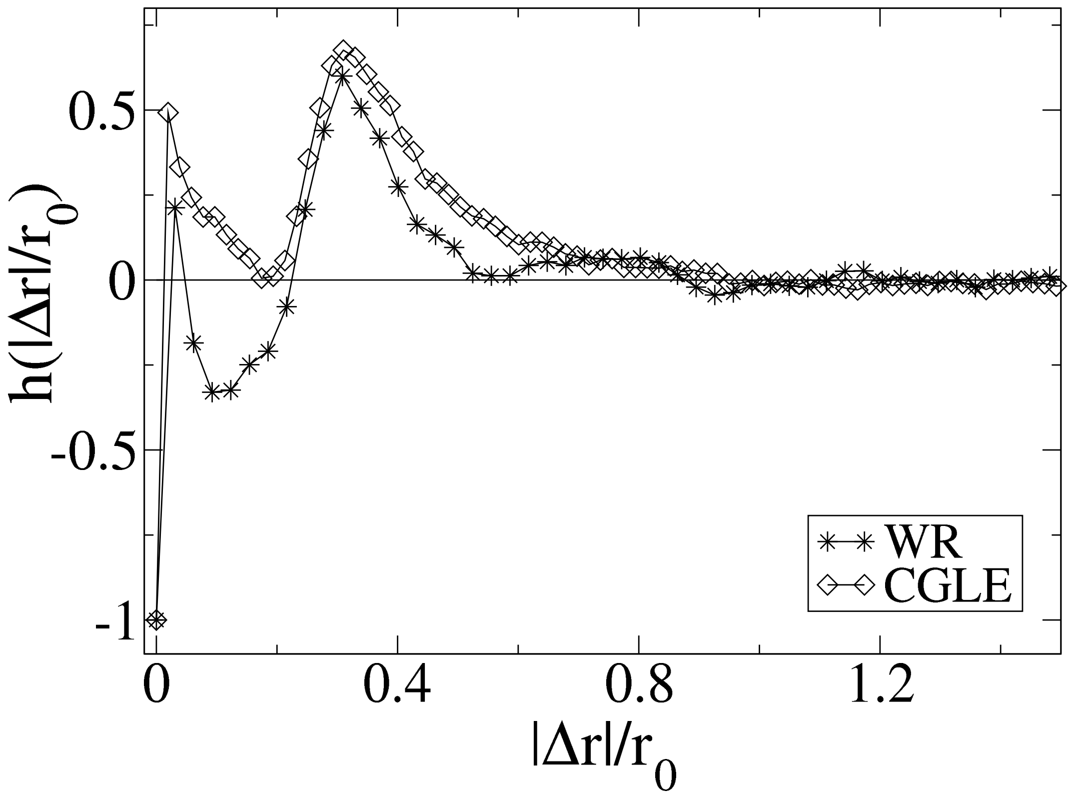




Medium with local deterministic chaos (Davidsen *et al.* ’03)



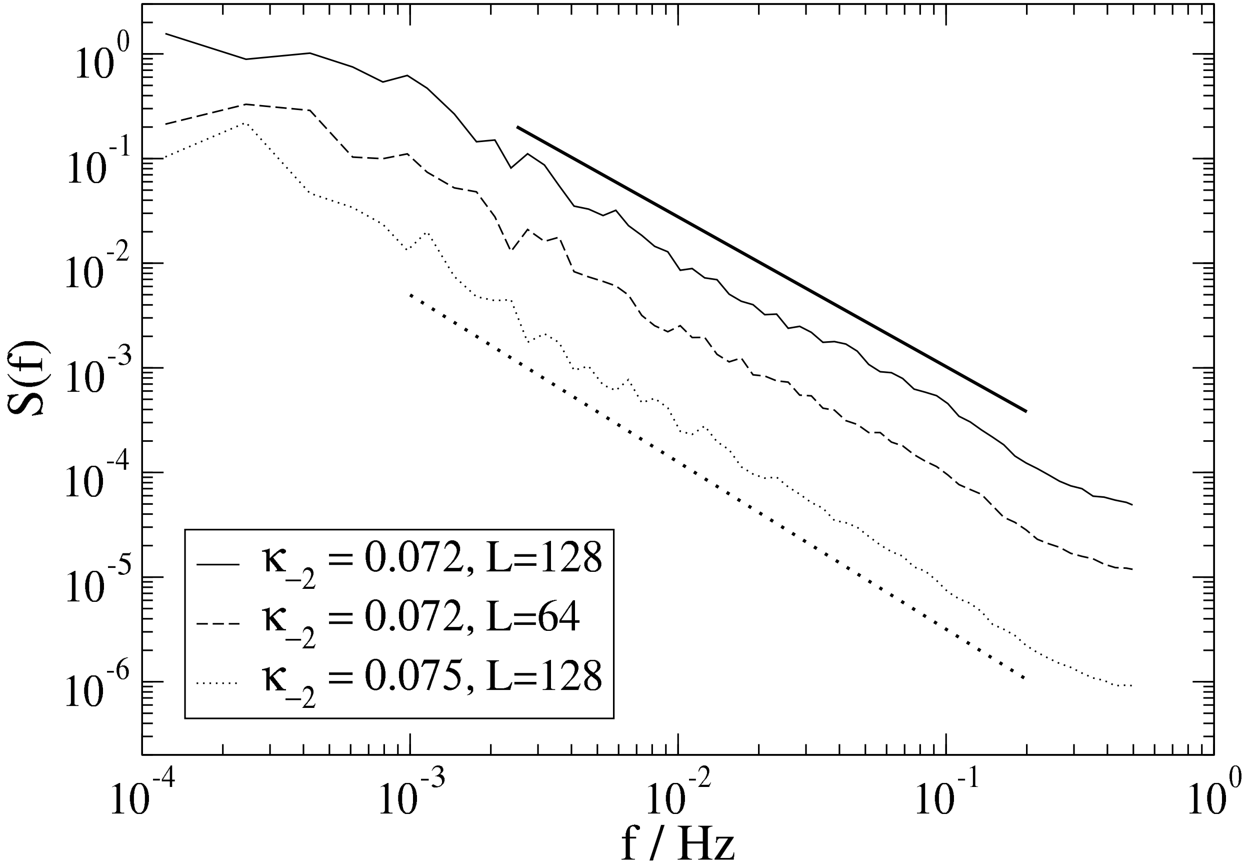
Pair correlation function



Normalized pair correlation function $h(|\mathbf{\Delta r}|/r_0)$ with $r_0 = \sqrt{L^2/\langle n \rangle}$ for WR and CGLE.

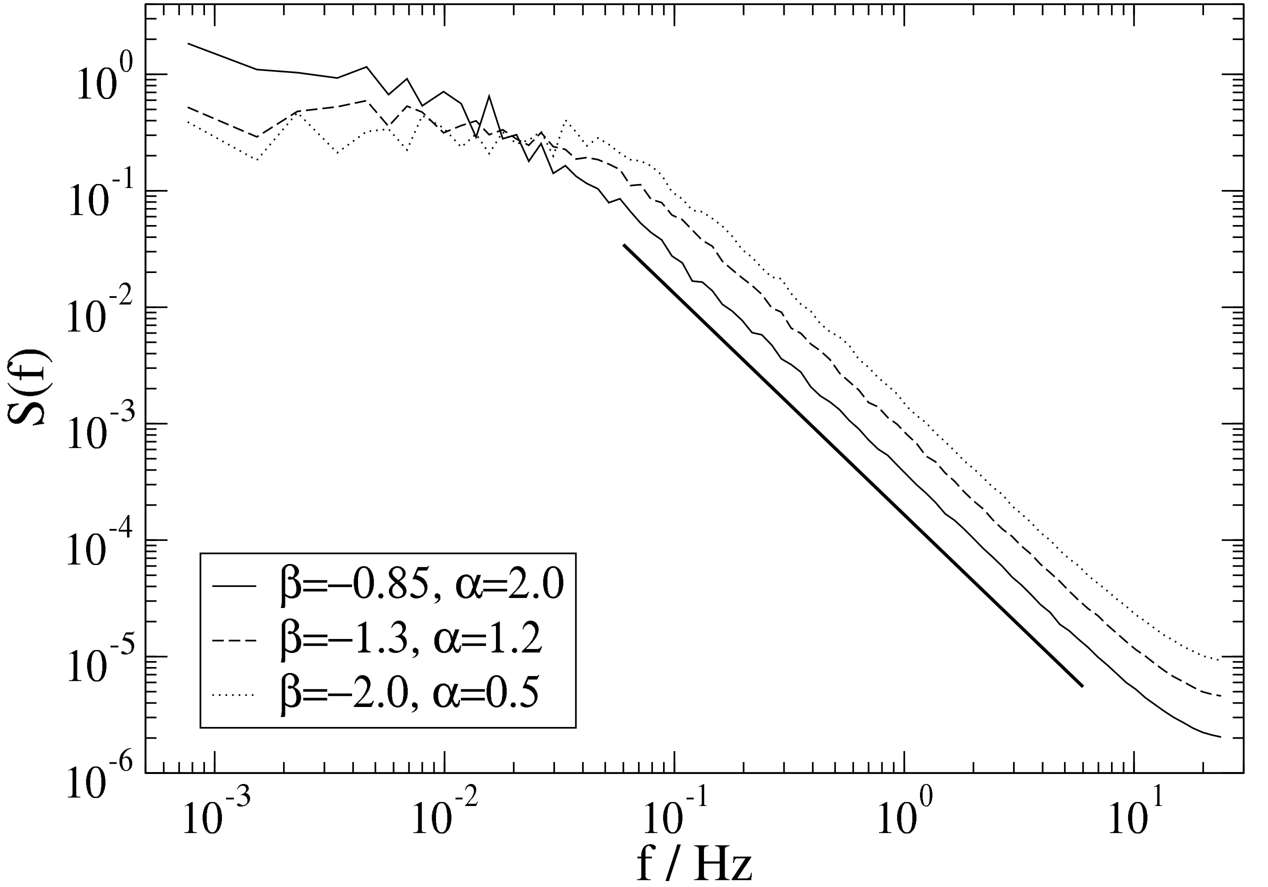
$$h(|\mathbf{\Delta r}|) \quad = \quad \frac{\langle n_+(\mathbf{r},t) n_-(\mathbf{r}+\mathbf{\Delta r},t)\rangle_{\mathbf{r},t}}{\langle n \rangle^2} - 1$$

Power spectrum of WR



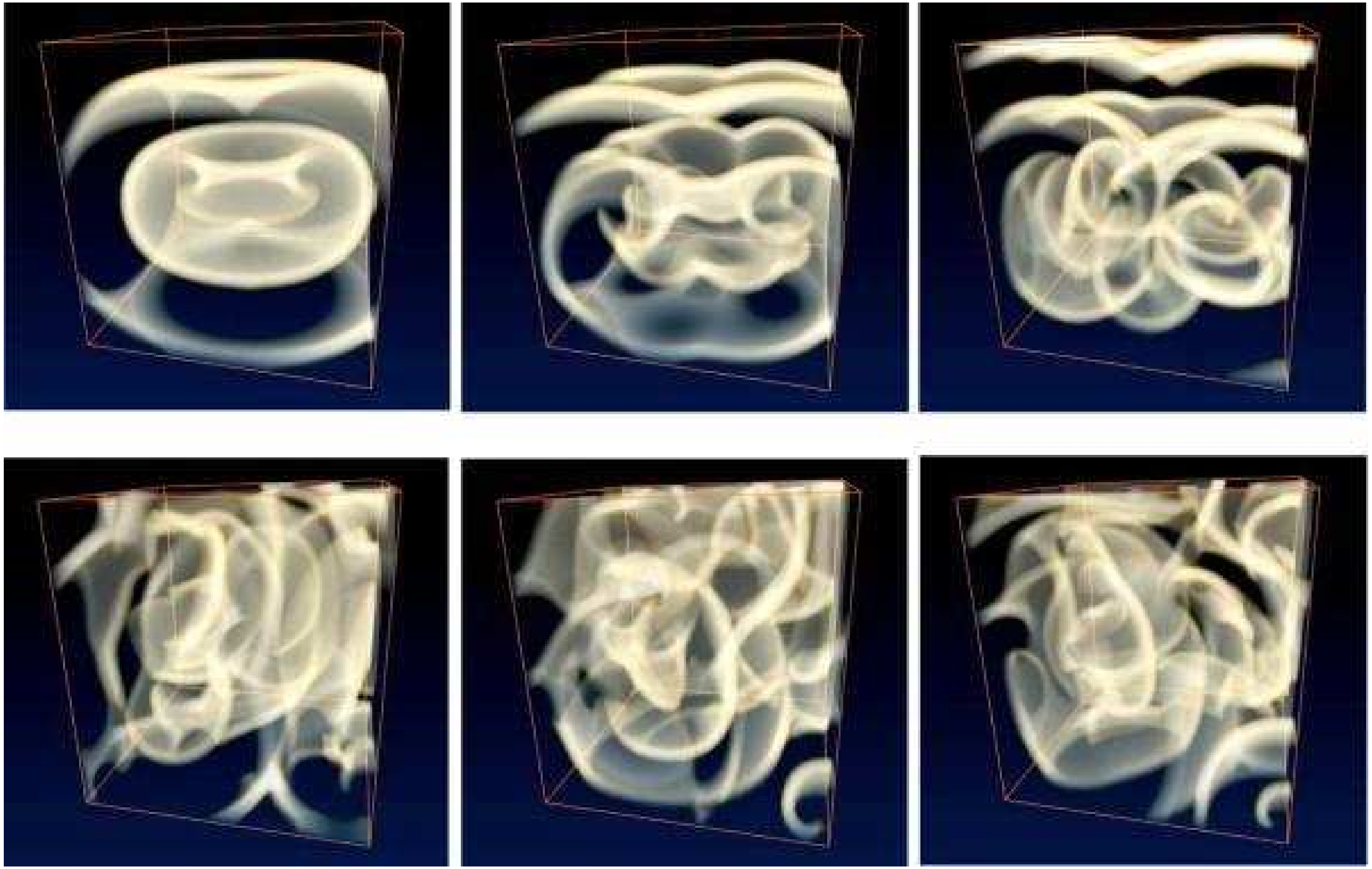
Power spectrum $S_L(f) = \lim_{T\to\infty} 1/2T \mid \int_{-T}^{T} dt \; n(t) \exp^{-i2\pi ft} \mid^2$. The thick lines are to guide the eye. $S_L(f) \propto 1/f^{1.43}$ for the thick solid line, and $\gamma = 1.60$ for the thick dotted line.

Power spectrum of CGLE



Power spectrum of $n(t)$ for different parameters in the CGLE and $L = 128$. The thick line is to guide the eye and decays with $\gamma = 1.9$. Note that $\bar{T} = 12.7, 8.40, 5.43$ from highest to lowest α.

Negative line tension instability (Winfree '94; Alonso *et al.* '03)

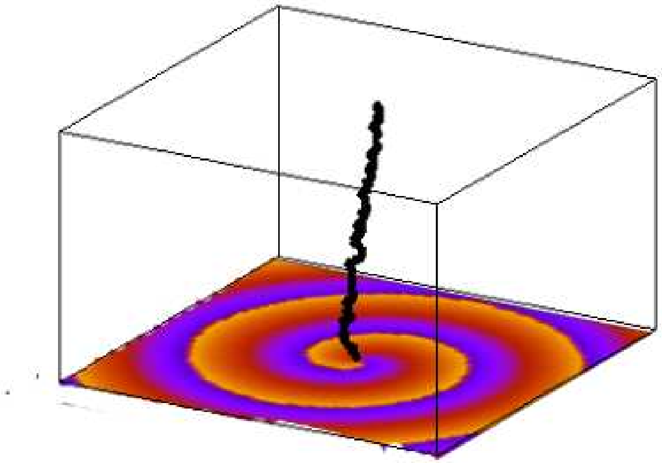


Filament turbulence: Excitable Barkley model in 3D

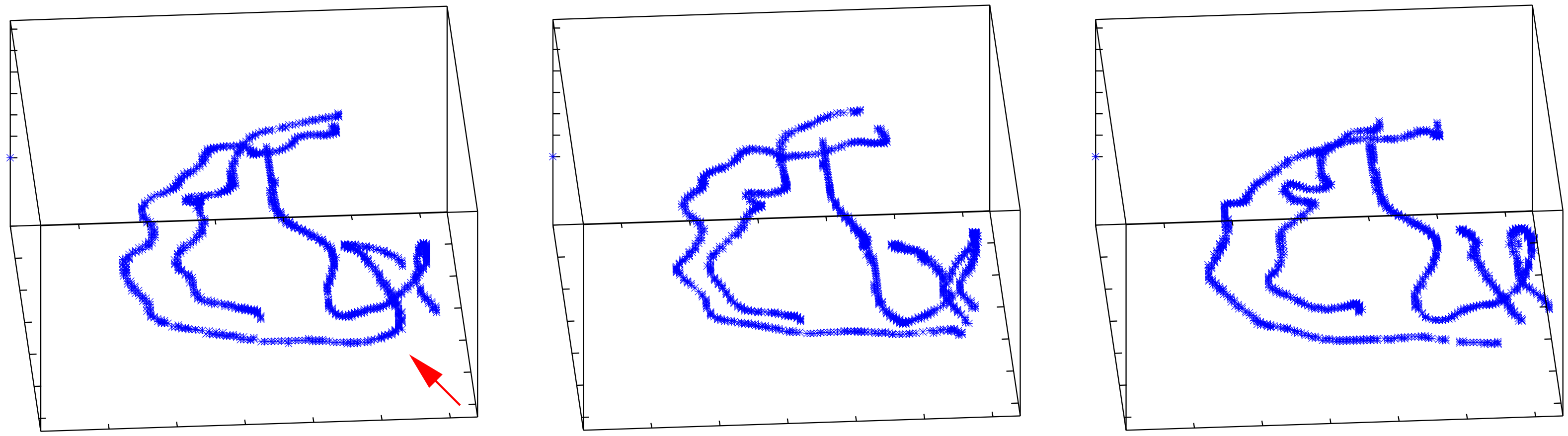
$$\partial_t u = D_u \nabla^2 u + \frac{1}{\epsilon} u(1-u)(u - \frac{v+b}{a}),$$
$$\partial_t v = D_v \nabla^2 v + u - v,$$

$\epsilon = 0.02$, $a = 1.1$, $b = 0.21$, $D_u = 1$, $D_v = 0$

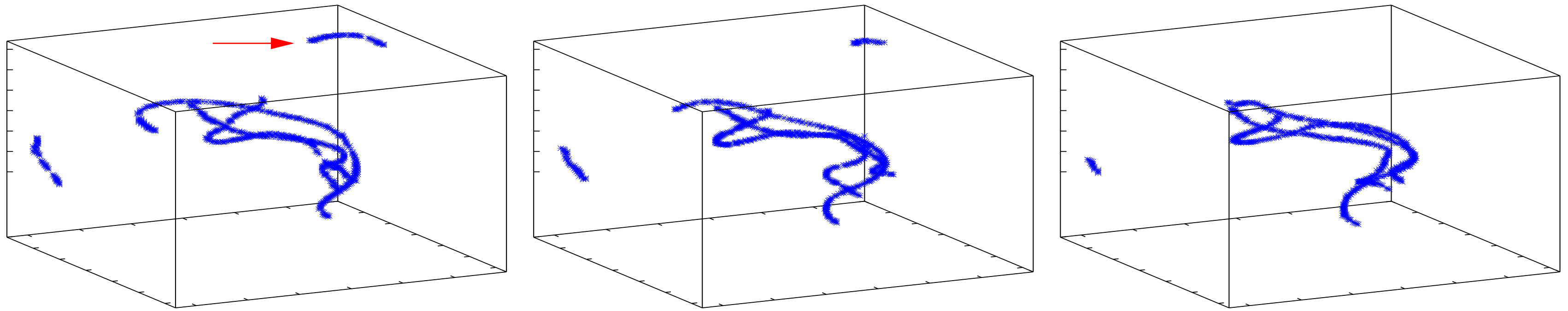
center of rotation: $u = 0.5$, $v = a/2 - b$



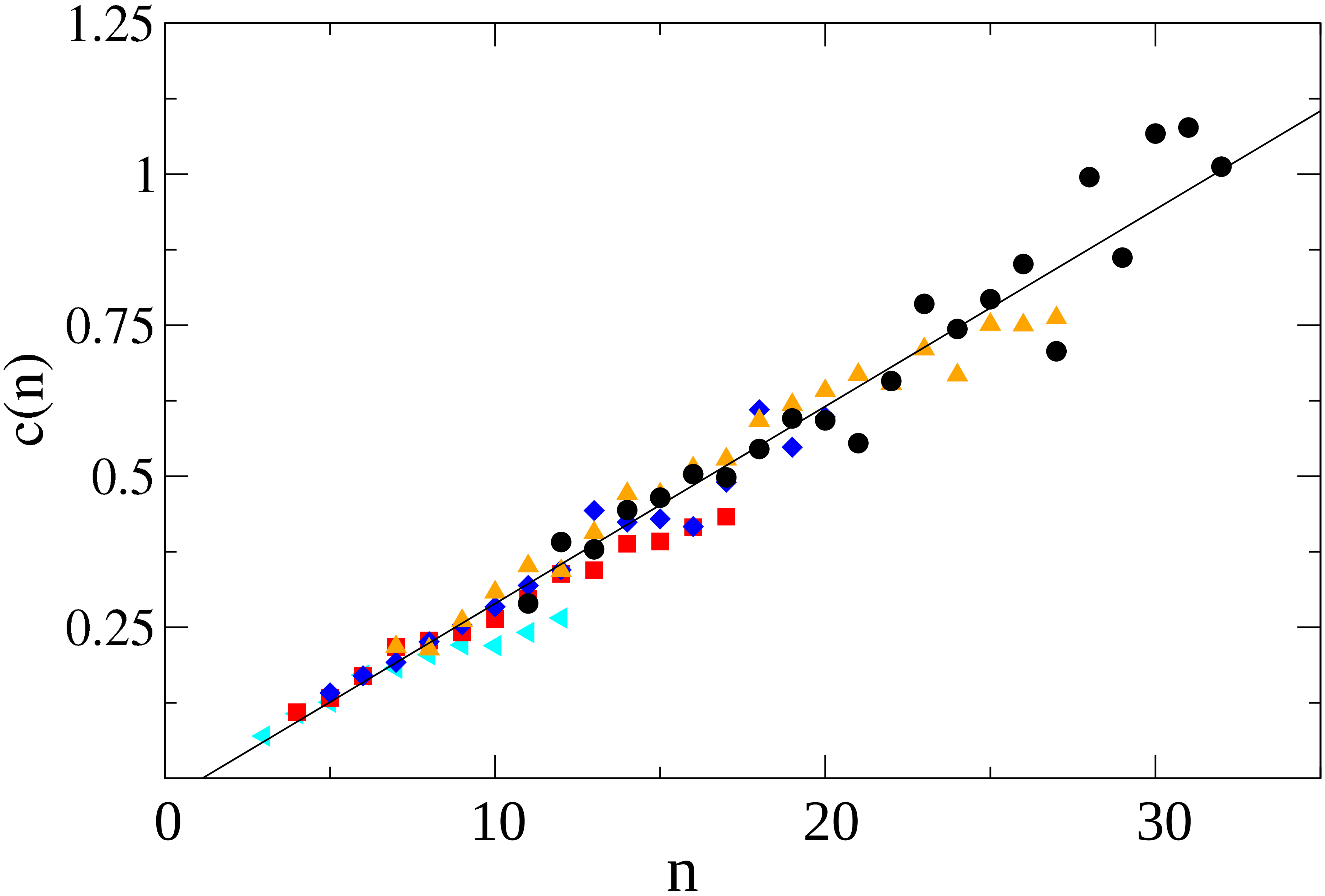
Creation of filaments



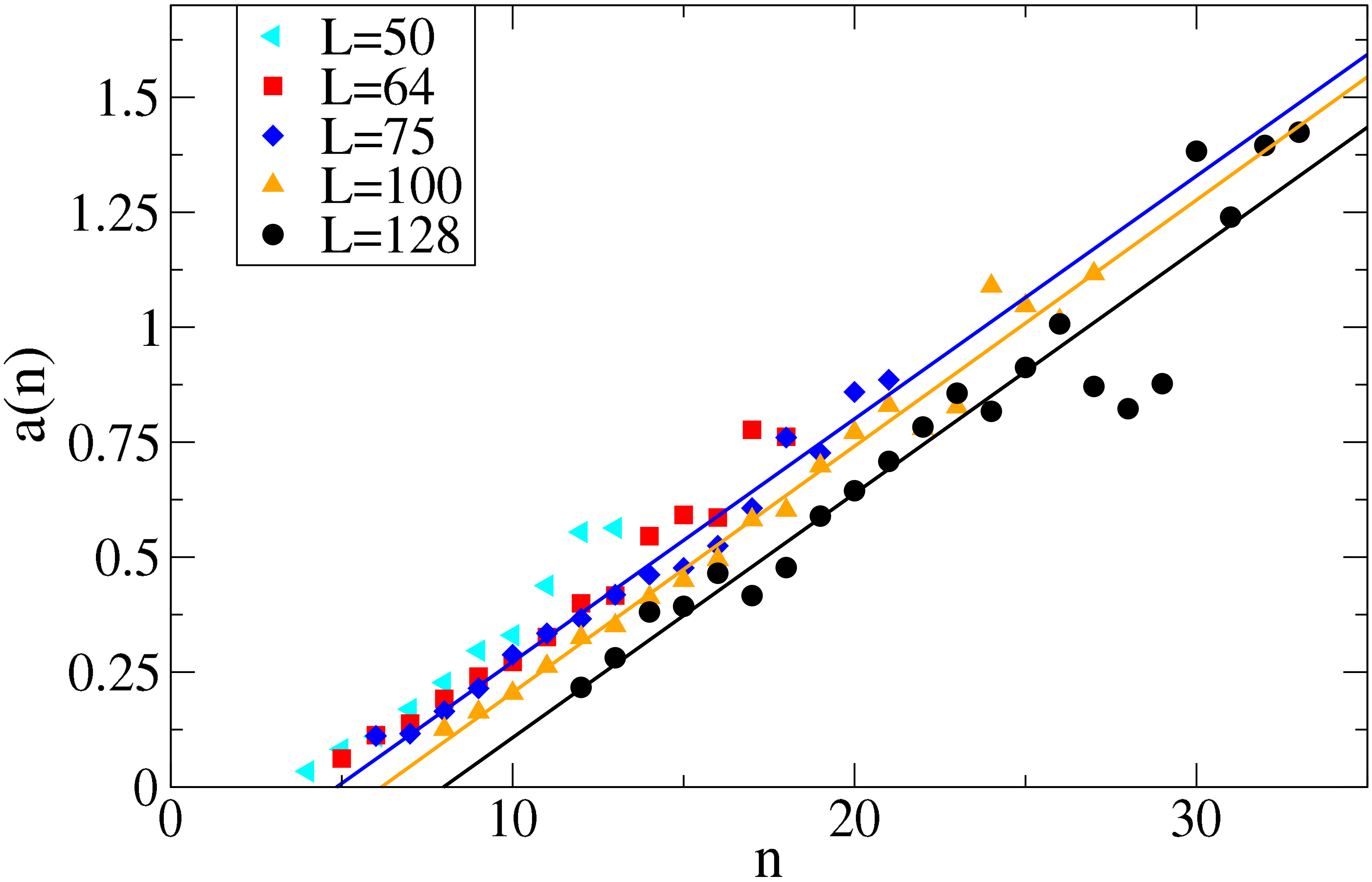
Annihilation of filaments



Creation rates



Annihilation rates



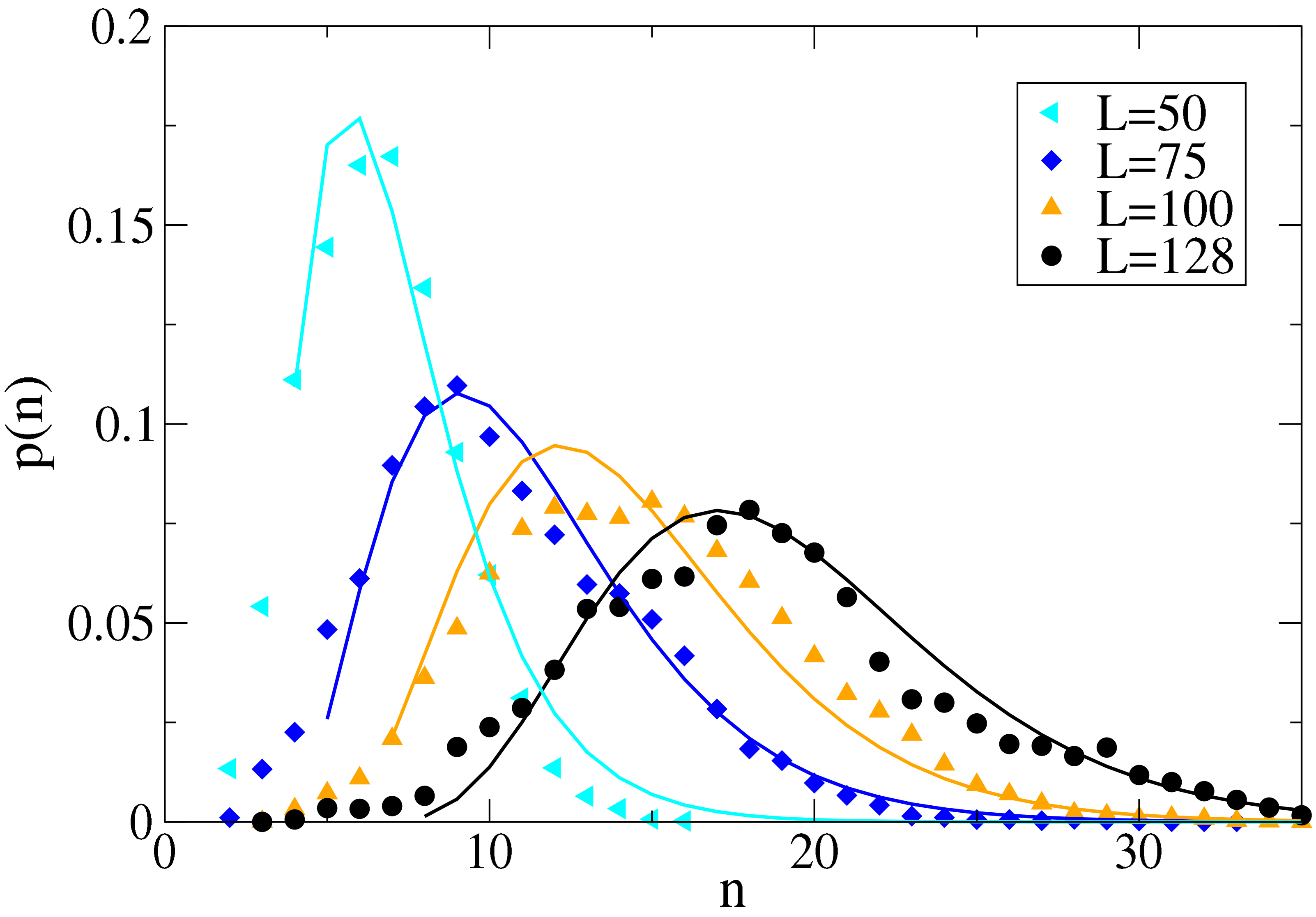
Markov model for filament turbulence

$$c(n) = \beta_1 + \beta_2 n, \qquad a(n) = \alpha_1 + \alpha_2 n.$$

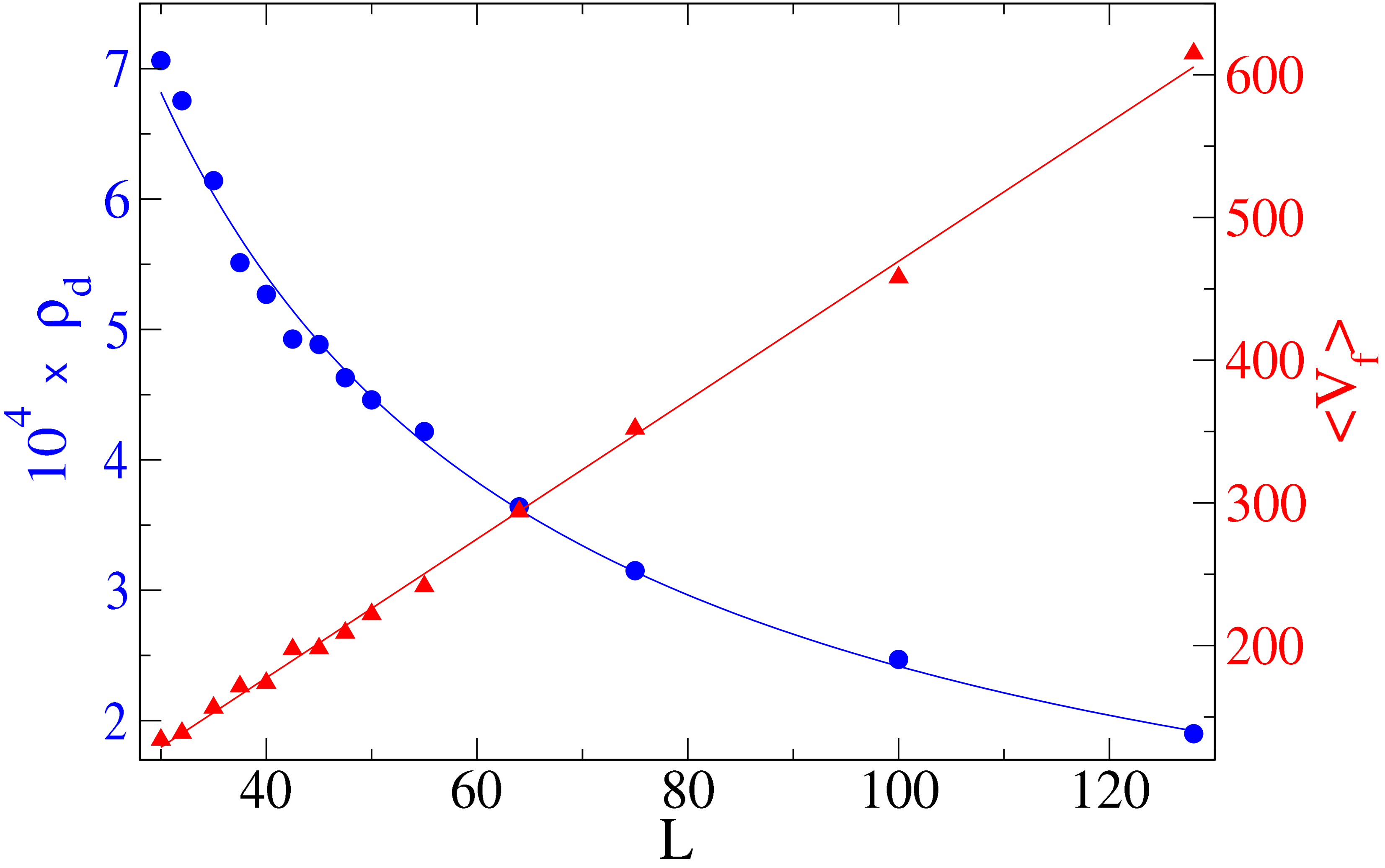
$$p(n) = p(n_0)\frac{z^{n-n_0}\Gamma(n+z_1)\Gamma(n_0+z_2+1)}{\Gamma(n+z_2+1)\Gamma(n_0+z_1)}$$

$$z_1 = \beta_1/\beta_2,\ z_2 = \alpha_1/\alpha_2,\ z = \beta_2/\alpha_2.$$

Distribution of surface defects

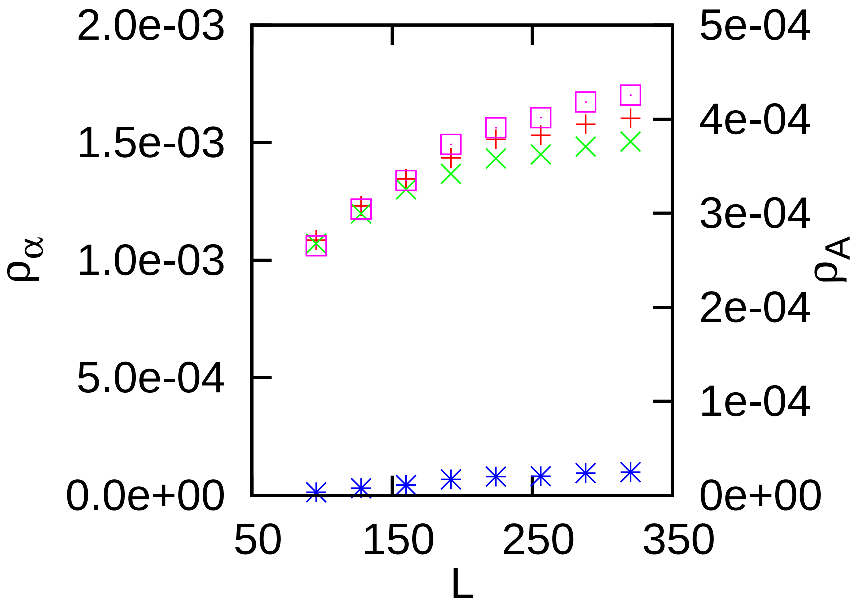


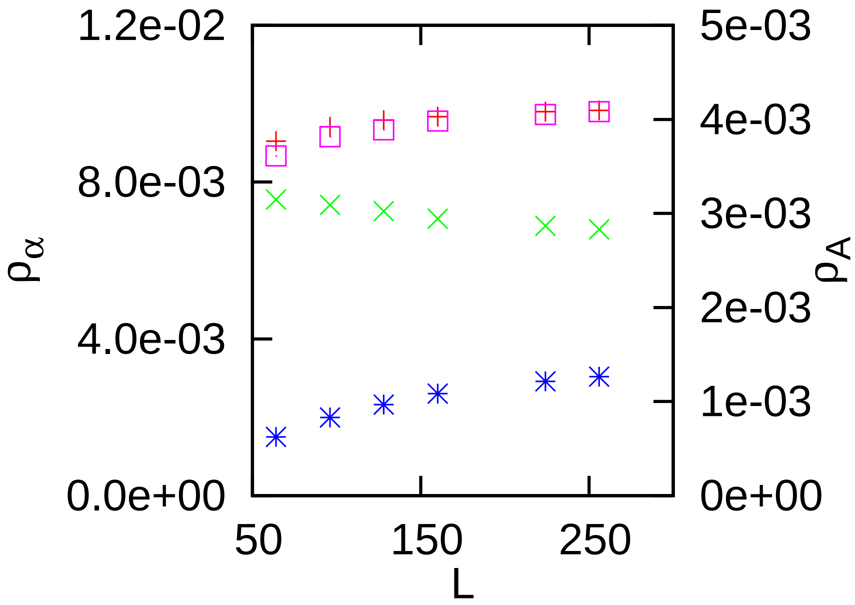
Average surface density & average volume



stronger interactions for small system sizes

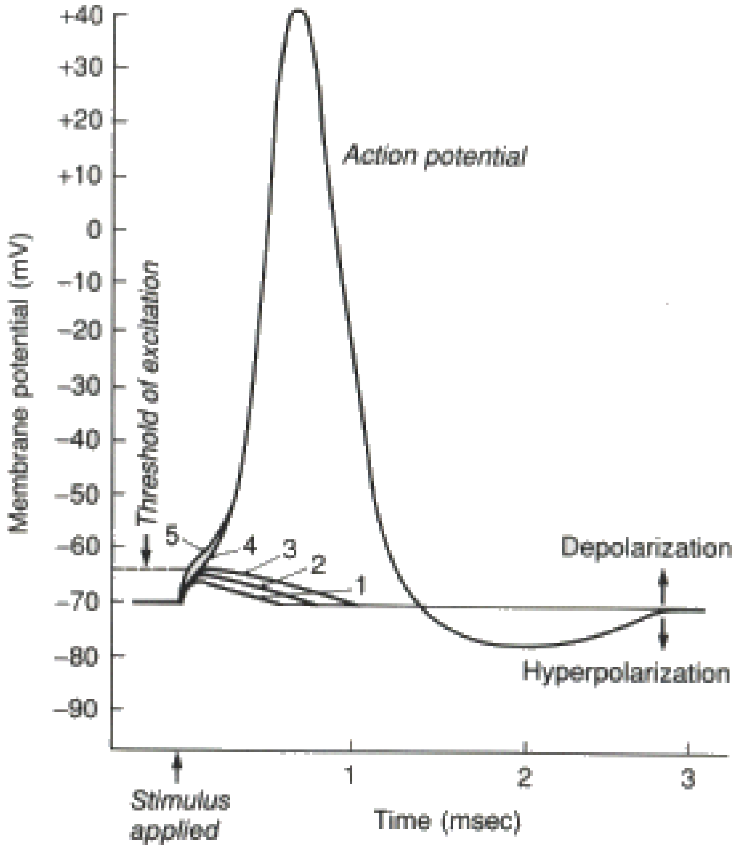
CGLE: Average densities





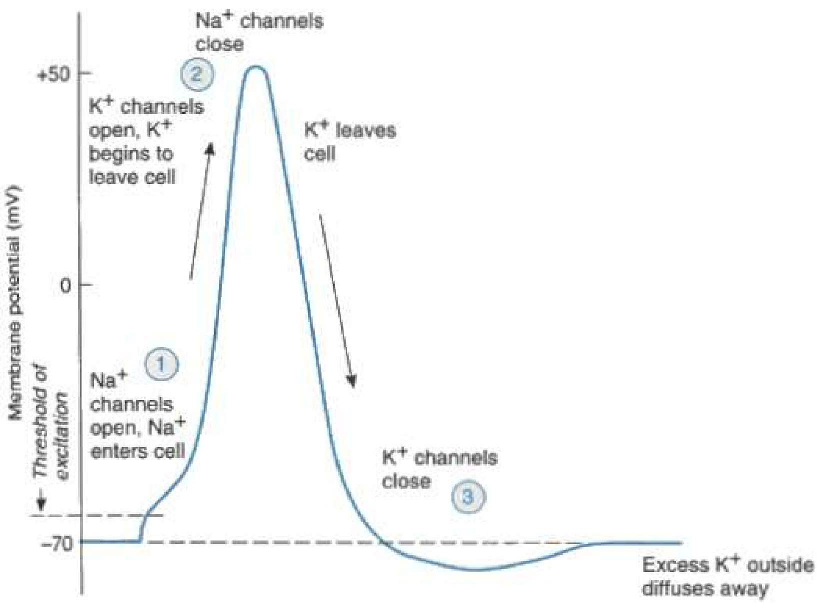
turbulence is extensive for $L \to \infty$

Action potential via patch clamp



- threshold of excitation
- amplification of stimulus
- refractory period
- action potential travels down the axon as a voltage spike
- excitatory signals
- inhibitory signals
- “negative” resting state maintained by ion pumps

Ion flow in action potential



I. Na^+ channels open, inflow of sodium ions, membrane potential becomes positive

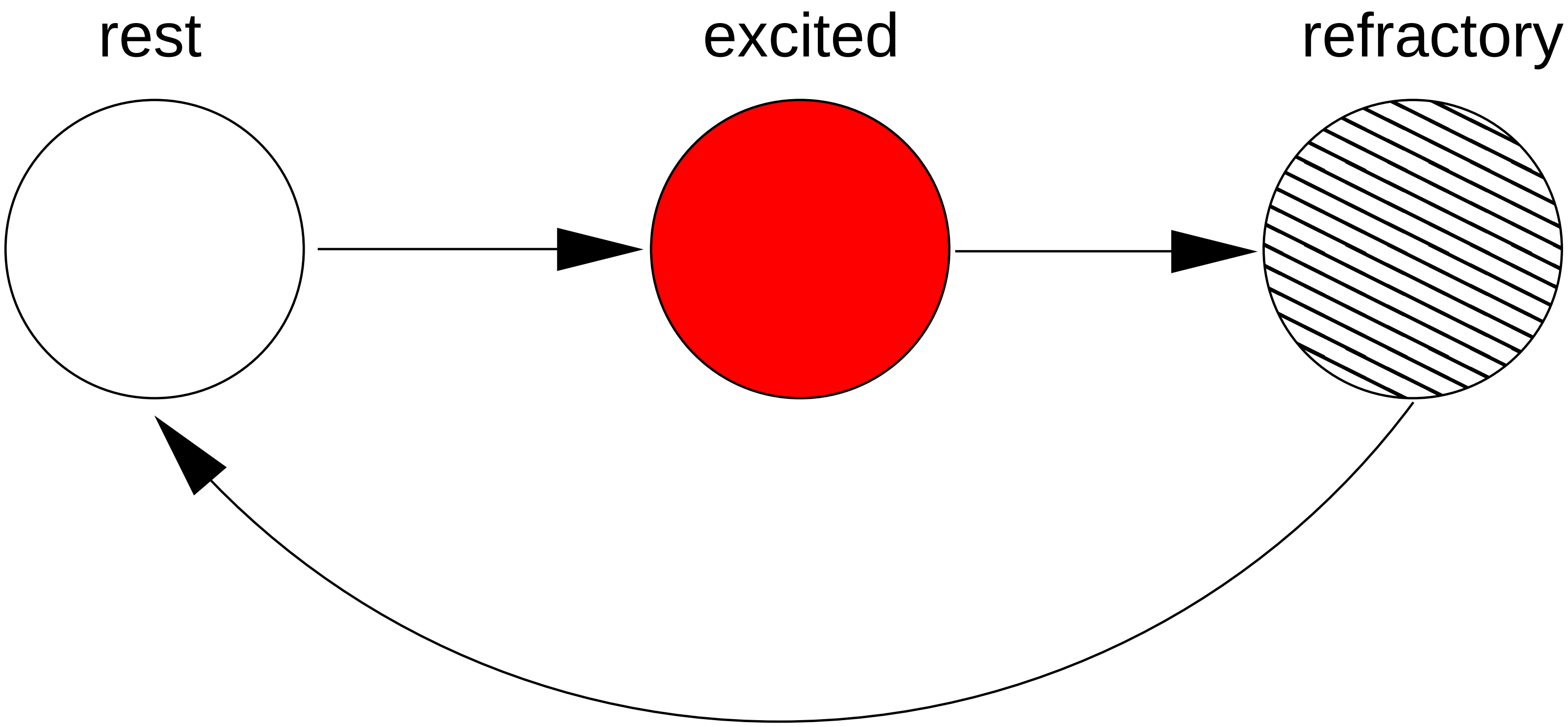
II. K^+ channels open, outflow of potassium ions

III. Na^+ channels close, membrane potential decays

IV. K^+ channels close

V. ion pumps restore rest state by transporting sodium out of the cell and potassium into the cell

Excitation dynamics



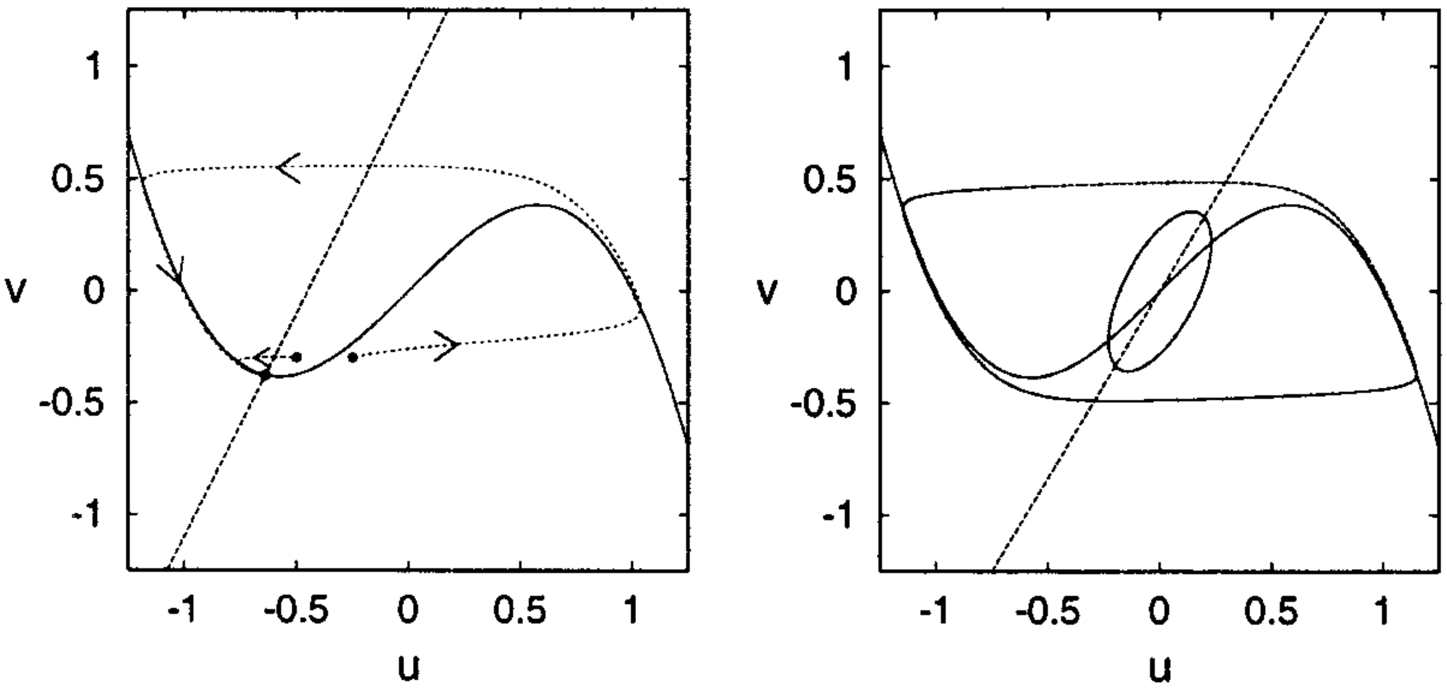
threshold of excitation: rest state is stable, sufficiently strong perturbation is required

Simple model: activator-inhibitor kinetics

$$
\begin{aligned}
\frac{du}{dt} &= -u^3 + u - v = R_u(u, v) \\
\frac{dv}{dt} &= \epsilon(u - \gamma v + \beta) = R_v(u, v)
\end{aligned}
$$

- ☞ u: concentration of fast activator (“sodium”)
- ☞ v: concentration of slow inhibitor or controller (“potassium”)
- ☞ slow means $\epsilon \ll 1$
- ☞ γ, β are constants determined by “chemical kinetics”
- ☞ generic vs. specific behavior

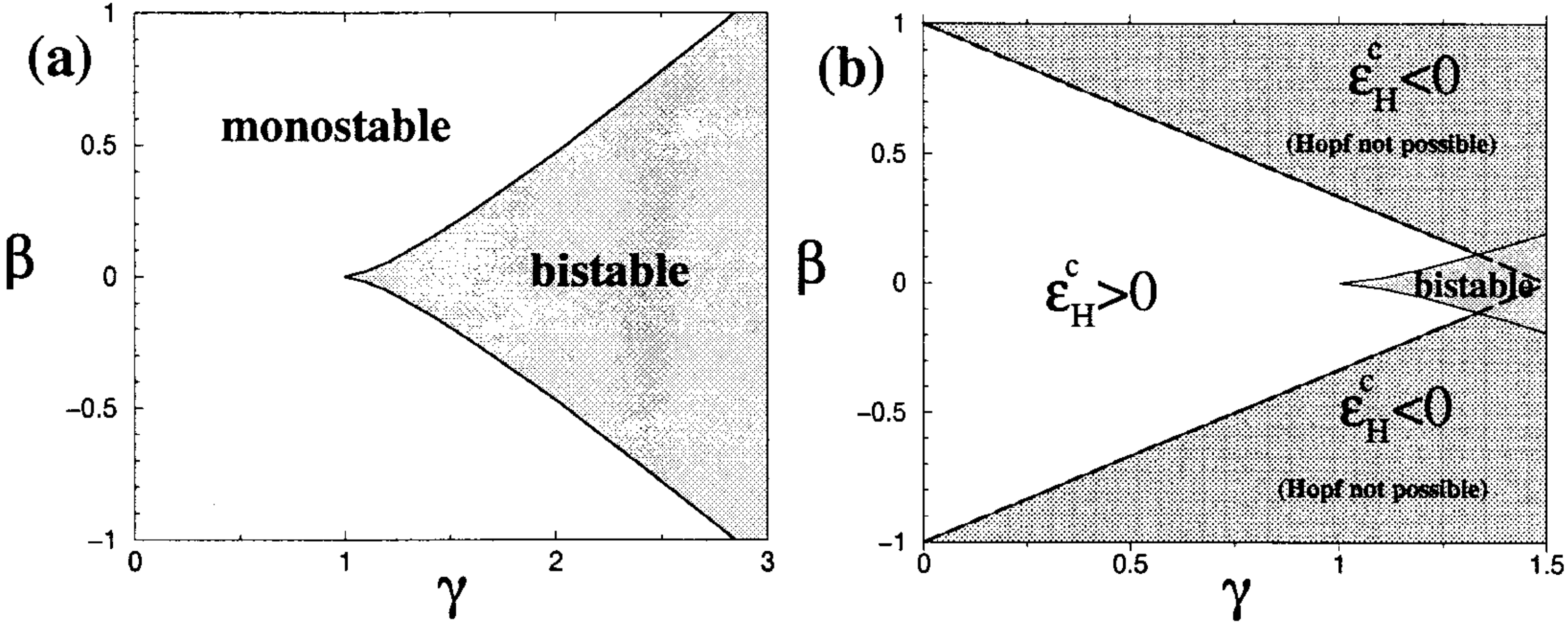
Nullclines ($\dot{u} = 0$; $\dot{v} = 0$) for FitzHugh Nagumo model



$$\frac{du}{dt} = -u^3 + u - v = R_u(u, v)$$

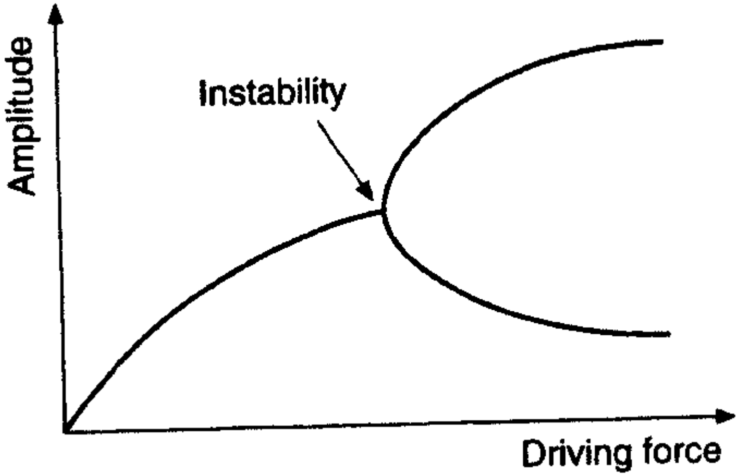
$$\frac{dv}{dt} = \epsilon(u - \gamma v + \beta) = R_v(u, v)$$

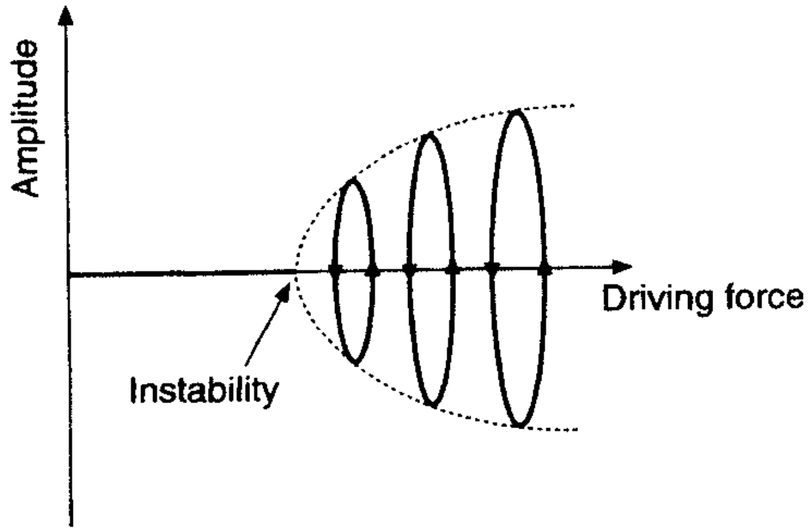
Stable equilibrium solutions of the FitzHugh Nagumo model



$$
\begin{aligned}
\frac{du}{dt} &= -u^3 + u - v = R_u(u,v) \\
\frac{dv}{dt} &= \epsilon(u - \gamma v + \beta) = R_v(u,v)
\end{aligned}
$$

Instabilities





pitchfork bifurcation

Hopf bifurcation