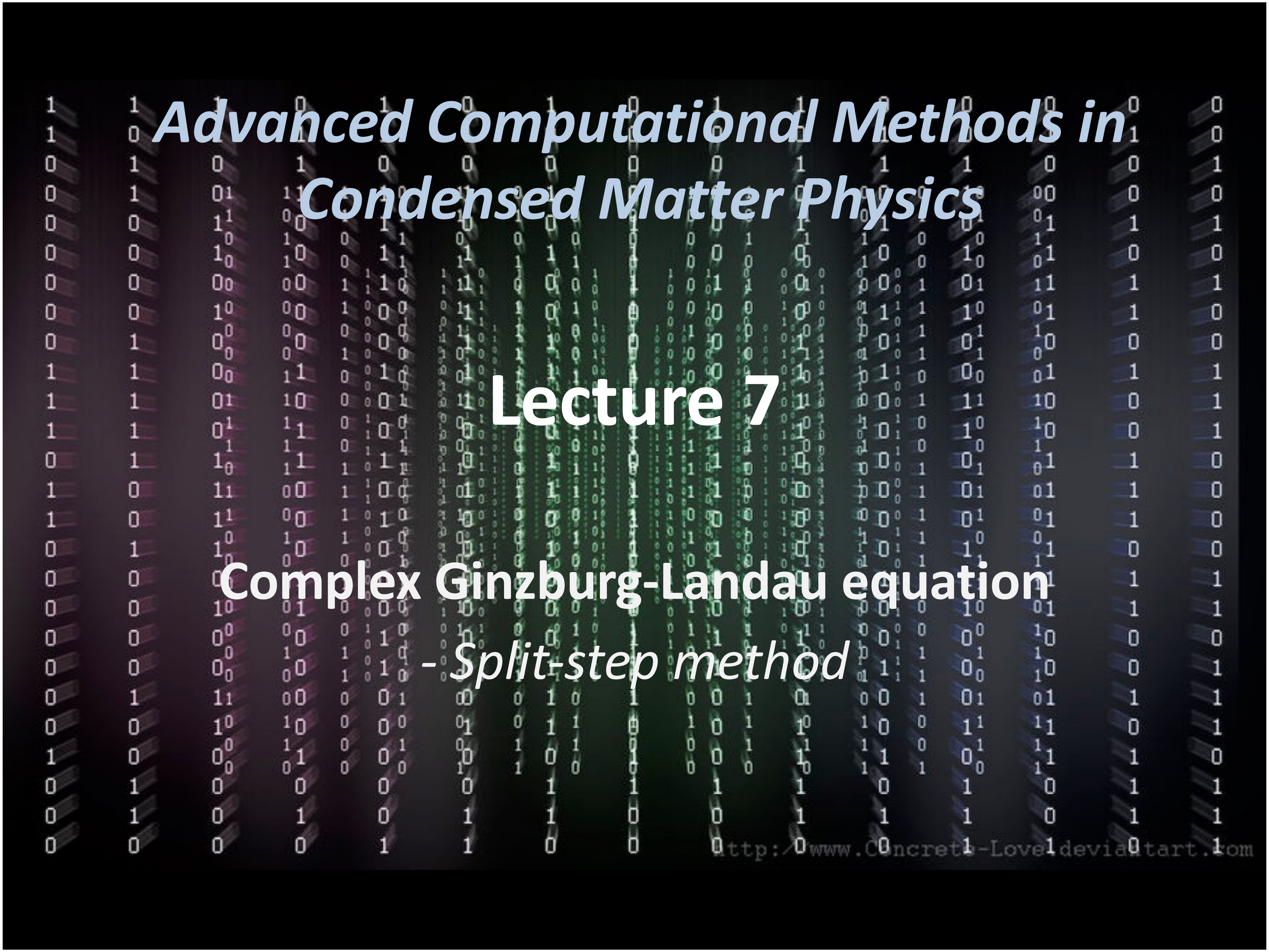
Advanced Computational Methods in Condensed Matter Physics

Lecture 7

Complex Ginzburg-Landau equation

- Split-step method



- The complex Ginzburg-Landau equation (CGLE) is one of the most-studied nonlinear equations in the physics community.
- It describes phenomena from nonlinear waves to second-order phase transitions, superconductivity, superfluidity and Bose-Einstein condensation etc.
- Here: overview of phenomena in 1D, 2D and 3D.

Lecture partially based on lectures by Igor Aronson

Historical

- Vitalii Ginzburg received Nobel Prize in Physics 2004 for the GL equation
- Alex Abrikosov received Nobel Prize in Physics 2004 for a particular stationary solution of the GL equation

Definition

- CGLE describes isotropic extended systems near the threshold of long-wavelength supercritical oscillatory instability
- Near the threshold the equation assumes a universal from
- The equation is written in terms of a complex amplitude of the most unstable oscillatory mode

Complex Ginzburg-Landau equation

$$\frac{\partial A}{\partial t} = A + (1+ib)\Delta A - (1+ic)\,|A|^2\, A$$

- *A(x,y,t)* –complex amplitude
- $\Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$ Laplace operator
- *b* – linear dispersion
- *c* – nonlinear dispersion

Example

- B-Z type chemical reactions (2D, 3D)
- Wide-aperture lasers (2D)
- Electro-convection in liquid crystals (1D)
- Hydrodynamic flows (1D)
- Flames (1D, 2D)
- Micro-organism colonies (2D)

Belousov Zhabotinsky reaction

Spiral pattern in an oscillatory BZ reaction

The oscillations are very well defined
(Hynne and Soerensen 1998)

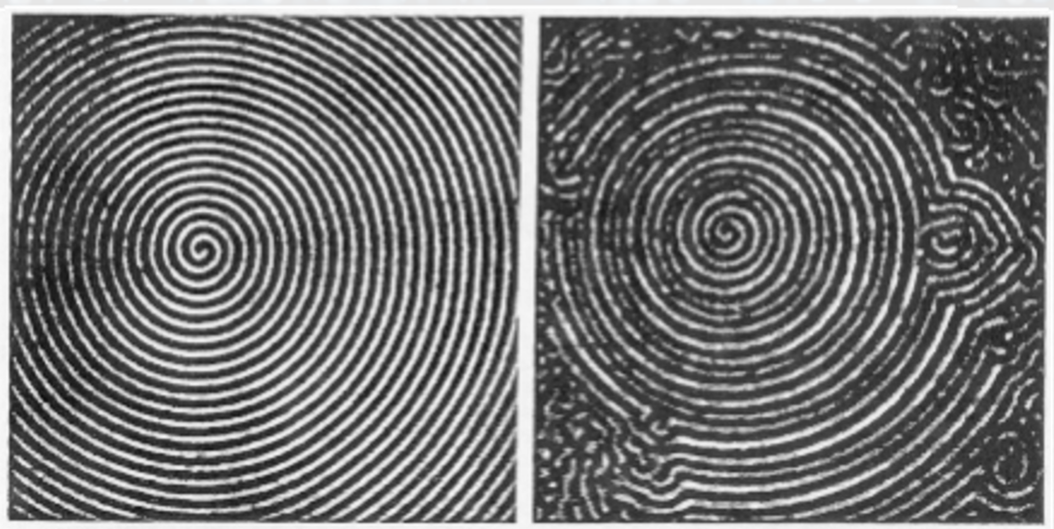
- Class of reactions that serve as a classical example of non-equilibrium thermodynamics, resulting in a nonlinear chemical oscillator
- Common element in these oscillating systems is the inclusion of bromine and an acid
- These reactions are far from equilibrium and remain so for a significant length of time.

→ chemical model of nonequilibrium biological phenomena

… more BZ

Oyang + Flesseles, Nature, 379 (1996)

B Z - Reaction



Chaotic spirals during aggregation of Dictyostelium
Siegert and Weijer, J. Cell Sci **93**, 325 (1989)

Connections to Condensed Matter

- (real) Ginzburg-Landau Equation (*b,c=0*)
  Superconductivity, superfluidity near T_c

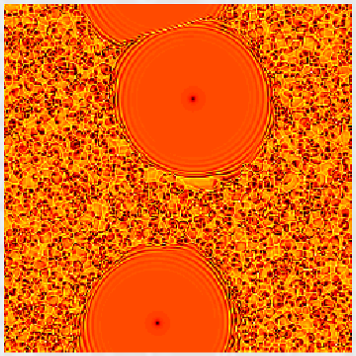
$$\frac{\partial A}{\partial t} = A + \Delta A - |A|^2 A$$

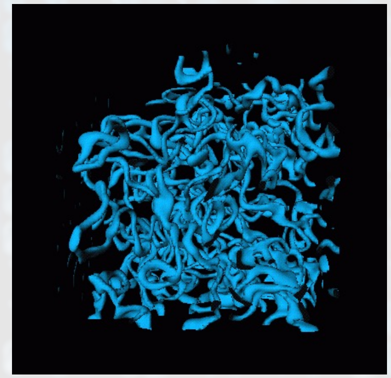
- Nonlinear Schrödinger Equations

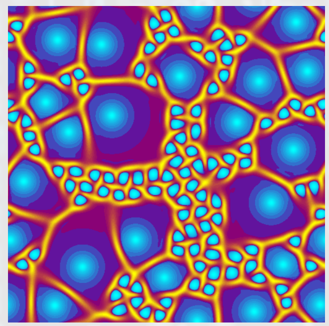
Superconductivity, superfluidity for T=0 , nonlinear optics

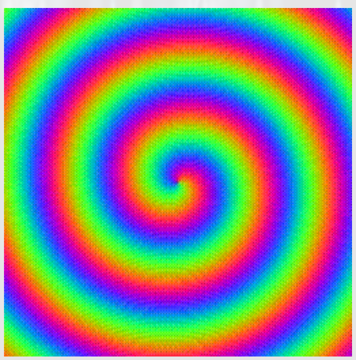
$$i\frac{\partial A}{\partial t} = \Delta A \pm |A|^2 A$$

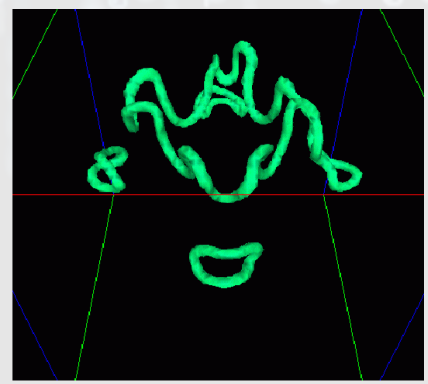
Observed patterns



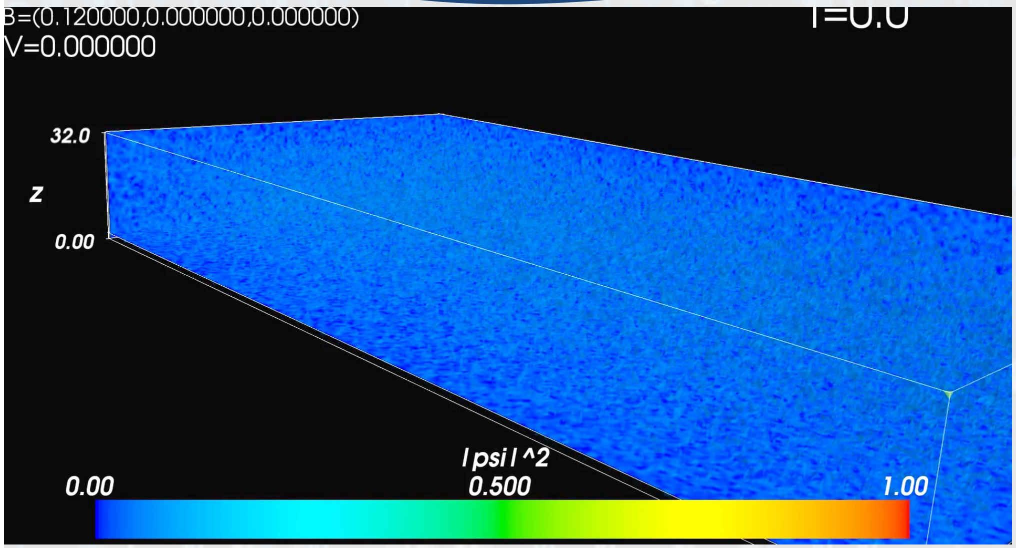






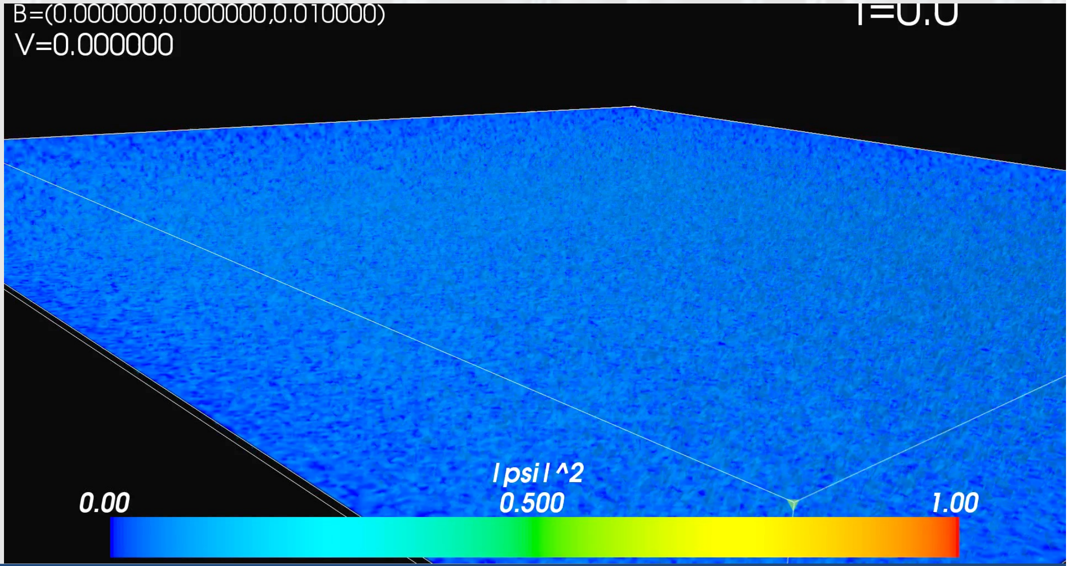


Ginzburg-Landau equation for SCs



Magnetic field and current are parallel + inclusions

Vortices moving over a step due to applied current



Numerical solution

$$\frac{\partial A}{\partial t} = A + (1 + ib)\Delta A - (1 + ic)|A|^2 A$$

Methods

- Explicit integration
- Implicit methods
    - Iterative solvers for parallel applications
- **(spectral) split step method**

First we rewrite the equation in terms of a linear (D) and a non-linear (N) operator:

$$\frac{\partial A}{\partial t} = [\hat{D} + \hat{N}]A$$

with $\hat{D} = 1 + (1 + ib)\Delta\,;\;\hat{N} = -(1 + ic)|A|^2$

Pseudo-spectral split step method

2. We split the equation and solve the linear and non-linear parts separately

$$\frac{\partial A_N}{\partial t} = -(1+ic)|A|^2 A = \hat{N} A$$

$$\frac{\partial A_D}{\partial t} = (1+(1+ib)\Delta)A = \hat{D} A$$

For the non-linear part we can write the formal solution for a small time step h:

$$A_N(t+h, r) = \exp\left[-(1+ic)|A|^2 h\right] A(t,r)$$

With Fourier transform

$$\tilde{A}_N(t,k) = \int d^3 r A_N(t,r) \exp[i\mathbf{k}\cdot\mathbf{r}]$$

….

Next, we solve the linear step in Fourier space

$$\tilde{A}(t+h,k) = \exp\left([1-(1+ib)k^2]h\right)\tilde{A}_N(t,k)$$

Finally the inverse Fourier transform yields A(t+h,r)
The small step in time, h, allows to treat these steps separately, but nevertheless has a numerical error

One could also solve the initial equation directly, by formally writing $\frac{\partial A}{\partial t} = [\hat{D}+\hat{N}]A$

$$A(t+h,r) \approx \exp\left[h(\hat{D}+\hat{N})\right]A(t,r)$$

Note: This is not exact, since we commuted the operators D and N. Using, a Baker-Hausdorff type formula for the commutator (e.g. for the non-linear Schrödinger equation) One can show that the error is of order h^2

…

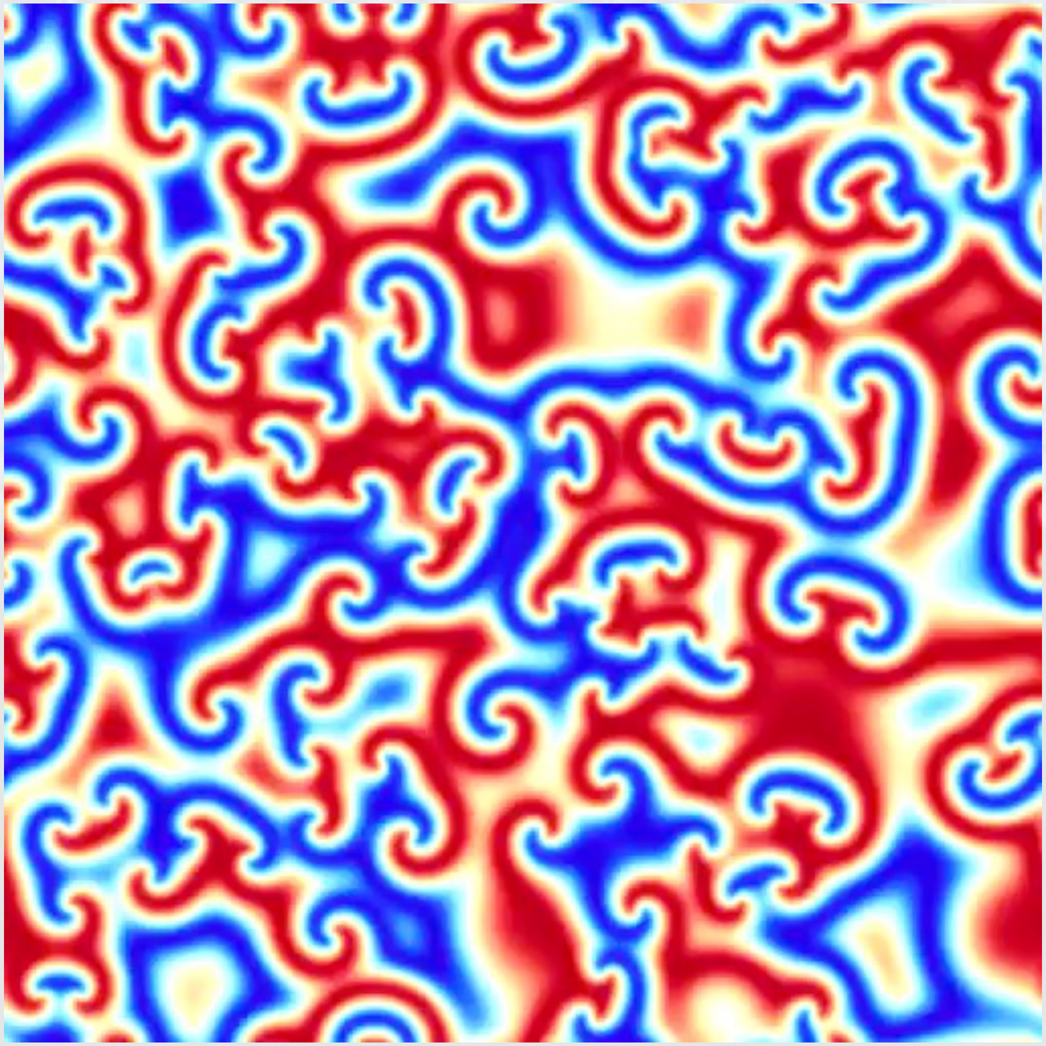
Finally, we compute the D operator in Fourier space and get the expression

$$A(t+dt,r) = F^{-1}[e^{h(1-(1+ib)k^2}F[e^{h\hat{N}}A(t,r)]]$$

If one takes half a step with one operator first, then a full step with the other, and the second half of the first again, the error of this method is of order h^3

Using the FFT for the Fourier transform results in a significantly faster (and more stable) integration than a finite difference method.

Solution for b=1, c=0



Coherent structures

- **Source:** group velocities directed outward of the defect
  sources dominate surrounding dynamics
  sources come in discrete families (except 1D Nozaki-Bekki holes)
  source select the wavenumber of emitted waves
- Sink (shock) are results of collisions of incoming waves
  shocks are determined by b.c. or other sources
  shocks come in continuous families and don't have specific structure
- Phason: group velocity does not change the sign
  bound state of shock and source

Classification of coherent structures from counting arguments
van Saarloos & Hohenberg, Physics D, 1992

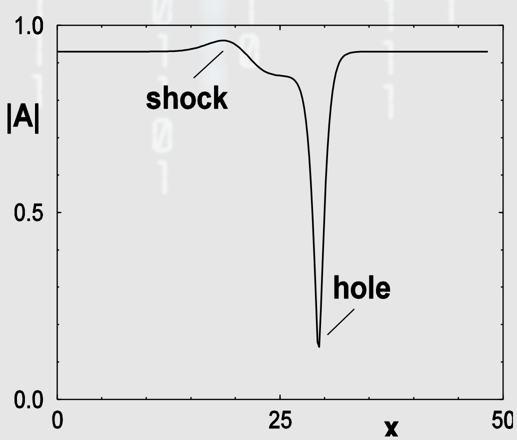
Topological defects

- Zeros of $A=|A|e^{i\theta}$ result in topological singularity for phase θ=arg$A$

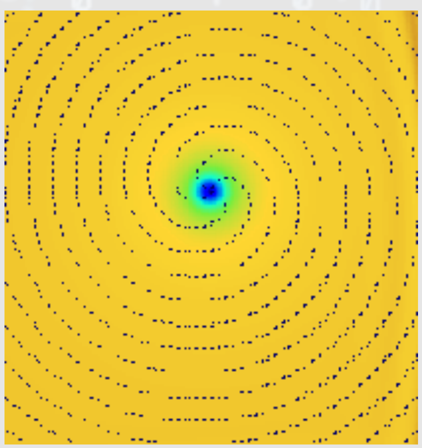
$$n = \frac{1}{2\pi}\oint_l \nabla\theta dl \text{ – topological charge, } n = \pm 1$$

- Defects: 1D – holes (phase slips) , 2D –spirals (vortices) , 3D – vortex lines or filaments

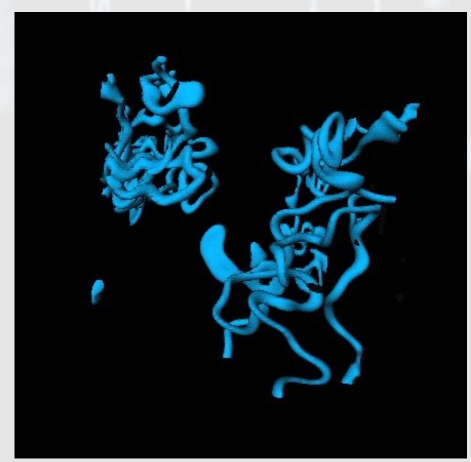
1D hole + shock



2D spiral



3D vortex lines



Importance of topological defects (TD)

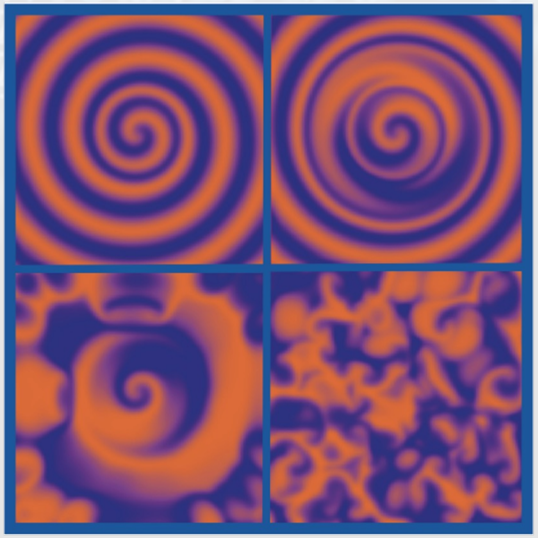
- Active TD (sources) dominate surrounding dynamics
- Stability of TD determine transition to chaos
- TD are "elementary excitation" of the medium. One can express the evolution of the CGLE in terms of a greatly simplified evolution of the "gas" of interacting TD
- TD can coexist with turbulence and exhibit spatio-temporal intermittency in 1D, 2D and 3D

Bulk and Core Instabilities of TD

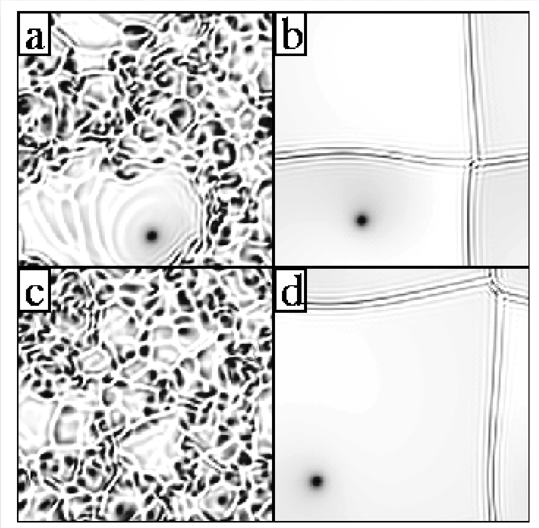
- Active TD select unique wavenumber and have a fixed core structure
- Bulk instability (BI) – emitted waves are unstable (continuum spectrum)
- Core instability (CI) : discrete localized mode are unstable
- Transitions to chaos can be related either to BI or CI, or both

Examples of BI and CI

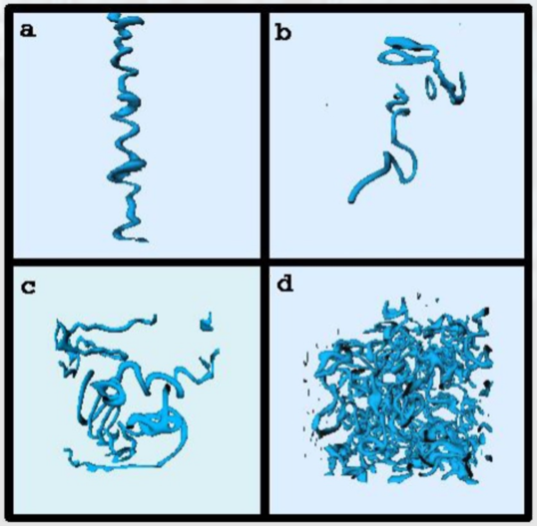
2D Spiral Breakup (BI)
b=1, c=-1



2D Spiral Intermittency
(BI+CI) , c=-0.4, b=40



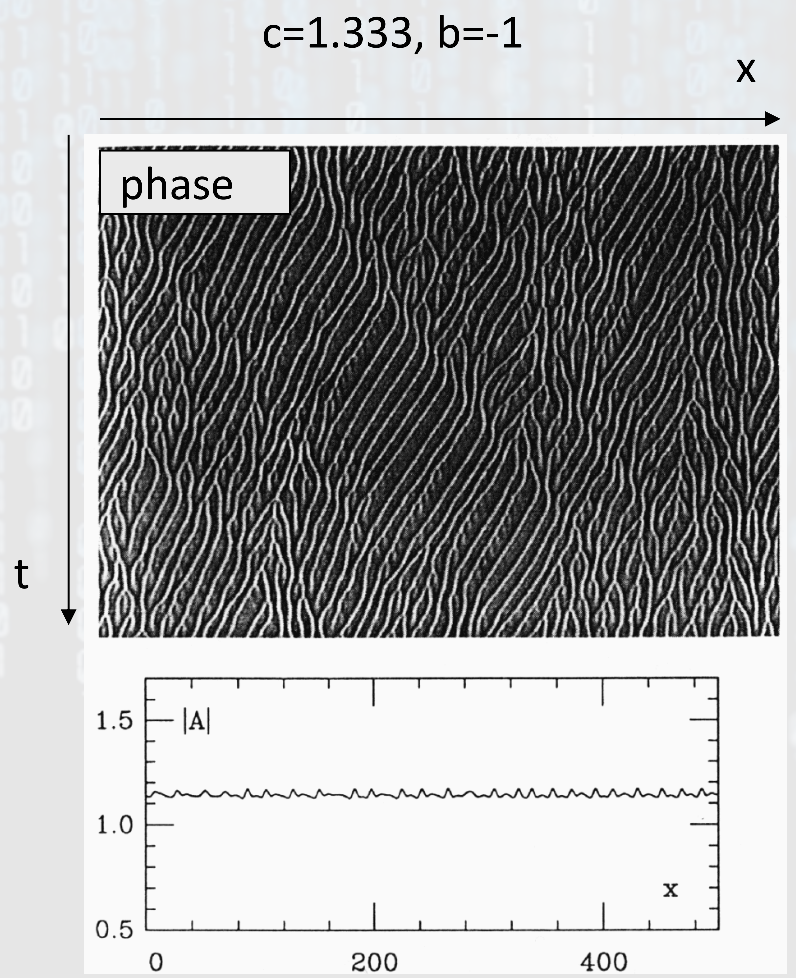
3D Vortex stretching
(CI) c=-0.03, b=50



Amplitude (or defect) and Phase chaos

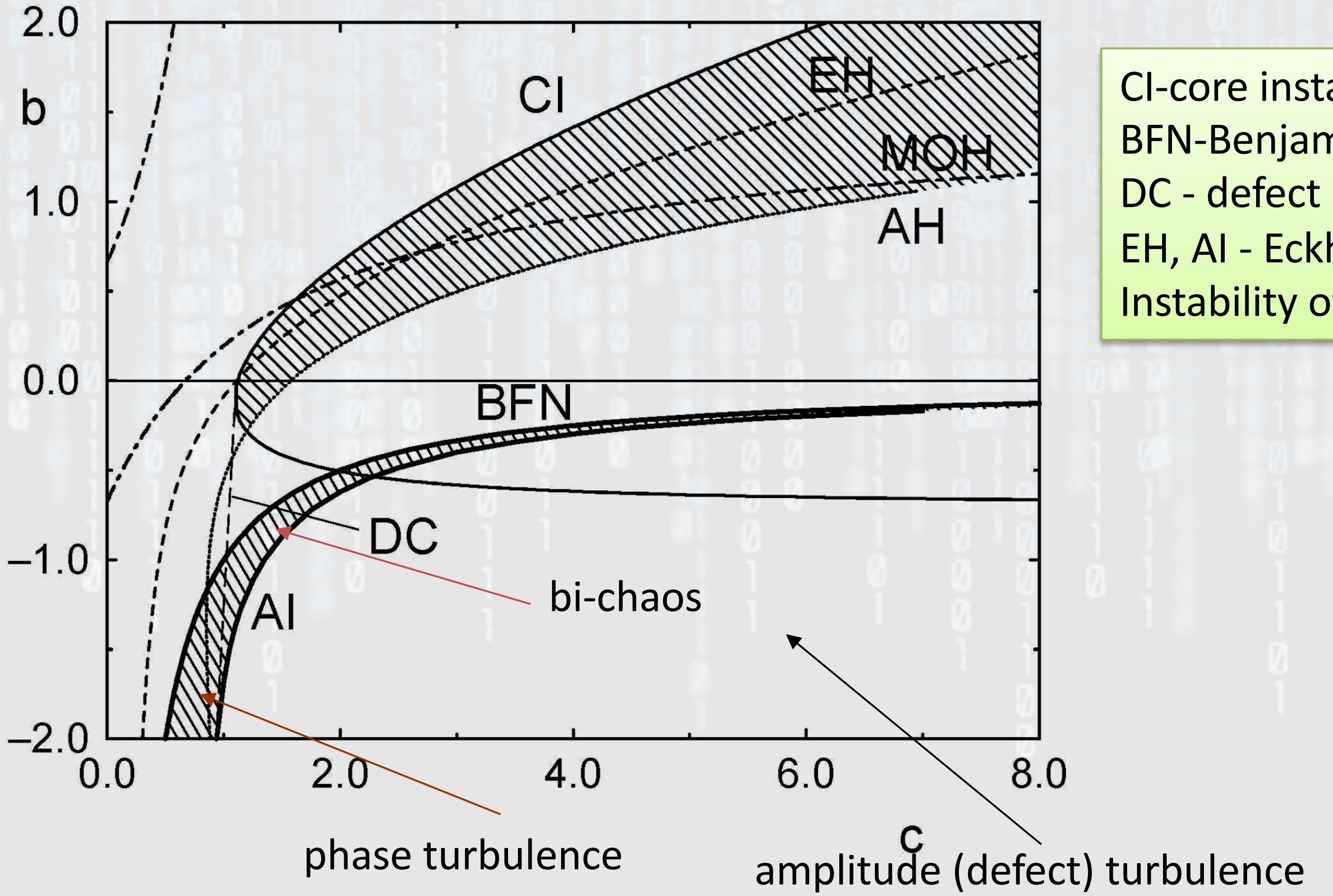
- ***Phase Chaos***

  |A|≈const>0, phase chaotic
- ***Amplitude Chaos:***
  amplitude *A* has zeroes



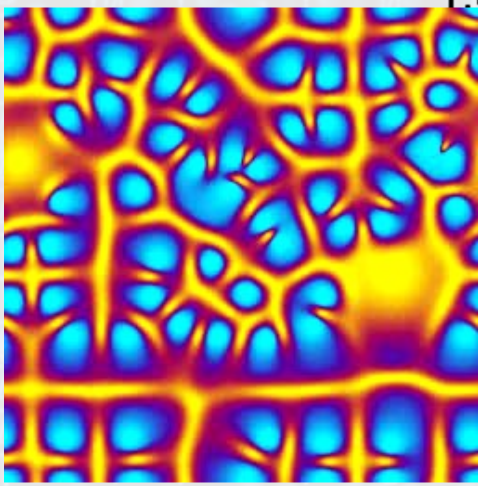
Chate et al, 1994

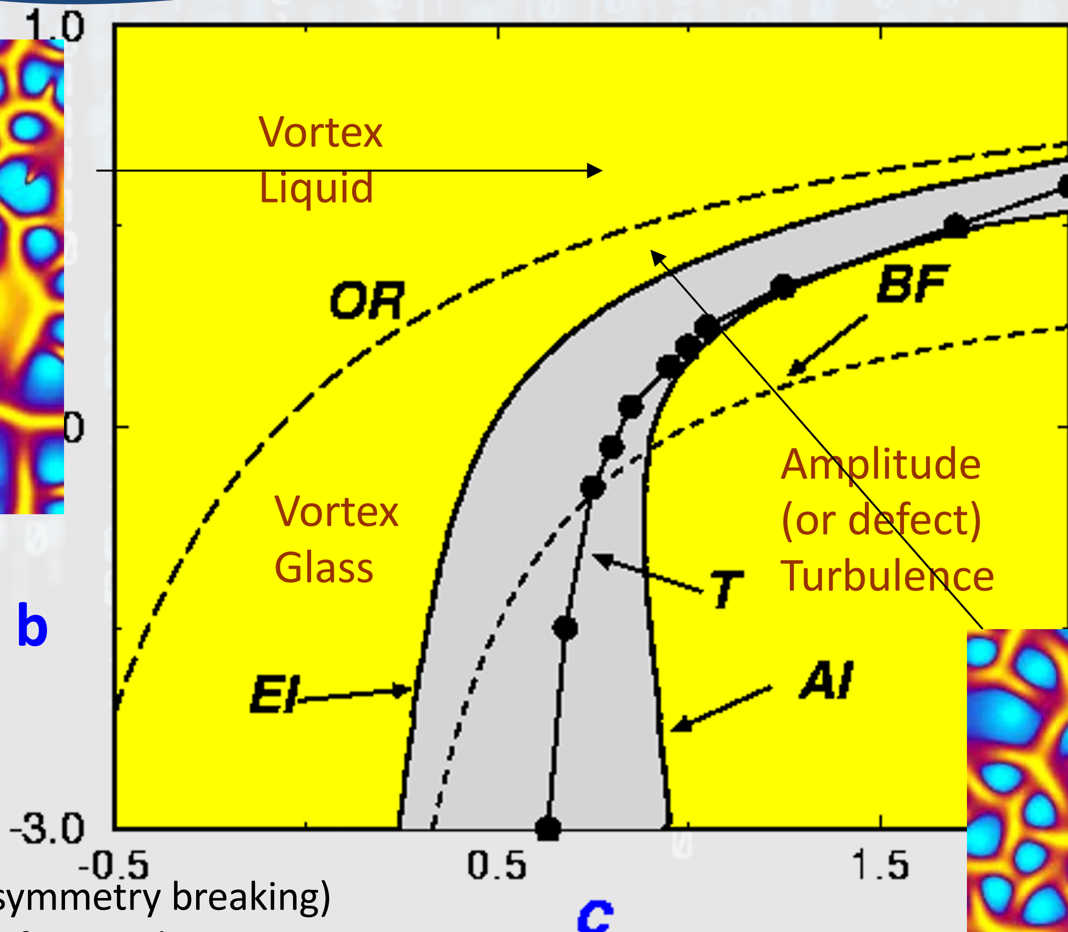
Very Rich Behavior even in 1D

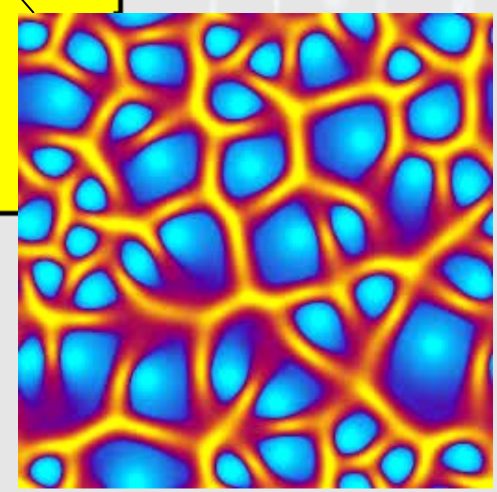


CI-core instability
BFN-Benjamin-Feir line
DC - defect chaos
EH, AI - Eckhaus and absolute
Instability of holes

Phase Diagram of 2D CGLE







- OR-oscillatory range (symmetry breaking)
- EI – Eckhaus instability for spirals
- BF – Benjamin-Fair limit
- AI- absolute instability for spirals and transition to chaos

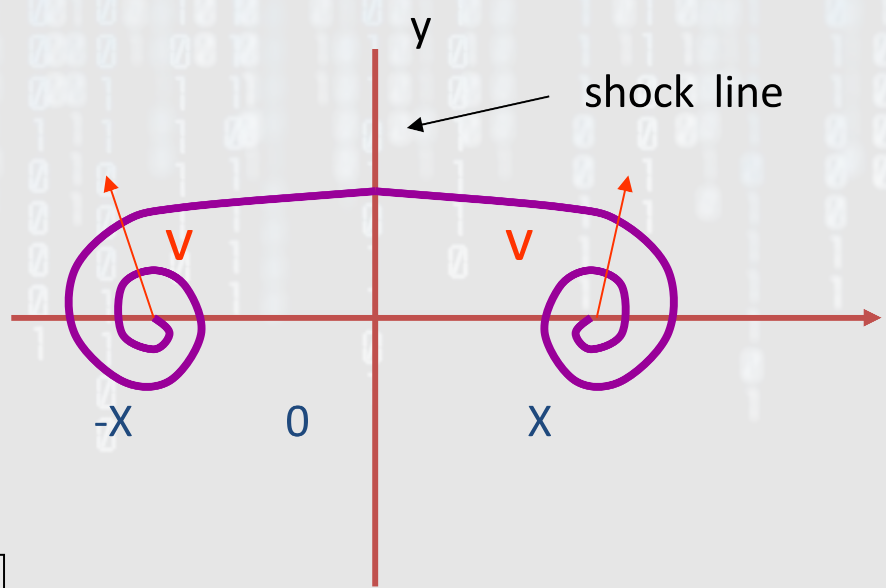
Interaction between two spirals

Exponential decay of interaction

- Monotonic range c<0.845 & b=0:
  - -weak repulsion irrespectively of charge
  - -no symmetry breaking
- Oscillatory range c>0.845:
  - -oscillatory interaction vs distance
  - -meta-stable bound states
  - -symmetry breaking

- Biktashev, 1989
- Aranson, Kramer & Weber, Phys Rev. E, 1993

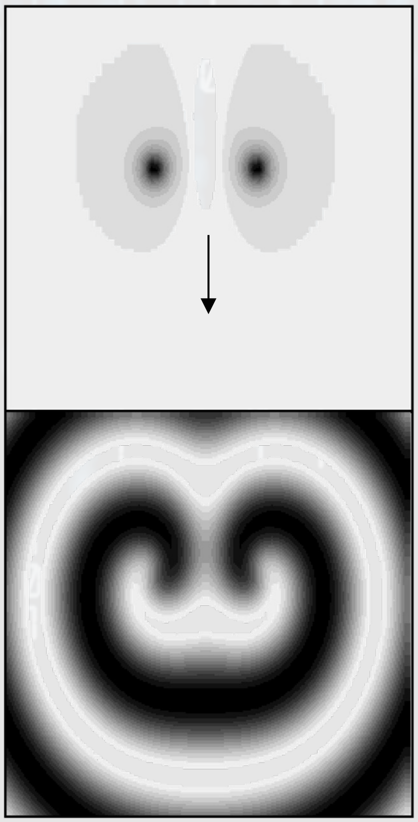
- v –velocity of the spiral core
- φ -phase of the spiral
- X -distance to the shock line



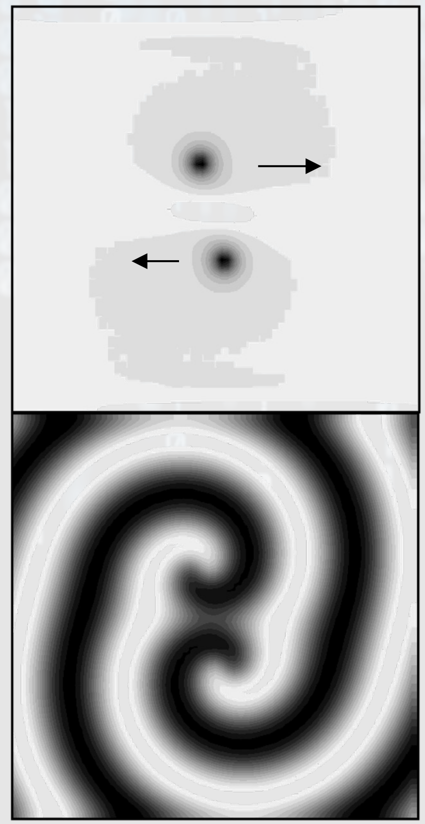
Examples of Bound States

Oppositely charged- drift

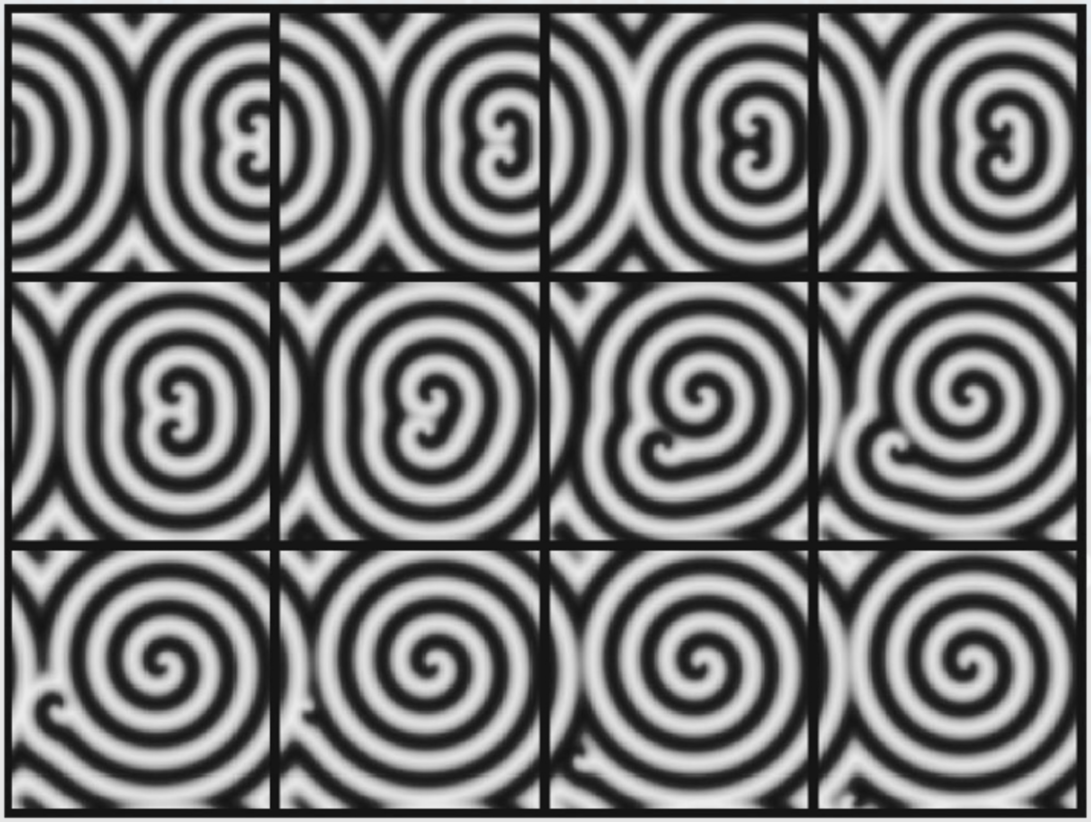
Likely charged-rotate



c=1.5,b=0

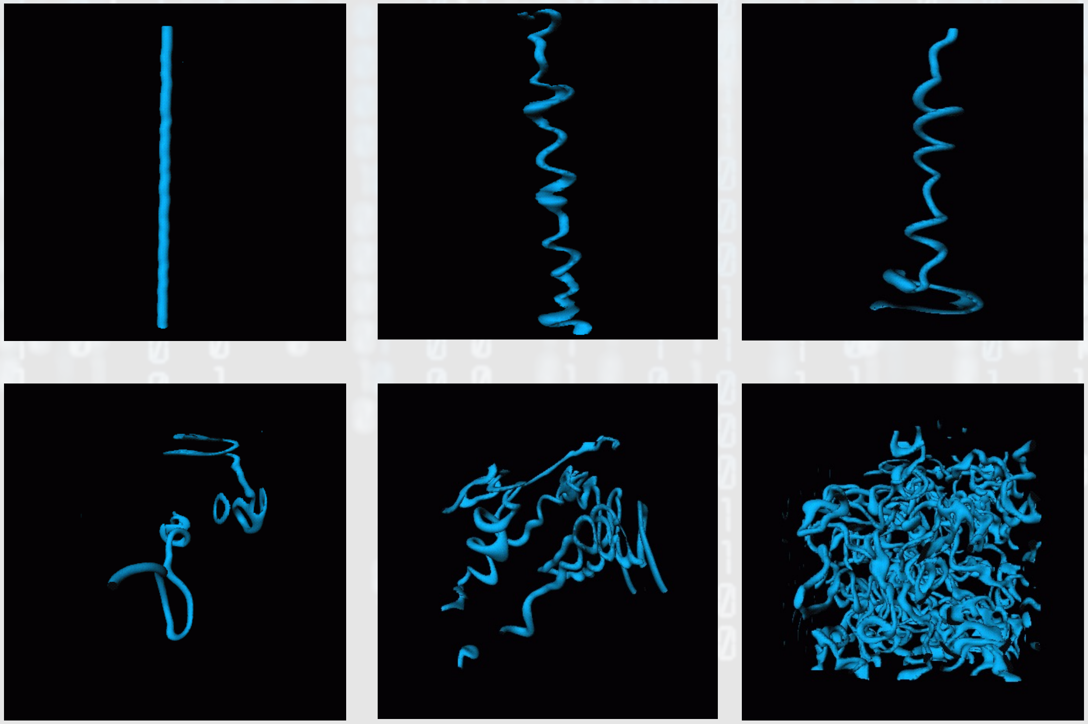


Symmetry breaking



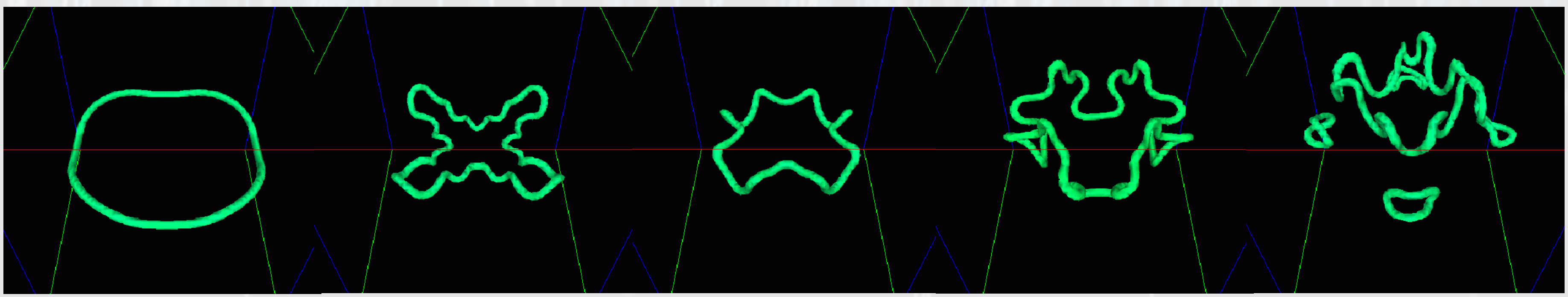
3D vortices more unstable than spirals

- Instability occurs at finite wavenumber in z-direction



Evolution of Vortex Ring

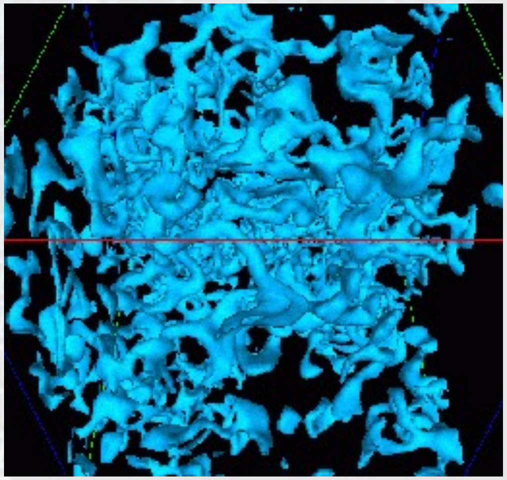
- Without CI vortex ring shrinks (Gabbay et al, 1997)
- With CI vortex rings breaks (Aranson & Bishop, 1997)

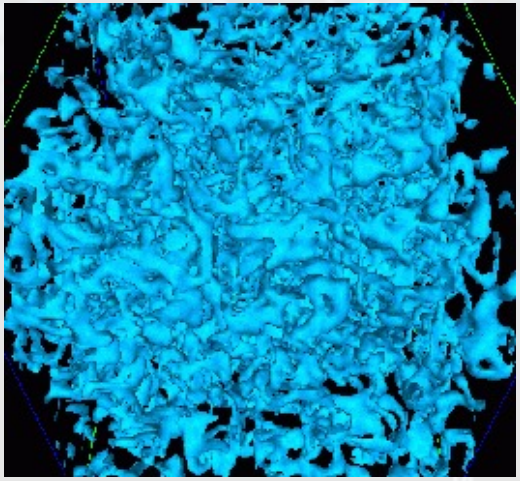


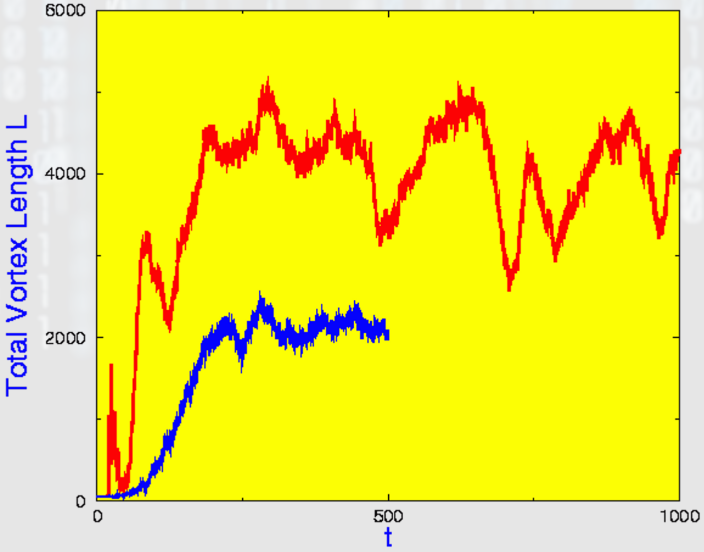
time

3D Core Instability and Symmetry Breaking

- Core Unstable Vortices in Oscillatory range show length oscillations







Conclusions

- CGLE describes broad range of phenomena on qualitative and quantitative levels
- CGLE is a universal model which can be rigorously derived from various physical, chemical or biological system
- CGLE is computationally efficient model and allows for some analytical treatment