

# Simulations in Statistical Physics

Course for MSc physics students

Janos Török

Department of Theoretical Physics

April 25, 2021

# Algorithmically defined models

- ▶ Self-Organized Criticality
  - ▶ Bak-Tang-Wiesenfeld model
  - ▶ Forest fire model
  - ▶ Bak-Sneppen model of evolution
- ▶ Traffic models
- ▶ SIR model
- ▶ Opinion models
- ▶ Flocking

# Agent based models

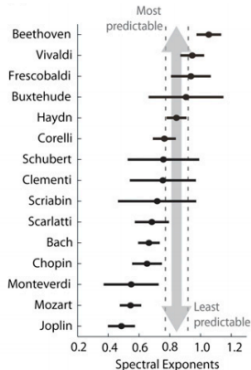
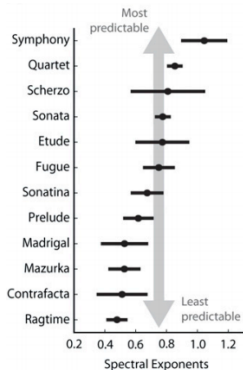
- ▶ Agents with well defined rules
- ▶ Interactions
  - ▶ Among all agents
  - ▶ Between neighbors (lattice or network)
  - ▶ Within a distance
- ▶ Complex emergent phenomena

# Self-Organized Criticality

- ▶ Critical state: inflection point in the critical isotherm
- ▶ Power law functions of correlation length, relaxation time
- ▶ Control parameter, generally temperature
- ▶ Critical point as an attractor?
- ▶ Why? Power law: We see many cases
  - ▶  $1/f$  noise (music, ocean, earthquakes, flames)
  - ▶ Lack of scales (market, earthquakes)
- ▶ Underlying mechanism?

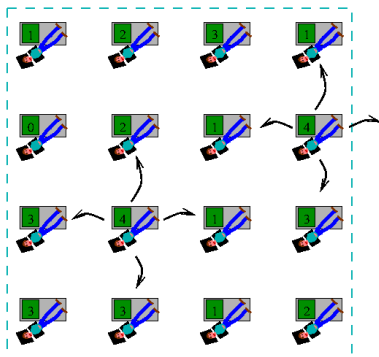
# $1/f$ spectrum

- ▶ Music, paintings, fire
- ▶ We seem to like it



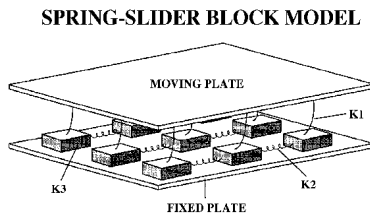
# Bak-Tang-Wiesenfeld model

- ▶ Originally a sandpile model
- ▶ Better explained as a *Lazy Bureaucrat model*:
  - ▶ Bureaucrats are sitting in a large office in a square lattice arrangement
  - ▶ Occasionally the boss comes with a dossier and places it on a random table
  - ▶ The bureaucrats do *nothing* until they have less than 4 dossiers on their table
- ▶ Once a bureaucrat has 4 or more dossiers on its table starts to panic and distributes its dossiers to its 4 neighbors
- ▶ The ones sitting at the windows give also 1 dossier to its neighbors and throw the rest out of the window.



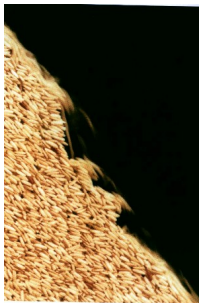
# Bak-Tang-Wiesenfeld model

- ▶ Originally a sandpile model
- ▶ Better explained as a *Lazy Bureaucrat model*:
- ▶ Best application: Spring block model of earthquakes:
  - ▶ Masses sitting on a frictional plane in a grid are connected with springs to each other and to the top plate
  - ▶ Top plate moves slowly, increasing the stress on the top springs slowly and randomly
  - ▶ If force is large enough masses move which increases the stress on the neighboring masses



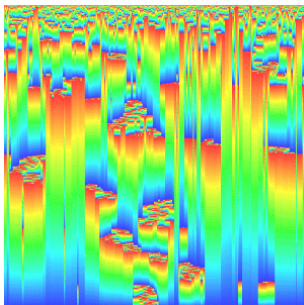
# Bak-Tang-Wiesenfeld model: Results

- ▶ Avalanche size distribution is a power law  $\rightarrow$  no scale
- ▶ No external parameter tuning for scale free state
- ▶ Hence the name: Self-organized criticality
- ▶ Lifetime distribution of avalanches:  $1/f$  (unfortunately for sand it is  $1/f^2$ )



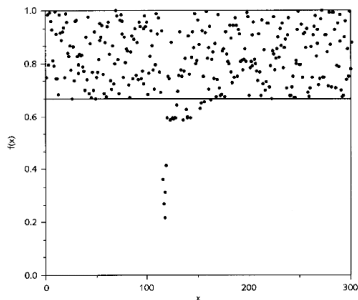
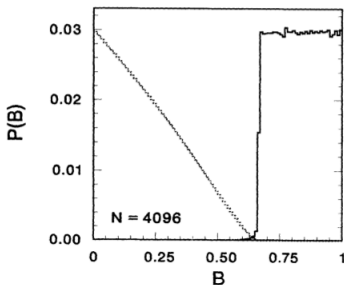
# Bak-Sneppen model of evolution

- ▶  $N$  species all depends on two other (ring geometry)
- ▶ Each species are characterized by a single *fitness*
- ▶ In each turn the species with the lowest fitness dies out and with it its two neighbors irrespective of their fitness
- ▶ These 3 species are replaced by new ones with random fitness
- ▶ Initial and update fitness is uniform between  $[0, 1]$



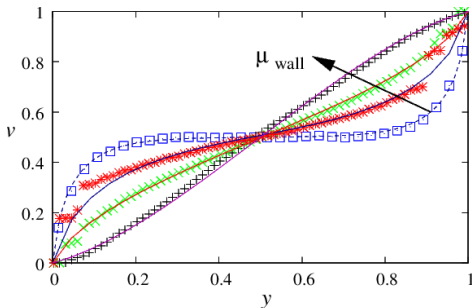
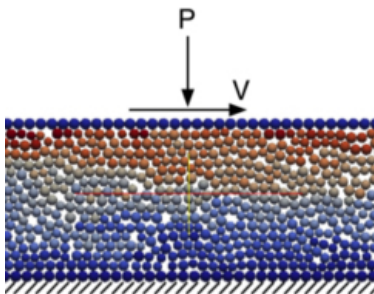
# Bak-Sneppen model of evolution: Results

- ▶ Steady state with avalanches
- ▶ Avalanches start with a fitness  $f > f_c \simeq 0.66$
- ▶ Avalanche size distribution power law
- ▶ Distance correlation power law



# Bak-Sneppen model of evolution an application: Granular shear

- ▶ Fitness  $\rightarrow$  Effective friction coefficient
- ▶ Specimen with lowest fitness dies out  $\rightarrow$  block is sheared at weakest position (shear band)
- ▶ Neighbors, related species die out and replaced by new species  $\rightarrow$  structure gets random around the shear band.

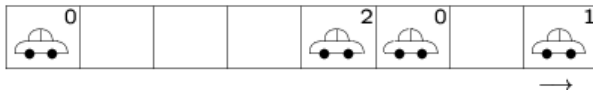


# Traffic models



# Nagel-Schreckenberg model

- ▶ Periodic 1d lattice (ring) Autobahn
- ▶ discretized in space and time
- ▶ Cars occupying a lattice moving with velocities  $v = 0, 1, 2, 3, 4, 5$
- ▶ Remark, if max speed is 126 km/h, then lattice length is 7 m, a very good guess for a car in a traffic jam
- ▶ It uses parallel update: at each timestep all cars move  $v$  sites forward



# Nagel-Schreckenberg model

## ► Algorithm:

1. **Acceleration:** All cars not at the maximum velocity increase their velocity by 1
2. **Slowing down:** Speed is reduced to distance ahead (1 sec rule)
3. **Randomization:** With probability  $p$  speed is reduced by 1
4. **Car motion:** Each car moves forward the number of cells equal to their velocity.

Configuration at time  $t$ :



a) Acceleration ( $v_{max} = 2$ ):



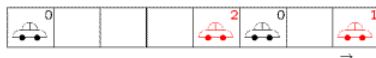
b) Braking:



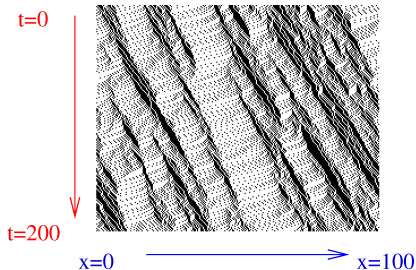
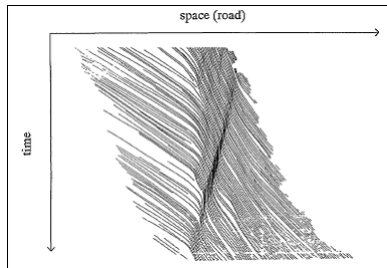
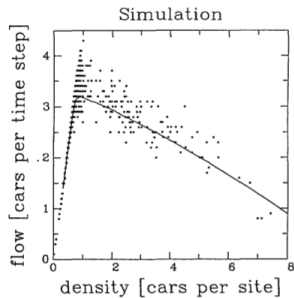
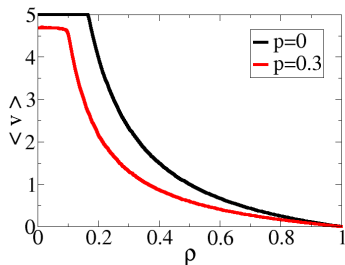
c) Randomization ( $p = 1/3$ ):



d) Driving (= configuration at time  $t + 1$ ):

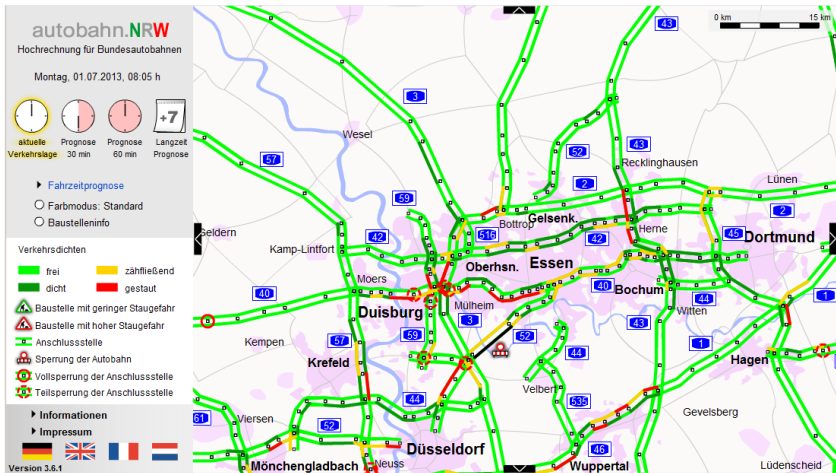


# Emergence of traffic jams



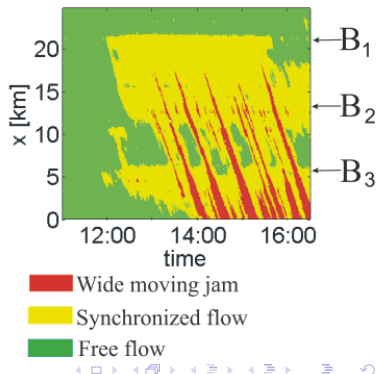
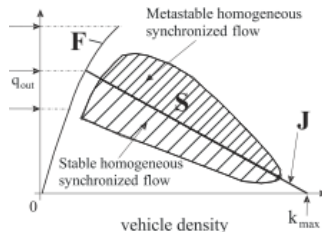
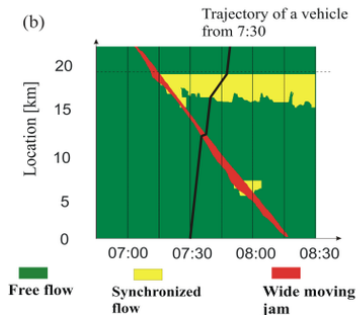
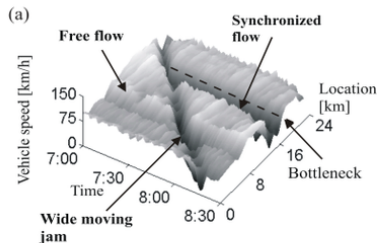
# Nagel–Schreckenberg model

- ▶ Transition from free-flow to jammed state
- ▶ Jammed state is a phase-separated phase
- ▶ Without randomization a sharp transition
- ▶ Had been used in NRW to predict traffic jams



# Three-phase traffic theory

Three traffic phases

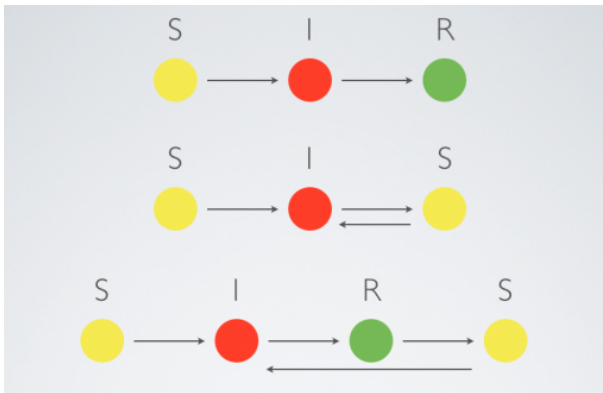


# Disease spreading, SIR model

- ▶ S: susceptible (can be infected with prob.  $\beta$  if meets an infected)
- ▶ I: Infected (may infect susceptible, but may recover with prob.  $\nu$ ).
- ▶ R: Recovered (Immune to the disease)
- ▶ Other versions:
  - ▶ SI: agents do not recover (e.g. information spreading)
  - ▶ SIS: recovered people can get disease again
  - ▶ SIRS: recovered agents may become susceptible (e.g. influenza)

# Disease spreading, SIR model

- ▶ S: susceptible
- ▶ I: Infected
- ▶ R: Recovered



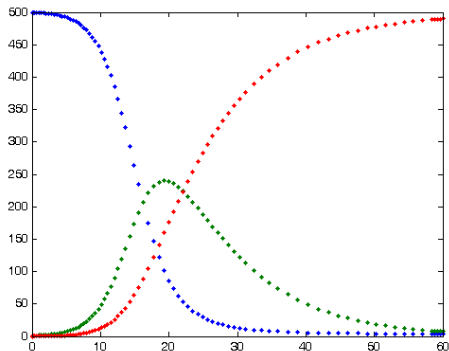
# SIR model, connected graph

Governing equations:

$$\dot{S} = -\beta IS$$

$$\dot{I} = \beta IS - \nu I$$

$$\dot{R} = \nu I$$



# SIR model, connected graph

Governing equations:

$$\dot{S} = -\beta IS$$

$$\dot{I} = \beta IS - \nu I$$

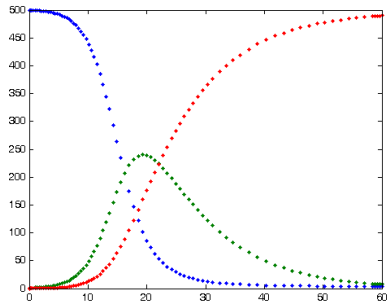
$$\dot{R} = \nu I$$

- ▶ Early stage  $S \simeq 1$

$$I \simeq I_0 \exp[(\beta - \nu)t]$$

- ▶  $R = \beta/\nu$  epidemic threshold
  - ▶  $R > 1$  outbreak
  - ▶  $R < 1$  localized

# SIR model vs. reality



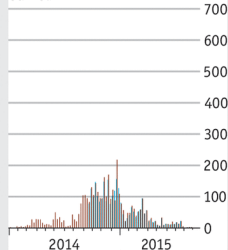
## New cases\* of Ebola infection per week

To August 23rd 2015

■ Patient database

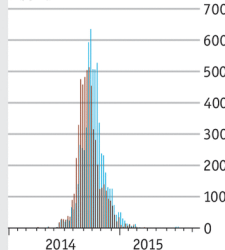
■ WHO Situation Report

Guinea



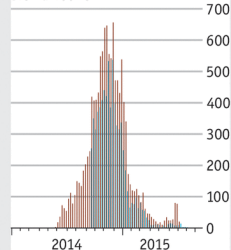
Source: WHO

Liberia



\*Confirmed and probable

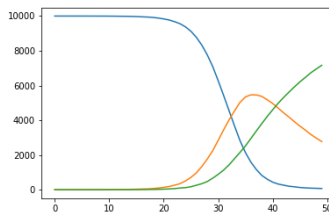
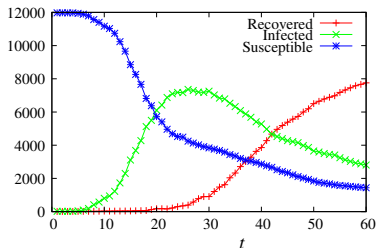
Sierra Leone†



†Patient database not published from July 5th 2015

# SIR reality vs. model

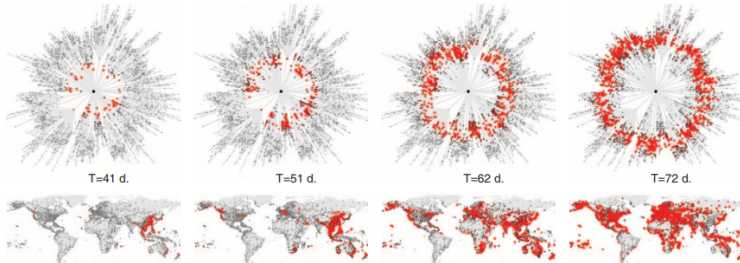
- ▶ Perfect mixing
- ▶ Everybody can meet everybody
- ▶ Covid-19, South Korea
- ▶ Susceptible approximated



# Algorithm for the SIR model

1. List of initially infected nodes is  $I$
2. Get a random (infected) node  $u$  from the list  $I$
3. For all neighbors  $w$  of  $u$  do 4.
4. If  $w$  is susceptible change it to infected with probability  $\beta$ , and enqueue it into list  $I$
5. With probability  $\nu$  change state of  $u$  to recovered otherwise put it back to  $I$
6. If  $I$  is not empty go back to 2.

# SIR on space and network



Brockmann-Helbing

# SIR and vaccination

- ▶ Epidemic threshold depends on the network:

$$\lambda_c = \beta/\nu \simeq \frac{\langle k \rangle}{\langle k^2 \rangle}$$

- ▶ where  $k$  is the degree of a node
- ▶ For lattices and random networks is finite
- ▶ For scale free networks  $P(k) \sim k^{-\gamma}$ , with  $2 < \gamma < 3$  this is infinite. Unfortunately many networks fall in this regime, e.g. transportation networks (especially flight), inside a country  $\gamma > 3$
- ▶ Vaccination: bring down  $\lambda_c$  to 1
  - ▶ Vaccinate hubs (doctors, shopkeepers, etc.)
  - ▶ Vaccinate large part of the society  $> 50\%$

# Predator prey model

- ▶  $N(t)$  number of predators
- ▶  $E(t)$  number of prey
- ▶ Model (Lotka 1925, Volterra 1926):

$$\begin{aligned}\dot{E}(t) &= \beta_E E(t) - [\mu_E N(t)] E(t) \\ \dot{N}(t) &= [\beta_N E(t)] N(t) - \mu_N N(t)\end{aligned}\tag{1}$$

- ▶ Solution  $\dot{E} = \dot{N} = 0$ :

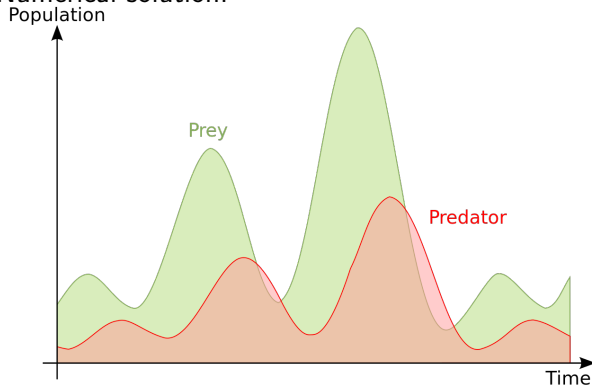
$$\begin{aligned}N &= E = 0 \\ N &= \beta_E / \mu_E, \quad E = \mu_N / \beta_N\end{aligned}\tag{2}$$

# Predator prey model

- Solution  $\dot{E} = \dot{N} = 0$ :

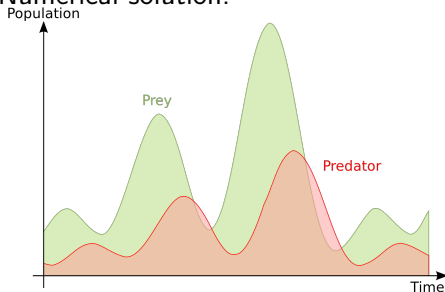
$$\begin{aligned} N &= E = 0 \\ N &= \beta_E / \mu_E, \quad E = \nu_N / \beta_N \end{aligned} \quad (3)$$

- Numerical solution:

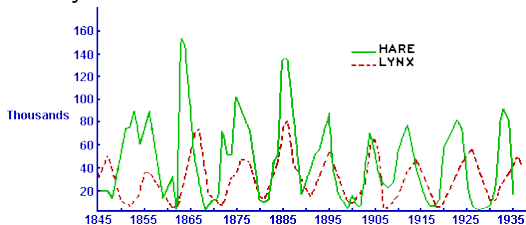


# Predator prey model

## ► Numerical solution:



## ► Reality:



# Other agent based models

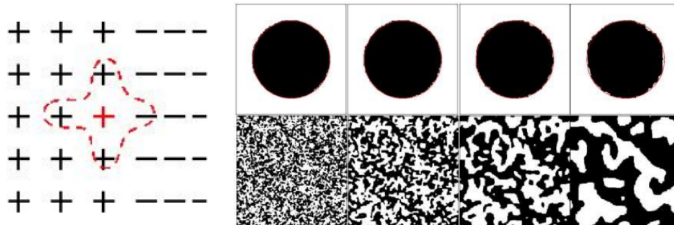
- ▶ Agents are nodes
- ▶ Interactions through links
- ▶ Any network:
  - ▶ Lattices
  - ▶ Random networks
  - ▶ Scale-free
  - ▶ Fully connected graphs
- ▶ Examples:
  - ▶ Opinion models
  - ▶ Game models

# Opinion models

- ▶ Agents have opinion  $x_i$ 
  - ▶ binary  $\pm 1$  (yes/no)
  - ▶ discrete (parties)
  - ▶ continuous (views)
  - ▶ vector (different aspects)
- ▶ Interaction with other agents
  - ▶ pairwise
  - ▶ global (with mean)

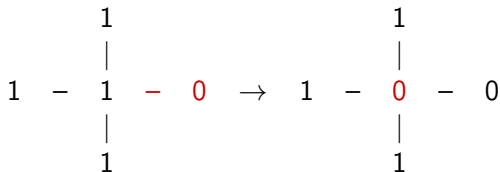
# Ising-model at $T = 0$

- ▶ Result depends on the lattice type (surface tension)
- ▶ Phase transition
- ▶ For larger systems probability to reach order goes to zero in  $d > 2$  (surface gets more important)
- ▶ Fully connected goes to order (no surface)

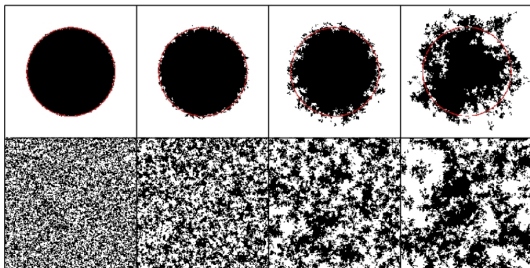


# Voter model

- Agents take opinion of random neighbor



- $d = 1, 2$  final state is consensus
- $d > 2$  final state is not consensus, but a finite system reaches consensus after a time  $\tau(N) \sim N$



# Variants

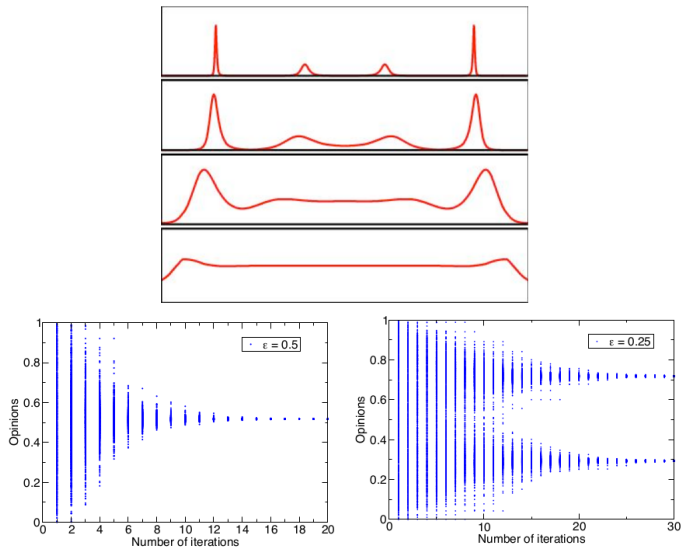
- ▶ Majority rule (with two neighbors (3 nodes) towards majority)
- ▶ Presence of zealots, i. e. agents that do not change their opinion
- ▶ Presence of contrarians
- ▶ Three opinion states with interactions only between neighboring states
- ▶ Noise (with some probability  $p$  agents change their state)
- ▶ Biased opinion in case of a tie

## Bounded confidence model: Deffuant model

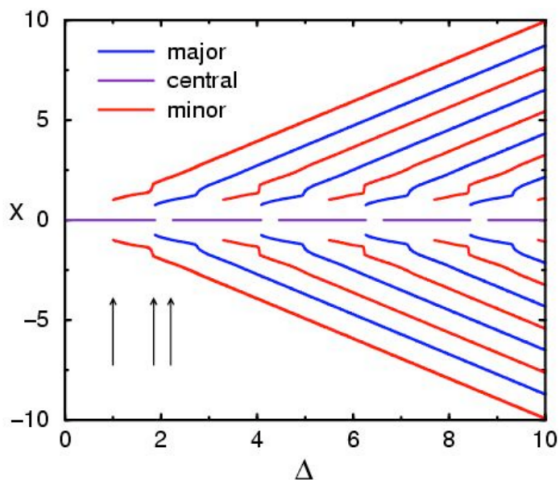
- ▶ Agents have opinion  $x_i$
- ▶ if  $|x_i(t) - x_j(t)| < \varepsilon$  then
  - ▶  $x_i(t+1) = x_i(t) - \mu[x_i(t) - x_j(t)]$
  - ▶  $x_j(t+1) = x_j(t) + \mu[x_i(t) - x_j(t)]$
- ▶  $\mu$  compromise parameter  $\mu = 1/2$  complete compromise
- ▶  $\varepsilon$  tolerance parameter
- ▶ Methods:
  - ▶ Monte-Carlo simulation
  - ▶ Master equation:

$$\frac{\partial P(x, t)}{\partial t} = \int_{|x_1 - x_2| < \varepsilon} dx_1 dx_2 P(x_1, t) P(x_2, t) \times$$
$$\times \left[ \delta \left( x - \frac{x_1 + x_2}{2} \right) - \delta(x - x_1) \right]$$

# Deffuant model: Opinion groups (fully connected graph)



## Deffuant model: Bifurcation diagram



$$\Delta = 2/\varepsilon, \mu = 1/2$$

# Flocking Model



# Flocking model

- ▶ Birds move with constant velocity ( $v_0$ )
- ▶ Align themselves to neighbors
- ▶ Some noise due to inaccurate averaging
- ▶ Differential equation

$$\theta_i(t + \Delta t) = \langle \theta(t) \rangle_{|r_i - r_j| < R} + \xi$$

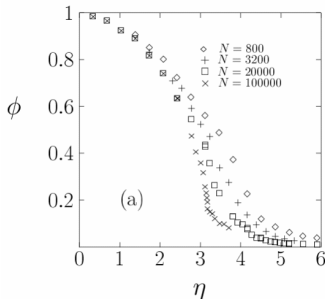
- ▶ Upgrade position:

$$r_i(t + \Delta t) = r_i(t) + v_0 e(\theta_i(t)) \Delta t$$

where  $e(\theta)$  is a unit vector in the direction of  $\theta$ .

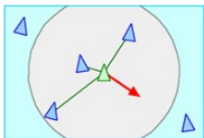
# Flocking model

- ▶ Birds move with constant velocity ( $v_0$ )
- ▶ Align themselves to neighbors
- ▶ Some noise due to inaccurate averaging
- ▶ Phase diagram 1d:

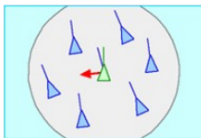


# Flocking model

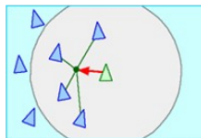
- ▶ Birds move with constant velocity ( $v_0$ )
- ▶ Align themselves to neighbors
- ▶ Some noise due to inaccurate averaging
- ▶ Non-physicist model:



**Separation:** steer to avoid crowding local flockmates



**Alignment:** steer towards the average heading of local flockmates



**Cohesion:** steer to move toward the average position of local flockmates

<http://www.red3d.com/cwr/boids/>

## Practice: SIR model

1. Create a network (random or lattice)
2. List of initially infected nodes is  $I$
3. Get a random (infected) node  $u$  from the list  $I$
4. For all neighbors  $w$  of  $u$  do 5.
5. If  $w$  is susceptible change  $w$  to infected with probability  $\beta$ , and enqueue it into list  $I$
6. With probability  $\nu$  change state of  $u$  to recovered otherwise put it back to  $I$
7. If  $I$  is not empty go back to 3.
8. Check the epidemic threshold
9. Check the effect of testing: if someone is infected with probability  $\mu$  it is discovered and all connected nodes go to quarantine for  $q$  timesteps under which they cannot be infected nor may infect