### Dynamic Ising Model: Reconstruction of Evolutionary Trees

#### INCT-SC 18-20/4/2011

Paulo Murilo Castro de Oliveira

pmco@if.uff.br

Instituto de Física, Universidade Federal Fluminense

## **One particle (confinement)**



#### One particle tied to the origin by a spring.

## **One particle (runaway)**



One particle repelled away from the origin by a anti-spring.

## **Two attracting particles**



Two particles tied to each other by a spring.

## **Two repelling particles**



Two particles repelling each other by a anti-spring.

 $E = \frac{1}{2} \sum_{i,j} J_{ij} (x_i - x_j)^2 \qquad F(x_i) = -\frac{\partial E}{\partial x_i}$ 

$$E = \frac{1}{2} \sum_{i,j} J_{ij} (x_i - x_j)^2 \qquad F(x_i) = -\frac{\partial E}{\partial x_i}$$

A distribution of positive and negative  $J_{ij}$  defines a complex and scape, peaks and valleys in the N-dimensional space.

$$E = \frac{1}{2} \sum_{i,j} J_{ij} (x_i - x_j)^2 \qquad F(x_i) = -\frac{\partial E}{\partial x_i}$$

A distribution of positive and negative  $J_{ij}$  defines a complex and scape, peaks and valleys in the N-dimensional space.

All particles start at  $x_i = 0$ , random initial velocities. The novement is traced by Molecular Dynamics (Newton's law).

$$E = \frac{1}{2} \sum_{i,j} J_{ij} (x_i - x_j)^2 \qquad F(x_i) = -\frac{\partial E}{\partial x_i}$$

A distribution of positive and negative  $J_{ij}$  defines a complex and scape, peaks and valleys in the N-dimensional space.

All particles start at  $x_i = 0$ , random initial velocities. The novement is traced by Molecular Dynamics (Newton's law).

preparation:  $\bar{x}_i(t + \Delta t) = x_i(t) + v_i(t)\Delta t + \frac{1}{2}F(x_i)\Delta t^2$ 

$$E = \frac{1}{2} \sum_{i,j} J_{ij} (x_i - x_j)^2 \qquad F(x_i) = -\frac{\partial E}{\partial x_i}$$

A distribution of positive and negative  $J_{ij}$  defines a complex and scape, peaks and valleys in the N-dimensional space.

All particles start at  $x_i = 0$ , random initial velocities. The novement is traced by Molecular Dynamics (Newton's law).

preparation: 
$$\bar{x}_i(t + \Delta t) = x_i(t) + v_i(t)\Delta t + \frac{1}{2}F(x_i)\Delta t^2$$

update: 
$$\begin{cases} x_i(t + \Delta t) = x_i(t) + v_i(t)\Delta t + \frac{1}{2}\frac{F(x_i) + F(\bar{x}_i)}{2}\Delta t^2 \\ v_i(t + \Delta t) = v_i(t) + \frac{F(x_i) + F(\bar{x}_i)}{2}\Delta t \end{cases}$$
 Verlet



## Why "Ising"?

sing (1925), most widespread model in Statistical Physics:

$$E = -\sum_{i,j} J_{ij} S_i S_j$$

where "spins" point only "up" ( $S_i = +1$ ) or "down" ( $S_i = -1$ ).

## Why "Ising"?

sing (1925), most widespread model in Statistical Physics:

$$E = -\sum_{i,j} J_{ij} S_i S_j$$

where "spins" point only "up" ( $S_i = +1$ ) or "down" ( $S_i = -1$ ).

Due to universality, many different systems can be described by this model: ferromagnetism or liquid gas ransition for  $J_{ij} > 0$ ; antiferromagnetism for  $J_{ij} < 0$  in pipartite lattices; spin glasses for both positive and negative, random  $J_{ij}$ ; and Boolean systems in general.

## Why "Ising"?

sing (1925), most widespread model in Statistical Physics:

$$E = -\sum_{i,j} J_{ij} S_i S_j$$

where "spins" point only "up" ( $S_i = +1$ ) or "down" ( $S_i = -1$ ).

Due to universality, many different systems can be described by this model: ferromagnetism or liquid gas ransition for  $J_{ij} > 0$ ; antiferromagnetism for  $J_{ij} < 0$  in pipartite lattices; spin glasses for both positive and negative, random  $J_{ij}$ ; and Boolean systems in general.

Onsager's exact solution (1944) for the thermodynamic behaviour of the uniform ferromagnet in two dimensions is a baradigmatic scientific achievement.

$$\frac{1}{2}J_{ij}(x_i - y_j)^2 = \frac{1}{2}J_{ij}x_i^2 + \frac{1}{2}J_{ij}x_j^2 - J_{ij}x_ix_j$$

"external" potential

$$\frac{1}{2}J_{ij}(x_i - y_j)^2 = \underbrace{\frac{1}{2}J_{ij}x_i^2 + \frac{1}{2}J_{ij}x_j^2}_{\text{interaction}} \underbrace{-J_{ij}x_ix_j}_{\text{interaction}}$$

"external" potential  

$$\frac{1}{2}J_{ij}(x_i - y_j)^2 = \frac{1}{2}J_{ij}x_i^2 + \frac{1}{2}J_{ij}x_j^2 - J_{ij}x_ix_j$$
interaction

The traditional <u>discrete</u> Ising model  $(-J_{\iota j} S_{\iota} S_{j})$  lacks a proper dynamics. Artificial rules based on thermodynamic equilibrium (Metropolis, etc) are generally adopted.

"external" potential  

$$\frac{1}{2}J_{ij}(x_i - y_j)^2 = \frac{1}{2}J_{ij}x_i^2 + \frac{1}{2}J_{ij}x_j^2 - J_{ij}x_ix_j$$
interaction

- The traditional <u>discrete</u> Ising model  $(-J_{ij} S_i S_j)$  lacks a proper dynamics. Artificial rules based on thermodynamic equilibrium (Metropolis, etc) are generally adopted.
- Now, the classical Newton's dynamics applies to the current continuous version.

"external" potential  

$$\frac{1}{2}J_{ij}(x_i - y_j)^2 = \frac{1}{2}J_{ij}x_i^2 + \frac{1}{2}J_{ij}x_j^2 - J_{ij}x_ix_j$$
interaction

- The traditional <u>discrete</u> Ising model  $(-J_{ij} S_i S_j)$  lacks a proper dynamics. Artificial rules based on thermodynamic equilibrium (Metropolis, etc) are generally adopted.
- Now, the classical Newton's dynamics applies to the current continuous version.
- That is why I called it Dynamic Ising Model.

## The first evolutionary tree



## The first evolutionary tree



La Phylosophie Zoologique

Lamarck (1809)

Darwin's birth year

#### Another evolutionary tree



#### **Another evolutionary tree**



 $J_{ij} = D - D_{ij}$ 

Parameter D is adjusted in between the two higher levels.

#### Rank plot, same tree



## **Tupian family, 43 languages**



Dynamic Ising Model: Reconstruction of Evolutionary Trees - p. 13/17

## Simulated tree, 63 languages



### **Measures for each real family**



#### **89 real families**



## **Our group at UFF**

# **Our group at UFF**

Suzana Moss Jorge Sá Martins Jürgen Stilck Marcio Argollo de Menezes PMCO Thadeu Penna(UFF-VR) Edgardo Brigatti (UFF-VR) Nestor Oiwa (UFF-Friburgo) Dietrich Stauffer (Köln)

# **Our group at UFF**

Suzana Moss Jorge Sá Martins Jürgen Stilck Marcio Argollo de Menezes PMCO

Gilney Zebende (UEFS) Solange Martins (UFLa) Adriano Sousa (Natal) Armando Ticona (La Paz) Karen Burgoa (UFLa) Veit Schwaemmle (Stüttgart) Klauko Mota Cinthya Chianca Carlos Eduardo Galhardo Thadeu Penna(UFF-VR) Edgardo Brigatti (UFF-VR) Nestor Oiwa (UFF-Friburgo) Dietrich Stauffer (Köln)

Nuno Crokidakis Peregrino Orahcio Felicio de Sousa Alexandre Pereira Lima Florencia Noriega Vargas Angelo Mondaine Calvão Pierre Amorim Soares Vitor Moraes Lara Marlon Ramos