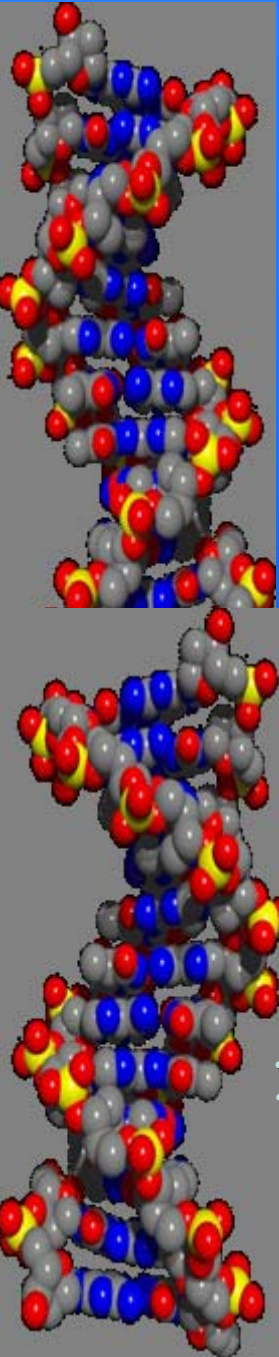


Molecular Dynamics Simulations using Intelligent Software Agents

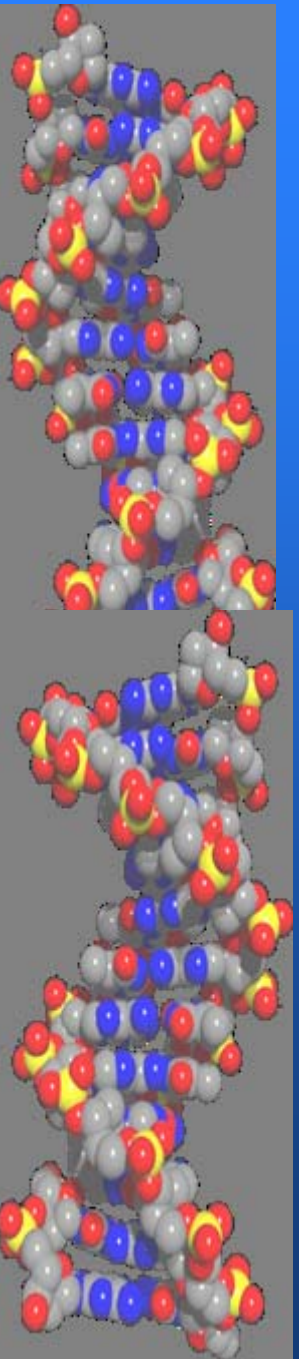
Ioanna Mprouza, Fotis Psomopoulos, Pericles Mitkas

Aristotle University of Thessaloniki
Dep. Of Electrical and Computer Engineering
Intelligent Systems and Software Engineering Lab (ISSEL)



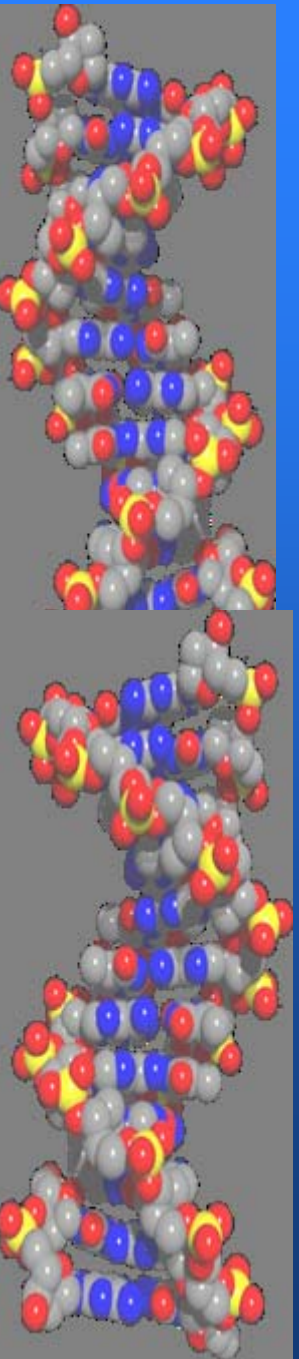
OUTLINE

- Introduction
- Problem Definition
- System Architecture
- Implementation
- Results
- Conclusions

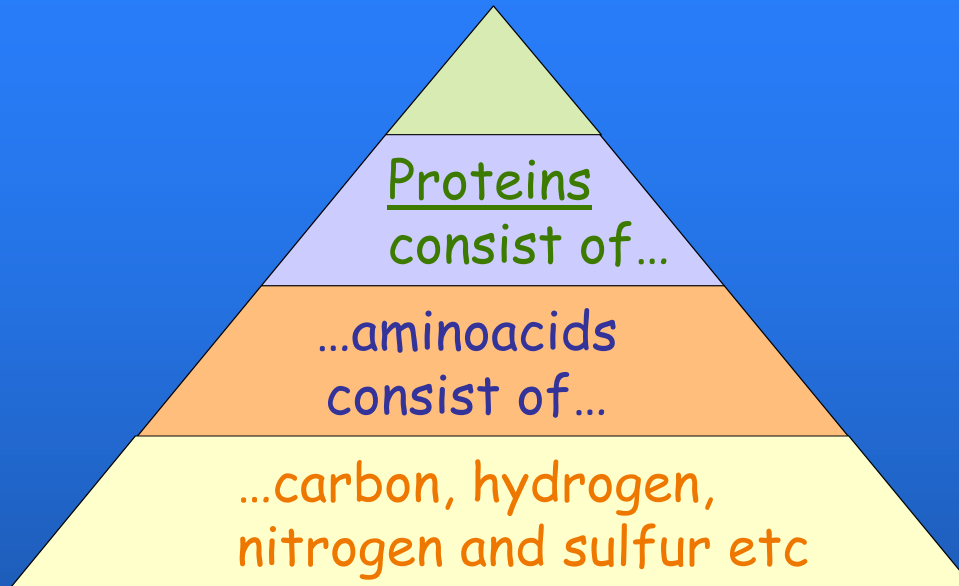


MOLECULAR DYNAMICS

- computer simulations at the atomic or molecular level
- employ numerical approaches based on
 - algorithms from computers
 - theories and concepts from:
 - mathematics
 - physics
 - chemistry
- depend on the use of force field / potential energy



PROTEINS



random conformation

ALA, GLU, GLN, ...
protein



native conformation

AGENTS??

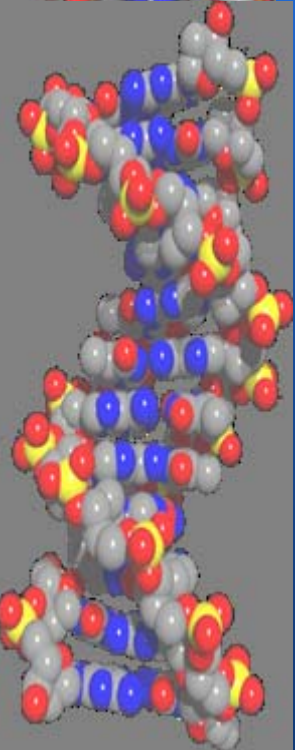
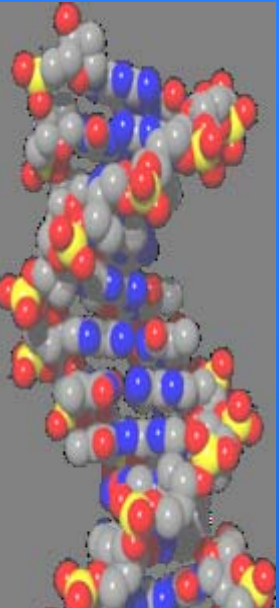
Agents are software programs or robots that:

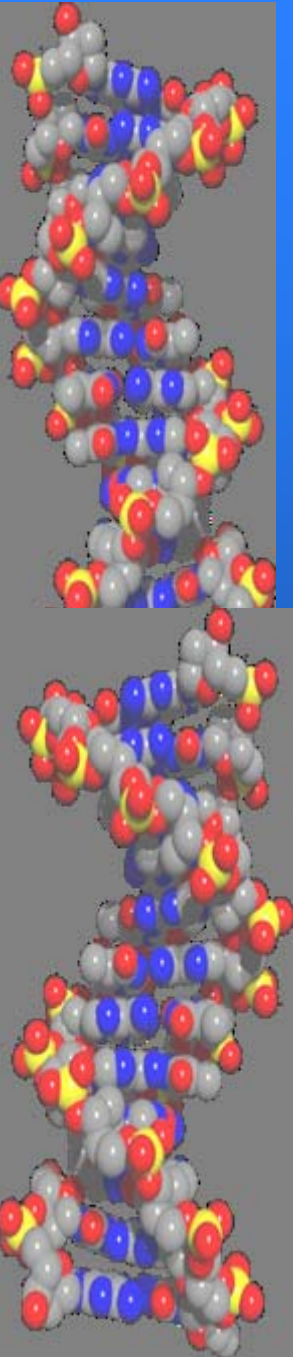
- act on behalf of a user or another program
- can activate themselves
- can adapt to their environment and modify their behavior

Such "action on behalf of" implies the authority to decide when (and if) an action is appropriate

Intelligent Agents

- autonomy
- communication
- mobility
- interaction with each other



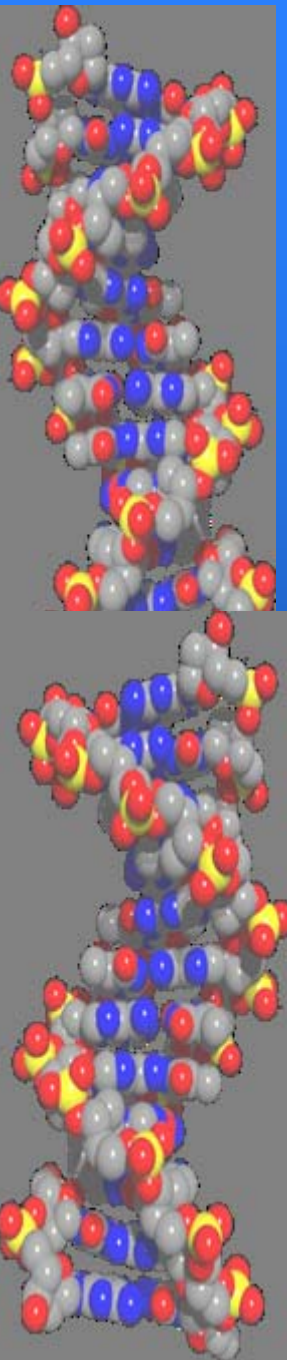


Multiagent Systems (MAS)

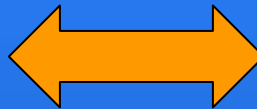
- many Intelligent Agents interact with each other.



PROTEINS AND AGENTS



Represent every Atom with an Agent



AtomAgent



The atoms that constitute the protein interact with each other



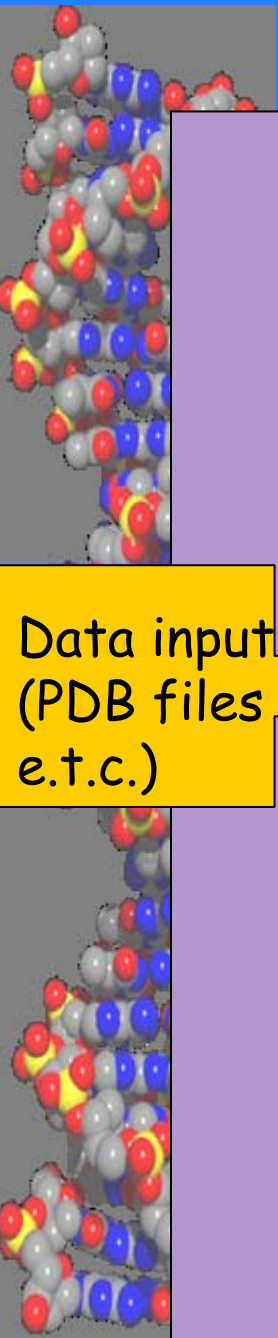
AtomAgents cooperate towards a common goal



the motion of the protein in space

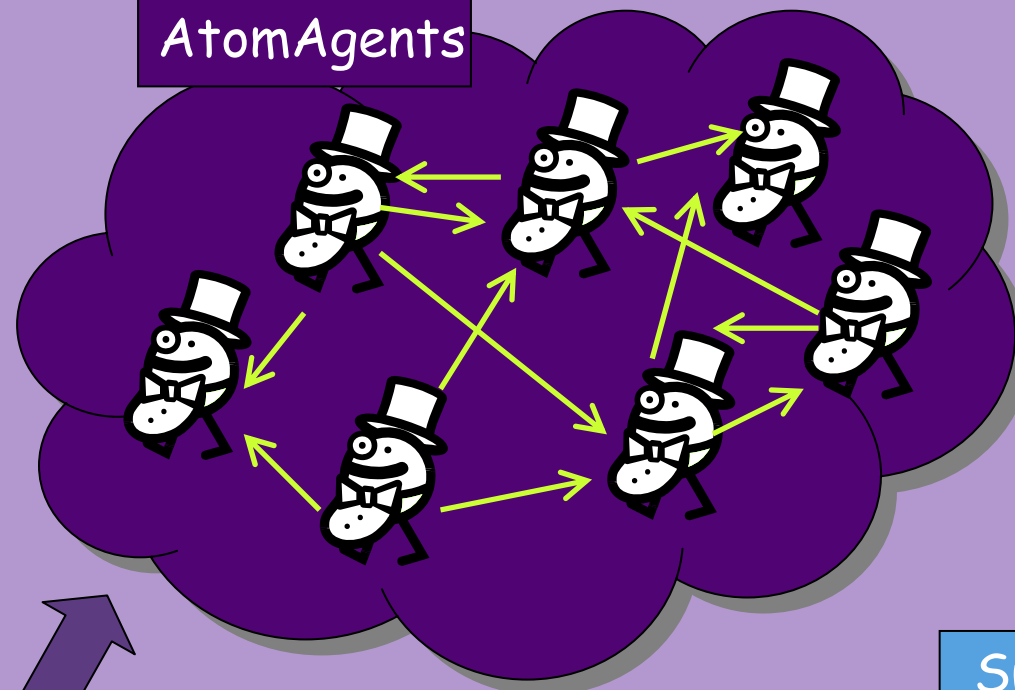
Protein is a MultiAgent System!!!

SYSTEM ARCHITECTURE (1)



Data input
(PDB files
e.t.c.)

AtomAgents

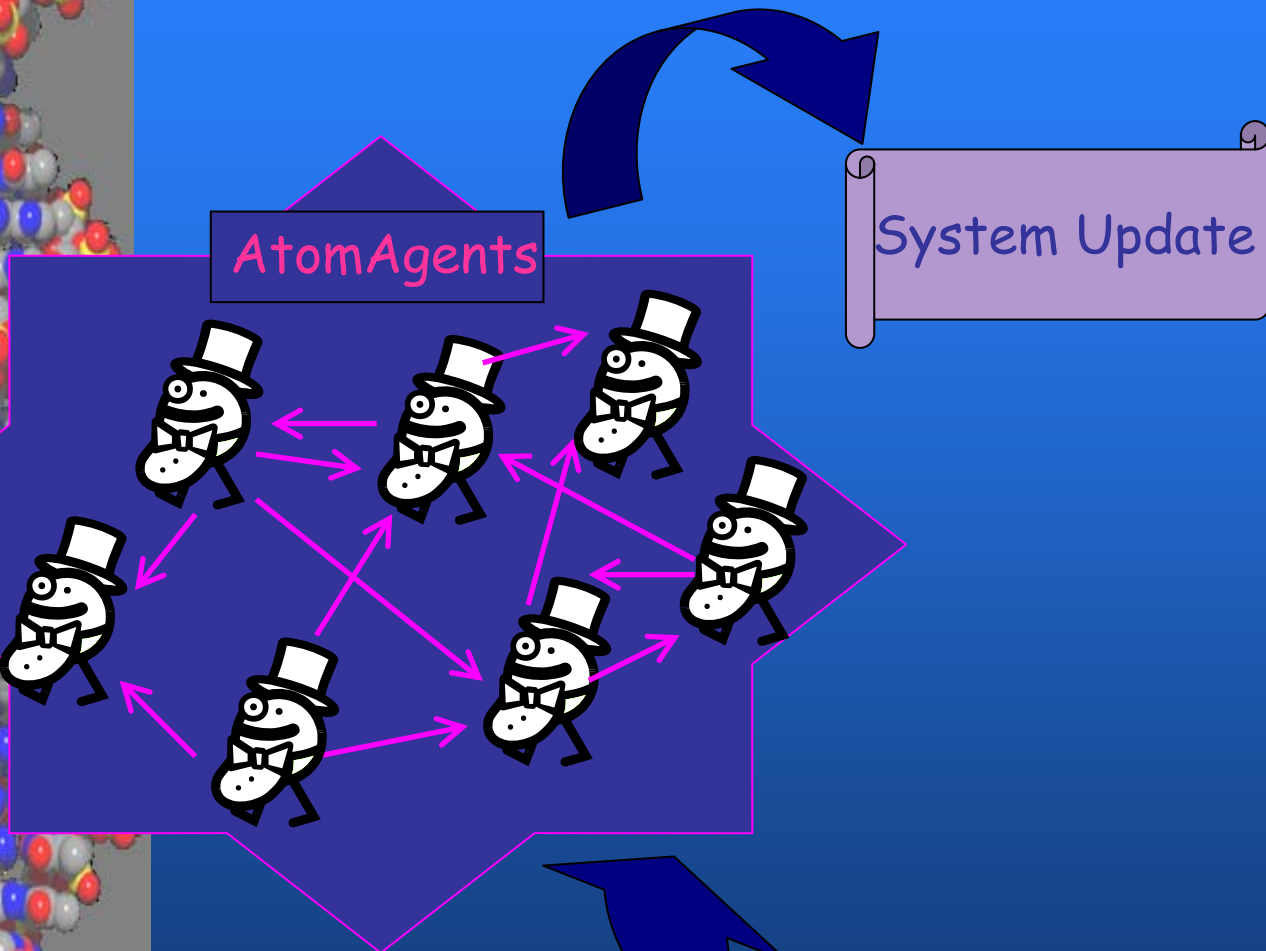
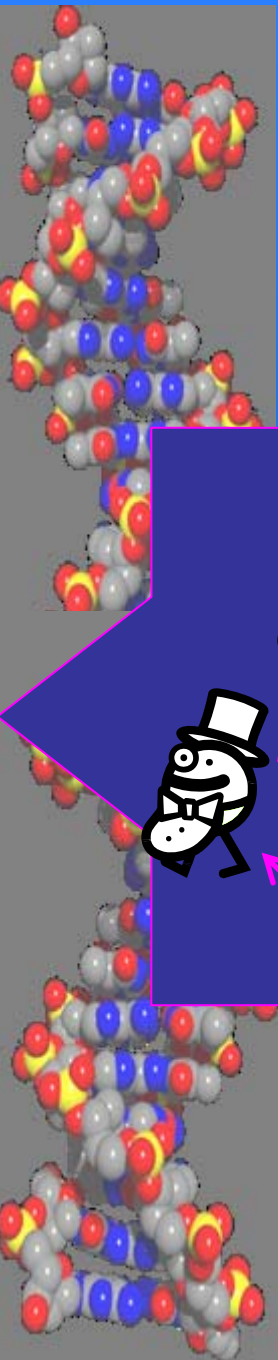


SYSTEM

coordinates, mass,
type of atom,
names,
connection with
others



SYSTEM ARCHITECTURE (2)



COORDINATOR
SuperAgent

EQUATIONS

- potential function

$$\begin{aligned}
 U = & \sum_{\text{Bonds}} K_b^i (b_i - b_0^i)^2 + \sum_{\text{Bond angles}} K_\theta^i (\theta_i - \theta_0^i)^2 \\
 & + \sum_{\text{Torsion angles}} K_\varphi^i \{1 - \cos[n^i(\varphi_i - \varphi_0^i)]\} \\
 & + \sum_{\substack{\text{Nonbonded pairs } i, j \\ \text{closer than cutoff}}} \left[A_{\text{sc}} \varepsilon^{ij} (r_0^{ij}/r_{ij})^{12} \right. \\
 & \quad \left. 2 \varepsilon^{ij} (r_0^{ij}/r_{ij})^6 - S_{\text{vdw}}^A(r_{ij}) \right] \\
 & + 332 \sum_{\substack{\text{Partial charges} \\ \text{closer than} \\ \text{cutoff}}} [q^i q^j / r_{ij} - S_{\text{els}}^A(r_{ij})]
 \end{aligned}$$

- force

$$F_i = -\partial U / \partial x_i$$

Levitt, Hirshberg, Sharon, Daggett, "Potential energy function and parameters for simulations of the molecular dynamics of proteins and nucleic acids in solution", Computer Physics Communications 91 (1995) 215-231

EQUATIONS

• Leapfrog method

$$v_{i,x}(t + h/2) = v_{i,x}(t - h/2) + ha_{i,x}(t) \quad (1)$$

$$r_{i,x}(t + h) = r_{i,x}(t) + hv_{i,x}(t + h/2) \quad (2)$$

$$v_{i,x}(t) = v_{i,x}(t - h/2) + (h/2)a_{i,x}(t) \quad (3)$$

$$v_{i,x}(t + h/2) = v_{i,x}(t) + (h/2)a_{i,x}(t) \quad (4)$$

$$r_{i,x}(t + h) = r_{i,x}(t) + hv_{i,x}(t + h/2) \quad (5)$$

$$v_{i,x}(t + h) = v_{i,x}(t + h/2) + (h/2)a_{i,x}(t + h) \quad (6)$$

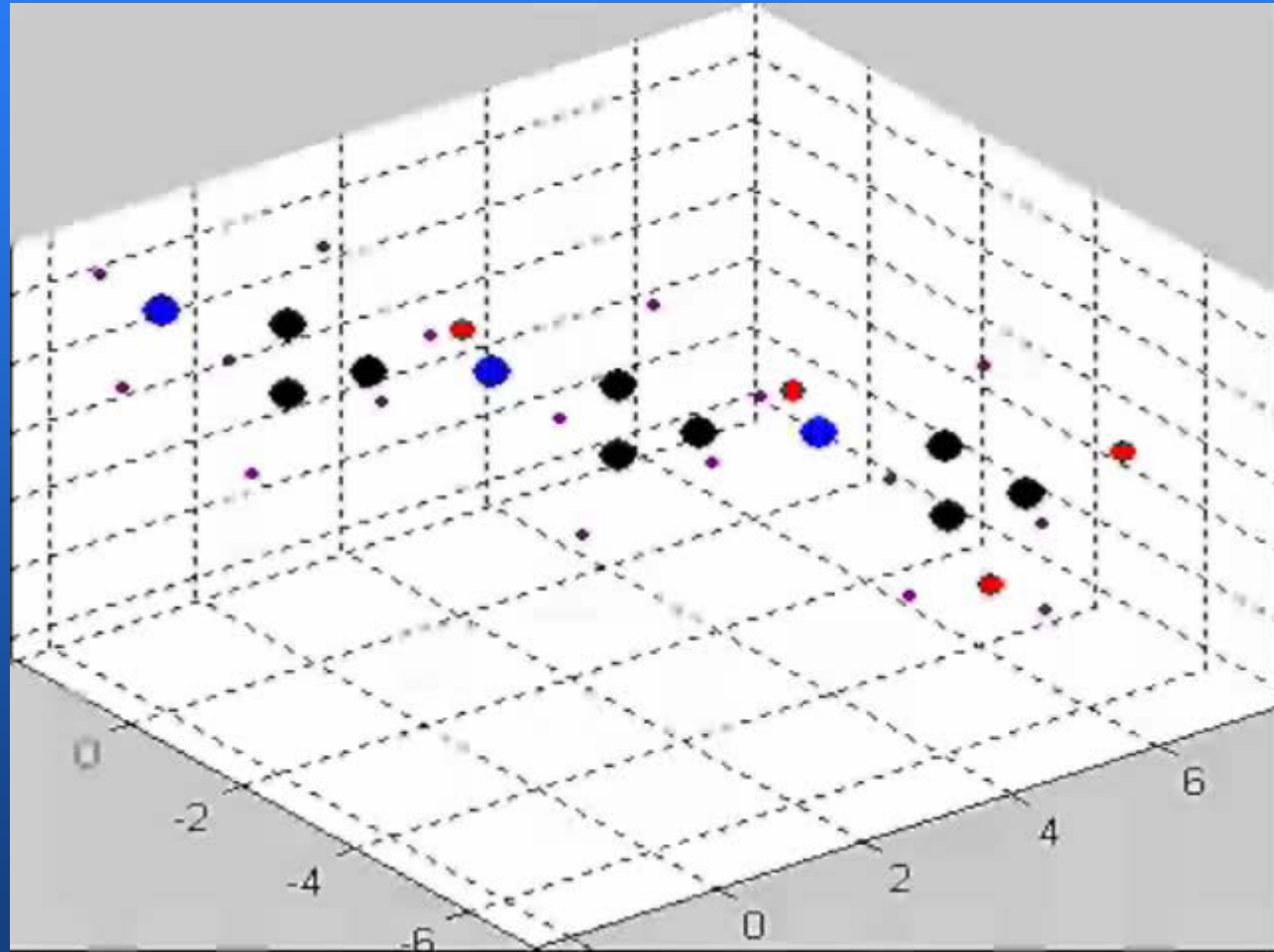
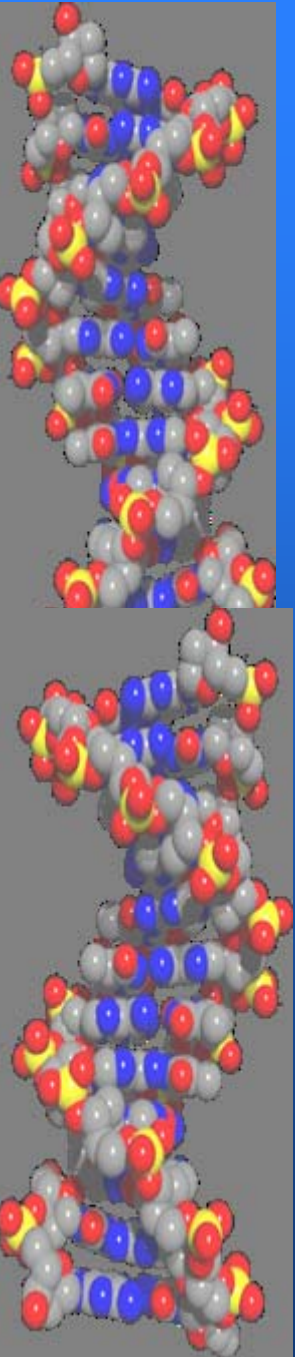
WHAT IS JADE AND HOW IS IT RELATED TO AGENTS?

JADE (Java Agent DEvelopment Framework)

- implemented in Java language
- software Framework
- library of classes
- implementation of
- multi-agent Systems
- complies with the FIPA specifications
- graphical tools

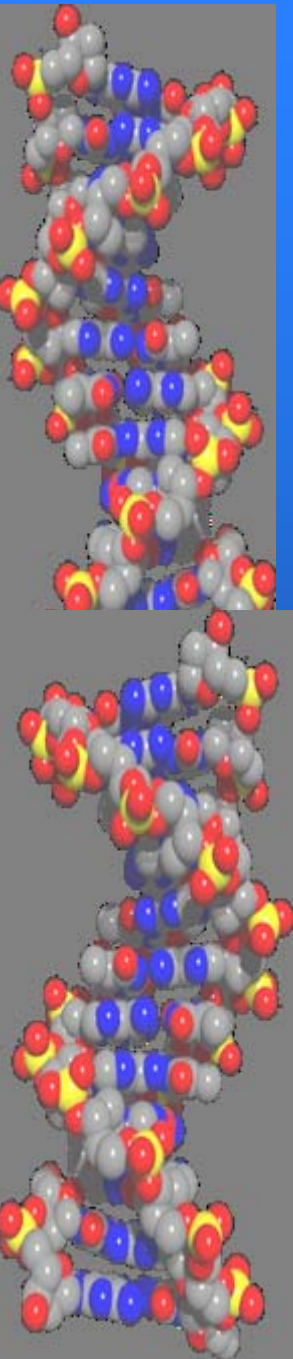
The latest version of JADE is JADE 3.5 released on 25th June 2007

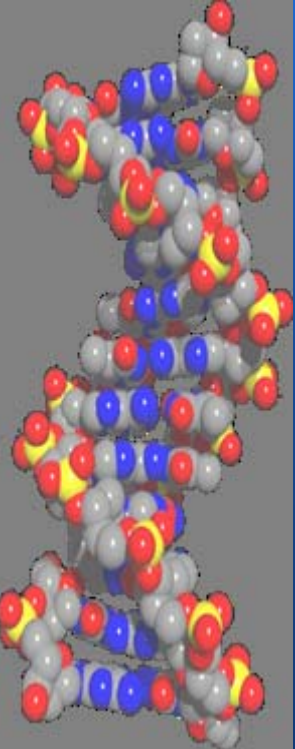
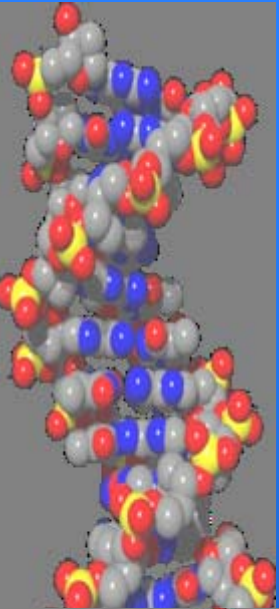
A FIRST SIMULATION



CONCLUSIONS

- We tried to combine a biological complex system, which is the motion of the protein and MAS in order to build a system that is
 - simple
 - quick
 - reliable
- The final goal is to great rules that will be used instead of potential function





THANK YOU