If we consider chemical systems, such as the crystal structure [1] or the supramolecular assembly [2] of an ensemble of molecule, a common question will arise: given N molecules, what is the lowest-energy organized structure that they can form?

This problem can be solved with the decomposition of the system in N agents.

An agent [3] is a computer system capable of exchanging information with other agents and its environment, taking decisions and performing autonomous actions (Fig.1).

Each agent can undertake one of the following actions (Fig.3):

- move to a new position on the lattice (stochastic rule);
- merge with another agent (deterministic rule);
- split into two different agents (adaptive rule).

The move of each agent resembles a Metropolis MC algorithm, with multiple attempted moves. If none of the attempted moves lowers the energy of the system, the algorithm chooses to keep the current configuration and an agent merges with the agent with which it has the largest attractive interaction.

If the energy of an agent made by several molecules is lower then the energy of the most stable agents of equal or smaller size, the agent split into two agents: in this way the rest of the agents “learn” this best arrangement.

The agent-based (AB) technique, previously used to study social phenomena, was recently applied to a chemical system [4]. With this technique a system of rigid shapes was allowed to evolve to the lowest-energy ordered structure on a 2-D lattice following a combination of stochastic, deterministic and adaptive rules with less computational effort than comparable Monte Carlo (MC) simulations (Fig.2).

The decomposition of the system into N agents, however, does not suffice to simulate the system. An agent (Fig.1) has a perception of its environment, taking decisions and performing autonomous actions (Fig.1).

An agent can be represented by a function:

\[ \text{action: } S \rightarrow A \]

where \( S = \{s_1, s_2, \ldots \} \) is the set of the environment states and \( A = \{a_1, a_2, \ldots \} \) is the set of the available actions.

This problem can be solved with the decomposition of the system in N agents.

Future Directions:

Because agents/molecules decide their move on the basis of energy calculations, an AB algorithm can be built for any molecular system for which the energy of a given configuration can be evaluated. Linking this algorithm to a molecular mechanics code (ie: Tinker, developed by J.Ponder), will allow us to compute the molecular interaction energies and model real systems [1, 2].

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