The additional particles approach for multiscale modelling of self-assembly

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THE PROBLEM

Biological system is requiring multiscale modelling, however there are no theoretical framework and trusted computational methods for that purpose. Self-assembly processes in multilevel systems are related with formation of complexes. That is why the problem of simplified mechanical analogs for modeled objects exists along with the problem of adequate complexation models.

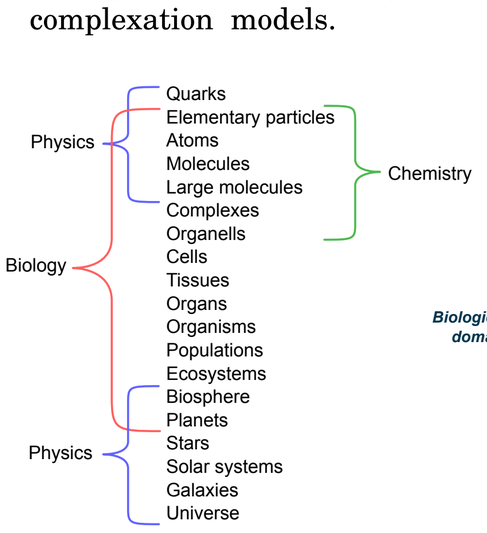

Fig. 1. Levels of organisation in different sciences [1]

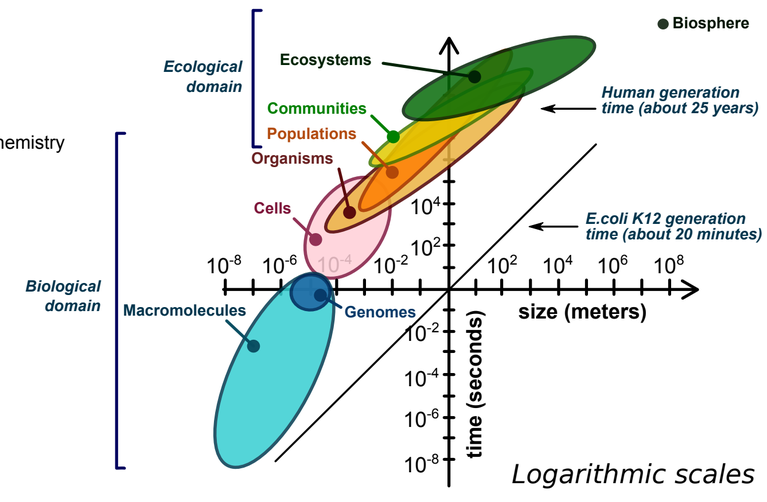

Fig. 2. Approximate relationship between characteristic times of interactions between elements of successive entities and characteristic scales of space along organisations levels [2]

In the molecular dynamics and various shape-based coarse-grain models [1] the effective potentials approach is used to parametrize formation and breaking of bonds. However there are some contraindications like entropic forces (depletion interaction and hydrophobic forces) and various mesoscopic electronic effects [2] on the supra-molecular level that are challenging for the search of the other bonds approximations. On the higher levels of organization the configuration of sub-levels can be dramatically changed during the bonding process what will make the analogy of effective potential even less credible.

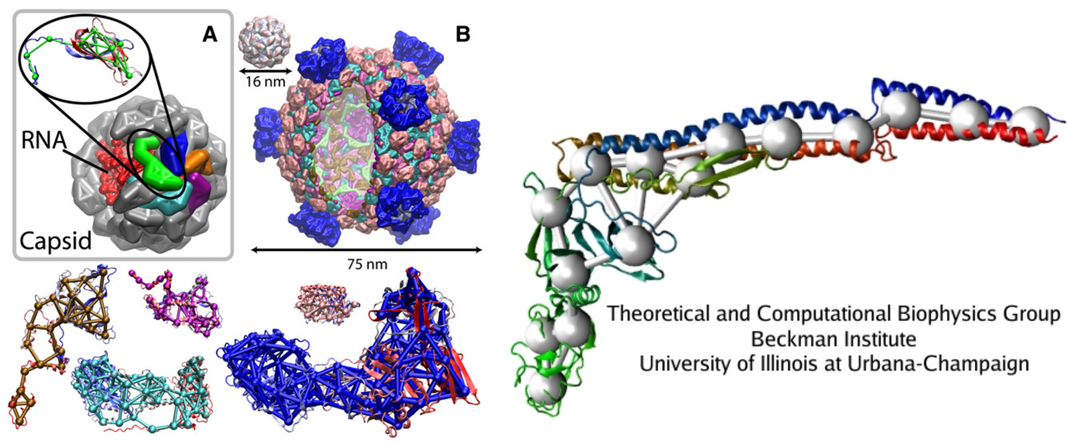

Fig. 3. Coarse-grained approach for supramolecular modelling [3]

THE SOLUTION

The scale-invariant method of additional particles for modeling bonds in self-assembly models and the theoretical frameworks for modeling multilevel systems were suggested. The formation and breaking of complexes were described by the multilevel derivative from the Langevin equation, that was called “reconstruction equation”. This equation describes evolution of system with variable amount of additional particles, which represent bonds and other new properties of complexes. Effective particles are emerging according to fixed local preconditions and forming potential for further system evolution.

For porpoise of the framework demonstration the artificial multilevel systems were generated with simple rules of properties succession from one level organization to another. The evolution of model multilevel systems were studied using Runge-Kutta-Merson numerical method in a specially developed computer application (http://levels.molpit.com). It was shown that reconstruction equations allows to study various stable periodic patterns, the dynamics of multilevel systems and the energy transfer through the levels of organization.

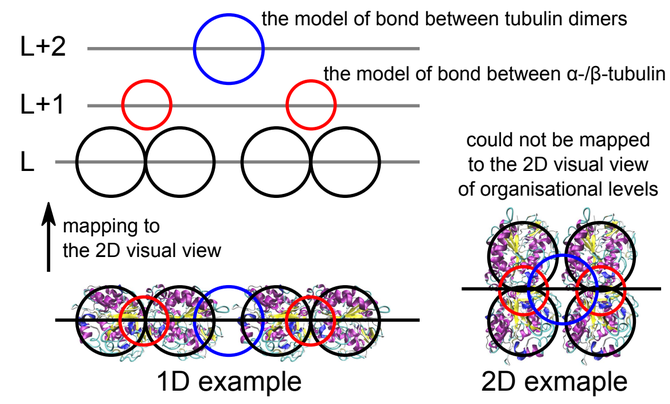

Fig. 4. Object of organisation is appearing when the distance between parent objects less threshold value

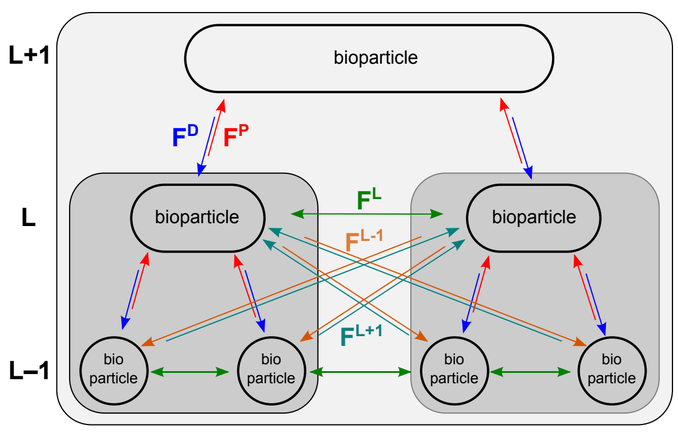

Fig. 5. Five-forces approach for describing of multi-level systems

$$m_j^i \frac{d^2 q_j^i}{dt^2} = \sum_{k \neq i} F_j^L(q_j^i, q_j^k) + \sum_{k \notin D_j^i} F_j^{L+1}(q_j^i, q_{j+1}^k)\mathcal{T}_{j+1}^k + \sum_{k \notin P_j^i} F_j^{L-1}(q_j^i, q_{j-1}^k)\mathcal{T}_{j-1}^k +$$
$$+ \sum_{k \in P_j^i} F_j^P(q_j^i, q_{j-1}^k)\mathcal{T}_{j-1}^k + \sum_{k \in D_j^i} F_j^D(q_j^i, q_{j+1}^k)\mathcal{T}_{j+1}^k - \gamma_j^i \dot{q}_j^i + \eta_j^i(t),$$

$$\mathcal{T}_j^i = \theta\left(\sum_{m,n \neq m, D_{j-1}^n \cup D_{j-1}^m = \varnothing} \sqcap\left(\frac{q_{j-1}^n - q_{j-1}^m}{2(r_{j-1}^n + r_{j-1}^m)}\right)\right)$$

Fig. 6. The equation of multi-level self-organisation. $\mathcal{T}$ — is a trigger function for switching of potentials

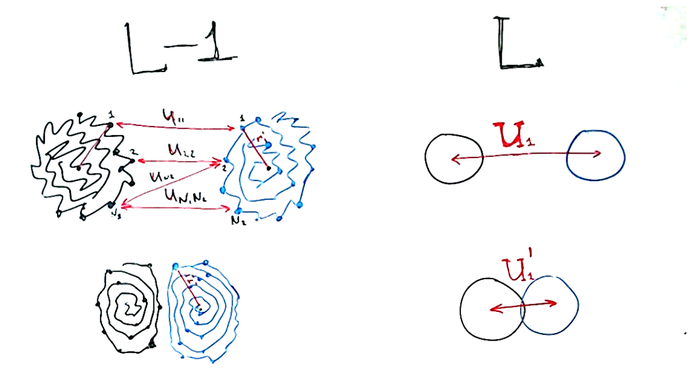

Fig. 7. The parameters that are hidden from the used mechanical analogy, lead to the changes of the potentials between model particles during the bonding process

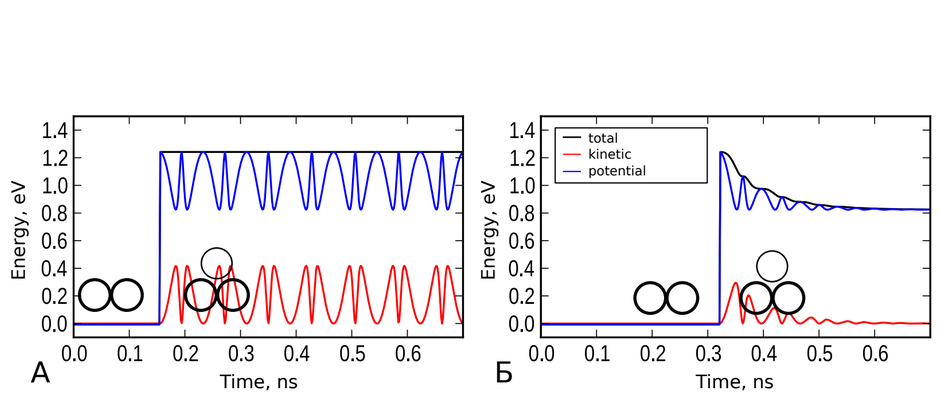

Fig. 8. The energy is skipping with appearing of new object and oscillate or decay in the case of dissipation

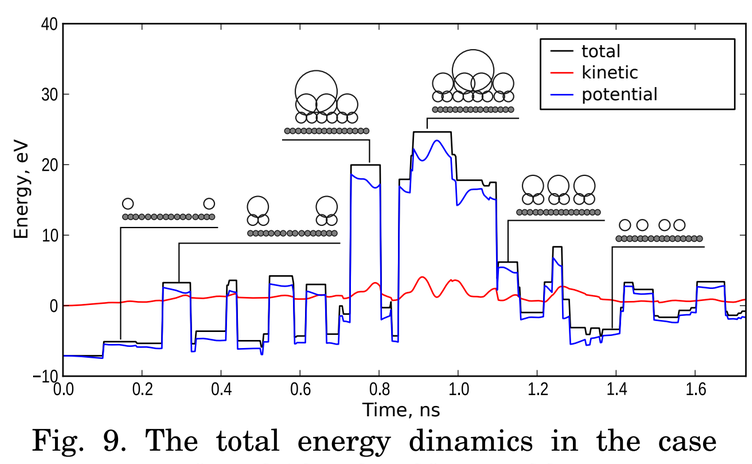

Fig. 9. The total energy dinamics in the case of multi-level self-assembly

CONCLUSION

The method of aditional particles was introduced for multiscale modelling of biological systems. The method of additional particles easier taking into account side effects for other particles in the system from the bond formation such us charge redistribution or conformational change. Suggested approach for complex formation can be used in multiscale theoretical frameworks such as coarse-grain models in a couple with effective potentials to increase accuracy of computations. The application for exploring of multi-level systems was developed (http://levels.molpit.com).

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Computations have been performed in **BlackBox Component Builder** http://blackboxframework.org
Poster prepared with the free vector graphics editor Inkscape

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