Aggregate, automate, assemble

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7 - Glossary

Molecular Dynamics

Molecular dynamics is a simulation technique in which positions of molecules are evolved over time by numerically integrating their equations of motions. These equations are based on classical mechanics and constructed using empirically derived pair-wise forces.

Topology (*molecular dynamics*)

A topology, in molecular dynamics, describes a molecule in the simulation. It contains all necessary information (*i.e.* parameters and functional forms) to calculate the forces acting on the molecule's particles based on the current conformation.

Force field

A force field describes all particle *types* available which can be used to parametrise molecules. These particle types define the parameters and functional forms used to calculate the non-bonded forces acting between particles in the simulation. In addition to the particle types a force field describes all bonded functional forms that can be used, as well as run parameters used by the molecular dynamics software, such as the time step. Finally, a force field usually describes a strategy for parametrising new molecules in such a way they are compatible with each other.

All atom

All atom force fields in molecular dynamics represent every single atom, including hydrogen atoms, as a separate particle in the simulation. For example: the CHARMM force field.

United atom

United atom force fields in molecular dynamics do not represent every single atom as a separate particle in the simulation. Instead, apolar hydrogens are grouped together with their parent carbon atom to form a single interaction site. For example: the GROMOS force field.

Coarse-grain

Coarse-graining is a technique in molecular dynamics in which multiple non-hydrogen atoms are grouped together to form a single interaction site in the simulation, also called a bead. For example: the Martini force field.

Martini

A coarse-grained molecular dynamics force field. Also a tasty cocktail made with 1 part Vermouth, 6 parts Gin and 1 or 2 olives to taste.

Supramolecular polymer

A polymer consisting of multiple molecules: the monomeric repeat units are not connected *via* covalent bonds.

Graph

A graph $G = (V, E)$ is a collection of nodes (V) connected by edges (E): $e_{ij} = (v_i, v_j) \in E$. In undirected graphs $e_{ij} = e_{ji}$. Unless specified otherwise all graphs in this thesis are undirected. The size of a graph is equal to the number of nodes: $|G| = |V|$.

Subgraph

Graph $H = (W, F)$ is a subgraph of graph $G = (V, E)$ if the following conditions hold:

$$
\begin{aligned}
&|H| < |G| \\
&W \subset V \\
&e_{ij} \in F \forall e_{ij} \in E \\
&e_{ij} \notin F \forall e_{ij} \notin E
\end{aligned}
$$

This means that all nodes in H are in G, and that nodes are connected in H if and only if they are connected in G.

Graph isomorphism

A graph isomorphism m between graphs $G = (V, E)$ and $H = (W, F)$ is a bijective mapping $m: V \mapsto W$ such that the following conditions hold:

$$
\begin{aligned}
|G| &= |H| \\
m(v) &\simeq w && \forall w \in W \\
(m(v_i), m(v_j)) &\simeq (v_i, v_j) && : (m(v_i), m(v_j)) \in F \forall (v_i, v_j) \in E
\end{aligned}
$$

This means that every node in H is mapped to exactly one node in G such that all connected nodes in H are connected in G. Note that labels on the nodes and edges, such as element or atom names, can affect the node and edge equivalence criteria.

Subgraph isomorphism

A subgraph isomorphism is as graph isomorphism, but without the constraint that $|G| = |H|$. Instead, $|H| \leq |G|$ if H is subgraph isomorphic to G.

Induced subgraph isomorphism

As subgraph isomorphism with the added constraint that equivalent nodes not connected in G are not connected in H: $(m(v_i), m(v_j)) \notin F \forall (v_i, v_j) \notin E$. We denote H being an induced subgraph of G as $H \subsetneq G$.

Maximal common induced subgraph

Also: Largest common induced subgraph.

The maximal common induced subgraph between G and H is the largest graph J such that $J \subsetneq G$ and $J \subsetneq H$. Commonly the answer is given as a mapping between G and H.