Physics > Chemical Physics

Continual Model of Medium II: Universal adaptive algorithm for triangulation of smooth molecular surface

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In the given paper the algorithm describing original and universal principles of a triangulation of a smooth molecular surface: solvent excluding solvent (SES), received by primary and secondary rolling, and solvent accessible surface (SAS) is presented. These surfaces are a boundary between molecule and solvent. Originality of the given paper consists in creation of the universal and adaptive algorithm of a triangulation. Universality of algorithm of a triangulation consists that it is suitable for not only for a surface, received by rolling and consisting of fragments of torus and sphere, but for any smooth surface, including any level surface. Adaptability of this algorithm consists in facts that the mesh size of a triangulation can vary depending on its location; reflecting even small, but smooth features of a surface; preventing "jump" to close, but not neighbor sites of the surface, excepting "cut off" of narrow necks and channels. It is reached by either decreasing triangulation lattice step to value smaller than two principal radiuses of curvature of the molecular surface or decreasing triangulation lattice step close to the active centre - closed, but not neighbor sites of the surface. The received triangulated surface can be used for the demonstration purposes in molecular editors (the algorithm is applicable for a triangulation of any smooth surface, for example, level surfaces) together with for calculation of solvation energy and its gradients for continual models of solvent.

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