

Molecular Geometry (MG) and MG Operating System: Software Engine Library for 2D- and 3D-sphere based Particle System

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Abstract: The geometry of atomic arrangement plays a critical role in understanding the structure of molecules in many fields. However, there exist no general mathematical/computational theory for the geometry of the atomic arrangement. This talk presents Molecular Geometry (MG) as the general mathematical/computational theory for the atomic arrangement accompanied by MG Operating System (MGOS) which implements the MG theory. MGOS allows the researchers to model their complicated structure problem as a geometric problem among spherical atoms in terms of elementary yet standard notions of volume, area, etc. and MGOS frees the researchers from hard and tedious work of developing and implementing the geometric algorithm so that they could focus on their primary research. MGOS is based on the Voronoi diagram of 3D spherical balls and consists of many useful callable functions in C++ language which could be embedded into user's application program. It turns out that the MG and MGOS could be applied to molecular structure problem and many other important applications such as the satellite conjunction prediction and the optimal design for 3D printing.

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