Prototyping of visualization styles of 3D scalar fields using POV-Ray rendering engine

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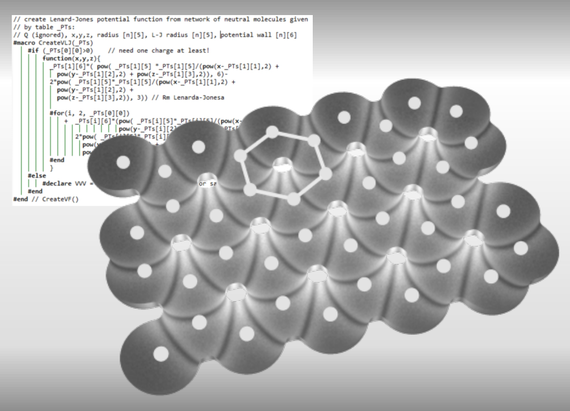
There is a persistent quest for novel methods of visualization in order to get insight into complex phenomena in scientific domains as various as physics, biomedicine or economics. Research teams involved achieved excellent results, however some problems with elaboration of novel visualization styles connected with flexibility of the software used and quality of the final images still persist.
In the paper results of inspection of four visualization styles of 3D static scalar field employing POVRay ray-tracing engine are discussed, i.e. equipotential surface method using direct implementation of isosurface{} object, cellular trilinear interpolation approach, application of texture and eventually pseudo-particles design.

All styles presented have been tested for hybrid visualizations and compared concerning computing time, informativeness and general appearance. It is shown in the work that Scene Description Language (SDL), domain specific language implemented in POV-Ray is flexible enough to use it as a tool for fast prototyping of novel visualization techniques. Visualizations discussed in the paper were computed using selected components of API of ScPovPlot3D, i.e. templates written in the SDL language.

To compare different visualization styles the same scalar field produced by selected molecular structure should be used for all tested styles. The structure chosen should obey at least two, contradictory, constraints. Firstly, it should be complex enough to reveal unknown properties, for example at boundary or in case of structural defects (e.g. lack of one of atoms). Secondly, it has to be as simple as possible to be computable in reasonable time on regular workstation. Based on these assumptions Lennard-Jones potential (often referred as L-J potential) around single layer hexagonal structure (thus referred in the paper as “graphene like”) composed from 40 neutral molecules, has been chosen. It should be mentioned, that electrostatic potential around real graphene flake is generated by electric charge distributed continuously due to the principles of the quantum mechanics and should be computed by integration over space using Coulomb’s Law.
Although in the paper electrostatic potential is taken into account conclusions remain the same for any static scalar field, e.g. tissue density restored from NMR or X-Ray DICOM images.

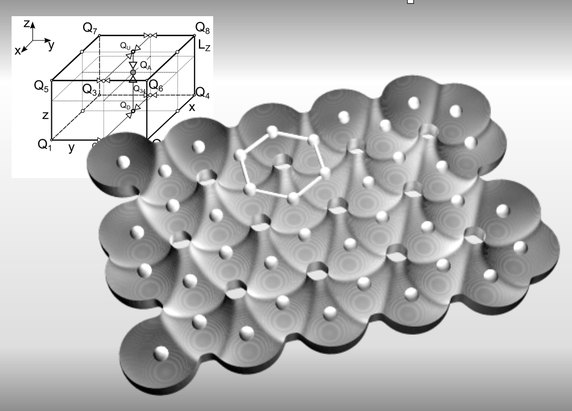
Below prototyping and search for optimal 3D visualization style of Lennard-Jones potential produced by “graphene like” flake is presented.

Isosurface - direct



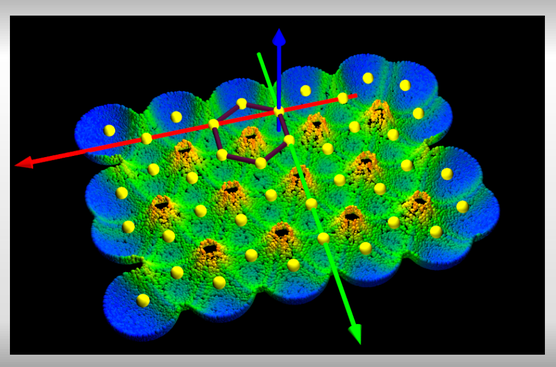
Hybrid representation of electrostatic L-J field around “graphene like” flake. Light gray circles marks “carbon” atoms, bonds of one hexagon are shown. The shape of the surface represents surface of constant potential and tint represents gradient of the potential: dark – low gradient, white-high gradient. Computation time was 1h 07m. Source: own.

Isosurface & Interpolation



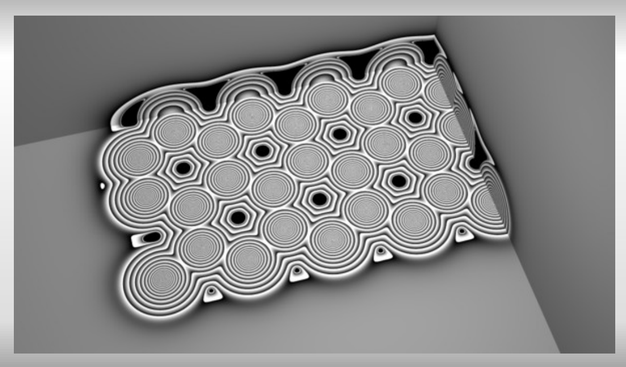
Hybrid representation of LJ potential and related gradient computed using multilinear interpolation over 300 x 150 x 60 grid of cells. The shape of the surface represents surface of constant potential and tint represents gradient of the potential: dark – low gradient, white-high gradient.
Computation time: 3h 18m. Source: own.

Random pseudoparticles

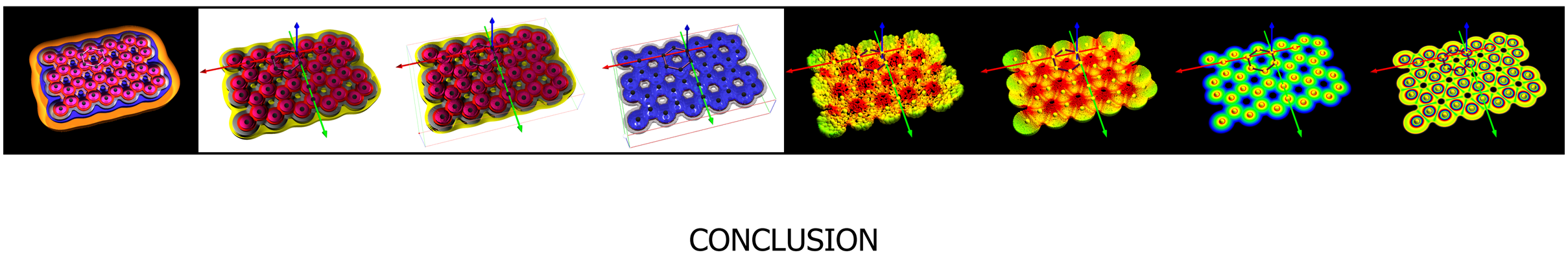


Hybrid representation of LJ potential and gradient using pseudoparticles approach employing 100'000 spheres. Due to small efficiency of drawing algorithm computation time was 4h 8m. Despite large number of spheres drawn, still same artifacts are visible. Source: own

Color maps



Color map representation of decimal logarithm of LJ potential painted on three perpendicular probe planes. BW stripes marks 10 times increase of potential value.
Computation time, 0h 2m. Source: own



CONCLUSION

High quality 3D render program equipped with efficient scripting language and supplementary API, like POV-Ray, may be used for fast prototyping of complex visualization styles.

Because of numerical efficiency problems in some cases external program should be used.

Due to relatively short computation time color map style is very well suited for fast introductory analysis of new structures.

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