Visualisation of molecules as rigid bodies

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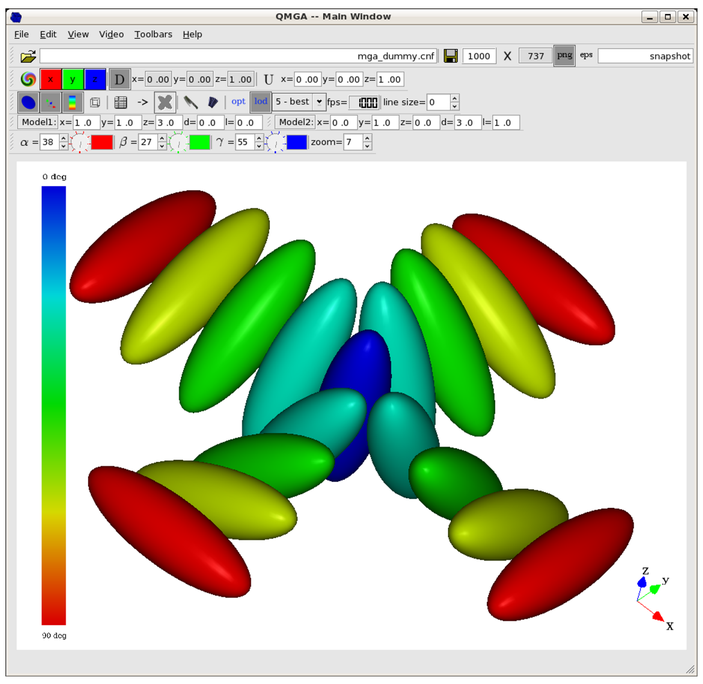
Coarse-grained modelling of molecules is often based on nonspherical convex rigid bodies like ellipsoids or spherocylinders representing groups of atoms. However, conventional molecular graphics programs are not able to visualise such objects, since they are conceived to display every single atom as a sphere, or maybe the secondary structure of a protein as a ribbon. Here we show a customised program to visualise ensembles of convex bodies in a fully rendered and interactive representation that was coded in C++ making use of the established toolkit Qt [1] for the graphic user interface. The code is distributed online as open source on SourceForge [2]. Sample graphics are presented from molecular dynamics simulations of model rodlike and platelike mesogens, with a focus on the latter, in bulk and confined inside a cylindrical nanopore.



A crucial features is coloring each molecule depending on its orientation.

Program features

Generating three dimensional pictures of molecular simulation output is useful if not mandatory for understanding the results and for presenting them in publications, talks and posters.

The following is a list of features that we deemed necessary for our visualisation program. The order in which they appear reflects to some extent their importance:

- a fully rendered view of the system
- a simplified stick representation of the system
- colour coding of each molecule
- zoom and rotation
- a convenient keyboard- and mouse-driven user interface
- folding and unfolding systems with periodic boundary conditions
- screenshot i.e. print functionality
- slicing of the system
- video functionality
- display mixtures of different objects
- adjustable lighting model
- adjustable render quality
- convenient save options

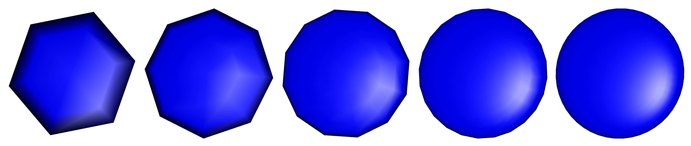
The configuration file format is conventional in molecular dynamics:

- header
  1 integer (number of molecules)
  3 doubles (unit box x, y, z side lengths)
  2 doubles (for moving boundary conditions)
- molecule information
  12 doubles ($\mathbf{r}_i, \mathbf{v}_i, \hat{\mathbf{e}}_i, \mathbf{u}_i$)
  1 or 2 integers (label, type tag; the latter optional)

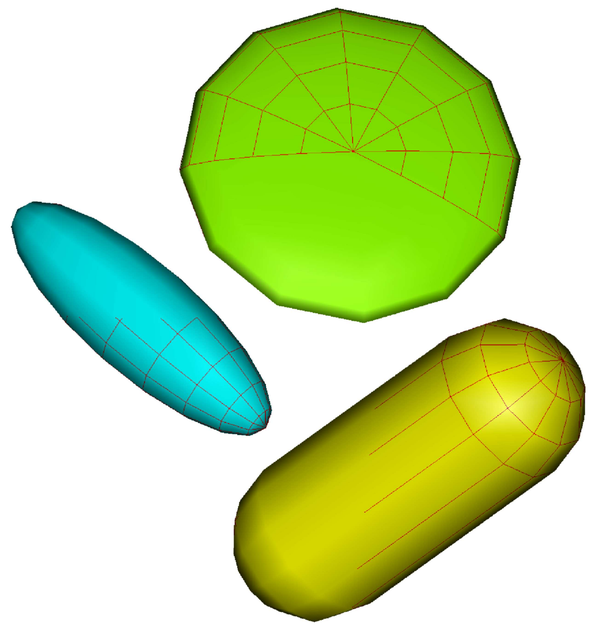
where $\mathbf{r}_i$ is the position of molecule i, $\mathbf{v}_i$ its velocity, $\hat{\mathbf{e}}_i$ its orientation and $\mathbf{u}_i$ its orientation velocity. Of these numbers, only the box sides, $\mathbf{r}_i$ and $\hat{\mathbf{e}}_i$ are used for visualisation purposes.

For example, the (artificially created) test file that results in the figure above in this column is (last four lines missing)

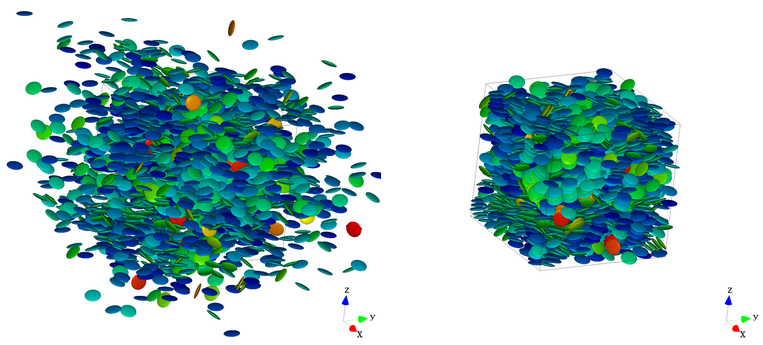
```
17
9.0
9.0
9.0
0.0 0.0
-4.0   0.0   0.0    0 0 0     0.0   1.0   0.0    0 0 0 1
-3.0   0.0   0.0    0 0 0     0.0   2.0   1.0    0 0 0 2
-2.0   0.0   0.0    0 0 0     0.0   1.0   1.0    0 0 0 3
-1.0   0.0   0.0    0 0 0     0.0   1.0   2.0    0 0 0 4
 0.0   0.0   0.0    0 0 0     0.0   0.0   1.0    0 0 0 5
 1.0   0.0   0.0    0 0 0     0.0  -1.0   2.0    0 0 0 6
 2.0   0.0   0.0    0 0 0     0.0  -1.0   1.0    0 0 0 7
 3.0   0.0   0.0    0 0 0     0.0  -2.0   1.0    0 0 0 8
 4.0   0.0   0.0    0 0 0     0.0  -1.0   0.0    0 0 0 9
 0.0  -4.0   0.0    0 0 0     1.0   0.0   0.0    0 0 0 10
 0.0  -3.0   0.0    0 0 0     2.0   0.0   1.0    0 0 0 11
 0.0  -2.0   0.0    0 0 0     1.0   0.0   1.0    0 0 0 12
 0.0  -1.0   0.0    0 0 0     1.0   0.0   2.0    0 0 0 13
```



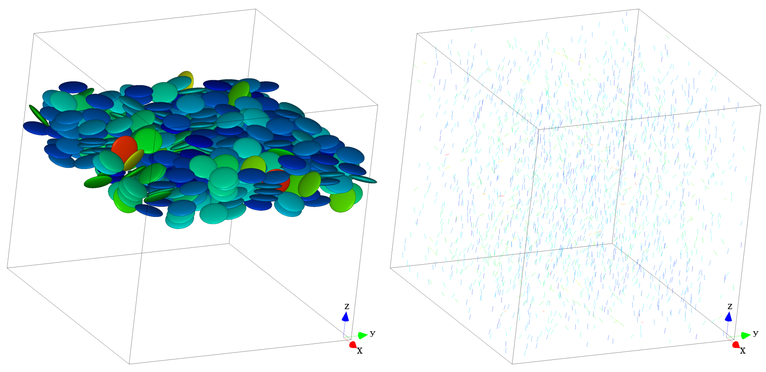
Different levels of rendering detail.



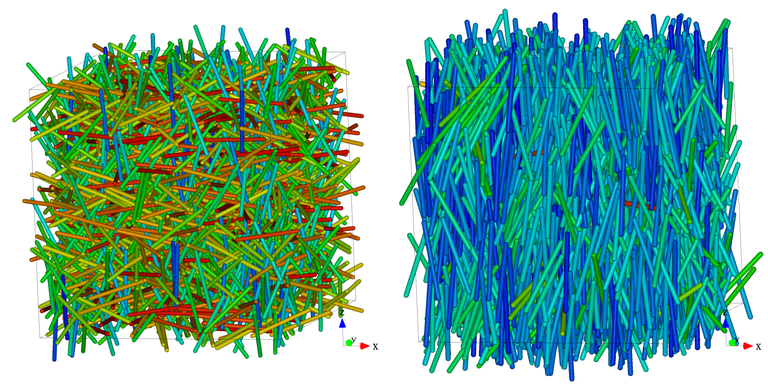
QMGA can display all common deformations of a sphere. Here we can see a prolate and an oblate ellipsoid as well as a spherocylinder. All models are partially overlayed with their wireframe for illustration purposes.



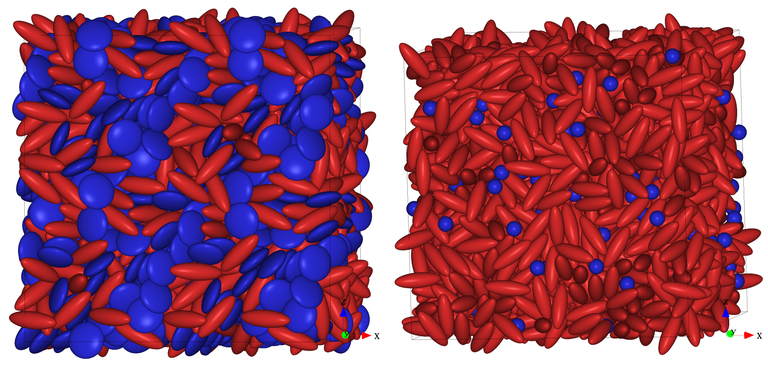
The same system with unfolded (left) and folded (right) periodic boundary conditions.



The same system again, sliced (left) and in simplified stick view (right).



Spherocylinders in an isotropic (left) and nematic (right) phase. The configurations were kindly provided by P. O'Brien, University of Warwick, UK.



Mixtures of different kinds of molecules can be shown too. The configurations were kindly provided by D. Cheung, University of Warwick, UK. There is no limit (except from hardware resources) to the number of different models that can be shown in a system.

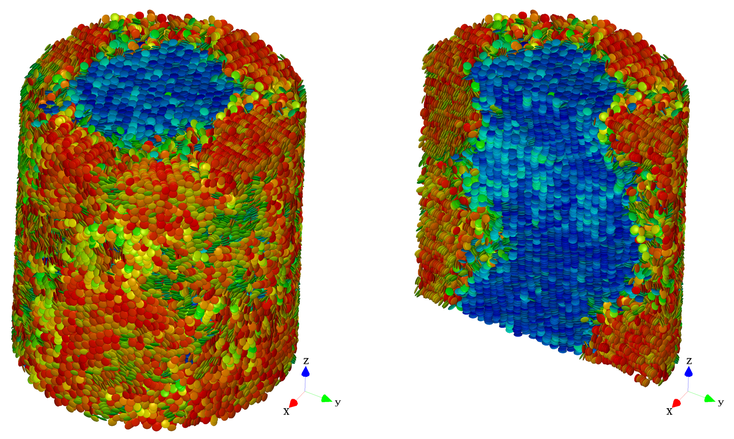
Case study: Model discotic mesogens confined inside a cylindrical nanopore

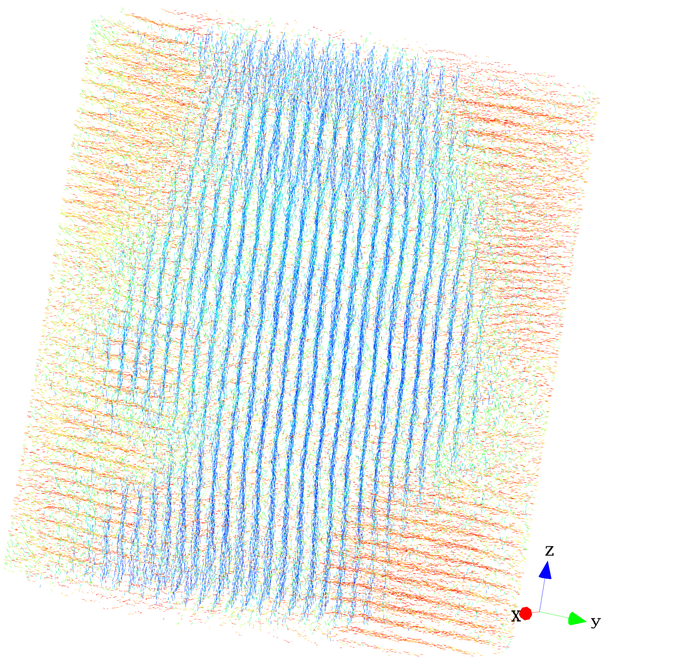
The confinement of discotic liquid crystals such as triphenylene derivatives in ordered porous templates such as alumina is a promising strategy to build organic optoelectronic devices, e.g. field-effect transistors and light-emitting diodes. There is experimental evidence that systems of this kind organise themselves in a columnar phase at the pore center, surrounded by a shell with a broad orientation distribution and planar anchoring on the pore walls [3]. Understanding the influence of the surface interaction and of the pore radius on the supramolecular architecture of the whole system has both a theoretical interest and a practical relevance for experimental work.

While there are many computer simulations of confined systems in slab geometry, simulations in cylindrical geometry are rare, and so far none of them have been performed with liquid crystals. The large amount of needed molecules rules out a description at atomic detail and makes rigid bodies more convenient. For the molecule-molecule interaction we used the Bates-Luckhurst extension of the Gay-Berne potential [4] to oblate shapes [5] with exponents $\mu = 1$, $\nu = 2$, shape anisotropy $\kappa = 0.2$ and energy anisotropy $\kappa' = 0.1$ [6]. For the molecule-surface interaction, only potentials in slab geometry have been developed so far: the integral over an infinite half-space for Lennard-Jones atoms [7] is easy and has been generalised to rodlike [8] and platelike [9] molecules, but the integral over an infinitely thick region outside a cylinder is awkward even for Lennard-Jones atoms, leading to elliptic type integrals and hypergeometric functions [10].

Though our simulations so far disregard surface curvature, they agree extraordinarily well with experimental results. Nevertheless, it is our aim to develop a specific potential for a cylindrical geometry. This should be important especially for small pores: there are experiments with diameters as little as three molecular lengths.

So far, QMGA has proved an essential tool to appreciate the results of the molecular dynamics runs of this confined core-shell system.





Slicing the nanopore or switching to stick view, it can be nicely seen that the system develops columns parallel to the cylinder axis in the middle of the confinement region.

References

[1] Qt homepage, `http://www.trolltech.de`.

[2] QMGA homepage, `http://qmga.sourceforge.net`.

[3] M. Steinhart, S. Zimmermann, P. Göring, A. K. Schaper, U. Gösele, C. Weder, J. H. Wendorff, Nano Lett. 5 (2005) 429–434.

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