CSCI596 Assignment 7: Visualizing Simulations
Due: November 13 (Mon), 2017

Part I: Molecular Dynamics Animation

Animate molecular dynamics (MD) simulation, choosing either of the following two options.

Option 1: Combine `md.c` and `atomv.c` to write a C/OpenGL program for *in situ* animation of simulation, following the lecture note on "*Visualizing Molecular Dynamics III—Animation*".

***Option 2*:** Use the VMD software (http://www.ks.uiuc.edu/Research/vmd) to post-process simulation data, following the lecture note on "*VMD Animation of Molecular Dynamics*". (For the simulation, use `lmd.c` instead of `md.c` for a better speed.)

Assignment: Demonstrate its execution on your laptop to me during the office hours.

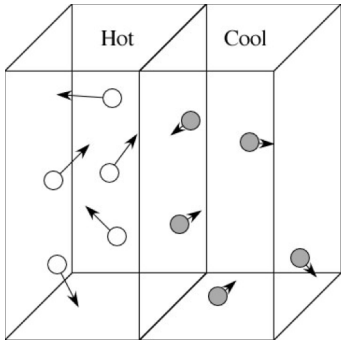
Part II: Visualizing an Electronic Wave Function

Visualize the wave function of a photo-excited hole (*i.e.*, absence of an electron) in the Gaussian-cube file, `http://cacs.usc.edu/education/cs596/src/viz/MoSe2-hole.cube`, as an isosurface, following the lecture note on "*VMD Animation of Molecular Dynamics*".

Assignment: Demonstrate its execution on your laptop to me during the office hours.

Final-Project Ideas

You may extend this assignment to your final project by adding additional features such as:



- Color-coding the atoms with their kinetic-energy values. (A nice visual demonstration of thermal equilibration may be obtained by initializing half the MD box at a high temperature and the other half at a low temperature and observing how these temperatures will equilibrate.)
- Color-coding the atoms by mapping their 3D velocities to points in the RGB color cube.
- Animate parallel MD code, `pmd.c`,[1,2] or your own application.
- How can you visualize (*e.g.*, color-code) the 3×3 stress tensor,[3-6]

$$\sigma_i^{\alpha\beta} = \frac{N}{\Omega}\left(v_i^\alpha v_i^\beta + \frac{1}{2}\sum_{j(\neq i)} r_{ij}^\alpha r_{ij}^\beta \left(-\frac{1}{r}\frac{du}{dr} \right)_{r=r_{ij}} \right) \quad (\alpha,\beta = x,y,z) \ ,$$

of the i-th atom (i = 0, ..., N-1), where N is the total number of atoms, $\Omega = L_x L_y L_z$ is the volume of the simulation box, r_{ij}^α is the α-th component of the vector $\vec{r}_{ij} = \vec{r}_i - \vec{r}_j$, and $u(r)$ is the Lennard-Jones potential function?

References

1. A. Sharma, *et al*., "Immersive and interactive exploration of billion-atom systems," *Presence: Teleoperators Virtual Env.* **12**, 85 (2003).
2. C. Zhang, *et al*., "ParaViz: a spatially decomposed parallel visualization algorithm using hierarchical visibility ordering," *Int'l J. Comput. Sci.* **1**, 407 (2007).
3. L. Hesselink, *et al*., "Research issues in vector and tensor field visualization," *IEEE Comput. Graphics Appl.* **14**, 76 (1993).
4. W. Ribarsky, *et al*., "Glyphmaker: creating customized visualizations of complex data," *IEEE Computer* **27(7)**, 57 (1994).
5. A. Sigfridsson, *et al*., "Tensor field visualisation using adaptive filtering of noise fields combined with glyph rendering," *IEEE Visualization 2002* (IEEE, 2002) p. 371.
6. C. Zhang, *et al*., "Glyph-based comparative visualization for diffusion tensor fields," *IEEE T. Vis. Comput. Graphics* **22**, 797 (2016).