CSCI596 Assignment 7: Visualizing Simulations
Due: November 5 (Fri), 2021

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*" (https://aiichironakano.github.io/cs596/Visual.pdf).

Option 2: Use the VMD software (http://www.ks.uiuc.edu/Research/vmd) to post-process simulation data, following the lecture note on "*VMD & OVITO Animation of Molecular Dynamics*" (https://aiichironakano.github.io/cs596/VMD.pdf). To simplify your task, pre-computed data file is provided as `lmd.xyz`.

Assignment: Demonstrate its execution on your laptop to me during office hours, or upload a movie file to Blackboard.

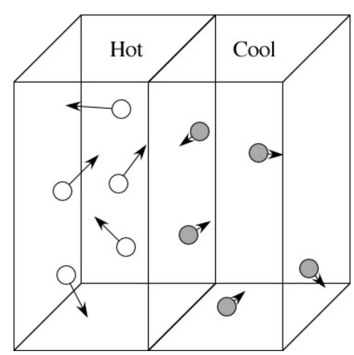
Part II: Visualizing an Electronic Wave Function

Visualize the wave function of a photo-excited hole (*i.e.*, absence of an electron) in the Gaussian-cube file, https://aiichironakano.github.io/cs596/src/viz/MoSe2-hole.cube, as an isosurface, following the lecture note on "*VMD & OVITO Visualization of Molecular Dynamics*".

Assignment: Demonstrate its execution on your laptop to me during office hours, or upload an image file to Blackboard.

Final-Project Ideas

(1) 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]

> Visualize (*e.g.*, color-code) the 3×3 stress tensor,[3-7]

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

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.

(2) Much better, visualize exciting data of your choice (*e.g.*, understanding how deep neural networks work by visualizing them).[8]

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. E. Zhang, *et al*., "Interactive tensor field design and visualization on surfaces," *IEEE Trans. Vis. Comp. Graphics* 13, 94 (2007).
7. C. Zhang, *et al*., "Glyph-based comparative visualization for diffusion tensor fields," *IEEE T. Vis. Comput. Graphics* **22**, 797 (2016).
8. J. Yosinski, *et al*., ",Understanding neural networks through deep visualization," *Proc. Int. Conf. Machine Learning, ICML* (2015).