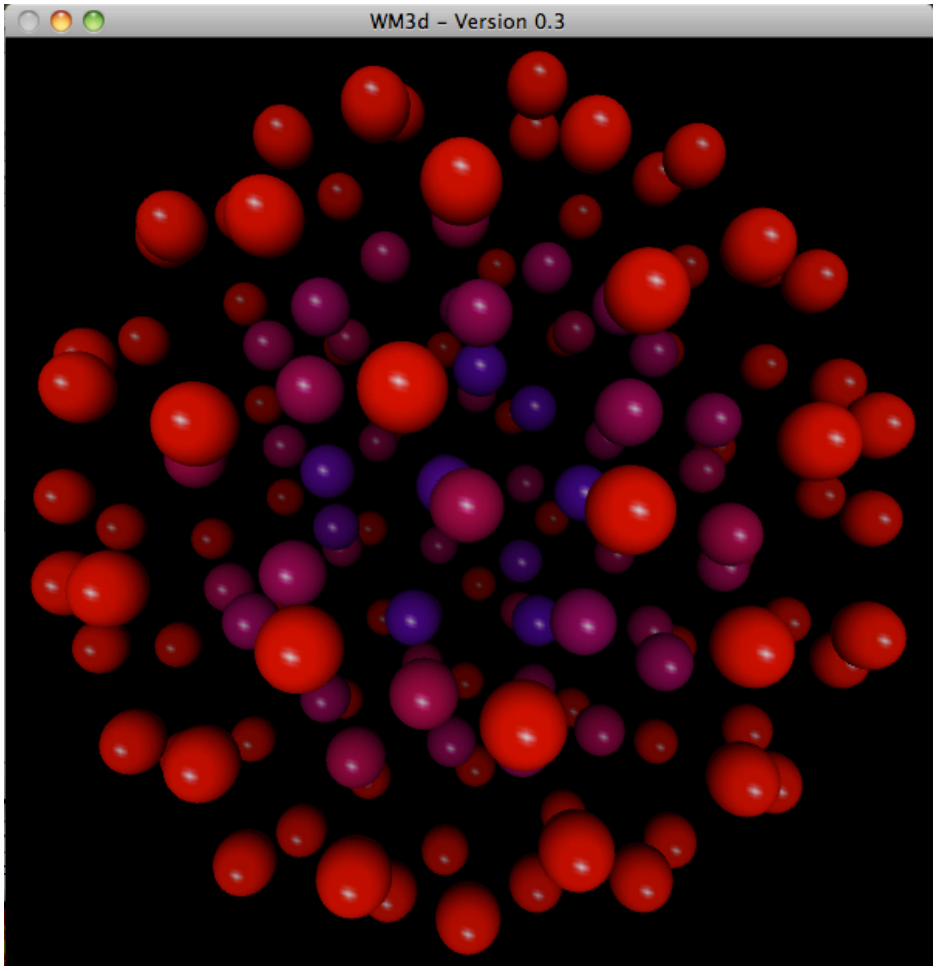
Wm3D

A real-time cluster exploration program

Wm3D is a freeware program to explore the structure of simple classical clusters such as 1D, 2D or 3D Wigner molecules of charges confined in a parabolical well under the mutual Coulomb repulsion, 3D Lennard-Jones clusters and the solutions of the Thomson problem.



The main window displays the cluster structure during its relaxation towards one of the minima of the energy landscape. For the Wigner molecule problem, a overdamped relaxation algorithm is employed, while for the Thomson and the Lennard-Jones problems a first minimization is performed via a zero-temperature Montecarlo algorithm followed by the relaxation method. In the auxiliary window, toggled with the ‘y’ key, several informations about the simulation are displayed. The molecule can be interactively rotated by clicking on it and moving the mouse. Alternatively, the keys ‘a’, ‘s’, ‘d’ and ‘w’ control the rotation. Zoom is controlled via the ‘z’ and ‘x’ keys. The simulation is restarted by pressing ‘r’. The number of particles is controlled with ‘+’ and ‘-’ (1x change) or ‘<‘ and ‘>’ (10x change). A fixed impurity can be added to the configuration by pressing ‘i’.
Several rendering options can be toggled: ‘f’ switches multisampling and ‘t’ controls the transparency. The size of the particles is controlled by ‘k’ and ‘l’, while ‘c’ toggles the colouring mode (energy-mode or flat-mode). Many of the above options can be selected via the contextual menu which can be invoked by right-clicking into the rendering window.

The keys ‘1’, ‘2’ and ‘3’ are a shortcut for the 1D, 2D and 3D Wigner molecule calculation respectively.

For feedback or comments, please contact me at fabio.cavaliere@gmail.com.