Coulomb Crystal Molecular Dynamics

Martin Bell, University of Oxford

1 Program description

The CCMD (Coulomb Crystal Molecular Dynamics) code provides a framework for performing molecular dynamics simulations of trapped ion clouds. Capabilities include:

- Simulation of microscope images for comparison with experimental data
- Ion clouds of complex compositions
- Variety of trapping potentials and radiofrequency waveforms
- Customisable ion type behaviours
- Extendable laser cooling models
- Chemical reaction simulations

A graphical user interface is supplied for 3D visualisation of the ion cloud, for optimising microscope and trap parameters and for generation of image data. Figure 1 shows a screenshot of the GUI in use.

2 Simulation details

Numerical integration of the ions' equations of motion is performed using the RESPA algorithm of Tuckerman, Berne and Martyna, which can be used to efficiently decouple the radiofrequency micromotion of the ions from their slower secular motion. The algorithm is modified to allow the inclusion of frictional forces and stochastic heating. See Refs:

1. M. Tuckerman, B. J. Berne and G. J. Martyna, *J. Chem. Phys.* **92**, 1990 (1992)
2. M. Tuckerman and B. J. Berne *J. Chem. Phys.* **95**, 4389 (1991)

The computational bottleneck for large-scale simulations of ion clouds in the strongly-correlated regime is the calculation of the long-range, many-body, Coulomb force. For large ion clouds (typically more than several thousand ions) only short integration times are possible and the inclusion of micromotion is too expensive. These problems are avoided in the current implementation using by calculating the many-body force in

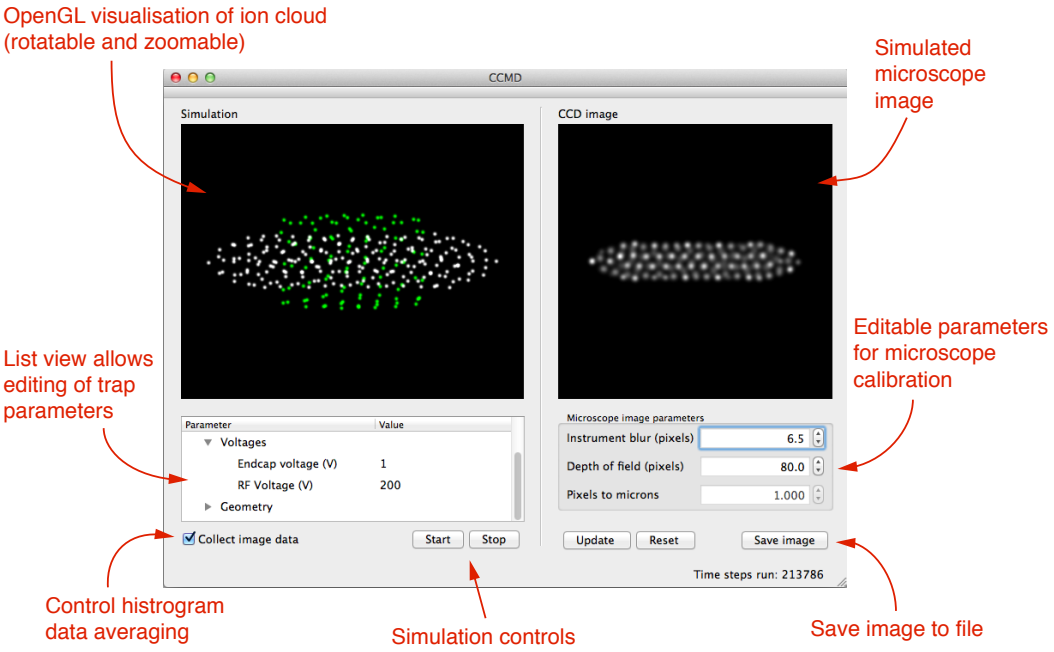

Figure 1: Screenshot of GUI showing real-time OpenGL visualisation of ion trajectories and microscope CCD image generation.

parallel using a graphics processor unit (GPU). In particular, the CUDA framework provided by NVIDIA is used to for *massively parallel* computation of the inverse-square forces, allowing speed-ups of more than an order of magnitude over typical single thread executions. Details of the CUDA framework are available at the NVIDIA website:

- http://developer.nvidia.com/

3 Requirements

Compilation of the CCMD requires the Boost library, whilst the GUI requires the Qt library and QtSDK to be installed. Use of the CUDA integrator requires a CUDA-compatible GPU to be installed along with the CUDA runtime library and CUDA-SDK.

4 Input files

In this current version, data input occurs by reading four text files in the config directory:

- `ion_types.txt`

  Definitions of the types of ion in the system based on: name, formula, mass, charge, is laser-cooled? laser-cooling parameter, is Heated?, heating parameter, colour in simulation, visibility in CCD images.

- `ion_numbers.txt`

  Composition of starting ion cloud using number of ions and formula

- `trap_config.txt`

  Trap parameters, voltages and geometry

- `integrator.txt`

  Parameters for numerical integration, currently using a RESPA-based integrator and Langevin-like single particle dynamics

5 Program structure

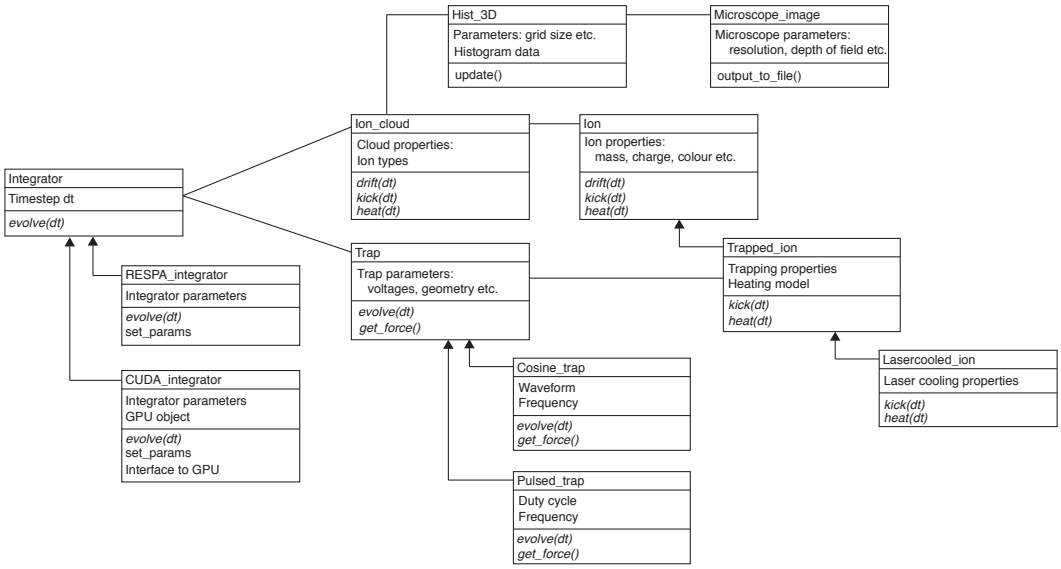

Figure 2: Diagram showing a simplified structure representing the relationships of classes used in a program to produce a simulated microscope image

6 Sample output

Figure 3 provides an example of a simulated microscope image using the experimental parameters typical for the ion trap system in Oxford.

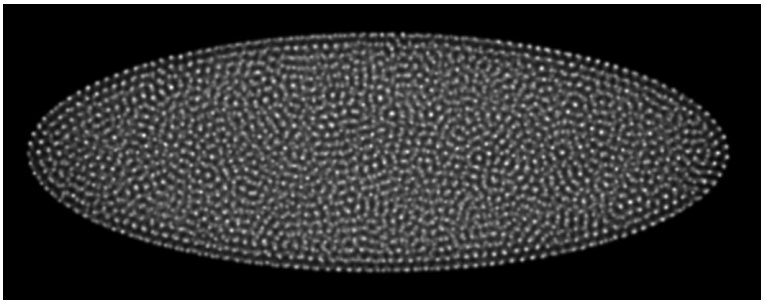

Figure 3: Example of simulated microscope fluorescence image for a Coulomb crystal consisting of 20,000 Calcium ions.

7 CUDA integrator speed-up

Illustrative data for the GPU simulation speed-up are given in Fig. 4. These simulations were performed on "tps24.chem.ox.ac.uk", which has a GeForce GT 440 GPU installed. Comparison is with single-thread execution on the 1 MHz AMD CPU.

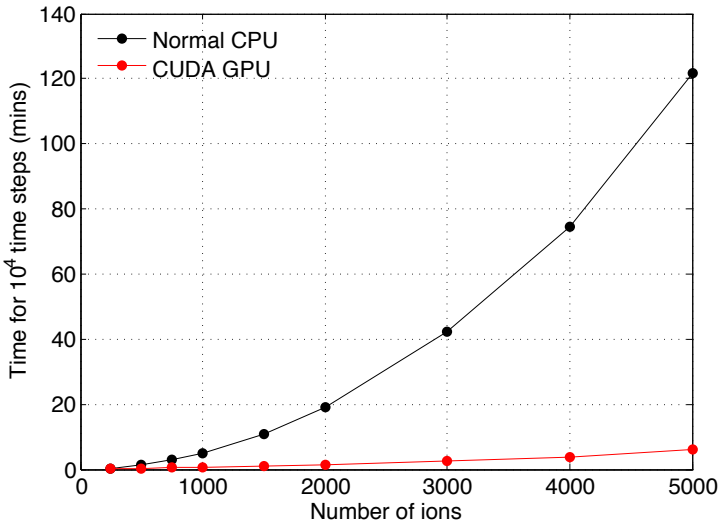

Figure 4: Speed up and scaling achievable using the CUDA-based integrator