Supplemental Online Materials

1. Quick Guide to FORCulator 3.0

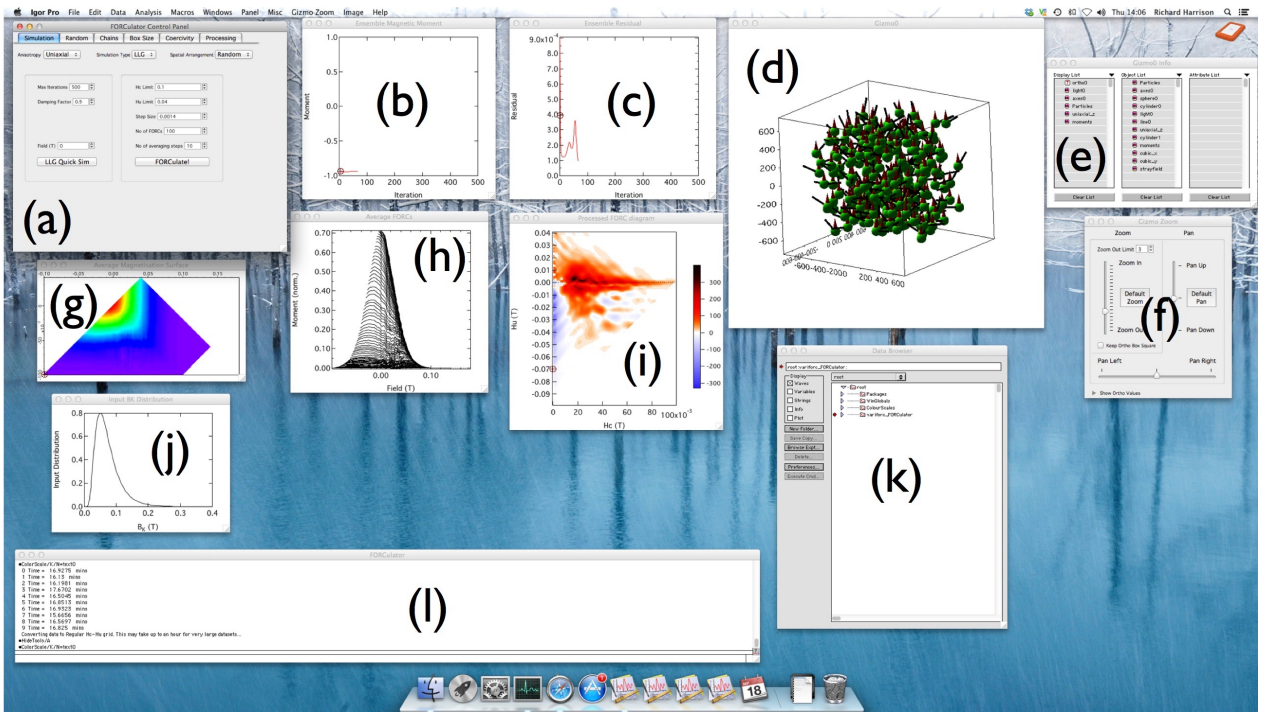
1.1 System Requirements

FORCulator is a self-contained package written using Igor Pro by WaveMetrics (www.wavemetrics.com). Although Igor Pro is a commerical package, a fully functioning demo version can be downloaded for free for Mac and Windows. This will allow you to explore FORCulator, but will not allow you to export results after 30 days. FORCulator has been written tested on a Mac running OSX v. 10.10.1 and Igor Pro version 7.02 (Build 28598). Although cross platform is usually trouble free, functionality cannot be 100% guaranteed on other systems using different software versions. It is recommended that you always use the latest version of Igor available from the WaveMetrics website.

FORCulator is processor intensive and simulations can take a long time (hours to days, depending on the parameters used and the number of repeat averaging steps required). Hence it is recommended that FORCulator is run on a desktop computer with multiple processors. All simulations presented in this paper were performed using an iMac with a 3.4 GHz Intel Quad Core i7 processor. Simulations were also tested successfully on a MacBook Pro with 2.2 GHz Intel Quad Core i7 processor and 4 GB RAM and a Mac Mini with 2.6 GHz Intel i7 processor and 16 GB RAM.

It is recommended that test runs are performed using smaller numbers of particles and fewer averaging steps before setting off longer simulations. This will allow preliminary results to be obtained in a matter of minutes, enabling the simulation parameters to be optimised.

1.2 Running FORCulator



After downloading the FORCulator.pxp file, simply double click to open it within Igor Pro. You should be presented with the FORCualtor control panel and a number of graphs, as shown in the screenshot above (window arrangement may be different if you have a different screen resolution). If not all the windows shown below are visible on your screen, go to Windows:Control:Retrieve all Windows in order to move them into visible positions. Note the screenshot above is from FORCulator 1.1, so may lack some of the newer features of version 3.0.

Windows are as follows:

a) FORCulator control panel. This panel contains multiple tabs that are used to specify all the parameters of the simulation. This panel is used to perform quick test simulations as well as set off a full FORC simulation.

b) Plot showing how the net magnetisation of the ensemble changes as a function of iteration number. This plot works only when performing quick test simulations using the "LLG Quick Sim" button. Use it to explore the convergence behaviour of the system for a given set of parameters.

c) Plot showing the average torque acting on the ensemble. Currently the simulation is considered to terminate when the average torque is less than 10^{-4}.

d) 3D (Gizmo) plot of the ensemble, showing particles (green spheres), magnetic moment vectors (red cones), stray field vectors (blue cones), uniaxial easy axes/cubic z axes (black lines), cubic x axes (red lines), and cubic y axes (blue lines). Click and drag in the window to rotate the display.

e) Gizmo display window. The left column (display list) contains those items that will appear in the 3D plot. To add an item to the display list, drag it from the middle column (object list) and drop it in the display list. To remove items from the 3D plot, select it in the display list and press the delete key.

f) Control panel allowing zooming and panning of the 3D plot (Igor 6 only).

g) Image plot of the running average magnetisation surface generated during the simulation.

h) Plot of the running average FORCs calculated during the simulation.

i) Final processed FORC diagram (calculated after simulation is finished).

j) Plot showing the input distribution of BK values (determined by the parameters in the 'coercivity' tab of the FORCulator control panel.

k) Data Browser. Red arrow should point at the FORCulator data folder.

1.3 The FORCulator control panel

1.3.1. Simulation

Anisotropy: Determines the type of anisotropy to be used in the simulations. Select either Uniaxial or Cubic <111>. Other options will be made available in future versions.

Simulation Type: Determines the method to be used to determine the magnetic configuration. SW refers to the quasi-static Stoner-Wohlfarth approach (uniaxial only). LLG refers to the approximate iterated solution to the Landau-Lifshitz-Gilbert equation. Use LLG for all but the most weakly interacting uniaxial systems.

Spatial Arrangement: Random packing, Chains, FCC and Cluster options are available. Other options will be made available in future versions (or on request).

Max Iterations: Maximum number of iterations of the LLG solver to be attempted before moving on to the next field step. Should be set to a value high enough to allow the vast majority of field steps to converge.

Damping factor: Value of the *f* factor used place moments close to the effective field. Use a value a close to $f = 1$ as possible, without producing oscillatory behaviour. Typical value is 0.9.

Field (T): Value of the applied field (parallel to the z axis of the simulation) used to perform a quick single-field calculation. Use different fields to explore hysteresis and convergence behaviour by examining plots (b) and (c).

LLG Quick Sim: Press this button to perform a quick simulation at the field specified above.

Hc limit: Specify the maximum coercivity desired for the FORC simulation.

Hu limit: Specify the upper limit of Hu for the FORC simulation.

Step size: Specify the field step size for the FORC simulation.

No of FORCs: The number of FORCs to be calculated in the simulation.

No of averaging steps: Specify the number of times the ensemble should be regenerated and its FORCs calculated in order to obtain the final averaged FORCs. For ensembles containing a small number of particles, the number of averaging steps should be increased in order to reduce noise in the final FORC diagram.

FORCulate!: Perform the FORC calculation. While the upper branch is being prepared, plots (b) and (c) will be updated (use this opportunity to double check that convergence is achieved). Once the FORC calculation proper begins, the updating will stop. After each set of FORCs is calculated, plots (g) and (h) will be updated, and the time taken to complete that set of FORCs will be printed in the command history area (l). After that the ensemble is regenerated and the process repeated the specified number of times.

1.3.2. Random

Use this tab to generate randomly packed, randomly oriented ensembles of particles.

No. of Particles: Specify the number of particles in the ensemble.

Diameter of Particles (nm): Specify the diameter of spherical particles to be generated.

Packing fraction: Specify the desired packing fraction of the ensemble. After choosing a number, press the Set Box Size button in order to automatically adjust the size of the ensemble box, based on

the specified number and size of spherical particles and the desired packing fraction. Alternatively, the box size can be specified manually.

Generate Particles: Press this button to test the parameters entered and see a 3D rendering of the ensemble in window (d). Press this button again to regenerate the ensemble.

1.3.3. Chains

Use this tab to generate random or aligned chains of particles.

Particles per chain: Specify the number of particles in each chain.

Number of chains: Specify the number of chains to be generated in the ensemble.

Diameter of Particles (nm): Specify the diameter of spherical particles to be generated.

Separation of Particles: Specify the centre-to-centre separation (in nm) of spherical particles in the chain.

Chain Collapse Factor: Specify the chain collapse factor ($0 \leq c \leq 1$). A value of $c = 0$ will generate straight chains. A value of $c = 1$ will generate the most collapsed chains.

Align easy axes with chain axis: Check this box in order to force the uniaxial easy axes (or cubic z axes) to follow a path that is tangential to the chain axis. If this is unchecked, the easy axes will be randomly generated.

Alignment vector: Specify the x, y and z components of a vector that will separate the first two particles in each chain. The vector can be specified in arbitrary relative units, and does not need to be a unit vector. For straight chains, this can be used to generate some degree of chain alignment. For collapsed chains this parameter has little effect. If a vector of 0, 0, 0 is entered, the first two particles in each chain are separated by randomly generated vectors.

Box size: Specify the size of the box into which the first particle in each chain is placed at random. Note that straight chains will typically extend far outside this box.

1.3.4. FCC

Use this tab to generate particles arranged in a face centred cubic array. This is particularly useful to generate very high packing fractions (up to 74% - the maximum value for spherical particles in contact with each other).

No of unit cells in x/y/z: An array of FCC unit cells is specified, with the given number of cells in each direction. There are 4 particles per unit cell.

Separation of particles: Centre to centre distance between particles. Set this equal to the diameter of the particles in order to make spheres in contact.

Fractional occupancy: Set to a value less that 1 in order to generate particle ‘vacancies’ in the close packed lattice.

1.3.5. *Clusters*

Use this tab to generate distributed small clusters of particles.

Particles per cluster: Specify the number of particles in each cluster

Number of clusters: Specify the number of individual clusters to be distributed inside the box.

Intra-particle packing fraction: Specify the packing fraction for particles within a cluster.

1.3.4. Coercivity

Alpha and Beta: Specify the parameters defining the log-normal input distribution of *intrinsic switching fields*. Alpha and beta parameters are defined according to Eqn. 15 in the FORCulator paper.

User Defined Coercivity: Click this box if you want to specify your own *coercivity* distribution (e.g. a coercivity distribution extracted from an experimental FORC diagram). You will need specify separate wave for the field values and the corresponding coercivity distribution. Note that coercivities are converted into corresponding intrinsic switching fields assuming uniaxial Stoner-Wohlfarth behaviour and the angle that each particle makes to the applied field. Only use this option if you are confident that this conversion between coercivity and switching field is appropriate for your system (e.g. **DO NOT USE** in conjunction with the Cubic Anisotropy option, as this conversion only applies to uniaxial systems).

1.3.5 Processing

Use this tab to format the simulation data, ready to be processed using the in-built FORCinel 3.0 software.

Format simulation data: Click this button and enter a name for the resulting data folder where the results will be stored. The simulation data will be formatted and stored in a standard FORCinel folder, ready to be processed and displayed in the same way you would for any experimental FORC diagram. Use the FORC Control Panel or the FORCinel menu to process and display your data.