

Connection Inspector:

The *Connection Inspector* contains the following options for use with connections:

Creating/Removing and Browsing the current Connections:

paste_56.tiff ↵

The *New Connection* button creates and adds another connection to the current list of connections and displays its default parameter settings. The user can create as many connections as possible within the memory limits of the machine.

The *Delete Connection* button deletes the current connection whose attributes are currently being displayed. If no more connections exist because of this action, certain buttons will become disabled until the *New Connection* button again creates a connection.

The arrow buttons allow the user to browse the connections and to change the currently displayed connection. When the arrows try to move before the first connection or after the last connection, the Inspector wraps around and displays the beginning or end of the list of connections.

Connection Attributes:

paste_57.tiff ↵ paste_0.tiff ↵

When a connection is created, the user may change the type of connection to be either a spring or a Lennard-Jones potential between the two attachments. The default type is a spring.

paste_59.tiff ↵

Each connection needs two endpoints to specify its extent. Each of the endpoints could be fixed points in the coordinate system or particles. The user chooses the attachment type using the pop-up lists. When the attachment is a fixed point, the fields specifying its position are editable and can be set. When the attachment is a particle, the fields display the initial position of that particle and cannot be edited here. If the initial position of the particle is not satisfactory, then the user can change the particle's initial position in the *Particle Inspector* only.

paste_60.tiff ↵

This field displays the current length of the connection given its attachments. When an attachment is changed, the initial length field will automatically be updated.

paste_61.tiff ↵

The color of a connection may be set by dragging in a new color using the *Color Panel* found in the *Tools* menu. The default color is light gray.

paste_62.tiff ↵

Even though a connection has a specified color, the user may choose to turn off the displaying of a connection by using the display connection: switch button. The default is to display the connection.

Spring attributes:

paste_63.tiff ↪ paste_64.tiff ↪

A spring type connection may be given a spring constant (k), a damping coefficient (c), and an unstretched length (x_0) which specify the force function which the spring imparts on its connections: $F(x) = -k(x-x_0) - c v$, where x is the length of the spring, x_0 is the unstretched length of the spring, and v is the net relative velocity of the attachments in the direction of the spring's extent.

Lennard-Jones potential attributes:

paste_3.tiff ↪

A Lennard-Jones potential connection is a potential used in molecular dynamics to simulate the interaction of electrically neutral atoms (Gould and Tobochnik, *An Introduction to Computer Simulation Methods: Applications to Physical Systems Part 1*, Addison-Wesley, Reading, 1988, Ch. 6).

paste_4.eps –

The Lennard-Jones potential is parameterized by a "length" σ and an "energy" ε . At $r = \sigma$, $V(r) = 0$. The parameter ε is the depth of the potential at the minimum of $V(r)$, and the minimum occurs at a separation $r = 2^{1/6} \sigma$. $V(r)$ is essentially zero for $r > 2.5\sigma$. The parameters ε and σ are expressed in units of 10^{-16} ergs and angstroms, respectively.

The *OK* button accepts all of the recent changes made to the current connection, reinitializes the simulation and closes the *Connection Inspector* panel.