

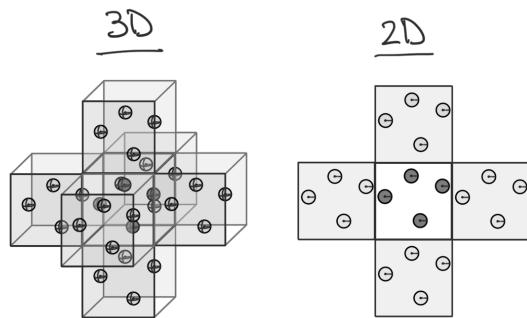
Shearing

Once you have created a system, we can apply flow and study the rheology, deformation, and particle structure.

A simple way to create flow is with a drag flow (e.g. Couette flow) using Lees-Edwards boundary conditions.

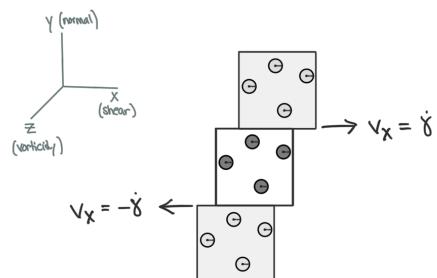
Lees-Edwards Boundary Conditions

Our DPD simulations use periodic boundary conditions to avoid wall effects and to generalize our system as one small region of a much larger (uniform) colloid-solvent system (e.g. a suspension, gel, crystal, etc.). This means that the system interacts across its boundaries with duplicate images of itself in all directions.

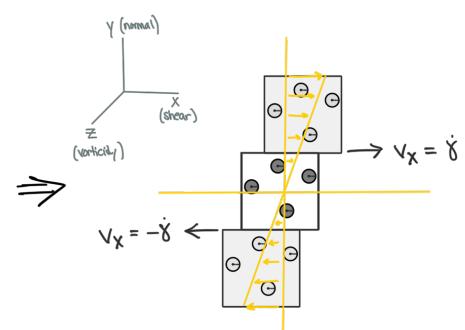
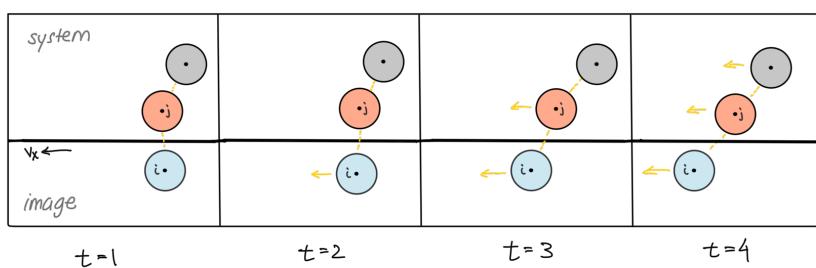


Therefore, to apply shear flow in a particular direction (the shear direction) we can just drag the normal-direction images in that direction across the system.

For example, we usually apply shear flow in the x -direction by dragging the y -images in opposite directions at the chosen shear rate ($\dot{\gamma}$), applying a shearing velocity at the top and bottom boundaries.



This velocity is propagated through the system by the interparticle pair interactions calculated at each timestep, creating the correct velocity profile.

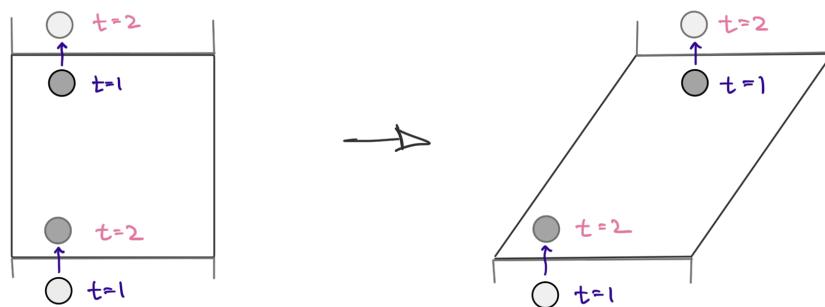


Box Tilting

What does this look like to the system? Essentially we deform the simulation box by a "tilt factor" theta. For shear in the x-direction and an xy tilt factor this looks like



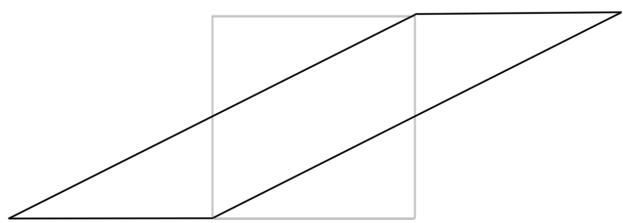
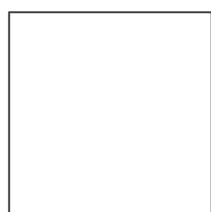
and automatically accounts for the change in position of any particle that crosses the y-boundaries without any nasty math.



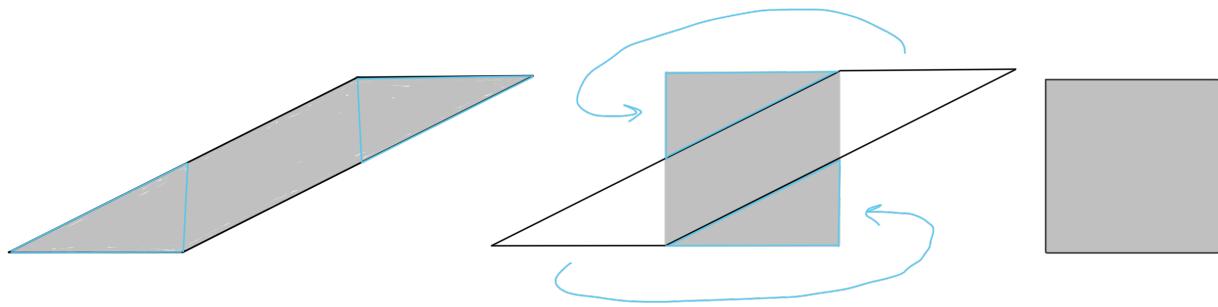
Box tilting is a common method of applying flow in molecular dynamics (MD) simulations, but we have to make some changes to how the box is rescaled (turning off a particle scaling step) to make sure we can retain all the information about a particle's interacting pairs when it crosses a simulation boundary.

We can then use the built in Box Resizer to tilt the box from

xy tilt factor theta=0 to xy tilt factor theta=1



acquire the sheared particles new positions relative to the tilted box, and then wrap those positions back into a cube and reset theta for the next step.

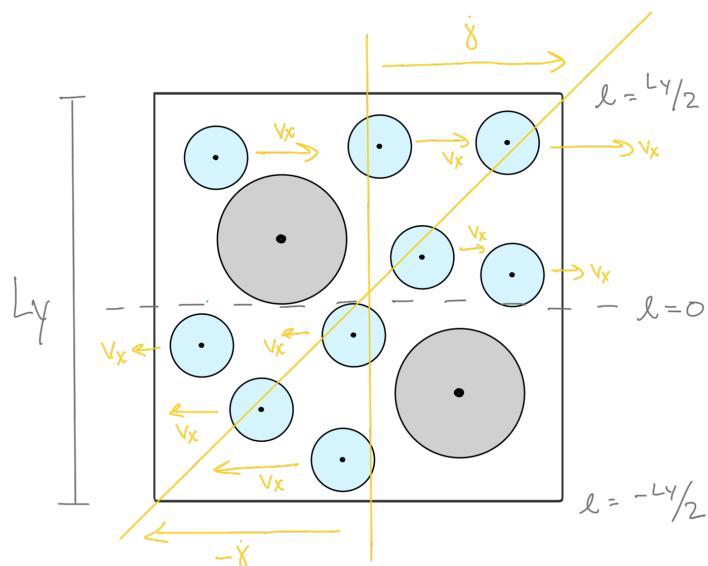


Each one of these box-tilt + wrapping steps acts as one strain. And because DED units are in and of themselves meaningless, we always report the shear stress of a system in terms of strain as the unit of time.

Velocity Modifications

One artifact of our shearing simulations starting at rest is that we get a large spike in the shear stress at the very beginning of the simulation. This is the result of a non-physical spike in the short-range lubrication force approximation as all our particles slowly begin moving.

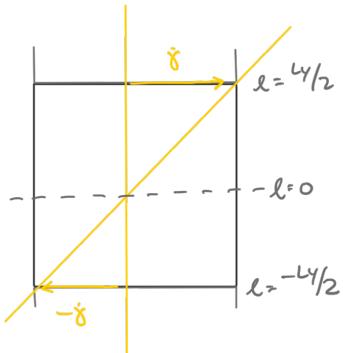
Although we can not fully remove this effect, we can mitigate it by initializing the solvent particles with a linear velocity profile matching the one we will generate with our drag flow: particle velocity in the x-direction $v_x = \gamma l$, where l is the y-position relative to the center of the box ($-\frac{L_y}{2} \leq l \leq \frac{L_y}{2}$).



When analyzing particle data we will often bin the velocities into slabs (e.g. size $(\gamma/2)/3$ for 10 slabs from $-\gamma/2$ to $\gamma/2$, finding the average velocity of each slab).

Finally, we also want to use this new y -axis reference frame ($-\gamma/2 \leq y \leq \gamma/2$) to update the velocity of any particle that crosses the y -boundary:

For shear rate $\dot{\gamma}$



$$v_x(t=2) = v_x(t=1) - \dot{\gamma}l$$

