Report a bug – YADE

AIM:

We would like to report a bug that we have observed while using the periodic simple shear in the tutorial examples. By executing the same script of the same sample on the same computer with a sequential utilization of Yade (one core used), results show unexpected variations.

THE SIMULATION :

The script is attached to this document. A periodic cloud of spheres configuration is taken for the sample, generated by the first block in the initial script. This same block is then taken away and the created sample is loaded. The simulation consists in an isotropic compression phase followed by a shearing phase in the xz direction. We fix the time step (below the value of the critical time step). The positions and velocities are saved before the simulation starts (manually), at the both end of the compression and shearing phase (script). The strain, stress, number of iteration and time values are also saved in a text document.

FACTS :

First, we try to run the same simulation four times from the control interface (i.e without closing Yade). The results presented by default in the Yade script are not the same (*image 1*).

On the *image* 1, the strain ε_{xz} (control parameter) is sightly different for the four different runs, even though it is the same simulation with the same arranged-particule packing. As the input is different, the output (stress σ_{zz} , stress σ_{xz}) are also different.

We have checked sphere positions and they are the same during the four runs, so the initial sample seems to be the same for each run.



Image 1: Graphs given by default by the periodic simple shear script, for 4 runs of the same simulation

In a second time, the simulation is saved and run four times by quitting and opening again Yade in the terminal. This other method should check if one or several parameters is/are not initialized in the same way when Yade is not closed between two simulations. We have also make sure that the spheres position are the same (the loading of the sample works, the packing is the same). Nevertheless the input and output are still diverging between the simulations.

The deformation-time graphs are not identical (*image 2*) which means the strain applied is not the same for the four supposed-equal simulations (whereas the test is driven by deformation). Moreover, the total duration and the duration of both parts of the simulation are slightly different from one run to another .



Image 2: Strain exz in function of simulation time for 4 same simulations

The fact that the four simulations unfold differently is also demonstrated is the *image 3*. The strain of one simulation is subtracted to the one of another simulation, so that the absolute value of this subtraction is drawn against the simulation time, for each simulation couple. If only the time of the beginning of the deformation was changing, the curve should be stair-shaped. In the *image 3*, there is indeed a jump around 4second which shows the difference in the beginning time of the strain phase, but the upper part of the stair-shaped curve is not flat, which shows that the strain velocity between two runs is also different.



Image 3: Normed subtraction of the strain of the four simulations (two by two) against time

In order to represent in the same formalism the input and the output as it is done in Yade script, a last graph is created depicting the stress components against the strain applied (*image 4*). The variations between the simulation while closing Yade are similar to the variations obtained while not closing Yade (*Image 1*). There is not any improvement between the two methods.



Image 4: Stress component against the applied strain

CONCLUSION :

We have noticed a variation in the results and demonstrated a variation in the input during a same Yade simulation (from the periodic simple shear example given in the web site).

We have been unabled to find the reason of such variations, and the only hypothesis we can formulated is that a or several parameters is / are not initialized in the same way between two runs of the same script. Strain and stress evolution have the same general behavior anyway between the four simulations, but the fact that they have not the same values for such identical runs (same sample, same script, same computer, same core) is puzzling...

If you know which are these parameters or what causes these variations, we would be pleased to know them. Thank you very much for your help.