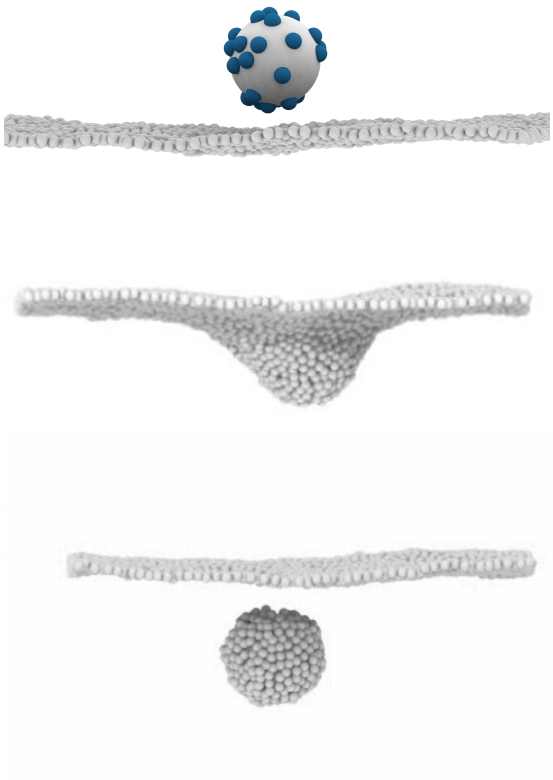
Wrap me tightly, *in simulations*

Let us consider a spherical nanoscale particle (virus, molecular condensate, synthetic nanoparticle) that is covered with sticky patches that bind to a fluid deformable membrane. The patches can be considered as point particles, the membrane can be considered as locally flat and its bending rigidity is ~22k*T*.

i) **Defined problem**: Measure the wrapping of the nanoparticle by the membrane as a function of the binding strength between the patches and the membrane and/or the number of patches. Is the wrapping continuous? At which total interaction energy is full wrapping achieved? Check your result against the membrane theory taught by Markus.

ii) Open-ended problem: Given a constant (and sufficient) number of patches & patch stickiness (i.e. the constant total binding energy), design the arrangement of patches that will provide the fastest full wrapping (endocytosis) of the membrane. Show us your designs and their performance (wrapping time). Your measurements should be a statistical average of several simulations with different initial conditions.

To execute these tasks we will use a coarse grained model for a membrane and a sticky nanoscale particle that can be downloaded here **https://github.com/Saric-Group/BSS2024_LAMMPS_Task** and can be run on any personal computer. The link contains explanations of all the files, the visualisations, some possible analysis scripts, and the lecturer will be around if help is needed. Each simulations should take a few minutes only.



Sticky patches (in blue) bind membrane particles (in gray).

Membrane partially wraps the particle.

Membrane fully wraps the particle and the wrapped particle detaches from mother membrane (budding).

Figure 1: Representative snapshots of simulations that will be run in this problem.