



Figure 1: Amount of RAM required per replica (in GB) as a function of the size of  $A_N^{n+}$  clusters ( $N$  = number of particles,  $n$  = number of charged particles,  $n \leq N$ ). Three types of clusters are tested: neutral ( $n/N = 0$ ) and “fully-charged” ( $n/N = 1$ ) clusters are plotted as filled black circles, other charged clusters ( $n/N = 0.5$  here) are plotted as filled red squares. Orange dashed lines are added to better identify the maximum cluster sizes on servers with 1 GB and 2 GB per CPU core, respectively. These tests have been performed on a HP Z800 workstation composed of 2 Intel Xeon X5670 2.93 GHz processors and 24 GB of RAM.