Canonical sampling through velocity rescaling GIOVANNI BUSSI, DAVIDE DONADIO, MICHELE PARRINELLO, ETH Zurich — We present [1] a new molecular dynamics algorithm for sampling the canonical distribution. In this approach the velocities of all the particles are rescaled by a properly chosen random factor. The algorithm is formally justified and it is shown that, in spite of its stochastic nature, a quantity can still be defined that remains constant during the evolution. In numerical applications this quantity can be used to measure the accuracy of the sampling. We illustrate the properties of this new method on Lennard-Jones and TIP4P water models in the solid and liquid phases. Its performance is excellent and largely independent on the thermostat parameter also with regard to the dynamic properties. [1] G. Bussi, D. Donadio and M. Parrinello, J. Chem. Phys. 126, 014101 (2007)

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