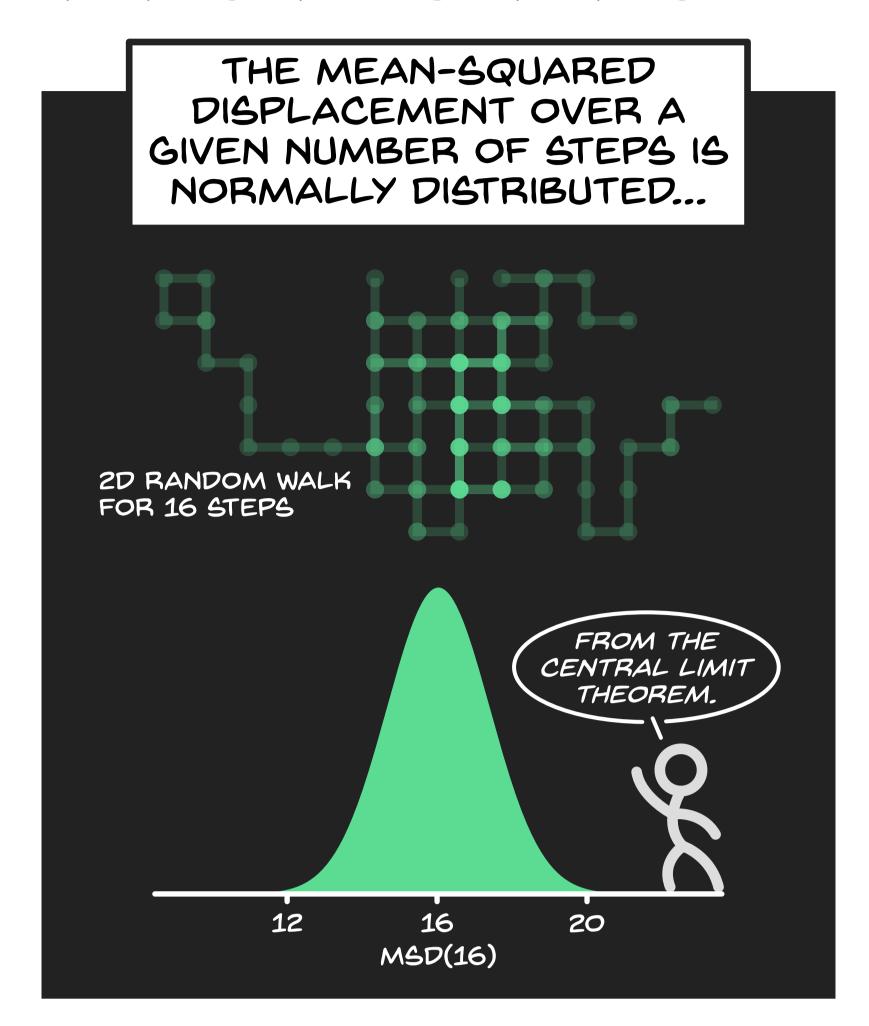
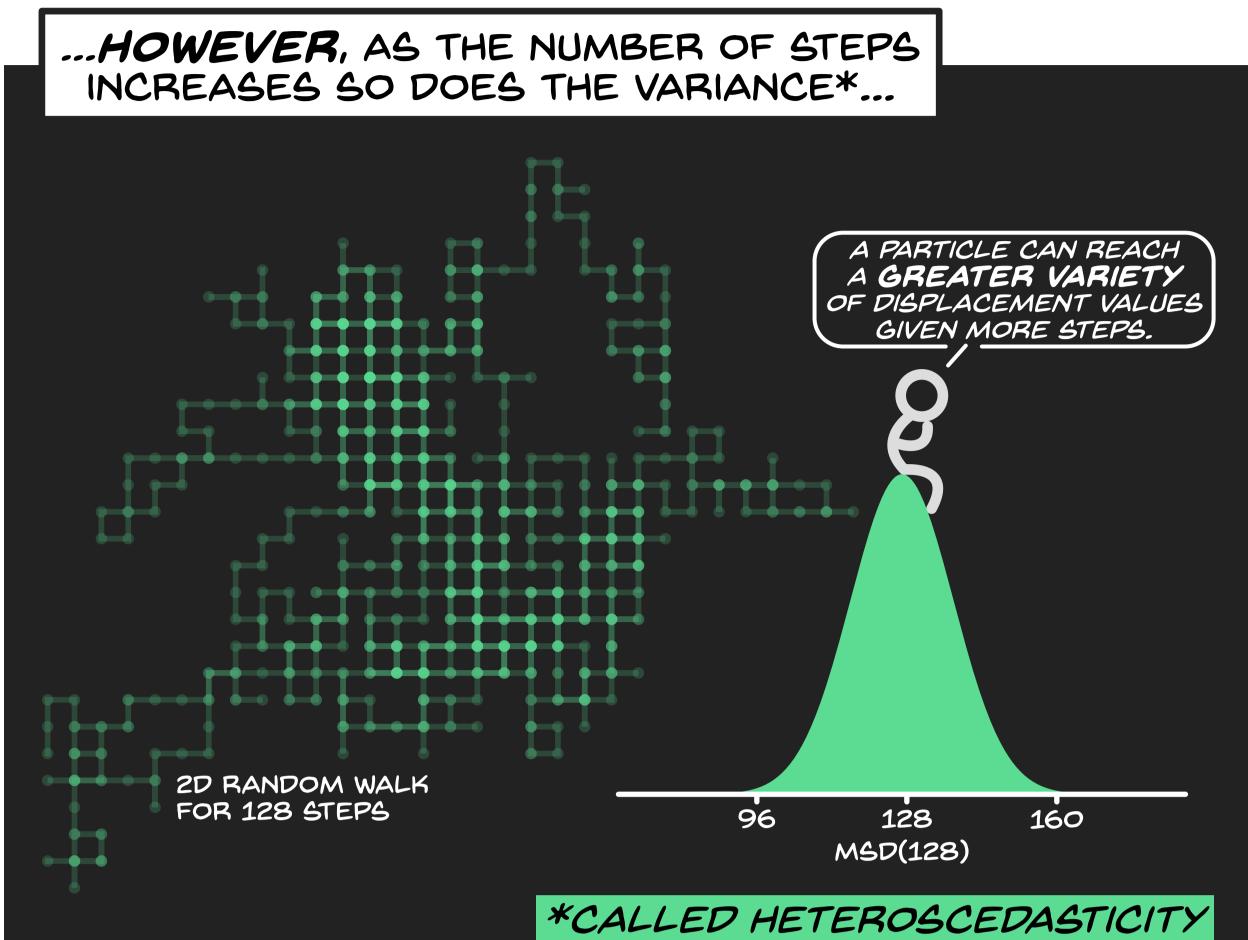
ACCURATE ESTIMATION OF DIFFUSION COEFFICIENTS AND THEIR UNCERTAINTIES FROM COMPUTER SIMULATION

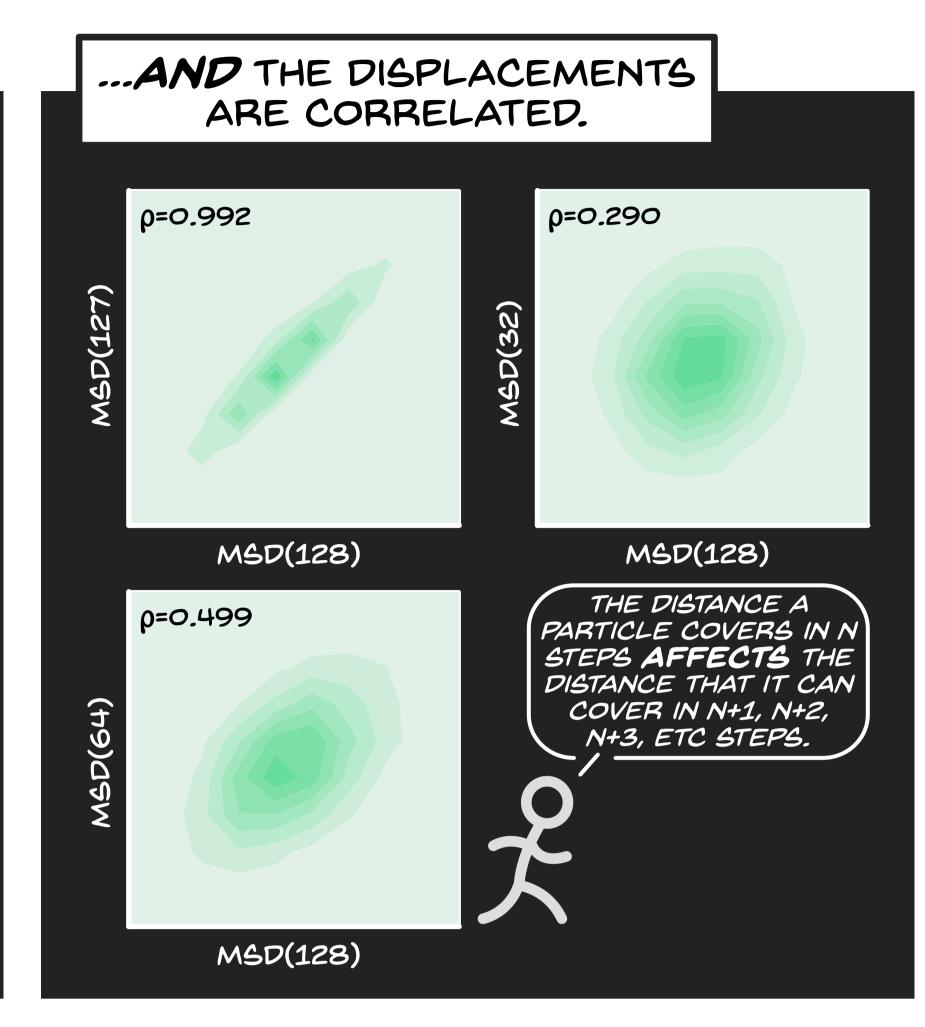
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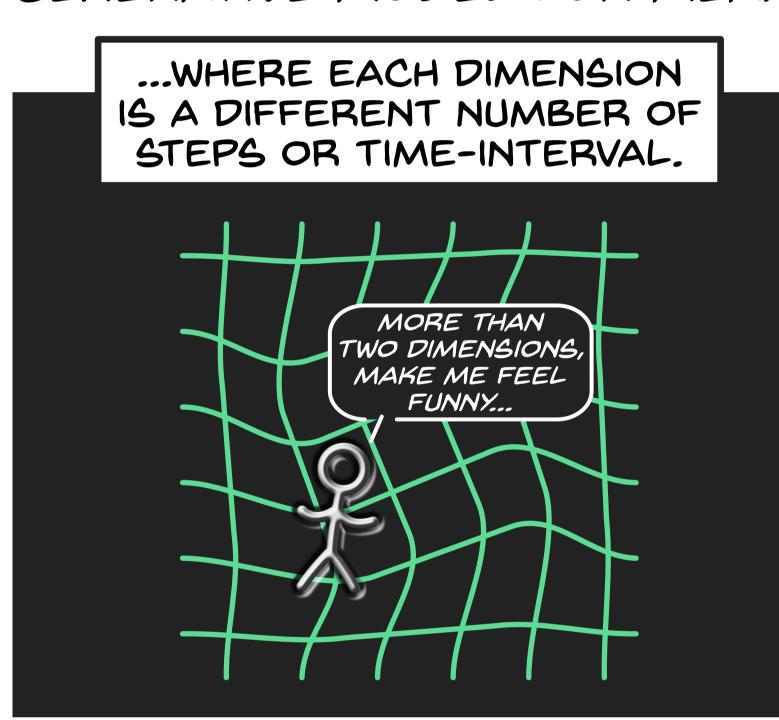
THE OPTIMAL SCHEME TO ESTIMATE THE DIFFUSION COEFFICIENT REQUIRES **BOTH** VARIANCE AND COVARIANCE TO BE CONSIDERED.

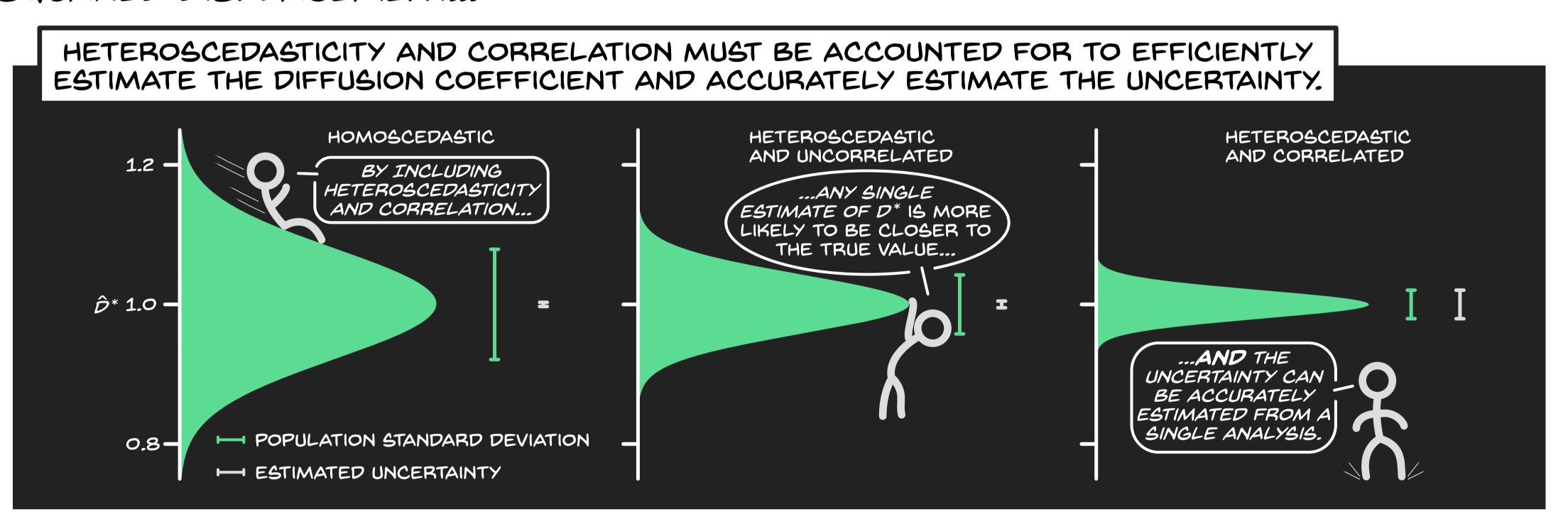




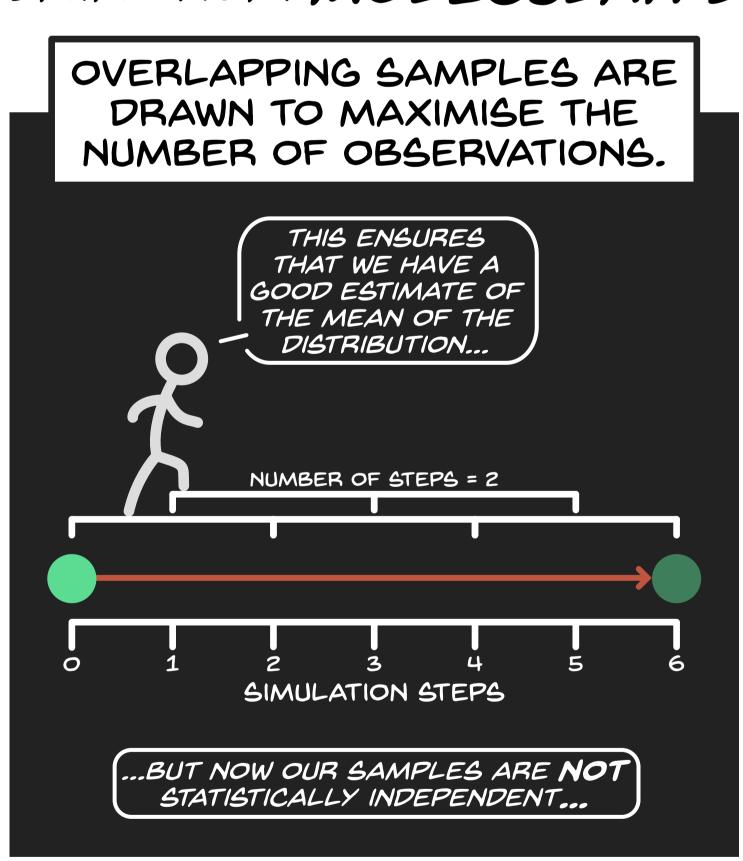


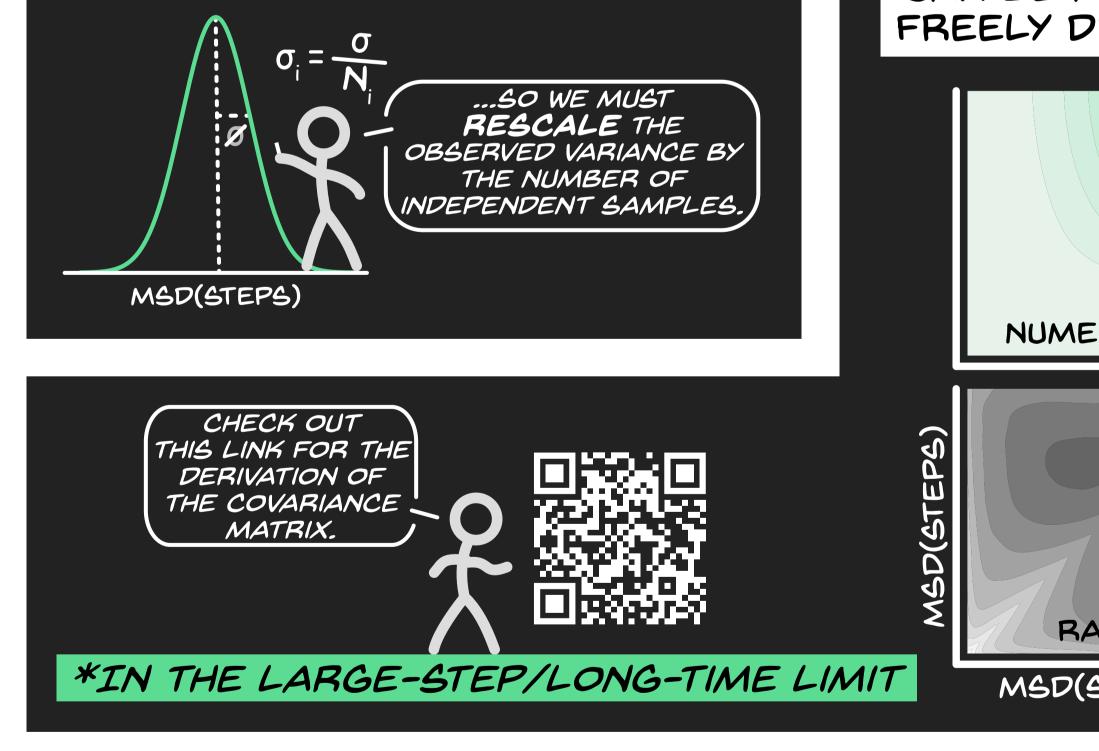
A COVARIANT MULTI-DIMENSIONAL NORMAL DISTRIBUTION CAN BE USED AS A GENERATIVE MODEL FOR MEAN-SQUARED DISPLACEMENT...

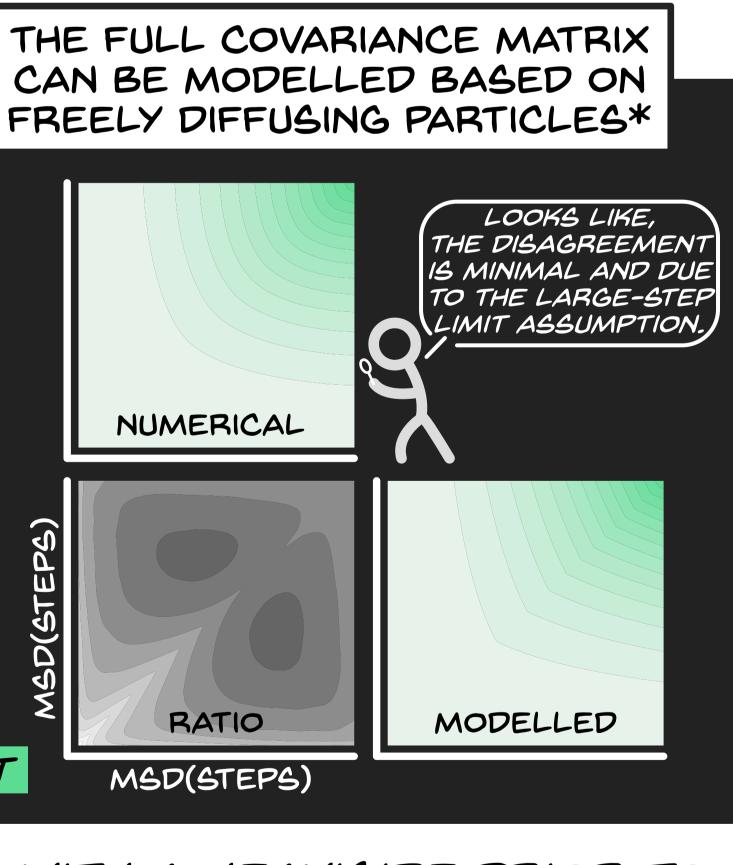




DATA FROM MOLECULAR DYNAMICS SIMULATION CAN BE USED TO PARAMETERISE THE MODEL.









WE CAN SAMPLE THE PARAMETERISED DISTRIBUTION LIKELIHOOD WITH A HEAVISIDE PRIOR TO GET AN ESTIMATE OF THE DIFFUSION COEFFICIENT DISTRIBUTION, WHICH WOULD TYPICALLY REQUIRE **MANY 1000**≤ **OF SIMULATIONS**.

