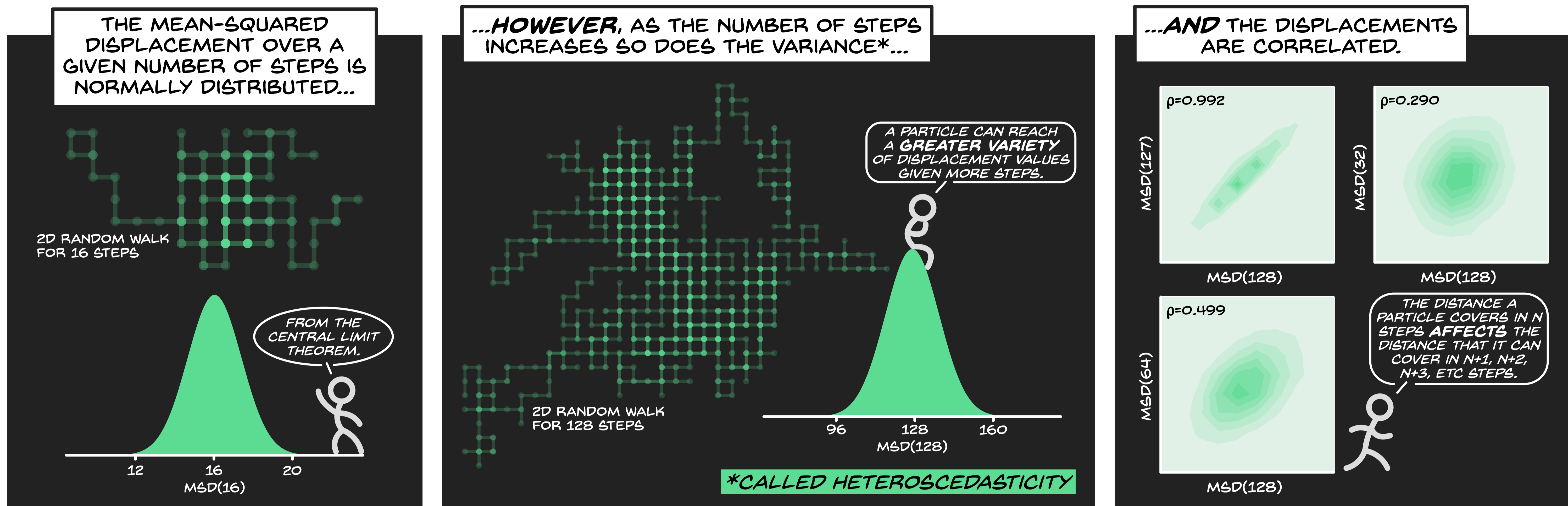


# ACCURATE ESTIMATION OF DIFFUSION COEFFICIENTS AND THEIR UNCERTAINTIES FROM COMPUTER SIMULATION

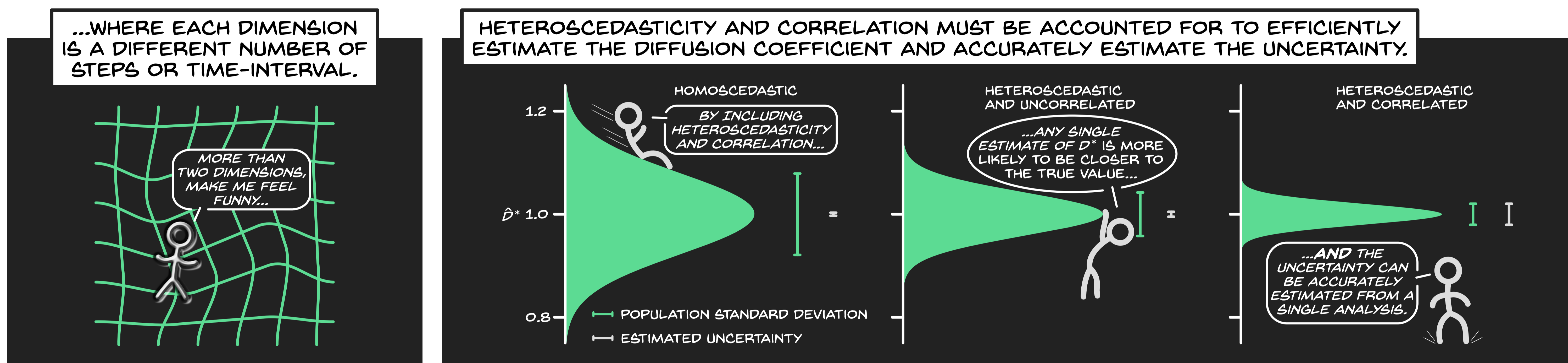
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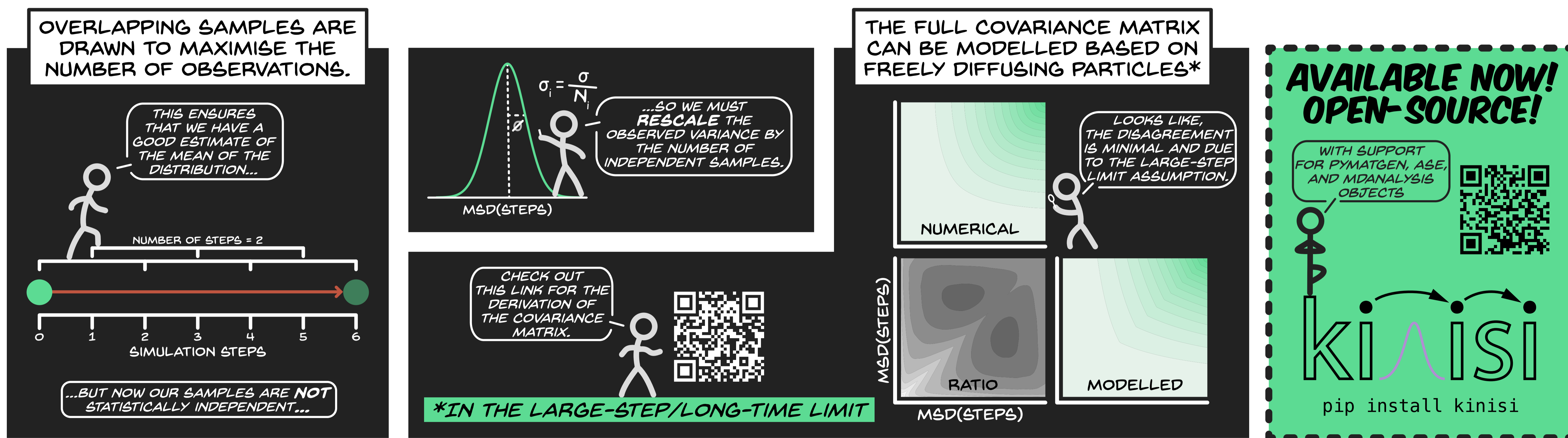
THE OPTIMAL SCHEME TO ESTIMATE THE DIFFUSION COEFFICIENT REQUIRES BOTH VARIANCE AND COVARIANCE TO BE CONSIDERED.



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 1000s OF SIMULATIONS.

