

STATISTICAL CHEMICAL ANALYSIS METHODS

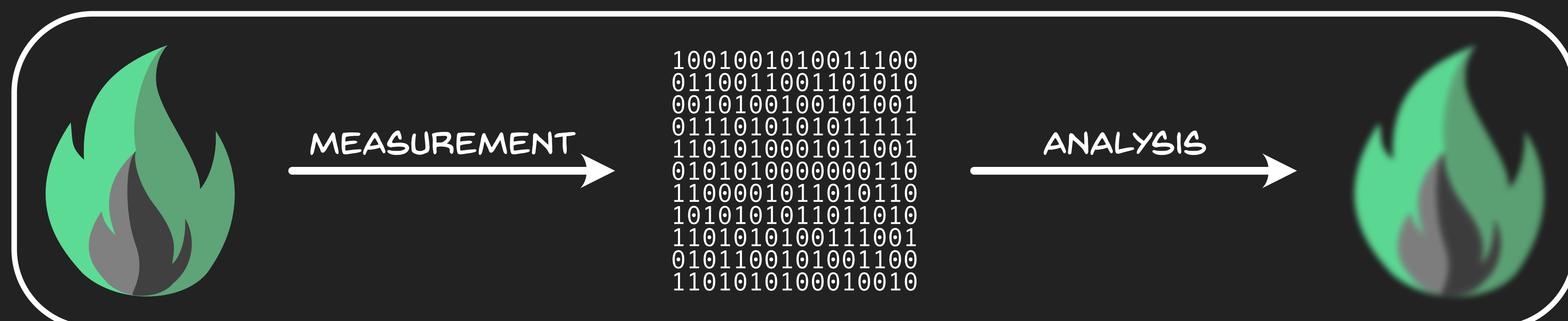
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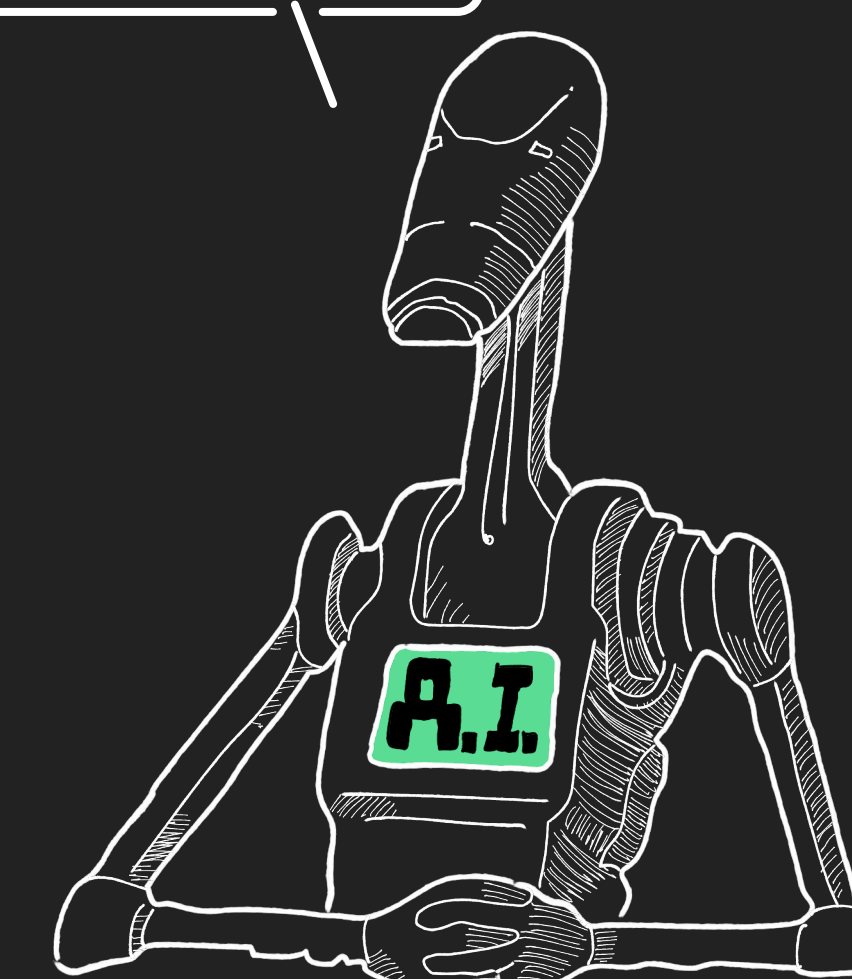
IN THE SCAMS@BRISTOL GROUP, WE ARE INTERESTED IN USING DATA-DRIVEN METHODOLOGIES TO IMPROVE ANALYSIS AND INCREASE AUTOMATION IN THE CHEMICAL SCIENCES.

THE MEASUREMENT PROCESS IS A **NOISY CHANNEL**; INFORMATION IS LOST. THE ROLE OF ANALYSIS IS TO TRY AND RECONSTRUCT THE PHYSICAL OBSERVABLE.

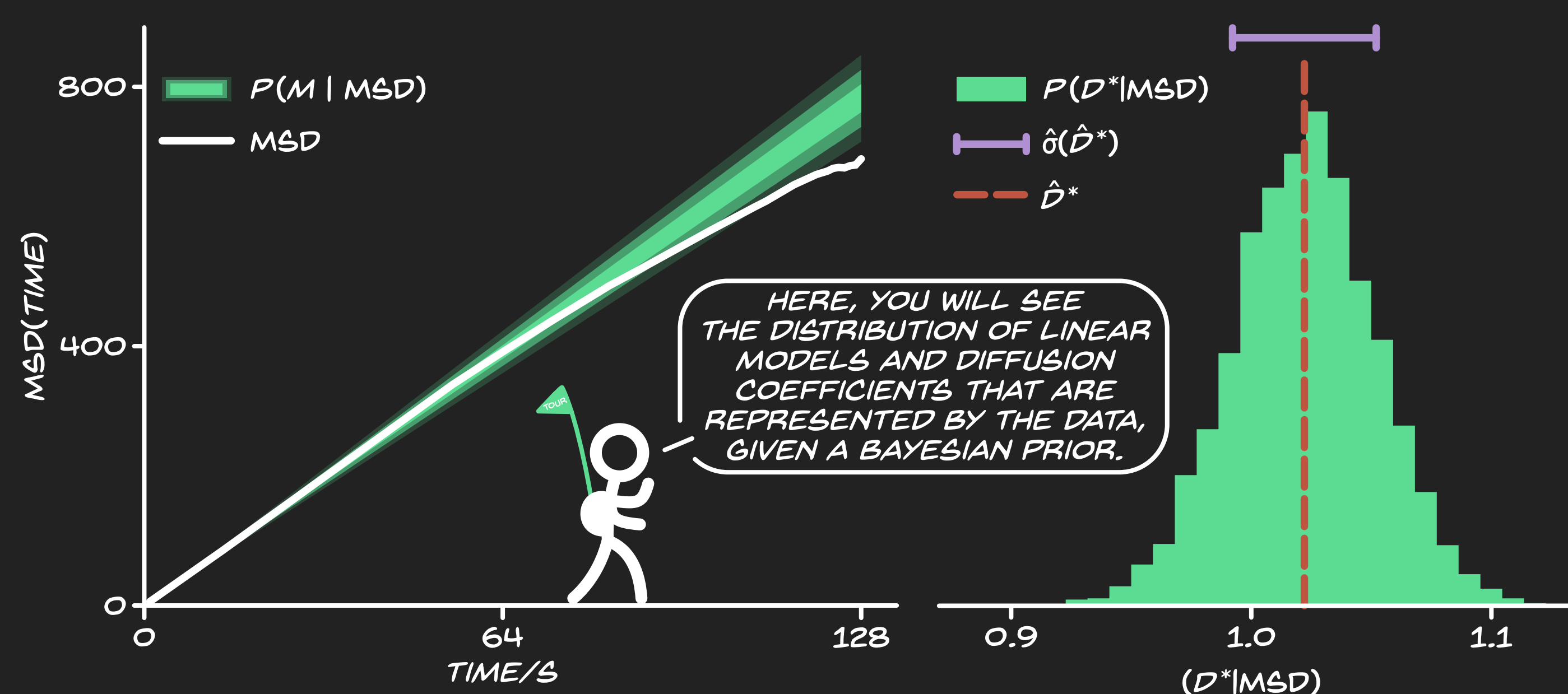


BETTER AND MORE AUTOMATED ANALYSES CAN FACILITATE RATIONAL DESIGN OF CHEMICALS AND MATERIALS, LEVERAGING ARTIFICIAL INTELLIGENCE.

ROGER ROGER.



WE HAVE DEVELOPED A NOVEL APPROACH TO ESTIMATE DIFFUSION PROPERTIES FROM ATOMISTIC SIMULATION WITH HIGH ACCURACY AND PRECISION...



...AND PRODUCED SOFTWARE TO MAKE THIS APPROACH WIDELY AVAILABLE.

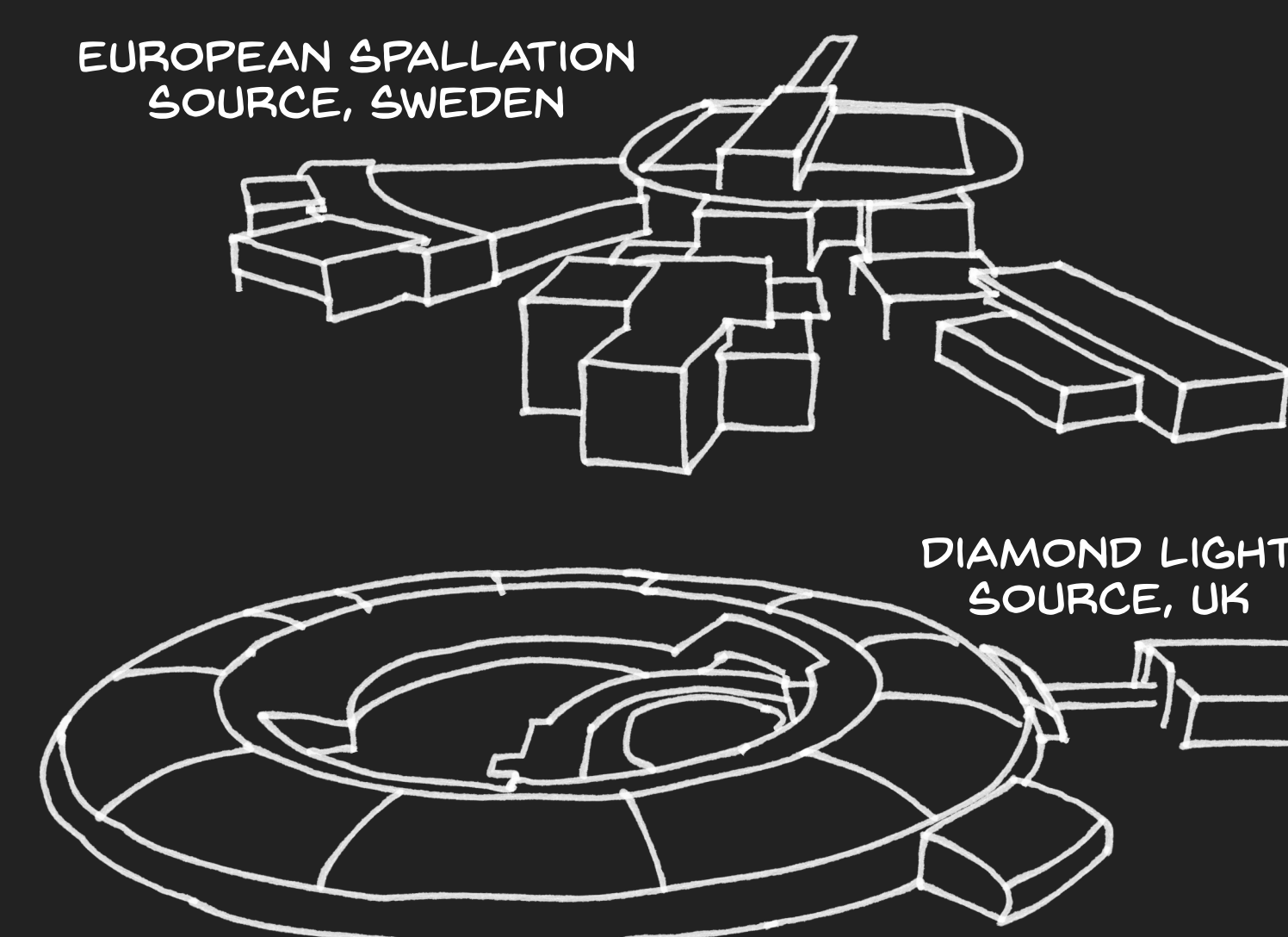
AVAILABLE NOW!
OPEN-SOURCE!

WITH SUPPORT
FOR PYMATGEN, ASE,
AND MDANALYSIS
OBJECTS



WE WORK CLOSELY WITH X-RAY AND NEUTRON SCATTERING FACILITIES..

EUROPEAN SPALLATION
SOURCE, SWEDEN



...TOWARDS DATA
STANDARDS AND NEW
ANALYSIS METHODS;...

WE WANT TO USE DATA-DRIVEN APPROACHES TO OPTIMISE SYNTHESIS AND FORMULATION.

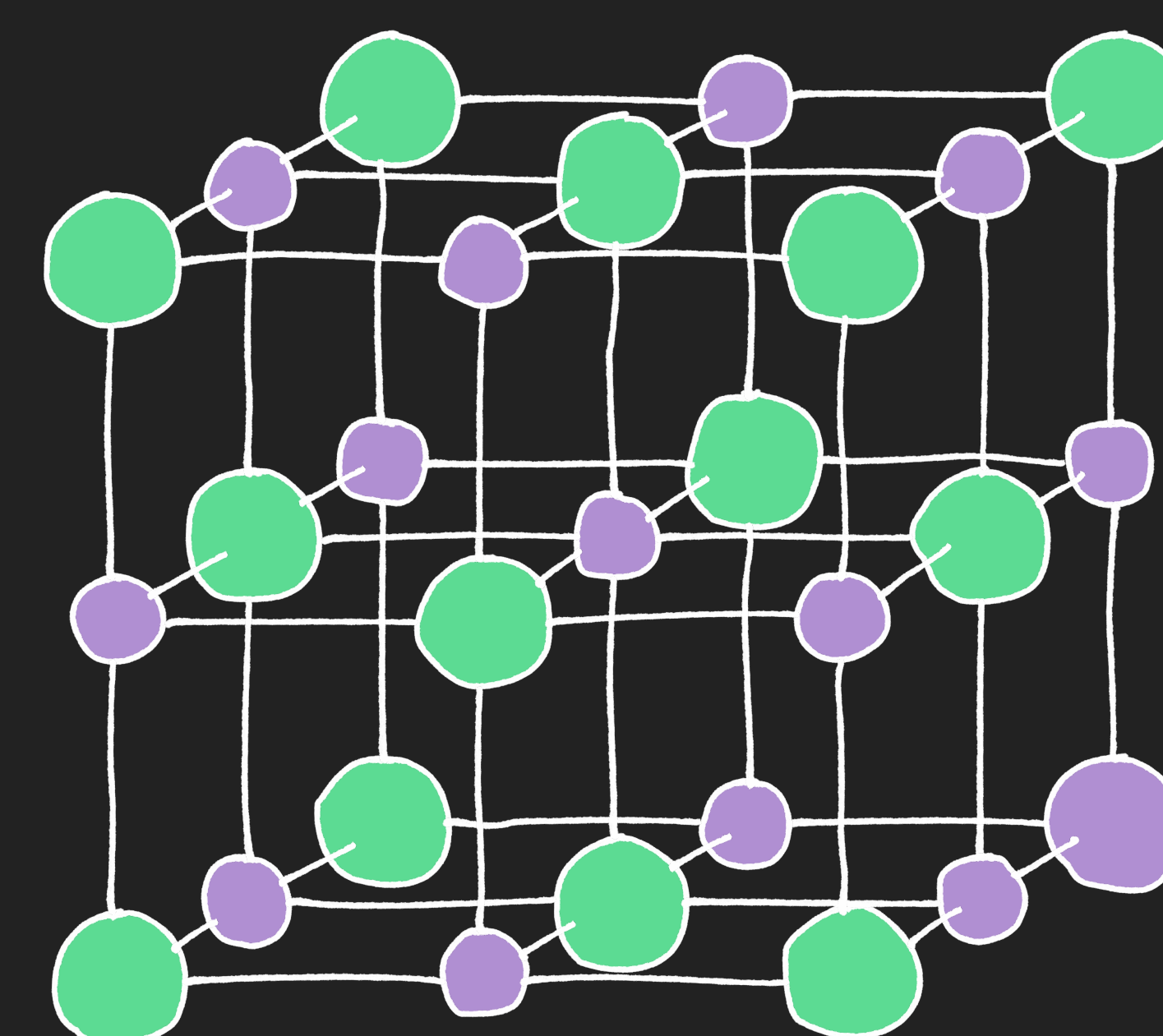
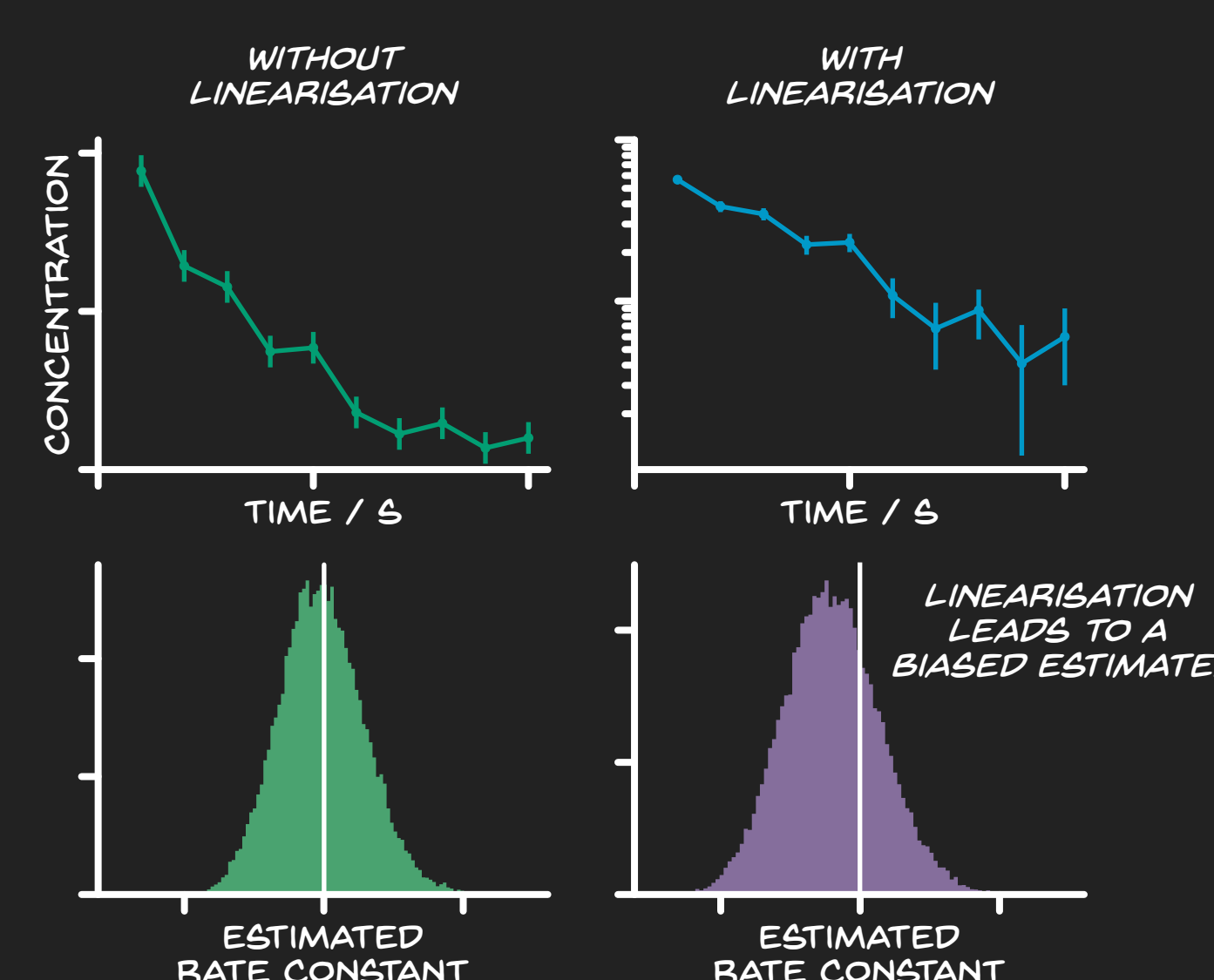
SYNTHETIC YIELD



HARNESSING
POWERFUL
OPTIMISATION
ALGORITHMS;
INCLUDING
BAYESIAN
OPTIMISATION
AND SWARM
INTELLIGENCE.

WE ARE PASSIONATE ABOUT EDUCATION, AND DEVELOPING EDUCATIONAL TOOLS.

ADVOCATING FOR DATA SKILLS
IN A CHEMISTRY EDUCATION.



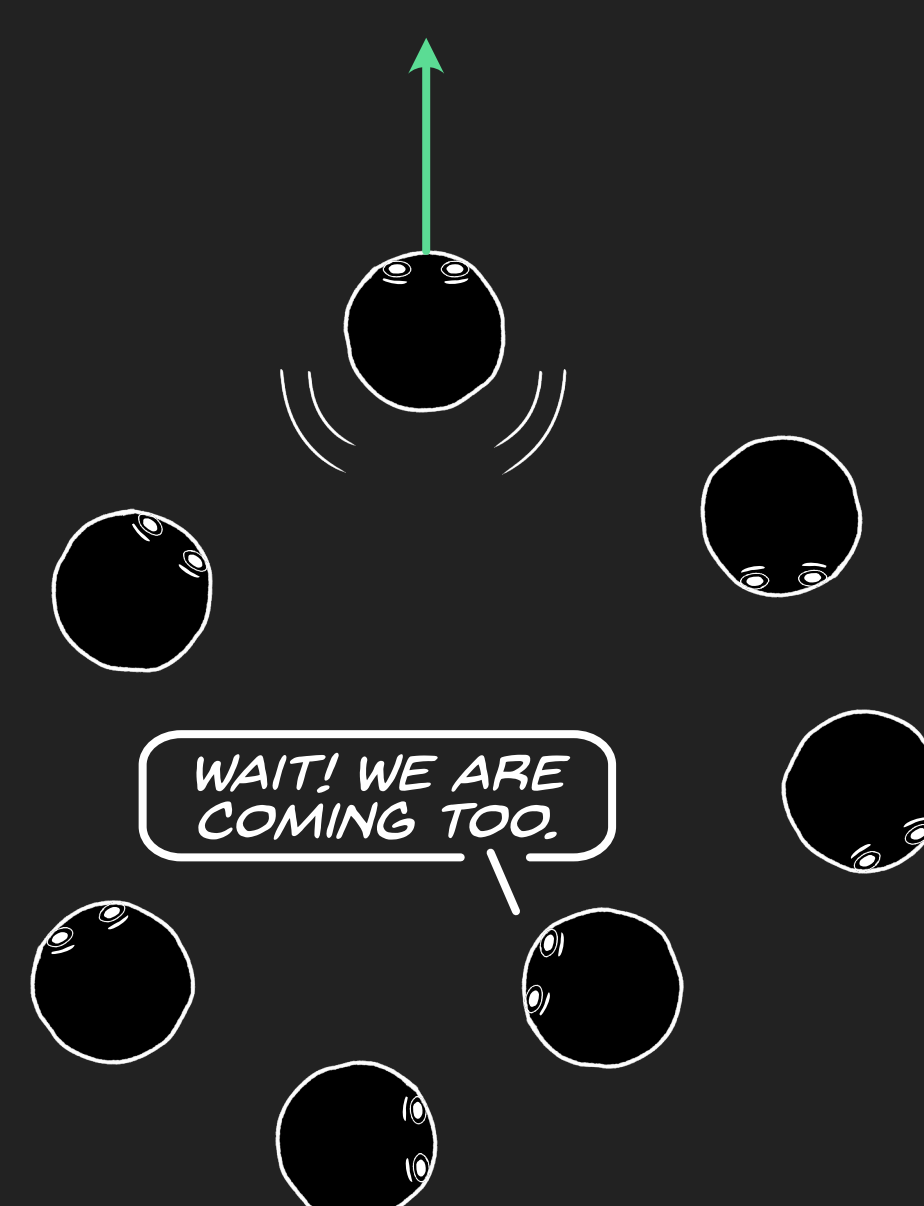
...INCLUDING USING
ATOMISTIC SIMULATION TO
UNDERSTAND EXPERIMENTS.

DO: 10.1039/C9CP00203K, 10.1088/2399-6528/AB12A9, 10.1088/2632-2153/AB94C4 & 10.1107/51600576722011426

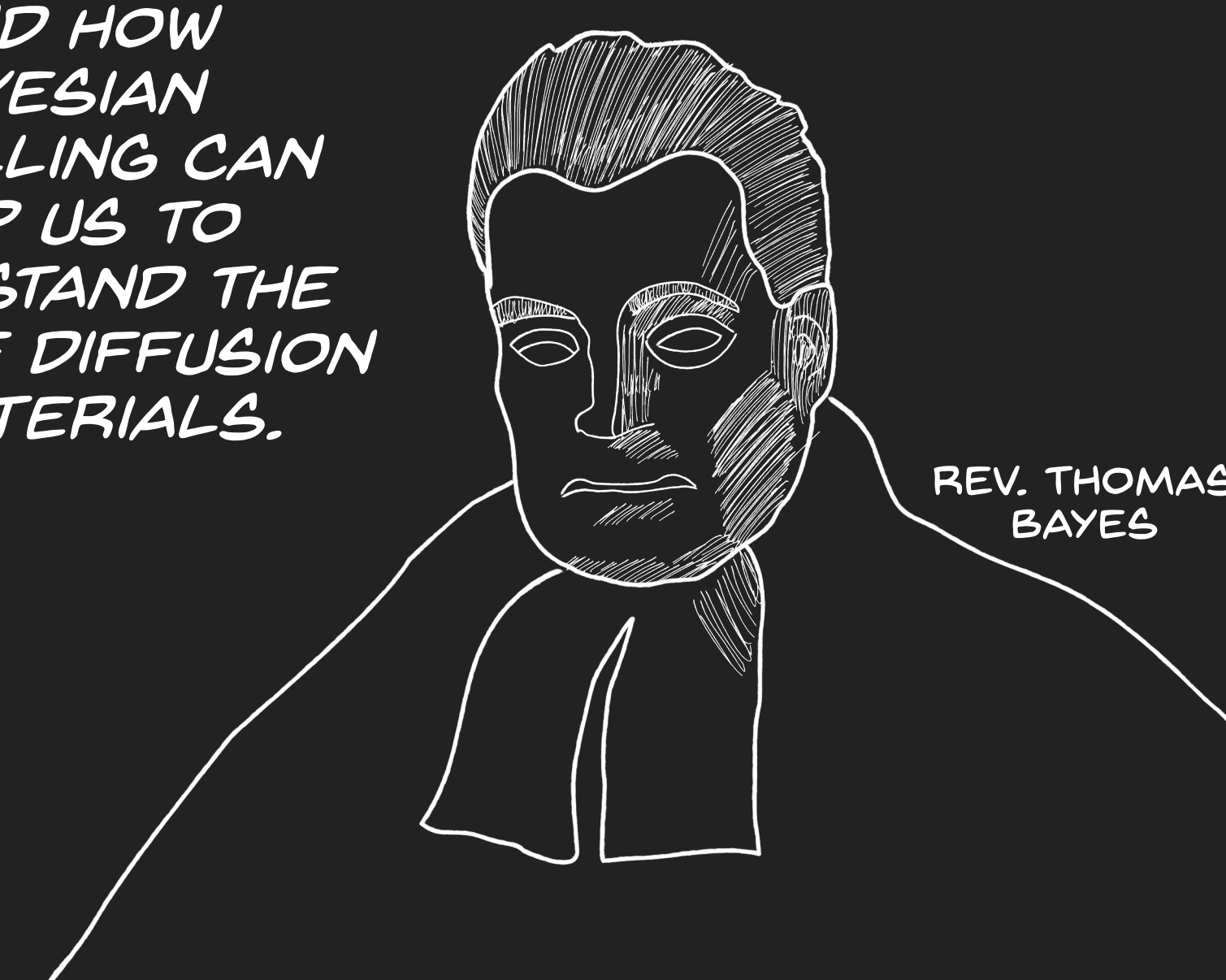
WE LOVE TO CONTRIBUTE TO OPEN SOURCE SOFTWARE PACKAGES AND PRACTICE OPEN SCIENCE.



RECENTLY, WE HAVE DEVELOPED AN INTEREST IN QUANTIFYING COLLECTIVE MOTION...



...AND HOW
BAYESIAN
MODELLING CAN
HELP US TO
UNDERSTAND THE
ROLE OF DIFFUSION
IN MATERIALS.



REV. THOMAS
BAYES