Swarm-based simulation strategy proves significantly shorter

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When the maths cannot be done by hand, physicists modelling complex systems, like the dynamics of biological molecules in the body, need to use computer simulations. Such complicated systems require a period of time before being measured, as they settle into a balanced state. The question is: how long do computer simulations need to run to be accurate? Speeding up processing time to elucidate highly complex study systems has been a common challenge. And it cannot be done by running parallel computations. That's because the results from the previous time lapse matters for computing the next time lapse. Now, Shahrazad Malek from the Memorial University of Newfoundland, Canada, and colleagues have developed a practical partial solution to the problem of saving time when using computer simulations that require bringing a complex system into a steady state of equilibrium and measuring its equilibrium properties.

These findings are part of a special issue on "Advances in Computational Methods for Soft Matter Systems," recently published in *EPJ E*.

One solution is to run multiple copies of the same simulation, with randomised initial conditions for the positions and velocities of the molecules. By averaging the results over this ensemble of 10 o 50 runs, each run in the ensemble can be shorter than a single long run and still produce the same level of accuracy in the results. In this study, the authors go one step further and focus on an extreme case of examining an ensemble of 1,000 runs—dubbed a swarm. This approach reduces the overall time required to get the answer to estimating the value of the

system at equilibrium.

Since this sort of massive multi-processor system is gradually becoming more common, this work contributes to increasing the techniques available to scientists. The solutions can be applied to computational studies in fields such as biochemistry, materials physics, astrophysics, chemical engineering, and economics.

More information: Shahrazad M. A. Malek et al, "Swarm relaxation": Equilibrating a large ensemble of computer simulations⋆, *The European Physical Journal E* (2017). DOI: 10.1140/epje/i2017-11588-2