chemisch
physikalische
gesellschaft

Gegründet im Jahre 1869 von H. Hlasiwetz, J. Loschmidt, J. Petzval und J. Stefan

EINLADUNG

zum

virtuellen Vortrag von

Ass.Prof. Dr. Carl Goodrich

Institute of Science and Technology (IST) Austria

Assembling function with differentiable simulations

am

Dienstag, 18. Jänner 2022, um 17:30 Uhr

Prof. Hinrich Grothe lädt zu einem geplanten Zoom-Meeting ein:
Zoom-Meeting beitreten:
https://tuwien.zoom.us/j/94356744318?pwd=aEkwcFBtS0htUnJ5T0o1ODNEeUVsdz09
Meeting-ID: 943 5674 4318
Passwort: 06P47nEA

Abstract

Solving inverse problems is a ubiquitous challenge spanning much of science. This is particularly relevant in the world of synthetic self-assembly, where we seek to create new materials by bringing together constituent building blocks whose size, shape, and interactions can be precisely controlled. But what collection of size, shape, and interactions will lead to the assembly of interesting materials with desirable properties? This inverse problem is challenging because even highly simplified models often contain 10s to 100s of parameters when there are more than just a few particle species. I will present a novel numerical approach for tackling this problem that directly connects experimentally relevant model parameters (e.g. sizes, shapes, interactions) with their effect on emergent material properties. This approach includes techniques borrowed from the machine learning community to differentiate over entire molecular dynamics simulations and other statistical physics calculations. In addition to enabling us to design self-assembled systems with complex properties and behavior, efficient and accurate gradient (and hessian) information presents a qualitatively different way of approaching classical physics simulations, with applications well beyond synthetic self-assembly.