Dansk Fysisk Selskab

Contribution ID: **11** Type: **Poster**

Predicting Scaling Properties From Individual Configuration

The dynamics and structural properties of several classes of highly viscous liquids are invariant during changing state points. These liquid classes, called Roskilde simple liquids, experience scaled invariant curves in their thermodynamics phase diagram, which are known as the isomorphs. The hidden scale invariant curves only appear at specified state points. Prior to that, exponent of the regression slope of potential and virial phase diagram was used to estimate these points. The scaled exponent method cannot be extended for the wide range of density and it is not efficient in terms of time and energy. We, therefore, presented scaled invariant dynamical methods, such as force and torque, to predict isomorphic state points. The asymmetric and symmetric dumbbell models with constraint and harmonic spring bonds were considered to test the new methods. Although each approach indicated different results in various models, predicted points revealed the proper isomorphs. In contrast, isomorphs are not supposed to be seen in harmonic spring bonded models. Evaluating the liquids system with harmonic spring bonds indicated the kind of isomorph-like behaviours through the scaling, which are called pseudomorphs. Generating pseudisoomorphs state points requires complex arithmetic methods, but it can provide appropriate temperatures, in which the pseudoisomorphs demonstrated. Overall, the new dynamical methods provided appropriate precise state points in both constraint and spring bonds models.

Primary author: SHEYDAAFAR, Zahraa (INM)

Presenter: SHEYDAAFAR, Zahraa (INM)