数学与系统科学研究院

计算数学所学术报告

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报告题目：

Solution Landscape: Algorithms and Applications

邀请人：徐劼 副研究员

报告时间：2021 年 8 月 9 日（周一）

上午：9：00-10：00

报告地点：科技综合楼

311 教室

Abstract:

How do we search for the entire family tree of possible intermediate states, without unwanted random guesses, starting from a stationary point on the energy landscape all the way down to multiple energy minima? Here we introduce a general numerical method that constructs the solution landscape, which is a pathway map connecting all stationary points of the energy. The solution landscape guides our understanding of how a physical system moves on the energy landscape. This method identifies multiple transition states between energy minima and the energy barrier associated with such a state.

As applications, we solve the Landau-de Gennes energy to model nematic liquid crystals confined in a square well; we illustrate the basic concepts by examining multiple stationary points and the connected pathway maps of the model; we further compare the results of the Erickson-Leslie energy. We also identify non-axisymmetric critical points of the Onsager model with different potential kernels. As another example, we find transition pathways connecting two-dimensional crystalline and quasicrystalline phases with a Lifshitz-Petrich free energy functional. The results reveal that phase transitions between the crystalline and quasicrystalline phases could follow two possible pathways, corresponding to either a one-stage phase transition or a two-stage phase transition, involving a metastable lamellar quasicrystalline state. As a constrained case, we also consider excited states of Bose-Einstein condensatio

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