数学与系统科学研究院

计算数学所学术报告

报告人： **Prof. Christoph Ortner**

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报告题目：

Hybrid Physics+Data-Driven Modelling of Interatomic Forces

邀请人： 周爱辉 研究员

报告时间：**2019** 年 **7** 月 **3** 日（周三）

上午 **10:00-11:00**

报告地点： 科技综合楼三层

311 报告厅

Abstract:

Accurate molecular simulation requires computationally expensive quantum chemistry models that makes simulating complex material phenomena or large molecules intractable. The past decade has seen a revival of interatomic potentials (IPs), fast but traditionally inaccurate surrogate models, re-casting their construction as a "machine learning" problem.

In the first part of the talk I will explain how this problem can be formalised as an unusual infinite-dimensional approximation problem, with many structures that can be exploited to make it tractable. In particular, our initial results indicate that the curse of dimensionality can be almost completely overcome.

In the second part of the talk I will introduce a practical regression scheme which (1) realises such an approximation and (2) at the same time resolves the long-standing challenge to construct such high-dimensional approximations for Its that "extrapolate well" outside of a limited training set.

欢迎大家参加！