universität wien

**FAKULTÄT FÜR MATHEMATIK**
Dekan Univ.-Prof. Dr. Radu Ioan Boţ

Einladung zur öffentlichen Defensio

## Manuel SEITZ

Thema der Dissertation

## Variational Modeling of Molecular Geometries

Abstract:
Deriving macroscopic properties from atomistic systems is a challenging yet rewarding task. In this thesis, we are concerned with three instances in this direction. First, we characterize three-dimensional ground states of a two dimensional mass-spring model featuring a three body potential preferring angles of Pi. The competition between closest nearest-neighbor interaction and the three-body potential causes flat squares to become kinked into the third dimension. This gives rise to the question of characterizing tilings with nonflat squares. We show that such arrangements admit ripples, bending and even roll-up, but essentially only in one dimension.

It has been shown that mass-spring models converge to classical linear elasticity in the simultaneous atomistic-to-continuum and linearization limit. In the second contribution, we extend this result to the dynamic setting. More precisely, we prove that solutions to the atomistic equation of motion featuring also viscosity effects converge to the momentum equation for the linear elastic energy.

Whereas in classical continuum mechanics stresses are described solely via contact forces, the atomistic approach has the advantage of featuring also long-range interactions. These two paradigms have been combined into a nonlocal continuum model, called Peridynamics. In some cases, it is possible to recover classical continuum-mechanics formulations in the nonlocal-to-local limit, i.e., when the horizon of the nonlocal interactions tends to 0. We present a dynamic nonlocal-to-local convergence result, considering the quasi static evolution of a viscoelastic peridynamic model with nonlocal viscosity potential. This can be interpreted as a nonlocal version of a Kelvin-Voigt rheological model. We prove that solutions of the nonlocal model converge to the solution of the local equation in the nonlocal-to-local convergence.

**Prüfungssenat**

Univ.-Prof. Mag. Dr. Andreas Cap
(Vorsitz, Universität Wien)

Univ.-Prof. Ulisse Stefanelli, PhD
(Universität Wien)

Prof. Dr. Thomas Hudson
(University of Warwick)

Prof. Dr. Roberto Alicandro
(Università degli Studi di Napoli)

**Zeit und Ort**

Dienstag, 28. Mai 2024, 10:00 Uhr

Online:

> https://univienna.zoom.us/j/68510970849?pwd=WVhPWC9mYkRvYytUaGI0dXJDUDdNdz09
>
> Meeting ID: 685 1097 0849
>
> Passcode: 635417