Post-doctoral/PhD position in the Chair of Applied Dynamics
at the Friedrich-Alexander-Universität Erlangen-Nürnberg

The position is part of a **DFG-funded project** 'A mechano-geometric framework to characterize macromolecular ensembles' at the interface of robotics and structural bioinformatics in collaboration with the Biosciences Division at SLAC National Accelerator Laboratory at **Stanford University**, and the Department of Bioengineering and Therapeutic Sciences at the **University of California, San Francisco**, California, USA.

Proteins perform an enormous variety of cellular functions on a broad range of spatio-temporal scales. Experimental and computational advances have increasingly enabled atomically detailed insights into their structure and dynamics. However, the molecular mechanisms of protein function, and how those mechanisms are perturbed by (disease) mutations and ligand interactions remain poorly understood. In this project we will develop and apply efficient robotics-inspired computational methods to resolve and study molecular mechanisms, with a view to redirect protein function. This is a unique opportunity to join a world-class interdisciplinary research team with **financial support for frequent travel between FAU and sunny California**.

The project focuses on aspects of

- kinematic/geometric modeling of proteins/nucleic acids
- optimized conformational sampling and motion planning/control
- protein design, data-driven modeling, and machine learning
- integrating crystallography, cryo-EM, and other data sources.
- opportunities to gain bench experience

The ideal candidate has obtained a MS degree (PhD preferred) in a quantitative discipline, like engineering, computational (bio-)physics or chemistry, applied mathematics, computer science, and an interest in structural biology. Proficiency in C++/Python, and fluency in English is required.

Representative publications:
Budday, Leyendecker, van den Bedem (2015) Geometric analysis characterizes molecular rigidity in generic and non-generic protein configurations. J. Mech. Phys. Solids 83:36-47
Budday, Leyendecker, van den Bedem (2018) Kinematic Flexibility Analysis: Hydrogen Bonding Patterns Impart a Spatial Hierarchy of Protein Motion. J. Chem. Inf. Model. 58:2108-2122
Dasgupta, Budday *et al* (2019) Cysteine modification can gate non-equilibrium conformational dynamics during enzyme catalysis. preprint at https://doi.org/10.1101/524751

For more information or to apply please contact:
Sigrid Leyendecker (sigrid.leyendecker@fau.de)
Henry van den Bedem (vdbedem@stanford.edu)