Contribution ID: **11**   Type: **not specified**

Knot classification in polymers through deep learning

Thursday, 7 April 2022 11:00 (15 minutes)

One of the fundamental open problems in knot theory is their classification, which aims to discriminate whether two given closed curves are topologically equivalent or not. The
problem might be tackled with knot invariants, such as the Alexander polynomial, quantities that are the same for equivalent knots. Nevertheless, algorithms implementing
knot recognition through invariants might take extremely large time or even fail.
In this work, we study the problem of knot classification in polymers by using deep learning. In particular, we resorted to long-short term memory (LSTM), a recurrent neural
network architecture usually used to process time-series data.
We simulated polymers, including different chain lengths and knots types. After the simulation, we computed a set of generalized dihedrals along the polymer chains and we
used them to train the LSTM.
Our preliminary results are encouraging and seem to lead to a flexible and quick method for detecting knots in polymers.

Presenter: BRAGHETTO, Anna (University of Padova)

Session Classification: Complex/Biological Systems