Contribution ID: **72** Type: **Poster**

Bridging Hydrodynamics and Non-Equilibrium Chemistry: The Feasibility of Deep Learning Surrogates in Simulations

Non-equilibrium thermo-chemistry plays a crucial role in shaping the properties of the interstellar medium, from galactic to protoplanetary scales, particularly within molecular clouds. However, accurately modeling its effects in numerical simulations remains a significant challenge due to the complexity of the associated systems of ODEs.

To address this, surrogate models—often based on deep learning—have been proposed as a means to accelerate on-the-fly calculations within simulations. While several surrogate models have been developed in recent years, their reliability remains an open question, and none have yet been integrated into full-scale simulations. In this talk, I will discuss a feasibility study on coupling hydrodynamics with surrogate models for chemistry, highlighting recent advances in controlling model approximation errors. Our findings suggest that these techniques hold great promise for achieving accurate and computationally efficient simulations of astrochemical environments.

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Session Classification: Session 6