TEMPLE UNIVERSITY
Department of Mathematics

Applied Mathematics and Scientific Computing Seminar

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Crystal Cutting and Radiative Moment Closures via Optimal Prediction

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Abstract.

The method of optimal prediction approximates a large system by a smaller one. More precisely, the mean solution of a complex system with respect to a measure is sought. For instance, in weather forecast, one can be interested in the average temperature of an ensemble of many possible tomorrows. The Mori-Zwanzig formalism applied to conditional expectations replaces the influence of the averaged unknown of the large system by a memory term.

We present two applications, for which optimal prediction successfully truncates a large system. In molecular dynamics, a large crystal is replaced by a smaller one. Optimal prediction yields a boundary layer condition that acts as if the crystal were continued to infinity, at least in equilibrium.

In moment methods for radiative transfer, an infinite system of partial differential equations has to be truncated. Various closures exist to incorporate the dynamics of the high moments on the ones of interest. An suitable adaptation of optimal prediction admits the re-derivation of, and thus a new perspective on, existing moment closures. In addition, new types of closure strategies can be derived, such as the crescendo-diffusion approximation.