Structure-preserving Neural Solver: from kinetic equations to mean-field games

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FMJH thematic post-doctoral fellowship

Mathématiques du calcul scientifique et de l'ingénierie (Maths-CSI)

Abstract

Many models in physics and economics are posed at a microscopic level, a distribution of particles or a population of optimising agents, while the quantities of interest are a few moments of a distribution. The equations governing these moments are in general not closed. A closure relation must then express the missing quantities in terms of the retained ones, and it must respect the constraints that the microscopic model satisfies automatically. This project studies closures fitted to microscopic simulations in which these constraints hold by construction, and compares them with penalised and with classical closures. Two model problems share this structure: the moment equations of the Bhatnagar–Gross–Krook (BGK) kinetic equation, and mean-field games in which each agent depends on the population only through a moment of its distribution.

1 Context

Moment closures in kinetic theory.

To describe a rarefied gas at a cost independent of the velocity variable, moment methods replace the kinetic equation by a system of balance laws for finitely many velocity moments of the distribution [1, 2]. The flux of the highest retained moment involves a moment of higher order, which the retained moments do not determine. A closure relation is therefore required. Not every vector is the moment vector of a nonnegative distribution, and a closure that leaves this realisable set yields a system without physical meaning. Closures by entropy minimisation preserve realisability and produce hyperbolic systems [2]. Their evaluation requires the solution of an optimisation problem in every cell and at every time step, and this problem becomes difficult to solve near the boundary of the realisable set [3].

Closures fitted to kinetic simulations.

To reduce this cost, closures fitted to kinetic simulations, typically with neural networks as solvers, have been proposed, for instance for polydisperse evaporating sprays [4]. Some of them reproduce by construction the structure of entropy-based closures, and inherit hyperbolicity and entropy dissipation [5, 6]. Others enforce hyperbolicity directly [7]. Imposing a property by construction and penalising its violation in the fitting objective are two distinct strategies. A penalty controls the violation only in the norm of the penalty term. For residual minimisation applied to partial differential equations, the penalised treatment of boundary values weakens the norm in which the error is controlled, and an exact treatment of the boundary values avoids this loss [8].

The same structure in mean-field games.

Mean-field games describe a large population of agents, each solving an optimal control problem whose data depend on the distribution of the population [9]. The value function of an agent solves a backward Hamilton–Jacobi–Bellman equation with a terminal condition. The distribution of the population has its own dynamics, given by a forward Fokker–Planck equation driven by the optimal control [10]. In many models an agent depends on the population only through a few moments: the mean trading rate in models of trade crowding [11], or aggregate quantities fixed by market clearing in heterogeneous-agent models of the economy [12, 13]. The evolution of these moments raises a closure problem of the same nature as in kinetic theory. It is closed in the linear–quadratic case. Otherwise it requires an approximation, by a few moments [12] or by moments fitted to simulations [14].

2 Objectives

The central question is whether closures fitted to microscopic simulations can satisfy by construction the constraints guaranteed by the microscopic model, and what this changes in stability, accuracy and cost relative to penalised and to classical closures. The project addresses it on two model problems for which reference solutions are available.

Moment equations of the BGK equation (first year).

The model is the BGK equation in one space and one velocity dimension [15], with a moment system closed by a relation for the first moment not retained. Closures are fitted to kinetic simulations over a range of Knudsen numbers, with the realisability of the moments imposed by construction. They are compared with penalised fits and with the entropy-based closure. The fitted closure is then inserted in a finite-volume solver for the moment system, and the resulting solution is compared with the moments of the kinetic solution. Three properties are examined: the stability of the scheme, its accuracy near the boundary of the realisable set, and its cost relative to the entropy-based closure.

Mean-field games with interaction through moments (second year).

The model is a mean-field game in which an agent depends on the population through the mean of the controls, as in trade crowding [11]. The linear–quadratic case, whose moment equations are closed, provides the reference solution. For a non-quadratic cost, the evolution of the mean is not closed, and a closure is fitted to simulations of the coupled system. The terminal condition of the value function, and the positivity and the mass of the distribution, are imposed by construction. The resulting solver is compared with a finite-difference solver of the coupled system [10].

Expected outcomes.

Two articles, one per model problem, and an open-source implementation. The numerical experiments use the computing resources of the HPC@Maths team.

3 Candidate profile

PhD in applied mathematics, with a background in the numerical analysis of partial differential equations and in at least one of the following: kinetic equations and moment methods, stochastic control and mean-field games, numerical optimisation or statistical learning. Programming skills in Python are expected, and C++ is appreciated.

4 Supervision and environment

- **Supervision:** Marc Massot (CMAP, HPC@Maths team) and Charles-Albert Lehalle (CMAP, MathsFi team).
- **Host laboratory:** Centre de Mathématiques Appliquées de l'École polytechnique (CMAP), Institut Polytechnique de Paris.

The project combines two research lines at CMAP: moment methods and high-performance computing for kinetic equations in the HPC@Maths team [16, 4], and stochastic control and mean-field games for market microstructure [11]. It builds on ongoing work at CMAP on fitted moment closures for kinetic equations and on residual minimisation with exactly imposed terminal conditions.

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