CRUNCH Seminars at Brown, Division of Applied Mathematics

Friday - January 14, 2022

Physics-informed machine learning using particle methods

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This talk explores the relation between particle methods and Artificial Neural Networks (ANNs). Firstly, particle methods like Molecular Dynamics (MD), Smooth Particle Hydrodynamics (SPH) and Discrete Element Method (DEM) are briefly introduced. Then, we define 'particle-neuron duals': mathematical objects that combine the ability of computational particles to model physical systems with the ability of artificial neurons to learn from data. Finally, a 'minimalistic' approach for incorporating physics constraints into ANNs is proposed. It is called 'minimalist' since, by using neighbour lists as physics-optimized convolution, it minimizes the complexity of the network. This approach is applied to three different inverse problems. Data from MD, SPH and DEM simulations are fed into the minimalistic model that 'extracts' their physics and reproduces the simulations with a high degree of accuracy. The model's capability for generalization is also noteworthy. As long as the underlying physics remains the same, the model can predict the dynamics of systems with geometries and boundary conditions very different from those of the training dataset.