Particle-in-Fourier Methods: A Promising Paradigm for Extreme-Scale Kinetic Plasma Simulations and Beyond

A major class of methods for fluid, kinetic plasma and fluid-structure interaction simulations involves particles governed by ordinary differential equations (ODEs) coupled to fields governed by partial differential equations (PDEs). Particle-in-cell type methods where the particles interpolate onto an underlying grid, field equations are solved on a grid and the field quantities are interpolated back from the grid to particle locations for advancing particle quantities are the current state-of-the-art approaches in these simulations. The use of a grid gives computational efficiency but also results in low-order of accuracy, instabilities and loss of conservation due to aliasing. Particle-in-Fourier (PIF) schemes where the particles interpolate back and forth directly with the Fourier space using nonuniform Fast Fourier Transforms (NUFFTs) and solve the field equations in the Fourier space are attractive in that aspect as we can eliminate or have explicit control of aliasing which leads to excellent accuracy, stability and conservation properties. Thanks to GPUs with massive computing power, these methods once considered not feasible for practical purposes are well suited to modern day computing architectures and can take full advantage of it.

In this talk we take electrostatic kinetic plasma simulations as an example and show many recent advances in PIF schemes which makes them a promising candidate for extreme-scale particle-field simulations. Specifically, we will talk about i) Extending PIF schemes to free space and Dirichlet boundary conditions while still maintaining semi-discrete energy and momentum conservation properties ii) Different distributed parallelization strategies for PIF schemes such as domain decomposition, particle decomposition and space-time decomposition and the suitable parameter regimes for each of them iii) Scaling and performance of PIF schemes compared to different flavors of PIC schemes and iv) Data-driven PIF schemes where we employ a Fourier neural operator based on nonuniform discrete Fourier transforms for the evaluation of fields towards fast surrogate models. Finally, we will mention our current and future works towards extending PIF schemes to other application domains as well as combining them with implicit time integration.