Performance comparison of the Numerical Flow Iteration to Lagrangian and Semi-Lagrangian approaches for solving the Vlasov equation in the six-dimensional phase-space

Rostislav-Paul Wilhelm*
Institute for Applied and Computational Math,
RWTH Aachen
Aachen, Germany
wilhelm@acom.rwth-aachen.de

Manuel Torrilhon
Institute for Applied and Computational Math,
RWTH Aachen
Aachen, Germany
mt@acom.rwth-aachen.de

In the context of high-temperature plasmas the velocity-distribution is often too far away from equilibrium to use fluid-dynamical models [1]. Thus one has to resort to the Vlasov equation

$$\partial_t f + \vec{v} \cdot \nabla_{\vec{x}} f + \vec{F} \cdot \nabla_{\vec{v}} f = 0, \tag{1}$$

modelling the dynamic in the probability distribution f arising from kinetic theory. The Vlasov equation is non-linearly coupled to the Poisson's or Maxwell's equations to compute the self-induced electro-static or electro-magnetic forces in $\vec{F}$ respectively. The probability distribution f is a function in t, $\vec{x}$ and $\vec{v}$ making it seven-dimensional. Additionally the non-linear coupling to electric or electro-magnetic forces introduces turbulences as well as fine structures called filaments. Thus the challenge is to resolve complicated dynamics with fine but physically relevant structures while working in a high-dimensional setting.

To tackle this problem one has to consider advanced discretization techniques but also potentials as well as limitations of modern high-performance hardware. Most schemes to solve the Vlasov equation rely on a direct discretization of the phase-space either using particles or a grid-based approach. This comes with the drawback of extensive memory-usage making these approaches heavily memory-bound and in the worst-case impossible to use for simulations due to limitations in terms of available hardware. In particular, grid-based approaches for the six-dimensional case allow only for low-resolution simulations and still come with significant overhead in terms of communication, leading to sub-optimal scaling results [2, 3].

Recently the authors suggested a new algorithm, the Numerical Flow Iteration (NuFI), which uses the Lagrangian framework to omit a direct discretization of the phase-space [4]. Instead one only saves the electro-magnetic forces, which are three-dimensional instead of six-dimensional functions, and uses these to evaluate f on the fly via a iterative reconstruction scheme. While from mathematical perspective this approach has favourable conservation properties, in the computational perspective this comes with a shift from heavily memory-bound algorithms to a compute-bound algorithm. For classical approaches the memory complexity essentially scales as $O\left(n^6\right)$ and computational complexity as $O\left(tn^6\right)$, neglecting the influence of non-uniform grids or higher order, where n is the number of discretization points per phase-space dimension and t is the total number of time-steps. For NuFI one gets a several orders lower memory complexity of $O\left(tn^3\right)$, however, has a higher computational complexity of $O\left(t^2n^6\right)$, i. e., trades the lower memory complexity for quadratic computational complexity in the number of time-steps. This is an unusual disparity allowing to run significantly higher resolution simulations on the same hardware. From a theoretical perspective, state-of-the-art high performance hardware profits from high flop/Byte-ratios and reduced data-communication in a scheme as is the case for NuFI, in contrast to classical approaches. Naturally the question arises whether one can see these effects in practical benchmarks and, in particular, whether the reduced memory complexity can actually justify the higher computational load when considering long time simulations, i. e., with a large number of time-steps N_T.

Theory and preliminary results suggest that while in lower dimensional cases classical approaches might still be overall favourable in terms of run-time for "practical resolutions", one expects NuFI to scale better with increasing number of degrees of freedom and dimensions due to the significantly lower memory complexity and therefore also lower communication overhead. This suggests potentially better suitability for high-dimensional Vlasov simulations.

To get a clearer picture, we want to discuss performance and scaling of NuFI and compare it to state-of-the-art algorithms currently employed to solve the Vlasov system, focussing on benchmarks in the six-dimensional case.

REFERENCES

[1] F. Chen. 2015. *Introduction to Plasma Physics and Controlled Fusion*. Springer Cham. ISBN: 978-3-319-22309-4. DOI: 10.1007/978-3-319-22309-4.

[2] Katharina Kormann, Klaus Reuter, and Markus Rampp. 2019. A massively parallel semi-Lagrangian solver for the six-dimensional Vlasov–Poisson equation. *The International Journal of High Performance Computing Applications*, 33, 5, 924–947. DOI: 10.1177/1094342019834644.

[3] Lukas Einkemmer and Alexander Moriggl. 2023. Semi-Lagrangian 4d, 5d, and 6d kinetic plasma simulation on large-scale GPU-equipped supercomputers. *The International Journal of High Performance Computing Applications*, 37, 2, 180–196. DOI: 10.1177/10943420221137599.

[4] Matthias Kirchhart and Rostislav-Paul Wilhelm. 2023. The Numerical Flow Iteration for the Vlasov-Poisson equation. (2023). arXiv: 2301.05581.