New perspectives in numerical methods for high-energy multiscale astrophysics

A joint PGI/PCTS Workshop at Princeton University
April 24 to 26, 2023
Workshop summary: Key themes and questions

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**Motivation:** Why do we innovate numerical methods?

**Evaluation:** How and in what context to evaluate the quality of methods?

**Generalization:** Are methods limited by requirements to input or output data?

**Physicality:** Do numerical techniques generate physical insight and conserve the relevant symmetries?
Motivation: Why do we innovate numerical methods?

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- Are there guiding principles to design neural networks, or do we rely exclusively on intuition?
- What advantages can machine learning or sub-grid acceleration generate beyond proof of concepts? Can neural networks outperform sub grid models to enhance fluid simulations?
- How can we exploit Vlasov-Fokker-Planck and parallel-kinetic descriptions for realistic problems in plasma- and astrophysics?
- When do hybrid approaches or domain decomposition, especially for PIC codes, enhance performance and mitigate scale separation?
**Evaluation:** How and in what context to evaluate the quality of methods?

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- How can the accuracy of machine learning-driven models be quantified, and how does it evolve with learning?
- How can machine learning models be compared to conventional models meaningfully?
- What is limiting long-term stability and accuracy of models in conventional vs. machine-learning models? Can multi-step training improve machine learning based models?
- Can you have a priori error estimates (like the discretization order in conventional methods) for machine-learning models?
- Different fields have different requirements for accuracy and completeness of information. How can we clarify which methods are good enough for a certain problem?
- What are good test problems to evaluate and compare the quality of new algorithms?
- Did we reach the break-even point for mesh refinement capacities of PIC codes in astrophysical applications? (Is refinement cheaper than a high-resolution global simulation?)
Generalization: Are methods limited by requirements to input or output data?

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• Does data reading for model training require special projections, processing, or distributions? Can the model use the raw data as input?
• Pre-conditioning for implicit PIC steps depends on the problem at hand. It is obtained from the linearized wave equations. How general can such strategies be?
• In hybrid methods, how does one separate the contribution by kinetic versus fluid processes when anisotropies appear in the problems? Often, an a priori choice has to be made.
• In hybrid codes, can the embedded PIC region have other geometries than rectangular?
• Can we make sure that machine learning models or sub grid prescriptions are generalizable? In other words, how can we extrapolate in the parameter space of our application?
**Physicality:** Do numerical techniques generate physical insight and conserve the relevant symmetries?

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- Can neural networks make predictions that conserve physical quantities (e.g., energy, phase space volume, etc.)? Can such models guarantee certain boundary conditions?
- Equally, can hybrid methods handle the conservation of relevant moments, such as charge?
- How complex can PDEs be that machine learning infers, is there a limit due to spatial and time-dependence of coefficients? How complete does the input data need to be?
- Can neural networks do implicit time-steps, like over-stepping the plasma frequency?
- How can tensor/model properties and the incorporated compression/approximation be interpreted with physical meaning?
- In hybrid approaches, how to exchange particles between fluid and non-thermal components? At the moment, they are treated separately, is there a unified treatment?
- What instabilities are preserved in hybrid formulations (e.g., ion-Weibel in the shock context)?
- Can AMR regions in PIC codes allow for improving particle statistics, for example by including other strategies like particle splitting/merging in the boundary level?
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Thank you!