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A Critical Review of Machine Learning of Energy Materials for POC (Particle in cell codes)

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Abstract: Given the numerous challenges, such as "low success probabilities, high time consumption, and high computational cost, inherent in the conventional approaches to developing energy materials, the screening of advanced materials in combination with the modelling of their quantitative structural-activity relationships has recently become one of the hot & trending topics in energy materials." This necessitates fresh ideas and tools for conducting scientific inquiry in the quest to advance the study of energy materials. Data-driven materials research is thought to change scientific findings and provide new paradigms for the production of energy materials, due to recent advances in artificial intelligence and machine learning. As data-driven materials engineering has advanced, it has become clear that machine learning can be used to significantly enhance these processes, making it possible to create and implement novel energy materials more quickly.

Keywords: machine learning, particle in cell code, artificial intelligence (AI), materials design, artificial intelligence.

I. INTRODUCTION

As environmental concerns mount throughout the world, there is now widespread agreement on the need to invest heavily in renewable energy research and development in order to create a carbon-free civilization within the next few generations. The creation of cutting-edge energy materials to facilitate efficient energy conversion and consistent power production is a vital step toward widespread use of green energy. Laboratory investigation and simulation exercises are the conventional means through which new energy materials are discovered and designed. It's a slow procedure, and there aren't that many untested samples of novel materials to begin with.

Recent advances in artificial intelligence (AI) technology have shown the huge potentials of using AI to the search for innovative and energy-efficient materials. The goal of machine learning (ML), a branch of AI, is to create artificial intelligence (AI) that can act like humans by learning from data or pre-existing knowledge. Therefore, ML may be utilised to expedite materials development because to its prowess in handling large data sets and high-dimensional analysis.

The field of materials science and engineering (MS&E) is one area where ML is being increasingly used in today's modern civilization. This review aims to provide an introduction to machine learning (ML) and its growing applications in the area of MS&E, and to delve further into some of the potential and problems connected with using ML to forecast materials' characteristics and speed up the design of novel materials. It is the sincere desire that this evaluation proves helpful to both beginners and experienced experts equally.

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A. Particle-In Cell (PIC) codes

Particles may be accelerated in a plasma because it is a nonlinear medium. It is important to have access to high-quality numerical simulation tools in order to accurately model this medium. Particle-In-Cell (PIC) programmes have established themselves as a robust and effective tool for kinetic plasma simulations during the last several decades. As their name implies, PIC codes are most effective when they closely resemble real-world plasma.

In actuality, the plasma is made up of a vast number of separate electrons and ions that interact with one another via fields that they produce themselves. While the structure of PIC codes is quite similar to that of real-world plasmas, the number of numerical particles or macroparticles that we track in the code may be substantially lower. A single numerical "macroparticle" might stand in for a cloud of many actual particles, occupying the same bounded region of space and travelling at the same rate. To represent the actual plasma's electrons and ions numerically, we may use heavy macroparticles with the same charge-to-mass ratio, but with each macroparticle standing in for a large number of their real-world counterparts.

Various approximations may be used, each with its own advantages and disadvantages, depending on the context. It is the complete electromagnetic PIC codes, which solve both the Maxwell equations and the relativistic equations of motion for the numerical particles, that offer the most basic approximation. The most accurate findings come from ab initio simulations, but they may be prohibitively costly. The quasi-static approximation is useful in the context of long-scale acceleration, when the driver propagates across lengths orders of magnitude larger than its own length.

The driver is supposed to remain stable across its expected propagation distance of about its own length. The laser pulse or any produced radiation cannot be represented directly by such codes; instead, an extra module for the laser pulse is needed, often in the envelope approximation, which allows for separation of fast and slow variables and hence substantial acceleration of the simulation.

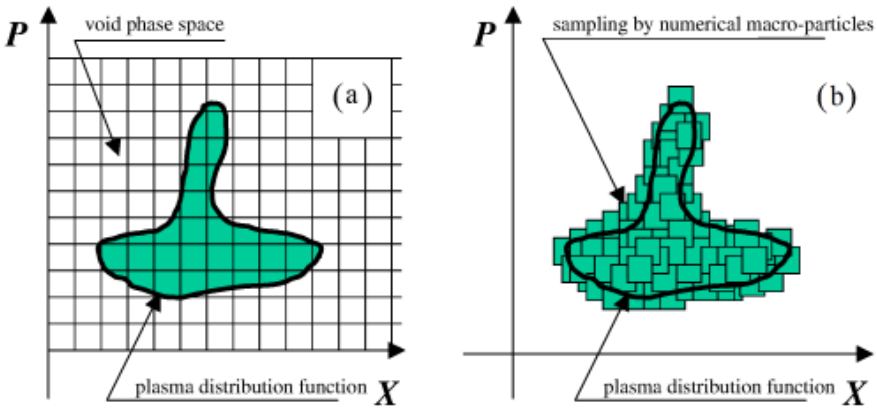

Fig. 1: Example of Kinetic plasma simulations: (a) Vlasov method, using an Eulerian grid in the phase space; (b) PIC method

B. Technical aspects

The traditional PIC approach developed by Buneman, Dawson, Hockney, Birdsall, Morse, and others is simple and uncomplicated to apply to many different situations. Due in large part to this, the following steps are often included in the approach for plasma simulation:

- Kinematic and dynamic equations integrated.
- Connecting the field's source terms for charge and current through interpolation.
- The fields are computed at each mesh node.
- The fields are interpolated to the particle positions from the mesh.

"PM" (particle-mesh) indicates the "particle-only average field" models. PP (particle-particle) interactions are direct binary interactions. PP-PM and P3M are the names given to models that include both kinds of interactions.

Discrete particle noise has been known to introduce inaccuracy into the PIC technique since its inception. Unlike with traditional fixed-grid methods like the Eulerian and semi-Lagrangian schemes, this statistical error has received less attention.

Algorithms for geometric PICs in the modern era are based on a distinct theoretical premise. To ensure “gauge invariance and conservation of charge,” energy-momentum, and most importantly the infinitely dimensional symplectic structure of the particle-field system, these algorithms employ tools of “discrete manifold, interpolating differential forms, as well as canonical or non-canonical symplectic integrators.” Geometric PIC algorithms provide the necessary properties because they are based on a more basic field-theoretic framework and are connected to the perfect form through the variational principle of physics.

C. ML-PIC interface

Recent efforts that use ML-based approaches to aid plasma kinetic simulations carry the potential in effectively addressing difficult sub-steps of the PIC algorithm. Future applications will likely combine plasma simulations with ML-based approaches. The work is on developing a streamlined interface for integrating modern PIC codes with ML-based approaches, especially NNs, for application in a wide range of contexts.

For example, although ML-based models are often built-in high-level environments like Python, PIC programmes are typically written in lower-level languages like Fortran, making the construction of an appropriate interface difficult. Although it might be difficult to maintain technically, people can take use of both settings.

When it comes to computing, Fortran is a quick and efficient choice. For massive scientific computations, its strong scalability in HPC computers means it is often employed. This is why OSIRIS, EPOCH, Tristan, and UPIC are only few of the numerous PIC codes written in Fortran. However, Python and other high-level languages are used for ML, and their ML libraries often interact with programmes written in lower-level, more efficient languages (such as C/C++). Users of Python may now construct and train ML models more quickly and easily. Training and inference may both be performed concurrently using these libraries on CPUs, GPUs, and other modern computing platforms.

It is difficult to incorporate ML-based models in highly scalable computational programmes due to the absence of an interface between the Fortran and Python environments. Efforts in recent times, however, have greatly reduced the complexity of this process. The neural-fortran micro-

framework was created to fill a need in the Fortran ecosystem by offering a library that could carry out the fundamental NN operations (such as gradient descent optimization and fully-connected dense layer computations). This library has now been developed into the "Fortran-Keras Bridge (FKB)."

By using the Keras package, FKB allows NNs to be trained in a Python environment and then their parameters exported to files that can be read and used for inference in FKB Fortran. To enable the use of NNs in highly scalable, computationally expensive Fortran algorithms, this package represents one of the first efforts at bridging both environments.

II. LITERATURE REVIEW

(Valdez & Melin, 2022) [1] In this work, we provide a survey of recent developments in the fields of "Quantum Computing (QC) and Deep Learning (DL)" and its implications for Computational Intelligence (CI). In order to solve issues, quantum algorithms (QAs) make use of the principles of quantum physics to manipulate quantum information about the state of a quantum system, which may then be processed in various ways. Numerous QAs have recently been presented, all of which have the common conclusion that classical algorithms may be significantly sped up (exponentials, polynomials, or super-polynomials) by making use of the effects of quantum physics. Because of this, QA may be able to provide answers to issues that have proven impossible to address with more conventional techniques. Machine learning methods are available, however, using DL algorithms.

(Badiali et al., 2022) [2] The work provides a mechanism for adding Machine Learning (ML) techniques into particle-in-cell (PIC) codes, with a focus on Monte- Carlo or statistical enhancements to the original PIC algorithm. The described method enables the development of neural networks in Python, where state-of-the-art ML tools are accessible for thorough training and testing. At runtime, the models are efficiently implemented into extremely scalable and completely parallelized PIC simulations. In the PIC code OSIRIS, we give proof-of-concept code for this technique by having a fully-connected neural network replace a section of a Compton scattering module.

(Xia et al., 2022) [3] The immediate need for sustainable energy to confront the fossil energy crisis and environmental problems has urged the rapid development of modern rechargeable metal-air batteries based on the redox reaction couples of gases, such as oxygen reduction and oxygen evolution, carbon dioxide reduction and carbon dioxide evolution. The conversion efficiency of these processes may be improved by using high-efficiency electrocatalysts, which is ideal for boosting battery performance. Significant improvements in electrocatalytic activities for "high-performance rechargeable Zn- and Li-air batteries" have been seen in recent years due to the introduction of single-atom catalysts (SACs) on carbon matrices as appealing and unique systems. This paper provides a concise overview of recent advances in the use of carbon-supported SACs in metal-air batteries, with an emphasis on the atomic-level electrocatalytic mechanism of SACs and their rational design. The potential and direction of SACs in the realm of metal-air batteries is also examined.

(Badiali et al., 2021) [4] To better characterise Compton scattering events in particle-in-cell (PIC) plasma simulations, we use an unique Machine Learning based approach. Instead of using

an analytical computation, we used a deep learning network to determine the probability density for Compton scattering events in this study. A comparison is made using OSIRIS's new Compton scattering module (1; 2). By adding a Neural Network component to OSIRIS, we were able to conduct a head-to-head evaluation. The findings point to an exciting new direction for the use of Machine Learning techniques in a wide variety of PIC code routines, not only Compton scattering.

(Liu et al., 2021) [5] Because traditional methods for developing energy materials have so many drawbacks, including low success probabilities, high time consumption, and high computational cost, one of the hottest and trendiest topics in the field right now is the screening of advanced materials in conjunction with the modelling of their quantitative structural-activity relations. This necessitates fresh ideas and tools for conducting scientific inquiry in the quest to advance the study of energy materials. Recent developments in AI and ML have sparked hopes that data-driven materials research may revolutionise how energy materials are created and how we understand their properties. What's more, the rise of data-driven materials engineering in recent years demonstrates that machine learning technology will greatly enhance the process of creating, discovering, and deploying novel energy materials. The article explains why it's crucial to create new energy materials that can help with global carbon neutrality. “Open-source databases, feature engineering, machine learning algorithms, and machine learning model analysis” are all covered in depth, as is an introduction to the principles of machine learning. Materials for alkaline ion batteries, photovoltaic cells, catalyst supports, and co2 capture are only few of the current subjects covered in data-driven materials science and engineering.

(Aguilar & Markidis, 2021) [6] Using “Deep Learning (DL)” to derive the electric field from the electron phase space, we create a novel “Particle-in-Cell (PIC)” approach for plasma simulations. To pass the two-stream instability test, we have developed a “Multilayer Perceptron (MLP) and a Convolutional Neural Network (CNN)”. By examining the projected growth rate of the two-stream instability, we confirm that the “DL-based MLP PIC approach” yields accurate findings. Total energy and momentum are not conserved in the DL-based PIC. In contrast to conventional PIC approaches, which are vulnerable to the cold-beam instability, the DL-based PIC approach is robust. This research demonstrates that building next-generation PIC algorithms by combining DL technology with conventional computational approaches is feasible.

(Keith et al., 2021) [7] Machine learning models are poised to revolutionise the chemical sciences by dramatically boosting the speed of computational algorithms and enhancing the insights available from computational chemistry methodologies. It will need the combined knowledge of computer scientists and physicists to make this a reality, however. New and seasoned scholars in any discipline will find useful information in this Review. It begins by providing brief introductions to both computational chemistry and machine learning techniques, illuminating how the two might be combined to provide deeper insights. We next critically analyse a selection of examples that show how molecular and materials modelling, retrosynthesis, catalysis, and drug design may all benefit from combining computational chemistry with machine learning.

(Chen et al., 2020a) [8] The landscape of physics and chemistry is shifting as a result of the fast transformation being effected by machine learning (ML). Given ML's ability to autonomously execute complex tasks, it is finally being put to use to aid in the finding of material correlations,

the comprehension of materials chemistry, and the acceleration of material discovery. Here, we provide a comprehensive overview of ML's use in the energy industry, including such areas as rechargeable alkali-ion batteries, photovoltaics, catalysts, thermoelectrics, piezoelectrics, and superconductors. First, we will provide a conceptual framework for ML in materials research, including a high-level review of various ML methods and recommended approaches. The applications of ML in energy materials are then critically discussed.

(Morgan & Jacobs, 2020) [9] Machine learning has already had a significant influence on materials research, influencing fields as diverse as material discovery and molecular simulation enhancement. Since this industry is always evolving, it may be difficult to keep up with the wide variety of possibilities and the greatest methods for using them. In order to address both of these concerns, researchers in this review first provide an overview of the areas where machine learning has recently had a major impact in materials science, after which they go into more depth about how to evaluate the validity and domain of suitability of some basic examples of machine learning models.

(Chen et al., 2020b) [10] The landscape of physics and chemistry is shifting as a result of the fast transformation being effected by machine learning (ML). With its ability to accomplish complex tasks on its own, ML is being used to help in the search for material correlations, to help understand materials chemistry, and also to speed up the production of innovative materials. Energy materials and the applications of ML in them are covered in depth, including rechargeable alkali-ion batteries, photovoltaics, catalysts, thermoelectrics, piezoelectrics, and superconductors. Furthermore, a conceptual framework is presented for ML in materials research, followed by a high-level review of various ML methods and recommended approaches. The use of ML in energy materials is then critically examined. Finally, some thoughts on some of the most pressing problems and most promising future developments in this dynamic sector round off our analysis.

(Zahid et al., 2020) [11] This article is dedicated to easing the integration of cutting-edge big data analytics (BDA) designs and infrastructures into the telecom industry. Every day, telecom businesses process anything from terabytes to petabytes of data. Internet of Things (IoT) applications in telecommunications also contribute to this data flood. New possibilities for extracting useful information from telecom big data have emerged as BDA has developed. Considering these advantages and the rapid evolution of BDA technology, it is crucial to examine the many current uses of BDA in the telecom industry. Additionally, we discuss about the positives and negatives that have been brought up in these pieces. We found no study that specifically addressed full-fledged BDA implementation in a live telecom setting; rather, all trials were proofs of concept (POC) on a severely constrained BDA technology stack (as opposed to the existing technology stack).

III. CONCLUSION

The dynamics of an ideal plasma may be roughly modelled using electromagnetic particle-in-cell algorithms. These programmes are unparalleled in their ability to anticipate the results of short pulse laser-plasma interactions, especially in the relativistic zone. Since electromagnetic PIC codes are most effective in this range, when binary collisions of plasma particles are either

insignificant or may be treated as a small disturbance. More than one PIC formulation has been suggested to increase PIC's modelling power by eliminating numerical instability, preserving energy, and integrating fluid dynamics into PIC codes. The outcomes of plasma simulations have been studied with the aid of machine learning. The ML-based PIC approaches require additional research, especially spectrum analysis of inaccuracy in electric field values.

In order to compete with existing PIC approaches in terms of physical correctness, an ML-based PIC should explicitly include the conservation rules in the scheme. Nothing from the governing equations or conservation laws, including total energy or conservation law, is used by the ML electric field solver.

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