Towards deep learning accelerated particle-in-cell simulations: application to Compton scattering

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Motivation

Implementation of a machine learning based collisions module in a particle-in-cell (PIC) code

➠Kinetic collisions in PIC codes are hard to efficiently implement and they are usually computationally expensive.

➠Machine learning models, and in particular deep learning models, can be efficiently used to learn complex functions such as the probability density of collisional processes.

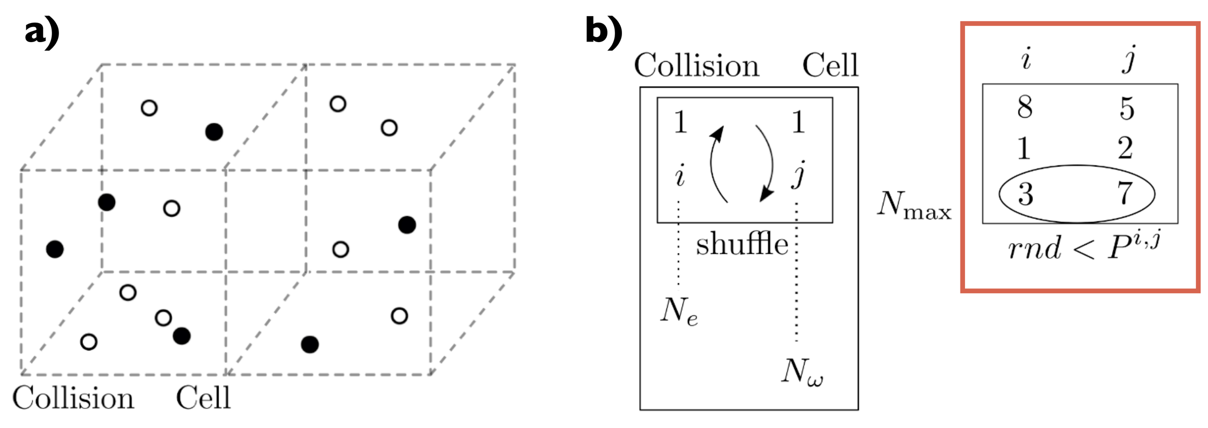
➠We employed a deep learning model to evaluate the probability density for Compton scattering events, replacing an analytical calculation [1].

➠An Artificial Intelligence (AI) module for the OSIRIS PIC code [2] (OSIRIS-AI) was developed. This module uses deep learning models trained in a different framework, namely the Keras Python library [3].

➠The advent of higher intensity laser experiments and the study of extreme astrophysical scenarios will require simulations including single Compton scattering. Thus, these research topics would benefit from reducing the computational cost of collisional processes in PIC codes.

Our Approach

We aimed to substitute a part of the single Compton scattering model [3] implemented in OSIRIS [2]



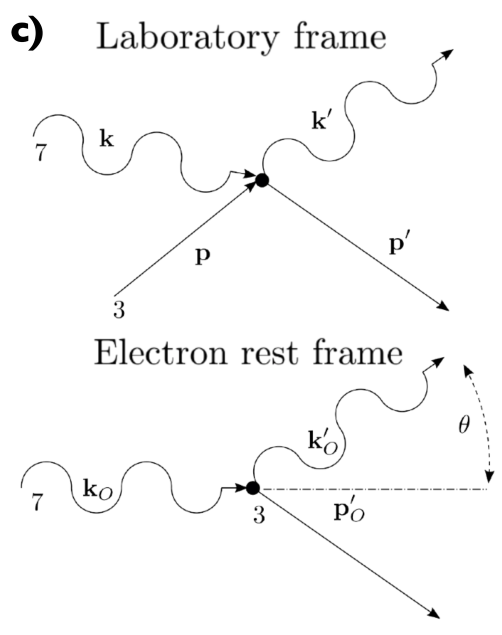


Figure 1: Overview of the Compton scattering algorithm implemented in OSIRIS **a)** Macro-particles are binned into collision cells. **b)** Particles are shuffled and paired through the no-time-counter-method. The probability of interaction for each pair is calculated. **c)** The momentum is then updated based on Compton frequency shift and momentum recoil.

The current algorithm calculates the probability of interaction for every potential collision pair $\{e^{\pm}, \gamma\}$ (red square in Figure 2.b)

➠ This is a computationally expensive computation that scales linearly with the number of particles.

➠ A machine learning based approach, in which a Neural Network (NN) is trained to learn the probability density distribution, could substitute this step and take full advantage of scalability of neural networks with respect to the number of particles.

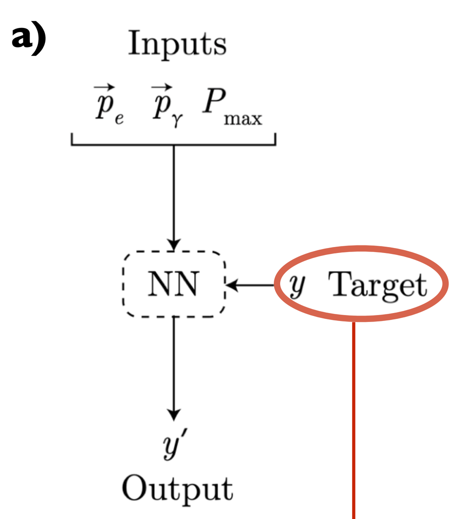
The development and implementation of a such a model into a production code was the main goal of this work.

Neural Network Training

➠ The momenta of the particles $(\vec{p}_\gamma, \vec{p}_e)$ and P_{max}, a normalisation factor dependent on simulation parameters.

➠ For an optimal training of the neural network, we balanced the data-set by weighting the less frequent events.

➠ The neural network comprises of 3 layers of size 6,8,1 with activation functions sigmoid, relu and sigmoid.



The neural network has as target the probability of interaction between the $\{e^{\pm}, \gamma\}$ pair, evaluated using an analytical model.

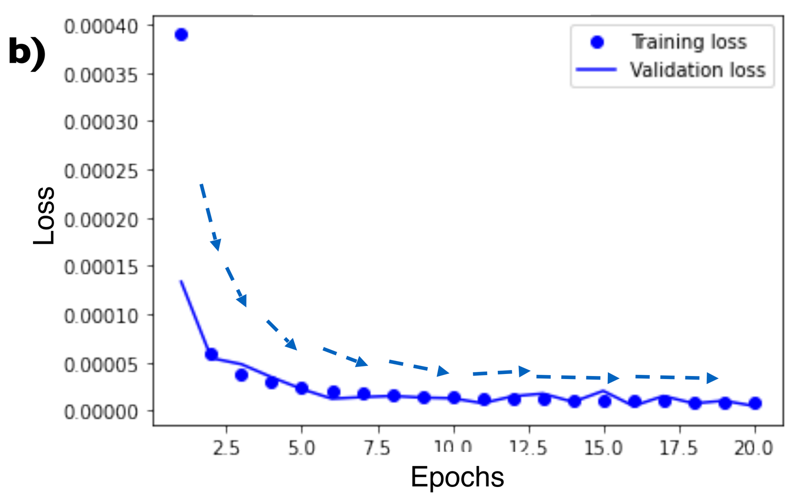


Figure 2: a) Neural Network input and output scheme. **b)** Loss score during training.

The predictive performance of the deep learning model is quantified by the loss function [4], which decreases during the training.

In this case, we used the Mean Square Error (MSE)

$$MSE = \frac{\sum_{i=1}^{n} (y_i - y_i^p)^2}{n}$$

Transfer learning application results in a generalised model, applicable in different energy regimes. Training in one regime and refining on others results on a good agreement with the conventional algorithm.

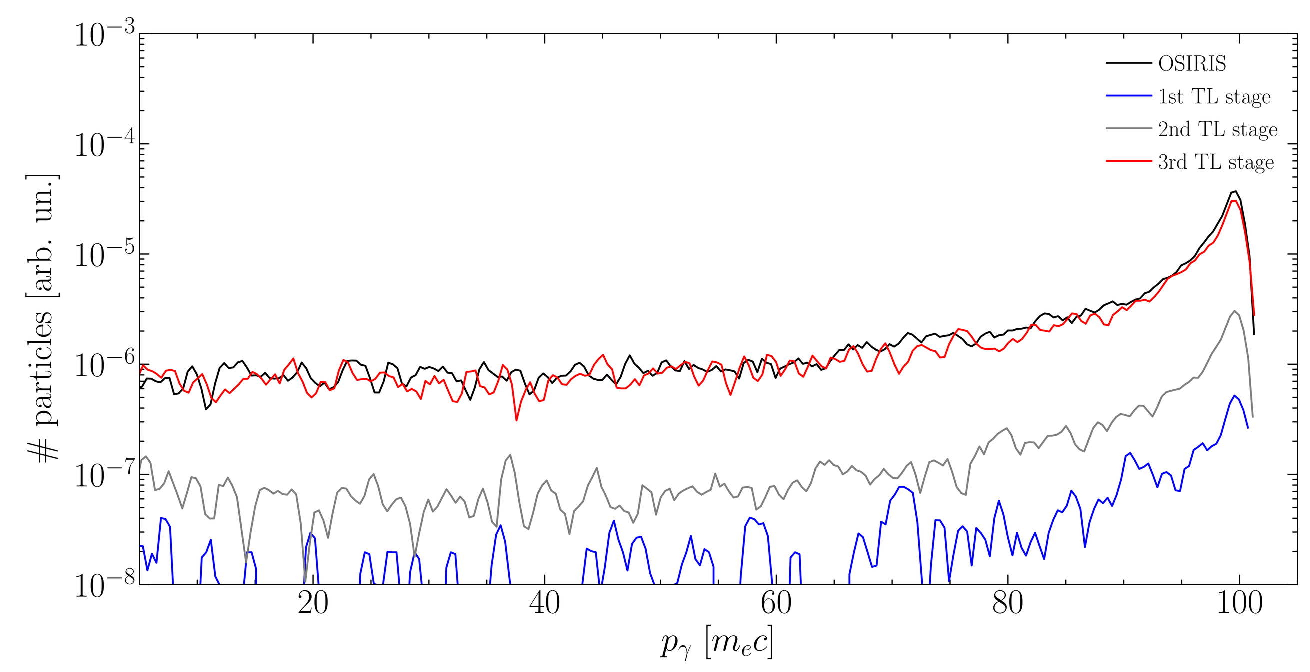


Figure 3: Photon Spectrum resulting from the interaction of a collimated electron beam and a photon gas undergoing Inverse Compton scattering ($\gamma = \hbar\omega/(m_e c^2)$).

OSIRIS-AI Results

The spectrum resulting from the AI-method and the analytical calculation agree within $\sim 10^{-5}$ particle count. A general overestimation of the number of scattered photons is observed.

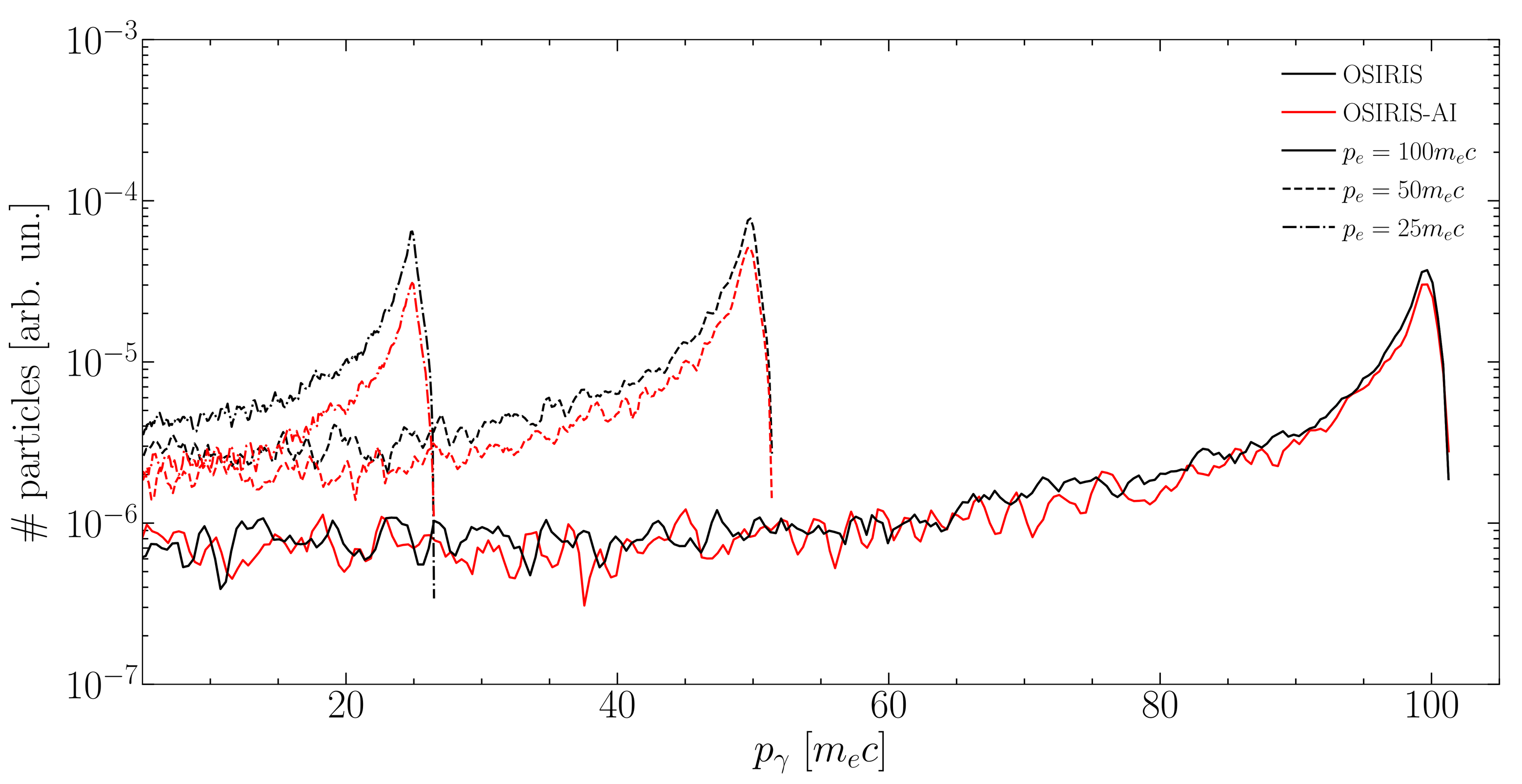


Figure 4: a) Photon spectrum from Inverse Compton scattering occurring at different energies.

The machine learning method outperformed the conventional algorithm, particularly when dealing with an higher number of particle per cell (ppc).

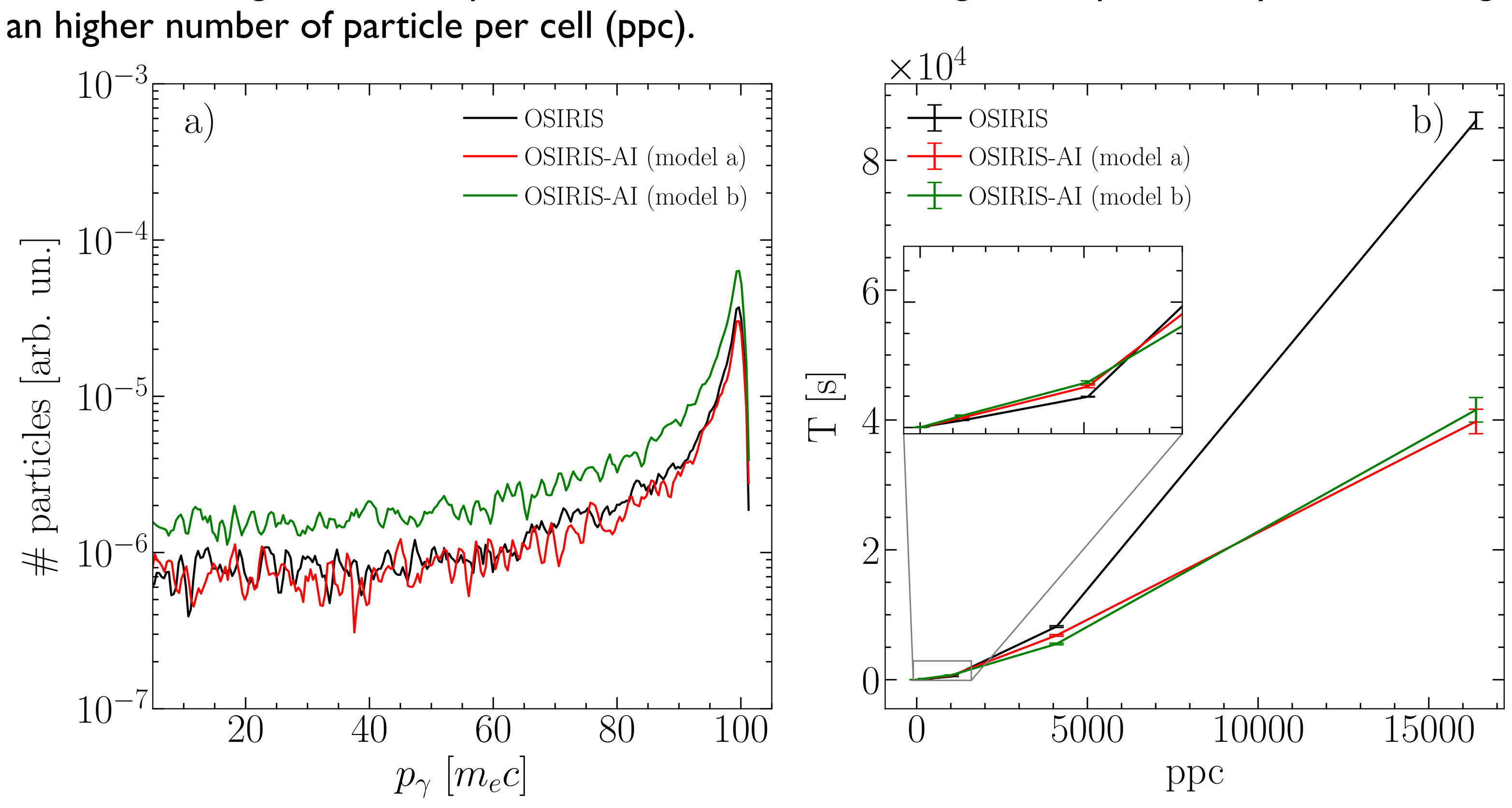


Figure 5: a) Photon spectrum from Inverse Compton scattering for two different models. **b)** Run-time comparison between the two methods and models as a function of ppc.

Conclusions & Future work

Proof-of-concept: neural networks can be employed to assist modelling of collisions in kinetic plasma simulations

➠Resulted in a good agreement with the conventional algorithm and faster run-time.

➠Exploiting state-of-art methods, such as transfer learning, was vital to achieve a general model.

Implementation of OSIRIS-AI module

➠It is now possible to easily utilise neural networks within OSIRIS simulations during run-time.

➠Further work is currently being done on optimising the AI library. Specially focused on taking advantage of the the parallelisation of matrix multiplication in HPC systems.

References

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