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ABSTRACT:

This document describes the collaboration of Dr Jian Fuh Ong from Extreme Light Infrastructure for Nuclear Physics, (ELI-NP), Romania, and Associate Prof. Vasilis Dimitriou, from the Institute of Plasma Physics & Lasers – IPPL of the Hellenic Mediterranean University-HMU in Crete, Greece, which started under the HPC-Europa3 transnational access visit. This visit resulted to the establishment of a Memorandum of Understanding (MoU) between the two institutes which was motivated by the need of optimizing the high-power laser experiments. The collaborative research work also advanced the modeling and simulations by using Graphics Processing Units (GPUs). The HPC-Europa3 project provided a strong international link and activated the collaboration between the two groups.

KEYWORD LIST: high-power laser-plasma, modeling, simulation, international collaboration, transnational access

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Executive summary

Dr Jian Fuh Ong from Extreme Light Infrastructure - Nuclear Physics (ELI-NP), Romania, visited the Institute of Plasma Physics and Lasers (IPPL) of the Hellenic Mediterranean University in Rethymnon, Greece, three times. The first two visits were partly funded by HPC-Europa3. These visits resulted to the establishment of a Memorandum of Understanding (MoU) between these two institutes which was motivated by the need of optimizing the high-power laser experiments with the help of advanced numerical models and simulations on High-Performance Computer (HPC) Infrastructures. These visits activated the collaboration of the two research Institutes. Moreover, the role of HPC-Europa3 in the collaboration is discussed.

Visits - joined forces and establishment of MoU

Dr Jian Fuh Ong from the Extreme Light Infrastructure - Nuclear Physics (ELI-NP) submitted a transnational access application in February 2019 in the 7th call of HPC-Europa3 to visit Associate Prof. Vasilis Dimitriou Institute of Plasma Physics & Lasers – IPPL of the Hellenic Mediterranean University-HMU. Associate Prof. V. Dimitriou leads the computational team of IPPL. The head of IPPL is Prof. M. Tatarakis. The research of the groups of ELI-NP and IPPL-HMU mainly focuses on the studying of the interaction of high-power laser-matter/plasma among other research topics.

To perform high-power laser-plasma experiments efficiently, several aspects such as possible outcomes, optimized configurations and the involved physical models have to be initially tested by numerical experiments. The use of Particle-In-Cell (PIC) simulations on HPC's offers reliable information on the processes within the plasma. The full PIC code solves Maxwell's equations and relativistic equations of motion of numerical particles and provides a close approximation to the real phenomena but demands extreme computational power. Therefore, attaining the optimum performance of the PIC codes on HPC infrastructures is of high importance. Associate Prof. V. Dimitriou aims to secure the efficiency and performance of the PIC code schemes on CPU and GPU architectures, for the simulation of two important experiments based on the high-power laser systems at IPPL-HMU and ELI-NP. The Target Normal Sheath Acceleration (TNSA) and the Laser Wakefield Acceleration (LWFA). These particles acceleration schemes serve as sources of radiation that subsequently lead to valuable applications. For example, high-quality x-ray and gamma-ray can be used for advanced medical treatments and diagnostics. Currently, such high-quality rays are normally generated by conventional km-sized accelerators. Development of compact particle acceleration schemes allows for the generation of high-quality radiation of tabletop size, making them cost-effective plasma devices.

The visits to IPPL were divided into two rounds under a single HPC-Europa3 application. The first visit was in June 2019 and the second visit was in October 2019, for three weeks each.

During the initial visit in June 2019, the team designed the setup of the experiments to simulate the TNSA and LWFA. The models are based on the 45 TW laser system of IPPL of HMU and the 100 TW and 10 PW laser systems of ELI-NP. Dr Jian Fuh Ong performed the LWFA simulations and the PhD candidate Giannis Tazes of IPPL performed the TNSA simulations. The reference numerical experiments were performed in two-dimensional (2D) domains, with the minimal computational resources demands. The scalability and performance of the simulations were then investigated. The optimal parameters derived by the 2D simulations were further used to the 3D simulations. The simulations were performed on the THIN nodes of the CPU architecture by using the EPOCH code developed by the plasma team at Warwick University, United Kingdom. Representative LWFA and TNSA 3D simulation results on the CPUs are depicted in Figure 1.
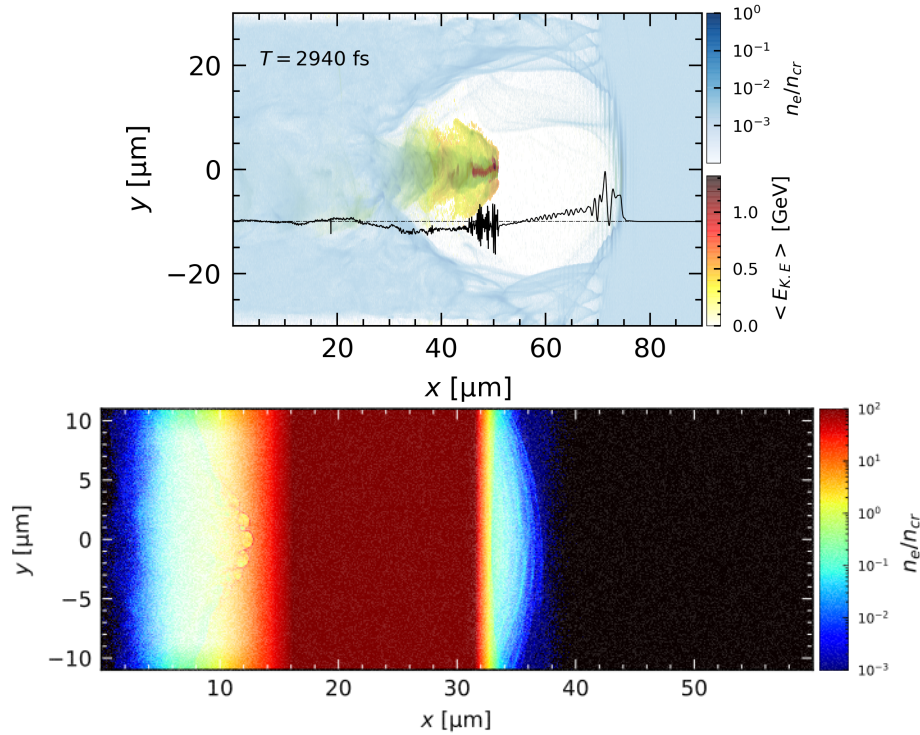
Figure 1: Simulation results of LWFA (top) and TNSA (bottom) on CPUs.

Furthermore, the PIC simulations models were set up on the GPUs architecture using the PIConGPU code. The models development and the setup of simulations on the GPUs was carried out in between the first and second HPC-Europa3 visits. In particular, Jian Fuh Ong received personal support from one of the developers of PIConGPU code, Axel Huebl, in a conference organized by European Physical Society in Milan, Italy. The installation of PIConGPU was further supported by the team of High-Performance Computer for Advanced Research Information System of the National Infrastructures for Research and Technology (HPC ARIS, GRNET), by creating a new module for PIConGPU.

It turned out that the collaboration and visit were successful and the leaders of both teams, Dr Ovidiu Tesileanu and Dr Vasilis Dimitriou agreed to propose signing a Memorandum of Understanding (MoU) between IPPL-HMU and ELI-NP.

During the second visit, in October 2019, Dr Jian Fuh Ong transferred the knowledge of GPU parallelization of the PIConGPU code to Giannis Tazes. The same reference numerical experiments were performed in two-dimensions (2D) with the minimum computational resource demands. Then, the scalability and performance of the PIC simulations were investigated. The parameters leading to the optimal performance in 2D simulations were used for the 3D simulations, as done for the CPUs architecture. Simulations were performed on GPU node island of ARIS using the PIConGPU code developed by the computational team at Helmholtz-Zentrum Dresden Rossendorf (HZDR), Germany.

The preliminary results of this study were presented in the TUMMIE, COST Action CA17126 meeting workshop held on February 17th & 18th 2020 at Warsaw, Poland [1,2].

This second visit marks the end of the HPC-Europa3 stage. However, further research work was needed for continuing the collaboration on the topics of mutual interest. This led Dr Jian Fuh Ong to apply for support from the COST Action TUMIEE that IPPL-HMU participates, supported by COST (European Cooperation in Science and Technology), as a Short-Term Scientific Mission (STSM) for a grant to visit again IPPL-HMU. The grant was approved and used for an STSM visit of one month during the March of 2020.

The 3D simulations produce a large amount of data and the post-processing becomes challenging. To simplify the processes, the simulation data were carefully selected. A Python script was written on Jupyter Notebook to visualize the data during the third visit. This script is based on the open-source visualization toolkits—openPMD, developed at HZDR by the same team of PIConGPU developers. At the moment, this script can only be used to visualize data generated from PIConGPU code. For the simulation using the EPOCH code, a different Python script was adopted.

In summary, optimal configurations and parameters for LWFA and TNSA simulations were identified for 2D and 3D models. On CPU architecture, we found sets of configuration parameters for which the simulations produced physically reliable results and the runtime of the simulations was significantly improved for the laser systems of 10, 100 PW of ELI-NP and 45TW of IPPL. On GPU architectures, the overall runtime was impressively reduced. These findings also apply for TNSA simulations with similar conclusions. The results are presented in the paper submitted for peer review entitled: "TNSA & LWFA PIC simulations performance on CPU & GPU architectures for high-power laser systems". These simulation findings provide the information needed for the choice of optimal parameters for modelling and simulations of laser/plasma accelerators with PIC codes on CPU and GPU HPC architectures.

An application for the 9th call on ARIS HPC system of GRNET, where Jian Fuh Ong participates as an external member, has already been submitted. Our common computational research findings will be applied to even more demanding computational models. The collaboration will be continued with the proposed new ideas for future experiments.

Role of HPC-Europa3

As a young scientist, Dr Jian Fuh Ong in Extreme Light Infrastructure - Nuclear Physics (ELI-NP), Romania, is expanding his research network in the field. It would be difficult for him to look for a host at foreign countries where they do not even know his scientific background and interests and since he is not aware of the scientific research and experience of his potential collaborators.

As an EC funded programme, HPC-Europa3 holds a large number of contacts and hosts with many success stories. Before the HPC-Europa3 application call, Jian Fuh and Vasilis had never met each other or collaborated in distance before. Their connection was achieved by the help of the support team of HPC-Europa3 in GRNET.

Vasilis and his research group were experienced users of the Greek HPC system (ARIS - High-Performance Computer for Advanced Research Information System of the National Infrastructures for Research and Technology). When Dr Jian Fuh Ong asked for advice while filling in his application for HPC-Europa3, Prof. Vasilis Dimitriou seemed to be a suitable collaborator. However, when proposing the collaboration, Dimitris Dellis, the head of HPC team in GRNET, could not imagine the matching of research interests of the two research institutes and the research confluence that finally come up. This is an excellent example of the HPC-Europa3 potentials, in bridging together two groups which had never met before, sharing the same passion in the same research field. Meeting up on site in turn, strengthens the collaboration between people, institutes and countries that work within the same research fields.

The collaboration initiated by HPCE3 does not end when the visits end. Active works are carrying on, in producing high quality research works and offering their outcomes to societies.

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