Application of the multicriterion optimization techniques and hierarchy of computational models to the research of ion acceleration due to laser-plasma interaction

I.N. Inovenkov, E.Yu. Echkina, V.V. Nefedov and L.S. Ponomarenko
Lomonosov Moscow State University, Department of Computational Math & Cybernatics, Leninskie gory, bld. 1/58, Moscow, 119991, Russian Federation
E-mail: vv_nefedov@mail.ru

Abstract. In this paper we discuss how a particles-in-cell computation code can be combined with methods of multicriterion optimization (in particular the Pareto optimal solutions of the multicriterion optimization problem) and a hierarchy of computational models approach to create an efficient tool for solving a wide array of problems related to the laser-plasma interaction. In case of the computational experiment the multicriterion optimization can be applied as follows: the researcher defines the objectives of the experiment - some computable scalar values (i.e. high kinetic energy of the ions leaving the domain, least possible number of electrons leaving domain in the given direction, etc). After that the parameters of the experiment which can be varied to achieve these objectives and the constrains on these parameters are chosen (e.g. amplitude and wave-length of the laser radiation, dimensions of the plasma slab(s)). The Pareto optimality of the vector of the parameters can be seen as this: \( \mathbf{x}^0 \) is Pareto optimal if there exists no vector which would improve some criterion without causing a simultaneous degradation in at least one other criterion. These efficient set of parameter and constrains can be selected based on the preliminary calculations in the simplified models (one or two-dimensional) either analytical or numerical. The multistage computation of the Pareto set radically reduces the number of variants which are to be evaluated to achieve the given accuracy. During the final stage we further improve the results by recomputing some of the optimal variants on the finer grids, with more particles and/or in the frame of a more detailed model. As an example we have considered the ion acceleration caused by interaction of very intense and ultra-short laser pulses with plasmas and have calculated the optimal set of experiment parameters for optimizing number and average energy of high energy ions leaving the domain in the given direction and minimizing the expulsion of electrons.

Keywords: computational experiment, mathematical modeling, multicriterion optimization problem, Pareto optimal set, laser pulse, laser-plasma interaction

Introduction
In the last twenty years laser-plasma interaction was a subject of a growing number of researches due to the theoretical and practical applicability of the results in medicine (e.g. hadronic therapy [1]), energy systems (e.g. nuclear fusion [2]) and some other applications. In this paper we discuss how a particles-in-cell computation code can be combined with the methods of multicriterion optimization (in particular the Pareto optimal solutions of the multicriterion optimization problem).
optimization problem) and a hierarchy of computational models approach to create an efficient tool for solving a wide array of problems related to the laser-plasma interaction. We also discuss some of the results obtain during the experimental runs of the computational system consisting of a relativistic PIC code (based on [3]) and a hierarchical Pareto-optimality based experiment scheduler.

1. Multicriterion optimization problem

The problem of multicriterion optimization is defined as follows: a vector of decision variables which satisfy constraints and optimizes a vector function whose elements represent the objective functions is to be found [4]. These functions form a mathematical description of performance criteria and they can be in conflict with each other. The solution of such a problem can be defined as follows: a vector of decision variables $x^0 \in X$ is Pareto optimal if there does not exist another $x \in X$ such that $f_i(x) \leq f_i(x^0)$ for all $i = 1, k$ and $f_j(x) < f_j(x^0)$ for at least one index $j$. Here, $X$ denotes the region of the problem where the constraints are satisfied. In most cases this definition will yield us not a single vector of decision variables but a set of Pareto optimal vectors, this set is called the Pareto optimal set.

In case of the computational experiment these definitions can be read as follows: the researcher defines the objectives of the experiment – some computable scalar values (i.e. high kinetic energy of the ions leaving the domain, least possible number of electrons leaving domain in the given direction, etc). In this paper it is assumed that all the objectives are equally significant to the researcher’s cause yet this restriction can be circumvented when needed to. After that the parameters of the experiment which can be varied to achieve this objectives and the constrains on these parameters are chosen (for example, amplitude and wave-length of the laser radiation, dimensions of the plasma slab(s)). The Pareto optimality of the vector of the parameters can be seen like this: vector $x^0$ is Pareto optimal if there exists no vector $x \in X$ which would decrease some criterion without causing a simultaneous increase in at least one other criterion.

These efficient set of parameters and constrains can be selected based on the preliminary calculations in the simplified models (one or two-dimensional) either analytical or numerical. As it can be seen the number of possible combinations of the parameter values in most cases will exceeds capabilities of the contemporary and near-future computers even with the most strict discretization of the parameter values (if we have $N$ parameters with 100 possible values for each we get $100^N$ possible variants) thus further optimization is still needed.

As a means of such an optimization the following approach can be chosen: we split the process of the problem solving into several stages. During the first stage we solve the problem with the coarse discretization of the parameters’ values and compute the Pareto optimal set. Then we add finer distributed parameter values in the vicinity of the vectors in the Pareto set and solve the problem for these finer distributed decision variables. The process can be repeated several times until we get the needed accuracy for the parameters’ distribution. For the $N$ parameters and 2 stages we can achieve nearly the same accuracy as with $100^N$ variants with just $2 \times 100^N$ calculations (or if the initial domain is wide and we expect serious deviations in results $C \times 100^N$ calculations where $C$ is the number of unique Pareto-optimal variants on all steps). As the finishing stage we can recompute some of the variants on the finer grids and/or with more particles to verify the results.

2. Some computational results of a laser-plasma interaction

We have tested the described experiment scheduling algorithm in the problem of finding a mode of interaction of the single pulse with the plasma foil which permits us to obtain the maximal energy of ions propagating in the same direction as the laser pulse with the constraint of keeping the energy of electrons leaving the vicinity of initial plasma domain as low as possible.
This problem can be interpreted as the problem of the multicriterion optimization with two criteria: 

\[ W_1 \rightarrow \max \quad \text{and} \quad W_2 \rightarrow \min, \]

where \( W_1 \) is the energy of ions blown out of the domain and \( W_2 \) is the electron energy.

In all computational experiments performed we have considered a laser with a wave length of 1.0 micron and wave period of 3.3 femtoseconds. Ratio of ion to electron mass has been set to 1836 and ratio of plasma electron frequency to pulse frequency has been set to 0.41. The domain in which we have performed our calculations had the size of \( 200 \lambda \times 60 \lambda \) and the initial plasma domain occupied a quarter of that.

We have chosen the following 3 parameters for variation – dimensionless amplitude of the pulse \( a_0 = eE_0 / m_e c \omega \) in \([0.5, 5.0]\) (corresponds to intensity around of \(10^{18} - 10^{19} W/cm^2\)), \( y\) - polarization of the impulse in \(OyZ\) \(([0.1, 0.9])\) and the time moment when the pulse is switched off (from 5 to 55 periods).

We have made 4 iterations. During the first three iterations of the Pareto optimization procedure we have performed 322 computational experiments with the \(10^6\) electrons and ions in the domain and \( \Delta_{x,y} = 0.1 \lambda \), for each parameter we have chosen 5 values at which it’s impact has been estimated by scheduler. Thus on the first iteration we have performed 125 experiments. Based on the results of these experiments a Pareto set has been formed and a single Pareto-optimal vector of parameters has been chosen – it was the following components \( a_0 = 2.75 \), \( y\) - polarization is 0.7, switch off time is 38.75 and \( W_1 / W_2 \) is approximately 2.

For the second iteration we have repeated all the action of the first step but we have redistributed the evaluation points around the Pareto-optimal vector from the previous step, i.e. we have been selecting our new evaluation points from the region \([1.625, 3.875] \times [0.5, 0.9] \times [27.5, 55.0]\). We do not change the computational model or accuracy of computation for this step thus we can safely omit the values computed during the previous iterations. Total number of experiments for this iteration is 98 (we evaluate each individual parameter in 5 points and some of the combinations are already computed during the previous step). After the second iteration the vector chosen for further investigation is \((a_0 = 3.03125, \quad y\) - polarization = 0.7, switch off time = 41.125\) and \( W_1 / W_2 \) exceeds 3.5 and gives \( W_1 \) of \(1.2 \times 10^8\).

On the third iteration another 98 experiments are performed but the vector \((a_0 = 3.03125, \quad y\) - polarization = 0.7, switch off time = 41.125\) is still in the Pareto set and is selected for the next iteration.

During the final fourth iteration the Pareto-optimal vector has been evaluated once more with higher precision – \(10^9\) electron and ion pairs are distributed in the plasma domain \( \Delta_{x,y} = 0.05 \lambda \).
The results of numerical computations are shown on the Figures 1 and 2. These figures demonstrate us the distribution of the electron and ion densities obtained for one of the Pareto optimal vectors and also the formation of jet streams of accelerated heavy ions is clearly visible. It can be seen on the Figure 2 that ion density is maximal along the axis of laser pulse propagation in the plasma with the slight sinusoidal variation in distance from the strait line through the domain. This propagating zone of high ion density is what leads to the high energy of ion beams which guarantee the high value of $W_I$.

3. Conclusions
The use of multicriteria optimization methods in selecting the conditions of a computational experiment makes it possible to effectively use the hierarchy of models and make the selection of the best values of the parameters using the Pareto optimal solution methodology. The experimental application of our computational approach confirmed its effectiveness with respect to the problem of optimizing a computational experiment on the interaction of ultra-short laser pulses with matter.

References
[1] Bulanov S.V., Esirkepov T.Zh., Khoroshkov V.S., Kuznetsov A.V. and Pegoraro F. Oncological hadrontherapy with laser ion accelerators // Physics Letters A. 2002. Vol. 299. Issues 2-3. P.P. 240-247.
[2] Terranova F., Bulanov S.V., Collier J.L., Kiriyama H., Pegoraro F. Enabling pulse compression and proton acceleration in a modular ICF driver for nuclear and particle physics applications // Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment. 2006. Vol. 558. Issue 2. P.P. 430-436.

[3] Esirkepov T.Zh. Exact charge conservation scheme for particle-in-cell simulation with an arbitrary form-factor // Computer Physics Communications. 2001. Vol. 135. N 2. P.P. 144–153.

[4] Zhukovskiy V.I., Salukvadze M.E. The Vector-Valued Maximin (In Series: Mathematics in Science and Engineering (Vol. 193), Edited by William F. Ames, Georgia Institute of Technology). New York: Academic Press, Inc. 1994. 404 P.