NEW COMPUTATIONAL PHYSICS APPLICATIONS: PARALLEL APPROACH TO NONLINEAR EFFECTS IN BEAM DYNAMICS *

M. GIOVANNOZZI†

INFN, Sezione di Bologna, V. Irnerio 46
Bologna, I-40126, Italy

E. MCINTOSH
CERN, IT Division
Geneva, CH-1211, Switzerland

G. FRANCHETTI
GSI, Planckstr. 1
Darmstadt, D-64291, Germany

G. TURCHETTI
Physics Dept. University of Bologna, V. Irnerio 46
Bologna, I-40126, Italy

We present the results obtained in the analysis of the motion of noninteracting charged particles under the influence of nonlinear forces in circular accelerators using parallel techniques. A key parameter in the definition of the machine performance is the so-called dynamic aperture (DA). This quantity represents the volume in phase-space where stable motion occur. The evaluation of such a volume requires CPU-intense numerical simulations. We show that it is possible to design parallel algorithms to speed-up the computations. Furthermore these algorithms are fully scalable.
Furthermore, we discuss possible applications of these new techniques in the computation of beam stability under the combined effect of nonlinear external forces and electromagnetic interaction between the particles.

1. INTRODUCTION

The new generation of particle accelerators can be divided into two groups: the first includes the high energy machines, such as the planned Large Hadron Collider [1], while the second includes the high intensity machines. The first class is intended to test the standard model. Due to the high energy, in order to reduce the overall size of the machine, it is mandatory to use superconducting magnets to

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†e-mail address: giovannozzi@bologna.infn.it

guide the charged particle along the machine circumference. This introduces strong nonlinear magnetic field errors, due to the rather poor field quality of superconducting magnets. Hence the motion becomes highly nonlinear and instabilities are generated, reducing the beam lifetime and the overall machine performance.
As far as the high intensity machines are concerned, they are mainly devoted to the study of inertial fusion or nuclear waste incineration. In this case the main source of concern is given by the strong interaction between particles in the beam. Once again this generates nonlinear forces and instabilities.
New tools are needed to study these complex nonlinear phenomena, and in the recent years, a big effort was devoted to the development of analytic tools to analyze the beam stability [2]. It turned out the the best technique is represented by normal forms. This is a perturbative approach allowing to analyse the phase-space topology and the dynamics in a neighbourhood of the origin. The main drawback of this approach, is that near the border of the so-called dynamic aperture (DA), i.e. the region in phase-space where stable motion occurs, the perturbative series defining normal forms start to show-up their divergent character. This is the most interesting region of phase-space, because in this domain originates the instability producing the particle losses. Therefore a detailed picture of this volume of phase-space allows some insight to the particle dynamics. This improved knowledge can be obtained by using numerical simulations in conjunction with sophisticated tools to reconstruct the phase-space properties, such as tune analysis [3].
In the first part of this paper we report on new results obtained in the evaluation of the dynamic aperture using parallel algorithms. As a first step we give a rigorous definition of DA, and then we propose a method to compute it in a sequential as well as in a parallel way. Furthermore we will show that the parallel algorithm is fully scalable.
The second part is devoted to a discussion on future applications which could benefit from the availability of parallel computers.

2. EVALUATION OF DYNAMIC APERTURE

2.1. *Definition and numerical computation*

The 4D nonlinear betatronic motion in a particle accelerator can be conveniently described by using 4D symplectic mappings[2]. If we use canonical coordinates $\mathbf{x} = (x, p_x, y, p_y)$ to express the particle position at a given section of the circular machine, then the coordinates after one turn $\mathbf{x}' = (x', p_x', y', p_y')$ are given by

$$\mathbf{x}' = \mathbf{F}(\mathbf{x}) \qquad \mathbf{x} = (x, p_x, y, p_y). \tag{1}$$

The position of the particle after N turns around the machine is simply obtained by the repeated application of equation (1) N times. The linear motion is given by the direct product of two constant rotations in the planes (x, p_x) and (y, p_y) by the

frequencies ν_x and ν_y also called the linear tunes of the machine.
To define the dynamic aperture, the first step is to consider the phase space volume of the initial conditions which are bounded after N iterations:

$$\int\int\int\int \chi(x, p_x, y, p_y)\, dx\, dp_x\, dy\, dp_y, \tag{2}$$

where $\chi(x, p_x, y, py)$ is the characteristic function of the set, i.e. it is unity if (x, p_x, y, p_y) is stable and zero otherwise.
To exclude the disconnected part of the stability domain in the integral (2), we have to use polar variables $(r_1, \vartheta_1, r_2, \vartheta_2)$: r_1 and r_2 are the linear invariants. It is customary to replace r_1 and r_2 with polar variables $r\cos\alpha$ and $r\sin\alpha$ (see Ref. [4] for more details). Having fixed α, ϑ_1 and ϑ_2, let $r_{last}(\alpha, \vartheta_1, \vartheta_2)$ be the last value of r whose orbit is bounded after N iterations. Then, the volume of the stability domain is

$$A_{\alpha,\vartheta_1,\vartheta_2} = \frac{1}{8}\int_0^{2\pi}\int_0^{2\pi}\int_0^{\pi/2} [r_{last}(\alpha, \vartheta_1, \vartheta_2)]^4 \sin(2\alpha)\, d\alpha\, d\vartheta_1\, d\vartheta_2. \tag{3}$$

In this way one excludes stable islands not connected to the main stable domain. The dynamic aperture will be defined as the radius of the hyper-sphere having the same volume as the stability domain:

$$r_{\alpha,\vartheta_1,\vartheta_2} = \left(\frac{2A_{\alpha,\vartheta_1,\vartheta_2}}{\pi^2}\right)^{1/4}. \tag{4}$$

To implement Eq. (3) as a computer code, one is forced to discretize the phase space variables $\vartheta_1, \vartheta_2, \alpha$ and r. If we consider a number of steps in the different variables given by $N_{\vartheta_1}, N_{\vartheta_2}, N_\alpha$ and N_r respectively, the dynamic aperture reads

$$r_{\alpha,\vartheta_1,\vartheta_2} = \left(\frac{\pi}{2N_\alpha N_{\vartheta_1} N_{\vartheta_2}} \sum_{i_\alpha=1}^{N_\alpha}\sum_{i_{\vartheta_1}=1}^{N_{\vartheta_1}}\sum_{i_{\vartheta_2}=1}^{N_{\vartheta_2}} [r_{last}(i_\alpha, i_{\vartheta_1}, i_{\vartheta_2})]^4 \sin(\frac{\pi i_\alpha}{N_\alpha})\right)^{1/4}, \tag{5}$$

where $r_{last}(i_\alpha, i_{\vartheta_1}, i_{\vartheta_2})$ is defined over a discrete set of values.
A detailed analysis of the errors introduced by the discretization of the phase-space variables was carried out in Ref. [4], together with a refined algorithm allowing to reduce the computational burden by avoiding the explicit scan on the variables (p_x, p_y).

2.2. *Parallel algorithms to evaluate the DA*

The computations needed to compute the Da, can be split into two stages: in the first one the last stable radius, as a function of the phase space parameters, is determined, and then the final formula (5) is evaluated, corresponding to the computation of an average value of r. This suggests that a possible approach to

implement a parallel algorithm would be to assign the initial conditions obtained by scanning over the phase-space variables to different processors, in order to determine the stability of each initial condition. Then, once all the processors have finished, the results could be gathered to evaluate the sums (5). In Ref. [5] we have discussed the issues involved in the design of a parallel algorithm to compute the DA, such as load-balance between the different processors and various options to implement the algorithm.
In Fig. 1 we present the main result obtained: it represents the total CPU-time used to compute the dynamic aperture, as a function of the number of processors. It is apparent how the algorithm implemented is perfectly scalable. Up to the maximum number of processors used in the simulations, we observe a reduction of the CPU-time in agreement with the expected value.
Different implementations have been tested, but they all show the same asymptotic behaviour. The main difference in the performance concerns the load-balance (see Ref. [5] for more details).

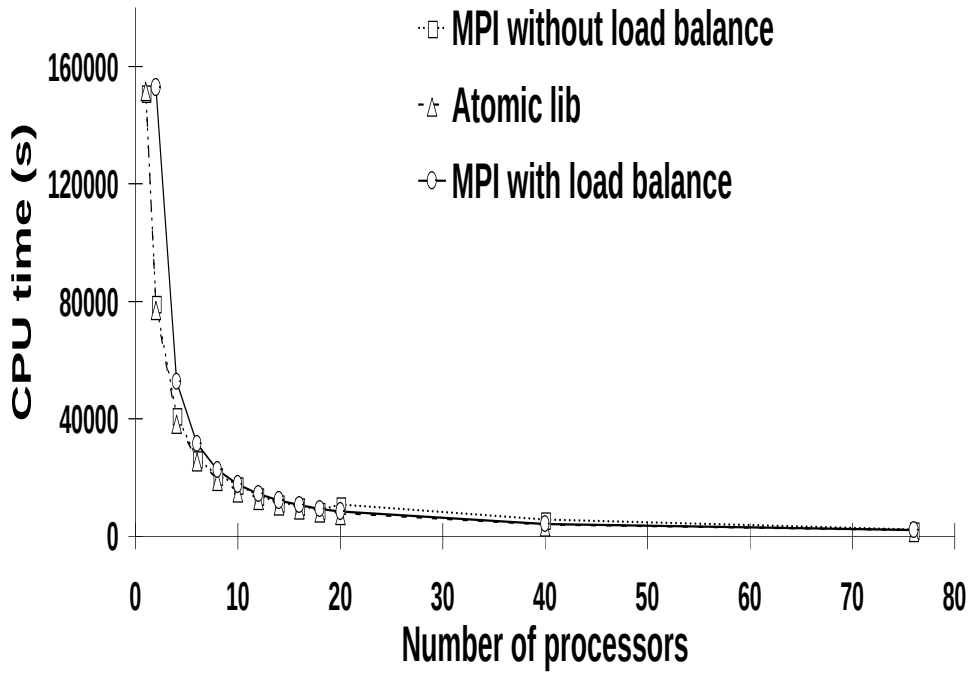

Figure 1: Performances of the first parallel algorithm. The total CPU-time is depicted as a function of N_{proc}. Different implementation schemes are shown.

3. NEW PERSPECTIVES

To compute the DA using the approach described in the previous Section the

typical values of the parameters are $N_{part} \approx 10^3 - 10^4$ and $T \approx 10^3$, where N_{part} stands for the number of particles used and T represents the number of iterations. In this Section we report on possible applications in different fields of accelerator physics, namely, the evaluation of the resonance network in the phase-space describing the particle motion, the study of transport phenomena due to deterministic or stochastic effects and the analysis of space-charge effects in particle accelerators.

3.1. *Analysis of nonlinear resonances*

A possible source of instability is given by nonlinear resonances. These occur when the frequencies of the motion in phase-space (which is a function of amplitude due to the presence of nonlinear effects [2]) satisfy a resonance condition of the type

$$n\nu_x + m\nu_y = p, \qquad \text{with } n, m, p \text{ integers.} \tag{6}$$

The resonance network, i.e. the plot of the initial conditions satisfying a resonant condition as a function of the phase-space amplitude or nonlinear invariants [6,7], proved to be a powerful tool in the analysis of the phase-space topology. This information can be obtained either using numerical simulations using refined tools to measure the nonlinear frequencies [3], or analytical computations based on normal forms [8,9]. In both cases, to obtain meaningful results it is necessary to use at least 10^4 initial conditions iterated for 10^3 turns in the case of numerical simulations. Therefore, the parameters are similar to the evaluation of the DA. Hence the same approach could be successfully applied to improve the efficiency in the computation of the resonance network.

3.2. *Transport problems*

Another interesting issue in the domain of nonlinear dynamics applied to circular machines is the study of particle transport due to variation of some parameters in the machine in conjunction with the presence of nonlinear effects. A typical example is the modulation of the quadrupolar strength due to a ripple in the power supply of the magnets. This induces a tune variation (also called tune modulation) which could lead to a substantial reduction of the DA of a machine. In the real case the modulation is produced by a superposition of a 50Hz component plus some harmonics. Therefore the perturbing effect is purely deterministic. In the case of a large number of periodic components, the overall effect tends to simulate a stochastic perturbation. For this reason, the analysis of the diffusion processes simulating the time evolution of an ensemble of noninteracting particles in a circular machine under the influence of periodic or stochastic perturbation [10,11], is of some interest. We would like to stress the fact that in parallel with the theoretical studies, some experiments have been carried out in recent years [12,13,14] to measure such effects in real machines.

The problem requires the solution of a Vlasov equation describing the evolution of the beam distribution. This can be performed by tracking a certain number of particles in the distribution to determine the global evolution. To ensure a good confidence level in the outcome of the computation it is mandatory to track no less than 10^4 particles. As far as the time evolution is concerned, the number of temporal steps depend on the phenomenon considered. In the case of stochastic perturbation 10^3 steps are enough as one can apply a rescaling to the time variable [11]. The situation is more delicate in the case of a deterministic modulation. In fact in this one has to take into account the different time scales. Hence the simulations must be performed for at least 10^4 turns. Once again the set of parameters is comparable with that used in the evaluation of the DA, and, furthermore, the particles are still noninteracting. This allows a simple generalisation of the approach described in the previous Section, namely each processor should take care of a different initial condition and should compute its evolution with time.

3.3. *Space-charge effects*

The analysis of space-charge effects in the particle motion represents the most challenging issue, amongst those described in this Section. In fact, in this case the particles are interacting with each other through the Coulomb force. Therefore, the straightforward generalization of the approach described to evaluate the DA does not work anymore. Some attempts to use a parallel approach to solve this problem can be found in the literature [15,16,17], but we believe there are still many open problems.

The starting point is the definition of the model, that, for simplicity will be considered two dimensional. The starting point is the definition a a set of N_{part} particles $x_1(0), \ldots x_{N_{part}}(0)$ representing the initial distribution. They will be called *superparticles*. The magnetic channel is made up by linear elements interleaved with nonlinear elements (which we will always represent in the kick approximation). The linear elements will be divided into a given number of slices, and the space-charge force will be evaluated at the entrance of every slice. The evolution of each superparticle will be given by

$$\begin{pmatrix} x_i(n+1) \\ p_i(n+1) \end{pmatrix} = \mathbf{M}_n \begin{pmatrix} x_i(n) \\ p_i(n) + \tau \sum_{j=1}^{N_{part}} F(|x_i(n) - x_j(n)|) \end{pmatrix} \tag{7}$$

where $\mathbf{M}_n$ represents the transfer matrix of the $n-th$ slice of the linear element $\mathbf{M}$, τ is an integration step related with the number of slices used to represent the element $\mathbf{M}$, and F gives the space-charge contribution from the different superparticles. For a model where the superparticles are considered as short charged segments of length $2L$ at a distance r and with charge density ρ, F takes the form

$$F = -\rho^2 \log(1 - \frac{4L^2}{r^2}). \tag{8}$$

In the limit $L/r \to 0$, F tends to the standard form of the Coulomb force. Eq. (7) actually represents a set of N_{part} coupled equations, giving the evolution of the set of superparticles.
To find an efficient parallel algorithm to determine the evolution of the particle distribution using Eq. (7) requires the solution of the following issues:

- one needs to find a criterion to define the number of slices to be used in the computation of the particle evolution. This is a critical parameter, because it determines the CPU-time per turn;

- it is customary to consider thick nonlinear magnetic elements using the so-called kick approximation (see Ref. [2] for more details), namely the considered element is replaced by a sequence of drift spaces and kicks. Although this approach generates only an approximate solution to the true equation of motion, it preserves the symplectic character of the dynamics. Furthermore the precision of the results can be tuned by increasing or decreasing the number of kicks used. In most applications, however, a single kick is enough to obtain accurate results. In the case of space-charge effects, one has to check whether a single kick approximation produces correct answers, and possibly one should define a criterion to determine the number of kicks needed in order to obtain a given precision in the simulation results;

- an efficient way to compute the space-charge term has to be found. A possible solution would be to interpolate F using the standard approach based, for instance, on splines. Therefore, one can build up a table to be used in the computation of the interaction term, thus reducing the number of function evaluations from N_{part}^2 to N_{part};

- to compute the space-charge force, one needs to know the coordinates of all the superparticles. This implies a global synchronisation of all processes and a good load balance when the the number of superparticles is large compared to the number of processors. Some tests have to be carried out to decide the best approach, namely a master slave structure of the algorithm (see for example Ref. [5]) based, for instance, on MPI [18,19,20], or a different technique based on the shared memory properties of the machine used for the simulations.

4. CONCLUSIONS

We have presented the results of a study aimed at applying a parallel approach to the analysis of the nonlinear motion in particle accelerators. As far as the computation of the dynamic aperture is concerned, we have shown that it is possible to design an efficient parallel algorithm.
Furthermore, we have pointed out a list of different topics in the field of nonlinear dynamics applied to accelerator physics, which could benefit from the parallel paradigm. In particular the analysis of space-charge effects seems to be extremely

promising for a fruitful application of parallel algorithms.

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