A FAST AND UNIVERSAL VLASOV SOLVER FOR BEAM DYNAMICS SIMULATUONS IN 3D*

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Abstract

The Vlasov equation can describe the evolution of a particle density under the effects of electromagnetic fields and thus it is possible to describe the evolution of a charged particle beam within an accelerator beam line. The Vlasov equation forms a partial differential equation in a 6D phase space witch renders it very expensive if it is solved via classical methods. A more efficient approach consists in representing the particle distribution function by a discrete set of characteristic moments. For each moment a time evolution equation can be stated. These ordinary differential equations can then be integrated efficiently by means of numerical methods if all acting forces together with a proper initial condition are given. The beam dynamics simulation tool V-Code has been implemented at TEMF on the basis of the moment approach. In this paper the numerical model, main features and designated use cases of the V-Code will be presented.

INTRODUCTION

The distribution of particles in the 6-dimensional (6D) phase space can be described by a density distribution function $f(\vec{r},\vec{p},\tau)$ with space coordinates $\vec{r}=(x,y,z)$, normalized momentum $\vec{p}=(p_x,p_y,p_z)$ and equivalent time $\tau = c\cdot t$. Their evolution in the phase space can then be expressed by the Vlasov equation

$$\frac{\partial f}{\partial \tau}+\frac{\partial f}{\partial \vec{r}}\cdot\frac{\vec{p}}{\gamma}+\frac{\partial f}{\partial \vec{p}}\cdot\frac{\vec{F}}{m_0c^2}=0 \qquad (1)$$

where γ represents the relativistic factor, $\vec{F}$ the applied forces, m_0 the particles rest mass and c the speed of light in free space.
Equation (1) is applicable for any forces $\vec{F}$ with slow variation in space [2]. Coulomb forces within an charged particle beam as well as forces from external electromagnetic fields meet this condition. Thus, the Vlasov equation is applicable for beam dynamics simulations of charged particle beams in accelerators.
It is very expensive to solve such a partial differential equation via classic numerical methods for a time varying 6D density distribution function.

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MOMENT APPROACH

A more efficient approach is to consider a discrete set of characteristic moments of the particle distribution function instead of the function itself [3]. Following this approach the problem can be reduced to a set of ordinary differential equations which can be evaluated by means of standard time integration methods.

Moment Definition

The classical raw moments $<\mu>$ are obtained from the distribution function f by a weighted integration over the whole phase space Ω

$$<\mu>=\int_\Omega \mu\ f(\vec{r},\vec{p},\tau)\ \mathrm{d}\Omega. \qquad (2)$$

Here, the normalized density distribution function to ensure

$$1\stackrel{!}{=}<1>=\int_\Omega f(\vec{r})\ \mathrm{d}\Omega \qquad (3)$$

has to be applied for proper algebraic relations.

A numerically advantageous choice of moments witch ultimately allows the determination of the overall position and the overall momentum of a particle distribution is given by the first order raw moments

$$\mu\in\{x,y,z,p_x,p_y,p_z\} \qquad (4)$$

in Cartesian coordinates.

By choosing the higher order moments in a centralized notation

$$\mu\in\{(x-<x>)^{l_1}\cdot\ \ldots\ \cdot(p_z-<p_z>)^{l_6},\ \ldots\} \qquad (5)$$

one automatically obtains a translatory invariant description of the shape of the particle distribution function.
For example, a subset of the second order moments

$$\begin{aligned}\sigma_x{}^2 &= <(x-<x>)^2>\\ \sigma_y{}^2 &= <(y-<y>)^2>\\ \sigma_z{}^2 &= <(z-<z>)^2>\end{aligned}$$

then identify the important variances of the underlying particle distribution.

Moment Evolution

The time evolution of the moment parameters can be expressed as follows:

$$\frac{\partial <\mu>}{\partial \tau} = \frac{\partial}{\partial \tau}\int \mu f \, \mathrm{d}\Omega = \int (f\frac{\partial \mu}{\partial \tau} + \mu \frac{\partial f}{\partial \tau}) \, \mathrm{d}\Omega. \quad (6)$$

Here, the Vlasov equation can be used to completely eliminate the time derivative of the distribution function and substitute it with a spatial expression instead:

$$\frac{\partial f}{\partial \tau} = -(\frac{\partial f}{\partial \vec{r}} \cdot \frac{\vec{p}}{\gamma} + \frac{\partial f}{\partial \vec{p}} \cdot \frac{\vec{F}}{m_0 c^2}). \quad (7)$$

Further, the time derivative of the moment parameter can be reformulated like

$$\frac{\partial \mu}{\partial \tau} = \frac{\partial \mu}{\partial <\vec{r}>} \frac{\partial <\vec{r}>}{\partial \tau} + \frac{\partial \mu}{\partial <\vec{p}>} \frac{\partial <\vec{p}>}{\partial \tau}. \quad (8)$$

Inserting (7) and (8) in equation (6) and applying a partial integration together with the moment definition (2) allows to state the following fundamental time evolution equation

$$\begin{aligned}\frac{\partial <\mu>}{\partial \tau} = &< \frac{\partial \mu}{\partial <\vec{r}>} >< \frac{\vec{p}}{\gamma} > + < \frac{\partial \mu}{\partial <\vec{p}>} >< \frac{\vec{F}}{m_0 c^2} > \\ &+ < \frac{\partial \mu}{\partial \vec{r}} \frac{\vec{p}}{\gamma} > + < \frac{\partial \mu}{\partial \vec{p}} \frac{\vec{F}}{m_0 c^2} > \end{aligned} \quad (9)$$

In order to enable the evaluation of (9) by means of a time integration method all arguments on the right hand side have to be expressed in terms of time dependent bunch parameters i.e. by moments of the settled form. This can be achieved by Taylor expanding $\frac{1}{\gamma}$ and $\vec{F}$ in an operation point defined by the particle distribution and utilizing a truncation according to the regarded order of moments.

If the energy spread is small compared to the mean energy of the whole bunch a linear approximation of γ is adequate

$$\gamma = \sqrt{1 + {p_x}^2 + {p_y}^2 + {p_z}^2} \quad (10)$$

but in general higher order forms are possible.

The series expansion for internal space charge forces and forces due to external fields can be performed independently. External fields are observed in radio frequency cavities (RF-cavities) or any kind of magnetic multipole for example.

External Field Representation

From the Maxwell equations in frequency domain and isotropic homogeneous linear media one can describe the fields within RF-cavities in cylindrical coordinates:

$$\begin{aligned} \underline{E}_r &= \frac{-1}{j\omega\varepsilon}\frac{\partial \underline{B}_\varphi}{\partial z}, & \underline{B}_r &= \frac{1}{j\omega}\frac{\partial \underline{E}_\varphi}{\partial z} \\ \underline{E}_\varphi &= \frac{1}{j\omega\mu\varepsilon}(\frac{\partial \underline{B}_r}{\partial z} - \frac{\partial \underline{B}_z}{\partial r}), & \underline{B}_\varphi &= \frac{-1}{j\omega}(\frac{\partial \underline{E}_r}{\partial z} - \frac{\partial \underline{E}_z}{\partial r}) \\ \underline{E}_z &= \frac{1}{j\omega\mu\varepsilon}\frac{1}{r}\frac{\partial (r\underline{B}_\varphi)}{\partial r}, & \underline{B}_z &= \frac{-1}{j\omega}\frac{1}{r}\frac{\partial (r\underline{E}_\varphi)}{\partial r} \end{aligned} .$$

In this formulation the field components $\underline{B}_r$, $\underline{E}_\varphi$, $\underline{B}_z$ are completely decoupled from $\underline{E}_r$, $\underline{B}_\varphi$, $\underline{E}_z$. Within accelerating cavities it is appropriate to consider the latter ones exclusively.
By defining $\vec{B} = \mathrm{curl}\vec{A}$ and applying Bernoulli's separation approach

$$\vec{\underline{A}}(r,z) = \vec{e}_z \underline{A}_z(r,z) = \vec{e}_z \sum_{i=0}^{\infty} \underline{A}_i(z) r^i \quad (11)$$

it is possible to describe $\underline{E}_r$, $\underline{B}_\varphi$, $\underline{E}_z$ solely with derivatives of the z-component of the vector potential $\vec{A}$

$$\underline{B}_\varphi = -2\underline{A}_2 \cdot r - 4\underline{A}_4 \cdot r^3 - 6\underline{A}_6 \cdot r^5 - \ldots \quad (12)$$

$$\underline{E}_r = \frac{1}{j\omega\mu\varepsilon}\left(2\underline{A}_2' \cdot r + 4\underline{A}_4' \cdot r^3 + 6\underline{A}_6' \cdot r^5 + \ldots\right) \quad (13)$$

$$\underline{E}_z = \frac{-1}{j\omega\mu\varepsilon}\left(4\underline{A}_2 + 16\underline{A}_4 \cdot r^2 + 36\underline{A}_6 \cdot r^4 + \ldots\right). \quad (14)$$

Evaluation on the axis ($r = 0$) results in

$$\underline{E}_z|_{r=0} = -\frac{4 \cdot \underline{A}_2}{j\omega\mu\varepsilon}, \quad (15)$$

which allows to determine the coefficients consecutively

$$\begin{aligned} \underline{A}_2 &= -\tfrac{1}{4} j\omega\mu\varepsilon \cdot \underline{E}_z|_{r=0} & (16)\\ \underline{A}_4 &= \tfrac{-1}{16} \cdot \left(\underline{A}_2'' + \omega^2\mu\varepsilon\underline{A}_2\right) & (17)\\ \underline{A}_6 &= \tfrac{-1}{36} \cdot \left(\underline{A}_4'' + \omega^2\mu\varepsilon\underline{A}_4\right) & (18)\\ &\vdots \quad . \end{aligned}$$

By successively inserting the coefficients in (12) - (14) one obtains the field components in cylindrical coordinates in terms of a series expansion

$$\underline{B}_\varphi = \tfrac{1}{2} j\omega\mu\varepsilon\, \underline{E}_{z0}\, r - \tfrac{1}{16} j\omega\mu\varepsilon\left(\underline{E}_{z0}'' + \omega^2\mu\varepsilon\, \underline{E}_{z0}\right) r^3 + \ldots \quad (19)$$

$$\underline{E}_r = -\tfrac{1}{2}\, \underline{E}_{z0}'\, r + \tfrac{1}{16}\left(\underline{E}_{z0}''' + \omega^2\mu\varepsilon\, \underline{E}_{z0}'\right) r^3 + \ldots \quad (20)$$

$$\underline{E}_z = \underline{E}_{z0} - \tfrac{1}{4}\left(\underline{E}_{z0}'' + \omega^2\mu\varepsilon\, \underline{E}_{z0}\right) r^2 + \ldots . \quad (21)$$

The function of this expansion constitute the paraxial approximation of the field distribution within a RF-cavity.

For multipole magnets a similar approach to approximate the three dimensional field distribution inside the source free vacuum tube is possible. The Maxwell equations for magnetostatic problems in source free vacuum areas can be reduced to the following equations:

$$\begin{aligned} \mathrm{curl}\ \vec{B} &= 0 & (22)\\ \mathrm{div}\ \vec{B} &= 0. & (23) \end{aligned}$$

This allows to state the scalar potential equation

$$\Delta V = \mathrm{div\ grad}\ V = 0 \quad \text{with} \quad \vec{B} = -\mathrm{grad}\ V. \quad (24)$$

Applying Bernoulli's separation approach together with a series expansion for magnetic 2n poles leads to

$$B_r = (r^{n-1}\,\alpha(z) - \frac{(n+2)\,r^{n+1}\,\alpha''(z)}{4(n+1)n} + \ldots)\cdot \sin(n\varphi) \tag{25}$$

$$B_\varphi = (r^{n-1}\,\alpha(z) - \frac{r^{n+1}\,\alpha''(z)}{4(n+1)} + \ldots)\cdot \cos(n\varphi) \tag{26}$$

$$B_z = (\frac{r^n\,\alpha'(z)}{n} - \frac{r^{n+2}\,\alpha'''(z)}{4(n+1)n} + \ldots)\cdot \sin(n\varphi) \tag{27}$$

with the multipole strength α along the longitudinal axis z.

Force Calculation

The forces resulting from the external fields can now be calculated by applying the Lorentz equation

$$\vec{F} = q(\vec{E} + \vec{v}\times\vec{B}). \tag{28}$$

As stated before the terms $<\vec{F}>$ and $<\mu\vec{F}>$ in (9) have to be expanded such that the resulting expression can be used to setup a moment description form.
A multipole expansion splits the force naturally in constant, linear, quadratic, etc. terms. By applying the moment definition (2) they can be expressed as follows:

- For constant forces $F_\nu = a$ one gets $<F_\nu>= a$ and $<\mu F_\nu>= 0$.
- For linear forces $F_\nu = b\mu$ one gets $<F_\nu>= 0$ and $<\mu F_\nu>= bM_{\mu\mu}$.
- For quadratic forces $F_\nu = c\mu^2$ one gets $<F_\nu>= cM_{\mu\mu}$ and $<\mu F_\nu>= cM_{\mu\mu\mu}$

Hence, the order of the moments has to be at least one order higher then that of the significant terms of the multipole expansion.

Space Charge Forces

In order to determine the space charge forces a model to reconstruct the charge distribution within the particle bunch from the moment description is needed. The simplest approach is to assume a homogeneously charged ellipsoidal bunch. Starting from the force acting between two particles moving together with constant speed one gets the space charge force $F(\vec{r})$ in an arbitrary point of observation $\vec{r}$ within the bunch by integrating over the bunch volume. In order to avoid the singularities of the integrand in the proximity of the point of observation one can omit a symmetric area surrounding this point when integrating. Within this area the space charge forces compensate themselves. Following this approach one gets

$$\vec{F}\,(\vec{r}) \approx G\left(\frac{2\gamma\sigma_z}{\sigma_x+\sigma_y}\right)\cdot\frac{eQ_0}{\gamma^2}\cdot\frac{\vec{r}-\langle\vec{r}\rangle}{V_\mathrm{G}} \tag{29}$$

with

$$G\,(u) = (1-\exp\,(-u))\cdot\begin{pmatrix}1&0&0\\0&1&0\\0&0&\gamma/u\end{pmatrix}. \tag{30}$$

The moment approach is not limited to this linear space charge model. The particle density reconstruction can also be done by other techniques like moment matching or the maximum entropy method.

Time Integration

The time evolution of all moments $<\mu>$ is specified by the stated set of fundamental differential equations (9). By defining a single comprehensive vector $\vec{\psi}$ which includes all considered moments one can state the new time dependent variable $\vec{\psi}(t)$. The whole physical model can then be written in the standard mathematical form

$$\vec{\psi}'(t) = \vec{\phi}(t,\vec{\psi}(t)),\ \vec{\psi}(t_0) = \vec{\psi}_0, \tag{31}$$

where $\vec{\psi}'$ denotes the time derivative and $\vec{\phi}$ summarizes all kinematic and kinetic effects of the forces mentioned above. If an initial set of moments $\vec{\psi}_0$ is provided the problem can be solved by standard time integration methods [1].

Multi Ensembles

In order to reproduce more complex particle interactions a multi ensemble model is possible. In this approach a particle distribution is represented by several sets of moments each of them defining an ensemble as shown in Fig. 1.

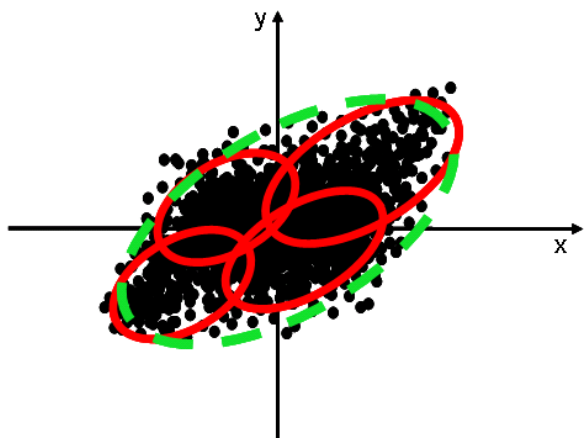

Figure 1: A 2D example of a multi ensemble setup. The red ellipsoids show four ensembles representing the particle distribution. The green dashed shape describes the set of moments obtained through weighted averages over the moments of the four single ensembles.

The time evolution of the several ensembles are calculated according to the procedure for single ensemble bunches described above. At any time a set of moments representing the whole bunch can be obtained from the moments of the

ensembles. The density distribution function for the whole bunch composed e.g. of two ensembles is defined as

$$f(\vec{r}) = f_1(\vec{r}) + f_2(\vec{r}). \quad (32)$$

This leads to the following equations for the charge Q:

$$Q = \underbrace{Q \int_\Omega f_1(\vec{r})\ \mathrm{d}\Omega}_{Q_1} + \underbrace{Q \int_\Omega f_2(\vec{r})\ \mathrm{d}\Omega}_{Q_2} \quad (33)$$

and defines the local density distribution functions via the relations

$$1 = \int_\Omega \frac{Q}{Q_1} f_1(\vec{r})\ \mathrm{d}\Omega \qquad 1 = \int_\Omega \frac{Q}{Q_2} f_2(\vec{r})\ \mathrm{d}\Omega. \quad (34)$$

The first order moments of the whole bunch can then be obtained from the first order moments of the individual ensembles $<\mu>_{f_1}$ and $<\mu>_{f_2}$ as follows:

$$<\mu> = \frac{Q_1}{Q}\ <\mu>_{f_1} + \frac{Q_2}{Q}\ <\mu>_{f_2}\ . \quad (35)$$

For the second order centralized moments

$$M_{uv} = <(u - <u>) \cdot (v - <v>)>$$

with $u, v \in \{x, y, z, p_x, p_y, p_z\}$ one obtains

$$M_{uv} = \frac{Q_1}{Q} \cdot M_{uv,f_1} + \frac{Q_1}{Q} \left(\langle u \rangle_{f_1} - \langle u \rangle\right) \cdot \left(\langle v \rangle_{f_1} - \langle v \rangle\right) + \frac{Q_2}{Q} \cdot M_{uv,f_2} + \frac{Q_2}{Q} \left(\langle u \rangle_{f_2} - \langle u \rangle\right) \cdot \left(\langle v \rangle_{f_2} - \langle v \rangle\right). \quad (36)$$

Additional higher order moments can be calculated similarly.

APPLICATIONS

Based on the moment approach the fast online beam dynamics simulation tool V-Code was implemented at TEMF. The aim of several further developments was to increase the application range to various accelerator designs. For example dipole bending magnets were introduced in [6] in order to simulate recirculating machines. The V-Code can be utilized for the design phase as well as during the accelerator operation.

Beam Line Design and Optimization

At the Superconducting Darmstadt Linear ACcelerator S-DALINAC the V-Code has been used during the design process of the injector for the new 100 keV polarized electron source. Starting from an initial ensemble issued from a simulation of the electron source with the CST code MAFIA [4] the entire beam line was modeled within the V-Code and simulated as a whole. The results of detailed simulations can be found in [5].

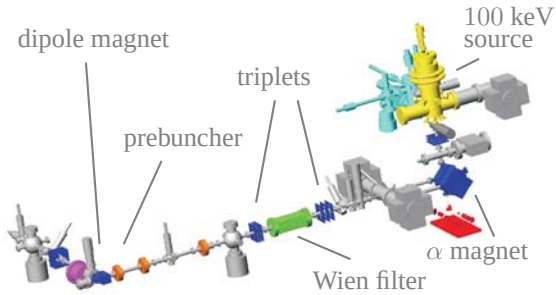

Figure 2: Schematic computational model of the compact injector design for the new polarized electron source at the S-DALINAC.

Operator Support

Fast beam dynamics simulations can advantageously assist the machine operators at various particle accelerator machines because of a flexible parameter variation combined with nearly simultaneous solution responses giving a detailed insight into the actual machine status. A user friendly front end was implemented for this purpose, giving the operator the possibility to comfortably change the parameter setup and receiving a well-arranged overview over the actual beam status.

Automatic Beam Adjustment

Finding an optimal parameter setup for an accelerator beam line is a tedious and laborious task as the number of variable parameters is typically very large. A fast simulation code opens the possibility to analyze a multitude of parameter sets in a reasonable time. By implementing objectives and valuation rules this procedure can be automated. Further, a connection between the simulation code and the accelerator diagnostic software allows to take into account measured parameters in the automated optimization process.

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