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DRIFTPIC, a Computer Program for the Calculation of Ion Trajectories in the Drift Section of Externally Applied-*B* Diodes

L. Feher, W. Schmidt, T. Westermann Hauptabteilung Daten- und Informationsverarbeitung

Kernforschungszentrum Karlsruhe

KERNFORSCHUNGSZENTRUM KARLSRUHE

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L. Feher, W. Schmidt, T. Westermann

Kernforschungszentrum Karlsruhe GmbH, Karlsruhe

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DRIFTPIC, a Computer Program for the Calculation of Ion Trajectories in the Drift Section of Externally Applied-B Diodes

Summary

The simulation program DRIFTPIC is introduced and described in this paper. DRIFTPIC is a particle-in-cell code for the drift section of pulsed power high current diodes (specifically for the externally applied-B ion diode) considering the self-magnetic field. By performing simulations with this program it is intended to achieve better knowledge about the processes in the drift section including an a priori current-neutralization model for a monopolar proton beam. The base for this work is the stationary particle-in-cell code BFCPIC.

DRIFTPIC - ein Computerprogramm zur Berechnung von Ionentrajektorien im Driftbereich von fremdmagnetisch isolierten Dioden.

Zusammenfassung

In diesem Bericht wird das Simulationsprogramm DRIFTPIC vorgestellt und beschrieben. DRFTPIC ist ein Particle-in-Cell Programm zur Berechnung des Eigenmagnetfeldes im Driftbereich von Hochstrom-Ionendioden (speziell für die fremdmagnetisch isolierte Ionendiode). Durch Simulationsrechnungen soll ein besseres Verständnis für die physikalischen Prozesse im Driftbereich gewonnen werden. Um die Stromneutralisierung zu berücksichtigen, wurde sowohl ein lokales als auch ein globales Modell entwickelt und implementiert. Die Basis für die numerischen Arbeiten bildet das stationäre Simulationsprogramm BFCPIC.

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L.Feher, W.Schmidt, T.Westermann Kernforschungszentrum Karlsruhe GmbH Hauptabteilung Daten- und Informationsverarbeitung Postfach 3640, D-7500 Karlsruhe 1

Summary

The simulation program DRIFTPIC is introduced and described in this paper. DRIFTPIC is a particle-in-cell code for the drift section of pulsed power high current diodes (specifically for the externally applied-*B* ion diode) considering the self-magnetic field B_{θ} . By performing simulations with this program it is intended to achieve better knowledge about the processes in the drift section including an a priori current-neutralization model for a monopolar proton beam. The basis for this work is the stationary particle-incell code BFCPIC [1], [2].

1 Introduction

Pulsed power ion diodes have been investigated [3] for producing intense beams of light ions. An important goal of ion diode research is to develop ion beams of sufficient power for inertial confinement fusion [4]. The required beam power and focal intensity at the target are larger than 100 TWand $100 TW/cm^2$, respectively. To reach sufficiently high power densities, the electric power supplied to the system has to be converted into focused ion beam energy.

At the Karlsruhe Nuclear Research Center the computational physics program continued to support the experiments with light ion beam diodes. Our aim is to simulate the main properties of these diodes for the ongoing experiments at KALIF [5] with stationary codes. With 3D time-dependent codes [6], the physics of pulsed power ion diodes are studied in detail [7]. However, these simulation results can only be achieved with an enormous computational effort resulting in high CPU-times on the order of 50 - 100 hours. In order to overcome these high CPU-times, phenomenological models are implemented into our stationary 2.5D particle-in-cell code BFCPIC [1], [2] and use the simulations from an engineering point of view.

Fig. 1 shows a schematic cross-section of a rotationally symmetrical externally applied-B ion diode in the (z, r)-plane developed at the Nuclear Research Center in Karlsruhe by Bluhm et al. [8]. The vacuum diode consists of a solid anode plate and a cathode ring. A mylar foil attached to the cathode ring seals the vacuum diode from the gas-filled drift space. Depending on the ion species to be produced, parts of the anode plate are coated with an appropriate material. These parts are shown dashed in the schematic diagram of the diode. The pulse length is typically about 50 to 100 ns, the applied voltage several MV, and the gap distance between the anode and the cathode tip is a few mm.



Figure 1: Schematic cross-section of the externally applied-B ion diode.

The electron current follows the outer conductor of the generator to the cathode area and to the cathode tip. Electric field enhancement causes electrons to be generated mainly at this edge. Due to a special preparation an anode plasma is generated in front of the anode. This anode plasma serves as an ion source. The ions are accelerated in the anode-cathode gap and leave the diode through a mylar foil into the gas-filled drift space. The electrons are influenced by magnetic fields induced by the movement of particles, themselves, and additionally by external magnetic fields perpendicular to the (z, r)-plane. This external magnetic field is produced by two magnetic coils. The electrons drift in the gap perpendicular to the electric and magnetic fields.

When the particles leave the diode region they enter the so-called drift section (cf. Fig. 1). The drift section is filled with a background gas (5 mb Ar) and separated from the diode region by a mylar foil. The electrons of the ionized background gas compensate fully the positive space charge of the ion beam. Due to the external magnetic field the electrons are prevented by directly following the ions. Hence, the ion beam is charge but not current neutralized. The current neutralization is only about 90 to 95 %. Although the magnetic field is primarily determined by the externally applied-*B* field, the rest current of 5 to 10 % of the original 500 kA ion current is not negligible. This uncompensated ion current leads to a B_{θ} -eigenfield which must be taken into account.

Several diagnostic tools were developed in order to extend the computational simulations to the drift section of the applied-B diode, too. A useful method for simulating charged particles in electromagnetic fields is the particle-in-cell method [9], [10]. In the case of the diode region, the 2.5D particle-in-cell simulation program BFCPIC was successfully applied. This model for simulating the diode physics was modified with respect to specific features of the drift section resulting in the program DRIFTPIC. Hence, with DRIFTPIC it is intended, to calculate trajectories of protons generated in a high current diode for a stationary beam, while the particles are propagating through a gas-filled drift section. Our main interest lies upon the effect of the beam's self-fields concerning its focussing. It is our further aim, to give the experimentalists an easy to handle simulation tool for ion propagation.

The organization of the paper is as follows: In Sec. 2 we discuss some general features of the kinetic theory applyable to the drift section of applied-B ion diodes. In Sec. 3 the physical models implemented in DRIFTPIC are introduced in order to compute the drift section in a self-consistent manner. In Sec. 4 the DRIFTPIC program is outlined and the input parameters are described. Examples of computations are discussed in Sec. 5. A trace program couples the diode region and the drift section, see Sec. 6. In its application, the position and the energy of ions can be chosen interactively and the trace of specific particles are computed. Summary and outlook are left to Sec. 7.

2 Theoretical Considerations of the Drift Section

The statements presented in this section are valid in general for a monopolar proton beam. In the experiment, additionally to the protons also carbon or (and) lithium components are present. In contrary to the protons, these other components can cause dissipative charge exchange in the cathode plasma. But we do not consider the properties of these particles in this investigation.

Invariants of ion motion

For the following consideration we assume that the Ar-background gas is fully ionized via scattering processes within timescales smaller than 1 nsec. For details of these ionization processes and charge neutralization effects see [11, Sec.4]. Furthermore, we assume that these electrons fully neutralize the space charge of the beam. Hence, enough electrons are generated by scattering processes for compensating the space charge of the beam. By means of the source equation

$$div ec{E} = rac{
ho}{\epsilon_0}$$
 ,

it yields that the electric field \vec{E} vanishes in the calculation area; and electric interactions have not to be considered. For a general formulation of the particle propagation we use the Lagrange function in cylindrical coordinates without the electric potential term:

$$L(r_i, z_i, \theta_i, \dot{r}_i, \dot{z}_i, \dot{\theta}_i, t) = \sum_i \frac{1}{2} m_i (\dot{r}_i^2 + (r_i \dot{\theta}_i)^2 + \dot{z}_i^2) + \sum_i q_i \vec{A}(r_i, z_i, t) \vec{v}_i \quad . (1)$$

We assign the vector potential to be zero sufficiently far away from the field generating coils and refer all other statements to this gauge. The equations of motion are obtained by means of the Euler-Lagrangeian differential equations

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_i} - \frac{\partial L}{\partial q_i} = 0 \quad . \tag{2}$$

The rotational symmetry of the diode and the choice of cylindrical coordinates implies that the cyclical variable θ leads to an important invariant, the canonical angular momentum:

$$p_{i_{\theta}} = \frac{\partial L}{\partial \dot{\theta}_{i}} = m_{i} r_{i}^{2} \dot{\theta}_{i} + q_{i} r_{i} A_{\theta}(r_{i}, z_{i}, t) = constant \quad . \tag{3}$$

Furthermore, we are interested in the adjusted stationary state, thus no explicit time dependence of the Lagrangeian equation is taken into account $\left(\frac{\partial L}{\partial t} = 0\right)$ and no dissipative effects (like interactions with plasma sheats within the diode) are considered.

Via the homogeneity of time, the stationary state yields energy conservation [14, p.17]

$$E = \sum_{i} \dot{q}_{i} \frac{\partial L}{\partial \dot{q}_{i}} - L = \sum_{i} \frac{1}{2} m_{i} \bar{v}_{i}^{2} = \sum_{i} q_{i} U \quad , \qquad (4)$$

where U is the potential between the anode and cathode, and q_i is the charge of each particle. Therefore, the energy of each particle in the drift section is constant and the velocity can directly be evaluated by means of

$$|\vec{v_i}| = \sqrt{2\frac{q_i}{m_i}U} \quad . \tag{5}$$

Influence of the initial conditions on the propagation of the ions

The quality of the beam focusing depends on the initial condition of the emission at the anode surface. The trajectory of a single ion (from the generation at the anode up to the focus) can be partitioned into the following sections:

- Generation of the particles at the anode surface and accelerated motion towards the virtual cathode.
- Deflection by magnetic fields between virtual cathode and the geometric cathode realized by the mylar foil.
- Crossing the mylar foil and entering the drift section.
- Ionisation by scattering in the gas-filled drift section and propagating to the focus.
- After reaching the focus further propagation until absorption in a Pbabsorber.

For each of these sections it yields

$$m_i r_i^2 \dot{\theta}_i + q_i r_i A_\theta(r_i, z_i, t) \Big|_{section \ l} = m_i r_i^2 \dot{\theta}_i + q_i r_i A_\theta(r_i, z_i, t) \Big|_{section \ m}$$
(6)
$$l, m: 1 \dots 5 \qquad .$$

If a particle reaches the axis $(r_i = 0)$, the canonical angular momentum involves the property:

$$p_{i_{\theta}} = m_i r_i v_{i_{\theta}} + q_i r_i A_{\theta}(r_i, z_i, t) \equiv 0 \quad . \tag{7}$$

Because of the conservation of the canonical angular momentum, the particle must have started at the anode with a momentum identical zero. By assigning the initial values of a particle at the anode wih $\tilde{r}_i, \tilde{z}_i, \ldots$, this relation is in general fulfilled, if

$$\tilde{v}_{\theta_i} = -\frac{q}{m} \tilde{A}_{\theta}(\tilde{r}_i, \tilde{z}_i) \Big|_{anode} \qquad (8)$$

Necessarily, the anode should represent an equipotential surface according to

$$\tilde{A}_{\theta}\Big|_{anode} \equiv 0, \qquad \Rightarrow \tilde{v}_{\theta_i} = 0 \qquad .$$
(9)

This is a neccessary condition for the ions in order to reach the axis. Furthermore, it is obvious, that a rotational drift can only be evolved by applying a B_z or B_r field, where the velocity v_{θ_i} is directly proportional to the local vector potential A_{θ} :

$$v_{\theta_i} = -\frac{q}{m} A_{\theta}(r_i, z_i) \quad . \tag{10}$$

The self-magnetic field B_{θ}

The positive charged particles of the ion beam are accelerated in the diode from the anode towards the virtual cathode. Behind the cathode plasma the ions enter the gas-filled drift section. Free electrons from the cathode plasma and from the ionized Argon atoms are available to neutralize the current density of the ion beam.

A local current neutralization factor f_i for each particle is introduced. The effective current is then given by

$$\vec{j}_{eff}(r_i, z_i) = q \sum_i \vec{v}_i \delta(\vec{r} - \vec{r}_i) (1 - f_i(r_i, z_i)) \quad . \tag{11}$$

By means of the Maxwell equation

$$rot\vec{H} = \vec{j} + \frac{\partial \vec{D}}{\partial t}$$
(12)

and by applying Stoke's theorem, the self-magnetic B_{θ} -field can be evaluated. Because of the assumed total charge neutralization in the drift zone and the stationarity of our problem, the term with \vec{D} can be left out and we find:

$$B_{\theta}(r,z) = \frac{\mu_0}{2\pi r} \iint \vec{j}_{eff} \quad d\vec{A} \quad . \tag{13}$$

This magnetic field generated by the motion of ions can feedback on the ions by changing the propagation and, hence, by changing the focusing properties of the beam. The main task of the numerical modelling of the drift section is to compute this B_{θ} -eigenfield in an appropriate way in order to describe the focusing behavior of the ion beam in a realistic manner.

3 The DRIFTPIC Models

In order to obtain more detailed information of particle trajectories and focusing behavior, the DRIFTPIC simulation model was developed. DRIFTPIC is a particle-in-cell code for the drift section of ion diodes taking into account externally as well as self-generated magnetic fields. The code is based on the stationary particle-in-cell code BFCPIC. In DRIFTPIC the current neutralization of the proton beam via the background gas is modelled considering the neutralization as a function of the externally applied-B field. By means of experimental measurements the degree of current neutralization is about 90 % of the proton beam. The remaining current density induces a self-generated B_{θ} -field which acts on the particles themselves.

In Fig. 2 the applied magnetic field profile as computed by PROFI [15] is shown. The corresponding magnetic field components (B_z, B_r) serve as an input for DRIFTPIC simulations. The two whirls of the magnetic field can clearly be identified. Near the field coils a strong magnetic field is induced. Apart from the coils the magnetic field decreases dramatically. Due to the spatial dependence of the applied-B field, the influence on the focusing of the ion beam is different for different parts of the drift section.



Figure 2: Magnetic field profile for the externally applied-B ion diode.

Moreover, due to this external magnetic field the electrons are prevented by directly following the ions. The ion beam is charge neutralized but not current neutralized. The current neutralization is only about 90 % to 95 %. Although the magnetic field is primarily determined by the applied-*B* field, the rest current of 5 % to 10 % of the original 500 kA ion current is not negligible. This uncompensated ion current leads to a B_{θ} -eigenfield which must be taken into account and computed in a self-consistent manner.

Hence, in the drift section the ions will not be accelerated by electric fields but deflected by externally applied- (B_z, B_r) fields and to a smaller degree by self-generated B_{θ} -fields.

If the external magnetic field increases the current neutralization decreases. Hence, the strength of the induced magnetic field B_{θ} becomes larger and the beam has a greater deflection towards the symmetry axis.

The aim of the simulations is to investigate this procedure numerically including the effects of the self-consistent magnetic fields in order to obtain a realistic description of the drift region. DRIFTPIC simulations follow BFCPIC computations. With BFCPIC not only the fields inside the anodecathode gap are computed but also ion trajectories along the gap. If the ions leave the diode, the positions as well as the velocities are stored. These phase space coordinates are the initial conditions for a DRIFTPIC-run.

The following physical conditions are implemented:

- Monopolar flow of protons. No electron dynamics is explicitly taken into account.
- No interaction throughout the electric potential.

Because of sufficient available electrons in the drift area, resulting by the total ionisation of the background gas, the beam is sufficiently fast charge neutralized in the whole calculating area, thus $div \vec{E} = 0$. This is equivalent to the lack of the potential term $U(r_i, z_i) = 0$ in the Lagrange formalism.

• No self-fields B_r and B_z : The self-generated diamagnetic fields B_z are

The self-generated diamagnetic fields B_r and B_z are small compared with the applied magnetic field and can be neglected.

• Current neutralization:

Current neutralization < 100% is taken into consideration by the use of a further discussed model, which is implemented for the self-consistent calculation of the B_{θ} self-magnetic field.

The current neutralization modell

After leaving the cathode, the protons propagate through a gas-filled drift section. In addition, the background gas is immediately ionized by the front of the beam. The positive charged ions interact with electrons, which are generated by scattering. We assume a sufficiently fast charge neutralization, thus

$$\rho_{electrones} + \rho_{protones} = 0 \quad . \tag{14}$$

Because of its motion, the current density of the proton beam can be written as

$$\vec{j}_{protones} =
ho_{protones} \, \vec{v}$$
 . (15)

By crossing the ionised drift section the electrons are torn to the direction of the proton beam, which leads to a return current. However, measurements at KALIF showed, that the current densities

$$\vec{j}_{effective} = \vec{j}_{protones} + \vec{j}_{elektrones}$$
 (16)

do not neutralize totally each other.

The degree of current neutralization has a dominant effect on the B_{θ} selfmagnetic field, resulting by the effective current density and is designed in the simulation as follows:

The effective current densities at time step $t = n\Delta t$ are evaluated with the proton's current densities of this time step as

$$\vec{j}_{eff}(r_i, z_i)\Big|_t = \vec{j}(r_i, z_i)\Big|_t (1 - f(r_i, z_i))$$
, (17)

with $f(r_i, z_i)$ describing an in general particle and therefore spatial depending current neutralization factor (i specifies the number of the macro-particle).

Furthermore, a coupling of current neutralization with applied magnetic fields should be taken into account. One imagines, that strong magnetic fields have an interfering effect on the electrons, not to be captured by the beam in the same way, as without a magnetic field leading to a worse current neutralization.

The following cases are considered:

1. $f(r_i, z_i) = f = constant$ in the whole simulation area

(global current neutralization factor).

For studying the particle propagation in the driftsection depending on the self-magnetic field B_{θ} without a coupling to the applied magnetic field. 2. $f(r_i, z_i) = f(|\vec{B}_{appl.}(r_i, z_i)|)$ (local current neutralization factor). The more strength the transversal B-fie

The more strength the transversal B-field has at the particle's location, the weaker is the beam neutralized, because of the gyro effects of the magnetic fields. For obtaining a specific model, we assume the following relation

$$1 - f(z_i, r_i) = \alpha \arctan(\beta \frac{\hat{v}_i \vec{B}_{appl.}(z_i, r_i)}{|vecB_{max}|} + \gamma) + \delta \quad . \tag{18}$$

 α is hereby a free parameter, responsible for the characteristic shape of the arctan function, while β, γ, δ are defined by the conditions:

$$f(B = 0) = 100\%$$

$$f(B = \frac{1}{2}B_{max}) = \frac{1 + f_{min}}{2} (symmetry \ condition)$$

$$f(B = B_{max}) = f_{min}$$

with f_{min} as the possible smallest degree of current neutralization.



Figure 3: Shape function of the current neutralization factor f.

The parameter β , γ , δ can be calculated via the ϵ_1 , and ϵ_2 explicitly by

$$\epsilon_1 = \tan\left(\frac{f_{max}}{\alpha}\right)$$
, $\epsilon_2 = \tan\left(\frac{f_{max}}{2\alpha}\right)$, (19)

$$\delta = \alpha \arctan\left(\frac{\epsilon_1 - 2\epsilon_2}{\epsilon_1 \epsilon_2}\right) ,$$
 (20)

$$\gamma = -\tan\left(\frac{\delta}{\alpha}\right)$$
 , (21)

$$\beta = \tan\left(\frac{f_{max} - \delta}{\alpha}\right) - \gamma \quad . \tag{22}$$

A possible shape of f for a given α $(\alpha = \frac{(1-f_{max})}{3})$ is shown in Fig. 3.

Particle emission

In the simulation, the particles start at the cathode taking their way through the drift section. For each particle the initial data for the starting location and velocity are needed. These are obtained from a former BFCPIC-run for the diode region. A new module had to be developped, to get proton emission from the cathode with the macro-particle concept. The use of macro-particles was motivated by the aim to save CPU-time. This emission scheme was realised in the subprogram KATRIN (KAThode Read and INitialize).

The center of mass of all in a cathode cell located particles defines the initial location and their averaged velocity the initial velocity of the macroparticle, respectively. The charge of this macro-particle is given by

$$Q_{macro} = \Delta t \iint \vec{j}_{cell} \ d\vec{A}_{cathode}$$
 (23)

 Δt is hereby the length of the time step, \vec{j}_{cell} is the current density situated in the cell and $d\vec{A}_{cathode}$ is the oriented surface element by the boundary coordinates of the examined cell. By it, all the demanded initial conditions of the macro-particles are known.

Calculation grid

As no specific geometric features have to be considered (open area), the region of interest has to be specified from only one input parameter. The user specifies the maximal z-value of the computational region. A parallel and nonequidistant 265×185 mesh is generated automatically extending the PROFI grid in the positive z-direction.

4 The DRIFTPIC Program

In this section the stationary, 2.5-dimensional, particle-in-cell code DRIFT-PIC is outlined and the input as well as output parameters are described. DRIFTPIC is organized as follows. Main input data are the

- externally applied-B field computed with the PROFI program package [15],
- the total ion current I_{tot} ,
- particle file from a former BFCPIC-run, (All ions leaving the diode region in a simulation with BFCPIC are written on a file.)
- the minimal degree of current neutralization f_{min} .

The simulation program DRIFTPIC then generates automatically a grid for the drift section and takes the ions from BFCPIC for the emission of ions on the cathode side. The electric charge of the macro-particles is adopted in such a way that the ion current emitted per time step corresponds to the input value I_{tot} . The degree of current neutralization is taken into account by introducing a current neutralization factor f and by modifying the current densities according to Eq. (17). The output data from DRIFTPIC are the fields and particle distribution in the drift section.

The program package DRIFTPIC consists of the three main components:

Initialization

- Input:

The boundary-fitted diode grid is read together with the extendable parallel PROFI grid and the applied magnetic field data. The particle data from a former diode simulation are read in for preparing the initial data of the macro-particles (ions).

- Maximal transversal $B_{appl.}$ -field:

In case of the local current neutralization model the knowledge of the possible maximum value of the transversal B_{appl} -field is necessary. This value $|B_{max}|$ is evaluated in a preprocessing routine, where the applied field alone interacts with the particles.

Main iteration cycle

- Calculation of the self-consistent magnetic field B_{θ} by use of the chosen current neutralization model.
- Particle pushing considering the influence of the self-field B_{θ} as well as the applied- (B_z, B_r) fields.

• Documentation of a simulation run

- Output:

The list directed output is made on a file, containing the following data: Particle matrix of the protons in the drift section as well as $j_r, j_z, j_\theta, \rho, B_\theta$. Output of the extended parallel calculation grid in a file for graphical postprocessing with the LIDIS program [13].

Appendix A1 shows the Job-Controll Language (JCL) for a typical run with DRIFTPIC for the drift section.

Input data sets are IFILEG (ft20), the computational grid for the diode simulation with BFCPIC and the corresponding data file IFILEI (ft22) of this simulation including the phase-space coordinates of the ions at the end of a BFCPIC-run. Moreover, IFILEB (ft21) serves as the input data for the externally applied-B field from PROFI calculations.

As output data sets have to be specified: IPROFI (ft40), it contains the computational grid which is generated by DRIFTPIC and which is required for the graphical display of the results with the LIDIS system. LOGD (ft30), it contains a protocol of the user defined input parameters as well as controll parameters at the end of the run (e.g. CPU-time of the modules, currents etc.). LOGP (ft31) includes the job output like the particle matrix of protons, the densities and the self-generated magnetic field B_{θ} . This file serves as the input for other diagnostic tools.

Further input and controll parameters for the simulation with DRIFTPIC are

- ZMAX: ZMAX (in mm) is the maximum value of the z-coordinate of the computational region to be considered.
- FWERT: FWERT means the minimal degree of rest current inducing an self-generated B_{θ} -field.

- NGLOB: NGLOB is the parameter which specifies whether the global current neutralization model (NGLOB = 1) or the local model (NGLOB = 0) is applied.
- DT: DT is the time step in seconds.
- NDT: NDT the number of time steps for the whole simulation.
- STROM: STROM (in A) specifies the total proton current entering the drift section. (It is possible to choose e.g. experimental values for STROM.)
- ITIMX: ITIMX is the expected CPU-time in minutes which is also specified in the JCL by the time parameter. If during a run the CPUtime pass over this value an internal interrupt occur and the data are stored in the files specified.
- DELTAZ: DELTAZ (in m) is the position of the PROFI grid relative to the boundary-fitted grid of the diode.
- F1: F1 (in kA) is the scaling factor of the externally applied-B field corresponding to the maximum coil current.

5 Results

In order to obtain a stationary state for the fields in the drift section on the parallel and nonequidistant 265×185 grid about 4000 time steps with a time step size of 2. 10^{-11} s are required. For the generation of particles, 39 cathode cells are used and one proton is emitted per time step and cell leading to about 19000 macro-particles in the computational region at the steady state.

The CPU-times on the IBM 3090 VF computer in a vectorized mode are listed in the following table. The time step was varied from 10^{-11} to 2. 10^{-10} s.

CPU-TIME					
time step [.]	# of time steps	# of particles	CPU-time		
$1.10^{-11} s$	8000	38000	100 min		
$2.10^{-11} s$	4000	19000	50 min		
$5.10^{-11} s$	2000	8600	13 min		
$1.10^{-10} s$	2000	6000	9 min		

Fig. 4 shows the particle map of protons at the steady state as the result of a DRIFTPIC-run using the local current neutralization model.





The calculation was made with a local current neutralization factor $f_{min} = 0.9$, meaning 10 % of the current densitiy of the proton beam can maximally contribute to the self-magnetic field B_{θ} . Such a neutralization degree is expected at the observed KALIF configuration. As input parameters for the simulation, characteristic values for KALIF-experiments were taken ($I_{tot} = 500$ kA). A ring focus for the protons occured in a distance of 2-3 mm to the z-axis by using the initial data from a former BFCPIC-run.

One has to note that the particle trajectories do not reach the symmetry axis since for the BFCPIC input parameters, the anode surface was not an equipotential line $A_{\theta} = 0$. From the analytic considerations of Sec. 2 it is clear that only for the condition $A_{\theta} = 0$ the beamlets are able to reach the symmetry axis.

The next graphic (Fig. 5) shows the particle map of protons using a local current neutralization model with f = 0.1 ($I_{tot}=500$ kA). This factor f is far to low for a realistic value, but demonstrates clearly the influence of the self-magnetic field B_{θ} on the trajectories, which are bended back to the z-axis.



Figure 5: Local current neutralization model. Neutralization factor f = 0.1.

The results for the global current neutralization model are shown in Figs. 6 and 7, where the current neutralization factor f was chosen to be 0.9 and 0.1, respectively.



Figure 6: Global current neutralization model. Neutralization factor f = 0.9.

Moreover, the effect of charge and current neutralization was subject of intensive investigation [11], concerning the time depending behavior [12], [13] of these effects and taking into account the focusing geometry of KALIF.

In order to demonstrate the influence of the time step, Fig. 8 indicates the result of a simulation with a time step size of 10^{-10} s. It clearly shows that the time step is to big. We found that the time step must be chosen smaller than 5. 10^{-11} s in order to obtain results which are independent of the time step size.



Figure 7: Global current neutralization model. Neutralization factor f = 0.1.



Figure 8: Global current neutralization model. f = 0.1. Time step $DT = 10^{-10}$.

6 Coupling the Diode Region with the Drift Section

In order to couple the diode region with the drift section, a trace program was developed. The TRAJEK program uses the diverse electromagnetic fields produced by BFCPIC, DRIFTPIC and PROFI in order to follow the trajectories of ions across the gap and along the drift section. In this application the position and the energy of ions can be chosen interactively and the trace of the specific particles is computed and plotted in an appropriate way.

In Fig. 6 a 3 dimensional plot of trajectories of some sample ions in the drift section is shown. Due to the externally applied-B field the motion obtains a slight deflection in θ -direction and due to the self-generated B_{θ} -field the traces are curved in the (z, r)-plane.



Figure 9: 3 dimensional plot of proton trajectories in the drift section. The traces of protons are curved due to the magnetic fields.

Three calculated trajectories of representative 1.7-MeV protons are shown in Figs. 6 and 6, respectively. The straight lines in Fig. 6 represent the ballistic trajectories of protons without magnetic field. For the traces in Fig. 6 the applied-B as well as the self-generated B_{θ} field are included in the computations. The program can also be used in the inverse direction: Given the position, energy and direction in the drift space, TRAJEK inverses time and computes the starting point of the specific ion at the anode. This application is used from experimentalists in order to determine the creation point of ions at the anode surface when the position and energy in the drift section are measured experimentally.



Figure 10: Ballistic movement of ions in the drift section.



Figure 11: Movement of ions in the drift section by taking into account the applied as well as self-generated magnetic fields.

7 Conclusions

In conclusion, for the simulation of our pulsed power ion diodes several stationary codes were developed simulating different aspects of these devices: The externally applied-B field is calculated by PROFI on a regular grid. BFCPIC computes on boundary-fitted grids the electromagnetic fields in the anode-cathode gap. It also produces particle files which serve as input for DRIFTPIC. DRIFTPIC models the drift section of applied-B diodes and TRAJEK couples the anode-cathode gap with the drift space using the information of BFCPIC, DRIFTPIC and PROFI.

The results discussed in this paper delivers nominal traces of protons in the drift section of externally applied-B diodes. These tools, however, are up to now not sufficient to reproduce the experimentally measured power densities on the target. It is demonstrated experimentally that the emission angle of an ion generated at a specific position at the anode surface varies about a nominal angle. Moreover, due to the electromagnetic instabilities between the anode and the virtual cathode the ion beam obtains a microdivergence of about 2° [17].

We have started to include these effects of micro-divergences: After evaluation of the experimental data the trajectories of ions will be imprinted by statistical fluctuations. Results in this direction will be reported in the near future.

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A Appendix

```
//ADI989DP JOB (0989,541,P0000),WESTERMANN,NOTIFY=ADI989,
11
          MSGCLASS=H, REGION=10M, TIME=(120,00)
//*MAIN LINES=55
// EXEC NEUFVCLG, SPACE=25,
11
         OPTC='OPT(3),DC(FELDER)',
11
        LIBL1='IMSL.MATH',
11
        OPTG='SIZE=10M'
//* JOB-CONTROLL-LANGUAGE FOR A RUN WITH THE
                                                           *
//*
                                                           *
//*
             DRIFTPIC-CODE
                           VERSION 1.1
                                                           炇
//*
//* A SIMULATION PROGRAM FOR THE MODELLING OF THE DRIFT SECTION
//* OF EXTERNALLY APPLIED-B ION DIODES.
                                                           늋
//*
                                                           ¥
//* AUTHORS: T. WESTERMANN, L. FEHER
                                                           嫁
//*
             KERNFORSCHUNGSZENTRUM KARLSRUHE GMBH. HDI
                                                           冰
//*
             3.6.1993
//C.SYSPRINT DD DUMMY
//C.SYSIN
           DD DISP=SHR, DSN=AD1989.DRIFTPIC.FORT(DRIFTPIC)
11
           DD DISP=SHR, DSN=AD1989.DRIFTPIC.FORT(SUBBLOCK)
11
           DD *
     FUNCTION FA04AS(IP)
С
     GENERATION OF RANDOM NUMBERS
     A = RNUNF()
     IF (IP.GT.O) THEN
     FA04AS=A
     ELSE
     FA04AS=2.*A-1.
     ENDIF
     RETURN
     END
     SUBROUTINE DATE (DAY)
     DETERMINATION OF DAY
С
     INTEGER
            NOW(8)
     CHARACTER DAY*8
     CALL DATIM (NOW)
```

```
WRITE (DAY(1:2),'(I2)') NOW(6)
      WRITE (DAY(4:5),'(12)') NOW(7)
      WRITE (DAY(7:8),'(12)') NOW(8)-1900
      DAY(3:3) = '.'
      DAY(6:6) = '.'
      END
      SUBROUTINE TIME (I)
      INTEGER NOW(8)
      CALL DATIM (NOW)
      I = 1000 * (3600 * NOW(5) + 60 * NOW(4) + NOW(3)) + NOW(2)
      END
      SUBROUTINE CLOCKM (I)
C .... CPU-TIME IN MICROSECONDS
      REAL * 8 RI
      CALL CPUTIME (RI, IRC)
      I = INT(RI/1000.)
      END
//*
//*
//* INPUT-DATA SETS
//G.FT20F001 DD DISP=SHR,DSN=ADI989.GRID.DATA(M2B)
//G.FT21F001 DD DISP=SHR,DSN=ADI989.BFELD2.DATA(WOF05A)
//G.FT22F001 DD DISP=SHR,DSN=ADI989.LOGP.BAP(BAP2)
//*
//* OUTPUT-DATA SETS
//G.FT30F001 DD DISP=SHR,DSN=ADI989.MAIN.LOGD(OUTG01)
//G.FT31F001 DD DISP=SHR,DSN=ADI989.LOGP.DPIC1(OUTG01)
//G.FT40F001 DD DISP=SHR,DSN=ADI989.GRID.DPIC(OUTF09)
/*
//G.SYSIN DD *
 &NAMEL1 IFILEG=20, IFILEB=21, IFILEI=22, LOGD=30, LOGP=31
                                                                 &END
 &NAMEL2
                                                                 &END
                                                                 &END
 &NAMEL3 IPROFI=40,ZMAX=.200,FWERT=0.9,NGLOB=0
 &NAMEL4 DT=2.E-11,NDT=4000,STROM=500000
                                                                 &END
 &NAMEL5 ITIMX=120
                                                                 &END
                                                                 &END
 &NAMEL6
                                                                 &END
 &NAMEL7 DELTAZ=-0.02,F1=40
ELEKTRISCHE REFERENZLISTE
5
```

MAGNETISCHE REFERENZLISTE

'RPN2'

'RPN2'

'RPDI'

'RPDI'

'FELD'

0.0

0.0

0.0

1.7E6

1111

1

4

3

2

1

0

28