BEAMPATH : A PROGRAM LIBRARY FOR BEAM DYNAMICS SIMULATION IN LINEAR ACCELERATORS

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Abstract

A structured programming technique was used to develop software for space charge dominated beams investigation in linear accelerators. The method includes hierarchical program design using program independent modules and a flexible combination of modules to provide a most effective version of structure for every specific case of simulation. A modular program BEAMPATH was developed for 2D and 3D particle-in-cell simulation of beam dynamics in a structure containing RF gaps, radio-frequency quadrupoles (RFQ), multipole lenses, waveguides, bending magnets and solenoids.

Introduction

High current beam dynamics simulation requires state-of-the art software which must be complete, efficient, flexible, accurate, reliable, modifiable, easy-to-use. The structured programming is a useful technique for a high quality program design [1-3] . The method is based on breaking a general problem into independent subtasks which are then combined to achieve the necessary versions of the structure. The structured-modular approach allows to resolve the contradiction between general goals of the project and efficiency of computing in every specific problem. The paper considers the results of application of the structured-modular principle to software design for beam dynamics simulation in linacs and transport systems.

Structured - Modular Programming

The structured programming is a number of rules to develop large programs running without mistakes. Only a few ideas which are essential for this project are discussed below.

The problem of beam dynamics simulation using a macroparticle method is a Cauchy problem:

$$\frac{d\bar{x}}{dt} = \bar{v} \qquad \bar{x}(t_0) = \bar{x}_0$$
$$\frac{d\bar{p}}{dt} = \bar{F} \qquad \bar{p}(t_0) = \bar{p}_0 \tag{1}$$

where $\bar{x}$, $\bar{v}$, $\bar{p}$ are position, velocity and momenta of the particle, respectively, t is time, $\bar{F}$ is an electromagnetic field acting on the particle. Solution of the problem can be presented as a sequence of execution of standard steps:

$$B_1 - B_2 - B_3 - \ldots\ldots - B_K \tag{2}$$

which include the initial distribution generation $\bar{x}_0$, $\bar{p}_0$, calculation of the electromagnetic field $\bar{F}$ and integration of the equations of motion. Every step in (2) can be subdivided. The most common method is a presentation of electromagnetic field as a sum of space charge field of the beam $\bar{F}_1$, RF field $\bar{F}_2$ and focusing field $\bar{F}_3$:

$$\bar{F} = \bar{F}_1 + \bar{F}_2 + \bar{F}_3 \tag{3}$$

Suppose every standard step of simulation is supported by M standard modules. The result is a modular library:

$$\begin{array}{ccccc} B_{11} & B_{12} & B_{13} & \ldots\ldots & B_{1K} \\ B_{21} & B_{22} & B_{23} & \ldots\ldots & B_{2K} \\ B_{31} & B_{32} & B_{33} & \ldots\ldots & B_{3K} \\ \ldots & \ldots & \ldots & \ldots & \ldots \\ \ldots & \ldots & \ldots & \ldots & \ldots \\ B_{M1} & B_{M2} & B_{M3} & \ldots\ldots & B_{MK} \end{array} \tag{4}$$

where B_{ij} is the i-th module for the j-th standard step of simulation. From (4) it follows that the total number of modules in the library is

$$P = M \cdot K \tag{5}$$

and the number of versions of a system is

$$H = M^K \tag{6}$$

From (5), (6) it follows, that $H \gg P$ can be easily achieved. It illustrates the well-known property of modular structure - the possibility to construct a large number of structure versions using relatively small number of basic modules. Usually a number of standard steps in simulation is between 3 and 10. To produce a flexible software a redundant modular structure is required.

One of the main principles of the structured programming is a "top-down" design technique. The project starts with the definition of the main objectivies of the problem and breaking the global program into independent subroutines corresponding to separate purposes. Each of these parts is subdivided into parts, etc. To keep the clarity of program a limited number of control programming structures are used: IF THEN ELSE structure, DO iteration, DO WHILE iteration, DO UNTIL iteration. The control structures can be combined according to the mentioned structures. This approach simplifies understanding, software support and updaiting .

Program Library

For systematic investigation of beam dynamics in linacs and transport systems the structured modular program library BEAMPATH was developed. The main characteristics of the program are the following:

Source language	FORTRAN 77
Storage requirement	0.5....5 MB
CPU running time for IBM 360 on 64 x 64 mesh	10^{-3} $\frac{\text{sec}}{\text{particle}\cdot\text{step}}$
on 32 x 32 x 16 mesh	10^{-2} $\frac{\text{sec}}{\text{particle}\cdot\text{step}}$

The program is used for particle-in-cell simulation of axial-symmetric, quadrupole-symmetric, ribbon and z-uniform beams in a channel containing the following elements: 1) RF gaps, 2) radio-frequency quadrupoles (RFQ), 3) multipole lenses (quadrupoles, sextupoles, octupoles, etc.), 4) waveguides, 5) bending magnets, 6) solenoids, 7) user defined elements. The beam of particles is assumed to be one-component. The problem is self-consistent with respect to space charge of the beam. The scattering of particles over residual gas is absent. The problem is solved in the right hand Cartesian coordinate system,the independent variable is time t.

Library organization

BEAMPATH is a set of basic computational subroutines developed according to structured programming rules. Subroutines are connected with the global program (see fig. 1). Every subroutine has the following features: solution of a well-identified problem, independence of external program, compatibility with other subroutines, portable, expandable, testable. For every module the purpose, usage, input and output parameters, error messages, names of other subroutines required are defined. Some other standard characteristics of the package are:

- all subroutines are free of input/output statements,
- subroutines do not contain fixed maximum dimensions for the data arrays named in their calling sequences,
- the COMMON statement is not used in the library because otherwise it will result in strong connection between independent parts of the program,
- all subroutines are uniformly documented.

```
      READ /DATA/         Data of the problem
      CALL PDS            Initial distribution

      DO 1 J=1,NSTEP      Main loop

                          External fields:
         CALL DTL         RF gaps
         CALL RFQ         Radio-frequency quadrupoles
         CALL MULTI       Multipole lenses
         CALL WAVE        Waveguides
         CALL BEND        Bending magnets
         CALL SOLEN       Solenoids
         CALL USER        User-defined element

                          Poisson solvers:
         CALL POTXY       Ribbon and z-uniform beams
         CALL POTRZ       Axial-symmetric beam
         CALL POTXYZ      Quadrupole-symmetric beam

         CALL INTEGR      Integration of equations of
                          motion
         CALL OUTPUT      Output results

    1 CONTINUE
      END
```

Fig. 1. Global structure of BEAMPATH program.

Numerical Techniques

The space charge field of the beam is calculated from Poisson equation on regular domains in various coordinate systems:

for z-uniform and ribbon beams

$$\frac{\partial^2 U}{\partial x^2} + \frac{\partial^2 U}{\partial y^2} = Q(x,y) \quad , \tag{7}$$

for axial-symmetric beam

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial U}{\partial r}\right) + \frac{\partial^2 U}{\partial z^2} = Q(r,z) \quad , \tag{8}$$

for quadrupole-symmetric beam

$$\frac{\partial^2 U}{\partial x^2} + \frac{\partial^2 U}{\partial y^2} + \frac{\partial^2 U}{\partial z^2} = Q(x,y,z) \quad . \tag{9}$$

The Dirichlet boundary conditiones for potential U are imposed on the surface of an infinite pipe and periodic conditions in longitudinal direction are assumed. The region is divided into uniform rectangular meshes of dimensions NX·NY, NR·NZ or NX·NY·NZ. The charge of every particle is area-weighted among the four (2D problem) or eight (3D problem) neighboring points. Poisson equation is replaced by a finite difference approximation and the resulting equations are solved by a method based on fast Fourier transform.

RF and focusing fields are approximated by smooth analytical functions using a certain potential distribution at the boundary of the channel:

RF gaps (similar to waveguides) :

$$U(r,z) = \sum_m U_m I_0(b_m r)\cos(k_m z) \quad ; \tag{10}$$

radio-frequency quadrupoles:

$$U(r,\Theta,z) = U_0 \left[X \left(\frac{r}{a}\right)^2 \cos 2\Theta + A\, I_0(kr)\cos(kz) \right] \quad ; \tag{11}$$

multipole lenses :

$$U(r,\Theta) = \sum_m U_m r^m \cos(m\Theta) \quad ; \tag{12}$$

bending magnets :

$$U(x,y) = -B_0\left(1-n\frac{x}{r_0}\right)y - B_0\frac{n}{6}\frac{y^3}{r_0^2} \quad ; \tag{13}$$

solenoids:

$$U(r,z) = f(z) - \frac{r^2}{4} f''(z) \quad . \tag{14}$$

Equations of motion are integrated using "leap-frog" method [4] . Input options for a continuous beam with uniform phase and limited energy spread include different distributions in 4D phase space: KV, waterbag, parabolic, Gaussian. The values of RMS beam emittances and orientation of ellipses on the phase planes are arbitrary. The output of the program is a file containing trajectories of particles, envelopes of the beam, RMS emittances evolution, capture efficiency, phase length of the bunch, energy spread, plots of the beam phase space (x,p_x), (y,p_y), (z,p_z) at the given points of the channel.

Numerical Example

Macroparticle method is a convenient tool to estimate the value of limited beam current in an accelerating structure. The alternative phase focusing principle [5] is characterized by high energy gain and relatively small transverse acceptance. The typical dependence of output current I_a versus input current I_i with fixed input for the beam has a maximum (see fig. 2). A similar maximum is observed in a beam spreading in a pipe of finite length and radius. With the space charge dominating, the smaller the initial value of the envelope of the beam R_0 , the larger the envelope of the spreading beam R :

$$\frac{dR}{dz} \sim \left(\ln \frac{R}{R_0} \right)^{\frac{1}{2}} \qquad (15)$$

As long as the final radius of the beam R_f is less than the aperture of the structure a the output current is proportional to the value of the input one. The output current reaches its maximum I_{max} when $R_f = a$. With the further increase of the input current the final radius of the beam remains constant $R_f = a$ and according to (15) the fraction of the beam passing through the structure is smaller than the maximum value I_{max} .

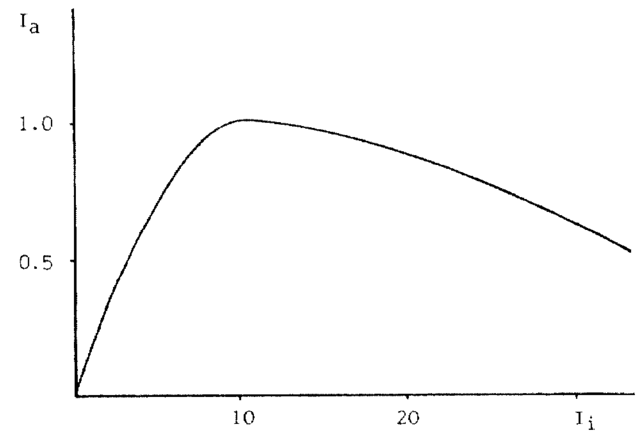

Fig. 2. Output beam current I_a versus input beam current I_i for linac with alternative phase focusing.

Conclusion

The structured programming technique was applied to the modular program library BEAMPATH to simulate a wide range of problems connected with linac design. The modularity is a useful tool for developing large programs. Every simulation step can be modified or substituted by another one without affecting the rest of the program. The application of this principle enables the user to develop his own version of the program. Tracking of macroparticles shows the typical dependence $I_a(I_i)$ with space charge dominating in alternative phase focusing accelerating structure and explains the maximum beam current.

References

1. E.Yourdon, Techniques of Program Structure and Design, Englewood Cliffs, N.J., Prentice-Hall,1975.
2. D.Tassel, Program Style, Design, Efficiency, Debugging and Testing, Englewood Cliffs, N.J., Prentice-Hall, 1978.
3. W.P.Lysenko, "An RFQ Simulation Code", Proceedings of the 1984 Linear Accelerator Conference, Seeheim/Darmstadt, West Germany, p.327-329.
4. J.P.Boris, "Relativistic Plasma Simulation - Optimization of a Hybrid Code", Proceedings of the 4th Conference on Numerical Simulation of Plasmas, Naval Res. Lab., Wash. D.C., 1970, p. 3-67.
5. J.D.Dreval, V.V.Kushin, Soviet Physics - Technical Physics, Vol. 17, No. 9, 1973.