ACCURATE PARTICLE TRACKING IN RF STRUCTURES

A. Adelmann, R. Geus, M. Zenon (Summer student from the ETHZ)

We report on a summer student project with the goal to couple the eigenmode solver femaXX with the particle tracking framework IPL (Independent Parallel Layer) in order to perform self-consistent (in the sense of paraxial approximation and in the electrostatic limit) particle tracking in RF structures. The Lorentz force equation is integrated in time and in the Laboratory frame. For the self fields (space charge) a Lorentz transformation in the co-moving frame allows us to compute the now electrostatic self fields easily [1]. The numerical solutions are validated using simple analytic test cases. By using femaXX we will be able to model large and complicated RF-structures accurately and efficiently.

IPL INDEPENDENT PARALLEL LAYER

IPL is a new software framework for 3D multiscale problems based on particles and has been developed at PSI. It is fully parallel and aimed at providing a high level of abstraction. In particular the underlying parallel layer, e.g. MPI (Message Passing Interface), is fully hidden. The main features of IPL are:

- Particles and particle manager (including ghost particles)
- Domain decomposition
- Cartesian grids, including semi unstructured grids
- Poisson solver [3]
- Efficient parallel I/O using HDF5 (hierarchical data format version 5) including checkpoint and restart features.

FEMAXX

femaXX is a parallel code developed by PSI and the Institute of Computational Science at ETH Zurich. It is intended to run very large scale eigenmode, quality factor and gap voltage computations for complicated RF structures. femaXX solves the time-harmonic Maxwell equations using a finite element approach and unstructured tetrahedral meshes. Nedelec finite elements and a subspace projection technique are used to avoid convergence to unwanted eigenmodes. A customised Jacobi-Davidson eigenvalue solver and a multilevel preconditioner are the main computational tools [2][4].

femaXX is a parallel code for execution on distributed memory architectures like e.g. workstation clusters. femaXX uses the MPI (Message Passing Interface) standard for communication between the processes.

COUPLING femaXX AND IPL

femaXX and IPL are two codes that were developed independently. Their data structures are incompatible and therefore an interface layer for passing data between the two codes is needed. For this purpose a new class *CavitySolver* has been implemented, providing the following public member functions:

runSolver Runs the eigenmode computation, steered by a single hierarchical parameter list.

getECavity Returns the amplitude of the electric field at an arbitrary location in the cavity.

getBCavity Returns the amplitude of the magnetic field at an arbitrary location in the cavity.

getLambda Returns the eigenvalue of the computed eigenmode.

The interface of *CavitySolver* uses only standard C++ types, i.e. all interfaces of Femaxx are completely hidden from IPL. This was necessary to avoid namespace clashes between the two packages.

Now consider the general Lorentz force equation with q the particle charge, m_0 the rest mass and γ the relativistic factor

$$F = \gamma\, m_0 \frac{d\vec{v}}{dt} = q[\vec{E} + (\vec{v} \times \vec{B})] \qquad (1)$$

with $\vec{E} \equiv \vec{E}_{\rm cav} + \vec{E}_{\rm other}$ and $\vec{B} \equiv \vec{B}_{\rm cav} + \vec{B}_{\rm other}$. Both the electric and the magnetic field are time and space dependent. In the above equation, $\vec{E}_{\rm cav}$ and $\vec{B}_{\rm cav}$ are obtained from femaXX. All other components of the E and B-field are zero in this particular case. The particle container of IPL stores the E and B-field of each particle into two additional vectors. This and a second order Leap Frog integration scheme constitutes our test program.

NUMERICAL EXPERIMENTS

We validate our code by tracking a single particle through a simple rectangular box cavity and compare the numerical solution with the analytic solution.

The eigenmodes for a box cavity $\Omega = [0, \pi a] \times [0, \pi b] \times [0, \pi c]$ are identified by the wave mode indexes k_x, k_y and k_z, which are all non-negative integers. With given k_x, k_y and k_z the corresponding eigenfrequency λ is calculated by: $\lambda = k_x^2/a^2 + k_y^2/b^2 + k_z^2/c^2$ and the associated eigenfunctions have the form

$$\vec{E} = [0, \quad 0, \quad e_z \sin(k_x x/a) \sin(k_y y/b)]^T . \qquad (2)$$

Note that this particular case holds only when exactly one wave mode index is equal to zero. Then the electric field is parallel to a coordinate axis in the entire domain Ω. Without loss of generality we assume $k_z = 0$,

which is exactly the case for the fundamental accelerating mode. The magnetic field is calculated analytically by scaling $\mathrm{curl}(E)$ appropriately.

The amplitude e_z can be chosen freely. It was determined by taking the normalisation of the electric field

$$\int_\Omega \vec{E}^2 \, d\Omega = \int_\Omega e_z^2 sin^2(\frac{k_x x}{a}) sin^2(\frac{k_y y}{b}) d\Omega = 1 \qquad (3)$$

into account. The resulting differential equation system is

$$\frac{d\vec{x}}{dt} = \vec{v}, \qquad (4)$$

$$\frac{\gamma m_0}{q} \frac{d\vec{v}}{dt} = \vec{E} + \vec{v} \times \vec{B}. \qquad (5)$$

To validate the tracking results equations (4) and (5) were solved using the symbolic algebra program Maple with appropriate initial conditions for $\vec{x}$ and $\vec{v}$.

For the tracking experiment we use a mesh with approximately 8'700 second order tetrahedral elements, representing a box-shaped cavity. A single particle with an initial velocity of roughly $0.4c$ in z-direction is integrated using a second order Leap Frog scheme. The particle's trajectory is off-axis, where the magnetic field is not zero (except at the initial position).

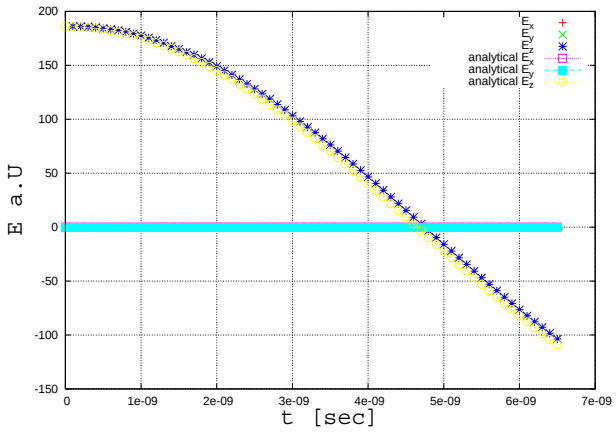

Fig. 1: E-Field computed analytically and numerically, evaluated at particle position.

Figs. 1 and 2 show that the E- and B-fields computed by femaXX agree well with the analytic solutions. The differences in the velocity shown in Fig. 3 is mainly caused by the discretisation error in the eigenmode computation and the integration error. Exact quantification of the errors are subject to further investigations.

CONCLUSIONS AND OUTLOOK

A first step towards self-consistent (in the sense of paraxial approximation and in the electrostatic limit) particle tracking in RF structures are done by validating single particle tracking against analytic solutions. By considering the general structure of the problem, namely the time integration of the Lorentz force equation, it is straight forward to include a more general

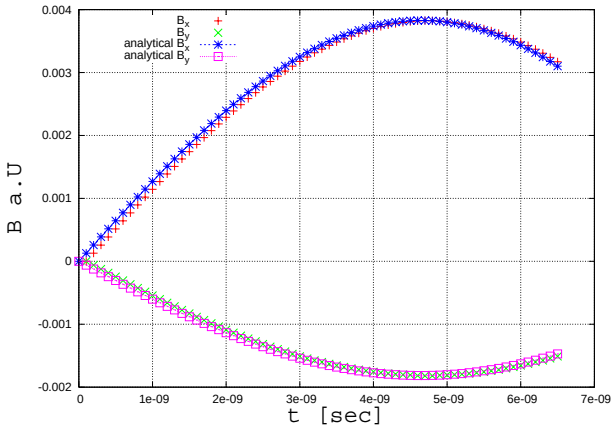

Fig. 2: B-Field computed analytically and numerically, evaluated at particle position.

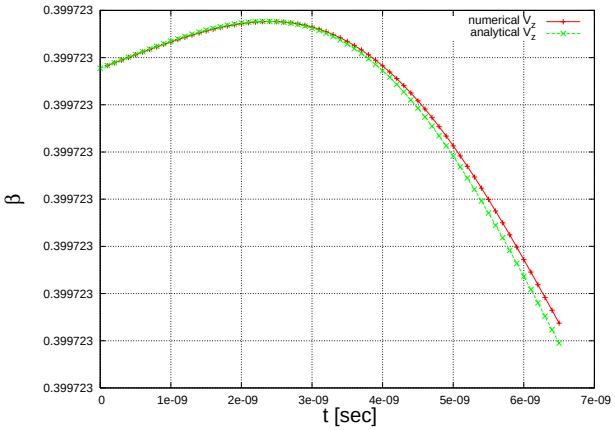

Fig. 3: z-component of particle's velocity for analytic and numerical solution.

magnetic field configuration and subsequently use the developed code in more complicated simulations, e.g. for Injector 2.

ACKNOWLEDGEMENTS

Fruitful discussions with Jean-Yves Raguin are acknowledged.

REFERENCES

[1] A. Adelmann, *3D Simulations of Space Charge Effects in Particle Beams*, PhD Thesis
ETHZ, October 2002, ISSN 1019-0643

[2] R. Geus, *Parallel eigenmode computations using femaXX*, PSI Scientific and Technical Report 2004 IV.

[3] A. Adelmann, C. Pflaum, *A Novel Massive Parallel Possion Solver for Beam Dynamics*, PSI Scientific and Technical Report 2004 IV.

[4] P. Arbenz, M. Becka, R. Geus, U. Hetmaniuk and T. Mengotti, *On a Parallel Multilevel Preconditioned Maxwell Eigensolver*, submitted to Parallel Computing.