Memo on simulation methods for the ILC Computational Grand Challenge – Cho Ng, 10-18-06

The ILC Computational Grand Challenge is stated as follows:

For a single three-cryomodule rf unit of the ILC Main Linac and by assuming realistic 3-D dimensions and misalignments, calculate multi-bunch beam dynamics effects, including wakefields and HOM excitations.

This memo is to address the computational method that is most suited and efficient to carry out the calculations for modeling the three-cryomodule rf unit, with each cryomodule consisting of 8 TDR cavities.

General Considerations

The main part of the calculation is to identify the trapped modes in the rf unit and determine their effects on the beam. The goal is to determine the frequency, impedance and damping factor (Q) of each mode. For electromagnetic calculations of accelerator structures, one can use the frequency or the time domain method. Generally speaking, for problems with high Q, the frequency domain method is preferred, while for problems where transient effects are important, the time domain method is the better choice. SLAC has developed a frequency domain code *Omega3P* and a time domain code *T3P*, both based on the finite element method, to address various aspects of field calculations in accelerator structures. We have opted to use the frequency domain code *Omega3P* for the dipole mode determination of the TDR cavity since the Q values of these modes can be as high as 10^6.

Frequency Domain Approach

Omega3P solves the Maxwell equations as an eigenvalue problem. The eigenvalue corresponds to the frequency of a (normal) mode of an accelerator component, which in our case is the cavity (here cavity is used as a generic term for the TDR cavity, cryomodule or the rf unit). The eigenvector corresponds to the field distribution of the mode. There are two types of cavity mode calculations,

(1) Closed cavity – One obtains the mode frequency by solving a real eigenvalue problem.
(2) Cavity with external coupling – An example is a cavity connected to a waveguide. In this case, fields can leak out through the external coupling (waveguide). The cavity can be modeled by a complex eigenvalue problem. The real part of the eigenvalue is the mode frequency and the imaginary part related to the damping (Q) of the mode.

The TDR cavity belongs to the latter category in that the cavity has external couplings through the HOM and fundamental couplers. The status of using *Omega3P* for the computation of the TDR cavities is,

(1) A number of modes can be obtained in a single run with all the required rf parameters, namely, the frequency, impedance and damping factor Q.
(2) The solution of eigenmodes is a scanning procedure in frequency, so it will guarantee that all possible modes in the system can be found.
(3) Using the same procedure, we have been able to obtain modes in a 4-cavity superstructure, and are now working toward a cryomodule of 8 cavities. In collaboration with computational scientists in ASCR SciDAC projects to improve the eigensolver efficiency, we are confident that we will achieve the goal of calculating wakefield effects in the 3-cryomodule rf unit outlined in the Grand Challenge.
(4) The linear solver used can scale to a thousand CPU's with fixed work-load per CPU. This is the so-called weak scaling, meaning that we increase the problem size as the number of CPU's increases in

the scalability measurement [see Ref. 1]. Note that the weak scalability is more appropriate for the ILC Grand Challenge as the problem size of modeling the rf unit is bigger than that we are currently simulating. The scalability of *Omega3P* on a peta-scale supercomputer will be tested when it is available. We will work with our SciDAC CET and Institutes partners on improving the scalability and performance on the peta-scale supercomputer that usually consists 10's of thousands of CPU's.

Time Domain Approach

TechX suggested using the time domain method to determine the mode spectrum and the Q values. A broadband pulse is first used to excite the mode spectrum, and then a narrow-band pulse is driven around a mode frequency to obtain the Q. We see some drawbacks in this approach.

(1) Mode identification – In the time domain, the modes have to be excited by a current source. One can only excite a mode which has non-vanishing field near the location of excitation. The rf unit is a fairly long structure, and some modes may localize in a small region of the entire structure. If the pulse is not applied accordingly in that region, those modes will not be found. Therefore, it is not certain that all the modes in the structure can be identified.

(2) Mode purity – For each dipole pair, the frequency difference between the two polarizations is small, of the order of 10's of kHz. To resolve the frequencies, the Qs and the field patterns of these modes for damping studies, a very narrow-band drive pulse of the order of 100's μs is needed. Let us take an educative guess. For a mesh step size of 0.5 mm, the time step is 1 ps. This means that 100's of millions of time steps are required to complete a time domain run, which is a very time consuming process. Furthermore, when one excites a drive pulse, it needs to be driven in the direction of a dipole mode polarization. However, the mode pattern is not known before one carries out the time domain simulation.

(3) Mode population – A rough estimate gives us about 1000 modes in the 3-cryomodule rf unit. In light of the above estimates, the time domain procedure does not seem practical.

Summary

The frequency domain approach using *Omega3P* is the clean and efficient method to calculate the trapped modes in the 3-cryomodule rf unit. We have successfully applied it to the TDR cavity, the LL cavity, the ILC crab cavity, and a superstructure consisting of 4 cavities. We will continue to collaborate with computational scientists to improve the performance of our parallel software. Solving the Grand Challenge problem with peta-scale computing is well within our reach.

Reference

[1] A. Gupta et.al., IEEE Trans. on Parallel and Distributed Systems, **8**(5), 502-520 (1997).