Scaling and Convergence of the Potential

Convergence of the iterative solution for the potential is not guaranteed is the SEMITIP calculations. Nevertheless, for suitable choice of parameters, all cases that have been investigated to date appear to have converged well. One important condition concering convergence is that, on the first scaling step in the computation, the number of grid points in each dimension not be too high. Typically 16 or 32 grid points in the radial direction and z direction into the semiconductor are suitable, with fewer points needed in the z direction into the vacuum or in the angular dimension (if used). In contrast, if say, 128 or 256 point are used in the first scaling step, then the convergence towards the solution may be very slow and the user could mistakenly assume that a correct solution have been achieved when actually the computation has not converged to the true solution.

Subsequent scaling steps in the solution for the potential are mainly intended to provide a finer mesh on which to evaluate the potential, i.e. without any significant global change in the potential compared to the first scaling step step.

Situations can arise when it is difficult to achieve near convergence of the solution on the first scaling step. For example, a small protrusion on the end of the tip forces the use of a fine grid, and hence many grid points may be needed to achieve a large enough simulation region. (Actually, tip protrusions have *not* been generally used in SEMITIP simulations, so they may lead to a variety of problems other than just limited convergence). Separately, in situations of self-consistency, the self-consistency loop is applied only in the *final* scaling step of the computation, so if significant changes in the solution are produced by the self-consistency, then care must to taken to use sufficiently tight convergence parameters for this loop.