In SEMITIP VERSIONS 2 and higher, grids with variable spacing were used for the r, ξ, and z coordinates. This variable spacing allowed the simulation to extend out to very large values of the coordinate, i.e. large enough so that the potential is essentially zero. Explicitly, the values of the grid points are assumed to be

$$r_i = \frac{2N_R\,\Delta r}{\pi}\tan\left(\frac{\pi\left(i-0.5\right)}{2N_R}\right) \qquad i = 1,2,3,\ldots,N_R\,, \tag{1a}$$

$$\xi_i = \sqrt{1+(r_i/a)^2}\,, \tag{1c}$$

and

$$z_j = -\frac{2N_S\,\Delta z}{\pi}\tan\left(\frac{\pi\,(j-0.5)}{2N_S}\right) \qquad j = 1,2,3,\ldots,N_S \tag{1c}$$

(the spacing shown for z_j is the one used for VERSIONS 4.2 and higher, prior to that it followed the form $z_j = -2N_S\,\Delta z\tan\left(\pi\,(j-1)/(2N_S)\right)/\pi$, $j = 1,2,3,\ldots,N_S-1$).

In VERSIONS 2 - 5, derivatives were calculated using the expressions

$$\frac{df}{dx} = \frac{f_{i+1}-f_{i-1}}{2\,\Delta x_i} \tag{2a}$$

and

$$\frac{d^2f}{dx^2} = \frac{f_{i+1}-2\,f_i+f_{i-1}}{\Delta x_i^2} \tag{2b}$$

for coordinate *x*, with the Δx_i values obtained by differentiation of Eqs. (1a) or 1(c),

$$\Delta r_i = \Delta r\left[\cos\left(\frac{\pi\left(i-0.5\right)}{2N_R}\right)\right]^{-2} \tag{3a}$$

$$\Delta z_j = -\Delta z\left[\cos\left(\frac{\pi\,(j-0.5)}{2N_S}\right)\right]^{-2}. \tag{3b}$$

While the expressions (2a) and (2b) are approximately correct, they can produce substantial errors when the Δx_i values vary with *i* as in Eqs. (3a) or (3b). Hence, in VERSIONS 6 and beyond, better forms for the derivatives are used:

$$\frac{df}{dx} = \frac{f_{i+1}-f_{i-1}}{(x_{i+1}-x_{i-1})} \tag{4a}$$

and

$$\frac{d^2f}{dx^2} = \left(\frac{f_{i+1}-f_i}{(x_{i+1}-x_i)} - \frac{f_i-f_{i-1}}{(x_i-x_{i-1})}\right)\frac{1}{(x_{i+1}-x_{i-1})/2}\,. \tag{4b}$$

Special considerations are required when i equals 1. For the radial derivatives, we assume a parabolic form for the function (potential) around $r = 0$ so that at $r = 0$ we have $f_0 = (9 f_1 - f_2)/8$ and $r_0 = 0$. The situation for the ξ derivatives is similar, although the value of ξ when $r = 0$ is $\xi = 1$. We again take this to be our zeroth grid point, so that $\xi_0 = 1$ and again $f_0 = (9 f_1 - f_2)/8$. The case of $j = 1$ is handled without any special attention since $j = 0$ corresponds to the surface (similarly, for the η parameter which extends to a value of N_V, the potential at $\eta = N_V + 1$ is simply the tip potential).

Special considerations are also needed when $i = N_R$ or $j = N_S$. It should be noted that, in almost all cases, the value of the potential is naturally zero at these boundaries of the grid, since the distance to the boundaries is so large that the potential falls to zero as a consequence of Poisson's equation. However, in situations where this does not occur, then values of the potential at $i = N_R + 1$ or $j = N_S + 1$ are needed, and some assumption is needed to establish those values. The program allows for two choices of boundary conditions: Dirichlet, in which the potential at $i = N_R + 1$ or $j = N_S + 1$ is taken to be zero, or Von Neumann in which the potential is taken to have the same value as at $i = N_R$ or $j = N_S$ (i.e. zero slope). This choice is controlled by the parameter IBC, which is set at the top of the semitip1.f, semitip2.f, or semitip3.f routine.. A value of IBC=0 corresponds to Dirichlet and IBC=1 to Von Neumann boundary conditions. The normal (default) setting is IBC=0.

The expressions for the derivatives in Eq. (4) have been compared to those of Eq. (2) for a two-dimensional test case of Laplace's equation $\nabla^2 f = 0$ with azimuthal symmetry. The analytic solution is $f(r) = c_1 \ln r + c_2$. Formulating a numerical solution using derivatives computed according to Eq. (4) yields results that agree exactly with this logarithmic dependence on *r*. However, with derivatives computed according to Eq. (2), the numerical solution deviates substantially from the logarithmic form (particularly for large *r*). Thus, the form of the derivatives given by Eq. (4) is found to be a substantial improvement for numerical solution of such problems. Similar agreement between theoretical expectation and computational results using the new form for the derivatives is found for 1-dimensional depletion, as discussed in example 2 of Uni1.f, and for a point charge on a surface, as discussed in example 6 of Uni2.f.