Screening:

There are two main types of screening, overlap screening and Coulomb screening. There is no broad consensus for either, so one simply does something that makes sense, and then uses user-defined threshholds to be sure nothing too bad happens.

In overlap screening, screening occurs at the atom level and the shell level. See the set of notes on this. This means that when one is looping over atoms (loop a) and shells (loop c) one may end up setting an integral to zero.

In the innermost loop (over primitives) one performs one last screening: set the integral to zero in the innermost loop if $s_{00}^{0} < \varepsilon$. (If that is true, then one can safely neglect the overlap/moment/kinetic-energy/derivatives integral.) Note that the "right" value for ε may be quite small, especially for moments. In general one can use a little bit coarser threshold for overlaps, and one needs potentially tighter threshholds for moments/derivatives (especially high-order moments/derivatives).

The basic strategy for overlap screening is that one first identifies a distance threshold beyond which atomic overlaps are negligible or shell-overlaps are negligible. After storing these thresholds, one can avoid computing certain integrals, which are set to zero. There are many ways to implement it, but one way would be to initialize the matrix of integrals one wishes to evaluate to "empty" or some placeholder, then fill zero's where one does not need to compute the integrals, and (finally) compute only integrals that had not (already) been assigned to zero.

In Coulomb screening for the 2-electron integrals, a nice method, with a nice trade-off between implementation difficulty and computational efficiency, was proposed by the Ochsenfeld group. See *J. Chem. Phys.* **147**, 144101 (2017).

The basic idea is that one forms an estimate for $I^{(0)}(\mathbf{a};\mathbf{b}\,|\,\mathbf{c};\mathbf{d})$ (the 2-electron integral) and then one neglects computing integrals where this estimate is sufficiently low. To do this, one first forms all the integrals where only two shells enter, namely,

$$Q_{\mathbf{ab}} = \sqrt{I^{(0)}(\mathbf{a};\mathbf{b}\,|\,\mathbf{a};\mathbf{b})} \tag{1}$$

and

$$M_{\mathbf{ac}} \equiv \sqrt{I^{(0)}(\mathbf{a};\mathbf{a}\,|\,\mathbf{c};\mathbf{c})} \tag{2}$$

Then the magnitude of the 2-electron integral can be estimated as (cf. Eqs. 11-13 in Ochsenfeld's paper)

$$\left|I^{(0)}(\mathbf{a};\mathbf{b}\,|\,\mathbf{c};\mathbf{d})\right| \approx \frac{Q_{\mathbf{ab}}Q_{\mathbf{cd}}}{\sqrt{Q_{\mathbf{aa}}Q_{\mathbf{bb}}Q_{\mathbf{cc}}Q_{\mathbf{dd}}}} \max\left(M_{\mathbf{ac}}M_{\mathbf{bd}}, M_{\mathbf{ad}}M_{\mathbf{bc}}\right) \tag{3}$$

If the predicted magnitude is small enough, then one can neglect the integral. Typically one choose a threshold of about 10^{-10} (which is typically good enough for microHartree accuracy) but sometimes smaller (or larger) thresholds are used.