算法 1 获取指定原子间 bcp 处电子密度

Input: $atomA(x^a, y^a, z^a)$: 原子 A 坐标; $atomB(x^b, y^b, z^b)$: 原子 B 坐标; $\rho(x_n, y_n, z_n)$: 离散空间电子密度; $eps1, eps2$: 条件阈值

转换原子 A 和 B 实际坐标到离散空间中坐标 $(x_n^a, y_n^a, z_n^a), (x_n^b, y_n^b, z_n^b)$
$grad(x_n, y_n, z_n) \leftarrow \nabla\rho(x_n, y_n, z_n)$
$hess(x_n, y_n, z_n) \leftarrow \nabla grad(x_n, y_n, z_n)$
$chg^{bcp} \leftarrow 0$
for x_n in range$(\min(x_n^a, x_n^b), \max(x_n^a, x_n^b))$ **do**
    for y_n in range$(\min(y_n^a, y_n^b), \max(y_n^a, y_n^b))$ **do**
        for z_n in range$(\min(z_n^a, z_n^b), \max(z_n^a, z_n^b))$ **do**
            $module \leftarrow \|grad(x_n, y_n, z_n)\|$
            if $module < eps1$ **then**
                $\lambda_1, \lambda_2, \lambda_3 \leftarrow \mathrm{eig}(hess(x_n, y_n, z_n))$
                $condition1 \leftarrow \bigwedge_{i=1}^{3} [\mathrm{abs}(\lambda_i) < eps2]$
                $condition2 \leftarrow \left[\sum_{i=1}^{3} \mathrm{sign}(\lambda_i)\right] = -1$
                if $condition1 \wedge condition2$ **then**
                    if $chg^{bcp} = 0 \vee module^{bcp} > module$ **then**
                        $chg^{bcp} \leftarrow chg(x_n, y_n, z_n)$
                        $module^{bcp} \leftarrow module$
                    end if
                end if
            end if
        end for
    end for
end for

Output: chg^{bcp}