

```
#include <stdio.h>
#include <vdwxc.h>

void main()
{
    double rho[] = {1.0, 2.0, 3.0, 4.0}; // input: density & gradient
    double sigma[] = {0.5, 1.5, 2.5, 3.5};
    double dedrho[] = {0.0, 0.0, 0.0, 0.0}; // output: derivatives
    double dedsigma[] = {0.0, 0.0, 0.0, 0.0};

    vdwxc_data vdw = vdwxc_new(VDWXC_DF1); // vdW-DF1 functional
    vdwxc_set_unit_cell(vdw, 1, 2, 2, // 1x2x2 grid; then cell vectors
                       1.0, 0.0, 0.0, 0.0, 2.0, 0.0, 0.0, 0.0, 2.0);
    vdwxc_init_serial(vdw);
    double energy = vdwxc_calculate(vdw, rho, sigma, dedrho, dedsigma);
    vdwxc_finalize(&vdw);
    printf("Energy %f Hartree\n", energy);
}
```