

Efficient evaluation of interatomic distances in large atomic scale models [Artivle v1.0]

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Abstract This article describes how lattice mathematical properties can be combined with the 3D space pixelation method to evaluate interatomic distances in large atomic scale 3D models. It aims to be an educative tool for students and researchers who want to develop structural analysis or 3D visualization tools that requires to implement and compute efficiently interatomic bond distances. Examples codes are provided in C, FORTRAN90 and Python.

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1 Introduction

Every student, every researcher in computational material science, has already spent time calculating interatomic distances. This problem is even likely to be the first one computational material scientists will spend some time over during their studies. As simple as the evaluation of a distance in 3D space could seem to be, the complexity of the problem increases considerably when dealing with the periodicity of non-cubic systems, and even more with the search for performance that is driving the analysis and the visualization of atomic scale models with more than tens of thousands of atoms.

This manuscript illustrates how lattice mathematical properties can be combined with the pixelation of the model box approach, to offer both a general, symmetry independent, methodology, and, an extremely efficient implementation of the search for first neighbor atoms.

2 Simulation box, lattice parameters and transformation matrices

Knowledge and understanding of the mathematics of lattice parameters and atomic coordinates is a prerequisite to the general formulation of the calculation of interatomic bond distances in 3D atomic scale models using periodic boundary conditions.

Note that this section can safely be ignored when dealing with non periodic systems.

2.1 Simulation box or lattice parameters

Box, or lattice parameters can be expressed with two different sets of parameters, using:

1. Using the box parameters A , B , C and the associated angles α , β and γ
2. Using the components of the lattice vectors $\vec{a}(a_x, a_y, a_z)$, $\vec{b}(b_x, b_y, b_z)$ and $\vec{c}(c_x, c_y, c_z)$

Then lattice vectors (2.1) can be calculated using box parameters (2.1) with:

$$\begin{bmatrix} A & 0.0 & 0.0 \\ \times \cos \gamma & B \times \sin \gamma & 0.0 \\ C \times \cos \beta & C \times L & C \times L^2 \end{bmatrix} \quad (1)$$

With:

$$L = \frac{\cos \alpha - \cos \beta \times \cos \gamma}{\sin \gamma} \quad (2)$$

While box parameters (2.1) can be calculated using lattice vectors (2.1) with:

$$A = |\vec{a}| \quad B = |\vec{b}| \quad C = |\vec{c}| \quad (3)$$

and:

$$\alpha = \frac{\vec{c} \cdot \vec{b}}{B \times C} \quad \beta = \frac{\vec{a} \cdot \vec{c}}{A \times C} \quad \gamma = \frac{\vec{a} \cdot \vec{b}}{A \times B} \quad (4)$$

The lattice volume:

$$V = \vec{a} \cdot (\vec{b} \wedge \vec{c}) = \vec{b} \cdot (\vec{c} \wedge \vec{a}) = \vec{c} \cdot (\vec{a} \wedge \vec{b}) \quad (5)$$

can then be calculated using:

$$V = A \times B \times C \times Z \quad (6)$$

With:

$$Z = \sqrt{1 - \cos^2 \alpha - \cos^2 \beta - \cos^2 \gamma + 2 \cos \alpha \cos \beta \cos \gamma} \quad (7)$$

Knowledge of these properties is a basic requirement, from there it possible to compute transformation matrices that allow the conversion from Cartesian r to Fractional f coordinates and the conversion from Fractional to Cartesian coordinates. These mathematical tools are extremely useful, if not almost mandatory prerequisites to the calculation, when dealing with non-cubic periodic systems.

2.2 From Cartesian to fractional coordinates

For an atom with Cartesian coordinates (r_x, r_y, r_z) , fractional coordinates (f_x, f_y, f_z) can be calculated using:

$$\begin{pmatrix} f_x \\ f_y \\ f_z \end{pmatrix} = T_f \times \begin{pmatrix} r_x \\ r_y \\ r_z \end{pmatrix} \quad (8)$$

Where the transformation matrix T_f is defined as:

$$T_f = \begin{bmatrix} \frac{1}{A} & -\frac{\cos \gamma}{A \sin \gamma} & \frac{\cos \alpha \cos \gamma - \cos \beta}{AZ \sin \gamma} \\ 0.0 & \frac{1}{B \sin \gamma} & \frac{\cos \alpha \cos \gamma - \cos \beta}{BZ \sin \gamma} \\ 0.0 & 0.0 & \frac{CZ}{\sin \gamma} \end{bmatrix} \quad (9)$$

2.3 From fractional to Cartesian coordinates

Similarly fractional coordinates (f_x, f_y, f_z) can be converted to Cartesian coordinates (r_x, r_y, r_z) using:

$$\begin{pmatrix} r_x \\ r_y \\ r_z \end{pmatrix} = T_c \times \begin{pmatrix} f_x \\ f_y \\ f_z \end{pmatrix} \quad (10)$$

Where the transformation matrix T_c is defined as:

$$T_c = T_f^{-1} = \begin{bmatrix} A & B \cos \gamma & C \cos \beta \\ 0.0 & B \sin \gamma & C \frac{\cos \alpha - \cos \beta \cos \gamma}{\sin \gamma} \\ 0.0 & 0.0 & \frac{CZ}{\sin \gamma} \end{bmatrix} \quad (11)$$

3 Pixelation of the model box

The idea of pixelation, or partitioning, of the model box illustrated in this section is mandatory to deal efficiently with searching for neighbor atoms in large atomic scale models. Indeed the intuitive way to implement the procedure would be to test every pair $i - j$ of atoms in the model: compute the interatomic distance D_{ij} between i (α) and j (β), and then compared this distance to a cutoff radius $R_{cut}(\alpha, \beta)$, that could appropriately be determined when looking at the radial distribution function $g_{\alpha\beta}(r)$. Then if D_{ij} is smaller or equal to $R_{cut}(\alpha, \beta)$ then atoms i and j are first neighbors, otherwise they are not. For a program which purpose is to render the atomic scale model in 3D space, the result of the analysis would be then to draw, or not, a bond between atoms i and j .

As intuitive and logical as this approach could seem to be, it requires to perform the testing for every pair of atoms in the model. Which, as long as the size of the system remains within the thousand or few thousands of atoms, could work in a seemingly efficient manner. The time order for the entire analysis is then proportional to $\frac{N \times (N-1)}{2}$, with N the total number of atoms in the model. However as the number of atoms increases, time required to performed the entire analysis increases even more dramatically, soon enough reaching a point where the program will likely seem to be completely frozen.

Therefore a step is required to optimize the procedure for large atomic scale models, and that is to distinguish atom(s) that are of interest for the purpose of the calculation from atom(s) that are not. This is done by dividing, or partitioning, the model box in smaller parts, or pixels.

Atomic coordinates will allow to associate an atom to a particular pixel. Then for this particular atom neighbors candidates will only be search for in that same pixel and its immediate surrounding pixel neighbors. The pixel dimension $a = R_{cut}$,

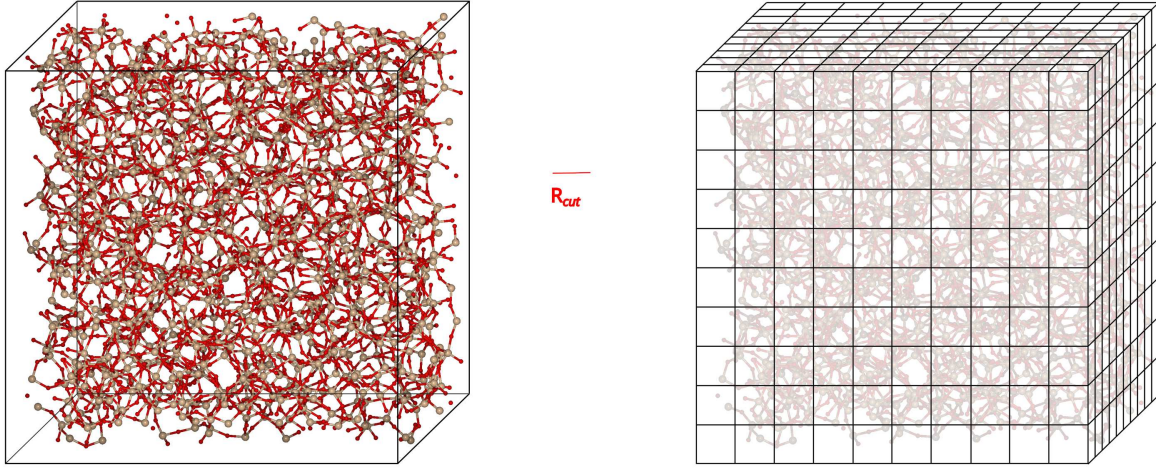


Figure 1. Pixelation of the model box

with R_{cut} is the cutoff radius used to search for first neighbors atoms.

This approach will limit the area of interest to the smallest possible size. Using this methodology the time order for the entire analysis becomes proportional to $N_p \times \frac{N_c \times (N_c - 1)}{2}$, with N_p is the total number of pixels in the grid, and N_c is the average number of atom(s) in the pixel and its 26 surrounding neighbor pixels: $N_c \ll N_p \ll N$.

The idea behind this approach is illustrated in figure 1.

3.1 Without Periodic Boundary Conditions

The number of pixels on each axis, $n_p(x)$, $n_p(y)$ and $n_p(z)$, are calculated using:

$$n_p(axis) = \left\lceil \frac{D_{max}(axis)}{R_{cut}} \right\rceil \quad (12)$$

Where $D_{max}(axis)$ is the maximum interatomic distance separating two atoms on *axis*, and R_{cut} is the cutoff distance that separates neighbor atoms.

Providing a model box, with parameters A, B, and C, encompassing the entire model could prove useful here, allowing the simplifications:

$$D_{max}(x) = A, \quad D_{max}(y) = B \quad \text{and} \quad D_{max}(z) = C \quad (13)$$

Otherwise calculations to determine D_{max} for each axis are needed. It is then required to test each pair of atomic coordinates in the model on *x*, *y* and *z*. However as long as only subtractions and min/max comparisons are involved calculation time will remain acceptable.

Then the total number of pixels in the model box, *pixels*, is calculated using:

$$pixels = n_p(x) \times n_p(y) \times n_p(z) \quad (14)$$

For an atom *at* with Cartesian coordinates (r_x , r_y , r_z) in the model, corresponding pixel indices in the pixel grid (p_x , p_y , p_z) can be calculated using:

$$p_{axis} = \left\lceil \frac{r_{axis} - \min_{axis}}{R_{cut}} \right\rceil \quad (15)$$

With:

$$p_{axis} \in [0, n_p(axis) - 1] \quad (16)$$

Where \min_{axis} is the lowest value for any atomic coordinates in the model on *axis*.

The pixel number for *at*, between 0 and *pixels* - 1, in entire the pixel grid, P_{id} is calculated using:

$$P_{id}(at) = p_x + n_p(x) \times p_y + [n_p(x) \times n_p(y)] \times p_z \quad (17)$$

With:

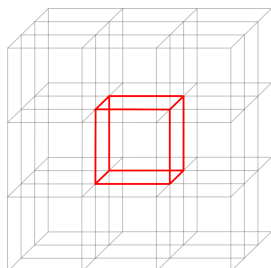
$$P_{id} \in [0, pixels - 1] \quad (18)$$

First neighbors list is calculated as follow:

1. The pixel position (p_x , p_y , p_z) for every atom (r_x , r_y , r_z) in the model is to be calculated so that each atom can be assigned a pixel number in the grid.
2. Accordingly a list of atom containing pixels is created, the list of atom(s) in each pixel being stored.
3. First neighbor(s) for an atom will then be search for in the pixel this atom belong to and in its surrounding pixel neighbors only, all other pixel(s) being safely ignored.

The list of pixel neighbors is constructed using the mathematical relationships between each pixel index in the grid, two cases must considered:

- Pixel inside the pixel grid:

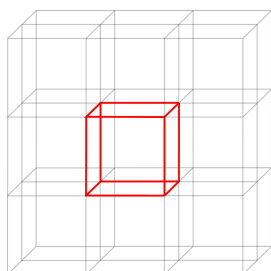


Self + 26 neighbors

- Pixel on the boundary of the pixel grid :

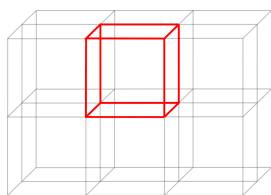
$$p_{axis} = 0 \text{ or } p_{axis} = n_p(axis) - 1$$

Face of the pixel grid



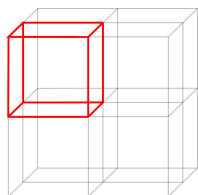
Self + 17 neighbors

Edge of the pixel grid



Self + 11 neighbors

Corner of the pixel grid



Self + 7 neighbors

Pixel neighbors are determined as illustrated in figure 2:

Note that this kind of approach only makes sense if the number of pixels in the grid is high enough so that all pixels are not neighbors.

3.2 With Periodic Boundary Conditions

Non-cubic symmetries make it more complicated to offer a general methodology to deal with periodic systems:

1. Evaluate the number of pixel(s) on each axis, $n_p(x)$, $n_p(y)$ and $n_p(z)$, using equations 12 and 13.
2. Convert atomic Cartesian coordinates to fractional coordinates using T_f .

Using the transformation to fractional coordinates is the easiest way to compute the distance between atoms in the model. The problem requires to consider the periodicity of the system, and, in the case of non-cubic symmetry transformations, could be tricky when using Cartesian coordinates. Working with fractional coordinates is much easier since in that case corrections are performed simply adding or subtracting multiples of 1.0 on any fractional direction.

- Convert Cartesian coordinates to fractional coordinates (f_x , f_y , f_z) using Eq. 8.
- Compute corrected fractional coordinates ($f_{c,x}$, $f_{c,y}$, $f_{c,z}$) inside the model box:

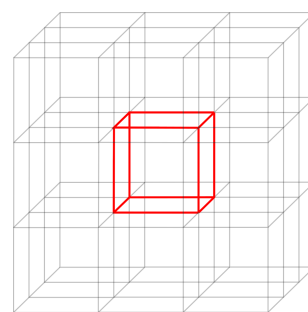
$$f_{c,axis} = f_{axis} - \lfloor f_{axis} \rfloor \quad \text{with} \quad 0 \leq f_{c,axis} < 1 \quad (19)$$

3. Pixel positions (p_x , p_y , p_z) are determined using the atom's corrected fractional coordinates ($f_{c,x}$, $f_{c,y}$, $f_{c,z}$):

$$p_{axis} = \lfloor f_{c,axis} \times n_p(axis) \rfloor \quad \text{with} \quad p_{axis} \in [0, n_p(axis) - 1] \quad (20)$$

4. Determine each pixel neighbors:

- Pixel inside the pixel grid:



Self + 26 neighbors, no PBC transformation required.

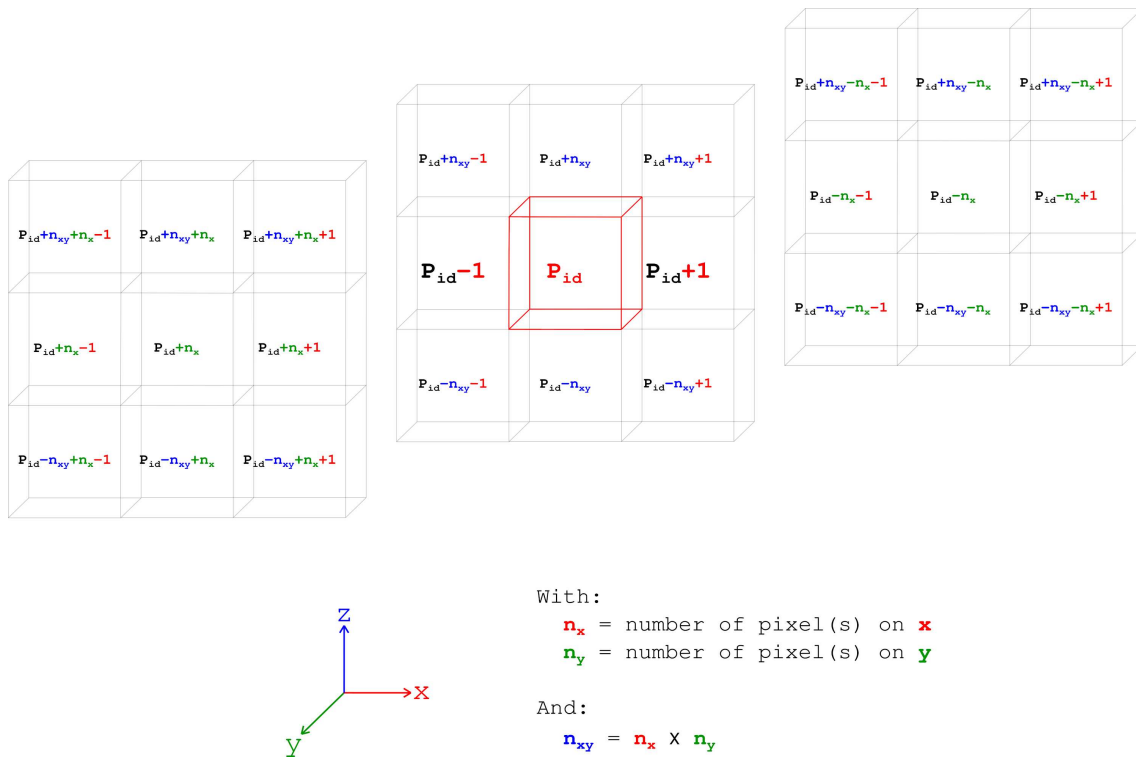
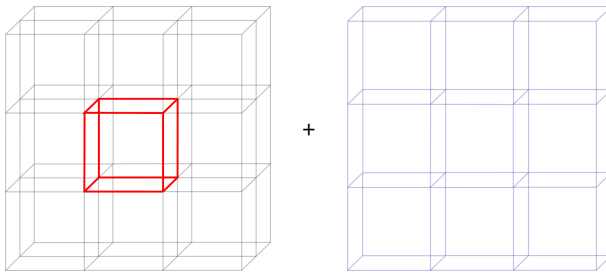


Figure 2. Finding pixel neighbors for pixel P_{id} : operation(s) on each axis are illustrated in the appropriate color(s)

- Pixel on the boundary of the pixel grid :

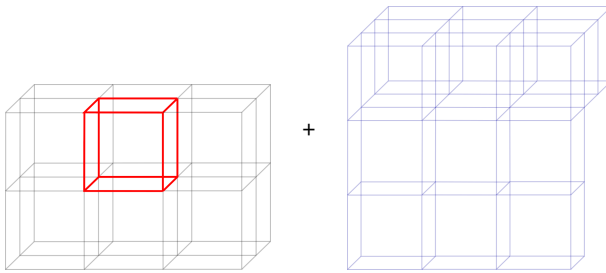
$$p_{axis} = 0 \text{ or } p_{axis} = n_p(\text{axis}) - 1$$

Face of the pixel grid:



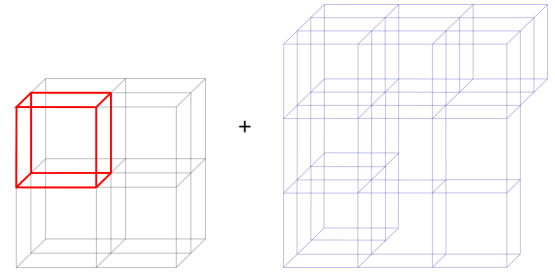
Self + 17 + 9 neighbors using PBC

Edge of the pixel grid:



Self + 11 + 15 neighbors using PBC

Corner of the pixel grid:



Self + 7 + 19 neighbors using PBC

For a pixel with number p_{id} with pixel coordinates (p_x, p_y, p_z) inside the pixel grid, pixel neighbors are determined as illustrated in figure 2. For pixel on the boundary of the grid, then adjustments are required to find the neighbors via PBC.

5. Compute the interatomic distance D_{ab} between 2 atoms a and b using corrected fractional coordinates:

$$f_{c,axis}(ab) = f_{c,axis}(a) - f_{c,axis}(b) \quad (21)$$

$$F_{axis}(ab) = \|f_{c,axis}(ab)\| \quad (22)$$

$$Fmin_{axis}(ab) = \min[F_{axis}(ab), 1.0 - F_{axis}(ab)] \quad (23)$$

$$f_{axis}(ab) = \frac{f_{c,axis}(ab)}{F_{axis}(ab)} \times Fmin_{axis}(ab) \quad (24)$$

$$\vec{r}(ab) = \mathbf{T_c} \times \vec{f}(ab) \quad (25)$$

$$\text{with } \vec{r}(ab) = \begin{pmatrix} r_x(ab) \\ r_y(ab) \\ r_z(ab) \end{pmatrix} \quad (26)$$

$$\text{and } \vec{f}(ab) = \begin{pmatrix} f_x(ab) \\ f_y(ab) \\ f_z(ab) \end{pmatrix} \quad (27)$$

$$D(ab) = |\vec{r}(ab)| \quad (28)$$

As mentioned in the previous section this approach only makes sense when the number of pixels in the grid is high enough so that all pixels are not neighbors. In the case where PBC are applied this means that the number of pixels on one dimension, x , y , or z should be higher than 3.

Commented codes that illustrate the entire work procedure are provided in:

- C codes: A.1 through A.7.
- FORTRAN90 codes: B.1 through B.7.
- Python codes: C.1 through C.7.

Note that this Python code is provided to illustrate the entire implementation in Python, but for that particular programming language several Python libraries already exist and can be used as fronted to simplify the complete coding (ex: [ASE](#), [Pysic](#), [MDAnalysis](#)), however in that case the pixelation approach is rarely coded in pure Python language ([Pysic](#) using Fortran, [MDAnalysis](#) using C).

4 Further optimizations

The analysis time can be reduced using MPI and/or OpenMP parallel programming. Several scenario, or approaches, can be envisioned depending on the size of the system in number of atoms and/or the number of configuration (MD steps):

- Single (MPI or OpenMP): atomic coordinates or pixels can be distributed over the CPU and/or CPU cores.
- Multiples (MPI or OpenMP): configurations can be distributed over the CPU and/or the CPU cores.

- Multiples (MPI and OpenMP): with hybrid parallelization configurations can be distributed over the CPU, and atomic coordinates or pixels can be distributed over the CPU cores.

Ideally the code would provide the option to switch to one or the other approach based on the number of configurations and or atoms in the system.

Note that this is the case of the **atomes** software [1] that implements an adaptive OpenMP programming distributing either the atomic coordinates or the MD steps on the CPU cores.

5 Conclusion

The general methodology behind efficient first neighbor(s) analysis in any kind of atomic scale models was described. It was illustrated that the understanding of lattice mathematics can simplify the evaluation of interatomic bond distances independently of the periodicity of the system, and that the particular idea of the pixelation, or partitioning, of the model box, is a prerequisite to any modern implementation of this analysis.

The methodology described in this article is the one implemented in the **atomes** software [1].

Checklist

For a more detailed description of author contributions, see the GitHub issue tracking and changelog at <https://github.com/Slookeur/Bonds>.

Potentially Conflicting Interests

No conflicting interests.

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References

- [1] Le Roux S. Comp. Mat. Sci.. 2025; 253:113805. <https://doi.org/10.1016/j.commatsci.2025.113805>.

SEARCHING FOR FIRST NEIGHBOR ATOMS

Non-periodic systems

- ☐ Choose a cutoff radius R_{cut} to determine first neighbor atoms
- ☐ Find the maximum distances, $D_{max}(x)$, $D_{max}(y)$ and $D_{max}(z)$ that separate 2 atoms on x , y and z
- ☐ Determine the number of pixels, $n_p(axis)$, on x , y and z using $n_p(axis) = \left\lceil \frac{D_{max}(axis)}{R_{cut}} \right\rceil$
- ☐ Create a pixel grid for a virtual box with dimensions $n_p(x)$, $n_p(y)$ and $n_p(z)$ on x , y and z axis respectively.
- ☐ Using its Cartesian coordinates, r_{axis} , associate each atom at with a pixel position in the grid
 - ☐ Pixel position on each $axis$: $p_{axis} = \left\lfloor \frac{r_{axis} - \min_{axis}}{R_{cut}} \right\rfloor$
 - ☐ Pixel ID number in the grid: $P_{id}(at) = p_x + n_p(x) \times p_y + [n_p(x) \times n_p(y)] \times p_z$
- ☐ Associate each pixel with its surrounding neighbors in the grid
- ☐ Search for bond candidates between the atoms of a pixel as well as the atoms of its surrounding pixel neighbors
- ☐ Evaluate distances using the atom's Cartesian coordinates

Periodic systems

- ☐ Choose a cutoff radius R_{cut} to determine first neighbor atoms
- ☐ Use the lattice parameters as maximum interatomic distances on x , y and z : $D_{max}(x) = A$, $D_{max}(y) = B$ and $D_{max}(z) = C$
- ☐ Determine the number of pixels, $n_p(axis)$, on x , y and z using $n_p(axis) = \left\lceil \frac{D_{max}(axis)}{R_{cut}} \right\rceil$
- ☐ Create a pixel grid with dimensions $n_p(x)$, $n_p(y)$ and $n_p(z)$ on x , y and z axis respectively.
- ☐ Convert all atom Cartesian coordinates to fractional coordinates f
- ☐ Compute the corrected fractional coordinates f_c to ensure that all are in the unit cell
- ☐ Using its correct fractional coordinates, $f_{c,axis}$, associate each atom at with a pixel position in the grid
 - ☐ Pixel position on each $axis$: $p_{axis} = \lfloor f_{c,axis} \times n_p(axis) \rfloor$
 - ☐ Pixel ID number in the grid: $P_{id}(at) = p_x + n_p(x) \times p_y + [n_p(x) \times n_p(y)] \times p_z$
- ☐ Associate each pixel with its surrounding neighbors in the grid, if needed apply PBC transformation(s)
- ☐ Search for bond candidates between the atoms of a pixel as well as the atoms of its surrounding pixel neighbors
- ☐ Evaluate distances using the atom's corrected fractional coordinates followed by a matrix transformation to Cartesian coordinates

Appendix A Commented C code

A.1 C code: data structures and global variables

```

1 // global data structures and variables used in the next code sections
2
3 #define TRUE 1
4 #define FALSE 0
5
6 // atom in pixel data structure
7 typedef struct pixel_atom pixel_atom;
8 struct pixel_atom
9 {
10     int atom_id;           // the atom ID
11     float coord[3];       // the atom coordinates on x, y and z
12 };
13
14 // pixel data structure
15 typedef struct pixel pixel;
16 struct pixel
17 {
18     int pid;               // the pixel number
19     int p_xyz[3];          // the pixel coordinates in the grid
20     bool tested;           // was the pixel checked already
21     int patoms;            // number of atom(s) in pixel
22     pixel_atom * pix_atoms; // list of atom(s) in the pixel, to be allocated
23     int neighbors;         // number of neighbors for pixel
24     int pixel_neighbors[27]; // the list of neighbor pixels, maximum 27
25 };
26
27 // pixel grid data structure
28 typedef struct pixel_grid pixel_grid;
29 struct pixel_grid
30 {
31     int pixels;            // total number of pixels in the grid
32     int n_pix[3];          // number of pixel(s) on each axis
33     int n_xy;              // number of pixels in the plan xy
34     pixel * pixel_list;    // pointer to the pixels, to be allocated
35 };
36
37 // bond distance data structure
38 typedef struct distance distance;
39 struct distance
40 {
41     float length;          // the distance in \AA\ squared
42     float Rij[3];          // vector components of x, y and z
43 };
44
45 /*
46  the following are considered to be provided by the user
47 */
48
49 // model description
50 int atoms;                 // the total number of atom(s)
51 float ** c_coord;          // list of Cartesian coordinates: c_coord[atoms][3]
52 float cutoff;              // the cutoff to define atomic bond(s)
53 float cutoff_squared;      // squared value for the cutoff
54
55 // model box description
56 float l_params[3];         // lattice a, b and c
57 float cart_to_frac[3][3];  // Cartesian to fractional coordinates matrix
58 float frac_to_cart[3][3];  // fractional to Cartesian coordinates matrix

```

A.2 C code: set periodic boundary condition pixel shift

```

1 void set_pbc_shift (pixel_grid * grid, int pixel_coord[3], int pbc_shift[3][3][3])
2 {
3     int x_pos, y_pos, z_pos; // loop iterators
4     for ( x_pos = 0 ; x_pos < 3 ; x_pos ++ )
5     {
6         for ( y_pos = 0 ; y_pos < 3 ; y_pos ++ )
7         {
8             for ( z_pos = 0 ; z_pos < 3 ; z_pos ++ )
9             {
10                 pbc_shift[x_pos][y_pos][z_pos] = 0;           // initialization without any shift
11             }
12         }
13     }
14     if ( pixel_coord[0] == 0 )                                // pixel position on 'x' is min
15     {
16         for ( y_pos = 0 ; y_pos < 3 ; y_pos ++ )
17         {
18             for ( z_pos = 0 ; z_pos < 3 ; z_pos ++ )
19             {
20                 pbc_shift[0][y_pos][z_pos] = grid->n_pix[0];
21             }
22         }
23     }
24     else if ( pixel_coord[0] == grid->n_pix[0] - 1 )          // pixel position on 'x' is max
25     {
26         for ( y_pos = 0 ; y_pos < 3 ; y_pos ++ )
27         {
28             for ( z_pos = 0 ; z_pos < 3 ; z_pos ++ )
29             {
30                 pbc_shift[2][y_pos][z_pos] = - grid->n_pix[0];
31             }
32         }
33     }
34     if ( pixel_coord[1] == 0 )                                // pixel position on 'y' is min
35     {
36         for ( x_pos = 0 ; x_pos < 3 ; x_pos ++ )
37         {
38             for ( z_pos = 0 ; z_pos < 3 ; z_pos ++ )
39             {
40                 pbc_shift[x_pos][0][z_pos] += grid->n_xy;
41             }
42         }
43     }
44     else if ( pixel_coord[1] == grid->n_pix[1] - 1 )          // pixel position on 'y' is max
45     {
46         for ( x_pos = 0 ; x_pos < 3 ; x_pos ++ )
47         {
48             for ( z_pos = 0 ; z_pos < 3 ; z_pos ++ )
49             {
50                 pbc_shift[x_pos][2][z_pos] -= grid->n_xy;
51             }
52         }
53     }
54     if ( pixel_coord[2] == 0 )                                // pixel position on 'z' is min
55     {
56         for ( x_pos = 0 ; x_pos < 3 ; x_pos ++ )
57         {
58             for ( y_pos = 0 ; y_pos < 3 ; y_pos ++ )
59             {
60                 pbc_shift[x_pos][y_pos][0] += grid->pixels;
61             }
62         }
63     }
64     else if ( pixel_coord[2] == grid->n_pix[2] - 1 )          // pixel position on 'z' is max
65     {
66         for ( x_pos = 0 ; x_pos < 3 ; x_pos ++ )
67         {
68             for ( y_pos = 0 ; y_pos < 3 ; y_pos ++ )
69             {
70                 pbc_shift[x_pos][y_pos][2] -= grid->pixels;
71             }
72         }
73     }
74 }

```

A.3 C code: add atom to pixel

```

1 void add_atom_to_pixel (pixel * the_pixel, int pixel_coord[3], int atom_id, float atom_coord[3])
2 {
3     int axis;
4     if (! the_pixel->patoms)
5     {
6         // if the pixel do not contains any atom yet, then save its coordinates in the grid
7         for ( axis = 0 ; axis < 3 ; axis ++ )
8         {
9             the_pixel->p_xyz[axis] = pixel_coord[axis];
10        }
11        // allocate the memory to store the first pixel_atom information
12        the_pixel->pix_atoms = malloc(sizeof*the_pixel->pix_atoms);
13    }
14    else
15    {
16        // otherwise reallocate memory to store the new pixel_atom information
17        the_pixel->pix_atoms = realloc(the_pixel->pix_atoms, (the_pixel->patoms+1)*sizeof*the_pixel->pix_atoms);
18    }
19    the_pixel->pix_atoms[the_pixel->patoms].atom_id = atom_id;
20    for ( axis = 0 ; axis < 3 ; axis ++ )
21    {
22        the_pixel->pix_atoms[the_pixel->patoms].coord[axis] = atom_coord[axis];
23    }
24    // increment the number of atom(s) in the pixel
25    the_pixel->patoms ++;
26 }

```

A.4 C code: preparation of the pixel grid

```

1 pixel_grid * prepare_pixel_grid (bool use_pbc)
2 {
3     pixel_grid * grid;           // pointer to the pixel grid to create
4     int axis;                    // loop iterator axis id (0=x, 1=y, 2=z)
5     int aid;                     // loop iterator atom number (0, atoms--1)
6     int pixel_num;               // pixel number in the grid
7     int pixel_pos[3];            // pixel coordinates in the grid
8     float cmin[3], cmax[3];      // float coordinates min, max values
9     float f_coord[3];           // float fractional coordinates
10
11     grid = malloc(sizeof*grid);
12
13     if ( ! use_pbc )             // without periodic boundary conditions
14     {
15         for ( axis = 0 ; axis < 3 ; axis ++ ) cmin[axis] = cmax[axis] = c_coord[0][axis];
16         for ( aid = 1 ; aid < atoms ; aid ++ ) // For all atoms
17         {
18             for ( axis = 0 ; axis < 3 ; axis ++ ) // For x, y and z
19             {
20                 cmin[axis] = min(cmin[axis], c_coord[aid][axis]);
21                 cmax[axis] = max(cmax[axis], c_coord[aid][axis]);
22             }
23         }
24         for ( axis = 0 ; axis < 3 ; axis ++ ) // For x, y and z
25         {
26             // Number of pixel(s) on axis 'axis'
27             grid->n_pix[axis] = (int)((cmax[axis] - cmin[axis]) / cutoff) + 1;
28         }
29     }
30     else // using periodic boundary conditions
31     {
32         for ( axis = 0 ; axis < 3 ; axis ++ ) // For x, y and z
33         {
34             // Number of pixel(s) on axis 'axis'
35             grid->n_pix[axis] = (int)(l_params[axis] / cutoff) + 1;
36         }
37     }
38     for ( axis = 0 ; axis < 3 ; axis ++ ) // For x, y and z
39     {
40         // correction if the number of pixel(s) on 'axis' is too small
41         grid->n_pix[axis] = (grid->n_pix[axis] < 4) ? 1 : grid->n_pix[axis];
42     }
43     grid->n_xy = grid->n_pix[0] * grid->n_pix[1]; // Number of pixels on the plan 'xy'
44     grid->pixels = grid->n_xy * grid->n_pix[2]; // Total number of pixels in the grid
45     grid->pixel_list = malloc (grid->pixels*sizeof*grid->pixel_list);
46     for ( pixel_num = 0 ; pixel_num < grid->pixels ; pixel_num ++ )
47     {
48         grid->pixel_list[pixel_num].pid = pixel_num;
49         grid->pixel_list[pixel_num].patoms = 0;
50         grid->pixel_list[pixel_num].tested = FALSE;
51     }
52     if ( ! use_pbc )             // without periodic boundary conditions
53     {
54         for ( aid = 0 ; aid < atoms ; aid ++ ) // for all atoms
55         {
56             for ( axis = 0 ; axis < 3 ; axis ++ ) // for x, y and z
57             {
58                 pixel_pos[axis] = (int)((c_coord[aid][axis] - cmin[axis])/cutoff);
59             }
60             pixel_num = pixel_pos[0] + pixel_pos[1] * grid->n_pix[0] + pixel_pos[2] * grid->n_xy;
61             add_atom_to_pixel (grid, pixel_num, pixel_pos, aid, c_coord[aid]);
62         }
63     }
64     else // using periodic boundary conditions
65     {
66         for ( aid = 0 ; aid < atoms ; aid ++ ) // for all atoms
67         {
68             // with 'matrix_multiplication' a user defined function to perform the operation
69             f_coord = matrix_multiplication (cart_to_frac, c_coord[aid]);
70             for ( axis = 0 ; axis < 3 ; axis ++ ) // for x, y and z
71             {
72                 f_coord[axis] = f_coord[axis] - floorf(f_coord[axis]);
73                 pixel_pos[axis] = (int)((f_coord[axis] * grid->n_pix[axis]);
74             }
75             pixel_num = pixel_pos[0] + pixel_pos[1] * grid->n_pix[0] + pixel_pos[2] * grid->n_xy;
76             add_atom_to_pixel (& grid->pixel_list[pixel_num], aid, f_coord);
77         }
78     }
79 }

```

```
78 }  
79 return grid;  
80 }
```

A.5 C code: finding pixel neighbors

```

1 // finding neighbor pixels for pixel in the grid
2 // - bool use_pbc          : flag to set if PBC are used or not
3 // - pixel_grid * the_grid : pointer to the pixel grid
4 // - pixel * the_pix       : pointer to the pixel with neighbors to be found
5 void find_pixel_neighbors (bool use_pbc, pixel_grid * the_grid, pixel * the_pix)
6 {
7     int axis; // loop iterator axis id (1=x , 2=y , 3= z)
8     int xpos, ypos, zpos; // neighbor position on x, y and z
9     int l_start[3] = { 0, 0, 0 }; // loop iterators starting value
10    int l_end[3] = { 3, 3, 3 }; // loop iterators ending value
11    int pmod[3] = { -1, 0, 1 }; // position modifiers
12    int nnp; // number of neighbors for pixel
13    int nid; // neighbor id for pixel
14    int pbc_shift[3][3][3]; // shift for pixel neighbor number due to PBC
15    bool boundary = FALSE; // is pixel on the boundary of the grid
16    bool keep_neighbor = TRUE; // keep or not neighbor during analysis
17
18    if ( use_pbc )
19    {
20        set_pbc_shift (the_grid, the_pix->p_xyz, pbc_shift);
21    }
22    else
23    {
24        for ( axis = 0 ; axis < 3 ; axis ++ )
25        {
26            if ( the_pix->p_xyz[axis] == 0 || the_pix->p_xyz[axis] == the_grid->n_pix[axis] - 1 ) boundary = TRUE;
27        }
28    }
29    for ( axis = 0 ; axis < 3 ; axis ++ )
30    {
31        if ( the_grid->n_pix[axis] == 1 )
32        {
33            l_start[axis] = 1;
34            l_end[axis] = 2;
35        }
36    }
37    nnp = 0;
38    for ( xpos = l_start[0] ; xpos < l_end[0] ; xpos ++ )
39    {
40        for ( ypos = l_start[1] ; ypos < l_end[1] ; ypos ++ )
41        {
42            for ( zpos = l_start[2] ; zpos < l_end[2] ; zpos ++ )
43            {
44                keep_neighbor = TRUE;
45                if ( ! use_pbc && boundary )
46                {
47                    if ( ( the_pix->p_xyz[0] == 0 && xpos == 0 ) || ( the_pix->p_xyz[0] == the_grid->n_pix[0] && xpos == 2 ) )
48                    {
49                        keep_neighbor = FALSE;
50                    }
51                    else if ( ( the_pix->p_xyz[1] == 0 && ypos == 0 ) || ( the_pix->p_xyz[1] == the_grid->n_pix[1] && ypos == 2 ) )
52                    {
53                        keep_neighbor = FALSE;
54                    }
55                    else if ( ( the_pix->p_xyz[2] == 0 && zpos == 0 ) || ( the_pix->p_xyz[2] == the_grid->n_pix[2] && zpos == 2 ) )
56                    {
57                        keep_neighbor = FALSE;
58                    }
59                }
60                if ( keep_neighbor )
61                {
62                    nid = the_pix->pid + pmod[xpos] + pmod[ypos] * the_grid->n_pix[0] + pmod[zpos] * the_grid->n_xy;
63                    if ( use_pbc ) nid += pbc_shift[xpos][ypos][zpos];
64                    the_pix->pixel_neighbors[nnp] = nid;
65                    nnp ++ ;
66                }
67            }
68        }
69    }
70    the_pix->neighbors = nnp;
71 }

```

A.6 C code: inter-atomic distance calculation

```

1 // evaluating the interatomic distance between 2 pixel atoms
2 // - bool use_pbc      : flag to set if PBC are used or not
3 // - pixel_atom * at_i : pointer to first pixel atom
4 // - pixel_atom * at_j : pointer to second pixel atom
5 distance evaluate_distance (bool use_pbc, pixel_atom * at_i, pixel_atom * at_j)
6 {
7     int axis;           // axis loop iterator
8     float u, v;         // float parameters
9     distance dist;      // distance data to store calculation results
10    for ( axis = 0 ; axis < 3 ; axis ++ )
11    {
12        dist.Rij[axis] = at_i->coord[axis] - at_j->coord[axis];
13    }
14    if ( use_pbc )
15    {
16        // then the pixel_atom's coordinates are in corrected fractional format
17        for ( axis = 0 ; axis < 3 ; axis ++ )
18        {
19            dist.Rij[axis] = dist.Rij[axis] - roundf(dist.Rij[axis]);
20        }
21        // transform back to Cartesian coordinates
22        // with 'matrix_multiplication' a user defined function to perform the operation
23        dist.Rij = matrix_multiplication (frac_to_cart, dist.Rij);
24    }
25    dist.length = 0.0;
26    for ( axis = 0 ; axis < 3 ; axis ++ )
27    {
28        dist.length += dist.Rij[axis] * dist.Rij[axis];
29    }
30    // returning the 'distance' data structure that contains:
31    // - the squared value for Dij: no time consuming square root calculation !
32    // - the components of the distance vector on x, y and z
33    return dist;
34 }

```

A.7 C code: pixel search for first neighbor atoms

```

1 // searching for first neighbor atoms using the grid pixelation/partitioning method
2 // - bool use_pbc : flag to set if PBC are used or not
3 void pixel_search_for_neighbors (bool use_pbc)
4 {
5     pixel_grid * all_pixels;    // pointer to the pixel grid for to analyze
6     int pix, pjx;              // integer pixel ID numbers
7     int aid, bid;              // integer loop atom numbers
8     int pid;
9     int l_start, l_end;        // integer loop modifier
10    pixel * pix_i, * pix_j;     // pointers on pixel data structure
11    pixel_atom * at_i, * at_j;  // pointers on pixel_atom data structure
12    distance Dij;               // distance data structure
13
14    all_pixels = prepare_pixel_grid (use_pbc);
15    // note that the pixel grid 'all_pixels' must be prepared before the following
16    // for all pixels in the grid
17    for ( pix = 0 ; pix < all_pixels->pixels ; pix ++ )
18    {
19        // setting 'pix_i' as pointer to pixel number 'pix'
20        pix_i = & all_pixels->pixel_list[pix];
21        // if pixel 'pix_i' contains atom(s)
22        if ( pix_i->patoms )
23        {
24            // search for neighbor pixels of 'pix_i'
25            find_pixel_neighbors ( use_pbc, all_pixels, pix_i );
26            // testing all 'pix_i' neighbor pixels
27            for ( pid = 0 ; pid < pix_i->neighbors ; pid ++ )
28            {
29                pjx = pix_i->pixel_neighbors[pid];
30                // setting 'pix_j' as pointer to pixel number 'pjx'
31                pix_j = & all_pixels->pixel_list[pjx];
32                // checking pixel 'pix_j' if it:
33                // - contains atom(s)
34                // - was not tested, otherwise the analysis would have been performed already
35                if ( pix_j->patoms && ! pix_j->tested )
36                {
37                    // if 'pix_i' and 'pix_j' are the same, only test pair of different atoms
38                    l_end = (pjx != pix) ? 0 : 1;
39                    // for all atom(s) in 'pix'
40                    for ( aid = 0 ; aid < pix_i->patoms - l_end ; aid ++ )
41                    {
42                        // set pointer to the first atom to test
43                        at_i = & pix_i->pix_atoms[aid];
44                        lstart = (pjx != pix) ? 0 : aid + 1;
45                        // for all atom(s) in 'pix_j'
46                        for ( bid = l_start ; bid < pix_j->patoms ; bid ++ )
47                        {
48                            // set pointer to the second atom to test
49                            at_j = & pix_j->pix_atoms[bid];
50                            // evaluate interatomic distance
51                            Dij = evaluate_distance (use_pbc, at_i, at_j);
52                            if ( Dij.length < cutoff_squared )
53                            {
54                                // this is a first neighbor bond !
55                            }
56                        }
57                    }
58                }
59            }
60            // store that pixel 'pix' was tested
61            pix_i->tested = TRUE;
62        }
63    }
64 }

```


Appendix B Commented FORTRAN90 code

B.1 FORTRAN90 code: data structures and global variables

```

1  ! global data structures and variables used in the next code sections
2  MODULE parameters
3
4  ! atom in pixel data structure
5  TYPE pixel_atom
6      INTEGER                :: atom_id           ! the atom ID
7      REAL, DIMENSION(3)     :: coord             ! the atom coordinates on x, y and z
8  END TYPE pixel_atom
9
10 ! pixel data structure
11 TYPE pixel
12     INTEGER                :: pid               ! the pixel number
13     INTEGER, DIMENSION(3)   :: p_xyz            ! the pixel coordinates in the grid
14     LOGICAL                 :: tested            ! was the pixel checked already
15     INTEGER                 :: patoms           ! number of atom(s) in pixel
16     TYPE(pixel_atom), DIMENSION(:), ALLOCATABLE :: pix_atoms ! list of atom(s) in pixel, to be allocated
17     INTEGER                 :: neighbors        ! number of neighbors for pixel
18     INTEGER, DIMENSION(27)  :: pixel_neighbors ! the list of neighbor pixels, maximum 27
19 END TYPE pixel
20
21 ! pixel grid data structure
22 TYPE pixel_grid
23     INTEGER                :: pixels            ! total number of pixels in the grid
24     INTEGER, DIMENSION(3)   :: n_pix           ! number of pixel(s) on each axis
25     INTEGER                 :: n_xy            ! number of pixels in the plan xy
26     TYPE (pixel), DIMENSION(:), ALLOCATABLE, TARGET :: pixel_list ! pointer to the pixels, to be allocated
27 END TYPE pixel_grid
28
29 ! distance data structure
30 TYPE distance
31     REAL                   :: length           ! the distance in Å squared
32     REAL, DIMENSION(3)     :: Rij              ! vector components of x, y and z
33 END TYPE distance
34
35 !
36 ! the following are considered to be provided by the user
37 !
38
39 ! model description
40 INTEGER                :: atoms                ! the total number of atom(s)
41 REAL, DIMENSION(atoms,3) :: c_coord           ! list of Cartesian coordinates
42 REAL                   :: cutoff              ! the cutoff to define first neighbors
43 REAL                   :: cutoff_squared      ! squared value of the cutoff to define first neighbors
44
45 ! model box description
46 REAL, DIMENSION(3)      :: l_params           ! lattice a, b and c
47 REAL, DIMENSION(3,3)    :: cart_to_frac      ! Cartesian to fractional coordinates matrix
48 REAL, DIMENSION(3,3)    :: frac_to_cart      ! fractional to Cartesian coordinates matrix
49
50 END MODULE parameters

```

B.2 FORTRAN90 code: set pixel periodic boundary condition shift

```

1 SUBROUTINE set_pbc_shift (grid, pixel_coord, pbc_shift)
2
3   USE parameters
4   IMPLICIT NONE
5
6   TYPE (pixel_grid), INTENT(IN)           :: grid           ! the pixel grid
7   INTEGER, DIMENSION(3), INTENT(IN)       :: pixel_coord    ! the pixel coordinates in the grid
8   INTEGER, DIMENSION(3,3,3), INTENT(INOUT) :: pbc_shift      ! the shift, correction, to be calculated
9
10  pbc_shift(:, :, :) = 0                                ! initialization without any shift
11
12  if ( pixel_coord(1) .eq. 1 ) then                    ! pixel position on 'x' is min
13    pbc_shift(1, :, :) = grid%n_pix(1)
14  else if ( pixel_coord(1) .eq. grid%n_pix(1) ) then   ! pixel position on 'x' is max
15    pbc_shift(3, :, :) = - grid%n_pix(1)
16  endif
17
18  if ( pixel_coord(2) .eq. 1 ) then                    ! pixel position on 'y' is min
19    pbc_shift(:, 1, :) = pbc_shift(:, 1, :) + grid%n_xy
20  else if ( pixel_coord(2) .eq. grid%n_pix(2) ) then   ! pixel position on 'y' is max
21    pbc_shift(:, 3, :) = pbc_shift(:, 3, :) - grid%n_xy
22  endif
23
24  if ( pixel_coord(3) .eq. 1 ) then                    ! pixel position on 'z' is min
25    pbc_shift(:, :, 1) = pbc_shift(:, :, 1) + grid%pixels
26  else if ( pixel_coord(3) .eq. grid%n_pix(3) ) then   ! pixel position on 'z' is max
27    pbc_shift(:, :, 3) = pbc_shift(:, :, 3) - grid%pixels
28  endif
29
30 END SUBROUTINE set_pbc_shift

```

B.3 FORTRAN90 code: add atom to pixel

```

1 SUBROUTINE add_atom_to_pixel (the_pixel, pixel_coord, atom_id, atom_coord)
2
3   USE parameters
4   IMPLICIT NONE
5
6   TYPE (pixel), INTENT(INOUT) :: the_pixel      ! pointer to the pixel
7   INTEGER, DIMENSION(3), INTENT(IN) :: pixel_coord ! the pixel coordinates in the grid
8   INTEGER, INTENT(IN) :: atom_id ! the atom ID number
9   INTEGER :: axis ! loop iterator axis id (1=x, 2=y, 3=z)
10  REAL, DIMENSION(3), INTENT(IN) :: atom_coord ! the atomic coordinates
11
12  if (the_pixel%patoms .eq. 0) then
13    ! if the pixel do not contains any atom yet, then save its coordinates in the grid
14    do axis = 1, 3
15      the_pixel%p_xyz(axis) = pixel_coord(axis)
16    enddo
17    ! allocate the memory to store the first pixel_atom information
18    allocate(the_pixel%pix_atoms(1))
19  else
20    ! otherwise reallocate memory to store the new pixel_atom informatio
21    the_pixel%pix_atoms = realloc(the_pixel%pix_atoms, the_pixel%patoms+1)
22  endif
23  ! increment the number of atom(s) in the pixel
24  the_pixel%patoms = the_pixel%patoms + 1
25  the_pixel%pix_atoms(the_pixel%patoms)%atom_id = atom_id
26  do axis = 1, 3
27    the_pixel%pix_atoms(the_pixel%patoms)%coord(axis) = atom_coord(axis)
28  enddo
29
30 END SUBROUTINE

```

B.4 FORTRAN90 code: preparation of the pixel grid

```

1  ! Preparation of the pixel grid
2  SUBROUTINE prepare_pixel_grid (use_pbc, grid)
3
4  USE parameters
5  IMPLICIT NONE
6
7  LOGICAL, INTENT(IN)           :: use_pbc           ! flag to set if PBC are used or not
8  TYPE (pixel_grid), INTENT(INOUT) :: grid          ! the pixel grid to prepare
9  INTEGER                      :: axis              ! loop iterator axis id (1=x, 2=y, 3=z)
10 INTEGER                      :: aid               ! loop iterator atom number (1, atoms)
11 INTEGER                      :: pixel_num         ! pixel number in the grid
12 INTEGER, DIMENSION(3)        :: pixel_pos        ! pixel coordinates in the grid
13 REAL, DIMENSION(3)           :: cmin, cmax        ! real precision coordinates min, max
14 REAL, DIMENSION(3)           :: f_coord          ! real precision fractional coordinates
15
16 if ( .not. use_pbc ) then      ! without periodic boundary conditions
17   do axis = 1 , 3
18     cmin(axis) = c_coord(1,axis)
19     cmax(axis) = c_coord(1,axis)
20   enddo
21   do aid = 2 , atoms          ! for all atoms
22     do axis = 1 , 3           ! for x, y and z
23       cmin(axis) = min(cmin(axis), c_coord(aid,axis))
24       cmax(axis) = max(cmax(axis), c_coord(aid,axis))
25     enddo
26   enddo
27   do axis = 1 , 3             ! for x, y and z
28     ! Number of pixel(s) on axis 'axis'
29     grid%n_pix(axis) = INT((cmax(axis) - cmin(axis)) / cutoff) + 1
30   enddo
31 else                          ! using periodic boundary conditions
32   do axis = 1 , 3             ! for x, y and z
33     ! Number of pixel(s) on axis 'axis'
34     grid%n_pix(axis) = INT(l_params(axis) / cutoff) + 1
35   enddo
36 endif
37 do axis = 1 , 3              ! for x, y and z
38   ! correction if the number of pixel(s) on 'axis' is too small
39   if ( grid%n_pix(axis) .lt. 4 ) then
40     grid%n_pix(axis) = 1
41   endif
42 enddo
43
44 grid%nx = grid%n_pix(1) * grid%n_pix(2)          ! Number of pixels on the plan 'xy'
45 grid%pixels = grid%nx * grid%n_pix(3)            ! Total number of pixels in the grid
46
47 allocate (grid%pixel_list(grid%pixels))
48 do pixel_num = 1 , grid%pixels
49   grid%pixel_list(pixel_num)%pid = pixel_num
50   grid%pixel_list(pixel_num)%patoms = 0
51   grid%pixel_list(pixel_num)%tested = .false.
52 enddo
53 if ( .not. use_pbc ) then      ! without periodic boundary conditions
54   do aid = 1 , atoms          ! for all atoms
55     do axis = 1 , 3           ! for x, y and z
56       pixel_pos(axis) = INT( (c_coord(aid,axis) - cmin(axis)) / cutoff)
57     enddo
58     pixel_num = pixel_pos(1) + pixel_pos(2) * grid%n_pix(1) + pixel_pos(3) * grid%nx + 1
59     call add_atom_to_pixel (grid%pixel_list(pixel_num), pixel_pos, aid, c_coord(aid,:))
60   enddo
61 else                          ! using periodic boundary conditions
62   do aid = 1 , atoms          ! for all atoms
63     f_coord = MATMUL ( c_coord(aid), cart_to_frac )
64     do axis = 1 , 3           ! for x, y and z
65       f_coord(axis) = f_coord(axis) - floor(f_coord(axis))
66       pixel_pos(axis) = INT(f_coord(axis) * grid%n_pix(axis))
67     enddo
68     pixel_num = pixel_pos(1) + pixel_pos(2) * grid%n_pix(1) + pixel_pos(3) * grid%nx + 1
69     call add_atom_to_pixel (grid%pixel_list(pixel_num), pixel_pos, aid, f_coord)
70   enddo
71 endif
72
73 END SUBROUTINE prepare_pixel_grid

```

B.5 FORTRAN90 code: finding pixel neighbors

```

1 SUBROUTINE find_pixel_neighbors (use_pbc, the_grid, the_pix)
2
3   USE parameters
4   IMPLICIT NONE
5
6   LOGICAL, INTENT(IN)           :: use_pbc           ! flag to set if PBC are used or not
7   TYPE (pixel_grid), INTENT(INOUT) :: the_grid       ! pointer to the pixel grid
8   TYPE (pixel), POINTER, INTENT(INOUT) :: the_pix     ! pointer to the pixel
9   INTEGER                      :: axis              ! loop iterator axis id (1=x, 2=y, 3=z)
10  INTEGER                      :: xpos, ypos, zpos    ! neighbor position on x, y and z
11  INTEGER, DIMENSION(3)        :: l_start = (/1, 1, 1/) ! loop iterators starting value
12  INTEGER, DIMENSION(3)        :: l_end = (/3, 3, 3/) ! loop iterators ending value
13  INTEGER, DIMENSION(3)        :: pmod = (/1, 0, 1/) ! position modifiers
14  INTEGER                      :: nnp                ! number of neighbors for pixel
15  INTEGER                      :: nid                ! neighbor id for pixel
16  INTEGER, DIMENSION(3,3,3)    :: pbc_shift         ! shift, correction, due to PBC
17  LOGICAL                      :: boundary=.false.    ! is pixel on the boundary of the grid
18  LOGICAL                      :: keep_neighbor = .true. ! keep or not neighbor during analysis
19
20  if ( use_pbc ) then
21    call set_pbc_shift (the_grid, the_pix%p_xyz, pbc_shift)
22  else
23    do axis = 1 , 3
24      if ( the_pix%p_xyz(axis) .eq. 1 .or. the_pix%p_xyz(axis) .eq. the_grid%n_pix(axis) ) then
25        boundary = .true.
26      endif
27    enddo
28  endif
29  do axis = 1 , 3
30    if ( the_grid%n_pix(axis) .eq. 1 ) then
31      l_start(axis) = 2
32      l_end(axis) = 2
33    endif
34  enddo
35  nnp = 0
36  do xpos = l_start(1) , l_end(1)
37    do ypos = l_start(2) , l_end(2)
38      do zpos = l_start(3) , l_end(3)
39        keep_neighbor = .true.
40        if ( .not. use_pbc .and. boundary ) then
41          if ( the_pix%p_xyz(1) .eq. 1 .and. xpos .eq. 1 ) then
42            keep_neighbor = .false.
43          else if ( the_pix%p_xyz(1) .eq. the_grid%n_pix(1) .and. xpos .eq. 3 ) then
44            keep_neighbor = .false.
45          else if ( the_pix%p_xyz(2) .eq. 1 .and. ypos .eq. 1 ) then
46            keep_neighbor = .false.
47          else if ( the_pix%p_xyz(2) .eq. the_grid%n_pix(2) .and. ypos .eq. 3 ) then
48            keep_neighbor = .false.
49          else if ( the_pix%p_xyz(3) .eq. 1 .and. zpos .eq. 1 ) then
50            keep_neighbor = .false.
51          else if ( the_pix%p_xyz(3) .eq. the_grid%n_pix(3) .and. zpos .eq. 3 ) then
52            keep_neighbor = .false.
53          endif
54        endif
55        if ( keep_neighbor ) then
56          ! evaluating neighbor pixel number in the grid
57          nid = the_pix%pid + pmod(xpos) + pmod(ypos) * the_grid%n_pix(1) + pmod(zpos) * the_grid%n_xy
58          if ( use_pbc ) then
59            ! correcting the value if PBC are used
60            nid = nid + pbc_shift(xpos, ypos, zpos)
61          endif
62          the_pix%pixel_neighbors(nnp) = nid
63          nnp = nnp + 1
64        endif
65      enddo
66    enddo
67  enddo
68  the_pix%neighbors = nnp
69
70 END SUBROUTINE find_pixel_neighbors

```

B.6 FORTRAN90 code: inter-atomic distance calculation

```

1  ! evaluating the interatomic distance between 2 pixel atoms
2  SUBROUTINE evaluate_distance (use_pbc, at_i, at_j, dist)
3
4  USE parameters
5  IMPLICIT NONE
6
7  LOGICAL, INTENT(IN)                :: use_pbc    ! flag to set if PBC are used or not
8  TYPE (pixel_atom), POINTER, INTENT(IN) :: at_i    ! first pixel atom
9  TYPE (pixel_atom), POINTER, INTENT(IN) :: at_j    ! second pixel atom
10 TYPE (distance), INTENT(INOUT)      :: dist      ! calculation results
11 INTEGER                            :: axis        ! loop iterator axis id (1=x, 2=y, 3=z)
12
13 do axis = 1, 3
14     dist%Rij(axis) = at_i%coord(axis) - at_j%coord(axis)
15 enddo
16 if ( use_pbc ) then
17     ! then the pixel_atom's coordinates are in corrected fractional format
18     do axis = 1, 3
19         dist%Rij(axis) = dist%Rij(axis) - AnINT(dist%Rij(axis))
20     enddo
21     ! transform back to Cartesian coordinates
22     dist%Rij = MATMUL( dist%Rij, frac_to_cart )
23 endif
24
25 dist%length = 0.0
26 do axis = 1, 3
27     dist%length = dist%length + dist%Rij(axis) * dist%Rij(axis)
28 enddo
29 ! returning the 'distance' data structure that contains:
30 ! - the squared value for Dij: no time consuming square root calculation !
31 ! - the components of the distance vector on x, y and z
32 END SUBROUTINE evaluate_distance

```

B.7 FORTRAN90 code: pixel search for first neighbor atoms

```

1 SUBROUTINE pixel_search_for_neighbors (use_pbc)
2
3   USE parameters
4   IMPLICIT NONE
5
6   LOGICAL, INTENT(IN)  :: use_pbc                ! flag to set if PBC are used or not
7   TYPE (pixel_grid)   :: all_pixels              ! the pixel grid to analyze
8   INTEGER             :: pix, pjx                ! integer pixel ID numbers
9   INTEGER             :: aid, bid                ! integer loop atom numbers
10  INTEGER             :: l_start, l_end           ! integer loop modifier
11  INTEGER             :: pid
12  TYPE (pixel_atom), POINTER :: pix_i, pix_j      ! pointers on pixel data structure
13  TYPE (atom), POINTER  :: at_i, at_j            ! pointers on pixel_atom data structure
14  TYPE (distance)       :: Dij                   ! distance data structure
15
16  call prepare_pixel_grid (use_pbc, all_pixels)
17  ! note that the pixel grid 'all_pixels' must be prepared before the following
18  ! for all pixels in the grid
19  do pix = 1, all_pixels%pixels
20    ! setting 'pix_i' as pointer to pixel number 'pix'
21    pix_i => all_pixels%pixel_list(pix)
22    ! if pixel 'pix_i' contains atom(s)
23    if ( pix_i%patoms .gt. 0 ) then
24
25      ! search for pixel neighbors of 'pix_i'
26      call find_pixel_neighbors (use_pbc, all_pixels, pix_i)
27
28      ! testing all 'pix_i' neighbor pixels
29      do pid = 1, pix_i%neighbors
30        pjx = pix_i%pixel_neighbors(pid)
31        ! setting 'pix_j' as pointer to pixel number 'pjx'
32        pix_j => all_pixels%pixel_list(pjx)
33        ! checking pixel 'pix_j' if it:
34        ! - contains atom(s)
35        ! - was not tested, otherwise the analysis would have been performed already
36        if ( pix_j%patoms .gt. 0 .and. .not. pix_j%tested ) then
37          ! If 'pix_i' and 'pix_j' are the same, only test pair of different atoms
38          if ( pjx .eq. pix ) then
39            l_end = 1
40          else
41            l_end = 0
42          endif
43          ! for all atom(s) in 'pix_i'
44          do aid = 1, pix_i%patoms - l_end
45            ! set pointers to the first atom to test
46            at_i => pix_i%pix_atoms(aid)
47            if ( pjx .eq. pix ) then
48              l_start = aid + 1
49            else
50              l_start = 1
51            endif
52            ! for all atom(s) in 'pix_j'
53            do bid = l_start, pix_j%patoms
54              ! set pointers to the second atom to test
55              at_j => pix_j%pix_atoms(bid)
56              ! evaluate interatomic distance
57              call evaluate_distance (use_pbc, at_i, at_j, Dij)
58              if ( Dij%length .lt. cutoff_squared ) then
59                ! this is a first neighbor bond !
60                endif
61              enddo
62            enddo
63          endif
64        enddo
65        ! store that pixel 'pix_i' was tested
66        pix_i%tested = .true.
67      endif
68    enddo
69  enddo
70 END SUBROUTINE pixel_search_for_neighbors

```

Appendix C Commented Python code

C.1 Python code: data structures and global variables

```

1 # Global data structures and variables used in the next code sections
2 import numpy as np
3
4 # Atom in pixel data structure
5 class PixelAtom:
6     def __init__(self, atom_id=0, coord=None):
7         self.atom_id = atom_id # the atom ID
8         self.coord = np.zeros(3) if coord is None else np.array(coord) # the atom coordinates on x, y and z
9
10 # Pixel data structure
11 class Pixel:
12     def __init__(self, pid=0, p_xyz=None, tested=False, patoms=0, pix_atoms=None, neighbors=0):
13         self.pid = pid # the pixel number
14         self.p_xyz = np.zeros(3) if p_xyz is None else np.array(p_xyz) # the pixel coordinates in the grid
15         self.tested = tested # was the pixel checked already
16         self.patoms = patoms # number of atom(s) in pixel
17         self.pix_atoms = [] if pix_atoms is None else pix_atoms # list of atom(s) in the pixel
18         self.neighbors = neighbors # number of neighbors for pixel
19         self.pixel_neighbors = np.zeros(27, dtype=int) # the list of neighbor pixels, maximum 27
20
21 # Pixel grid data structure
22 class PixelGrid:
23     def __init__(self, pixels=0, n_pix=None, n_xy=0, pixel_list=None):
24         self.pixels = pixels # total number of pixels in the grid
25         self.n_pix = np.zeros(3, dtype=int) if n_pix is None else np.array(n_pix) # pixel(s) on each axis
26         self.n_xy = n_xy # number of pixels in the plan xy
27         self.pixel_list = [] if pixel_list is None else pixel_list # pointer to the pixels, to be allocated
28
29 # Bond distance data structure
30 class Distance:
31     def __init__(self, length=0.0, Rij=None):
32         self.length = length # the distance in Å squared
33         self.Rij = np.zeros(3) if Rij is None else np.array(Rij) # vector components of x, y and z
34
35 # Model description
36 atoms = 0 # the total number of atom(s)
37 c_coord = None # list of Cartesian coordinates: c_coord[atoms][3]
38 cutoff = 0.0 # the cutoff to define atomic bond(s)
39 cutoff_squared = 0.0 # squared value for the cutoff
40
41 # Model box description
42 l_params = np.zeros(3) # lattice a, b and c
43 cart_to_frac = np.zeros((3, 3)) # Cartesian to fractional coordinates matrix
44 frac_to_cart = np.zeros((3, 3)) # fractional to Cartesian coordinates matrix

```


C.2 Python code: set pixel periodic boundary condition shift

```

1 # adjust, if needed, shift to search for pixel neighbor(s) using PBC
2 # - grid pixel_grid           : the pixel grid
3 # - int pixel_coord[3]       : the pixel coordinates in the grid
4 # - int pbc_shift[3][3][3]   : the shift, correction, to be calculated
5 def set_pbc_shift(pixel_grid : PixelGrid, pixel_coord : np.ndarray, pbc_shift : np.ndarray):
6     # Initialize pbc_shift to zero
7     for x_pos in range(3):
8         for y_pos in range(3):
9             for z_pos in range(3):
10                 pbc_shift[x_pos][y_pos][z_pos] = 0           # initialization without any shift
11
12     if pixel_coord[0] == 0:                                   # pixel position on 'x' is min
13         for y_pos in range(3):
14             for z_pos in range(3):
15                 pbc_shift[0][y_pos][z_pos] = pixel_grid.n_pix[0]
16
17     elif pixel_coord[0] == pixel_grid.n_pix[0] - 1: # pixel position on 'x' is max
18         for y_pos in range(3):
19             for z_pos in range(3):
20                 pbc_shift[2][y_pos][z_pos] = -pixel_grid.n_pix[0]
21
22     if pixel_coord[1] == 0:                                   # pixel position on 'y' is min
23         for x_pos in range(3):
24             for z_pos in range(3):
25                 pbc_shift[x_pos][0][z_pos] += pixel_grid.n_xy
26
27     elif pixel_coord[1] == pixel_grid.n_pix[1] - 1: # pixel position on 'y' is max
28         for x_pos in range(3):
29             for z_pos in range(3):
30                 pbc_shift[x_pos][2][z_pos] -= pixel_grid.n_xy
31
32     if pixel_coord[2] == 0:                                   # pixel position on 'z' is min
33         for x_pos in range(3):
34             for y_pos in range(3):
35                 pbc_shift[x_pos][y_pos][0] += pixel_grid.pixels
36
37     elif pixel_coord[2] == pixel_grid.n_pix[2] - 1: # pixel position on 'z' is max
38         for x_pos in range(3):
39             for y_pos in range(3):
40                 pbc_shift[x_pos][y_pos][2] -= pixel_grid.pixels

```

C.3 Python code: add atom to pixel

```
1 def add_atom_to_pixel(the_pixel: Pixel, pixel_coord: np.ndarray, atom_id: int, atom_coord: np.ndarray):
2     if not the_pixel.patoms:
3         # if the pixel do not contains any atom yet, then save its coordinates in the grid
4         for axis in range(3):
5             the_pixel.p_xyz[axis] = pixel_coord[axis]
6
7     new_atom = PixelAtom(atom_id, atom_coord)
8     the_pixel.pix_atoms.append(new_atom)
9
10    # increment the number of atom(s) in the pixel
11    the_pixel.patoms += 1
```

C.4 Python code: preparation of the pixel grid

```

1 # preparation of the pixel grid
2 # - bool use_pbc : flag to set if PBC are used or not
3 def prepare_pixel_grid(use_pbc : bool):
4     grid = PixelGrid()                # create a new pixel grid
5     cmin = [float('inf')] * 3         # initialize to infinity
6     cmax = [-float('inf')] * 3        # initialize to negative infinity
7     pixel_pos = np.zeros(3, dtype=int)
8
9     if not use_pbc:                    # without periodic boundary conditions
10         for axis in range(3):
11             cmin[axis] = cmax[axis] = c_coord[0][axis]
12         for aid in range(1, atoms):   # for all atoms
13             for axis in range(3):     # for x, y and z
14                 cmin[axis] = min(cmin[axis], c_coord[aid][axis])
15                 cmax[axis] = max(cmax[axis], c_coord[aid][axis])
16         for axis in range(3):         # for x, y and z
17             # number of pixels on axis 'axis'
18             grid.n_pix[axis] = int((cmax[axis] - cmin[axis]) / cutoff) + 1
19     else:                              # Using periodic boundary conditions
20         for axis in range(3):         # for x, y and z
21             # number of pixels on axis 'axis'
22             grid.n_pix[axis] = int(l_params[axis] / cutoff) + 1
23
24     for axis in range(3):              # for x, y and z
25         # correction if the number of pixels on 'axis' is too small
26         grid.n_pix[axis] = 1 if grid.n_pix[axis] < 4 else grid.n_pix[axis]
27
28     grid.n_xy = grid.n_pix[0] * grid.n_pix[1]    # number of pixels on the plan 'xy'
29     grid.pixels = grid.n_xy * grid.n_pix[2]      # total number of pixels in the grid
30
31     grid.pixel_list = [Pixel(pid=i) for i in range(grid.pixels)]
32
33     if not use_pbc:                    # without periodic boundary conditions
34         for aid in range(atoms):       # for all atoms
35             for axis in range(3):      # for x, y and z
36                 pixel_pos[axis] = int((c_coord[aid][axis] - cmin[axis]) / cutoff)
37                 pixel_num = pixel_pos[0] + pixel_pos[1] * grid.n_pix[0] + pixel_pos[2] * grid.n_xy
38                 add_atom_to_pixel(grid.pixel_list[pixel_num], pixel_pos, aid, c_coord[aid])
39     else:                              # using periodic boundary conditions
40         for aid in range(atoms):       # for all atoms
41             # with 'matrix_multiplication' a user defined function to perform the operation
42             f_coord = matrix_multiplication(cart_to_frac, c_coord[aid])
43             for axis in range(3):      # for x, y and z
44                 f_coord[axis] = f_coord[axis] - np.floor(f_coord[axis])
45                 pixel_pos[axis] = int(f_coord[axis] * grid.n_pix[axis])
46                 pixel_num = pixel_pos[0] + pixel_pos[1] * grid.n_pix[0] + pixel_pos[2] * grid.n_xy
47                 add_atom_to_pixel(grid.pixel_list[pixel_num], pixel_pos, aid, f_coord)
48
49     return grid

```

C.5 Python code: finding pixel neighbors

```

1 # Finding neighbor pixels for pixel in the grid
2 # - bool use_pbc      : flag to set if PBC are used or not
3 # - grid * the_grid   : pointer to the pixel grid
4 # - pixel * the_pix   : pointer to the pixel with neighbors to be found
5 def find_pixel_neighbors(use_pbc : bool, the_grid : PixelGrid, the_pix : Pixel):
6     boundary = False                                # is pixel on the boundary of the grid
7     keep_neighbor = True                            # keep or not neighbor during analysis
8     l_start = [0, 0, 0]                             # loop iterators starting value
9     l_end = [3, 3, 3]                               # loop iterators ending value
10    pmod = [-1, 0, 1]                                # position modifiers
11    pbc_shift = np.zeros((3, 3, 3), dtype=int)       # shift for pixel neighbor number due to PBC
12
13    # check if PBC are used
14    if use_pbc:
15        set_pbc_shift(the_grid, the_pix.p_xyz, pbc_shift)
16    else:
17        for axis in range(3):
18            if the_pix.p_xyz[axis] == 0 or the_pix.p_xyz[axis] == the_grid.n_pix[axis] - 1:
19                boundary = True
20
21    # adjust the loop start and end based on the grid dimensions
22    for axis in range(3):
23        if the_grid.n_pix[axis] == 1:
24            l_start[axis] = 1
25            l_end[axis] = 2
26
27    nnp = 0 # number of neighbors
28    for xpos in range(l_start[0], l_end[0]):
29        for ypos in range(l_start[1], l_end[1]):
30            for zpos in range(l_start[2], l_end[2]):
31                keep_neighbor = True
32
33                if not use_pbc and boundary:
34                    if the_pix.p_xyz[0] == 0 and xpos == 0:
35                        keep_neighbor = False
36                    elif the_pix.p_xyz[0] == the_grid.n_pix[0] and xpos == 2:
37                        keep_neighbor = False
38                    elif the_pix.p_xyz[1] == 0 and ypos == 0:
39                        keep_neighbor = False
40                    elif the_pix.p_xyz[1] == the_grid.n_pix[1] and ypos == 2:
41                        keep_neighbor = False
42                    elif the_pix.p_xyz[2] == 0 and zpos == 0:
43                        keep_neighbor = False
44                    elif the_pix.p_xyz[2] == the_grid.n_pix[2] and zpos == 2:
45                        keep_neighbor = False
46
47                if keep_neighbor:
48                    # calculate the neighbor id
49                    nid = the_pix.pid + pmod[xpos] + pmod[ypos] * the_grid.n_pix[0] + pmod[zpos] * the_grid.n_xy
50                    if use_pbc:
51                        nid += pbc_shift[xpos][ypos][zpos]
52                    the_pix.pixel_neighbors[nnp] = nid
53                    nnp += 1
54
55    the_pix.neighbors = nnp

```

C.6 Python code: inter-atomic distance calculation

```

1 # evaluating the interatomic distance between 2 pixel atoms
2 # - bool use_pbc      : flag to set if PBC are used or not
3 # - pixel_atom * at_i : pointer to first pixel atom
4 # - pixel_atom * at_j : pointer to second pixel atom
5 def evaluate_distance(use_pbc : bool, at_i : PixelAtom, at_j : PixelAtom):
6     dist = Distance()          # Placeholder for the distance data structure
7     Rij = np.zeros(3)          # Initialize the distance vector
8     # calculating the distance components between atoms
9     for axis in range(3):
10         Rij[axis] = at_i.coord[axis] - at_j.coord[axis]
11
12     if use_pbc:
13         # then the pixel_atom's coordinates are in corrected fractional format
14         for axis in range(3):
15             Rij[axis] = Rij[axis] - round(Rij[axis])
16
17         # transform back to Cartesian coordinates
18         # matrix_multiplication is assumed to be defined elsewhere
19         Rij = matrix_multiplication(frac_to_cart, Rij)
20
21     # calculating the squared distance (no square root for efficiency)
22     dist.length = np.sum(Rij ** 2)
23     dist.Rij = Rij             # store the distance vector components
24
25     # returning the 'distance' data structure that contains:
26     # - the squared value for Dij
27     # - the components of the distance vector on x, y, and z
28     return dist

```

C.7 Python code: pixel search for first neighbor atoms

```

1 def pixel_search_for_neighbors(use_pbc : bool):
2     # pointer to the pixel grid for analysis
3     all_pixels = prepare_pixel_grid(use_pbc)
4
5     # for all pixels in the grid
6     for pix in range(all_pixels.pixels):
7         # setting pix_i as pointer to pixel number pix
8         pix_i = all_pixels.pixel_list[pix]
9
10        # if pixel pix_i contains atom(s)
11        if pix_i.patoms:
12            # search for neighbor pixels
13            find_pixel_neighbors(use_pbc, all_pixels, pix_i)
14
15            # testing all pix_i neighbor pixels
16            for pid in range(pix_i.neighbors):
17                pjax = pix_i.pixel_neighbors[pid]
18                # Setting pix_j as pointer to pixel number pjax
19                pix_j = all_pixels.pixel_list[pjax]
20
21                # checking pixel pix_j if it:
22                # - contains atom(s)
23                # - was not tested, otherwise the analysis would have been performed already
24                if pix_j.patoms and not pix_j.tested:
25                    # If pix_i and pix_j are the same, only test pair of different atoms
26                    end = 0 if pjax != pix else 1
27
28                    # for all atom(s) in pix_i
29                    for aid in range(pix_i.patoms - end):
30                        # Set pointer to the first atom to test
31                        at_i = pix_i.pix_atoms[aid]
32                        start = 0 if pjax != pix else aid + 1
33
34                        # for all atom(s) in pix_j
35                        for bid in range(start, pix_j.patoms):
36                            # Set pointer to the second atom to test
37                            at_j = pix_j.pix_atoms[bid]
38
39                            # evaluate interatomic distance
40                            Dij = evaluate_distance(use_pbc, at_i, at_j)
41
42                            if Dij.length < cutoff_squared:
43                                # This is a bond!
44                                pass
45
46            # store that pixel pix_i was tested
47            pix_i.tested = True

```