PorosityPlus

Version 1.0.1

Contents

1   Overview

The PorosityPlus code can be used to calculate the surface area, volume and pore size distribution (PSD) of particle networks. These particles can be multiscale ranging from atoms to nanoparticles to grains with the assumption that they can be modelled by spheres. It works on multi-frame xyz movies with up to 10 particle types defined by different particle type pair cutoff distances. Applied to gas adsorption studies, these particles can model atoms and the Monte Carlo routine uses a spherical probe useful for simulating pore accessibility of gases like helium and argon.

In the following manual, bold text represents either filenames or simulation parameters from the simulation controlling file **PorosityPlus.inp**.

The code along with citation information is located at the CSIRO Data Access Portal:

[FIX]

Please report all errors and issues to Dr George Opletal

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1.2   Installation

PorosityPlus is written in Fortran 90 and has been tested for compilation using the GNU Fortran 6.3 (GFortran) compiler and the Intel Fortran Compiler.

PorosityPlus requires a compilation of the **Porosityplus.f90** main code file and the **Porosityplus_mod.f90** module file in addition to numerous input files. Below are steps to compiling and running the code on a Unix based machine using the Intel Fortran Compiler.

- Type

```
ifort Porosityplus_mod.f90 Porosityplus.f90 -o Porosityplus.exe
```

A successful compilation will create the executable file **Porosityplus.exe**.

When running simulations, **Porosityplus.inp** must always be present and contains the simulation parameters. Additionally, a **.xyz** input file, which is to be analysed, must also be present (see section 2). All the input files need to be in the same directory and the generated output files write out to the same directory.

2   File I/O

A file naming convention is employed for input and output files in order to simplify the use of the code. A prefix is used for filenames as follows,

in_	Input files that may be needed by the code. This excludes the **PorosityPlus.inp** file and any input files whose names are defined within this file.
od_	Output data file in the comma-separated file (.csv) format
ov_	Output visualization file in an xyz format (.xyz) with possible additional particle data contained in the fifth column and beyond.

The visualization outputs have been tested using the Ovito visualization package found at,

https://www.ovito.org/

Table 1 Input and output files

FILE	DESCRIPTION
Porosityplus.inp	Input file for simulation variables
Use defined XYZ file	The name of the input xyz file that is to be analysed should be input in the **Porosityplus.inp** file. The user-defined **.xyz** input file needs to be in the form,
	number of particles
	space or comment
	two letter label, location along the x-axis, y-axis, z-axis of particle 1 in frame 1
	two letter label, location along the x-axis, y-axis, z-axis of particle 2 in frame 1
	..
	..
	Below is an input example of a two-frame **.xyz** file for an atomic system with the first frame containing 3 hydrogen atoms and the second frame having 2 hydrogen atoms.
	3
	H 5.456 2.435 4.435
	H 3.454 3.667 6.544
	H 4.345 1.234 4.326
	2

H 3.454 4.343 5.454

H 2.458 5.197 3.693

The total number of atoms in each frame does not have to be constant and up to ten element types are tracked.

od_data.csv	Analysis for each frame (rows) consisting of the following columns, • Accessible surface area (in units of $Å^2$)and accessible specific surface area (m^2/g) using the surface calculation routines. • Total pore volume ($Å^3$) and total bulk volume ($Å^3$), total specific pore volume (cm^3/g) and porosity (zero probe radius) and accessible variants of these quantities with a finite probe radius selection.
od_psd.csv	Specific pore volume (cm^3/g.Å) versus pore diameter (Å). The integral of this graph is the total specific pore volume (cm^3/g).
od_gr.csv	Total radial distribution function as a function of particle separation (Å).
ov_surf.xyz	The location of accepted insertion points from the Surface Area routine which provides a graphical view of the surfaces in the system. Only a single frame is output (last frame of multi-frame movie).
ov_vol.xyz	The location of all accepted insertion point positions into the network using the Pore Volume routine. Only a single frame is output (last frame of multi-frame movie).
ov_psdI.xyz	The location of all accepted insertion point positions into network using the Accessible Pore Volume and PSD routine. The number of points is equal to the total number of accepted insertions. Only a single frame is output (last frame of multi-frame movie).
ov_psdF.xyz	**.xyz** coordinate file of all accepted insertion points in their final positions after random walks used in the PSD calculation. These points are also the origin of all maximum spheres for each insertion point which encompass the original insertion point and does not overlap the network particles. These points represent the sphere locations from which their diameters are binned for the calculation of the PSD. The fifth column represents the radius value for each point. Only a single frame is output (last frame of multi-frame movie).

3 Input File

A sample test input file (**Porosityplus.inp**) is shown below with explanations. The value(s) at the start of the line is the variable that is read in before the code jumps to the next line while the text following the values are ignored. The number of lines in the input file remains constant. The rest is a description to assist the user including the name of the parameter at the end of each line in square brackets. A detailed explanation of each line follows this example file.

```
test.xyz            Name of xyz input file                              [file_xyz]
1                   No. of frames in xyz file                           [frames]
1                   Start frame                                         [frame_begin]
1                   End Frame                                           [frame_end]
1                   Frame frequency for analysis                        [frame_freq]

12.011              Avg. atomic weight of network particles (a.m.u)     [atomic_w]
10.0                x cell length (Angstrom) of xyz input file          [xl]
10.0                y cell length                                       [yl]
10.0                z cell length                                       [zl]
0                   PBCs (1=3D periodic, 0=not periodic)                [pbc_option]
172                 Seed for random number generator                   [iseed]

1                   Surface Area                  (0=off, 1=on)         [opt_sur]
1                   Total Pore Volume             (0=off, 1=on)         [opt_vol]
1                   Accessible Pore Volume and PSD (0=off, 1=on)        [opt_psd]

100000              Samples – Surface Area              -Surface Area…     [por_sample1]
100000              Samples – Total Pore Volume         -Total Pore Volume…  [por_sample2]

100000              Samples – Accessible Pore Volume and PSD  -Accessible Pore…  [por_sample3]
100                 Number of attempts from each point                 [por_attempt]
100                 Number of move attempts from each point            [por_move]
2.0                 Max attempted move distance (Angstrom)             [max_walk]

0.1                 PSD resolution for diameter (angstrom)             [bin_res]

C   1.70            Label of particle type 1, radius of particle …  [input_label(1), input_rad(1)]
H   1.20            Label of particle type 2, radius of particle …  [input_label(2), input_rad(2)]
N   1.55            Label of particle type 3, radius of particle …  [input_label(3), input_rad(3)]
S   1.00            Label of particle type 4, radius of particle …  [input_label(4), input_rad(4)]
T   1.00            Label of particle type 5, radius of particle …  [input_label(5), input_rad(5)]
U   1.00            Label of particle type 6, radius of particle …  [input_label(6), input_rad(6)]
V   1.00            Label of particle type 7, radius of particle …  [input_label(7), input_rad(7)]
W   1.00            Label of particle type 8, radius of particle …  [input_label(8), input_rad(8)]
X   1.00            Label of particle type 9, radius of particle …  [input_label(9), input_rad(9)]
Y   1.00            Label of particle type 10, radius of particle … [input_label(10), input_rad(10)]

1.00                Radius of probe particle (Angstrom)                [input_radp]

1                   Calculate g(r)                                     [opt_g2]
1                   Write out xyz files                                [opt_writeout
```

```
test.xyz            Name of xyz input file                              [file_xyz]
1                   No. of frames in xyz file                           [frames]
1                   Start frame                                         [frame_begin]
1                   End Frame                                           [frame_end]
1                   Frame frequency for analysis                        [frame_freq]
```

file_xyz is the user-defined file name of the input **.xyz** file. **frames** specifies how many xyz frames there are in the **.xyz** file. **frame_begin** and **frame_end** control at which frame the analysis begins and ends. **frame_freq** controls how many frames between each analysis.

```
12.011              Avg. atomic mass of network particles (a.m.u)        [atomic_m]
10.0                x cell length (Angstrom) of xyz input file           [xl]
10.0                y cell length                                        [yl]
10.0                z cell length                                        [zl]
0                   PBCs (1=3D periodic, 0=not periodic)                 [pbc_option]
172                 Seed for random number generator                     [iseed]
```

atomic_m is the average atomic mass in atomic mass units of the network particles used in the calculation of the total specific pore volume. The average is simply the average of all the individual particle atomic masses. **xl**, **yl** and **zl** are the cell lengths and **pbc_option** is for selecting periodic boundary conditions. **iseed** is a positive integer used as a seed for the random number generator.

```
1                   Surface Area                    (0=off, 1=on)        [opt_sur]
1                   Total Pore Volume               (0=off, 1=on)        [opt_vol]
1                   Accessible Pore Volume and PSD (0=off, 1=on)         [opt_psd]
```

opt_sur, opt_vol, opt_psd determine if the surface area, total pore volume and accessible pore volume/PSD should be calculated. See section 4.0.

```
100000              Samples - Surface Area                  -Surface Area…   [por_sample1]

100000              Samples - Total Pore Volume             -Total Pore Volume [por_sample2]

100000              Samples - Accessible Pore Volume and PSD  -Accessibl…    [por_sample3]
100                 Number of attempts from each point               [por_attempt]
100                 Number of move attempts from each point          [por_move]
2.0                 Max attempted move distance (Angstrom)           [max_walk]
```

por_sample1 is the total number of insertion attempts around a particle used to calculate the surface area. **Por_sample2** is the total number of insertion attempts into the cell used to calculate the pore volume. **por_sample3** is the total number of insertion attempts into the cell used by the PSD routines. **por_attempt** is the total number of attempts to move away from a successful (non-overlapping) insertion location to find the maximum pore size encompassing the original insertion point. **por_move** is the total number of moves for each attempt in search of this maximum pore size. **max_walk** is the maximum displacement for each attempted move.

```
0.1                 PSD resolution for diameter (Angstrom)               [bin_res]
```

bin_res is the spacing of the PSD histogram.

```
C   1.70    Label of particle type 1, radius of particle…    [input_label(1), input_rad(1)]
H   1.20    Label of particle type 2, radius of particle…    [input_label(2), input_rad(2)]
N   1.55    Label of particle type 3, radius of particle…    [input_label(3), input_rad(3)]
S   1.00    Label of particle type 4, radius of particle…    [input_label(4), input_rad(4)]
T   1.00    Label of particle type 5, radius of particle…    [input_label(5), input_rad(5)]
U   1.00    Label of particle type 6, radius of particle…    [input_label(6), input_rad(6)]
V   1.00    Label of particle type 7, radius of particle…    [input_label(7), input_rad(7)]
W   1.00    Label of particle type 8, radius of particle…    [input_label(8), input_rad(8)]
X   1.00    Label of particle type 9, radius of particle…    [input_label(9), input_rad(9)]
Y   1.00    Label of particle type 10, radius of particle…   [input_label(10), input_rad(10)]

1.00        Radius of probe particle (Angstrom)              [input_radp]
```

input_label(1), **input_label(2)**,..are one or two letter designation (usually elemental for atomic systems) for the particle type which should match the labels in the xyz input file. **input_rad(1)**, **input_rad(2)**,… are the associated particle radii. **input_radp** is the probe particle radius.

1	Calculate g(r)	[opt_g2]

opt_g2 turns on and off the calculation and output of the total g(r). Since this calculation scales as N^2, it can take a lot of time for very large systems.

1	Write out .xyz files	[opt_writeout]

A flag for allowing the write out of xyz files

4   Theory/Operation

The code is based upon the geometric determination of the pore volume and pore size distribution (PSD) as outline by L. D. Gelb and K. E. Gubbins[1,2].

The code uses Metropolis Monte Carlo integration to determine the surface area, pore-volume, and PSD of a connected network of particles.

A critical consideration in these calculations is the choice of the radius of the inserted probe particle called the probe radius (**input_radp**). In the literature and as illustrated in figure 1, if some probe particle radius is used, two different types of surfaces can be defined. The Connolly surface (shown in red) is obtained by rolling the probe particle (shown in blue) along the network particles (shown in green whose radii are given by the choices of **input_rad**) while the Accessible surface is defined as the centre of the probe rolling along the Connolly surface (shown as dashed yellow line). If the probe particle radius is zero (**input_radp**=0), the two surface definitions become identical. As an example, a particle of radius 1Å has a Connolly surface area of $\frac{4}{3}\pi(1^3) = 4.189$Å^2. However, using a probe particle of radius 1Å (**input_radp** = 1), the accessible surface area is $\frac{4}{3}\pi(2^3) = 33.51$Å^2 since the particle and probe can't approach closer than 2Å. PorosityPlus only outputs accessible surface areas and the Connolly surface area is obtained by setting **input_radp** to zero.

Quantities within the program that uses the accessible surface definition have the label 'accessible' in front of their title (accessible surface area for example) while quantities using the Connolly surface definition, use the 'total' label in front of their title (total pore volume for example). Note that in terms of porosity, the total pore volume which is the empty space surrounding network particles is always larger than the accessible pore volume since the probe particles might not be able to fit into small pores.

Within the program, there are three main calculation routines,

SURFACE AREA - selected by the **opt_sur** option, calculates the accessible surface area by randomly picking a point around some random particle at a particular radius (radius equal to the particle radius + probe radius) and checking if that point overlaps any neighbouring particles. If it does not, the move is accepted. The acceptance fraction is then multiplied by the total surface area of the individual particles (spheres of radius of particle + probe) to obtain an estimate of the internal surface area. Quantities calculated with this routine as output to the **od_data.csv** include the accessible surface area (Å) and accessible specific surface area (m^2/g).

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[1] L. D. Gelb, K. E. Gubbins, Langmuir **14**, 2097 (1998).

[2] L. D. Gelb, K. E. Gubbins, Langmuir **15**, 305 (1999).

TOTAL PORE VOLUME – selected by the **opt_vol** option, calculates the total pore volume via the repeated insertion of a probe particle of zero radius into the cell checking to ensure that it does not overlap any other particles. If it does not, its position is accepted. The number of accepted moves divided by the total attempted moves is the porosity or pore volume fraction. Quantities calculated with this routine as output to the **od_data.csv** include the total pore volume ($Å^3$), total bulk volume ($Å^3$), total specific pore volume (cm^3/g) and total porosity.

ACCESSIBLE PORE VOLUME AND PSD – selected by the **opt_psd** option, the calculation of the PSD begins with the acceptance of a trial point insertion. If there is no overlap, a determination of the maximum sphere size which both encompasses the original insertion point and which does not overlap any network particles needs to be found. This code finds this maximum sphere diameter by a random walk away from the original insertion point. Once found, a check is made to ensure that this maximum sphere is larger than the pore particle and if so, the diameter is binned into a histogram. This is repeated over many trials to determine the PSD.   A grid cell nearest neighbour routine is used to speed up the code. Quantities calculated with this routine as output to the **od_data.csv** include the accessible pore volume ($Å^3$), accessible bulk volume ($Å^3$), accessible specific pore volume (cm^3/g) and accessible porosity.
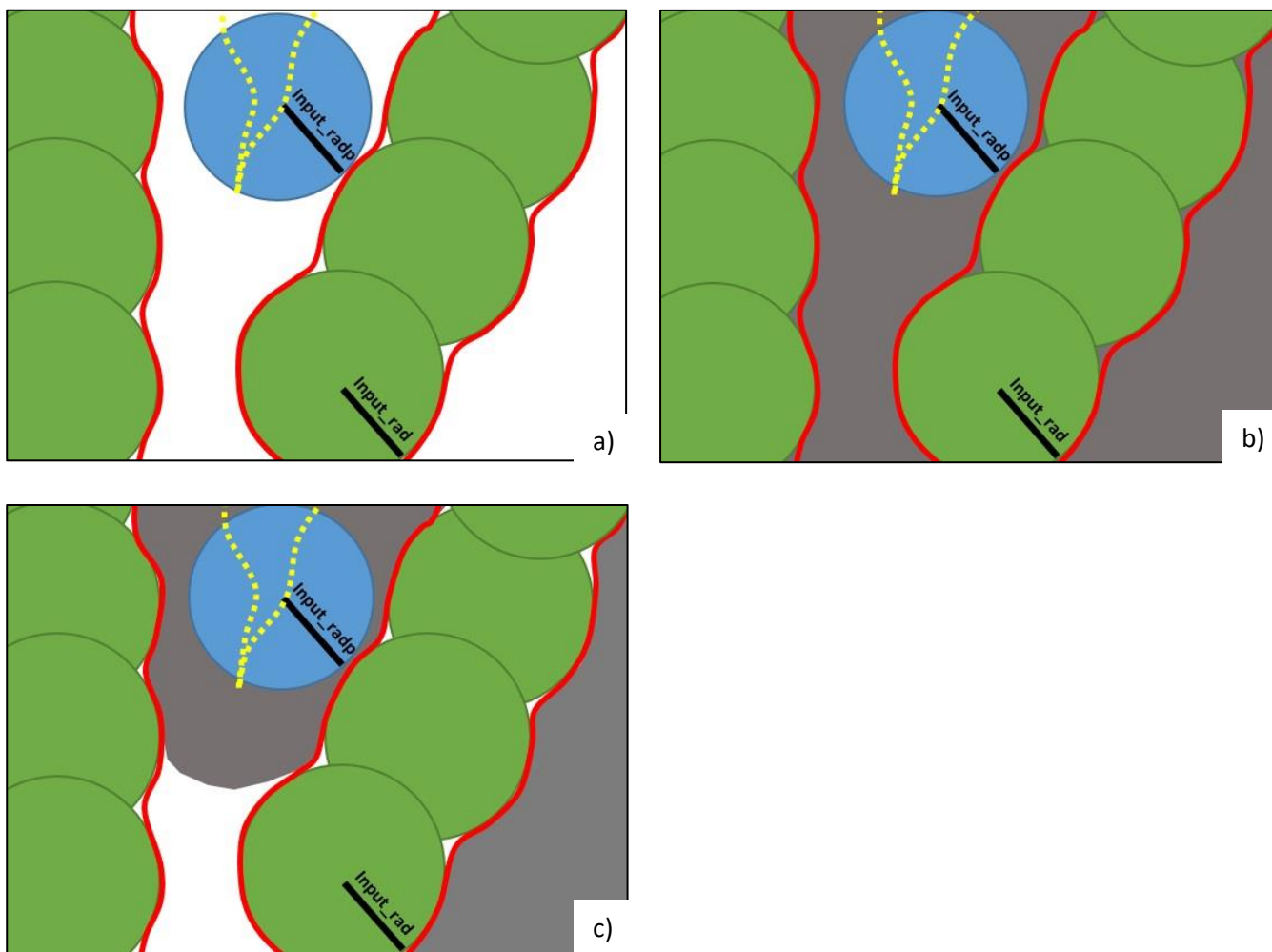
Figure 1 (a) Representation of the different definitions of molecular surfaces and pore volumes. As a spherical probe (blue) is rolled along the network particles (green), its edges trace out the Connolly surface (red lines) while its centre traces the accessible surface (yellow dotted lines). (b) the total pore volume shown in grey is always larger than (c) the accessible pore volume shown in grey. Note that if the probe radius goes to zero, the two surface definitions become equivalent.

Defining
S_T is the total number of attempted insertions.
S_A is the total number of accepted insertions.

The total porosity is given by $P = S_A/S_T$
The pore volume is given by $V_p = xl \cdot yl \cdot zl \cdot P$ where xl, yl, zl are the cell boundary lengths in Angstrom.
The bulk volume is given by $V_b = xl \cdot yl \cdot zl \cdot (1 - P)$

The mass of the simulation cell in grams is given by,
$M = N \cdot A / N_A$ where N is the total number of particles, A is the average atomic weight of the particles and N_A is Avogadro's number (6.022141523^{23} mol^{-1}).

The total specific pore volume (in units of cm^3/g) is $V_{p\,spec} = V_p \cdot 1 \times 10^{-24}/M$ where the numerical factor is a conversion from Angstrom to centimetres.

Finally, the pore size distribution PSD(d), is constructed from the accepted binned maximum pore diameters H(d) by,

$$PSD(d) = \frac{H(d) \cdot V_{p\,spec}}{S_A \cdot \delta}$$

where δ is the PSD bin spacing. The PSD has the units of $\frac{cm^3}{g \cdot \mathring{A}}$

4.1 Particle Radius

While PorosityPlus allows for application to arbitrary particle systems such as nanoparticles and macroscopic grains, many applications involve analysis of atomic configurations. As such, it is instructive to comment on the choice of atomic radii. Being a geometric technique, accuracy is limited but a common choice for the atomic radii (values of **input_rad**) is that of the element's Van der Waals radius. A similar choice is often made for the probe particle radius **input_radp** (if wanting accessible surface quantities) although more complicated techniques can be used to determine **input_radp**, based on a minimum potential energy distance between the probe and bulk atoms.[3]

An illustrative application can be found in a study of nanoporous carbons[4]. Here the carbon radius used the Van der Waals radius of 1.7Å while the particle probe radius was varied to simulate the use of Argon, Helium and a point of zero radius. The effects on the calculation of the total specific pore volume (which is just the integral of the PSD) is shown in figure 2 and shows a convergence of the pore volume to a maximum value (0.62 cm^3/g) as the probe radius is reduced to near zero.

[3] L. Sarkisov, A. Harrison, Mol. Simul. **37**(15), 1248–1257 (2011).
[4] A. H. Farmahini, G. Opletal, S. K. Bhatia, J. Chem. Phys. C **117**(27), 14081-14094 (2013).
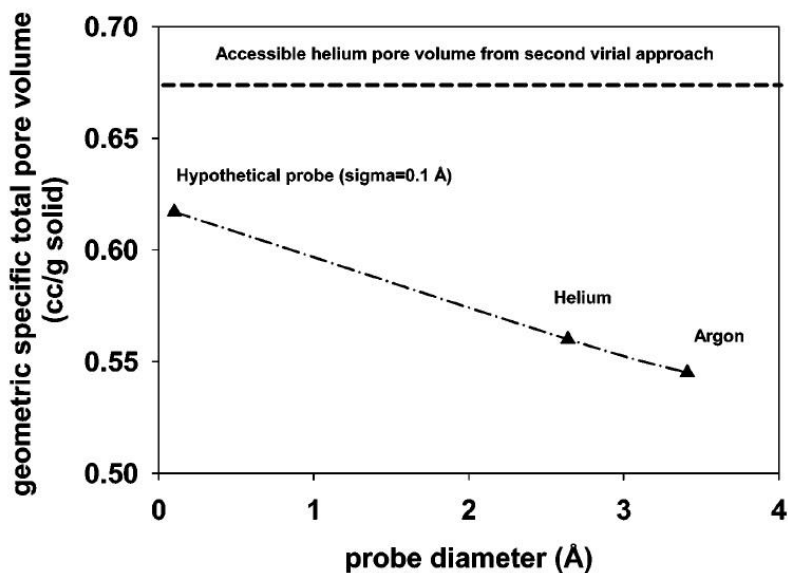
Figure 2 Variation of total pore volume with probe diameter (figure 7 of Ref 4).

Looking at the PSD using the helium particle probe in figure 3, it can be seen that its lower pore volume (0.56 cc/g) is the result of a truncation of pores from the PSD which have a radius smaller than the helium probe radius.
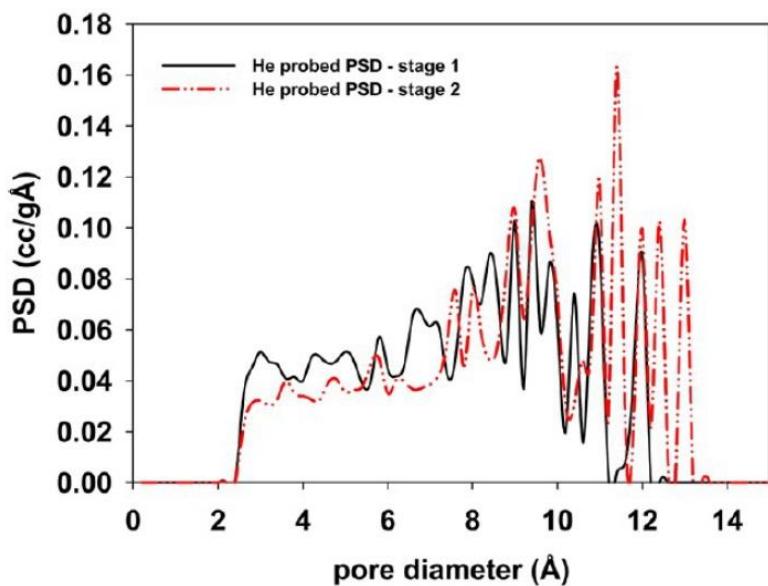

Figure 3 Geometric PSD of structures illustrating the truncation of micro-pores that are smaller than the Helium probe particle (figure 5 of Ref 4).

5   Examples

Applications of the code with numerous examples are found in the **/Example/** directory. These are detailed below.

5.1   /Examples/Intro1

The **/Example/Intro1** directory contains the **PorosityPlus.inp** file and the **intro1.xyz** file containing a single particle located at the origin (x=y=z=0.0) of radius 1Å. The accessible surface area and total bulk volume are calculated using a 10Å cubic simulation cell with and without periodic boundary conditions (PBC) using a particle probe radius of zero (point probe) and 1Å. The **PorosityPlus.inp** file is set up for case 1 with 100,000 steps below and should be adjusted to reproduce the other cases.

Case	Scenario	Accessible surface area (Å^2)	Total bulk volume (Å^3) (cell volume - total pore volume)
1	input_radp = 0.0 pbc_option = 0	1.589 (0.1) 1.574 (1) 1.570 (10) 1.571 (100) **1.571 (expected)**	0.490 (0.1) 0.501 (1) 0.525 (10) 0.525 (100) **0.524 (expected)**
2	input_radp = 0.0 pbc_option = 1	12.566 (0.1) 12.566 (1) 12.566 (10) 12.566 (100) **12.566 (expected)**	4.140 (0.1) 4.102 (1) 4.209 (10) 4.186 (100) **4.189 (expected)**
3	input_radp = 1.0 pbc_option = 0	6.356 (0.1) 6.298 (1) 6.281 (10) 6.284 (100) **6.283 (expected)**	0.490 (0.1) 0.501 (1) 0.525 (10) 0.525 (100) **0.524 (expected)**
4	input_radp = 1.0 pbc_option = 1	50.265 (0.1) 50.265 (1) 50.265 (10) 50.265 (100) **50.265 (expected)**	4.140 (0.1) 4.102 (1) 4.209 (10) 4.186 (100) **4.189 (expected)**

Table 1 – Scenarios illustrating the effects of a combination of periodic boundaries and probe radii. The bracket value is the number of sample steps in millions with the expected theoretical value in bold.

In case 1, the spherical particle sits at the origin and without periodic boundaries and only 1/8th of the sphere is located within the simulation cell. Thus an area of $\frac{4\pi(1^2)}{8} = 1.571\ \text{Å}^2$ and bulk volume of $\frac{\frac{4}{3}\pi(1^3)}{8} = 0.524\ \text{Å}^3$ is expected. In case 2, the periodic boundaries are turned on and thus the entire sphere is now within the simulation cell. The expected area and bulk volume now become 12.566 Å^2 and 4.189 Å^3.   In case 3, the periodic boundaries are turned off and thus only 1/8 of the sphere is contained within the cell again similar to case 1. Here, however, the probe particle radius is equal to 1Å instead of being point-like as in cases 1 and 2. As such, the 1Å probe

particle gives the lone particle at the origin an accessible surface radius of 2Å. Thus, the expected surface area is $\frac{4\pi(2^2)}{8} = 6.383$ Å^2. The total pore volume remains unchanged.

In case 4, the periodic boundaries are on and thus the probe particle is entirely in the simulation cell. With the accessible surface at 2Å radius, the expected surface area is equal to 50.265 Å^2.

The PSD for cases 1 and 3 are identical as well as cases 2 and 4. These are shown in figure 4 along with the graphical outputs of case 1 and 2 (using 100000 samples). A cubic 10Å cell has a cross cell diagonal length of $\sqrt{300} = 17.32$Å. A single particle of 1Å radius is located at the origin. Thus, with no PBCs and using the Connolly surface definition (case 1), the largest pore would be of the order 17.32-1.00 = 16.32Å in radius or 32.6Å in diameter which is the approximate location of the green peak in the PSD. The distribution in space of these maximum pore centres in the PSD sampling is shown in green and they are located along the cell boundaries. Note that this pore would extend outside the 10Å simulation cell.

With PBCs present, the pores can run into the lone atom through the periodic boundaries. Thus, the maximum pore diameter is now 17.32-2.00 = 15.32Å which is the location of the red peak. The locations of the maximum pore centres shown in red are now found towards the centre of the cell.
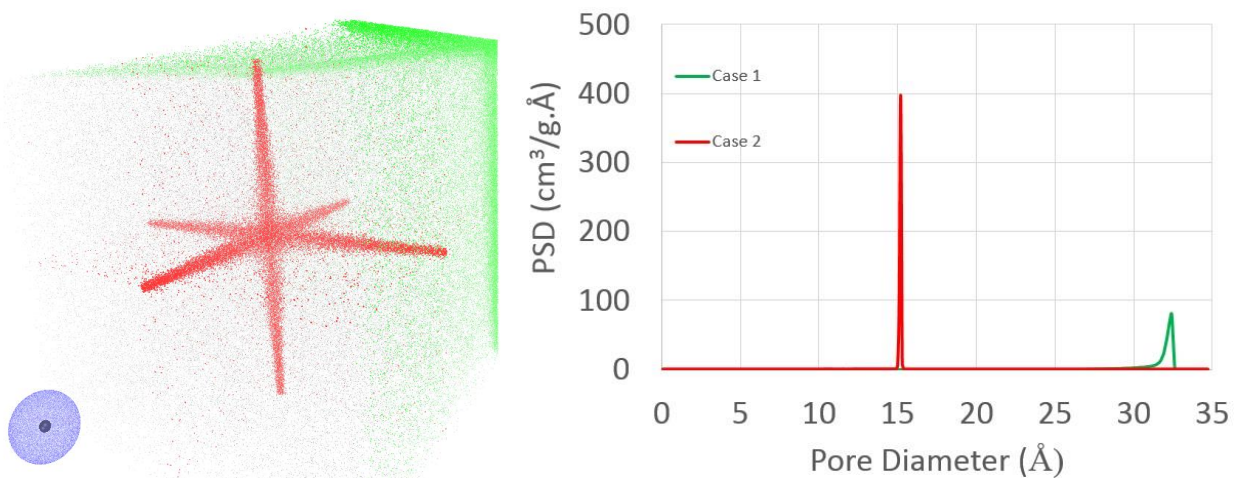

Figure 4 Illustration the PSD and graphical output of case 1 and 2. **ov_surf.xyz** output is shown in blue and represents the surface area sampling (black sphere within is the particle centre). **ov_psdI.xyz** represents the initial random insertion locations used to calculate the accessible pore and bulk volumes. **ov_psdF.xyz**, shows the final pore centre locations after the random walk from the initial position which is used to calculate the PSD where the green locations are case 1 while the red locations are case 2.

5.2   /Examples/Intro2

The **/Example/Intro2** directory contains the **PorosityPlus.inp** file and the **intro2.xyz** file containing a 4 particle configuration for analysis using periodic boundary conditions (**pbc_option**=1) with 100,000 samples in a 10Å cubic cell.
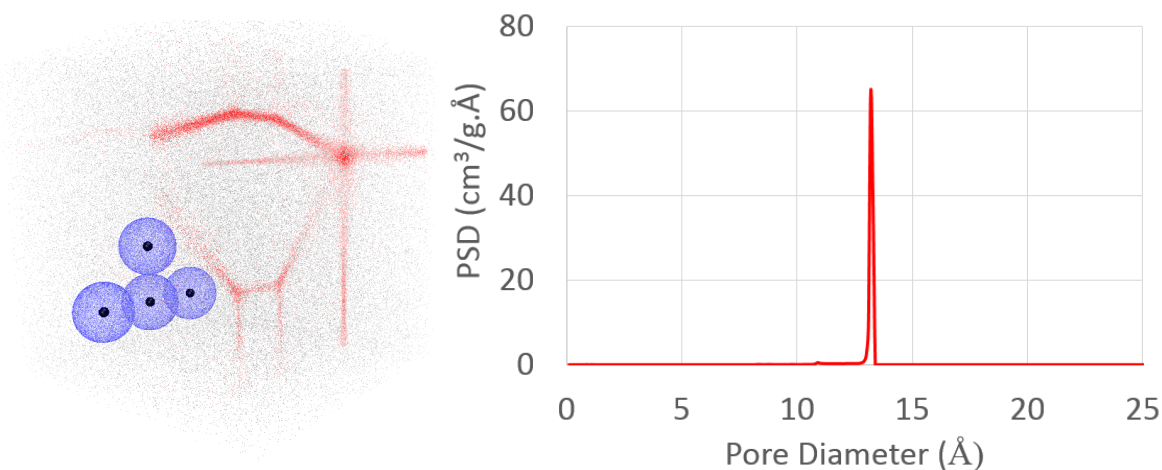

Figure 5 Illustration of the xyz output files in the code along with the PSD when using a zero radius probe particle. **ov_surf.xyz** output is shown in blue and represents the surface area sampling (black sphere within are the particle centres). **ov_psdI.xyz** is shown in grey and represents the initial and random insertion locations used to calculate the accessible pore and bulk volumes. **ov_psdF.xyz**, shown in red, are the final pore centre locations after the random walk used to calculate the PSD.

If we assume a probe particle radius of zero (point-like probe), the four network particles of radius 1Å are not overlapping (just touching) and the resulting surface area and bulk volume should be that of four spheres (50.3 Å^2 and 16.8 Å^3 giving a total pore volume of 983.2 Å^3) as illustrated in figure 5. The example, however, is set up with a probe particle radius of 1Å and therefore there is a significant overlap of the accessible surface as shown in figure 6. The **od_data.dat** file results in an accessible area of 119.7 Å^2 while the total pore volume remains the same at 983.3 Å^3 since it always uses the Connolly surface. The accessible pore volume, however, is lower at 979.9 Å^3 since although it still uses the Connolly surface, there are volumes near the four spheres where the 1Å radius probe particle cannot access.
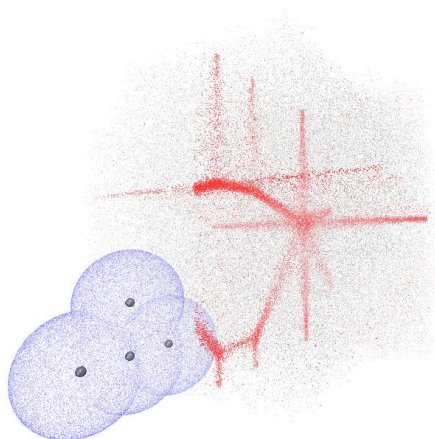

Figure 6 Outputs using a particle probe size of radius 1Å illustrating the overlapping accessible surface.

5.3   /Examples/Intro3

The **/Example/Intro3** directory contains the **PorosityPlus.inp** file and the **intro3.xyz** file which holds a 1237 carbon atom, 5 frame configurations of a Monte Carlo based simulation from a random configuration into a porous amorphous carbon. Note that the graphical outputs only ever occur for the last frame in the analysis.

Using a probe diameter of 1.5Å and a carbon radius of 1.8Å with periodic boundaries in a 30Å cubic cell, the **od_data.dat** file contains the analysis for the 5 frames.

Frame,Accessible surface area (A^2),Accessible specific surface area (m^2/g),Total pore volume (A^3),Total bulk volume (A^3),Total specific pore Volume (cm^3/g),Total porosity,Accessible pore volume (A^3),Accessible bulk volume (A^3),Accessible specific pore volume (cm^3/g),Accessible porosity

  1, 0.255225E+03, 0.103451E+03, 0.788103E+04, 0.191190E+05, 0.319445E+00, 0.291890E+00, 0.705510E+03, 0.262945E+05, 0.285967E-01, 0.261300E-01

  2, 0.473131E+04, 0.191776E+04, 0.136941E+05, 0.133059E+05, 0.555070E+00, 0.507190E+00, 0.104849E+05, 0.165151E+05, 0.424989E+00, 0.388330E+00

  3, 0.516995E+04, 0.209556E+04, 0.140910E+05, 0.129090E+05, 0.571157E+00, 0.521890E+00, 0.114305E+05, 0.155696E+05, 0.463315E+00, 0.423350E+00

  4, 0.513224E+04, 0.208027E+04, 0.142255E+05, 0.127745E+05, 0.576607E+00, 0.526870E+00, 0.116597E+05, 0.153403E+05, 0.472606E+00, 0.431840E+00

  5, 0.526639E+04, 0.213465E+04, 0.142835E+05, 0.127165E+05, 0.578960E+00, 0.529020E+00, 0.119686E+05, 0.150314E+05, 0.485126E+00, 0.443280E+00

One can see the accessible surface area increases as the random distribution of atoms starts to move together forming bonds. The porosity also increases. Notice that for the first frame (random distribution of atoms), the porosity using the total pore volume routines is equal to 29% but the accessible pore volume porosity is only equal to 2.5%. This is due to the fact that the probe particle cannot fit into the network without overlap.

The **od_psd.dat** file contains the 5 columns for the PSD in each frame and is graphed in figure 7.
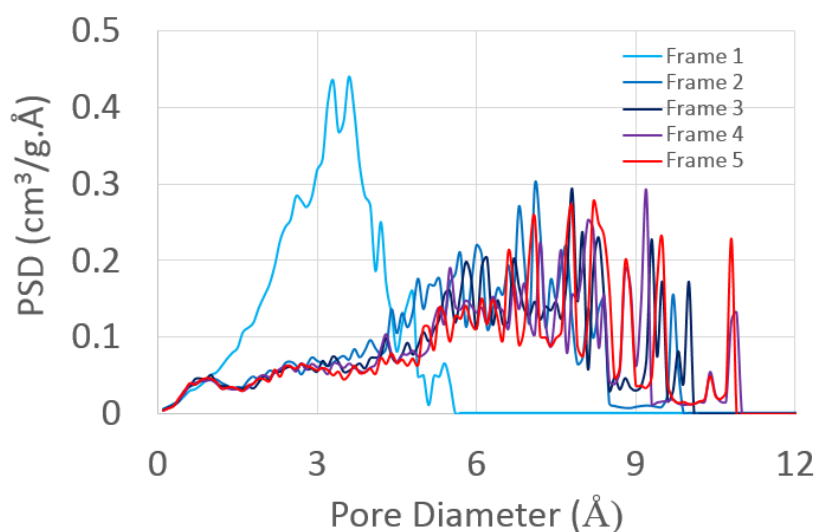

Figure 7 Pore size distributions of the five frame carbon system.

Focusing on the last configuration in frame 5, there are number of ways to visualize the analysis outputs.
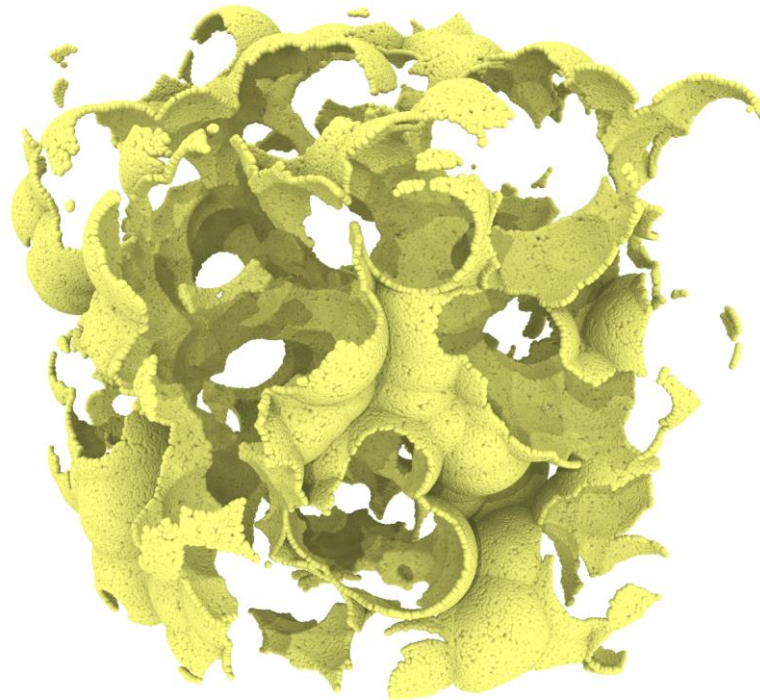

Figure 8 Surface area accepted sample points from **ov_surf.xyz** defining the accessible surface (visualized in Ovito).
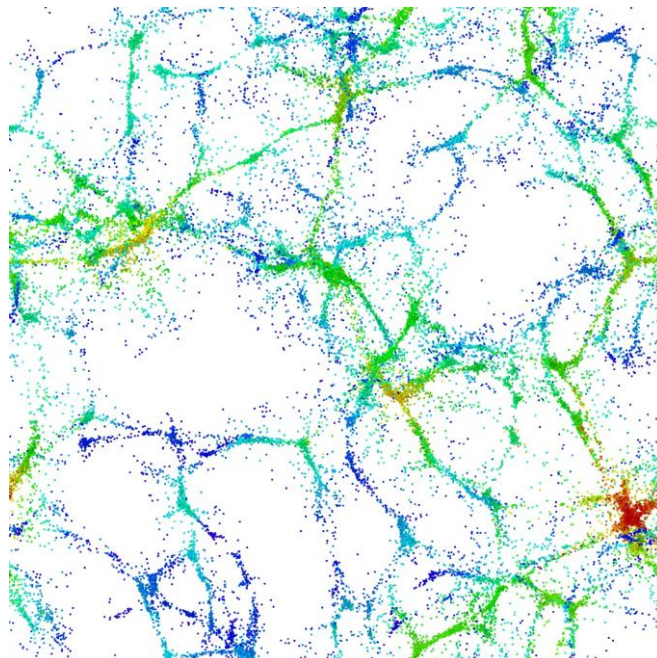

Figure 9 The final positions of point insertions to calculate the PSD from the **out_psdFs.xyz** output file. This shows the locations of the centre of the maximum sized spheres encompassing the initial insertion point where the fifth column detailing the radius shows up as colors in Ovito.