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1 PCBM-CG

Continuuing the Girifalco CG C60 simulation work, the idea is to supplement the single point forcefield by an interaction site to 'kinda' represent PBM.

This is done by defining a couple of atomtypes — the C60 is standard Girifalco:

```
[ atomtypes ]
;type    mass    charge       ptype          sigma      epsilon
 C60    720.60   0.00           A           0.89535      26.822830
 PBM    190.00   0.00           A           0.5          10.0
```

You then connect these things together with 'bonds' to specify their location, and build up the bis / tris by specifying angles between the sidechains to preserve the correct structure.

1.1 Pymol Rendering

Overlapping the two representations, and drawing spheres at the vdW radii (hard sphere approximation) of the two coarse grain atoms, you get something a little like this:

In Pymol, going from the output PDB files, which open as orange and green blobs, you want to:

```
show spherse, all
alter elem P, vdw=2.5
alter elem C, vdw=4.47675
rebuild
```

All together, with 10 mono PCBM on a wall, this looks something like:

1.2 Parameterisation

So, we basically have three free parameters with this paramterisation: Strength of 'PBM' LJ potential, eqm distance of PBM LJ potential, and size of bond for fullere—PBM.

LJ potentials are combined by geometric average of the r^6 and r^{12} parameters (multiply them together + then sqrt) [type 1], or by the Lorentz-Beerthelot rules (arithmetic avg for σ, geometric for ϵ) [type 2]. But one can also define the pairs explicitly in gromacs.

I guess what we really want to do is make use of the atomistic monoPCBM forcefield, and fit the 3 parameters to reproduce similar CoM RDFs between the CG representation and the atomistic. That should get the distances correct, ish, at least.

1.3 RDFs

So let's see how they compare currently...

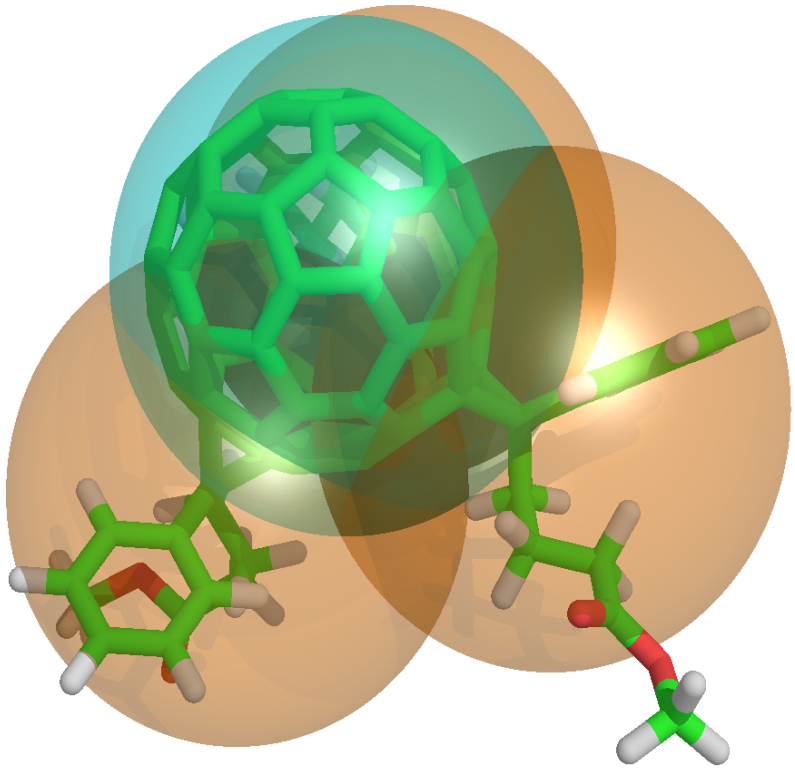

Figure 1: Render of atomistic EEE Tris with superimposed vdW radii balls with the same parameters as the FF (well, the fullerene one might be off by 10%, think this is the old incorrect reading of the Girifalco force field)

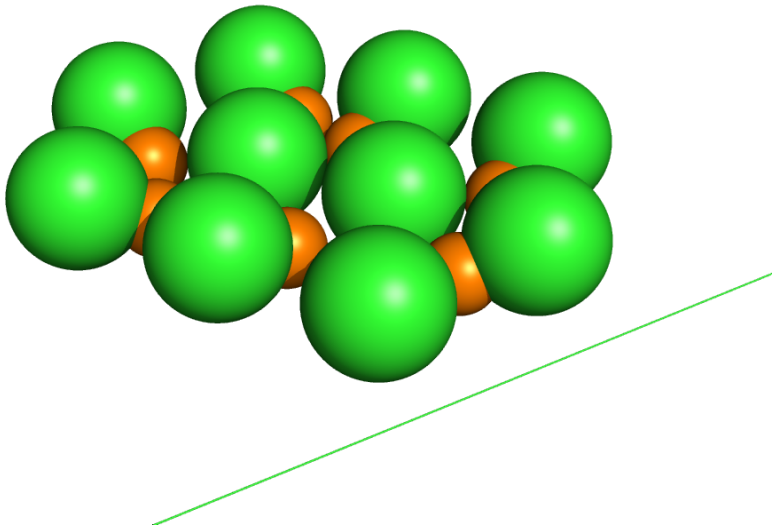

Figure 2: 10 mono PCBM of the new build forecfield, with a dense wall of C60 sites below them. MD at 300K, just to show behaviour and packing arrangement.

1.4 CG-RDF

So make an index with 'a C' to 'make_ndx -f confout.gro'.

And it looks quite interesting, you see the clear C60-C60 peak at just over 1nm, and then a 2nd peak which I imagine is from fullerene-fullerene with a PBM stuck in the way. Perhaps. This is C60-C60 centre distance don't forget, no contri from PBM:C60 or PBM:PBM.

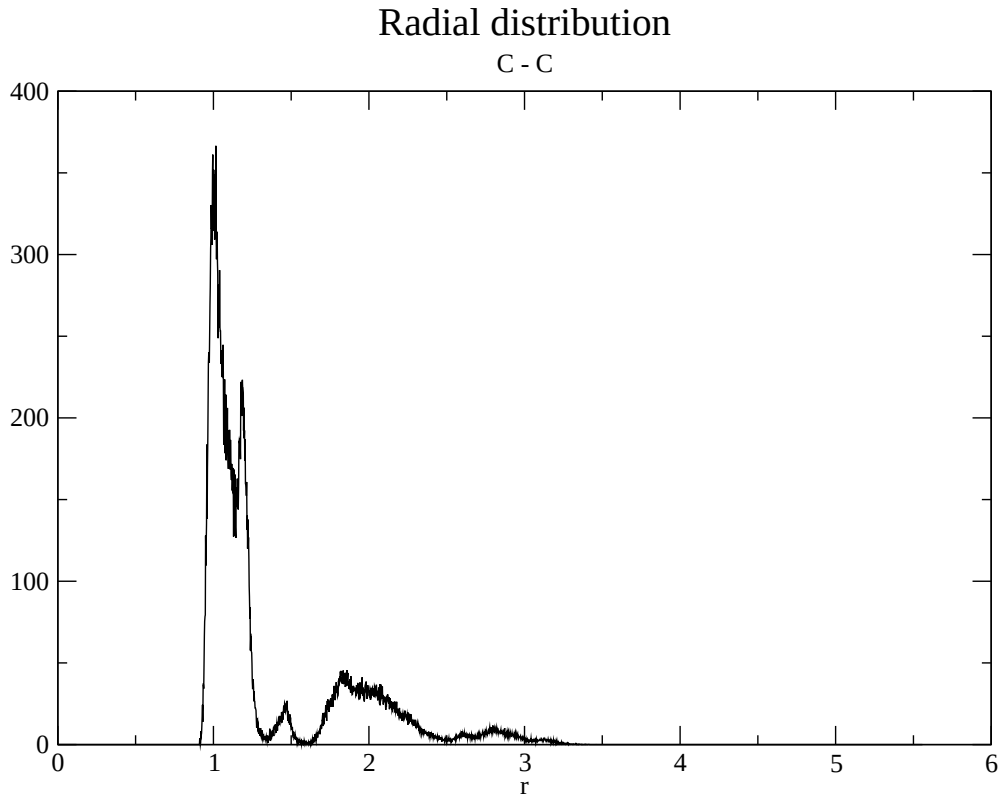

Figure 3: Just a little simulation, 10 CG monoPCBM on a sticky wall. More or less arbitrary guess parameters. Lots of issues with this data—more of less squashed on 2D wall, only a couple of neighbours at most etc. Need to do a proper 3D volume simulation...

1.5 3D CG sim

So the FF with the three variables are: $\sigma = 0.5$, $\epsilon = 10.0$, bond $= 0.5$

Looks like:

And running under MD, it looks like:

Ok, did 10ns of MD, the RDF is now:

Just realised I'd be in remiss if I didn't do equiv. for a pure C60 simulation. Rather than reuse the stuff with Joe, I may as well restart a job from exact same initial conditions as this one...

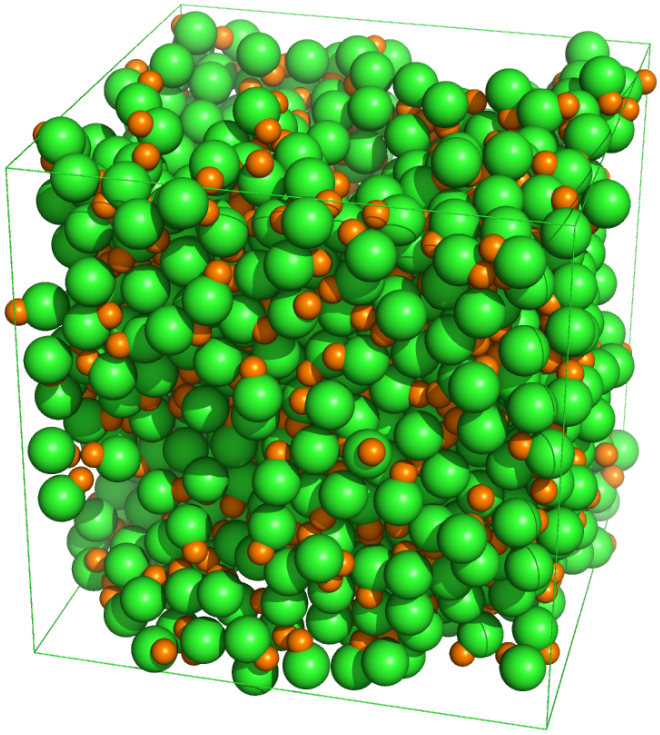

Figure 4: Starting configuration (after steepest descents relax) for 1000 CG monoPCBM in 10x10x10 box.

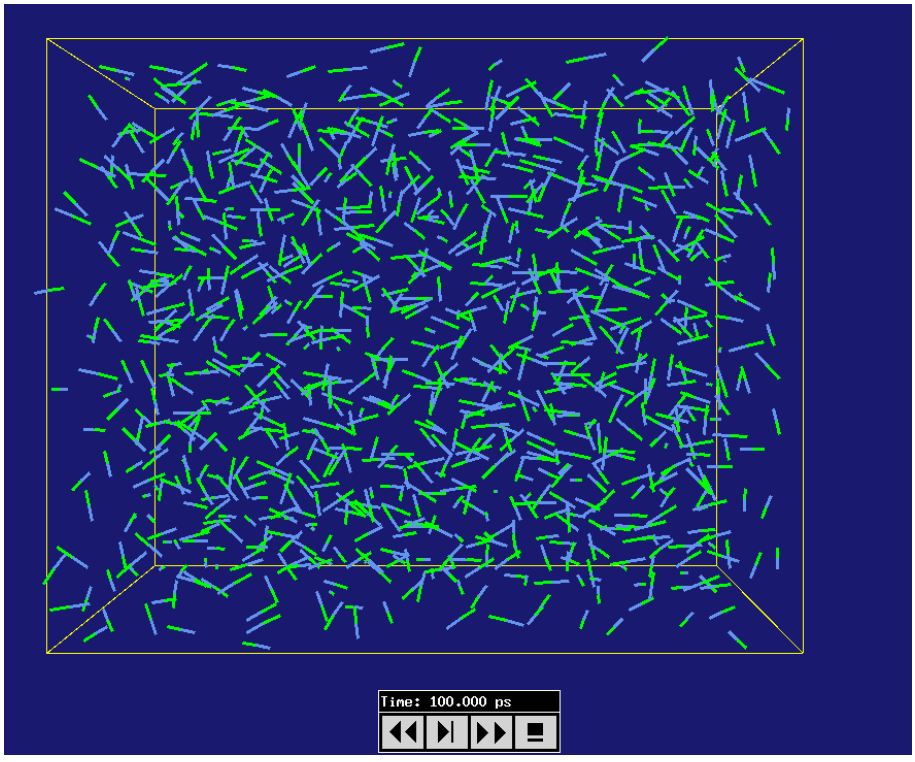

Figure 5: Nothing to do while running MD, so thought I'd capture a picture of the sim running in ngmx. Look like little fishies.

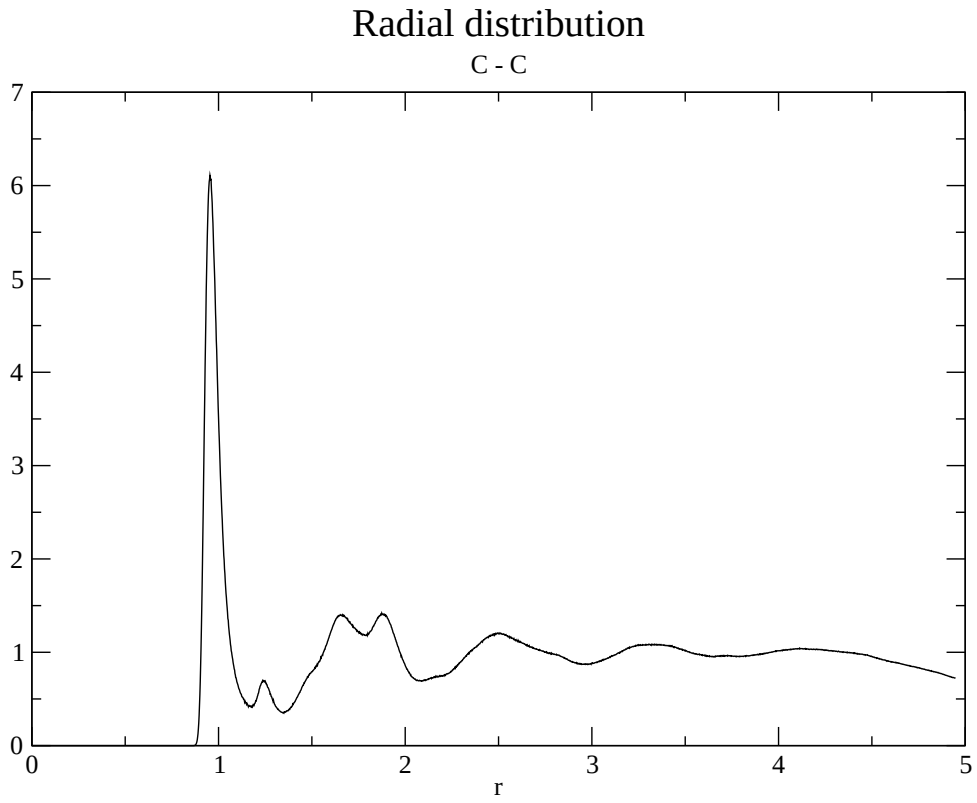

Figure 6: 1000 mono PCBM CG force field, first stab... rdf from C60 sites - C60 sites, 10ns MD run with barostat + thermostat @ STP

1.6 Initial monoPCBM vs. C60 Girifalco

1.7 Compare to Atomistic...

Hmm, bit challenging — need to build index files.

PCBM has 88 atoms (therefore, 60 C60, 28 PBM).

Awk script to make index for C60 looked like:

```
BEGIN{
  for (i=0;i<99;i++)
     for (a=1;a<61;a++)
         print i*88+a
}
{}

for PBM:
BEGIN{
  for (i=0;i<99;i++)
     for (a=1;a<=28;a++)
         print 60+i*88+a
}
{}
```

And so now we go back to the CG simulations and reproduce the same:

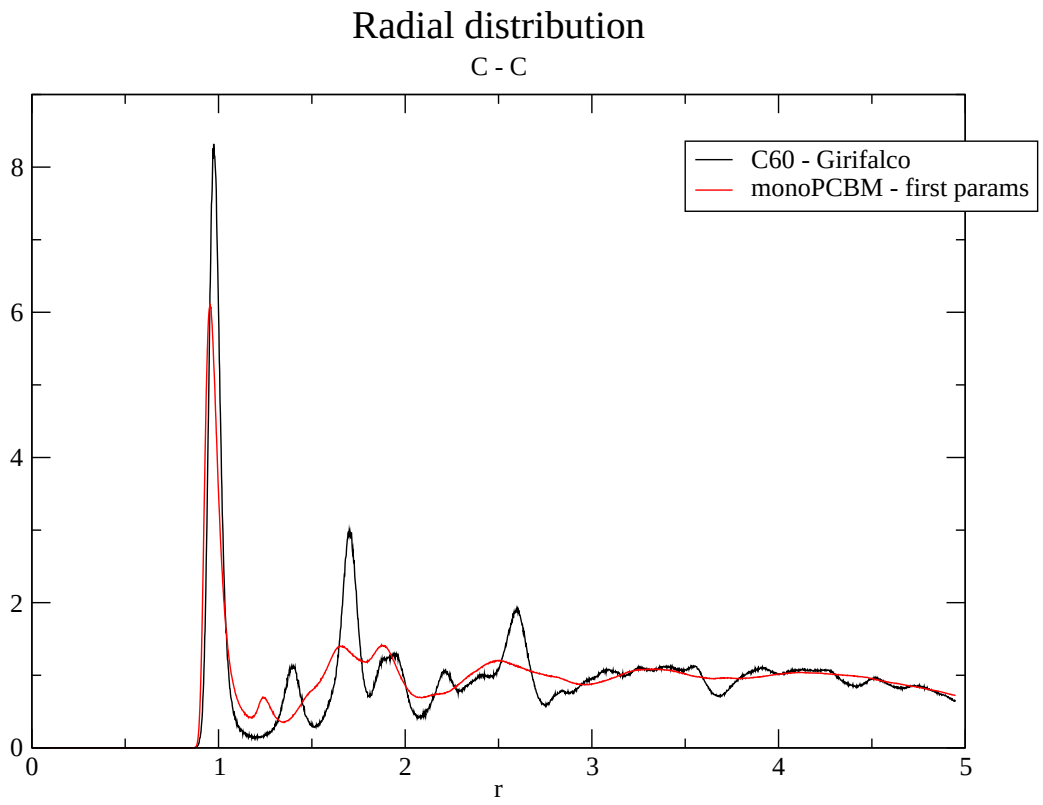

Figure 7: 5ns of C60 Girifalco vs. 10ns of monoPCBM first param.. Same starting conditions, barostat 1 atm, thermo 300K.

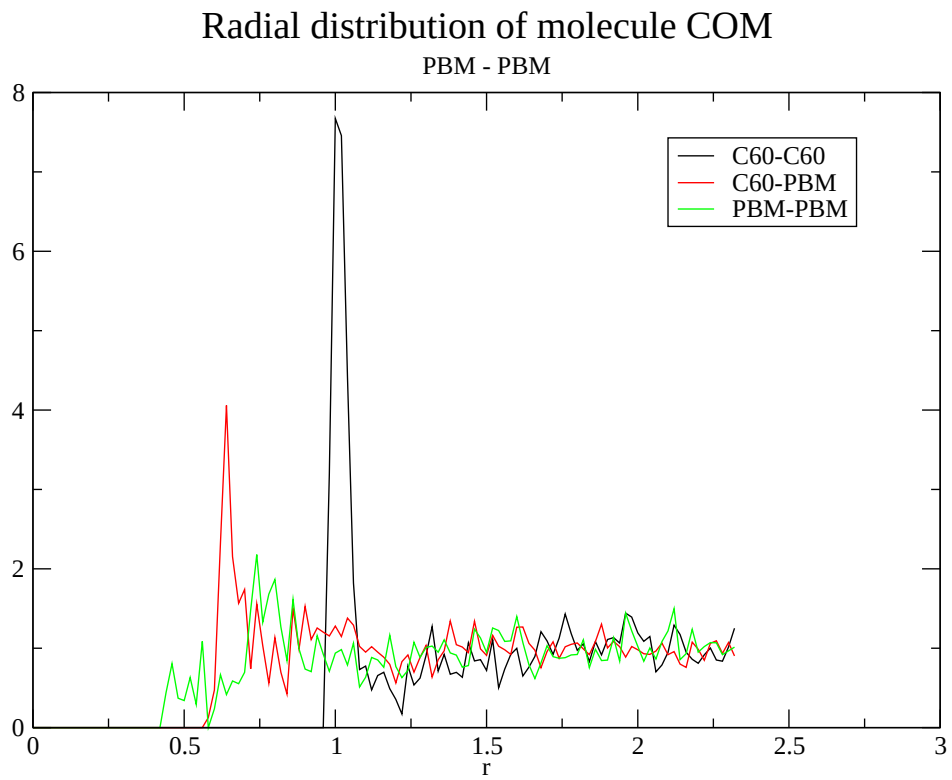

Figure 8: From a single frame of a 99-PCBM atomistic simulation, then steepest descents relaxation. Indexes composed with awk script, centre of mass molecular RDF for the components.

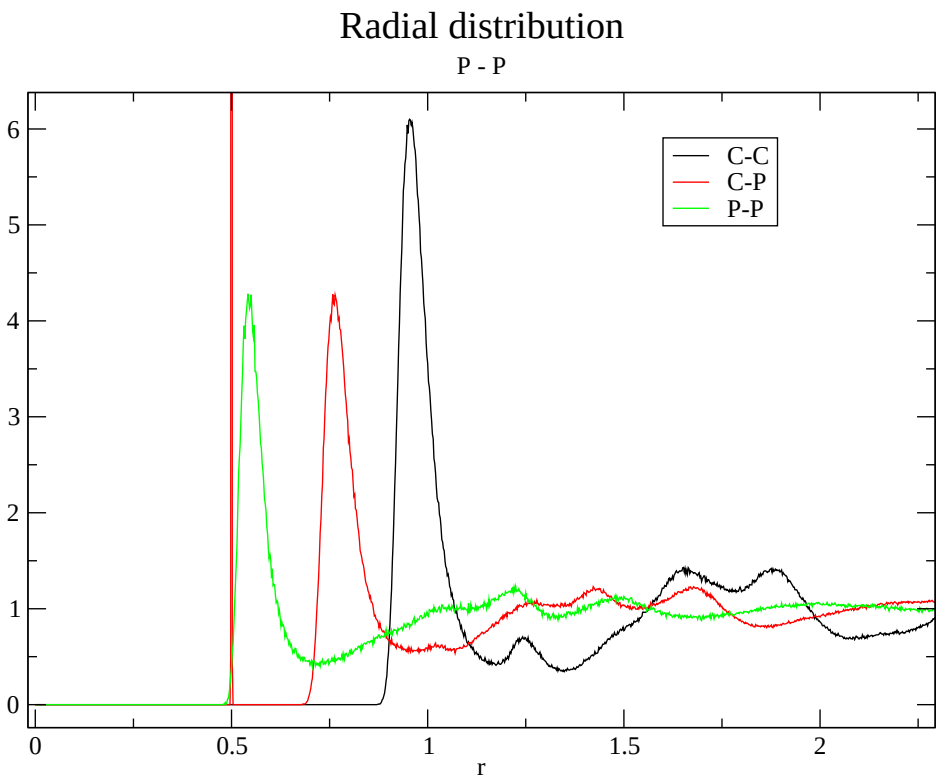

Figure 9: Comparison for the atomistic simulations, RDF from the 10ns early CG mono PCBM run, showing distances between the P(BM) + C(60) units, and amongst themselves. Note the large peak for the bonded part of the PCBM.

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0.8 Single monoPCBM-atomistic

To check whether the RDFs included within single molecule contributions, I looked at the C–C, C–P, P–P distances for a single PCBM from the atomistic simulation (with -rdf mol_com, and building an index with 1–60, 61–88).

This gave null results for C–C and P–P (as expected), and a value of 6.34 Åfor C–P, which is therefore the characteristic 'bonded' length.