

Loops in LAMMPS

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Percolation problem

two components: solvent + particles
particles bond to form network

What is percolation structure? bond fraction
How depend on solvent quality (i.e. solvent-particle interaction)?

System: binary LJ; density = $0.7\sigma^3$
 $c_S=0.7$ $c_P=0.3$
vary ϵ_{SP}

cf. Plitschke PRE 03

Need 1000-10000 runs for percolation analysis
Systems are small (<100000).

Want to run do 100-1000 runs within single LAMMPS script



Needs

fix bond/create

perform adding bonds in percolation simulation

What output is needed for percolation analysis?

Need to do cluster analysis on bond data

Need to determine if percolation occurs (requires positions)

need positions and bonds

config config.bonds

Need dumps periodically done in run (standard)

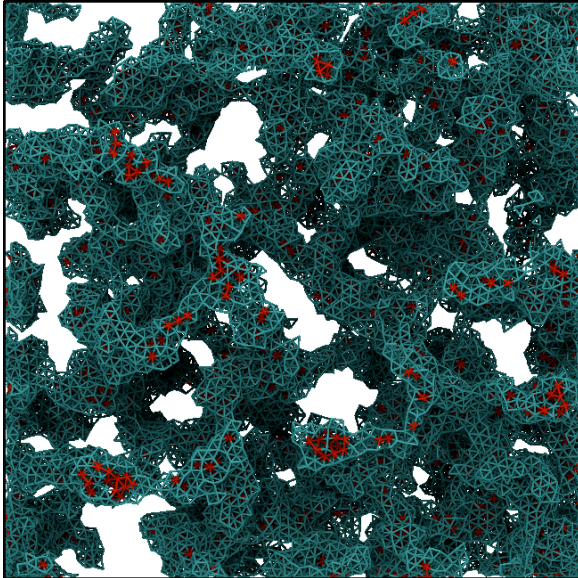
Need 1000s of run

Want the names to be config.1 config.2

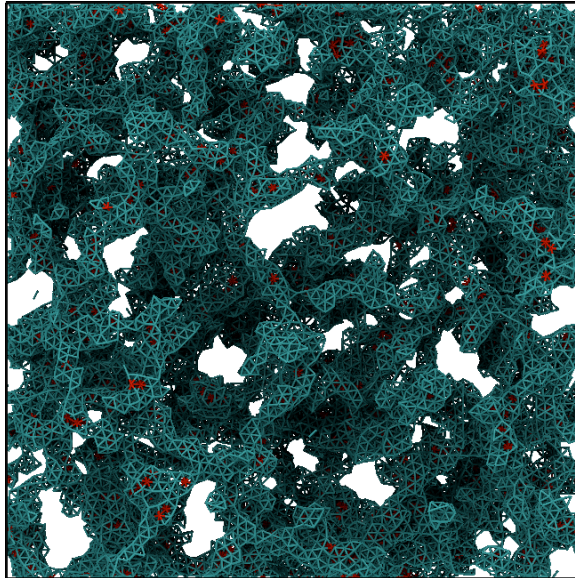
for a perl script to automatically read files and do analysis



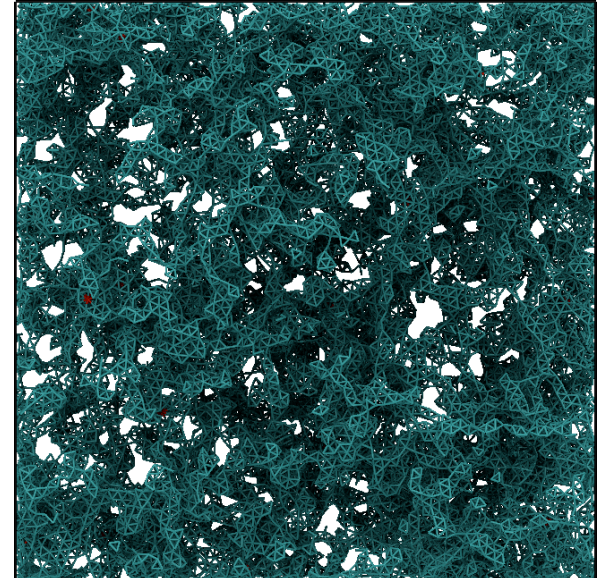
Percolation clusters



$\epsilon_{SP}=0.75$



$\epsilon_{SP}=1.0$



$\epsilon_{SP}=1.5$



LAMMPS input script: part 1

```
variable      f equal 12      # functionality of crosslinker
variable      steps equal 80000      # number of steps in each xlink iteration
variable      dtime equal 2000      # number of steps in each dump

echo      screen
units      lj
atom_style  full
special_bonds      lj/coul 0.0 1.0 1.0 extra ${f}

read_data    input

...                                # equilibration run

run      10000

# Bonding part _____

# BOND bond/create Nevery itype jtype Rmin bondtype      iparam f newtype jparam f newtype
fix      3 all bond/create 100 2      2      1.1      1      prob 0.1 912759 iparam ${f} 3      jparam ${f} 3

thermo      100                                #same as Nevery in fix bond/create
thermo_style      custom step temp etotal evdwl ebond press f_3[1] f_3[2]
thermo_modify      norm no

dump      d1 all custom ${dtime} config.0 id type x y z ix iy iz
dump      d2 all bond ${dtime} config.bonds.0
run      ${steps}
```

```

variable    n loop 1000          # number of iterations
label      here

# Reset bonds and atom types
delete_bonds all multi remove special # remove all bonds (why this is 2nd iteration)
set          group particles type 2   # reset all the maximally bonded to type 2

unfix       3                     # turn off bond making

# must have new thermo since no longer have fix bond/create
thermo      1000
thermo_style custom step temp etotal evdwl ebond press
thermo_modify norm no

undump      d1
undump      d2
run       10000

# Bonding part _____
# BOND bond/create Nevery itype jtype Rmin bondtype iparam f newtype jparam f newtype
fix         3 all bond/create 100 2 2 1.1 1 prob 0.1 912759 iparam ${f} 3 jparam ${f} 3

thermo      100 #same as Nevery in fix bond/create
thermo_style custom step temp etotal evdwl ebond press f_3[1] f_3[2]
thermo_modify norm no          # BTW: this normalization sucks

dump        d1 all custom ${dtime} config.$n id type x y z ix iy iz
dump        d2 all bond ${dtime} config.bonds.$n
run       ${steps}

next n
jump     thisinputscriptname here # read THIS input file and go to label above

```

<goo|~/Data/pv/run39> ls config.? config.?? config.???

config.0	config.189	config.279	config.369	config.459	config.549	config.639	config.729	config.819	config.909
config.1	config.19	config.28	config.37	config.46	config.55	config.64	config.73	config.82	config.91
config.10	config.190	config.280	config.370	config.460	config.550	config.640	config.730	config.820	config.910
config.100	config.191	config.281	config.371	config.461	config.551	config.641	config.731	config.821	config.911
config.101	config.192	config.282	config.372	config.462	config.552	config.642	config.732	config.822	config.912
config.102	config.193	config.283	config.373	config.463	config.553	config.643	config.733	config.823	config.913
config.103	config.194	config.284	config.374	config.464	config.554	config.644	config.734	config.824	config.914
config.104	config.195	config.285	config.375	config.465	config.555	config.645	config.735	config.825	config.915
config.105	config.196	config.286	config.376	config.466	config.556	config.646	config.736	config.826	config.916
config.106	config.197	config.287	config.377	config.467	config.557	config.647	config.737	config.827	config.917
config.107	config.198	config.288	config.378	config.468	config.558	config.648	config.738	config.828	config.918
config.108	config.199	config.289	config.379	config.469	config.559	config.649	config.739	config.829	config.919
config.109	config.2	config.29	config.38	config.47	config.56	config.65	config.74	config.83	config.92
config.11	config.20	config.290	config.380	config.470	config.560	config.650	config.740	config.830	config.920
config.110	config.200	config.291	config.381	config.471	config.561	config.651	config.741	config.831	config.921
config.111	config.201	config.292	config.382	config.472	config.562	config.652	config.742	config.832	config.922
config.112	config.202	config.293	config.383	config.473	config.563	config.653	config.743	config.833	config.923
config.113	config.203	config.294	config.384	config.474	config.564	config.654	config.744	config.834	config.924
config.114	config.204	config.295	config.385	config.475	config.565	config.655	config.745	config.835	config.925
config.115	config.205	config.296	config.386	config.476	config.566	config.656	config.746	config.836	config.926
config.116	config.206	config.297	config.387	config.477	config.567	config.657	config.747	config.837	config.927
config.117	config.207	config.298	config.388	config.478	config.568	config.658	config.748	config.838	config.928
config.118	config.208	config.299	config.389	config.479	config.569	config.659	config.749	config.839	config.929
config.119	config.209	config.3	config.39	config.48	config.57	config.66	config.75	config.84	config.93
config.12	config.21	config.30	config.390	config.480	config.570	config.660	config.750	config.840	config.930
config.120	config.210	config.300	config.391	config.481	config.571	config.661	config.751	config.841	config.931
config.121	config.211	config.301	config.392	config.482	config.572	config.662	config.752	config.842	config.932
config.122	config.212	config.302	config.393	config.483	config.573	config.663	config.753	config.843	config.933
config.123	config.213	config.303	config.394	config.484	config.574	config.664	config.754	config.844	config.934
config.124	config.214	config.304	config.395	config.485	config.575	config.665	config.755	config.845	config.935
config.125	config.215	config.305	config.396	config.486	config.576	config.666	config.756	config.846	config.936
config.126	config.216	config.306	config.397	config.487	config.577	config.667	config.757	config.847	config.937
config.127	config.217	config.307	config.398	config.488	config.578	config.668	config.758	config.848	config.938
config.128	config.218	config.308	config.399	config.489	config.579	config.669	config.759	config.849	config.939
config.129	config.219	config.309	config.4	config.49	config.58	config.67	config.76	config.85	config.94
config.13	config.22	config.31	config.40	config.490	config.580	config.670	config.760	config.850	config.940
config.130	config.220	config.310	config.400	config.491	config.581	config.671	config.761	config.851	config.941
config.131	config.221	config.311	config.401	config.492	config.582	config.672	config.762	config.852	config.942
config.132	config.222	config.312	config.402	config.493	config.583	config.673	config.763	config.853	config.943
config.133	config.223	config.313	config.403	config.494	config.584	config.674	config.764	config.854	config.944
config.134	config.224	config.314	config.404	config.495	config.585	config.675	config.765	config.855	config.945
config.135	config.225	config.315	config.405	config.496	config.586	config.676	config.766	config.856	config.946
config.136	config.226	config.316	config.406	config.497	config.587	config.677	config.767	config.857	config.947
config.137	config.227	config.317	config.407	config.498	config.588	config.678	config.768	config.858	config.948
config.138	config.228	config.318	config.408	config.499	config.589	config.679	config.769	config.859	config.949
config.139	config.229	config.319	config.409	config.5	config.59	config.68	config.77	config.86	config.95
config.14	config.23	config.32	config.41	config.50	config.590	config.680	config.770	config.860	config.950
config.140	config.230	config.320	config.410	config.500	config.591	config.681	config.771	config.861	config.951
config.141	config.231	config.321	config.411	config.501	config.592	config.682	config.772	config.862	config.952
config.142	config.232	config.322	config.412	config.502	config.593	config.683	config.773	config.863	config.953
config.143	config.233	config.323	config.413	config.503	config.594	config.684	config.774	config.864	config.954

...

Some Results

Run perl script to do analysis; Run some more; and run some; and

10,000 particle systems

