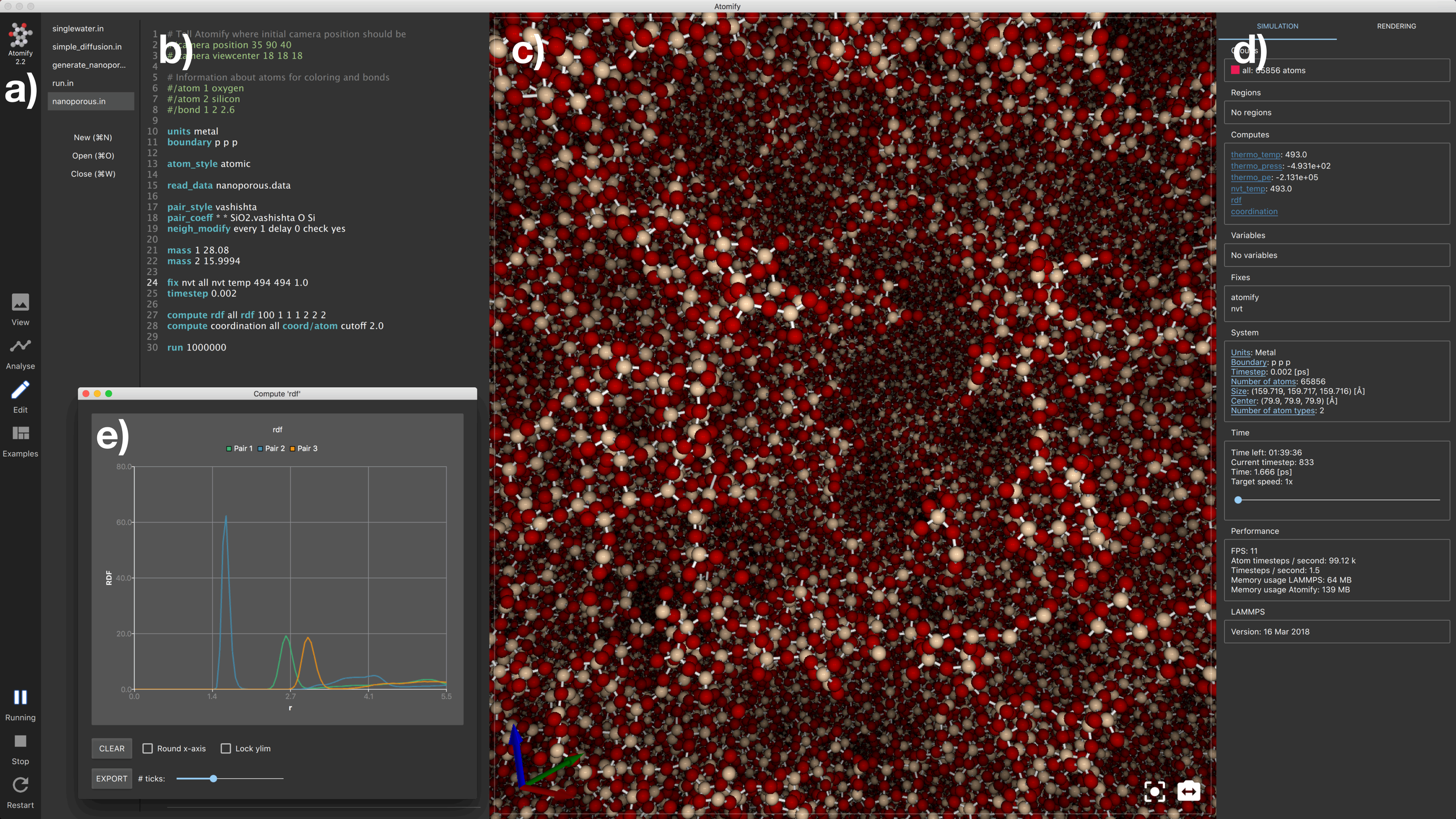
Atomify
Atomify 2.2
a)
singlewater.in
simple_diffusion.in
generate_nanopor...
run.in
nanoporous.in
New (⌘N)
Open (⌘O)
Close (⌘W)
View
Analyse
Edit
Examples
Running
Stop
Restart
b)
Tell Atomify where initial camera position should be
camera position 35 90 40
camera viewcenter 18 18 18
Information about atoms for coloring and bonds
#/atom 1 oxygen
#/atom 2 silicon
#/bond 1 2 2.6
units metal
boundary p p p
atom_style atomic
read_data nanoporous.data
pair_style vashishta
pair_coeff * * SiO2.vashishta O Si
neigh_modify every 1 delay 0 check yes
mass 1 28.08
mass 2 15.9994
fix nvt all nvt temp 494 494 1.0
timestep 0.002
compute rdf all rdf 100 1 1 1 2 2 2
compute coordination all coord/atom cutoff 2.0
run 1000000
c)
d)
SIMULATION
RENDERING
Groups
all: 65856 atoms
Regions
No regions
Computes
thermo_temp: 493.0
thermo_press: -4.931e+02
thermo_pe: -2.131e+05
nvt_temp: 493.0
rdf
coordination
Variables
No variables
Fixes
atomify
nvt
System
Units: Metal
Boundary: p p p
Timestep: 0.002 [ps]
Number of atoms: 65856
Size: (159.719, 159.717, 159.716) [Å]
Center: (79.9, 79.9, 79.9) [Å]
Number of atom types: 2
Time
Time left: 01:39:36
Current timestep: 833
Time: 1.666 [ps]
Target speed: 1x
Performance
FPS: 11
Atom timesteps / second: 99.12 k
Timesteps / second: 1.5
Memory usage LAMMPS: 64 MB
Memory usage Atomify: 139 MB
LAMMPS
Version: 16 Mar 2018
Compute 'rdf'
e)
rdf
Pair 1
Pair 2
Pair 3
RDF
r
80.0
60.0
40.0
20.0
0.0
0.0
1.4
2.7
4.1
5.5
CLEAR
Round x-axis
Lock ylim
EXPORT
ticks: