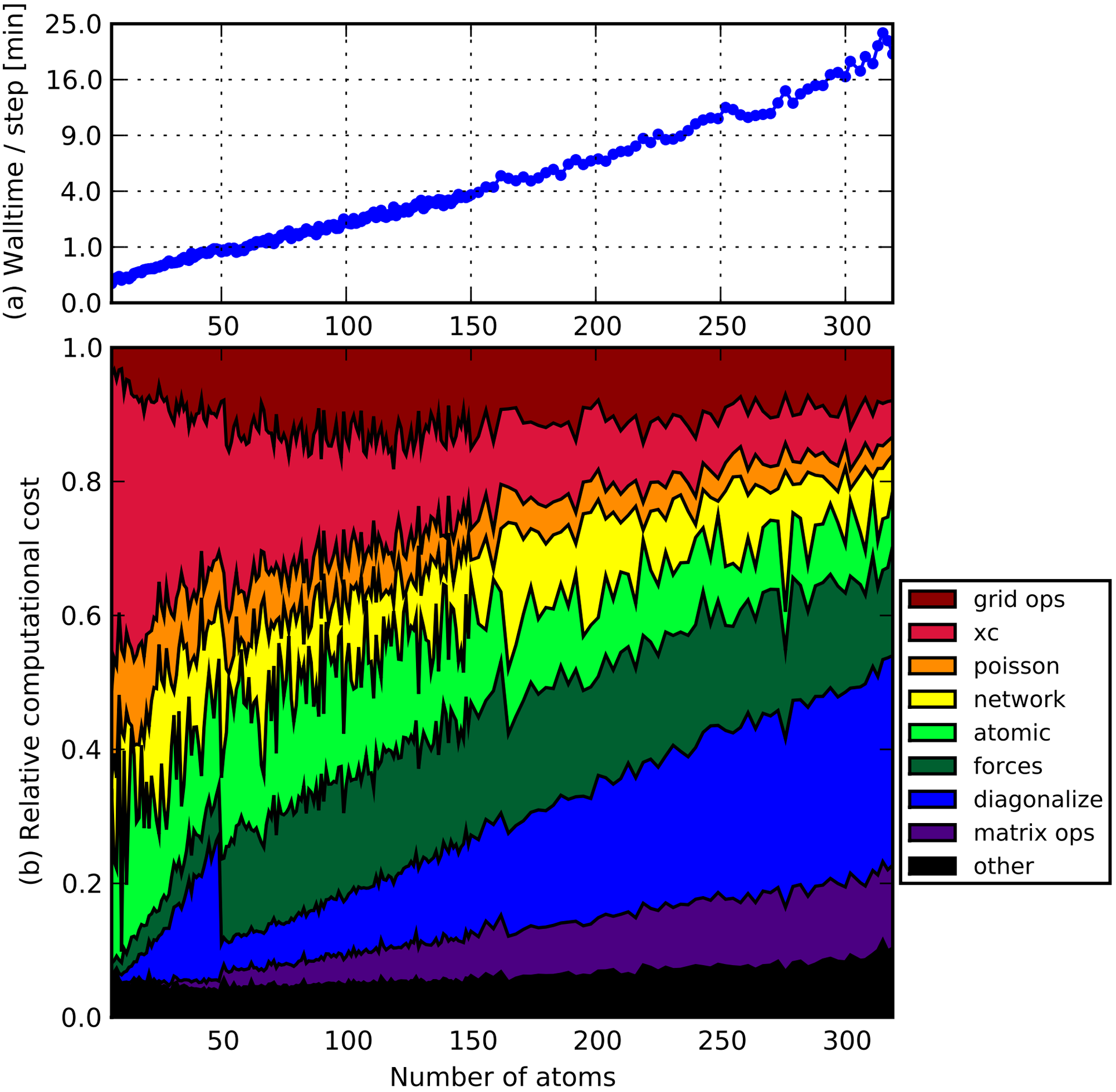
(a) Walltime / step [min]
25.0
16.0
9.0
4.0
1.0
0.0
50
100
150
200
250
300
(b) Relative computational cost
1.0
0.8
0.6
0.4
0.2
0.0
Number of atoms
grid ops
xc
poisson
network
atomic
forces
diagonalize
matrix ops
other