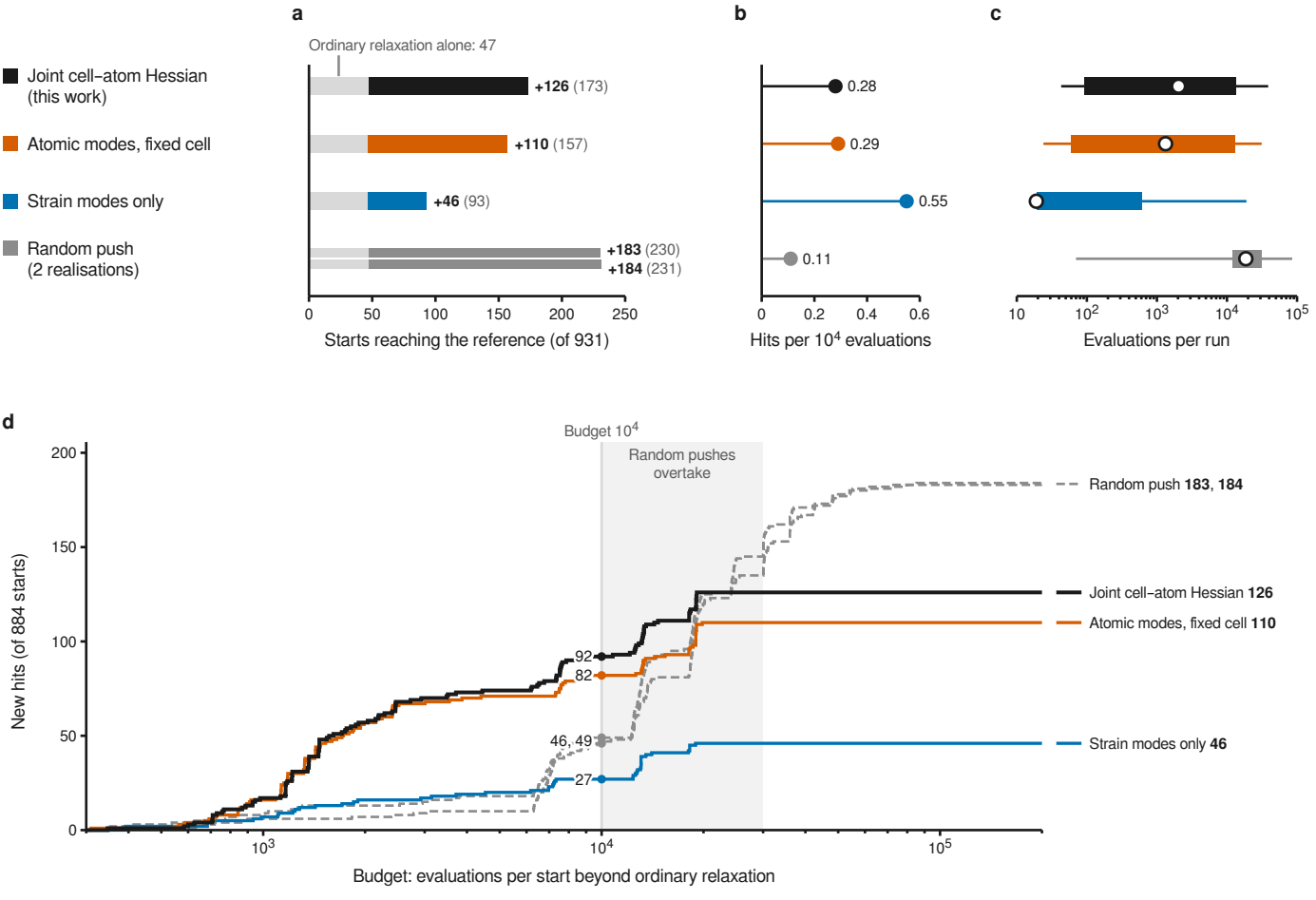
a
b
c
d
Joint cell–atom Hessian (this work)
Atomic modes, fixed cell
Strain modes only
Random push (2 realisations)
Ordinary relaxation alone: 47
+126 (173)
+110 (157)
+46 (93)
+183 (230)
+184 (231)
0
50
100
150
200
250
Starts reaching the reference (of 931)
0.28
0.29
0.55
0.11
0
0.2
0.4
0.6
Hits per 10^4 evaluations
10
10^2
10^3
10^4
10^5
Evaluations per run
Budget 10^4
Random pushes overtake
200
150
100
50
0
New hits (of 884 starts)
92
82
46, 49
27
10^3
10^4
10^5
Budget: evaluations per start beyond ordinary relaxation
Random push 183, 184
Joint cell–atom Hessian 126
Atomic modes, fixed cell 110
Strain modes only 46