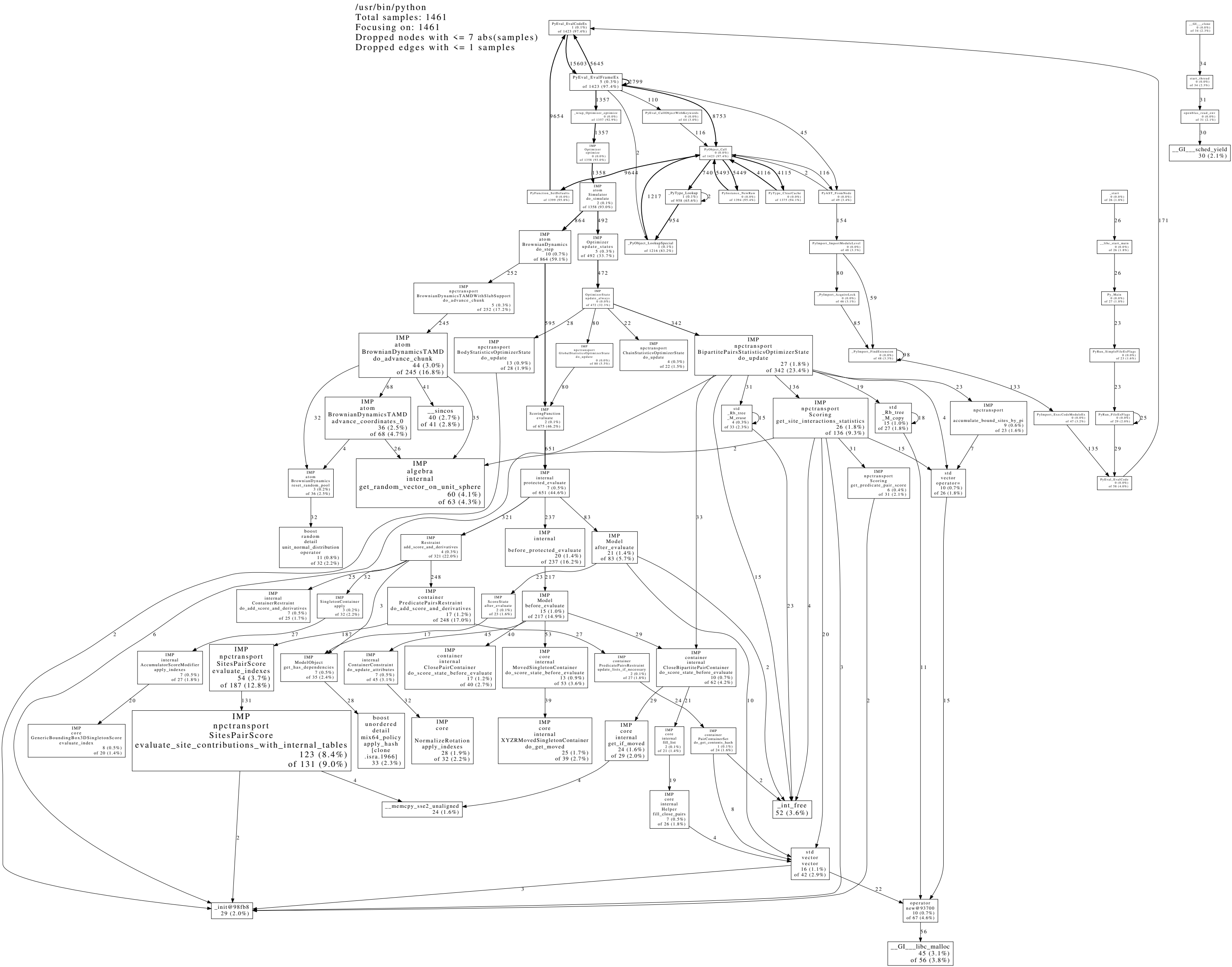
/usr/bin/python
Total samples: 1461
Focusing on: 1461
Dropped nodes with <= 7 abs(samples)
Dropped edges with <= 1 samples
PyEval_EvalFrameEx 5 (0.3%) of 1423 (97.4%)
IMP atom BrownianDynamics do_step 10 (0.7%) of 864 (59.1%)
IMP Optimizer update_states 5 (0.3%) of 492 (33.7%)
IMP npctransport BrownianDynamicsTAMDWithSlabSupport do_advance_chunk 5 (0.3%) of 252 (17.2%)
IMP atom BrownianDynamicsTAMD do_advance_chunk 44 (3.0%) of 245 (16.8%)
IMP npctransport BodyStatisticsOptimizerState do_update 13 (0.9%) of 28 (1.9%)
IMP npctransport ChainStatisticsOptimizerState do_update 4 (0.3%) of 22 (1.5%)
IMP npctransport BipartitePairsStatisticsOptimizerState do_update 27 (1.8%) of 342 (23.4%)
IMP atom BrownianDynamicsTAMD advance_coordinates_0 36 (2.5%) of 68 (4.7%)
__sincos 40 (2.7%) of 41 (2.8%)
IMP npctransport Scoring get_site_interactions_statistics 26 (1.8%) of 136 (9.3%)
std _Rb_tree _M_copy 15 (1.0%) of 27 (1.8%)
IMP npctransport accumulate_bound_sites_by_pi 9 (0.6%) of 23 (1.6%)
IMP algebra internal get_random_vector_on_unit_sphere 60 (4.1%) of 63 (4.3%)
IMP internal protected_evaluate 7 (0.5%) of 651 (44.6%)
IMP npctransport Scoring get_predicate_pair_score 6 (0.4%) of 31 (2.1%)
std vector operator= 10 (0.7%) of 26 (1.8%)
boost random detail unit_normal_distribution operator 11 (0.8%) of 32 (2.2%)
IMP internal before_protected_evaluate 20 (1.4%) of 237 (16.2%)
IMP Model after_evaluate 21 (1.4%) of 83 (5.7%)
IMP container PredicatePairsRestraint do_add_score_and_derivatives 17 (1.2%) of 248 (17.0%)
IMP Model before_evaluate 15 (1.0%) of 217 (14.9%)
IMP npctransport SitesPairScore evaluate_indexes 54 (3.7%) of 187 (12.8%)
IMP container internal ClosePairContainer do_score_state_before_evaluate 17 (1.2%) of 40 (2.7%)
IMP core internal MovedSingletonContainer do_score_state_before_evaluate 13 (0.9%) of 53 (3.6%)
IMP container internal CloseBipartitePairContainer do_score_state_before_evaluate 10 (0.7%) of 62 (4.2%)
IMP npctransport SitesPairScore evaluate_site_contributions_with_internal_tables 123 (8.4%) of 131 (9.0%)
boost unordered detail mix64_policy apply_hash [clone .isra.1966] 33 (2.3%)
IMP core NormalizeRotation apply_indexes 28 (1.9%) of 32 (2.2%)
IMP core internal XYZRMovedSingletonContainer do_get_moved 25 (1.7%) of 39 (2.7%)
IMP core internal get_if_moved 24 (1.6%) of 29 (2.0%)
_int_free 52 (3.6%)
__memcpy_sse2_unaligned 24 (1.6%)
std vector vector 16 (1.1%) of 42 (2.9%)
_init@98fb8 29 (2.0%)
operator new@93700 10 (0.7%) of 67 (4.6%)
__GI___libc_malloc 45 (3.1%) of 56 (3.8%)
__GI___sched_yield 30 (2.1%)