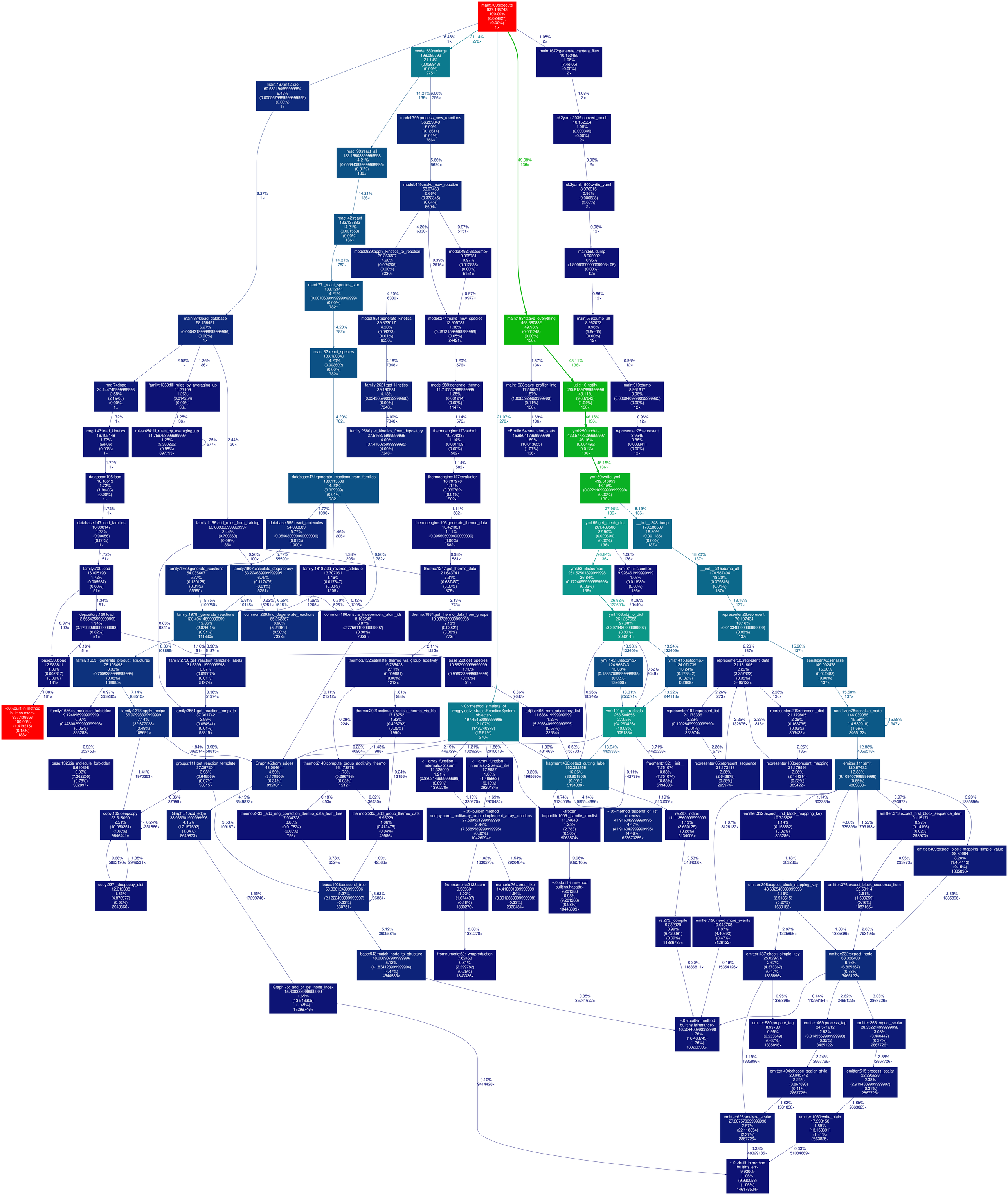
main:709:execute
937.136743
100.00%
(0.029827)
(0.00%)
1×
model:589:enlarge
198.085792
21.14%
(0.028943)
(0.00%)
275×
main:1672:generate_cantera_files
10.153485
1.08%
(7.4e-05)
(0.00%)
2×
main:467:initialize
60.532194999999994
6.46%
(0.000567999999999999)
(0.00%)
1×
model:799:process_new_reactions
56.229349
6.00%
(0.12614)
(0.01%)
756×
ck2yaml:2039:convert_mech
10.152534
1.08%
(0.000345)
(0.00%)
2×
react:99:react_all
133.19608399999998
14.21%
(0.056943999999999995)
(0.01%)
136×
model:449:make_new_reaction
53.07468
5.66%
(0.372345)
(0.04%)
6694×
ck2yaml:1900:write_yaml
8.976915
0.96%
(0.000628)
(0.00%)
2×
react:42:react
133.137882
14.21%
(0.001558)
(0.00%)
136×
model:929:apply_kinetics_to_reaction
39.363327
4.20%
(0.024265)
(0.00%)
6330×
model:492:<listcomp>
9.068781
0.97%
(0.012835)
(0.00%)
5151×
main:560:dump
8.962092
0.96%
(1.8999999999999998e-05)
(0.00%)
12×
react:77:_react_species_star
133.12141
14.21%
(0.00106099999999999)
(0.00%)
782×
main:374:load_database
58.756491
6.27%
(0.000421999999999999996)
(0.00%)
1×
model:951:generate_kinetics
39.323017
4.20%
(0.09373)
(0.01%)
6330×
model:274:make_new_species
12.905787
1.38%
(0.461215999999999996)
(0.05%)
24421×
main:1934:save_everything
468.386882
49.98%
(0.001748)
(0.00%)
136×
main:576:dump_all
8.962073
0.96%
(5.6e-05)
(0.00%)
12×
react:82:react_species
133.120349
14.20%
(0.003692)
(0.00%)
782×
rmg:74:load
24.144745999999998
2.58%
(2.1e-05)
(0.00%)
1×
family:1360:fill_rules_by_averaging_up
11.77109
1.26%
(0.014254)
(0.00%)
36×
family:2621:get_kinetics
39.190981
4.18%
(0.034305999999999996)
(0.00%)
7348×
model:889:generate_thermo
11.710557999999999
1.25%
(0.031214)
(0.00%)
1147×
main:1928:save_profiler_info
17.560071
1.87%
(1.0085929999999999)
(0.11%)
136×
util:110:notify
450.81897899999996
48.11%
(9.687642)
(1.04%)
136×
main:910:dump
8.961617
0.96%
(0.00604099999999999995)
(0.00%)
12×
rmg:143:load_kinetics
16.105148
1.72%
(9e-06)
(0.00%)
1×
rules:454:fill_rules_by_averaging_up
11.756758999999999
1.25%
(5.380222)
(0.58%)
897753×
family:2580:get_kinetics_from_depository
37.516875999999996
4.00%
(37.416025999999995)
(4.00%)
7348×
thermoengine:173:submit
10.708385
1.14%
(0.001109)
(0.00%)
582×
cProfile:54:snapshot_stats
15.880417999999999
1.69%
(10.013655)
(1.07%)
136×
yml:250:update
432.57773299999997
46.16%
(0.064492)
(0.01%)
136×
representer:78:represent
8.9549
0.96%
(0.003341)
(0.00%)
12×
database:105:load
16.10512
1.72%
(1.8e-05)
(0.00%)
1×
database:474:generate_reactions_from_families
133.115568
14.20%
(0.069599)
(0.01%)
782×
thermoengine:147:evaluator
10.707276
1.14%
(0.089782)
(0.01%)
582×
yml:59:write_yml
432.519953
46.15%
(0.022116999999999998)
(0.00%)
136×
database:147:load_families
16.098147
1.72%
(0.00056)
(0.00%)
1×
family:1166:add_rules_from_training
22.839899999999997
2.44%
(0.799863)
(0.09%)
36×
database:555:react_molecules
54.093889
5.77%
(0.054030999999999996)
(0.01%)
1090×
thermoengine:106:generate_thermo_data
10.421021
1.11%
(0.00559599999999999999)
(0.00%)
582×
yml:65:get_mech_dict
261.489508
27.90%
(0.020604)
(0.00%)
136×
__init__:248:dump
170.588539
18.20%
(0.001135)
(0.00%)
137×
family:700:load
16.095193
1.72%
(0.005987)
(0.00%)
51×
family:1769:generate_reactions
54.035407
5.77%
(0.120125)
(0.01%)
55590×
family:1907:calculate_degeneracy
63.224689999999995
6.75%
(0.117479)
(0.01%)
5251×
family:1818:add_reverse_attribute
13.707061
1.46%
(0.017847)
(0.00%)
1205×
thermo:1247:get_thermo_data
21.643741
2.31%
(0.687457)
(0.07%)
876×
yml:82:<listcomp>
251.52561899999998
26.84%
(0.172409999999999998)
(0.02%)
136×
yml:81:<listcomp>
9.926461999999999
1.06%
(0.011989)
(0.00%)
136×
__init__:215:dump_all
170.587404
18.20%
(0.379816)
(0.04%)
137×
depository:128:load
12.565425999999999
1.34%
(0.179935999999999998)
(0.02%)
51×
family:1978:_generate_reactions
120.404148999999999
12.85%
(2.876915)
(0.31%)
111630×
common:226:find_degenerate_reactions
65.262367
6.96%
(5.243611)
(0.56%)
7238×
common:186:ensure_independent_atom_ids
8.162646
0.87%
(2.775611999999999997)
(0.30%)
7238×
thermo:1884:get_thermo_data_from_groups
19.937359999999998
2.13%
(0.03821)
(0.00%)
773×
yml:108:obj_to_dict
261.267682
27.88%
(3.3973489999999997)
(0.36%)
303014×
representer:26:represent
170.197434
18.16%
(0.0133499999999999999)
(0.00%)
137×
base:203:load
12.983811
1.39%
(0.002317)
(0.00%)
181×
family:1633:_generate_product_structures
78.105498
8.33%
(0.705928999999999999)
(0.08%)
108885×
family:2730:get_reaction_template_labels
31.539911999999998
3.37%
(0.055073)
(0.01%)
51974×
thermo:2122:estimate_thermo_via_group_additivity
19.735423
2.11%
(0.009881)
(0.00%)
1212×
base:293:get_species
10.862900999999999
1.16%
(0.956033999999999999)
(0.10%)
51×
yml:142:<listcomp>
124.966743
13.33%
(0.189370999999999998)
(0.02%)
132609×
yml:141:<listcomp>
124.071739
13.24%
(0.173342)
(0.02%)
132609×
representer:33:represent_data
21.181606
2.26%
(3.257322)
(0.35%)
3465122×
serializer:46:serialize
149.002478
15.90%
(0.042482)
(0.00%)
137×
~:0:<built-in method builtins.exec>
937.138868
100.00%
(1.419215)
(0.15%)
188×
family:1686:is_molecule_forbidden
9.124896999999999
0.97%
(0.478002999999999996)
(0.05%)
393262×
family:1373:apply_recipe
66.929983999999999
7.14%
(32.677028)
(3.49%)
108691×
family:2551:get_reaction_template
37.361742
3.99%
(0.064541)
(0.01%)
58815×
thermo:2021:estimate_radical_thermo_via_hbi
17.18752
1.83%
(0.428792)
(0.05%)
1990×
~:0:<method 'simulate' of 'rmgpy.solver.base.ReactionSystem' objects>
197.45150099999998
21.07%
(148.740378)
(15.91%)
270×
adjlist:465:from_adjacency_list
11.685419999999999
1.25%
(5.298840999999999995)
(0.57%)
22664×
yml:101:get_radicals
253.504855
27.05%
(94.263426)
(10.08%)
509133×
representer:191:represent_list
21.173336
2.26%
(0.120284999999999999)
(0.01%)
293974×
representer:206:represent_dict
21.179865
2.26%
(0.163736)
(0.02%)
303422×
serializer:78:serialize_node
146.039056
15.58%
(14.539918)
(1.56%)
3465122×
base:1326:is_molecule_forbidden
8.610398
0.92%
(7.262205)
(0.78%)
352897×
groups:111:get_reaction_template
37.297201
3.98%
(0.648569)
(0.07%)
58815×
Graph:45:from_edges
43.004641
4.59%
(3.170506)
(0.34%)
932481×
thermo:2143:compute_group_additivity_thermo
16.173878
1.73%
(0.296793)
(0.03%)
1212×
<__array_function__ internals>:2:sum
11.325929
1.21%
(0.830314999999999999)
(0.09%)
1330270×
<__array_function__ internals>:2:zeros_like
17.5887
1.88%
(1.465663)
(0.16%)
2920484×
fragment:466:detect_cutting_label
152.382756
16.26%
(86.851806)
(9.29%)
5134006×
fragment:132:__init__
7.751074
0.83%
(7.751074)
(0.83%)
5134006×
representer:85:represent_sequence
21.173118
2.26%
(2.643878)
(0.28%)
293974×
representer:103:represent_mapping
21.179591
2.26%
(2.144314)
(0.23%)
303422×
emitter:111:emit
120.67432
12.88%
(6.109407999999999)
(0.65%)
4063066×
copy:132:deepcopy
23.515099
2.51%
(10.060251)
(1.08%)
9646441×
Graph:81:add_edge
38.936901999999996
4.15%
(17.197692)
(1.84%)
8649873×
thermo:2433:_add_ring_correction_thermo_data_from_tree
7.934328
0.85%
(0.017824)
(0.00%)
798×
thermo:2535:_add_group_thermo_data
9.95229
1.06%
(0.412475)
(0.04%)
49586×
~:0:<built-in method numpy.core._multiarray_umath.implement_array_function>
27.589221999999998
2.94%
(7.658558999999999995)
(0.82%)
10426094×
<frozen importlib:1009:_handle_fromlist
11.74648
1.25%
(2.783)
(0.30%)
9063574×
~:0:<method 'append' of 'list' objects>
41.916042999999995
4.47%
(41.916042999999995)
(4.48%)
623673285×
re:227:finditer
11.113560999999999
1.19%
(2.650125)
(0.28%)
5134006×
emitter:392:expect_first_block_mapping_key
10.725526
1.14%
(0.158862)
(0.02%)
303286×
emitter:373:expect_first_block_sequence_item
9.115171
0.97%
(0.14196)
(0.02%)
293973×
emitter:409:expect_block_mapping_simple_value
29.95684
3.20%
(1.404113)
(0.15%)
1335896×
copy:237:_deepcopy_dict
12.612808
1.35%
(4.870977)
(0.52%)
2949366×
base:1026:descend_tree
50.336124999999996
5.37%
(2.122249999999999997)
(0.23%)
630751×
fromnumeric:2123:sum
9.535601
1.02%
(1.674497)
(0.18%)
1330270×
numeric:76:zeros_like
14.418391999999999
1.54%
(3.091266999999999998)
(0.33%)
2920484×
~:0:<built-in method builtins.hasattr>
9.201286
0.98%
(9.201286)
(0.98%)
10446899×
emitter:395:expect_block_mapping_key
48.632543999999996
5.19%
(2.518615)
(0.27%)
1639182×
emitter:376:expect_block_sequence_item
23.50114
2.51%
(1.509259)
(0.16%)
1087166×
re:273:_compile
9.232979
0.99%
(6.420081)
(0.69%)
11886789×
emitter:120:need_more_events
10.043768
1.07%
(4.40393)
(0.47%)
8126132×
emitter:437:check_simple_key
25.029776
2.67%
(4.373367)
(0.47%)
1335896×
emitter:232:expect_node
63.326403
6.76%
(6.865367)
(0.73%)
3465122×
base:943:match_node_to_structure
48.006907999999996
5.12%
(41.834123999999996)
(4.47%)
4544585×
fromnumeric:69:_wrapreduction
7.62463
0.81%
(2.299782)
(0.25%)
1343326×
Graph:75:_add_or_get_node_index
15.438336999999999
1.65%
(13.546305)
(1.45%)
17299746×
~:0:<built-in method builtins.isinstance>
16.504400999999998
1.76%
(16.483743)
(1.76%)
139232906×
emitter:580:prepare_tag
8.93733
0.95%
(6.233649)
(0.67%)
1335896×
emitter:469:process_tag
24.571612
2.62%
(3.314556999999999998)
(0.35%)
3465122×
emitter:266:expect_scalar
28.352214999999998
3.03%
(3.440442)
(0.37%)
2867726×
emitter:494:choose_scalar_style
20.945742
2.24%
(3.867893)
(0.41%)
2867726×
emitter:515:process_scalar
22.295928
2.38%
(2.919438999999999997)
(0.31%)
2867726×
emitter:626:analyze_scalar
27.867570999999998
2.97%
(22.118354)
(2.37%)
2867726×
emitter:1080:write_plain
17.298158
1.85%
(13.153391)
(1.41%)
2663825×
~:0:<built-in method builtins.len>
9.93009
1.06%
(9.930053)
(1.06%)
146178504×