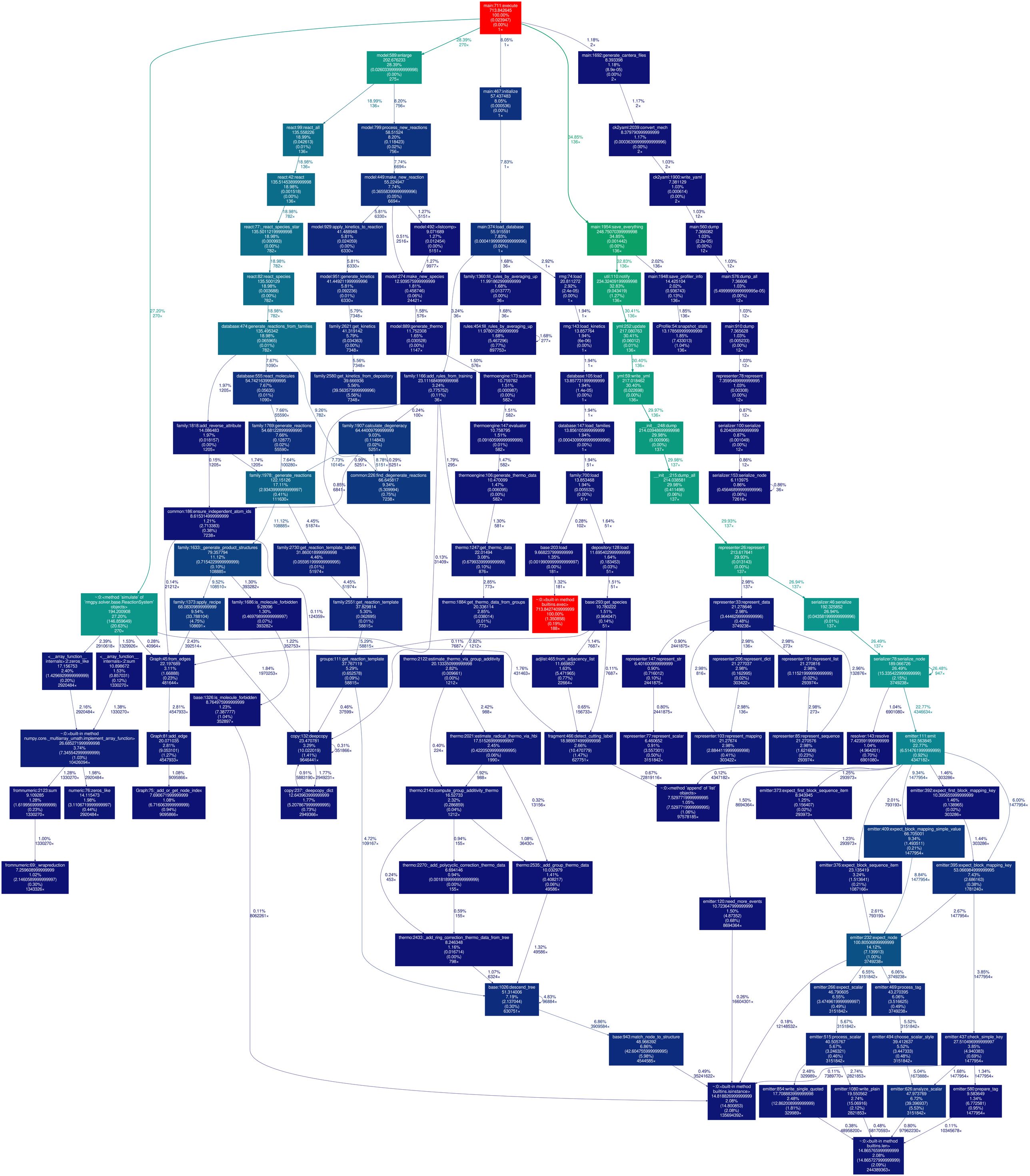
main:711:execute
713.842645
100.00%
(0.023947)
(0.00%)
1×
model:589:enlarge
202.676233
28.39%
(0.026033999999999998)
(0.00%)
275×
main:467:initialize
57.437483
8.05%
(0.000536)
(0.00%)
1×
main:1692:generate_cantera_files
8.393398
1.18%
(8.9e-05)
(0.00%)
2×
ck2yaml:2039:convert_mech
8.379790999999999
1.17%
(0.00036399999999999996)
(0.00%)
2×
ck2yaml:1900:write_yaml
7.381129
1.03%
(0.000614)
(0.00%)
2×
main:560:dump
7.366082
1.03%
(2.2e-05)
(0.00%)
12×
main:576:dump_all
7.36606
1.03%
(5.4999999999999995e-05)
(0.00%)
12×
main:910:dump
7.365628
1.03%
(0.005233)
(0.00%)
12×
representer:78:represent
7.3595489999999995
1.03%
(0.00308)
(0.00%)
12×
serializer:100:serialize
6.204085999999999
0.87%
(0.001049)
(0.00%)
12×
serializer:153:serialize_node
6.113975
0.86%
(0.45646899999999996)
(0.06%)
72616×
main:1954:save_everything
248.75070399999998
34.85%
(0.001442)
(0.00%)
136×
main:1948:save_profiler_info
14.425104
2.02%
(0.936743)
(0.13%)
136×
util:110:notify
234.32409199999998
32.83%
(9.043419)
(1.27%)
136×
rmg:74:load
20.811272
2.92%
(2.4e-05)
(0.00%)
1×
main:374:load_database
55.915591
7.83%
(0.00041999999999999996)
(0.00%)
1×
model:492:<listcomp>
9.071689
1.27%
(0.012454)
(0.00%)
5151×
model:929:apply_kinetics_to_reaction
41.488948
5.81%
(0.024059)
(0.00%)
6330×
model:449:make_new_reaction
55.224947
7.74%
(0.36558399999999996)
(0.05%)
6694×
model:799:process_new_reactions
58.51524
8.20%
(0.118423)
(0.02%)
756×
react:99:react_all
135.558226
18.99%
(0.042613)
(0.01%)
136×
react:42:react
135.51453899999998
18.98%
(0.001518)
(0.00%)
136×
react:77:_react_species_star
135.50112199999998
18.98%
(0.000993)
(0.00%)
782×
react:82:react_species
135.500129
18.98%
(0.003688)
(0.00%)
782×
model:951:generate_kinetics
41.449211999999996
5.81%
(0.092236)
(0.01%)
6330×
model:274:make_new_species
12.939575999999999
1.81%
(0.458746)
(0.06%)
24421×
family:1360:fill_rules_by_averaging_up
11.991862999999999
1.68%
(0.013777)
(0.00%)
36×
database:474:generate_reactions_from_families
135.495342
18.98%
(0.065965)
(0.01%)
782×
family:2621:get_kinetics
41.319142
5.79%
(0.034363)
(0.00%)
7348×
model:889:generate_thermo
11.752308
1.65%
(0.030528)
(0.00%)
1147×
rules:454:fill_rules_by_averaging_up
11.978012999999999
1.68%
(5.467296)
(0.77%)
897753×
rmg:143:load_kinetics
13.857764
1.94%
(6e-06)
(0.00%)
1×
yml:252:update
217.080763
30.41%
(0.06012)
(0.01%)
136×
cProfile:54:snapshot_stats
13.178569999999999
1.85%
(7.433013)
(1.04%)
136×
database:555:react_molecules
54.74216399999995
7.67%
(0.05635)
(0.01%)
1090×
family:2580:get_kinetics_from_depository
39.666936
5.56%
(39.56357399999996)
(5.56%)
7348×
family:1166:add_rules_from_training
23.111684999999998
3.24%
(0.775752)
(0.11%)
36×
thermoengine:173:submit
10.759782
1.51%
(0.000987)
(0.00%)
582×
database:105:load
13.857731999999999
1.94%
(1.4e-05)
(0.00%)
1×
yml:59:write_yml
217.018462
30.40%
(0.022698)
(0.00%)
136×
family:1818:add_reverse_attribute
14.086483
1.97%
(0.018157)
(0.00%)
1205×
family:1769:generate_reactions
54.68122899999995
7.66%
(0.12877)
(0.02%)
55590×
family:1907:calculate_degeneracy
64.44009799999999
9.03%
(0.114843)
(0.02%)
5251×
thermoengine:147:evaluator
10.758795
1.51%
(0.09160599999999999)
(0.01%)
582×
database:147:load_families
13.856105999999999
1.94%
(0.00043099999999999996)
(0.00%)
1×
__init__:248:dump
214.039486999999998
29.98%
(0.000906)
(0.00%)
137×
family:1978:_generate_reactions
122.15126
17.11%
(2.9343999999999997)
(0.41%)
111630×
common:226:find_degenerate_reactions
66.645817
9.34%
(5.309994)
(0.75%)
7238×
thermoengine:106:generate_thermo_data
10.470099
1.47%
(0.006095)
(0.00%)
582×
family:700:load
13.853468
1.94%
(0.005532)
(0.00%)
51×
__init__:215:dump_all
214.038581
29.98%
(0.411498)
(0.06%)
137×
common:186:ensure_independent_atom_ids
8.615314999999999
1.21%
(2.713383)
(0.38%)
7238×
family:1633:_generate_product_structures
79.357794
11.12%
(0.71542299999999999)
(0.10%)
108885×
family:2730:get_reaction_template_labels
31.860018999999998
4.46%
(0.05595199999999999995)
(0.01%)
51974×
thermo:1247:get_thermo_data
22.01494
3.08%
(0.67993399999999999)
(0.10%)
876×
base:203:load
9.668237999999999
1.35%
(0.00199099999999999997)
(0.00%)
181×
depository:128:load
11.695402999999999
1.64%
(0.183453)
(0.03%)
51×
representer:26:represent
213.617641
29.93%
(0.013143)
(0.00%)
137×
~:0:<method 'simulate' of 'rmgpy.solver.base.ReactionSystem' objects>
194.200908
27.20%
(146.859649)
(20.63%)
270×
family:1373:apply_recipe
68.08309899999999
9.54%
(33.788104)
(4.75%)
108691×
family:1686:is_molecule_forbidden
9.28096
1.30%
(0.46979899999999997)
(0.07%)
393282×
family:2551:get_reaction_template
37.829814
5.30%
(0.062695)
(0.01%)
58815×
thermo:1884:get_thermo_data_from_groups
20.336114
2.85%
(0.038014)
(0.01%)
773×
~:0:<built-in method builtins.exec>
713.8427409999999
100.00%
(1.350858)
(0.19%)
188×
base:293:get_species
10.780222
1.51%
(0.964047)
(0.14%)
51×
representer:33:represent_data
21.278646
2.98%
(3.4446299999999996)
(0.48%)
3749238×
serializer:46:serialize
192.325852
26.94%
(0.043581999999999996)
(0.01%)
137×
<__array_function__ internals>:2:zeros_like
17.156753
2.40%
(1.4296929999999999)
(0.20%)
2920484×
<__array_function__ internals>:2:sum
10.898672
1.53%
(0.857031)
(0.12%)
1330270×
Graph:45:from_edges
22.197689
3.11%
(1.66888)
(0.23%)
481644×
groups:111:get_reaction_template
37.767119
5.29%
(0.652578)
(0.09%)
58815×
thermo:2122:estimate_thermo_via_group_additivity
20.133350999999998
2.82%
(0.009661)
(0.00%)
1212×
adjlist:465:from_adjacency_list
11.669837
1.63%
(5.471965)
(0.77%)
22664×
representer:147:represent_str
6.401600999999999
0.90%
(0.716012)
(0.10%)
2441875×
representer:206:represent_dict
21.277037
2.98%
(0.162995)
(0.02%)
303422×
representer:191:represent_list
21.270816
2.98%
(0.11521999999999999)
(0.02%)
293974×
serializer:78:serialize_node
189.066726
26.49%
(15.335422999999999)
(2.15%)
3749238×
base:1326:is_molecule_forbidden
8.764975999999999
1.23%
(7.387777)
(1.04%)
352897×
~:0:<built-in method numpy.core._multiarray_umath.implement_array_function>
26.685271999999998
3.74%
(7.345542999999999)
(1.03%)
10426094×
Graph:81:add_edge
20.071035
2.81%
(9.053101)
(1.27%)
4547933×
copy:132:deepcopy
23.470781
3.29%
(10.022019)
(1.41%)
9646441×
thermo:2021:estimate_radical_thermo_via_hbi
17.515269999999997
2.45%
(0.42205099999999995)
(0.06%)
1990×
fragment:466:detect_cutting_label
18.989974999999998
2.66%
(10.470779)
(1.47%)
627751×
representer:77:represent_scalar
6.460652
0.91%
(3.557301)
(0.50%)
3151842×
representer:103:represent_mapping
21.27674
2.98%
(2.8844119999999998)
(0.41%)
303422×
representer:85:represent_sequence
21.270576
2.98%
(1.621608)
(0.23%)
293974×
resolver:143:resolve
7.423591999999999
1.04%
(4.964201)
(0.70%)
6901080×
emitter:111:emit
162.563845
22.77%
(6.514761999999999)
(0.92%)
4347182×
fromnumeric:2123:sum
9.109285
1.28%
(1.6199569999999999)
(0.23%)
1330270×
numeric:76:zeros_like
14.115473
1.98%
(3.1106719999999997)
(0.44%)
2920484×
Graph:75:_add_or_get_node_index
7.690671999999999
1.08%
(6.716069999999999)
(0.94%)
9095866×
copy:237:_deepcopy_dict
12.643963999999999
1.77%
(5.207867999999995)
(0.73%)
2949366×
thermo:2143:compute_group_additivity_thermo
16.52733
2.32%
(0.286859)
(0.04%)
1212×
~:0:<method 'append' of 'list' objects>
7.5297719999999995
1.05%
(7.5297719999999995)
(1.06%)
97578185×
emitter:373:expect_first_block_sequence_item
8.943945
1.25%
(0.156407)
(0.02%)
293973×
emitter:392:expect_first_block_mapping_key
10.395655999999999
1.46%
(0.138965)
(0.02%)
303286×
emitter:409:expect_block_mapping_simple_value
66.705001
9.34%
(1.493511)
(0.21%)
1477954×
fromnumeric:69:_wrapreduction
7.259608999999999
1.02%
(2.1460589999999997)
(0.30%)
1343326×
thermo:2270:_add_polycyclic_correction_thermo_data
6.694146
0.94%
(0.00181899999999999999)
(0.00%)
155×
thermo:2535:_add_group_thermo_data
10.032979
1.41%
(0.408217)
(0.06%)
49586×
emitter:376:expect_block_sequence_item
23.135419
3.24%
(1.513641)
(0.21%)
1087166×
emitter:395:expect_block_mapping_key
53.066984999999995
7.43%
(2.686163)
(0.38%)
1781240×
emitter:120:need_more_events
10.723647999999999
1.50%
(4.87352)
(0.68%)
8694364×
thermo:2433:_add_ring_correction_thermo_data_from_tree
8.246348
1.16%
(0.016714)
(0.00%)
798×
emitter:232:expect_node
100.80506899999999
14.12%
(7.139913)
(1.00%)
3749238×
base:1026:descend_tree
51.314006
7.19%
(2.137044)
(0.30%)
630751×
emitter:266:expect_scalar
46.790605
6.55%
(3.4749619999999997)
(0.49%)
3151842×
emitter:469:process_tag
43.270395
6.06%
(3.516625)
(0.49%)
3749238×
base:943:match_node_to_structure
48.966392
6.86%
(42.604755999999995)
(5.98%)
4544585×
emitter:515:process_scalar
40.505767
5.67%
(3.246321)
(0.46%)
3151842×
emitter:494:choose_scalar_style
39.412637
5.52%
(3.447333)
(0.48%)
3151842×
emitter:437:check_simple_key
27.510499999999997
3.85%
(4.940383)
(0.69%)
1477954×
~:0:<built-in method builtins.isinstance>
14.818826999999999
2.08%
(14.800853)
(2.08%)
135694392×
emitter:854:write_single_quoted
17.708883999999998
2.48%
(12.862008999999999)
(1.81%)
329989×
emitter:1080:write_plain
19.550562
2.74%
(15.06916)
(2.12%)
2821853×
emitter:626:analyze_scalar
47.973769
6.72%
(39.396937)
(5.53%)
3151842×
emitter:580:prepare_tag
9.583649
1.34%
(6.772581)
(0.95%)
1477954×
~:0:<built-in method builtins.len>
14.865765999999999
2.08%
(14.865727999999999)
(2.09%)
244389363×