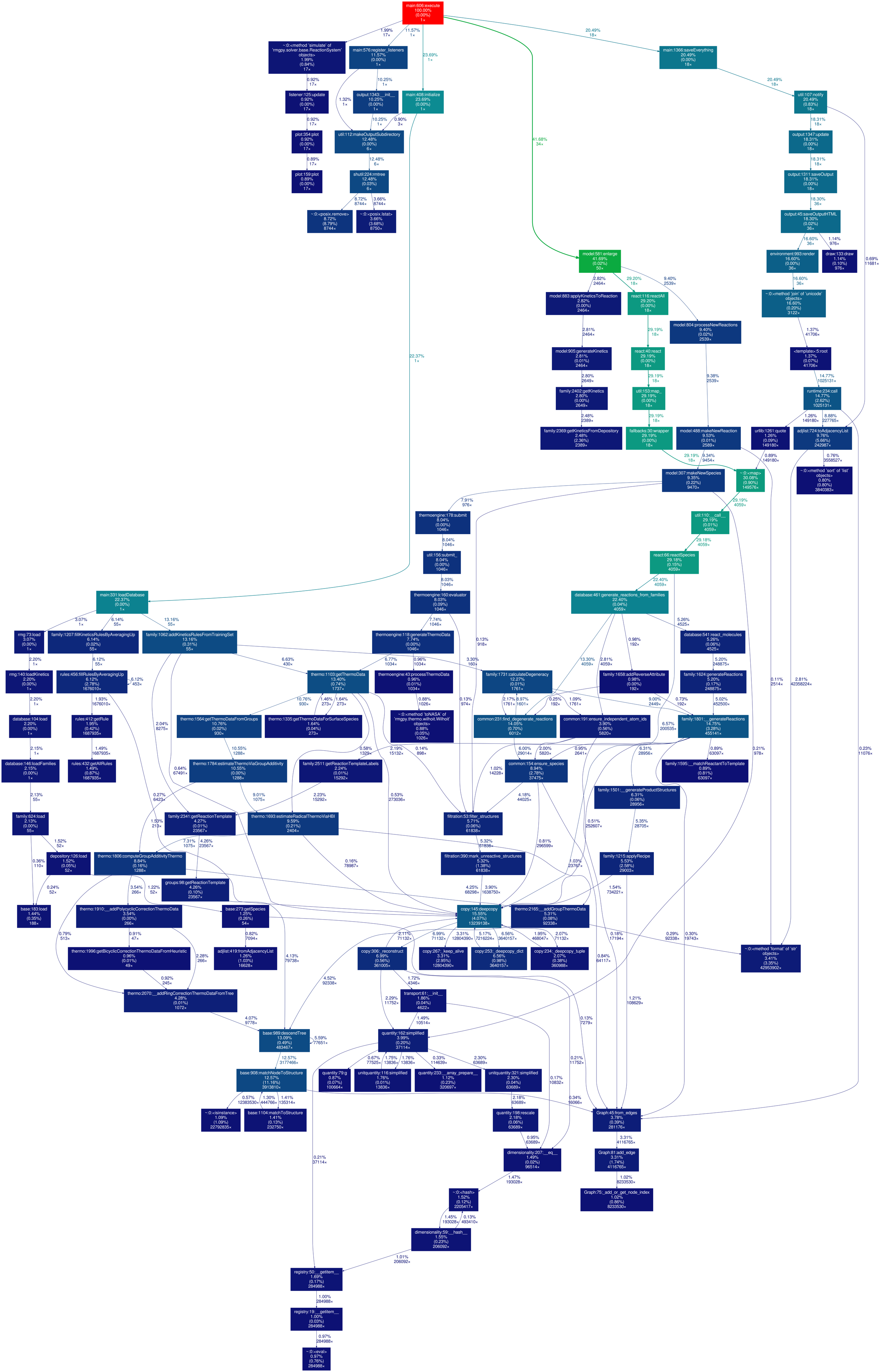
main:606:execute 100.00% (0.00%) 1×
~:0:<method 'simulate' of 'rmgpy.solver.base.ReactionSystem' objects> 1.99% (0.84%) 17×
main:576:register_listeners 11.57% (0.00%) 1×
main:1366:saveEverything 20.49% (0.00%) 18×
listener:125:update 0.92% (0.00%) 17×
output:1343:__init__ 10.25% (0.00%) 1×
main:408:initialize 23.69% (0.00%) 1×
util:107:notify 20.49% (0.83%) 18×
plot:354:plot 0.92% (0.00%) 17×
util:112:makeOutputSubdirectory 12.48% (0.00%) 6×
output:1347:update 18.31% (0.00%) 18×
plot:159:plot 0.89% (0.00%) 17×
shutil:224:rmtree 12.48% (0.03%) 6×
output:1311:saveOutput 18.31% (0.00%) 18×
~:0:<posix.remove> 8.72% (8.79%) 8744×
~:0:<posix.lstat> 3.66% (3.68%) 8750×
output:45:saveOutputHTML 18.30% (0.02%) 36×
model:581:enlarge 41.69% (0.02%) 50×
environment:993:render 16.60% (0.00%) 36×
draw:133:draw 1.14% (0.10%) 976×
model:883:applyKineticsToReaction 2.82% (0.00%) 2464×
react:116:reactAll 29.20% (0.00%) 18×
~:0:<method 'join' of 'unicode' objects> 16.60% (0.20%) 3122×
model:804:processNewReactions 9.40% (0.02%) 2539×
model:905:generateKinetics 2.81% (0.01%) 2464×
react:40:react 29.19% (0.00%) 18×
<template>:5:root 1.37% (0.07%) 41706×
family:2402:getKinetics 2.80% (0.00%) 2649×
util:153:map_ 29.19% (0.00%) 18×
runtime:234:call 14.77% (2.62%) 1025131×
family:2369:getKineticsFromDepository 2.48% (2.36%) 2389×
fallbacks:30:wrapper 29.19% (0.00%) 18×
model:488:makeNewReaction 9.53% (0.01%) 2589×
urllib:1261:quote 1.26% (0.09%) 149180×
adjlist:724:toAdjacencyList 9.76% (5.66%) 242987×
model:307:makeNewSpecies 9.35% (0.22%) 9470×
~:0:<map> 30.08% (0.90%) 149576×
~:0:<method 'sort' of 'list' objects> 0.80% (0.80%) 3840383×
thermoengine:178:submit 8.04% (0.00%) 1046×
util:110:__call__ 29.19% (0.01%) 4059×
util:156:submit_ 8.04% (0.00%) 1046×
react:66:reactSpecies 29.18% (0.15%) 4059×
main:331:loadDatabase 22.37% (0.00%) 1×
thermoengine:160:evaluator 8.03% (0.09%) 1046×
database:461:generate_reactions_from_families 22.40% (0.04%) 4059×
rmg:73:load 3.07% (0.00%) 1×
family:1207:fillKineticsRulesByAveragingUp 6.14% (0.02%) 55×
family:1062:addKineticsRulesFromTrainingSet 13.16% (0.31%) 55×
thermoengine:118:generateThermoData 7.74% (0.00%) 1046×
database:541:react_molecules 5.26% (0.06%) 4525×
rmg:140:loadKinetics 2.20% (0.00%) 1×
rules:456:fillRulesByAveragingUp 6.12% (2.78%) 1676010×
thermo:1103:getThermoData 13.40% (0.74%) 1737×
thermoengine:43:processThermoData 0.96% (0.01%) 1034×
family:1731:calculateDegeneracy 12.27% (0.01%) 1761×
family:1658:addReverseAttribute 0.98% (0.00%) 192×
family:1624:generateReactions 5.20% (0.17%) 248875×
database:104:load 2.20% (0.00%) 1×
rules:412:getRule 1.95% (0.42%) 1687935×
thermo:1564:getThermoDataFromGroups 10.76% (0.02%) 930×
thermo:1335:getThermoDataForSurfaceSpecies 1.64% (0.04%) 273×
~:0:<method 'toNASA' of 'rmgpy.thermo.wilhoit.Wilhoit' objects> 0.88% (0.05%) 1026×
common:231:find_degenerate_reactions 14.05% (0.70%) 6012×
common:191:ensure_independent_atom_ids 3.90% (0.56%) 5820×
family:1801:__generateReactions 14.75% (3.28%) 455141×
database:146:loadFamilies 2.15% (0.00%) 1×
rules:432:getAllRules 1.49% (0.87%) 1687935×
thermo:1784:estimateThermoViaGroupAdditivity 10.55% (0.00%) 1288×
family:2511:getReactionTemplateLabels 2.24% (0.01%) 15292×
common:154:ensure_species 8.94% (2.78%) 37475×
family:1595:__matchReactantToTemplate 0.89% (0.81%) 63097×
family:1501:__generateProductStructures 6.31% (0.06%) 28956×
family:624:load 2.13% (0.00%) 55×
family:2341:getReactionTemplate 4.27% (0.01%) 23567×
thermo:1693:estimateRadicalThermoViaHBI 9.59% (0.21%) 2404×
filtration:53:filter_structures 5.71% (0.06%) 61838×
depository:126:load 1.52% (0.05%) 52×
thermo:1806:computeGroupAdditivityThermo 8.84% (0.16%) 1288×
filtration:390:mark_unreactive_structures 5.32% (1.38%) 61838×
family:1215:applyRecipe 5.53% (2.58%) 29003×
groups:98:getReactionTemplate 4.26% (0.10%) 23567×
base:183:load 1.44% (0.35%) 188×
thermo:1910:__addPolycyclicCorrectionThermoData 3.54% (0.00%) 266×
base:273:getSpecies 1.25% (0.26%) 54×
copy:145:deepcopy 15.55% (4.07%) 13239138×
thermo:2165:__addGroupThermoData 5.31% (0.08%) 92338×
~:0:<method 'format' of 'str' objects> 3.41% (3.35%) 42953902×
thermo:1996:getBicyclicCorrectionThermoDataFromHeuristic 0.96% (0.01%) 49×
adjlist:419:fromAdjacencyList 1.26% (1.03%) 16628×
copy:306:_reconstruct 6.99% (0.56%) 361005×
copy:267:_keep_alive 3.31% (2.95%) 12804390×
copy:253:_deepcopy_dict 6.56% (0.98%) 3640157×
copy:234:_deepcopy_tuple 2.07% (0.38%) 360988×
thermo:2070:__addRingCorrectionThermoDataFromTree 4.28% (0.01%) 1072×
transport:61:__init__ 1.86% (0.04%) 4622×
base:989:descendTree 13.09% (0.49%) 483467×
quantity:162:simplified 3.99% (0.20%) 37114×
base:908:matchNodeToStructure 12.57% (11.16%) 3913810×
quantity:79:g 0.87% (0.07%) 100664×
unitquantity:116:simplified 1.76% (0.01%) 13836×
quantity:233:__array_prepare__ 1.12% (0.23%) 320697×
unitquantity:321:simplified 2.30% (0.04%) 63689×
~:0:<isinstance> 1.09% (1.09%) 22792835×
base:1104:matchToStructure 1.41% (0.13%) 232750×
quantity:198:rescale 2.18% (0.06%) 63689×
Graph:45:from_edges 3.78% (0.39%) 281176×
dimensionality:207:__eq__ 1.49% (0.02%) 96514×
Graph:81:add_edge 3.31% (1.74%) 4116765×
~:0:<hash> 1.52% (0.12%) 2205417×
Graph:75:_add_or_get_node_index 1.02% (0.86%) 8233530×
dimensionality:59:__hash__ 1.55% (0.23%) 206092×
registry:50:__getitem__ 1.69% (0.17%) 284988×
registry:19:__getitem__ 1.00% (0.03%) 284988×
~:0:<eval> 0.97% (0.76%) 284988×