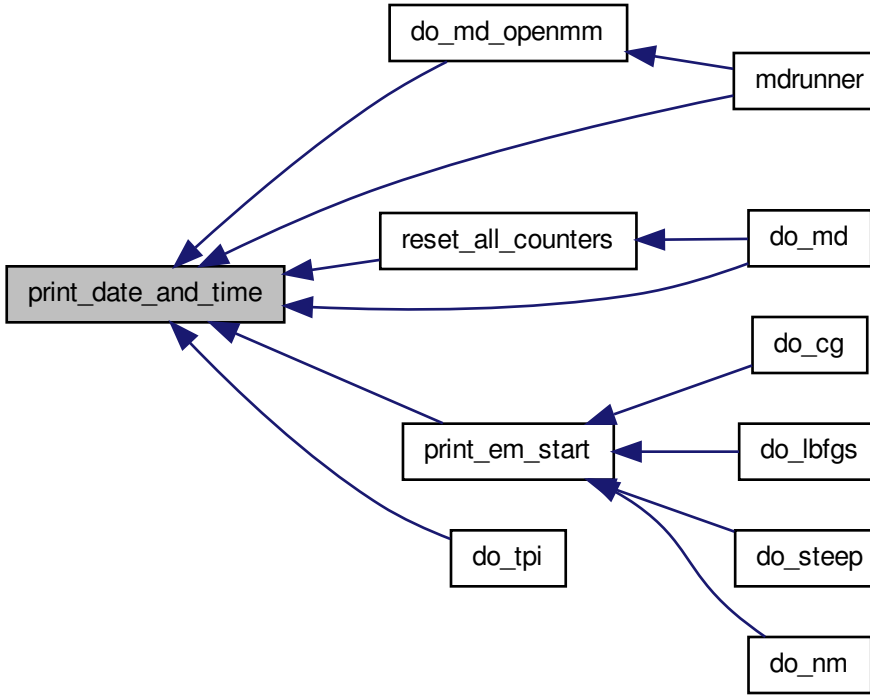
do_md_openmm
mdrunner
reset_all_counters
do_md
print_date_and_time
do_cg
print_em_start
do_lbfgs
do_tpi
do_steep
do_nm