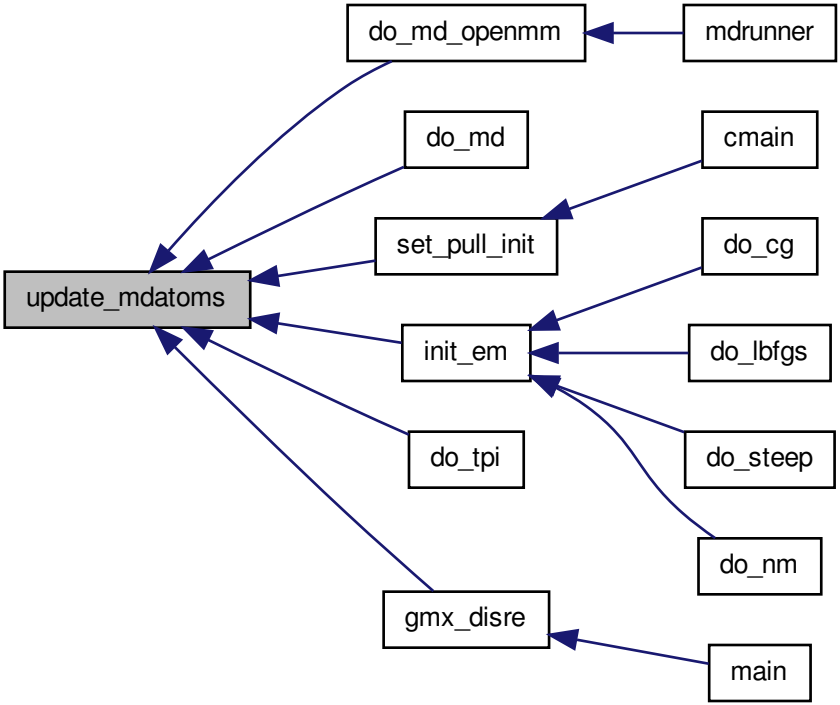
do_md_openmm
mdrunner
do_md
cmain
set_pull_init
do_cg
update_mdatoms
init_em
do_lbfgs
do_tpi
do_steep
do_nm
gmx_disre
main