Debug report CP2K

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Situating the problem

We are trying to run a QM MD simulation with the GPW-method, combined with some classical force-field like energy terms of the form $A\exp(-Br)$.

For this, we make use of the MULTIPLE_FORCE_EVALS option in CP2K. We would like to conduct the MD run in the isothermal-isobaric ensemble (NPT). Since the studied molecular systems are rather big (e.g. a methanol system of 128 molecules), it is necessary to make use of multiple computing units, i.e. run the simulation in parallel mode.

With these combinations (MULTIPLE_FORCE_EVALS, NPT, parallel), CP2K always stops after the first QM step: there is no error to be found in the output files, the CPUs keep on using memory, but no output is written anymore after the first (succesfully converged) QM step. When a canonical ensemble (NVT) is considered, the MD simulation with the MULTIPLE_FORCE_EVALS runs as it should. Note that with the combination of NPT and MULTIPLE_FORCE_EVALS, but with only one CPU (serial mode), the simulation also runs smoothly, so it is probable that this is an MPI-problem.

Situating the bug

For two cpu's.

- process 1 (P1) → goes into the function *force_env_set_cell* (integrator.F, line 1129-1130) and this function ends without error, after which P1 goes in the function *force_env_calc_energy_force* (force_env_methods.F)

  → *mixed_energy_forces* (force_env_methods.F)

  → *mp_sync* (message_passing.F) (*)

- process 2 (P2) also goes into the function *force_env_set_cell* (integrator.F, line 1129-1130), but does not end:

  → *qs_env_rebuild_pw_env* (qs_environment_methods.F)

  → *pw_env_rebuild* (pw_env_methods.F)

  → *destroy_gaussian_gridlevel* (gaussian_gridlevels.F)

  → *mp_sum_l* (message_l_passing.F). This latter happens on the same MPI-group as mp_sync of P1 (i.e. P1 and P2 are in the same MPI-group) (**). This causes a deadlock: P1 waits for P2 and vice versa.

(*) mp_sync waits until (or rather: it expects that) that P2 is at the same point (i.e. the function *mp_sync*. This is a 'barrier' that has to be crossed for CP2K to be able to continue.

(**) function *mp_sum_l* does a summation, and waits for P1 for input, but P1 is never going to send this info, because it waits for P2...

Backtraces

P1:

```
(gdb) bt
#0  0x00002aaaad1cc313 in __GI___poll (fds=<optimized out>,
    nfds=<optimized out>, timeout=<optimized out>)
    at ../sysdeps/unix/sysv/linux/poll.c:87
#1  0x00002aaaadb64ab0 in ?? () from /usr/lib/libopen-pal.so.0
#2  0x00002aaaadb638ff in ?? () from /usr/lib/libopen-pal.so.0
#3  0x00002aaaadb58221 in opal_progress () from /usr/lib/libopen-pal.so.0
#4  0x00002aaaac63e655 in ?? () from /usr/lib/libmpi.so.0
#5  0x00002aaab2fa8c94 in ?? ()
   from /usr/lib/openmpi/lib/openmpi/mca_coll_tuned.so
#6  0x00002aaaac652ee9 in PMPI_Allreduce () from /usr/lib/libmpi.so.0
```

```
#7  0x00002aaaac3f8b58 in pmpi_allreduce__ () from /usr/lib/libmpi_f77.so.0
#8  0x000000000071eed1 in message_passing::mp_sum_l (msg=50339, gid=0)
    at /home/marc/doctoraat/build/cp2k/cp2k/makefiles/../src/message_l_passing.f90:
    809
#9  0x000000000122010c in gaussian_gridlevels::destroy_gaussian_gridlevel (
    gridlevel_info=...,
    para_env=<error reading variable: Cannot access memory at address 0x0>,
    error=...)
    at /home/marc/doctoraat/build/cp2k/cp2k/makefiles/../src/gaussian_gridlevels.F:
    93
#10 0x000000000152e00a in pw_env_methods::pw_env_rebuild (pw_env=0x3e9fec0,
    qs_env=0x3e731c0,
    external_para_env=<error reading variable: Cannot access memory at
    address 0---Type <return> to continue, or q <return> to quit---bt
x0>, error=...)
    at /home/marc/doctoraat/build/cp2k/cp2k/makefiles/../src/pw_env_methods.F:226
#11 0x000000000082920b in qs_environment_methods::qs_env_rebuild_pw_env (
    qs_env=0x3e731c0, error=...)
    at /home/marc/doctoraat/build/cp2k/cp2k/makefiles/../
    src/qs_environment_methods.F:447
#12 0x000000000052f803 in force_env_types::force_env_set_cell (
    force_env=0x584a670, cell=0x3bc7a90, error=...)
    at /home/marc/doctoraat/build/cp2k/cp2k/makefiles/../src/force_env_types.F:816
#13 0x0000000000530bfa in force_env_types::force_env_set_cell (
    force_env=0x3e29190, cell=0x3bc7a90, error=...)
    at /home/marc/doctoraat/build/cp2k/cp2k/makefiles/../src/force_env_types.F:854
#14 0x00000000013c3d80 in integrator::npt_i (md_env=0x584b610,
    globenv=0x3f7ba30, error=...)
    at /home/marc/doctoraat/build/cp2k/cp2k/makefiles/../src/integrator.F:1129
#15 0x0000000000bb8202 in velocity_verlet_control::velocity_verlet (
    md_env=0x584b610, globenv=0x3f7ba30, error=...)
    at /home/marc/doctoraat/build/cp2k/cp2k/makefiles/../
    src/velocity_verlet_control.F:84
```

P2:

```
(gdb) bt
#0  0x00002aaaad1cc2d8 in __GI___poll (fds=0x24d2320, nfds=6,
    timeout=<optimized out>) at ../sysdeps/unix/sysv/linux/poll.c:83
#1  0x00002aaaadb64ab0 in ?? () from /usr/lib/libopen-pal.so.0
```

```
#2  0x00002aaaadb638ff in ?? () from /usr/lib/libopen-pal.so.0
#3  0x00002aaaadb58221 in opal_progress () from /usr/lib/libopen-pal.so.0
#4  0x00002aaaac63e655 in ?? () from /usr/lib/libmpi.so.0
#5  0x00002aaab2fa6afa in ?? ()
   from /usr/lib/openmpi/lib/openmpi/mca_coll_tuned.so
#6  0x00002aaab2fae58f in ?? ()
   from /usr/lib/openmpi/lib/openmpi/mca_coll_tuned.so
#7  0x00002aaaac6540ed in PMPI_Barrier () from /usr/lib/libmpi.so.0
#8  0x00002aaaac3f91d3 in pmpi_barrier__ () from /usr/lib/libmpi_f77.so.0
#9  0x0000000000739b62 in message_passing::mp_sync (group=0)
    at /home/marc/doctoraat/build/cp2k/cp2k/makefiles/../
    src/message_passing.F:810
#10 0x00000000005244f6 in force_env_methods::mixed_energy_forces (
    force_env=0x3e1d8d0, calculate_forces=.TRUE., error=...)
    at /home/marc/doctoraat/build/cp2k/cp2k/makefiles/../
    src/force_env_methods.F:1087
#11 0x000000000052cee0 in force_env_methods::force_env_calc_energy_force (
    force_env=0x3e1d8d0,
    calc_force=<error reading variable: Cannot access memory at address 0x0>,
    consistent_energies=<error reading variable:
    Cannot access memory at address---Type <return> to continue, or q <return> to qui
 0x0>,
    skip_external_control=<error reading variable:
    Cannot access memory at address 0x0>,
    eval_energy_forces=<error reading variable:
    Cannot access memory at address 0x0>, error=...)
    at /home/marc/doctoraat/build/cp2k/cp2k/makefiles/../
    src/force_env_methods.F:245
#12 0x00000000013c3dae in integrator::npt_i (md_env=0x3e71ce0,
    globenv=0x3b46730, error=...)
```