```
&GLOBAL
  SEED        897163
  WALLTIME    20000
  PROJECT     MD-H2O-64-RI-MP2-TZ
  RUN_TYPE    MD
  PRINT_LEVEL LOW
&END GLOBAL
&MOTION
  &MD
    &RESPA
       FREQUENCY 6
    &END RESPA
    ENSEMBLE     NVE
    STEPS        50
    TIMESTEP     1.5
    TEMPERATURE  300
  &END MD
  &PRINT
    &RESTART
      &EACH
         MD  1
      &END
    &END
    &RESTART_HISTORY
      &EACH
         MD  10
      &END
    &END
    &FORCES
      &EACH
         MD  1
      &END
    &END
    &VELOCITIES
      &EACH
         MD  1
      &END
    &END
  &END
&END MOTION
&MULTIPLE_FORCE_EVALS
  FORCE_EVAL_ORDER  2  1
  MULTIPLE_SUBSYS
&END
                    ⋮
```

```
                                    ⋮
&FORCE_EVAL
  METHOD Quickstep
  &DFT
    BASIS_SET_FILE_NAME    ./BASIS
    &MGRID
      CUTOFF    290
      REL_CUTOFF 40
    &END MGRID
    &QS
      EPS_DEFAULT   1.0E-12
    &END QS
    &SCF
      SCF_GUESS RESTART
      EPS_SCF 1.0E-7
      MAX_SCF  30
      &OT
        MINIMIZER       CG
        PRECONDITIONER  FULL_SINGLE_INVERSE
      &END
      &OUTER_SCF
        EPS_SCF 1.0E-7
        MAX_SCF 2
      &END
      &PRINT
        &RESTART OFF
        &END
      &END
    &END SCF
    &XC
      &XC_FUNCTIONAL
        &LIBXC
          FUNCTIONAL  XC_GGA_XC_PBE1W
        &END LIBXC
      &END XC_FUNCTIONAL
      &VDW_POTENTIAL
         POTENTIAL_TYPE PAIR_POTENTIAL
         &PAIR_POTENTIAL
            TYPE DFTD3
            R_CUTOFF 16
            D3_SCALING 1.0618  1.3371  0.2319
            PARAMETER_FILE_NAME  ./dftd3.dat
         &END
      &END
    &END XC
  &END DFT
  &SUBSYS
@INCLUDE 'input.geometry'
    &KIND H
      BASIS_SET    cc-DZ-refit
      &POTENTIAL
        1
          0.20000000  2     -4.07311634      0.68070153
        0
      &END
    &END KIND
    &KIND O
      BASIS_SET    cc-DZ-refit
      &POTENTIAL
        2 4
             0.26099935  2    -14.15180600      1.97829510
        NLCC  1
             0.252338420313492 1 44.0109866619909
        2
             0.22308282  1     18.37181432
             0.26844098  1      0.10003633
      &END
    &END KIND
  &END SUBSYS
&END FORCE_EVAL
                                    ⋮
```

```
                                    ⋮
&FORCE_EVAL
  METHOD Quickstep
  &DFT
    BASIS_SET_FILE_NAME    ./BASIS
    POTENTIAL_FILE_NAME    ./POTENTIALS
    &MGRID
      CUTOFF    500
      REL_CUTOFF 50
    &END MGRID
    &QS
      EPS_DEFAULT 1.0E-15
      EPS_PGF_ORB 1.0E-18
    &END QS
    &SCF
      SCF_GUESS RESTART
      EPS_SCF 1.0E-7
      MAX_SCF 30
      &OT
        MINIMIZER       CG
        PRECONDITIONER  FULL_SINGLE_INVERSE
      &END
      &OUTER_SCF
        EPS_SCF  1.0E-7
        MAX_SCF  2
      &END
      &PRINT
        &RESTART OFF
        &END
      &END
    &END SCF
    &XC
      &XC_FUNCTIONAL NONE
      &END XC_FUNCTIONAL
      &HF
        FRACTION  1.0
        &SCREENING
          EPS_SCHWARZ          1.0E-9
          EPS_SCHWARZ_FORCES   1.0E-9
          SCREEN_ON_INITIAL_P  FALSE
        &END SCREENING
        &INTERACTION_POTENTIAL
          POTENTIAL_TYPE TRUNCATED
          CUTOFF_RADIUS  6.0
          T_C_G_DATA     ./t_c_g.dat
        &END
        &MEMORY
          MAX_MEMORY 8000
        &END
      &END HF
      &WF_CORRELATION
        METHOD  RI_MP2_GPW
        &RI_MP2
          EPS_CANONICAL 1.0E-7
          FREE_HFX_BUFFER
        &END
        &CPHF
          EPS_CONV  1.0E-6
          MAX_ITER  50
        &END
        &WFC_GPW
          CUTOFF      300
          REL_CUTOFF  50
          EPS_FILTER  1.0E-12
          EPS_GRID    1.0E-10
        &END
        MEMORY    8000
        NUMBER_PROC  1
      &END
    &END XC
  &END DFT
  &SUBSYS
@INCLUDE 'input.geometry'
    &KIND H
      BASIS_SET          cc-TZ
      RI_AUX_BASIS_SET   RI_TZ
      POTENTIAL      GTH-HF-q1
    &END KIND
    &KIND O
      BASIS_SET          cc-TZ
      RI_AUX_BASIS_SET   RI_TZ
      POTENTIAL      GTH-HF-q6
    &END KIND
  &END SUBSYS
&END FORCE_EVAL
```

Figure 41. Input example for running an MD simulation at the RI-MP2 level using a multiple timestep scheme. See text below for more information.