in the high level function call of `tdksman()`. The parameters for RT-TDDFT calculations are parsed and stored in `tdks_desc`, then the correct type of TDKS orbital is selected by the `tdks_selector()`. The `td_ks` is pointed to either `td_ks_r` or `td_ks_u`. The proper propagator algorithm is selected in a similar way by the `propagator_selector()`, and the `propagator` is then pointed to the desired class (`euler_1st_order`, `mmut_2nd_order` , `lflppc_3rd_order` or `eppc_3rd_order`). Then set the initial state. The propagation starts and keep iterates until is done. Each class focus on their properties and functionalities. Such as in the propagator derived class `mmut_2nd_order`, it is all about the algorithm for the propagator. It does not depend on which orbital type is using, how the CAP is constructed, and which external field is selected. For future implementations of the propagator algorithms, for example, developers do not need to know how restricted/unrestricted is implemented, how CAP is integrated, or the details of which field. Other classes appeared in the propagator classes (base and derived) are the base classes that act as interfaces.

3 Manual

Fig.2.3 shows a basic RT-TDDFT job for H_2O. Fig.2.4 shows an unrestricted RT-TDDFT job for H_2O incorporate with PCM. The RT-TDDFT calculation is performed after the SCF calculation if in `$rem` section `TDKS` is set `true`. `INCFOCK` need to be `0`, and `PURECART` need to be `2222`. Below are control variables in the `$tdks` section. We provide each with their description, type and default value.

DT

the value for the time step Δt in a.u.

TYPE: double

```
$molecule
   0 1
   O  0.000000  0.000000  0.000000
   H  0.758602  0.000000  0.504284
   H  0.758602  0.000000  -0.504284
$end

$rem
   METHOD    pbe0
   BASIS     6-31G*
   TDKS      true
   INCFOCK   0
   PURECART 2222
   SCF_CONVERGENCE    7
$end

$tdks
   DT              0.05
   MAXITER         30000
   PROPAGATOR      MMUT
   FIELD_VECTOR    1 1 1
   FIELD_TYPE      delta
   FIELD_AMP       0.001
$end
```

Figure 2.3: Q-Chem basic RT-TDDFT job for H_2O.

```
$molecule
   0 1
   O  0.000000  0.000000  0.000000
   H  0.758602  0.000000  0.504284
   H  0.758602  0.000000  -0.504284
$end

$rem
   METHOD   pbe0
   BASIS    6-31G*
   TDKS     true
   INCFOCK  0
   PURECART 2222
   UNRESTRICTED       true
   SCF_CONVERGENCE    7
   SOLVENT_METHOD     PCM
$end

$pcm
   Theory          CPCM
   Method          SWIG
   Solver          Inversion
   HeavyPoints     194
   HPoints         194
   Radii           Bondi
   vdwScale        1.2
$end

$solvent
   Dielectric 78.39
$end

$tdks
   DT             0.05
   MAXITER        30000
   PROPAGATOR     MMUT
   FIELD_VECTOR   1 1 1
   FIELD_TYPE     delta
   FIELD_AMP      0.001
$end
```

Figure 2.4: Q-Chem unrestricted RT-TDDFT job for H_2O incorporate with PCM.

DEFAULT: 0.02

MAXITER

the max number of time steps.

TYPE: integer

DEFAULT: 15000

DO_CAP

include complex absorbing potential

TYPE: logical

DEFAULT: false

CAP_TYPE

the CAP type

TYPE: string

DEFAULT: atom_centered_spherical

CAP_R0

the cut off radius r_0 for CAP

TYPE: double

DEFAULT: 0

CAP_ETA

the curvature η for CAP

TYPE: double

DEFAULT: 1.0

PROPAGATOR

the propagator algorithm

TYPE: string

DEFAULT: MMUT

OPTIONS: EULER, MMUT, LFLPPC, EPPC

PC_FOCK_THRESH

the Fock matrix threshold for consistency checking in PC methods

TYPE: integer

DEFAULT: 7 (for 10^{-7})

PC_DEN_THRESH

the density matrix threshold for consistency checking in PC methods

TYPE: integer

DEFAULT: 7 (for 10^{-7})

PC_MAX_ITER

the max number of iterations for PC methods

TYPE: integer

DEFAULT: 20

FIELD_TYPE

the external field type

TYPE: string

DEFAULT: delta

OPTIONS: delta, cw, impulse, static,none

FIELD_VECTOR

the field vector for the external field

TYPE: vector with elements in double

DEFAULT: 1.0 1.0 1.0

FIELD_AMP

the external field amplitude in a.u.

TYPE: double

DEFAULT: 0.0001

FIELD_FREQUENCY

the external field frequency in e.v.

TYPE: double

DEFAULT: 0.001

FIELD_PEAK

the t_{peak} in the Gaussian envelope for impulse field (in a.u.)

TYPE: double

DEFAULT: 0.0

FIELD_TAU

the σ in the Gaussian envelope for impulse field (in a.u.)

TYPE: double

DEFAULT: 0.7