Instruction

There are in total 6 folders and one library file for the simulation code.

1. Libslatec.a
The libslatec.a file is suited for the gfortran (free fortran compiler) compiler.
If you use ifort (not free) compiler you can use libslatec.a or slatec.a library file.

Slatec is originally a fortran77 library and was later on implemented in fortran90, it contains a large amount of numerical methods for the calculation.

The relevant method for our simulation is DDERKF which Solve an initial value problem in ordinary differential using a Runge-Kutta-Fehlberg scheme.

2. input
The input folder contains three different type of files.
(1). The *.pa potential file generated by simion
This file is generated directly from simion and will be used later on by the pot2acc.for code to calculate the acceleration file. You can use other software based on the finite element method to generate the potential file from the electrodes then you should modify the pot2acc.for code
(2). The input*.dat file (for example: inputOH.dat) which defines the parameters for the simulation
This file contains a lot of parameters……
There are parameters for the potential array to be used for trajectory calculation, these parameter are not supposed to be changed!!!
Parameters for the molecules……
Parameters for the Stark decelerator……
Parameters for the molecular beam……
……
(3). The molecule and potential parameter file *.dat (for example: OH_M32_K32.dat)
This file contains three sets of parameters. The first set is for the decelerated molecules like mass (in amu), lambda-doubling (in cm-1), dipole moment (in Debye), the orientation parameter (MK/J(J+1)). The second set is for the dimensions of the potential array, which are used for the fitting of the potential to get the analytical solution. They are not supposed to be changed!!! The third set is the scaling factor for converting the units (gu) of the potential derived from simion to mm for calculation. The other factor is the scaling factor of the high voltage applied on the electrode to 10kV.

3. pot2acc
In this folder there is the pot2acc.for file which is used for the acceleration calculation. The code is based on the readpa.for written by Hendrik. L. Bethlem to read the potential value from the .pa file.
To compile this code:
gfortran –o2 pot2acc.for ../libslatec.a –o pot2acc.exe
To run the code:
./pot2acc.exe –i1 ../input/decel10kV.pa –i2
../input/OH_M32_K32.dat
then you will get the acceleration files in the output folder.

4. timeseq
In this folder you have the timeseq.for code file which is used to calculate the time sequence to switch the high voltage on the electrodes.
To compile:
gfortran –o2 timeseq.for ../libslatec.a –o timeseq.exe
To run:
./timeseq.exe –i ../input/inputOH.dat
After running, you get two files in the output folder. The first one is called T2jump.out. This file can be sent directly to the pulse generator to generate the trigger pulses for the switches. The second file is called T2jump.dat, in this file you will find the detailed information about the velocities, energies and timings at each switching point. It is useful to for checking, like the final velocity and so ever.

5. fly
In this folder, there is the fly.for code file which is used to run the fully trajectory simulation for a bunch of molecules.
To compile:
gfortran –o2 fly.for ../libslatec.a –o fly.exe
To run:
./fly.exe –i1 ../input/inputOH.dat –i2 ../output/T2jump.out
You will get the phase space distribution after the decelerator and the data are stored in the output folder in the file called ff.dat.