Introduction to Full Multiple Spawning using MOPAC

Todd J. Martínez

August 11, 2006

The Full Multiple Spawning (FMS) code calculates the nuclear dynamics using electronic energies and gradients calculated on the fly, in this case using a development version of MOPAC.

The following input files are required:
Control.dat (provides the control values and sets up the dynamics calculation)
Geometry.dat (provides the geometry at the ground state minimum)
Frequencies.dat (provides the normal modes at the ground state minimum)
ethylene.dat (MOPAC input file with key words for the electronic structure calculations)
set5 (needed if using a customized parameter set)

Make a directory for the first dynamics simulation in which we will excite ethylene to S_1 and then watch the dynamics for 500 fs. For this simulation we will be using the standard PM3 parameter set.

Copy these files from the following directory:
~train18/martinez/Tests/PM3

Run the dynamics code using the following command:
~train18/FMS/FMSMopacAmber.e >& FMS.out &

The job should take a few minutes or less. Once the job is complete you will have many more files in your directory that provide all the information about the run. The first column is usually time in atomic units. Here are a few of the more important ones:

Traj.*x* (*x* is the trajectory number)	Includes the position, momentum, population and state of the x^{th} trajectory at each timestep
E.dat	Provides the classical and QM energies at each time
N.dat	Provides the population on each state as well as the total population
Traj.*x*I	Gives the energy of each electronic state along this trajectory
Coup.*x*	Provides the value of the non-adiabatic coupling between the given trajectory and the other electronic states in the calculation
Spawn.*x*	Gives the geometry at which the x^{th} trajectory spawned

To look at the behavior of each trajectory, create a movie file by using the command:
~train18/FMS/trajtoxyz
and enter the number of the trajectory to convert. It will make a file Traj.*x*.xyz from the Traj.*x* file that includes a geometry every fs in the calculation. You can visualize this movie using molden or vmd.

You might want to plot some of the following information to analyze the dynamics run in gnuplot.

plot 'N.dat' u 1:2	(Shows the population of the ground state as a function of time)
plot 'N.dat' u 1:3	(Shows the population of the excited state as a function of time)
plot 'Traj.*x*' u 1:41	(Shows the population of trajectory *x* as a function of time)
plot 'Traj.*x*I' u 1:4	(Shows the energy gap between the ground and excited state for trajectory *x* as a function of time)
plot 'Coup.*x*' u 1:2	(Shows the non-adiabatic coupling between trajectory *x* and the ground state as a function of time. If trajectory *x* is on the ground state this value will always be zero.)
plot 'Coup.*x*' u 1:3	(Shows the non-adiabatic coupling between trajectory *x* and the excited state as a function of time. If trajectory *x* is on the excited state this value will always be zero.)

You might want to try to plot some of these on top of each other using.

Now make a new directory for the second dynamics simulation in which we will excite ethylene to S_1 and then watch the dynamics for 500 fs. For this simulation we will be using a reoptimized parameter set for the C atoms.

Copy these files from the following directory:
~train18/martinez/Tests/Reopt1

Run the dynamics code using the following command:
~train18/FMS/FMSMopacAmber.e >& FMS.out &

Analyze this dynamics run as you did the previous.
What do you notice is different?