In order to generate and visualize the transition densities of a particular state, you have to run the mdM_th program (the same that you use for NAESMD) choosing as initial state the one you want to calculate (X=1,2, and so) but with 0 steps and the option 1 in the line of "write view files to generate cubes" in the input.ceon file.

If you run mdM_th in that way, you will generate a file view-0000-000X.DATA, being X the number of the singlet excited state Sx.

Once you have these files view-0000X.DATA for all the X states you want to analyze, you need to modify them. First, you have to make a cont1 file with the list of files (view-0000-000X.DATA) but without the end .DATA. See attached an example.

After that, you have to execute the file ./correr, that it is an script that build the .cube files using a small fortran program cubemain.f and then you have to compress them (because the .cube files could be very large) using a c program, trimcube.c

So, in that way you generate the *.cube files that can be visualize using VMD.

Open VMD, file → new molecule and in the browse rea done of the view0000-00XX.cube that you have generated and push load.

After thatm in the Main window go to Graphics → Representations.

There, choose CPK in "Drawing Method".

Then press "Create Rep" (Up) and below "Drawing Method" choose Isosurface. You are going to se a grid. Down on the right, at Show, choose only "Isosurface" (without Box).

Then, also Down at the right, in "Draw" choose "Solid surface".

Then, you have to see the slider that say "Isovalue". Move it more or less to -0.02 aprox and in "Coloring Method", here it says "Name" choose "ColorID", the 0 is the blue.

Then, press again "Create Rep" (Up), and change the color to 1. And where it said "isovalue" change the sign "-" by "+" (you have top ut the cursor inside the box with the number) and press enter.

If you want to change the iscontorn, you can chage the small number at "isovalue". For example, +0.002 and -0.002 makes everything bigger respect to +0.02 y -0.02. In order to change these values you always have to select the corresponding "Rep", that is, look that you have 3 Rep: CPK, Isosurface with ColorID 0 and Isosurface with ColorID 1, so, for example, in order to change the Isovalue of -0.02 to -0.002, you first have to select the Isosurface with ColorID 0. I hope you understand that, otherwise…, just ask!

The idea is to visualize the differen transition densities of the different SX states in order to see where they are spatially localized. The pictures can be saved using Main →File→Render…and there you have to choose the Browse saving the file with .bmp extension.