This program is very similar to the original SOP program in terms of setup and running, there are just a few extra parameters to define.

1 - In the “def_param.h” file, you can set the fixed_beads and pulled_bead (which determines the pulling vector), as well as the integration time step (h), eH, deltax, R_limits and spring constants.

Lines 40 t0 54 are the parameters that define the interaction between the protein and the nucleotide. Line 50 is the eH for this interaction (0.2 for Hsp70). On line 54, you need to define the number of residues in the protein, as the program will count the nucleotide as a second chain starting where the protein chain stops. On line 55 you need to define the type of nucleotide you want to model. 0 = rigid/static, 1 = normal, 2 = rigid but COM moves. 2 is the standard option for Hsp70.

2 - In the protein pdb file, after the protein chain atoms are listed, you need to include the nucleotide coordinates. Each atom needs to be listed as a “CA” type atom. Additionally, each atom needs to be listed as a valid amino acid type, “VAL” or similar. The chain label should be different than the protein chain label, and the atom and residue numbers need to go in order. See example below.

Atom Number (column 2)
| Atom Type (3)
| | Amino Acid Type (4)
| | | chain label (5)
| | | | Amino Acid Number (6) X, Y, Z coordinates (columns 7-9)
| | | | | |

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ATOM   2894  N   THR A 383      86.461  93.710  98.574  1.00 78.54           N
ATOM   2895  CA  THR A 383      85.604  94.293  97.553  1.00 81.73           C
ATOM   2896  C   THR A 383      84.127  94.147  97.920  1.00 87.92           C
ATOM   2897  O   THR A 383      83.321  95.042  97.667  1.00 93.10           O
ATOM   2898  CB  THR A 383      85.868  93.675  96.165  1.00 79.19           C
ATOM   2899  OG1 THR A 383      85.939  92.252  96.276  1.00 78.83           O
ATOM   2900  CG2 THR A 383      87.176  94.194  95.589  1.00 72.24           C
ATOM   2901  N   GLY A 384      83.789  93.014  98.524  1.00 86.36           N
ATOM   2902  CA  GLY A 384      82.421  92.718  98.896  1.00 77.50           C
ATOM   2903  C   GLY A 384      81.921  91.470  98.200  1.00 79.55           C
ATOM   2904  O   GLY A 384      80.842  90.970  98.498  1.00 96.10           O
ATOM   2905  CA  VAL D 385     107.345  78.748 100.059  1.00 29.94           P
ATOM   2906  CA  VAL D 386     105.874  79.100 100.230  1.00 26.91           O
ATOM   2907  CA  VAL D 387     107.966  79.197  98.771  1.00 21.55           O
ATOM   2908  CA  VAL D 388     108.314  79.192 101.283  1.00 27.47           O
ATOM   2909  CA  VAL D 389     106.758  76.040  99.541  1.00 36.86           P
ATOM   2910  CA  VAL D 390     105.484  75.859 100.294  1.00 37.56           O
ATOM   2911  CA  VAL D 391     106.688  76.306  98.061  1.00 42.90           O
ATOM   2912  CA  VAL D 392     107.624  77.172 100.297  1.00 29.89           O
ATOM   2913  CA  VAL D 393     107.794  74.840  99.809  1.00 33.13           O
ATOM   2914  CA  VAL D 394     109.022  74.729  99.085  1.00 25.69           C
ATOM   2915  CA  VAL D 395     109.990  73.959  99.974  1.00 25.89           C
ATOM   2916  CA  VAL D 396     109.443  72.652 100.191  1.00 48.19           O
ATOM   2917  CA  VAL D 397     111.342  73.754  99.346  1.00 46.64           C
ATOM   2918  CA  VAL D 398     112.273  73.658 100.427  1.00 32.55           O
ATOM   2919  CA  VAL D 399     111.189  72.397  98.690  1.00 49.75           C
ATOM   2920  CA  VAL D 400     112.432  71.743  98.448  1.00 41.64           O
ATOM   2921  CA  VAL D 401     110.353  71.666  99.718  1.00 53.18           C
ATOM   2922  CA  VAL D 402     109.631  70.546  99.086  1.00 46.97           N
```

3 - You need to obtain a contact map of your pdb file to input to the program. The "get_contacts_PDB_nucl.c" gives the command to make the executable "run_contacts". This produces four files, "Contact_map_" for the inter- and intra-chain contacts. There are two of each, one with backbone only contacts (labeled "b") and one with backbone and side-chain contacts (labeled "sc_and_b"). To get the correct contacts for the program, you need to cat the inter and intra-chain backbone only contact files into one file. This is the file you will pass to the SOP program when running. If using a different version of the contact program, just be sure that your file contains the correct contacts (inter and intra-chain, backbone only), the output formats are pretty standard (exception: compare contacts program output has an extra column).

4 - The pbs script is set up the same as for a normal SOP run, with the compile and run commands the same, only using the SOP-nucleotide program files. The run command is:

./run_protein_Fene <pdb_file>.pdb <Contacts_file> <run_number>

5 - The output file you will want to use for plotting the force vs. extension curve is the "out<pdb_file>_<k_trans>_<deltax>_<h>.dat". Column 3 is the extension in A, column 4 is the force (*70 to convert to pN). The other file ends in "_d.dat", which Ji Young programed to print, not sure what's in this file exactly.