Comments for TWEEZ13E simulation

This folder contains source code, data files and compiler tools for the Brownian dynamics simulation of an optical trap. The code is written using Borland Turbo-Pascal, so it must be compiled and run on a 32-bit computer capable of running in MS-DOS mode. Any PC computer with Microsoft-XP usually works OK. Place the entire folder including all files on the desktop. Then there are 2 ways to run the simulation. Either click on the pre-compiled application file TWEEZ13E or else click on the application TPX which launches the Pascal compiler and loads the simulation source code. You may need to pull down the FILE menu, select OPEN and choose file TWEEZ13E.PAS. Then you can see the source code, edit it and re-compile. When the simulation is running you will be asked to select a DNA sequence by entering a genome name. Ten such sequences are provided in the GENOME sub-folder. For example, if you wished to load the lambda-phage sequence you would enter the word LAMBDA. Note such sequences are always read from the 5' end of a single strand so your LAMBDA hairpin will start near the left end of lambda and run toward the right. If you want to start at the opposite end of the genome with the opposite orientation, you must create a separate file by inverting the base sequence order and complimenting each base. For instance, the file named REVLAM will make a hairpin starting near the right end of lambda and running toward the left. Next specify how far into the file to start your hairpin (maybe a restriction site location) and finally specify the length of the hairpin (maybe size of a restriction fragment). Suppose you want to unzip a hairpin cut from the right end of lambda by BamH1 restriction enzyme. Then enter text as follows:

Choose genome REVLAM
Starting where? 1
Hairpin length? 6770

After selecting a sequence, a screen should appear with a blue cross, a wiggly green line, and a text label 'm = menu'. Press the M key to see the menu of various functions. Then, for example, press the R key and a "Readings" window will open with current variable values. Press the B key and see a picture of the trap bead and the pipette bead positions. Press the right-arrow key and see the pipette bead move to the right away from the trap position. Also see the wiggly green line starts to climb and the <avForce> variable start to increase in the readings window. Continue pushing the right-arrow key until the force passes ~18 pN and then you will see the force drop suddenly when the hairpin starts to rip open. Now press the F7 key in order to automate the pulling process and record data at simulated temperatures. Now you must answer some questions. Suppose you want to pull at 3 evenly-spaced temperatures (5 deg. 25 deg. and 45 deg.) and record the results in a file called ANYNAME with 7 or fewer letters. Your entries would be as follows:

minimum temperature 5
maximum temperature 45
temperature increment 20
maximum force (pN) 50
minimum force (pN) 5
pull rate (nm/sec) 100
file name ANYNAME

This simulation takes ~10 hours to run and writes 3 files into the OUTPUT sub-folder, one file for each temperature, and each about 3MB in size. To speed things up I suggest turning off the readings window and turning off the pipette-bead display and using a smaller hairpin, say 1000 bp. Then it will take under 2 hrs for the simulation and make smaller output files. Also, turn off the power-save options in the XP control panel if you want the simulation to continue running for hours unattended. Push the letter Q to quit the program anytime.

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