Grishchuk Lab
https://www.med.upenn.edu/grishchuklab/
January 2016

Software 2. Molecular-mechanical model of the dynamic microtubule.
(Zakharov et al., 2015)

Programming language: C++, OpenMP library.

Files: Constants.h, MT.cpp, Protofilament.cpp

Compilation (using Microsoft Intel compiler): icc -openmp MT.cpp Protofilament.cpp Constants.h -o MT.

Input parameters are all in the Constants.h file in order as they appear in the Table 1 (Model Parameters) with comments describing what each parameter means.

Output files: Position of i^{th} monomer in j^{th} protofilament is defined by three coordinates $(x^{ij},y^{ij},\tau^{ij})$ as described in the paper. Coordinates are written in one line in MT_coords.txt file and nucleotide states of corresponding monomers are saved in Type_mon.txt file (0 for "D"-monomers, 1 for "T"- monomers and -1 for absent subunits). Each line in both files represents one time moment. Default time period between saving is 14 ms.

One line in MT_coords.txt file consists of coordinates ordered as follows: $\{x^{i1}\},\{y^{i1}\},\{\tau^{i1}\}$, $\{x^{i2}\},\{y^{i2}\},\{\tau^{i2}\},\ldots$, $\{x^{ij}\},\{y^{ij}\},\{\tau^{ij}\}$, … ,$\{x^{iN}\},\{y^{iN}\},\{\tau^{iN}\}$, where $\{a^{i1}\}\equiv\{a^{i1}\}|_{i=1,2,..,50}$. Corresponding line in the Type_mon.txt file consists of nucleotide states $\{f^{i1}\},\{f^{i2}\}$, … ,$\{f^{iN}\}$. Here N=13; i =1,2,…,49,50.