Documentation for Code to Simulate AJ and FA Friction Clutch Models

Contents

I. Overview

The MATLAB (Mathworks) code in this software package can be used to simulate the AJ and FA friction clutch models that were described in Shoyer et al. 2023 (hereafter referred to as the publication). Simulations were run using MATLAB R2019b. Please refer to the publication and its supporting information (especially SI Appendix, Supplementary Note 1) for description of the model formulation, parameters, analysis, and additional background information. Additionally, refer to the publication for all citations related to the development, implementation, and validation of the models.

The code repository is organized into three sub-directories, which pertain to the AJ friction clutch model ("AJFrictionClutch"), FA friction clutch model ("FAFrictionClutch"), and the friction clutch validation configuration ("FrictionClutchValidation"). Section II of this document covers the main functions that simulate timecourses of the AJ or FA friction clutch models for a specified parameter combination. Section III of this document covers scripts that perform example parameter sweeps, analyze outputs to generate summary tables, and generate plots of the summary tables.

II. Main Functions to Simulate AJ or FA Friction Clutch Models

The functions "runSimulation_AJClutch.m" (in folder "AJFrictionClutch") and "runSimulation_FAClutch.m" (in folder "FAFrictionClutch") simulate a timecourse of the AJ or FA friction clutch model for a specified parameter combination and set of initial conditions. These parameters and initial conditions are defined in the model formulation found in the publication (SI Appendix, Supplementary Note 1). In the context of their implementation in the code, they are defined in the "INPUTS" section of the comments at the top of each function. The functions output logs of timecourse data as well as linkage state transitions. All outputs are defined in the "OUTPUTS" section of the comments at the top of each function and, for convenience, are also reproduced in the spreadsheets "Definitions_OutputVariables_AJFrictionClutch.xlsx" and "Definitions_OutputVariables_FAFrictionClutch.xlsx". Parameters for unbinding rate constants of bonds are defined in "DefineForceDepRateConstantModels_AJ.m" and "DefineForceDepRateConstantModels_FA.m", for the AJ and FA models, respectively. The unbinding rate constant models, parameters, citations, and plots of the mean lifetime

for each unbinding rate constant model with the data points from the respective single molecule paper are provided in the publication.

III. Script Packages to Perform, Analyze, and Plot Example Parameter Sweeps

Three sub-folders are set up with MATLAB scripts to (1) perform an indicated parameter sweep (simulate the clutch model for a set of parameter combinations), (2) analyze the outputs to generate time-averaged statistics from time course data (e.g. average number of engaged linkages or average total force) as well as statistics on the linkage transitions (e.g. average engaged linkage lifetime), and (3) generate plots of the summary data. The code repository is organized into three sub-directories, which pertain to the AJ friction clutch model ("AJFrictionClutch"), FA friction clutch model ("FAFrictionClutch"), and the friction clutch validation configuration ("FrictionClutchValidation").

A. Example Velocity Sweep of AJ Friction Clutch

"AJFrictionClutch" contains the following code, with commented headers providing more information. This performs a velocity sweep on the AJ Friction Clutch in various different linkage configurations (defined at the top of the first script).

1. "ParamSweep_AJFrictionClutch_Velocity.m": runs indicated parameter sweep calling "runSimulation_AJClutch.m" and "DefineForceDepRateConstantModels_AJ.m"
2. "PostProcess_AnalyzeTimescouse_AJFrictionClutch.m": analyzes the outputs to generate time-averaged statistics from timecourse data (e.g. average number of engaged linkages or average total force) as well as statistics on the linkage transitions (e.g. average engaged linkage lifetime)
3. "MakePlots_AJFrictionClutch_VelocitySweep.m": makes summary plots from the anlayzed data as well as trajectory plots of representative timecourse.

When this example parameter sweep is run, analyzed, and plotted by running the above three scripts in this sequence, summary plots and timecourses similar to those shown in the publication for the AJ Friction Clutch will be generated. Examples of these plots have been generated using the code in this package and stored in the subfolder "Example_SummaryOutputs".

B. Example Velocity Sweep of FA Friction Clutch

"FAFrictionClutch" contains the following code, with commented headers providing more information. This performs a velocity sweep on the FA Friction Clutch in various different linkage configurations (defined at the top of the first script).

1. "ParamSweep_FAFrictionClutch_Velocity.m": runs indicated parameter sweep calling "runSimulation_FAClutch.m" and "DefineForceDepRateConstantModels_FA.m"
2. "PostProcess_AnalyzeTimescouse_FAFrictionClutch.m": analyzes the outputs to generate time-averaged statistics from timecourse data (e.g. average number of engaged linkages or average total force) as well as statistics on the linkage transitions (e.g. average engaged linkage lifetime)
3. "MakePlots_FAFrictionClutch_VelocitySweep.m": makes summary plots from the anlayzed data as well as trajectory plots of representative timecourse.

When this example parameter sweep is run, analyzed, and plotted by running the above three scripts in this sequence, summary plots and timecourses similar to those shown in the publication for the FA Friction Clutch will be generated. Examples of these plots have

been generated using the code in this package and stored in the subfolder “Example_SummaryOutputs”.

C. Friction Clutch Validation: Velocity Sweep of Friction Clutch w/ Single Bond Interface

“FrictionClutchValidation” contains the following code, with commented headers providing more information. This performs a velocity sweep on the Friction Clutch in a validation configuration in which each linkage has only a single bond interface that exhibits an ideal or Bell Model slip bond characteristic.

1. “ParamSweep_AJFrictionClutch_Velocity.m”: runs indicated parameter sweep calling “runSimulation_AJClutch.m“ and “DefineForceDepRateConstantModels_AJ.m” with a modification of bond parameters to realize the validation configuration in which each linkage has only a single bond interface that exhibits an ideal or Bell Model slip bond characteristic.
2. “PostProcess_AnalyzeTimescouse_AJFrictionClutch.m”: analyzes the outputs to generate time-averaged statistics from timecourse data (e.g. average number of engaged linkages or average total force) as well as statistics on the linkage transitions (e.g. average engaged linkage lifetime)
3. “MakePlots_FrictionClutchValidation.m”: makes summary plots from the analyzed data as well as trajectory plots of representative timecourse.

When this example parameter sweep is run, analyzed, and plotted by running the above three scripts in this sequence, summary plots and timecourses similar to those shown in the publication for the Validation Friction Clutch will be generated. Examples of these plots have been generated using the code in this package and stored in the subfolder “Example_SummaryOutputs”.

IV. License and Disclaimers

Furthermore, if any errors are found during use of the code, please report them to Brenton D. Hoffman (Brenton.Hoffman@Duke.edu).