# Code and data manual

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This document contains a short manual of how to use the c code and Mathematica analysis file that Jeremy has used to obtain all data for our article on “Mechanical interplay between cell shape and actin cytoskeleton organization”. It also describes which data can be found where.

## The main folder structure

The main folder "Code" contains several different versions of the c code and corresponing Mathematica file. In the c code Jeremy has briefly written in each version what is new with respect to the previous version. The final and correct version of the code and corresponding Mathematica file and data, used for the Figures in the article, are found in the folder labelled "Bulk\_7v3".

## The simulation data

The folder "Bulk\_7v3" contains a number of subfolders and files. The simulation data is found in:

- The data for Figure 4 is found in the folder "shape8". The subfolders indicate the values of the parameters that they are named after, except for the subfolder "run" which indicates that the simulation has been performed several times with the same parameters. The final subfolders contain the following files: The file "vertex" contains the location of the cell edge, "bulk" contains the location and nematic tensor of the cell interior, "force" contains the forces on the adhesion sites, and “global” contains a number of global parameters that are defined in the C code. Here, q\_difference\_total and shape\_difference\_total are the last iterations where the nematic tensor Q and the shape of the cell change with more than some predefined value. In the case of the paper data, this is Q<0.1 and a change of one pixel. Both quantities need to be multiplied by the “period” (which stores after how many timesteps a configuration is saved) to obtain the total number of iterations. The number behind each of these names in the file name indicates the time during the simulation. The final files are labeled with a number “11”. Finally, the file whose name starts with “input” stores all the input parameters as defined in the “gcyto\_2018\_12\_18.pl” file, and the “prints.dat” contains the output of the terminal.

- The data for Figure 5 if found in the folder "shape9", which contains the same structure as “shape8”.

- The simulations of the real cell shapes, used for Figures 6 and 7, are found in folders "shape100" through "shape105", where each number represents a different experimental cell. The cell numbers correspond to the cell numbers in Wim’s database and the figs. in the paper as follows:

|  |  |  |
| --- | --- | --- |
| cell number simulations | Cell number database Wim | Displayed in figure |
| 100 | 253 | Fig. 6 |
| 101 | 258 | Fig. 7d,i,n |
| 102 | 267 | Fig. 7c,h,m |
| 103 | 303 | Fig. 7e,j,o |
| 104 | 312 | Fig. 7B,g,l |
| 105 | 792 | Fig. 7a,f,k |

The file structure is the same as described above for “shape8”, with the following exceptions: the final files are labeled with number “21”, and the final subfolder contains three more files: “exp\_border\_shape\_100\_linepoints\_65.dat” (the number 100 is an example”) contains the shape of the cell edge as extracted from the experimental data, the same file with “bulk” contains the processed, coarse-grained experimental data on the cytoskeleton, and the file with “comparison” compares the theoretical and experimental shape. These processed experimental data files are also stored together for all six cells in the subfolder “experimental” of the folder “Bulk\_7v3”.

-The experimental cell shape simulations have been performed with a range of anchoring numbers. The table below shows which anchoring number is used for each figure:

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Figure | Anchoring W | W/K (1/μm) | K/W(μm) | An |
| 6 D | 1 | 0.0141 | 70.656 | 0.333796 |
| 6e | 5 | 0.0708 | 14.1312 | 1.66898 |
| 6F | 24 | 0.3397 | 2.944 | 8.0111 |
| 7k | 18 | 0.2548 | 3.92533 | 4.41137 |
| 7l | 12 | 0.1698 | 5.888 | 4.13717 |
| 7m | 33 | 0.4671 | 2.14109 | 18.6125 |
| 7n | 13 | 0.1840 | 5.43508 | 4.57433 |
| 7o | 13 | 0.1840 | 5.43508 | 4.65224 |

In order to translate this to a dimensionless anchoring number, the area of the cells have been calculated by counting how many pixels are inside the experimental cell, multiplied by the area 0.138 micron x 0.138 micron of a pixel. A typical length scale *R* has than be extracted using the square root of this area. This has been performed in Mathematica using the notebook “calculating\_area\_and\_length\_experimental\_cells.nb”.

|  |  |  |
| --- | --- | --- |
| Figure | Area | Length scale *R* |
| 6 | 556.237 | 23.5847 |
| 7a | 299.848 | 17.3161 |
| 7b | 593.392 | 24.3596 |
| 7c | 1588.1 | 39.8509 |
| 7d | 618.111 | 24.8618 |
| 7e | 639.345 | 25.2853 |

## The experimental data

The files in the main folder “Bulk\_7v3” with names shape(#)cell(#)(bulk/border/coherency/orientation).txt contain raw experimental data from ImageJ. These files store for each pixel in the microscope image the local orientation and coherence and whether or not is part of the cell boundary and part of the cell bulk. The files in the main folder with names “coherence\_shape\_#.dat” are the coherence data where all the pixels that are not inside the cell have been assigned a value equal to zero for the coherence.

## The C code

A simulation, or a sequence of simulations, are performed by running the “gcyto” file in the terminal. The most recent version is named “gcyto\_2019\_08\_13.pl”. This file also contains the values of all input parameters. When run, this file calls on “cyto”, “cyto.C”, “cyto.h”, and “makefile”, and automatically creates new folders for storing the generated data.

## Data analysis

The data is analyzed and plotted in Mathematica. The most recent version of the analysis file is called “continuum\_simulation\_19\_02\_13.nb”. The functions that need to be used for plotting are called:

-Fig.4 (phase diagram): plotbulkorientationcolourbackgroundpaper  
  
- Fig.5 (rectangles): plotbulkorientationcolourbackgroundpaper

- fig. 6B,7f-j (coarse grained experimental data): plotbulkorientationcolourbackgroundexperimental

- - fig. 6B,7f-j (coarse grained experimental data with adhesion sites plotted): plotbulkorientationcolourbackgroundexpsimadhesions2

- fig. 6D, 6e, and 6F, and fig. 7k-o (simulated data, without circles on the adhesion sites): plotbulkorientationcolourbackgroundexpsim

- fig. 6D, 6e, and 6F, and fig. 7k-o (simulated data, the adhesion points as overlay): plotbulkorientationcolourbackgroundexpsimadhesionsonly

## Calculating Delta squared

The data containing the value of Delta squared for a given simulation is stored in the file exp\_comparison\_"shapenumber"\_linepoints\_"linepoints".dat which is stored in the lowest order maps that also contain the other run data such as bulk\_#.dat, vertex\_#.dat, etc. In Mathematica, the data is automatically plotted as a function of W/K using the function

'anchchisquaredplotshapesjackknife'.