New lattice Boltzmann simulations plan

I have developed the code to rotate the plates in the seeder file by any degrees specified as input by the user. I used matrix transformation methods to cut and reorient the matrix values based on the desired rotation. This method is different from the code developed by Dr. Hugh Daigle, which requires intrinsic knowledge of the center of each platelet in the matrix. Since the dimensions of clay particles were not changed in Dr. Daigle’s study, the centers of the platelets were hard-coded into the rotation algorithm. I could not implement this method as we constant change the matrix configuration based on input clay platelet dimensions and fluid injection.

Below are two examples for matrix rotation of a clay with input length of 20 nm (4 voxels) and aspect ratio of 20.

Example 1: Initial porosity =0.26



Implemented rotation = 20 degrees

Z-direction:

Y-direction:

X-direction:

Example 2: Initial Porosity 0.65

Rotation = 45 degrees

Z direction:

Y direction:

X direction:

I think the code works quite well. There are changes to the porosity as we rotate the sample because new layers are added to the seed matrix. The size of the seed matrix remains consistent during rotation of grains.

Using the new code, I propose running 2 sets of simulations that I think would benefit our project:

1. Analyze effect of fabric: I can think of two key ways of implementing rotation of clay platelets in our models:
   1. Develop generalized mudstone models with different initial rotations (45, 35, 25, 15, 5 degrees) and simulate compaction on them. The developed porosity-permeability trends will explicitly analyze the effect of bedding direction on horizontal and vertical permeability. This would be methodology like Daigle and Dugan, 2011.
   2. Implement a simplistic particle orientation model: Develop initial smectite, kaolinite and generalized mudstone models with rotation of 45 degrees. Reduce particle orientation (from 45 to 0 degrees) in a step wise fashion as compaction is simulated on the initial models with rotation. Thus, we will go from high porosity initial models (45 degrees grain rotation) to low porosity final models (with 0 degrees grain rotation). This methodology will help analyze the effect of increase in bedding character during compaction on vertical and horizontal permeability.

While I think both methods (a) and (b) have their merits, I don’t think conducting both of them is beneficial.

1. Analyze effect of aspect ratio: In our paper we suggest that aspect ratio is the key controlling factor for vertical permeability. I can run some simple models to test this. I propose using the length of grains corresponding to the generalized mudstone model (length of 2 micron) and changing the aspect ratios of the particles. These models will not incorporate particle rotation. I can run two test cases, developing porosity-permeability relationships during compaction:
   1. Using a high aspect ratio of 50 (this is the aspect ratio of smectite)
   2. Using a low aspect ratio of 20 (this is the aspect ratio of kaolinite)

These tests will help us to relative importance of aspect ratio vs length of clay platelets and can be presented as a new figure in our discussions section.

Let me know what you think. I can get started on proposed work #2 while we decide what is the best way to incorporate rotation in the new models.