Conclusions

Approximate Simulations of Dynamical Graph Grammars using the DGG Modeling Library

- An approximation of the exact simulation algorithm has been designed using the novel Expanded Cell Complex (ECC) and improved by making use of a semi-online match data structure with incremental updates.

- A new modeling library DGGML and a graph library YAGL have been developed.

  - The building blocks of DGGML each have their own unique contribution.

- Conducted three experiments for the CMA DGG, observing long-time behaviors of cytoskeletal network-like formation and localized alignment in the simulated array, and the approximate algorithm outperforming the exact.

- In the PCMA we explored the effects that different face shapes and boundary conditions have on local and global alignment.

  - In the case of a square face shape, we find the evidence to indicate array orientation may be multi-modal.

  - In the case of a rectangular face shape, we find that different boundary conditions may reorient the array mainly between the long and short axes.

  - The periclinal CMA DGG demonstrates the flexibility and utility of DGGML and highlights its viability to be used as a computational means of testing, screening or inventing hypotheses to explain emergent phenomena.

Future Paths

DGGML and Beyond.

- Extending the expanded cell complex to 3D.

- Including reaction diffusion equations.

- Upgrading DGGML to a compiler for the DGG language, including automatic parallelization and more sophisticated grammar analysis.

- Theoretical bounding of the commutator error.

- Mutliscale modeling and DGG meta-rules.

- As a future modeling path, we could instead simulate the top periclinal face of the cell using different domain shapes.

- More experiments can also be added with different variations of parameters and rules.

- Machine Learning DGG(ML)[2]

- And much more!