Simulation of Lipid Membrane Rupture via Cellular Automation

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ABSTRACT

Biological cell membranes consist of many organized phospholipid molecules. Rupture, i.e. the forceful opening of large area pores, in these membranes is a common form of cell damage, and irreversible rupture has been implicated in disease, e.g. muscular dystrophy. Understanding and perhaps controlling membrane pore formation would be promising not only in disease treatment and prevention, but also in applications such as gene therapy and drug delivery. Previously, only circular pores were known to form in biological membranes. However, recent experimental study of model bi-layer lipid membranes spreading on solid supports has led to the discovery of two new rupture modes: fractal and floral [1]. These modes share at least a qualitative similarity to the interaction of immiscible fluids in porous media (e.g., viscous fingering and invasion percolation).

What is poorly understood are the reasons a membrane might prefer to form one type of fracture pattern rather than another. It is hypothesized that heterogeneous mechanical pinning (i.e., adhesion) between lipid bilayers governs this preference. Unfortunately, the very small fluid volume entrapped between the layers, as well as the difficulty in controlling the number of pinning sites, poses limits on the experimental investigation of rupturing.

To investigate these different rupture morphologies, we developed a numerical model based on cellular automation (CA). A cellular automation consists of a grid of that are assigned a specific state (e.g., a 0 or 1). These states evolve through the application of a few very simple rules. Despite their simplicity, CA are able to capture a range of complex behavior, even emergent behavior, in the areas of growth, aggregation, segregation, and percolation [2]. While CA have been of particular interest to, for example, the geological science and spatial simulation communities, its application to lipid rupture mechanics is novel. Our new CA combines rules from both standard percolation models and particle-based fracture methods. We demonstrate the CA via simulations of circular, floral, and fractal morphologies and show how these can be obtained through simple alterations of pinning density and behavior.

REFERENCES

[1] Gözen, I. et al. Fractal avalanche ruptures in biological membranes. Nature Materials 9, 908-912 (2010).

[2] O'Sullivan, D. and Perry, G.L.W., Spatial Simulation: Exploring Pattern and Process, Wiley-Blackwell, 2013.