Bruce MacLennan, University of Tennessee, Knoxville, TN, USA

Mathematical Principles of Morphogenesis Applied to Nanoscale Self-Assembly

Our research is applying the mathematical principles of embryological morphogenesis to the self-assembly of complex, hierarchically structured physical systems. Current approaches to nanoscale self-assembly are limited to homogeneous or highly regular structures. On the other hand, future applications of self-assembly (such as sophisticated autonomous robots) will require the ability to assemble physical systems that are structured from the nanoscale up to the macroscale. The best example we have of such a process is morphogenesis in the developing embryo.

Our approach is to take known or hypothesized processes of biological morphogenesis, to extract their mathematical structures, and to apply them to the synthesis of artificial systems. Our goal is to develop morphogenetic algorithms that apply to very large numbers of agents (hundreds of thousands to hundreds of millions), and so we use partial differential equations (PDEs) as our primary expressive medium (as is also common in the biological morphogenesis literature). In order to accommodate the visco-elastic properties of large numbers of connected microscopic agents, we use the theoretical framework of continuum mechanics in a Lagrangian reference frame. One goal is to develop techniques that mimic or replace the fundamental morphogenetic processes described by Salazar-Ciudad, Jernvall, and Newman (2003).

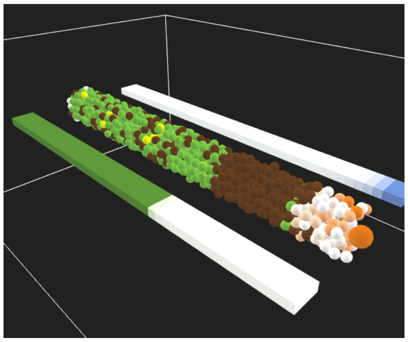

Figure 1: Clock-and-Wavefront Process

As one particular case we have extracted documented morphogenetic processes out of their biological developmental context, and applied them to the simulated synthesis of a complex structure: a segmented “spine” with a opposed pairs of segmented “legs.” To accomplish this we have applied the “clock and wavefront” process of Cooke and Zeeman (1976) to generate both the spine — which is analogous to embryological somitogenesis — but also to the generation of the legs. By controlling the parameters of the process we can independently control the number and length of the segments of both the spine and the legs. The legs grow out of imaginal disks whose placement is controlled by morphogen gradients from the anterior and posterior boundaries of the spinal segments.

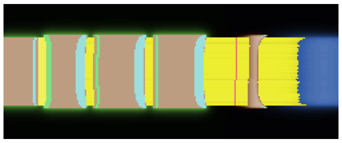

Figure 2: Development of Spine

To facilitate the description of morphogenetic processes, whether implemented by biological or artificial agents, we have developed a sort of programming language suited to the description of “tissues” composed of differing substances characterized by their properties and active behavior, defined by stochastic PDEs. The formal properties of the notation permit the equations to be implemented in a variety of physical media, both living and nonliving.

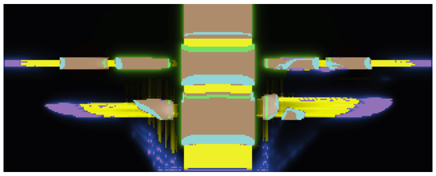

Figure 3: Development of Legs

J. Cooke, E.C. Zeeman (1976). A clock and wavefront model for control of the number of repeated structures during animal morphogenesis, *Journal of Theoretical Biology* **58**: 455–476.

I. Salazar-Ciudad, J. Jernvall, S. Newman (2003). Mechanisms of pattern formation in development and evolution, *Development* **130**: 2027–2037.