Modelling and simulation of the effect of diffusion and flow on growth processes

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Abstract

In this paper a method for modelling nutrient distributions, caused by a combination of diffusion and flow, will be discussed. The nutrient distributions are simulated using the lattice Boltzmann model of transport. From the nutrient distributions it is possible to model growth processes, which are driven by the local amount of available nutrients.

Keywords:  morphogenesis; lattice Boltzmann method; diffusion and flow limited growth

1 Introduction

In many biological systems the distribution of chemical agents and nutrients, caused by a combination of flow and diffusion, plays a fundamental role. An example is morphogenesis where the external distribution of nutrients [2], as well as the internal distribution of morphogens [6] in the organism, can induce certain growth patterns. For filter-feeding marine sessile organisms, as for example sponges, stony-corals, and hydro-corals, the growth process is strongly affected by the local availability of suspended material. In a model of the morphogenesis of an organism, in which suspension feeding represents a significant part of the energy intake, two components are relevant. The first component is a model of the growth process and the second is a model of the influence of the nutrient distribution on the local growth velocities.

In the absence of flow the distribution of nutrients around the growth form can be modelled as a diffusion process in a steady state: there is a source of suspended material and the organism consumes continuously nutrients from its environment. In general, in a marine environment, there will be a significant contribution of the hydrodynamics to the dispersion pattern of the suspended material around the growth form. In this case the distribution of nutrients around the organism will be determined by a combination of flow and diffusion. The contribution of flow to the nutrient distribution of nutrients can be quantified by the Péclet number:

\[ Pe = \frac{\bar{u}l}{D} \]  

(1)

where \( \bar{u} \) is the average flow velocity, \( l \) a characteristic length in the system, and \( D \) the diffusion coefficient. In the diffusion limited case \( Pe \) is very small (nearly zero), while in the flow dominated case \( Pe \) is large.

In this paper we will discuss a method to model a nutrient distribution determined by a combination of diffusion and flow, and we will show how this nutrient distribution can be included in a model of a growth process. The flow pattern around the growth form is modelled using the lattice Boltzmann method, this method can be combined with a tracer step, in which populations of “particles” move over the nodes of the lattice. In this tracer step the joint effect of flow and diffusion on the nutrient distribution can be studied. We will give a brief introduction to the method in section 2.1, a more detailed account of this method is given in [1] [5] [4]. This method is especially suitable for modelling diffusion and flow phenomena in biological systems. In this method boundary conditions with a complex geometry can be easily specified. The Péclet number and the Reynolds number can be varied independently [5]. In addition we can take advantage of the fact that the method is very suitable for scalable implementations on Massive Parallel Computers [7], which allows for the required large scale simulations of biological systems. The growth process is modelled using the aggregation model [8] in which growth is modelled by the addition of particles and where the growth form is represented in discrete space.
2 Methods

2.1 Modelling the nutrient distribution

In the simulations a cubic lattice is used, where each node is connected with 18 other nodes. There are 6 links with the length of one lattice unit and 12 links with the length of $\sqrt{2}$ units. All parameters and variables in the lattice Boltzmann method are expressed in lattice units. The mean populations of particles travel simultaneously from one node to one of the 18 neighbours. The evolution of the lattice is described by the following dynamical rule:

$$n_i(r + c_i, t + 1) = n_i(r, t) + \Delta_i(r, t)$$  \hspace{1cm} i = 1, ..., 18 \hspace{1cm} \hspace{1cm} (2)

where $n_i(r, t)$ is the continuous velocity distribution function, which describes the number of particles of particles at a node at position $r$, at time $t$ and with direction $c_i$. The moments of the distribution function $n_i(r, t)$:

$$\rho = \sum_i n_i$$

$$j = \sum_i n_i c_i = \rho u$$

$$\Pi = \sum_i n_i c_i c_i$$

correspond to the hydrodynamic fields mass density $\rho$, momentum density $j$ ($u$ is the flow group velocity at node $r$), and momentum flux $\Pi$.

A linearized collision operator $L_{ij}$ about an appropriate equilibrium $n^eq$ can be constructed:

$$\Delta_i(n) = \Delta_i(n^eq) + \sum_j L_{ij}(n_j - n^eq_j)$$ \hspace{1cm} \hspace{1cm} (4)

where $\Delta_i(n^eq) = 0$ by definition since the equilibrium is collision invariant, and where $n^eq$ is the Maxwell Boltzmann distribution for a gas. The distribution function can be splitted into an equilibrium and a non-equilibrium part:

$$n_i = n_i^eq + n_i^{neq} \hspace{1cm} \hspace{1cm} (5)$$

The momentums of the particles are changed by adding an external force, the driving force $F$, to the system. The particle collisions conserve mass and momentum but change the non-equilibrium part of the momentum flux:

$$\Pi^{neq} = \Pi + \Pi^eq$$ \hspace{1cm} \hspace{1cm} (6)

By using properties as conservation of mass, momentum, and symmetry, it is possible to construct a number of equations (see for a more detailed account of the collision process [5] ) for the moments of $L_{ij}$.

One computational update of the lattice now involves a propagation step where $n_i$ particles travel from node $r$ to node $r + c_i$ and a collision step in which the post-collision distribution $n_i + \Delta_i(n)$ is determined in the following three steps. First at each node $\rho$, $j$, and $\Pi$ are calculated and the equilibrium momentum flux $\Pi^eq$ is determined. In the second step the momentum flux, including the equilibrium and nonequilibrium part, can be updated using the equations constructed for the moments of the linearized collision operator $L_{ij}$. In the third step, after the post collision momentum is computed, the post-collision distribution $n_i + \Delta_i(n)$ can be calculated.
In the simulations two types of boundary conditions are used: at the borders of the lattice periodic boundary conditions are applied, while in the nodes adjacent to the nodes representing the obstacle, solid boundary conditions are used. Periodic boundary conditions can be implemented by exchanging the \( n_i \)'s of the links at the borders of the lattice. Solid boundary conditions can be represented by exchanging the \( n_i \)'s between the adjacent node and a neighbouring fluid node.

After the lattice Boltzmann iteration a tracer step is applied where populations of tracer particles are released from well defined source nodes, while the tracer particles are absorbed by the sink nodes: the nodes adjacent to the growth form. The tracer particles can move from a node at site \( r \) in the lattice to one of the 18 adjacent nodes \( r + c_i \), where the Péclet number determines if flow or diffusion dominates. In the simulations diffusion coefficient \( D \) varies, and \( \tau \) is kept constant by the adjusting the driving force \( F \) of the system. Due to the growth of the aggregate, without adjustment of the driving force, the velocity in the free fluid would gradually decrease.

### 2.2 Modelling the growth process

The growth process is modelled in a similar way as done in the Diffusion Limited Aggregation model [8]. In Fig. 1 the basic construction of the aggregate is shown. The cluster is initialized with a “seed” positioned at the bottom plane of the lattice. The bottom plane, “the substrate”, is positioned at the \( xz \)-plane at \( y = 1 \), while the seed is one lattice site, located at the position \( (z_{max}/2, 2, z_{max}/2) \). In both the cluster and substrate sites solid boundary conditions are applied. The flow in the lattice is directed from the \( yz \)-plane at \( x = 0 \) to the \( yz \)-plane at \( x = z_{max} \). The flow velocity in the free fluid nodes is kept to a constant value \( \Upsilon \). The flow pattern about the obstacle (substrate and cluster) is determined in the lattice Boltzmann iteration, followed by a tracer step. In the last step tracer particles are released from the source plane, the lattice sites in the \( xz \)-plane at \( y = y_{max} \). The tracer particles are absorbed by the nodes adjacent to the sites in the substrate plane (the \( xz \)-plane at \( y = 1 \)) and the aggregate. In the sink nodes the amount of absorbed tracer particles is determined and a new node is added to the cluster. The probability \( p \) that \( k \), an element from the set of open circles \( \circ \) (the adjacent sink nodes) will be added to the set of black circles (the aggregate nodes) is given by

\[
p(k \in \circ \rightarrow k \in \bullet) = \frac{(a_k)}{\sum_{j\in\circ}(a_j)} \tag{7}
\]

where \( a_k = \) absorbed amount of tracer particles at position \( k \)

**Figure 1:** Basic construction of the aggregate.
3 Results

In Fig. 2 the aggregate and the nutrient distribution, in a section made in the $zy$-plane, through the middle of the lattice, are shown. In this simulation $Pe$ was set to the value 0.0150. The colour shift black to white indicates a decrease in tracer particle concentration. The shape of the basins of equal nutrient ranges is displayed by colouring the adjacent basins black. In Fig. 3 a similar section is shown through the nutrient distribution in an experiment in which $Pe$ is set to the value 0.250.

![Figure 2: Nutrient distribution around an Aggregate where $Pe$ is set to the value 0.0150 (the diffusion limited case).](image)

4 Discussion

In Figs. 2 and 3 it is demonstrated that the influence of hydrodynamics on the nutrient distribution occurs at higher $Pe$ numbers. In the case of a low $Pe$ number the diffusion limited situation is obtained: an irregular object that is branching towards the nutrient source. At a higher $Pe$ number the influence of the flow becomes visible: the object start to develop branches in the opposite direction of the flow, in the stream shadow of the aggregate an area depleted from nutrients occurs. Furthermore it can be observed that the degree of compactness increases for higher $Pe$ numbers. The results presented in this paper show the feasibility to study the combined effect of diffusion and flow on growth processes in three dimensions by applying the lattice Boltzmann method.

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Figure 3: Nutrient distribution around an Aggregate where $Pe$ is set to the value 0.250.

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