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Before the endless forms: embodied model of transition from single cells to aggregates to ecosystem engineering

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The emergence of complex multicellular systems and their associated developmental programs is one of the major problems of evolutionary biology. The advantages of cooperation over individuality seem well known but it not clear yet how such increase of complexity emerged from unicellular life forms. Current multicellular systems display a complex cell-cell communication machinery, often tied to large-scale controls of body size or tissue homeostasis. Some unicellular life forms are simpler and involve groups of cells cooperating in a tissue-like fashion, as it occurs with biofilms. However, before true gene regulatory interactions were widespread and allowed for controlled changes in cell phenotypes, simple cellular colonies displaying adhesion and interacting with their environments were in place. In this context, models often ignore the physical embedding of evolving cells, thus leaving aside a key component. The potential for evolving pre-developmental patterns is a relevant issue: how far a colony of evolving cells can go? Here we study these pre-conditions for morphogenesis by using CHIMERA, a physically embodied computational model of evolving virtual organisms. Starting from a population of single cells moving in a fluid, closed space, and exploiting one nutrient source from a given repertoire of food particles falling from the top of their environment, it is shown that cells undergo major transitions as they evolve their metabolism and adhesion properties in order to exploit resources and occupy space. At some point, some cells "discover" the energy-rich top of their world and the whole population flips towards the upper layer. At this point they act as ecosystem engineers, modulating the flow of nutrients and creating opportunities for new niches to form, as illustrated by the subsequent emergence of a specialized level of detritivores.

Keywords: Multicellularity, hierarchical evolution, evodevo, major transitions, embodied simulation

I. INTRODUCTION

A key problem in evolutionary biology is the emergence of complex life forms under the cooperation of several interacting cells [1,2]. Multicellularity emerged through evolution several times (at least 25) and has been a prerequisite for the generation of complex types of development [3-6]. This major transition brought division of labour and opened the door for the emergence of development and body plans [7-9]. But for many reasons, and in spite of its obvious importance, the evolution of multicellularity is not yet well understood. The fossil traces of the transition are still incomplete, although rapidly improving. However, dedicated efforts to unravel the phylogeny of multicellular living forms, the analysis of special model organisms and the cues provided by the presence of potential genetic toolkits predating the emergence of complex metazoans are defining the potential minimal requirements for the transition towards complex multicellular life forms.

This transition is particularly relevant for the critical changes took place around 560 Myr ago, associated to the so called Cambrian event [1,10] but its roots predate a much earlier time window, as indicated by the analysis of ancestral genomes. Moreover, the picture gets more complicated as we consider additional components related to the physical environment and the constraints and opportunities posed by ecological interactions. Actually, the multiple facets of the debate on the origins of multicellular organisms have to do with the role played by the different potential shapers of the event. These multiple factors are not independent, and are likely to have interacted in complex ways.

In general terms, the multicellular state is characterized by the existence of cell-cell interactions of some sort that provide a source for collective adaptation to energy limitations, physical fluctuations and eventually division of labor. In multicellular organisms, lower-level entities (cells) have relinquished their ability to reproduce as independent units and instead replicate exclusively as part of the larger whole. But long before a developmental body plan was even defined, several layers of complexity were required. This as a particularly relevant problem deeply tied with the problem of hierarchies in evolution [11-13]. Before developmental programs allowed true multicellular organisms to emerge, single cells developed into monomorphic aggregates and later on into differentiated aggregates [12]. Moreover, cell adhesion mechanisms required for the emergence of multicellularity have a much early origin [14]. In this context, long before complex metazoans appeared, some key components of the toolkit were already in place. How did these

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components affected the transition to multicellularity is an open question, and theoretical models can help to address it.

Most mathematical and computational models dealing with early evolution of development assume that either genetic networks or even body plans are already in place (thus Darwin’s endless forms are available) or instead deal with pattern-forming colonies and their potential to form structures under given spatial and nutrient constraints [15-17]. However, less attention has been given to the physics associated to these processes, in spite of their obvious importance (see [18] and references cited). By physics we refer to two different levels. One level involves cellular interaction forces, which can be sometimes properly captured by cell sorting models based on energy minimization functionals [19,20]. By properly defining an optimization algorithm, it is possible to evolve morphologies and see the interplay between cell differentiation, growth and communication [21]. The other level deals with the embedding of cells and organisms within a physical medium. Here the forces are closer to standard physics. The way cells might displace in their three-dimensional environment, how they interact with the substrate or how they find nutrients in a fluctuating medium are here key components of the problem. Previous work on such embedded artificial systems was pioneered by Karl Sims who used evolutionary rules to obtain best solutions based on evolved ”organisms” composed by a number of connected blocks linked to (and controlled by) a simple neural network. Further work has considered the interplay between genetic networks and morphogenesis [25,26].

In this paper we would like to address, under a well defined framework, some questions related to the pre-multicellular world were cell aggregates (but not true organisms or body plans) could develop, providing some key preconditions for multicellularity to emerge. In particular, we would like to understand how the physical context, cell-cell adhesion properties, ecological and genetic factors concur to favor the emergence of cell aggregates and how does the environment modify or influence the evolution of cell diversity and cell-cell interactions under a given spatial framework. By introducing an explicit three-dimensional embodiment, we also try to see if there how it can play a role in favoring the emergence of innovations. Here such a pre-body plan scenario and its potential to form structures under given spatial and nutrient constraints [15-17]. However, less attention has been given to the physics associated to these processes, in spite of their obvious importance (see [18] and references cited). By physics we refer to two different levels. One level involves cellular interaction forces, which can be sometimes properly captured by cell sorting models based on energy minimization functionals [19,20]. By properly defining an optimization algorithm, it is possible to evolve morphologies and see the interplay between cell differentiation, growth and communication [21]. The other level deals with the embedding of cells and organisms within a physical medium. Here the forces are closer to standard physics. The way cells might displace in their three-dimensional environment, how they interact with the substrate or how they find nutrients in a fluctuating medium are here key components of the problem. Previous work on such embedded artificial systems was pioneered by Karl Sims who used evolutionary rules to obtain best solutions based on evolved ”organisms” composed by a number of connected blocks linked to (and controlled by) a simple neural network. Further work has considered the interplay between genetic networks and morphogenesis [25,26].

II. ENVIRONMENT. CELLS AND PHYSICAL SIMULATION

In our model, evolution takes place within a spatially confined environment where physical forces play a role as external constraints. Organisms are also spatially embedded structures and their embodiment is relevant as it provides the proper link with the external world and the biotic scenario where other organisms inhabit. Our starting point here is a population of single-cell organisms, where each cell in the initial population is identical. The spatial domain is a cube with floor and walls. In figure 1 we display a basic scheme of the system considered here along with the different components of the physical interactions that will be taken into account.

A. Cell and particles

Cells and particles are simulated with rigid bodies moving within a fluid-like environment. A cell (particle) has spherical geometry with radius $R_i$, mass $M_i$, spatial position $r_i$, and velocity $v_i$. The motion of a cell is described by the standard second law:

$$M_i \frac{dv_i}{dt} = F_i$$  \hspace{1cm} (1)

Numerical integration of equation (1) gives cell velocity at time $t + \Delta t$:

$$v_i(t + \Delta t) = v_i(t) + \frac{F_i}{M_i} \Delta t$$  \hspace{1cm} (2)

where $\Delta t$ is the size of the integration step, and the total force acting on $M_i$ will be:

$$F_i = F_c + F_{r} + F_{n} + F_{w} - k_d v_i + M_i g$$  \hspace{1cm} (3)

applied to any cell is the sum of environmental forces $F_c$, the gravitational field $g$, the collision force $F_{r}$, the cell-wall adhesion $F_{w}$ and the cell-cell adhesion $F_{n}$ term.

B. Environmental forces

For simplicity, we assume that the external environment exerts the same force to every cell or particle, i. e.:

$$F_c = k_n n$$  \hspace{1cm} (4)
FIG. 1 Basic scheme of the components of the CHIMERA model. The system is confined within a rigid cube with a floor where particles fall and to which cells can attach. Five additional square boundaries are also present which cannot be crossed. The upper boundary allows a flow of nutrient particles (here small spheres) at a constant rate. Particles fall under gravity and experience local turbulence as a random velocity field. As they reach the floor, they can keep moving under the same flow and also disappear as they degrade into detritus particles.

where \( \mathbf{n} \) is a random vector with \(|\mathbf{n}| = 1\) and \( k_e > 0 \) is a constant parameter that indicates the strength of the external field. This choice implies that external fluctuations in the fluid medium are homogeneous, thus affecting all parts of the system uniformly. This approximation thus neglects potential effects played by small-scale eddies, which might actually play a role in adaptational changes.

Movement of particles in a fluid is subject to viscous drag \((-k_d \mathbf{v}_i)\) where \( k \) is the drag coefficient associated to the surrounding fluid. The effect of drag is to resist motion, making the particle gradually come to rest in the absence of other influences.

C. Cell-cell collisions

We apply the discrete element method [28] to the computation of collision forces between the \( i \)-th cell and all its interpenetrating cells, that is, cells located at a distance below a given threshold (see figure 2):

\[
F_i^c = \sum_{i \neq j} \nu \left[ \mathbf{v}_{ij} - \frac{\mathbf{r}_{ij}}{||\mathbf{r}_{ij}||} \left( \mathbf{v}_{ij} \frac{\mathbf{r}_{ij}}{||\mathbf{r}_{ij}||} \right) \right] + \xi \mathbf{v}_{ij} - \nabla \Phi_{ij}(\mathbf{r}_{ij}; R_i, R_j) \tag{5}
\]

where \( \nu \) is the shear coefficient, \( \xi \) is the damping coefficient, \( k \) is the spring coefficient, \( \mathbf{x}_{ij} = \mathbf{x}_j - \mathbf{x}_i \) is the offset vector between the \( \mathbf{x}_i \) and \( \mathbf{x}_j \) cell positions, and \( \mathbf{v}_{ij} = \mathbf{v}_j - \mathbf{v}_i \) is the difference between cell velocities. The last term in the right-hand side gives the force resulting from a potential function associated to a soft-core interaction, namely

\[
\Phi_{ij}(\mathbf{r}_{ij}; R_i, R_j) = \frac{1}{2} k (R_i + R_j - ||\mathbf{r}_{ij}||)^2 \tag{6}
\]

Computation of spatial interaction forces requires \( N(N-1)/2 \) possible collision checks for \( N \) bodies in the worst-case scenario. In order to reduce this computational cost we use a spatial partitioning scheme. Here, a 3-D uniform grid subdivides the entire container volume in equally-sized square voxels [29]. All the bodies (cells and particles) are sorted by a mapping function \( h(\mathbf{r}) \) that computes their voxel index:

\[
h(\mathbf{r}) = \frac{1}{d}(\mathbf{r} - \mathbf{o}) \tag{7}
\]

where \( \mathbf{o} \) is the grid origin and \( d \) is the voxel size. For each cell or particle, we only check its collisions with close particles and cells, i.e., having the same or a neighboring
Each cell has an intrinsic probability $E$. Cell-cell adhesion will see, cells can evolve cell-wall adhesion if $|x_{ij}|$ is above the maximal length, i.e., with certain probability $1$.

D. Cell-substrate adhesion

Attachment of cells to surfaces may provide a favorable micro-environment (e.g., biofilms). Let us indicate by $ax+by+cz+d=0$ the plane equation for the closest wall to the cell located at $r_i=(x_i,y_i,z_i)$. Cell-plane distance $D(r_i)$ is described by:

$$D(r_i) = \frac{ax_i + by_i + cz_i + d}{\sqrt{a^2+b^2+c^2}}$$

When a cell with adhesion strength to the substrate $J_i^f > 0$ is close enough, i.e., $D(x_i) < \delta_w$, we will add a spring connecting the center of the cell $x_i$ with its projection on the wall $x_{iJ}$ (see figure 3B). Here, $\delta_w$ specifies the cell-wall adhesion range. The wall spring attached to any cell exerts the following attraction force:

$$F_n^i = -k_s \left( ||r_i - r_{iJ}|| - d_s \right) \frac{r_i - r_{iJ}}{||r_i - r_{iJ}||}$$

where $d_s$ is the spring equilibrium distance, $k_s$ is the spring constant and $F_n^i = 0$ when the cell is not attached to any spring. Existing cell-wall links can be removed with certain probability $1-\eta(t)$ or when the spring length is above the maximal length, i.e., $||r_i - r_{iJ}|| > d_{wJ}$. As we will see, cells can evolve cell-wall adhesion $J_i^f$ in order to maximize the intake of nutrient particles.

E. Cell-cell adhesion

Cells can form aggregates by attaching to other cells. Each cell has an intrinsic probability $J_i^c$ to create a new adhesion link. Given two close cells located at $r_i$ and $r_j$, we will set an adhesion string connecting them with probability $(J_i^c + J_j^c)/2$. The adhesion force to any cell is the sum of forces contributed by all the active cell-cell adhesion springs:

$$F_i^c = -\sum_j k_l (||r_i - r_j|| - d_l) \frac{r_i - r_j}{||r_i - r_j||}$$

where $d_l$ is the spring equilibrium distance, and $k_l$ is the spring constant. Adhesion springs break spontaneously with rate $\delta \approx 0.001$ or when the spring is very large, i.e., $||r_i - r_j|| > d_l$.

On the other hand, Interpenetration collisions between cells and walls are not resolved with explicit forces (see figure 3A). When a body interpenetrates a wall, it bounces along its opposite velocity direction, i.e., $\nu(t + \Delta t) = \mu \nu(t)$ by a constant factor $\mu < 0$. In addition, we relocate the body outside the wall (see below). This approximation ensures that particles will never move beyond container limits and does not change the main results presented here. The final cell (or particle) position is obtained from:

$$r_i(t + \Delta t) = r_i(t) - \delta n + \nu_i(t + \Delta t) \Delta t$$

where $\delta > 0$ is the cell-wall interpenetration distance and $n$ is the normal of the wall at the collision point with $|n|=1$ (see figure 3A).

Finally, the computation of particle force $f_i$ is more simple than in the case of cells. Particles collide with boundary walls, other particles and with cells. Particles can not adhere to the walls, or to any other body. The total force exerted on a particle is

$$f_i = F_e + F_n^p + F_n^c - k_d \nu_i + g$$

where $F_e$ is the environmental force (as defined for cells, see above), $\nu_i$ is the particle velocity and $g$ is the gravity field. The force $F_n^p$ applied to particle collisions follows the same equation used to compute cell-cell collision responses (5) but using particle mass ($M$) and radius ($r$). Similarly, the term $F_n^c$ accounts for the collision response between any pair of interpenetrating particles and it has the same form as in (5).

We have calibrated the parameters associated to the physics as described above in order to avoid numerical instabilities. We have used small integration steps, i.e., $\Delta t = 0.03$ and fixed several physical parameters, including the cell and particle masses and the spring constants, to suitable values. An exhaustive exploration of the physical parameter space will be investigated elsewhere.

III. EVOLUTIONARY RULES

Once our embodied, physical description of how interactions take place within our environment, we need to further extend our model by including evolutionary
rules. Mechanical interactions, for example, can be understood in terms of predefined mechanisms (constrains derived from the nature of physical laws) together with sets of parameters that tune their relevance in terms of how different forces influence dynamics. In this paper we explore the impact of such parameter changes once the basic laws are already in place. The introduction of physical constraints as part of the framework defining our cells and their interactions allows us to integrate different factors emerging at the boundaries between physics and biology [30].

Moreover, the explicit nature of selection pressures associated with gathering nutrients from a spatially explicit, fluctuating environment is introduced under a population-level (and thus ecological) framework. In summary, the model takes into account physical embodiment, ecological and evolutionary constraints and allows interaction parameters among cells to change. Although no developmental programs emerge at this level, we will see how the degrees of freedom included in our approximation allow cell aggregates to emerge, along with innovation and the creation of niches and specialization.

Let us define the initial conditions and basic rules of evolutionary and dynamical change used in our computational model. A key component that requires full description is how cells grow and divide. Moreover, each time a cell replicates, mutations affecting different parameters can modify the phenotypes of the newly created offspring. At the beginning, we start from an homogeneous population of $N_0$ cells, each having mass $M_0$ and feeding on the same resource, i.e., $E_1 > 0$ and $E_2 = 0$ for all $j > 1$. At every simulation step, we introduce $N_p$ new particles in the system, starting at the top of the simulated volume. Eventually, cells collide with nutrient particles and consume them according to a cell-specific relative efficiency $\hat{E}_j$ (a given nutrient particle is consumed only when $\hat{E}_j > 0$, otherwise the particle is deflected and does not enter into the cell body). Consumed particle contributes to the corresponding molecule mass:

$$M_j^t(t + \Delta t) = M_j^t(t) + E_j(t)m$$

(13)

where $m$ is the particle mass. Once consumed, the particle is removed from the system. Nutrient particles have a characteristic lifetime and degrade with rate $\mu_p$. The total cell mass $M_i(t)$ is the sum of all molecular masses, i.e.:

$$M_i(t) = \sum_j M_j^t(t)$$

(14)

At each time step, cells consume a constant amount of energy $e_s > 0$ to sustain themselves,

$$M_j^t(t + \Delta t) = \left[1 - \frac{e_s}{M_i(t)}\right] M_j^t(t)$$

(15)

When the total cell mass is below a critical threshold $M_i < M_c$, the cell dies. If enabled, disintegration of the cell releases $(M_i(t)/m) \approx (M_c/m)$ residual particles to the medium. These residual particles will be consumed by detritivores when their relative efficiency is $E_d > 0$. Residuals have a characteristic lifetime and degrade with a slower degradation rate, here fixed to $\mu_p2$.

Cells divide once their total mass is at least twice their initial mass, $M_i(t) \geq 2M_0$. After reproduction, the mother cell reduces its mass by $M_0$:

$$M_j^t(t + \Delta t) = \left[1 - \frac{M_0}{M_i(t)}\right] M_j^t(t)$$

(16)

However, cell division is limited by the available surrounding space. Here, we allow the mother cell to reproduce only when its number of neighboring cells (i.e., within a radius of size $2R_c$) is below a given density threshold $N_c$. The new offspring is placed at a random location close to the mother cell, and specific rules ensure that this new cell is within the boundaries of the simulated medium.

The offspring cell (with index $k$) has initial mass $M_0$ and inherits the cell mother (with index $i$) mutated efficiency $E^{k}_j = E^{i}_j(t) + \nu$ with probability $\mu \approx 0.01$ or $E^{k}_j = E^{i}_1(t)$ otherwise. Here, the random $\nu$ perturbation follows a Gaussian distribution with zero mean and standard deviation $\sigma_m = 0.3$.

In addition, the offspring cell inherits both the (mutated) mother’s cell-floor adhesion and cell-cell adhesion coefficients, respectively. That is, $J^k_i(t) = J^i_j(t) + \nu$ with probability $\mu$ or $J^k_i(t) = J^i_j(t)$ otherwise; $J^k_i(t) = J^i_j(t) + \nu$ with probability $\mu$ or $J^k_i(t) = J^i_j(t)$. After mutation, the offspring coefficients are normalized to ensure that the following conditions: $\sum_j E^{k}_j = 1$, $\hat{\mathcal{E}}J^k_i \in [0, 1]$, $\hat{\mathcal{E}} J^k_i \in [0, 1]$ and $\hat{\mathcal{E}} J^k_i \in [0, 1]$ are satisfied.

IV. RESULTS

As a result of the previous set of rules and initial condition, we have a simple ecological food web involving a set
FIG. 4 Cell (black) and particle (red) growth curves can be described with a superposition of processes, in different stages. Inset: During the transition to the inverted population, cells grow with successive lag, growth and asymptotic phases. Cell placed at the source of nutrients growth at a super-exponential rate, which is limited by the amount of available resources, i.e., space and nutrients (notice the peak). The shape of these curves is associated to the emergence of an inverted cell population in the simplest configuration of the CHIMERA model (no cell-cell adhesion, no exchange, no predation). This behavior is very robust and it has been observed in all the scenarios explored in this paper. From left to right, time evolution (A) t=17000, (B) t=170000, (C) t=200000 and (D) t = 300000 of an initial population of homogeneous cells that evolve floor adhesion by following the vertical gradient of nutrient particles. Bright cells have high floor adhesion (where yellow indicates maximum adhesion) and darker colors correspond to free-moving cells. Notice that adhesion evolves first in cells close to the wall boundaries. Here: Φ = 25 particles per timestep, Δt = 0.03, δw = 0.05, då = 0.01, ν = 80, ξ = 80, k = 400, Me = 20, Rj = 0.08, mπ = 3.35, ri = 0.025, ke = 2, kd = 0.001 (see text).

of resources and a single specialist grazer, which takes E1 particles and grows at the expense of metabolizing them. Further degradation of particles leads to waste that is removed from the virtual tank and moreover death of cells also generates an additional resource (the detritus compartment, E₂). Ecologically, this is our starting point, which will evolve as organisms change their feeding preferences and as a consequence of interactions between organisms and their physical environment.

Given the potential for evolving physical parameters as well as nutrient intake-related parameters, our cells will be able to evolve within a range of possible adaptations. For example, given the number of potential food sources to be consumed, we will observe a spread from the original parameter set defined by

\[ E_1 = 1 \cap E_j > 1 = 0 \]

to a continuum space of efficiencies

\[ \mathcal{E} = \{(E_1, ..., E_n) \mid E_i \in [0, 1]\} \tag{19} \]

As we will see below, these spread leads to a predictable outcome in a first phase of the evolution process, while it leads to an unexpected innovation later on.
A. Transition to generalism epoch

The first trend observed in all our simulations is a tendency from the starting specialization (all cells exploiting one source with maximal efficiency) to generalism: mutations allow to exploit other resources with less efficiency but overall this is a better strategy given the finite amount of energy particles. Since nutrient enters the system from the upper layer at a constant rate $p$ at the upper layer and degraded into waste at a rate $\delta_k$, under the absence of grazers the time evolution of the number of energy particles of class $k$, namely $N_k$, will follow a linear model $dN_k/dt = p - \delta_k N_k$ (for $k = 1, \ldots, n_p$) and thus each component will have an average steady value of $N_k^* = p/\delta_k$. Thus the overall number of particles at the beginning (before grazing starts) will be $N^* = n_p p/\delta$, which is achieved under a logistic growth pattern. Here we use $n_p = 4$ nutrient sources, together with a fifth one (the detritus particles). This occurs at the very early stages, where only one source is being exploited. However, since we are interested in the long-term evolution, we would like to see how the particle-grazer population dynamics. One of the first trends easily observed in the model is the tendency towards generalism: the payoff given by the exploitation of a variety of resources outweighs the loss of efficiency as more resources are grazed.

The degree of generalism of a given individual is measured by means cell entropy $H(C_i)$ defined as the normalized diversity of efficiencies:

$$H(C_i; E_{1i}, \ldots, E_{ni}) = -\frac{1}{\log(n_p + 1)} \sum_{1 \leq j \leq n_p + 1} E_{ji} \log[E_{ji}]$$

where $E_{ji} = E_{ji}/E_{ji}$ is the relative efficiency of the $i$-th cell when feeding on the $j$-th nutrient resource and $n_p$ is the number of different resources. Notice that, in the initial configuration, all cells have entropy $H(C_i) = 0$. As defined, the degree of generalism will be zero when only one source is used (specialized diet) and will reach a maximum value for individuals grazing on multiple sources. This measure is color-coded in our snapshots of the system. The average efficiency for each cell is given by $\langle E_i \rangle = \sum_j E_{ji}/n_p(i)$ where $n_p(i)$ indicates the number of nutrient sources exploited by $C_i$.

The simulation shows a steady increase of cell-wall attachment and cell-cell adhesion followed by a steady increase in number of cells. This is a consequence of the fact that, in order to get access to falling particles, a larger surface is needed. Cells that attach to the surface can climb up the walls. Having a moderate cell-cell adhesion also helps in avoiding them to fall down. In this way, we have formed aggregates that are moving up as cells divide. The impact of this, along with the simultaneous tendency towards generalism, can be seen in figure 4. The cell population (blue curve) grows rapidly as the aggregates start to emerge and expand, eventually covering the top layer. During the process, groups of cells, often forming layers parallel to the floor, become larger and larger.

As cells start exploiting Figure 4 shows a typical example of cell and particle growth curves. Cell growth curve (blue) can be described as the superposition of different processes. The amount of available resources (black) is related to the efficiency and the cell population size. During the exponential phase cells colonize the source of nutrients at a super-exponential rate (see figure 5). However, the population cannot sustain this pace of growth indefinitely because of spatial constraints and limited nutrients in an accelerated way, until they reach the maximum. Accordingly, the amount of available nutrient particles stabilizes in a well-defined mean value.

![Figure 5](image.png)

**FIG. 5** Sharp transition in the time evolution of average cell-floor adhesion. This transition is associated to the increasing height (inset) of the cell populations as further cells climb the walls towards the upper layer (see text).

B. Transition to ecosystem engineering epoch

The first most interesting and relevant result of our study is a seemingly inevitable innovation made by our evolving cells as they "discover" that gathering particles is easier if they attach to the top floor of the system. Cells reach the nutrient source by evolving cell-floor adhesion (see figure 5). Here, collision with particles happens more frequently and nearby cells have a higher reproduction rate (and thus a higher fitness) because the sustained intake of nutrients. Eventually, cells with high floor adhesion ($J^f \approx 1$) colonize the source of nutrients in a brief burst of super-exponential growth. This is illustrated by figure 4d, where we can see a snapshot of our system soon after cells have "discovered" the roof. In terms of the population dynamics, it is also observed that the number of free nutrient particles declines as they are more efficiently found and removed from the system.

The fast adoption of this innovation and how it relates with cell-substrate adhesion if obvious if we look at figure
FIG. 6 Convergence and path dependence in CHIMERA simulations. Here we display the evolution of the average cell entropy in three different simulations while keeping the same parameters. Notice that the transient evolutions can be very different but all of them converge to a similar average entropy. Sometimes the transition is abrupt but it can also follow a more smooth trajectory (black line).

5, were we can see how this adhesion strength sharply increases as soon as the first aggregates start to emerge. In the same figure (inset) we also plot the average height of cells, measured in terms of distance to the top layer (located at the $z = 0$ coordinate. Within this process (data not shown) we have a slower increase in the cell-cell adhesion strength, which helps to maintain the coherence of the aggregates and further prevents cells from falling to the floor.

In spite of its rapid adoption, it is worth noticing that this transition does not always take place at the same time nor following the same pattern. The previous plots are the representative runs, but the convergence to the final state take longer in some cases, and it can follow rather different paths (figure 6). Although the same final result is always achieved.

A major consequence is derived from this innovation. As cells in the top layer start to dominate the whole flow of nutrients, something new happens. After the colonization is completed, cells die and their waste material falls to the bottom. The resulting detritus stays for a while and is eventually removed by degradation. But some cells have already developed a mild efficiency to exploit these particles, so some of them after falling from the roof, will find themselves inhabiting a niche that is rich in a given type of energy source. After a while, they develop a higher efficiency and eventually become specialists. This is illustrated in figure 7a-b, where we can see that the efficiency of detritivores grows fast after the top floor population has been established. In the inset of figure 7a we display an example of the stationary state.

This transition defines an instance of so-called ecosystem engineering [31-33]. By changing the flow of nutrients, the top floor population causes a physical change in the environment due to their spatial distribution.

As it occurs with freshwater phytoplankton organisms, which intercepts light by placing themselves on the top of the water column or with higher plants, producing litter form dead leaves, our ecosystem provides a clever example of this scenario. By modulating the flow of nutrients, which eventually shifts from nutrient-rich to detritus-dominated flows, an effective asymmetry is generated.

The process of niche creation and the emergence of
ecosystem engineering promote a new feedback towards the way detritivores behave. If cell-cell adhesion is allowed to evolve, it can be shown that the detritivore compartment evolves significant adhesion among individual cells, which can be described as a new form of cell aggregate. It is interesting to notice that our aggregates do not cooperate in terms of sharing resources, but instead they emerge from selection constraints imposed by the requirement of an expanded area, which can only be obtained by attaching to the vertical surfaces. An additional advantage is obtained by living in higher locations: energy particles are falling near there and in fact, in the presence of fluctuations, it is likely that particles hitting the walls are captured by cells adhered to them. But the process has a discontinuity: by covering the roof, an accelerated transformation takes place, modifying the whole organization of the ecological assembly and allowing the emergence of an additional trophic compartment.

In figure 8 we summarize the changes experienced by our system as we cross through the different regimes. Here we have indicated the flows of matter from the external energy sources to waste. In fig. 8a, the initial state of our system is shown, with several sources of particles but only one being exploited by the single specialist. Such scenario is slowly replaced by a heterogeneous one (fig. 8b) marked by an increasing tendency to generalism: mutations affect efficiency rates and the potential for exploiting several resources. As evolution proceeds and cell develop adhesion (here indicated as small protrusions) along with a complete generalism (c). Here we indicate with \( \{ E_i \} \) that cells use equally all types of nutrients with the same coupling. Eventually (d) the new niche of detritus-rich particles triggers the evolution of a specialized population of detritivores. This result
is predictable, provided that the abundance of incoming particles is large enough.

V. DISCUSSION

The challenge for biologists is to explain how a population of cells becomes a single entity capable of self-reproduction; that is, how an evolutionary transition that involves a shift in the level at which selection operates, from individual entities to groups of entities, can occur. From the point of view of our picture of early stages of the evolution of development, the generation of simple interactions among cells and between cells and their physical medium needs to be considered. In particular, we might consider the problem of a pre-developmental scenario where true multicellularity has not yet emerged but the preconditions for multicellular-like assemblies are already in place.

If the initial steps towards life took place in water, an appropriate model considering the role of physical interactions must take into account (a) events taking place within a fluid and (b) those associated to physical exchanges between individuals and individuals with the boundaries of the system (such as the sea bottom or a pond floor). By considering these basic forces, we introduce a minimal set of (possible) rules of interaction that can evolve through time. Such rules allow our artificial cells to explore their environment, interact and make decisions. But it also provides a very basic framework to explore the potential for finding patterns of pre-developmental pathways based on interactions among single-celled entities.

The transition from the floor to the top layer defines an instance of so-called \textit{ecosystem engineering} [27]. By changing the actual flow of nutrients to the system, they cause a physical change in the environment due to their physical distribution. Moreover, by doing so they also allow the emergence of a specialized, spatially segregated compartment of detritivores. Following [31] classification scheme, our artificial creatures are autogenic engineers: they change their environment mainly via their own physical structures. As it occurs with freshwater phytoplankton organisms, which intercept light by placing themselves on the top of the water column, or in higher plants, producing litter from dead leaves, our system provides a simple example of this scenario. By modulating the flow of nutrients, which eventually shift from nutrient-rich to detritus-dominated flows, an asymmetry is generated, thus actually creating a new niche for detritivores to appear. Here the main structure created is a cell barrier associated to cell-floor interactions.

Future work should consider the explicit introduction of minimal genetic networks, the potential for cooperation in terms of nutrient sharing, an active role of our organisms in modifying their environmental conditions (thus adding an additional layer to the potential for ecosystem engineering) and variability of spatial conditions. These in silico experiments could be compared in some cases with evolutionary sequences of growth and selection observed in microbial communities [35-38]. Moreover, help designing and interpreting experimental approaches based on the introduction of selection favoring given traits. All these extensions of the CHIMERA model will allow us to approach relevant questions concerning the tempo and mode of the transition to multicellularity and how the different players (ecology, genetic interactions, physical embodiment and path dependence) affect the final outcome.

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VI. REFERENCES


