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Abstract In this chapter, we advocate a *domain specific language* (DSL) approach to overcome the difficulties of modeling and simulating morphogenetic processes. A careful discussion of the design goals of a DSL leads to the development of an experimental programming language called MGS. Its declarative approach is based on the notion of *topological collection* originating from algebraic topology. Topological collections arise naturally when modeling a "dynamical system with a dynamic structure", or $(DS)^2$, as the state of the system. The evolution function of the system is specified by a *transformation*, which is a set of rewriting rules where each rule defines a local interaction. We illustrate these notions through different models of the same morphogenetic process: the growth of a T-shaped structure. The objective is to show how a variety of models can be consistently handled within the MGS framework.

1 Introduction

Most research works presented in this book rely on *simulation* to model, explore and analyze the behavior of engineered morphogenetic processes. Computer simulation is a tool of choice, if not the only systematically available one, for their design. In this context, making the implementation of computer simulation faster, easier, and reusable is absolutely crucial. Yet, the modeling and simulation of such systems remain today difficult and error-prone for at least two reasons:

 The spatial organization of morphogenetic systems is dynamic and requires advanced computer representations, often at different scales.

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• Models of morphogenetic processes require a coupling between *patterning* and *development*: the evolution of a system's spatial structure depends on its state, while at the same time the evolution of its state depends on its spatial structure.

This situation often leads to the development of ad hoc simulation frameworks, which are dedicated to a particular problem and rely on a particular spatial representation. In contrast, this chapter advocates a domain specific language (DSL) approach to cope with the difficulties encountered when elaborating a computer simulation of natural and engineered morphogenesis.

Designing a DSL for the Simulation of Morphogenesis

DSLs are specially tailored programming languages designed to solve problems in a particular domain [41]. To this end, they provide useful abstractions and notations for the domain at hand. They are more attractive than general-purpose languages for programming in a dedicated domain due to their ease of coding, systematic reuse, better productivity, reliability, maintainability, and flexibility [61]. Furthermore, DSLs are usually small and declarative¹ as opposed to imperative.

Compared with *ad hoc* simulation platforms, a language dedicated to the modeling and simulation of morphogenesis offers more expressive power and wider applicability. For instance, it can facilitate the comparison of various morphogenetic models by providing a uniform and consistent environment for their description and simulation. It can also leverage the "know-how" gathered from various models by enabling model sharing, reuse and coupling.

Yet, the DSL approach must also face difficulties similar to the ad hoc approach. While it addresses the need for generality, there is no unifying formalism that can include all morphogenetic processes. The "wholesale" modeling of morphogenesis would mobilize a great number of models of many types (genetic, mechanical, chemical, etc.) requiring a wide range of formalisms (from continuous to discrete, from deterministic to stochastic) and styles (for example, some models adopt a space-centric view, while others rely on an agent-centric view).

Short of integrating this diversity at a theoretical level, it is nevertheless possible to develop a framework to unify *programming* for simulation purposes. The feasibility of code-level unification is based on three key findings:

- Despite the variety of formalisms and styles used in the simulation of morphogenesis, the vast majority of them capture morphogenetic processes as dynamical processes. However, the *structure* of these dynamical systems is itself dynamic.
- Space-centered or entity-centered modeling can be reconciled through an *interaction-oriented* view. The problem is then to offer sufficiently expressive means of specifying sophisticated interactions.

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¹ Declarative programming focuses on *what* should be computed instead of *how* it must be done. Objects and constructions are close to the mathematical standards that enable an easier mathematical reasoning on programs. Thus a declarative program is an executable specification not burdened by the implementation details and remains close to the mathematical model.

• The various spatial organizations that underlie the state of a developmental system can be subsumed under the abstract viewpoint of *topological chains*. However, this does not presume the difficulties of achieving an effective implementation.

Based on these observations, the MGS project started in the early 2000's with the goal of elaborating a DSL dedicated to the modeling and simulation of morphogenesis [22]. Since then, the notions investigated in MGS have been validated by the simulation of numerous examples of processes involved in morphogenesis, such as self-assembly [53, 28, 5], models of gene regulatory networks [21], systems biology (mainly at a cellular level) [25, 50, 42, 54], synthetic biology [19], plant growth [48] and other natural developmental cases [51, 30].

Outline of the Chapter

In the rest of this introductory section, we elaborate upon the above three findings, as they constitute the rationale behind MGS. However, this discussion is not a prerequisite for understanding the self-contained presentation of the MGS language exposed in Section 2. This presentation focuses on the notions of *topological collections* and *transformations* used to represent respectively the state of a morphogenetic process and its evolution function. Section 3 illustrates these constructions with different models of the same example: the development of a T-shaped structure. The objective is to show how a variety of models can be handled consistently within the MGS framework.

1.1 (DS)²: Coupling Patterning and Development

In his famous last publication from 1952 entitled "The Chemical Basis of Morphogenesis" [60], Alan Turing elaborates a dynamical systems view of morphogenesis, where he characterizes a developing organism as a set of variables that change over time and capture the state of the system along with its developmental changes. He also conducts a study of the set of all possible trajectories of this system. With a great vision of the fundamental challenges posed by morphogenesis, he writes:

The interdependence of the chemical and mechanical data [describing the state of a growing embryo] adds enormously to the difficulty, and attention will therefore be confined, so far as is possible, to cases where these can be separated.

Accordingly, Turing decides to focus his attention on simplified cases in which mechanical aspects can be ignored and chemical aspects are the most significant.

Since Turing, it has become a widespread idea that dynamical systems offer general principles for formalizing, understanding and designing self-organization processes such as the ones encountered in morphogenesis. However, in the great majority of models proposed to describe developmental processes, the *shape* (mechanical data) and the *content* (chemical data) are clearly decoupled, making these models usually fall into two categories²:

- formalisms that focus on pattern formation in an initially homogeneous but static substrate, and
- generative formalisms that specify the creation and the evolution of a dynamic shape, irrespective of the processes that may take place within the shape.

Examples of the first category are given by reaction-diffusion systems, activatorinhibitor models, or random Boolean networks. They rely on various model of dynamical systems (Table 1). Examples of the second category include Lindenmayer systems (L-systems) [36], membrane computing [46], graph grammars [49], selfassembly systems, and others (Table 2).

Table 1 Formalisms that can be used to specify structured dynamical systems according to (a) the underlying space in which the patterning process takes place, (b) a continuous or discrete representation of time, and (c) the state variables of the system's components. "Numerical Solutions" refer to explicit numerical solutions of partial differential equations (PDE) or systems of coupled ordinary differential equations (ODE).

C: continuous D: discrete	PDE	Coupled ODE	Numerical Solutions	Cellular Automata
(a) Space	С	D	D	D
(b) Time	С	С	D	D
(c) States	С	С	С	D

Table 2 Generative formalisms that can be used to specify the evolution of a shape, according to the *topology* connecting the components of the shape. In a *multiset*, all elements are considered connected to each other. In a *sequence*, elements are ordered linearly: this case includes lists and extends to tree-like structures (lists of lists). *Uniform* structures involve a regular neighborhood, e.g., a rectangular lattice where each element has exactly four neighbors. Group-Based Fields (GBF, Section 2.1.4) are a powerful tool relying on mathematical groups to represent such structures. The first four cases describe spatial structures that can be accurately depicted by a graph. Beyond graphs, *nD combinatorial structures* are used to define arbitrary connections between components of various dimensions. The MGS language (next section) can handle all these types of shapes.

Topology:	multiset	sequence	uniform	arbitrary graph	nD combinatorial structures
Formalism:	membrane system	L-systems	GBF	map L-systems, graph-grammars	MGS

 $^{^2}$ This distinction is somewhat contrived. For instance, cellular automata have been devised to study self-reproduction of distinct entities, but these entities are represented by specific patterns in a predefined medium.

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Dynamical Systems with a Dynamic Structure $(DS)^2$

Naturally, various extensions of existing formalisms have been proposed to address the coupling of patterning and development, and blur the above distinction. For example, the original L-systems have been later extended with the notion of *parameters* [47]. This enabled models of plant growth and differentiation, such as *Anabaena Catenula*, based on a chemical paradigm of reaction-diffusion by activation-inhibition. On the one hand, a growth model specifies where diffusion and reaction are possible while, on the other hand, concentrations of chemicals control growth rate and shape change.

This extended L-system can be seen as a dynamical system, yet the set of variables characterizing its state (i.e., the concentration of the chemicals in each cell of the organism) itself changes in time due to the development of new cells. We call such systems *dynamical systems with a dynamic structure*, denoted in short $(DS)^2$, to stress their specificity [18].

Today, using the widespread availability of inexpensive computing power, it is possible to build computational simulations of very large, coupled models. It remains, however, that the simulation of processes that modify themselves due to their own activity—a distinctive feature of morphogenesis—is a problem of great complexity. From the viewpoint of programming, a main challenge is to come up with a *local description* of the shape *and* the evolution of the state. In fact, if the set of variables that describes the system cannot be known in advance, it is impossible to specify a *global* evolution function. It does not mean that there is no such function, but simply that it cannot be defined explicitly. This is especially the case when the individual (local) interactions between the system's entities are well characterized but the corresponding global evolution function cannot be deduced from these interactions. The macroscopic (global) evolution of the system must be computed as the "temporal and spatial integration" of all the various local and dynamic interactions between the system's elements.

1.2 Space-Centric, Agent-Centric and Interaction-Oriented Modeling

The seminal article of Turing introduces two models: a set of coupled ordinary differential equations (ODEs) and a formulation based on partial differential equations (PDEs). In the former, each cell is characterized by the concentration of two morphogens and the corresponding equations describe the exchange of morphogens between two adjacent cells due to diffusion and the reactions within a cell. In the latter, there are no cells: the system is described as a continuous medium where morphogens diffuse and react in each point of the domain. In both cases, the spatial structure (whether a set of cells or a continuous domain) is fixed *a priori*. If this where not the case, Turing would have faced the "interdependence" problem that he himself stressed, namely the coupling between the spatial structure and the processes that take place in this domain.

There are two ways of looking at this coupling: from the viewpoint of the *spatial structure* or from the viewpoint of the *processes* within this structure. In discrete models, this is the well-known difference between space-centric and agent-based models. For example, a prey-predator model can be instantiated using cellular automata in which the state of a cell represents the presence of a prey, the presence of a predator or the absence of both [16]. This is the spatial viewpoint. The model can also be instantiated by a population of individuals that represent preys or predators, and are able to interact if they are in the same neighborhood. This is the agent-centric viewpoint.

The same distinction arises in continuum mechanics models between the Eulerian and the Lagrangian formulations (Fig. 1). The Eulerian formulation focuses on what is occurring at a fixed point in a reference frame as time progresses (as in cellular automata). In the Lagrangian formulation, an observer follows the position (and other properties) of a spatial element of the system's structure as it moves through a reference space and time (as in agent-based models).

Unifying the Agent-Centric and the Space-Centric Approaches

This distinction has a significant impact on the programming style of the simulation: object-oriented languages and multi-agent systems have been developed to support the agent-centric view, while spatial computing languages [3, 1] support the space-



Fig. 1 In fluid dynamics, the Eulerian specification of a flow field describes how the fluid flows over time at each point of a *fixed reference frame*. In a Lagrangian description, the properties (position, stress, etc.) of a local piece of changing shape follow the piece *as it moves*.

centric view. Leaving apart the difference of entities ("elementary piece of space" vs. "agent"), the essential difference between the two approaches resides in the expression of the system's evolution:

- in the agent-centric view, an entity evolves by receiving a message from another entity, whereas
- in the space-centric view, an entity evolves by querying its neighborhood.

If the spatial structure is static, this neighborhood can be fixed a priori, but if it is dynamic, then the difference between the two points of view starts to vanish. "Elementary pieces of space" become agents that can be dynamically created and rearranged through time. Thus with respect to the simulation of morphogenesis, the two styles diverge only in the expression of the local evolution of an elementary entity: triggered by the entity itself or triggered by another entity.

Neither framework is satisfactory because they both focus on the local evolution of a single entity, which is not expressive enough. For example, to handle the problem of collision of particles in cellular automata, one must either consider a two-phase evolution step (propagation and collision) [55] or turn to lattice gas automata, a variant that considers the coupled evolution of more than one cell [9]. In agent-based modeling, the problem of coordinating synchronously several agents also leads to the development of more flexible schemes [39, 38, 34].

We propose to overcome the limitation of both agent-based and space-based approaches by focusing on the *interactions* between entities (whether agents or elements of space). Interactions specify the simultaneous evolution of a (usually small) subset of the entities composing the system (Fig. 2).

1.3 A Unifying View of Spatial Organization

Viewing a system through the interactions of its elements, instead of its decomposition into elements or the location of these elements, brings forth a new struc-



Fig. 2 (a) In *space-centric interactions*, the state of a spatial element (black) evolves by following the state of its neighbors (gray). (b) In *agent-based modeling*, the evolution of an agent A (black) is triggered by another agent (gray) that includes A in its relationships. In these first two cases, an elementary evolution step is limited to an individual entity. (c) More generally, *interaction-based modeling* enables the simultaneous evolution of arbitrary subsets of entities.



Fig. 3 The interaction structure of a system *S* resulting from the subsystems of elements in interaction at a given time step. In the interaction view, the decomposition of a system *S* into subsystems S_1, S_2, \ldots, S_n is *functional*: the state $s_i(t+1)$ of subsystem S_i depends solely on the previous state $s_i(t)$. However, the decomposition of *S* into the S_i 's can itself depend on the time steps. Thus we write $S^t = \{S_{i_1}^t, S_{2_2}^t, \ldots, S_{n_i}^t\}$ for the decomposition of system *S* at time *t* and we have: $s_i(t+1) = h_i^t(s_i(t))$ where h_i^t is the "local evolution function" of S_i^t corresponding to an interaction between the elements of S_i^t . The successive decompositions S^t, S^{t+1}, \ldots can be used to capture the *elementary parts*, i.e., the smaller sets created by intersection between the S_i^t 's. These elementary parts corresponds to the agents in agent-based modeling (Fig. 2b) or to elementary pieces of space in space-centric approaches (Fig. 2a). The *interaction structure* \mathscr{A} is the lattice of inclusions. The leaves $V(\mathscr{A})$ of the lattice are the elementary parts of *S*.

ture [23, 26, 27]. The main idea is the following: if an element *s* interacts with a subsystem $S_i = \{s_1, ..., s_n\}$ (a subset of other elements), then it also interacts, at least conceptually, with any subset S'_i included in S_i . This is a *closure* property, which derives an abstract structure from the subsets of elements. These subsets form a *lattice*, and it is possible (and fruitful) to view this lattice in topological terms as an "abstract simplicial complex" [26] (Fig. 3).

The notion of cellular complex is introduced more formally in the next section. It corresponds to a space built by appropriately gluing cells³, which represent elementary pieces of space of various dimensions. This space is very abstract: it consists of subsets of elements that compose the system and are involved in local interactions. We call this space \mathscr{A} to distinguish it from \mathbb{R}^3 where the elements are physically located. Spaces \mathscr{A} and \mathbb{R}^3 are a priori different. However, if the interactions satisfy a *locality property*⁴, only elements that are neighbors in physical space \mathbb{R}^3 can interact directly. In this case, space \mathscr{A} is strongly related to \mathbb{R}^3 .

We can illustrate via several examples the relevance of considering arbitrary subsets of basic elements as "cells" with a given dimension, both in space-based and in agent-based descriptions. Some physical quantities are naturally linked with pieces of space of a given dimension. For instance, chemical concentration, heat, magnetic or electric charges are all associated to volumes; flux are associated to surfaces; tension to lines; temperature, potential, displacement are associated to points. In a biological tissue, the biological cells are volumes that exchange signals through their 2D manifold membranes. The shape of the membrane is constrained by the

³ The term "cell" refers here to a topological notion, not to a biological cell.

⁴ The locality property states that matter/energy/information transmissions happen at a finite speed. This property is not always relevant, even for physical systems, for instance because processes may occur on two distinct time scales: changes on the fast time scale may appear instantaneous with respect to the slow time scale, enabling the interaction of arbitrarily far elements.

cytoskeleton which is a 1D branching structure. Signaling between cells is achieved by the exchange of molecules (which are points at this level of abstraction; but if one is interested in the way they interact, the DNA or the proteins are themselves linear sequences folded into 3D shapes), and so on.

A Shift of Perspective

The interaction-based programming style reverses the perspective adopted in the agent-based and spatial approaches⁵. Instead of proceeding by first specifying the elements in the system, one must define the topological structure \mathscr{A} (i.e., the neighborhood relationships) allowing their interactions. The subsystems (in particular, the components of the system) are then identified with the cells of \mathscr{A} .

In this framework, the state of a $(DS)^2$ simply corresponds to the assignation of a (local) state to each component. The topology of \mathscr{A} restricts the possible transition functions of a subsystem *S*, as the current state of *S* only depends on the previous state of *S* and its neighbors. Now, however, *S* is not restricted to be one agent or one spatial element: it can be any arbitrary *population of agents* or an arbitrary *subspace*. Furthermore, the evolution function not only specifies the evolution of local states but also their coupled evolution with the topology itself.

Such a structure is well-known in algebraic topology: the state of a $(DS)^2$ can be represented by a *topological chain* that associates some values with each cell of the cellular complex [33].

Over the past half-century, there have been notable efforts to develop comprehensive formulations from physics and geometry based on topological chains. The use of chains and cochains to structure the modeling and simulation of physical systems can be traced back to at least the 1960's with Branin [6], who applied these notions to network analysis and circuit design. Later, Tonti and co-authors [56, 57] developed comprehensive discrete formulations of physical laws from first principles [40, 58]. Several studies have subsequently developed this approach in the field of physical modeling and computer-aided design (CAD), notably by Shapiro using the Chain programming language [45] and various follow-up works [8, 15, 12, 13]. Chains have also been used in numerical computation as a tool to structure and generalize the notion of "mesh" [4].

One major goal of these studies is to unravel a proper set of definitions and differential operators that make it possible to operate the machinery of multivariate calculus in a finite discrete space. The motivation is to find an equivalent calculus that operates intrinsically in discrete space, without the reference to the discretization of an underlying continuous process. This line of research is particularly developed in the field of "geometric modeling", with several recent achievements [11, 31].

However, these works do not focus on the modeling of dynamical structures in the way developed here. Their technical apparatus focuses on uniform computations and metric structures, whereas the MGS language (presented in the next section) re-

⁵ Although the interaction-based view could also be qualified as "spatial" because of the topological structure of \mathscr{A} , the term "spatial" will be used in this section to qualify only space-centered models referring to the physical space.

lies only on *combinatorial structures*. We believe that the combinatorial approach is less constrained, therefore potentially more amenable to algorithmic computations.

1.4 The MGS Approach to the Simulation of Morphogenesis

The discussion in the previous sections can be summarized by a simple slogan: *the specification of morphogenetic processes must be*

- *local*,
- interaction-based,
- on topological chains.

The idea is to describe the global dynamics of morphogenesis by summing up local evolutions triggered by local interactions that modify quantities associated to the topological cells of a cellular complex as well as the topological organization of these cells. In this setting, two subsystems S and S' do not interact because they are identified *per se* but because they are neighbors. This property enables the potential interaction of components that do not yet exist in the beginning of the simulation and do not know each other at their time of creation.

This approach has been instantiated in an experimental DSL for the modeling and simulation of morphogenesis, called MGS (which stands for "encore un Modèle Général de Simulation" in French, meaning "yet another general model of simulation"). For technical reasons, the algebraic structure needed on topological chains has been relaxed and the resulting structure is called a *topological collection*.

Transformations are used to define the interactions that make the system evolve. Transformations are functions acting on collections and defined by a specific syntax using rewriting rules. The mechanics of rewriting systems are familiar to anyone who has done arithmetic simplifications: an arithmetic expression can be simplified by repeatedly replacing parts of the expression, called *subexpressions*, with other subexpressions. For example, using the rule

$$\frac{x}{y} \cdot \frac{y}{z} \Rightarrow \frac{x}{z}$$

(where *x*, *y* and *z* are pattern variables representing arbitrary non-null numbers), the expression $\frac{7}{3} \cdot \frac{3}{11} \cdot \frac{11}{5}$ can be rewritten by successive applications of this rule as follows:

$$\frac{7}{3} \cdot \frac{3}{11} \cdot \frac{11}{5} \Longrightarrow \frac{7}{11} \cdot \frac{11}{5} \Longrightarrow \frac{7}{5}.$$

A "transformation" generalizes this process to topological collections with rules based on local interactions:

- the left-hand side of the rule (the "pattern") defines the elements in the system that interact;
- the right-hand side of the rule defines the fate of the elements in interaction.



Fig. 4 A *topological collection* is used to represent the state of a $(DS)^2$ at time *t*. An MGS transformation gathers one or several *rules* that specify the local evolution functions of the $(DS)^2$: the left-hand side of a rule defines a sub-collection of elements in interaction using a pattern matching mechanism; the right-hand side defines the evolution of this sub-collection. "Topological surgery" extends the notion of *substitution* used in rewriting systems to build the new state.

(Fig. 4). MGS rules are able to specify the evolution of the quantities associated to the cells of the underlying space as well as the cells and their topological organization.

2 Short Introduction to MGS

MGS embeds the idea of *topological collections* and *transformations* into the framework of a *dynamically typed, applicative* language. In our context, dynamically typed means that there is no static type-checking and that type errors are detected at run-time during evaluation. MGS is an applicative programming language: operators acting on values combine values to yield new values, they do not act by side-effect.

Collections constitute the only data structure available in MGS, i.e., the unique way of aggregating values with respect to some neighborhood relationship. Transformations are functions acting on collections and defined by a specific syntax using rules.

2.1 Topological Collections

A topological collection can be viewed as a slight generalization of the notion of *field*. In physics, a field is the assignment of a quantity to each point of a spatial domain [35]. MGS handles spatial domains defined by *abstract cellular complexes* [59].

We start by introducing the notion of abstract cellular complex (Section 2.1.1) and its use to implement topological collections. Then, we present *specific* instantiations of topological collections as different kinds of graphs:

- graphs without neighbors via *records* (Section 2.1.2)
- complete graphs via (*multi*)sets, and linear structures via sequences as members of the category of *monoidal collections* (Section 2.1.3)
- regular graphs via group-based fields (GBFs, Section 2.1.4)
- irregular graphs via *proximal collections*, i.e., neighborhood relationships generated by a distance function between elements (Section 2.1.5).

MGS provides topological collections based on abstract cellular complexes. This type of topological collections includes all the above types and extends to higher dimensions. Yet, specific types (such as monoidal collections, GBFs, or proximal collections) also have a usefulness because they correspond to specific topologies that can be implemented more efficiently.

Finally, we introduce a way to "glue" multiple collections of the same type, as it is often the case in nested topological collections, using *subtyping* (Section 2.1.6).

2.1.1 Abstract Cellular Complexes

An abstract cellular complex (ACC) is a formal construction that builds a space in a combinatorial way from simpler objects called *topological cells*. Each topological cell abstractly represents a part of the whole space: points are cells of dimension 0, lines are 1D cells, surfaces are 2D cells, etc. The structure of the whole space, corresponding to a partition into topological cells, is described by *incidence relationships*, which relate a cell to the other cells *in* its boundary.

More formally, an abstract cellular complex $K = (C, \prec, [\cdot])$ is a set C of abstract elements, called *cells*, provided with a partial order \prec , called the *incidence relation*, and with a *dimension* function $[\cdot] : C \to \mathbb{N}$ such that, for each *c* and *c'* in C: $c \prec c' \Rightarrow [c] < [c']$. We write $c \in K$ when a cell *c* is a cell of C. A cell of dimension *p* is called a *p*-cell. For example, graphs (which are made of only 0- and 1-cells) are examples of one-dimensional ACCs. Another example is depicted in Fig. 5.



Fig. 5 On the left, the Hasse diagram of boundary relationship of the ACC given in the middle: it is composed of three 0-cells (c_1, c_2, c_3) , of three 1-cells (e_1, e_2, e_3) and of a single 2-cells (f). The three edges are the faces of f, and therefore f is a common coface of e_1 , e_2 and e_3 . On the right, a topological collection associates data with the cells: positions with vertices, lengths with edges and area with f.



Fig. 6 The 0-cells *A* and *B* are 1-neighbors because they are faces of the 1-cell *E*. The 1-cells *E* and *F* are 0-neighbors because the 0-cell *B* is a common face. The sequence of 0-cells "A,B,C" is a (0,1)-path of length 3, and the sequence of 1-cells "E,F" is a (1,0)-path of length 3.

A *p*-cell *c* and a *q*-cell *c'* are said *incident* if one lies in the boundary of the other, i.e., $c \prec c'$ or $c' \prec c$. Particularly, *c* is a *face* of *c'*, which is denoted c < c', if they are incident and p = q - 1. Conversely, the cell *c'* is called a *coface* of *c*. An example of incidence relationship is commented in Fig. 5.

More elaborated neighborhoods can be defined from the incidence relationship. In MGS, the (n, p)-neighborhood is used: two cells c and c' are q-neighbor either if they have a common border of dimension q or if they are in the boundary of a qcell (of higher dimension). If the two cells are of dimension p, we say that they are (p,q)-neighbors. A (p,q)-path is a sequence of p-cells such that two consecutive cells are q-neighbors. For example, the usual notion of "path" in a graph, i.e., a sequence of vertices such that from each of them there is an edge to the next vertex in the sequence, corresponds to the notion of (0, 1)-path (Fig. 6).

Topological Collection of an ACC

Similar to a field that associates some quantity with the points of a spatial domain, a topological collection *C* of an ACC is a finite function labeling the cells of the ACC with a value (Fig. 5). Thus the notation C(c) refers to the value of *C* on cell *c*. Since a cellular complex may contain an infinite number of cells, we restrict ourselves to collections labeling a finite number of cells. We write |C| for the set of cells for which *C* is defined. The collection *C* can be written as a formal sum

$$\sum_{c \in |C|} v_c \cdot c, \text{ where } v_c \stackrel{\text{\tiny df}}{=} C(c).$$

With this notation, the underlying ACC is left implicit but can usually be recovered from the context. By convention, when we write a collection *C* as a sum

$$C = v_1 \cdot c_1 + \dots + v_p \cdot c_p,$$

we stress that all c_i are distinct. Notice that this addition is associative and commutative. The above notation is used directly in MGS to build new topological collections on arbitrary ACCs of any dimension.

Topological collections are a weakened version of the notion of *topological chain* developed in algebraic topology [43]. They were introduced in [24] to describe arbitrary complex spatial structures that appear in biological systems [25], and other dynamical systems with a time varying structure [18, 29]. From the viewpoint of computer science, topological collections are reminiscent of *data-fields*, studied e.g. by B. Lisper [32]. Data-fields are a generalization of the "array" data structure, in

which the set of indices is extended to finite subsets of \mathbb{Z}^n (see also [20]). With topological collections, in contrast, the underlying space is arbitrary. In fact, the type of a topological collection is determined by the chosen ACC.

Graphs are a particularly important class of ACCs in MGS since it has been showed in [23] how customary data structures (sets, lists, vectors, trees) can be seen as graph-based topological collections: the elements in a data structure are the quantities assigned by the collection to the nodes of a graph; the incidence relationship correspond to the edges of the graph and allows the usual data traversal.

In addition to scalar values (such as symbols, Booleans, integers, floats, strings, or lambda-expressions), the current implementation of MGS allows the programmer to handle several types of collections. The elements in a collection can be any type of values, including collections, thus achieving complex objects in the sense of [7]. Through examples, we informally sketch out in the next sections the collection types that we use.

2.1.2 Records

An MGS record is a map that associates a value with a name called a *slot*. The value can be of any type, including other records or collections. Accessing the value of a slot from a record is achieved with the dot notation: expression $\{a=1, b="red"\}$.b evaluates to the string "red". New types of records can be defined using a specific syntax: for instance, record $T = \{a:int, b:string\}$ defines a type T of records in which slots a and b are respectively labeled by an integer and a string.

The topologies associated with records are the "totally disconnected" ones: slots in records have no neighbors. Seen as graphs, records' vertices correspond to the slots and labels to the values associated with the slots—but they have no edges.

2.1.3 Monoidal Collections

A specific neighborhood relationship that plays an important role in the rest of this chapter is the *full relation*. With this relation, every element in the collection is a neighbor of all the other elements. This corresponds to the *multiset* data structure.

Multisets, along with sets and sequences, are called *monoidal collections* because they can be built as monoids equipped with the *join* operator. A sequence corresponds to a join operation that has no special property except associativity; multisets are obtained with an associative and commutative join; and sets when the join operator is associative, commutative and idempotent. The join operator with its properties induces the topology of the collection and its associated neighborhood relationship. It is a linear graph for sequences and a complete graph for sets and multisets.

We write a::m to add a value a in a monoidal collection m. The notations seq:(), bag:() and set:() refer to the empty sequence, the empty multiset and the empty set, respectively.



Fig. 7 (Left) A GBF defining a NEWS grid, with two generators e and n. (Right) A GBF defining an hexagonal grid with three generators e, n and nw, and a constraint n - nw = e.

2.1.4 Group-Based Fields

Topological collections can be defined as *Group-Based Fields* (GBF), which are considered as associative arrays whose indices are elements of a group [17]. The latter is defined by a *finite presentation*, i.e., a set of generators together with some constraints on their combination. Thus a GBF can be pictured as a labeled graph where the underlying graph is the Cayley graph of the finite presentation. The labels are the values associated with the vertices and the generators are associated with the edges.

For instance, in order to define a NEWS grid (a rectangular lattice in which each node has four neighbors) we may use two generators e (east) and n (north), supporting addition, difference and multiplication by an integer, as illustrated in Fig. 7a.

Similarly, an hexagonal grid (6 neighbors for each vertex) can be defined by means of three generators n, e and nw (north-west) and a constraint n - nw = e, as illustrated in Fig. 7b. Notice that such grid is adequate to represent cells with a hexagonal shape, since the grid can be paved with hexagons centered on the positions in the grid. As shown by the dashed path, we have $2 \cdot n + e = 2 \cdot e + n + nw$, which can be also checked in an algebraic way, by substituting nw with n - e in this equality as allowed by the constraint.

The GBF structure is thus adequate to define the arrangement of a grid, in any number of dimensions. A GBF type is specified by the presentation of the underlying group: a list of generators and a list of equations. For example, in the case of the hexagonal grid:

gbf H = < n, e, nw; nw + e = n >

MGS only handles Abelian groups, thus the commutation equations are implicit and we use an additive notation.

The relationships between Cayley graphs and group theory are pictured in Fig. 8. A word (a sum of generators) is a path. Path composition corresponds to the group addition. A closed path (a cycle) is a word equal to 0 (the identity of the group). An equation v = w can be rewritten v - w = e and corresponds to a cycle in the



Fig. 8 Graphical representation of the relationships between Cayley graphs and group theory. The GBF pictured here is G = <n, e> (the equations specifying the commutation between the generators are implicit). A node in this graph is an element of the group *G*. A path is a sum of generators and their inverses. The empty path is 0 and corresponds to the null displacement. In any Cayley graph, backtracking paths are closed paths. An equation corresponds to a closed path specific to the group structure. On the right, the diagram shows a closed path corresponding to the commutation between n and e, that is: n + e = e + n or, equivalently, n + e - e - n = 0.

graph. There are two types of cycles in the graph: cycles that are present in all Cayley graphs and correspond to group laws (intuitively: a backtracking path such as e + n - n - e) and closed paths specific to the group's own equations (e.g., e - n - e + n). In this framework, a graph connectivity property such as "there is always a path going from any node *P* to any node *Q*" is equivalent to saying that "there is always a solution *x* to equation P + x = Q".

2.1.5 Proximal Collections

Proximal collections are graphs whose neighborhood relationship is specified by a relation given on the elements of the collection (Fig 9). For example, let r be a relation on integers such that

fun r(x, y) = abs(y - x) < 10

Then, we are able to define a proximal collection as follows:

proximal MyProx = r

It means that two integers n and m are neighbors in a collection of type MyProx if and only if (iff) their "distance", as specified by r, is less than 10. We call r the *indicator relation* of a proximal collection such as MyProx.

2.1.6 User-Defined Subtypes

There is often a need to distinguish between collections of the same type (e.g., several multisets nested in another multiset). This can be accomplished by vari-



Fig. 9 A *proximal* collection is a set of elements equipped with a relation that defines which elements are neighbors. This sketch shows a set of 7 elements located in the 2D plane, in which two elements are neighbors iff the distance between them is below some constant.

ous means, among which we chose *subtyping*. The subtype of a collection can be thought of as a "color" that does not change the structure of the collection. A collection subtype declaration may look like:

```
collection MySet = set
and collection AnotherSet = set
and collection AnotherMySet = MySet[int]
```

This example specifies a hierarchy of three subtypes: *AnotherMySet* is a subtype of *MySet*, itself a subtype of set, and *AnotherSet* is also a subtype of set but is not comparable with *MySet*. Note that the above declaration allows restriction on the types of the elements: a set of subtype *AnotherMySet* can only contain integers.

For each type T, there is an associated predicate with the same name that can be used to check if a value has type T. For example, the expression MySet("thisis a string") returns false. Extra utility functions, such as querying the size, "pretty-printing", constructors or accessors, can also be instantiated when a type is defined.

2.2 Transformations

Usually in physics, fields and their evolution are specified using differential operators. MGS generalizes these operators in a rewriting mechanism called *transformation*. A transformation is the application of some local rules following some strategy. A transformation T is written as a set of rules:

trans $T = \{ \dots rule; \dots \}$

When there is only one rule in the transformation, the enclosing braces can be dropped. A rule is a basic transformation taking the following form:

 $pattern \implies expression$

It specifies a local evolution of the field: the left-hand side (lhs) of the rule typically matches elements in interaction, and the right-hand side (rhs) computes local updates of the field (Fig. 4). The application of a local rule $a \Rightarrow b$ in a collection *C*

- 1. selects a subcollection A that matches the pattern a,
- 2. computes a new subcollection *B* as the result of the evaluation of the expression *b* instantiated with the collection *A*, and
- 3. substitutes *B* for *A* in *C*.

This type of rewriting removes the part matched by the left-hand side and replaces it with the part computed by the right-hand side.

Transformations are a powerful way to define functions on topological collections that comply with the underlying spatial structure. For instance, a discrete analog of differential operators can be defined using transformations [29]. For multisets, transformations simply reduce to associative-commutative rewriting [10] also called multiset rewriting.

2.2.1 Patterns

We present here a subset of the MGS pattern language. These expressions have a generic meaning, i.e., they can be interpreted in any collection type. The grammar of these pattern expressions is:

$$pat := x \mid \{...\} \mid x, y \mid x < y \mid x: P \mid x/exp,$$

where *pat* and *pat'* are patterns, *x* ranges over the pattern variables, *P* is a predicate and exp is an expression evaluating to a Boolean value. The explanation below provides an informal semantics for these patterns.

Variables

A pattern variable x matches exactly one element in the topological collection. The variable x can then occur elsewhere in the rest of the rule to denote the value associated to the matched cell. The notation \hat{x} is used in the rest of the rule to denote the cell itself. Patterns are *linear*: two distinct pattern variables always refer to two distinct cells.

Record Patterns

The construction $\{...\}$ is used to match a record. The content of the braces can be used to match records with or without a specific field (eventually constrained to a given field type or field value). For instance, $\{a, b: string, c=3\}$ is a pattern that matches a record with fields a, b of type string and c with value 3.

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Neighborhoods

A pattern is a *composition* of pattern variables. There are three composition operators:

- 1. The composition denoted by a simple juxtaposition (such as "x y") does not constrain the arguments of the composition.
- 2. a. When two pattern variables are composed using a comma (as in "x, y"), it means that the cells matched by x and y must be *p*-neighbors. The default value for *p* is 1 and can be explicitly specified during the application of the transformation if needed.
 - b. When the collection is a GBF, it is possible to specify a particular direction for the neighborhood relationship: the pattern $x \mid n > y$ matches two elements x and y such that: if x labels the cell \hat{x} , then y labels the cell $\hat{x} + n$.
- 3. The last composition operator corresponds to the face operator: a pattern "x < y" (resp. "x > y") matches two cells \hat{x} and \hat{y} such that $\hat{x} < \hat{y}$ (resp. $\hat{x} > \hat{y}$).

Guards

The expression pat/exp matches the subcollections matched by pat verifying exp. Pattern pat: P is a syntactic shortcut for (pat as x)/P(x). For instance, x:int matches an element x provided that x is an integer and y/y > 3 matches an element y provided that y > 3 holds (the operator > is overloaded and denotes the numeric comparison as well as the incidence relationship).

2.2.2 Rules, Transformations and Application Strategies

A transformation is a set of rules. When a transformation is applied to a collection, the default strategy is to apply the first rule as many times as possible in parallel (a rule can be applied if its pattern matches a subcollection). In the remaining collection, the second rule is applied as many times as possible in parallel with the first rule, and so on. This strategy is the *maximal parallel application strategy* used in L-systems or in Paun systems [46]. Several other strategies are available in MGS such as the *Gillespie application strategy* based on Gillespie's stochastic simulation algorithm used to model chemical reactions [52]. Strategies provide a fine control over the choice of the rules applied within a transformation. They are often non-deterministic, i.e., when applied to a collection *C*, only one of the possible outcomes (randomly chosen) is returned by the transformation.

A transformation T is a function like any other function and also a *first-class* value. It means that, e.g., a transformation can be passed as an argument to another function or returned as a result. This allows to compose transformations very easily, leading to a higher-order functional programming style.

The expression T(c) denotes the application of one transformation step to the collection *c*. A transformation step consists of applying the rules according to a specific rule application strategy. A transformation step can be effortlessly iterated:

T[iter = n](c) denotes the application of *n* transformation steps to *c*,

T[fix](c) applies the transformation T until a fixed point is reached.

Note that transformations are first class functions (which are first class value).

3 Growth of a T-Shape in MGS

In this section, we show MGS at work by elaborating three different versions of the same problem: the development of a T-shaped structure. This challenge has been proposed as a benchmark example in [3] to compare different *spatial computing* languages with each other, in particular how they behaved in three paradigmatic tasks: (a) the creation of a coordinate system, (b) the growth of a structure of a given shape, and (c) the patterning of this structure. Our interest here is to demonstrate the benefits of a DSL approach such as the MGS language, i.e., how the flexibility brought by the notions of "topological collection" and "transformation" makes it possible to accommodate various modeling styles and program reuse. To this aim, we will develop three models:

- one based on *cellular automata*'s regular space-time lattice (Section 3.1),
- one based on *proximal collections*, corresponding to an "amorphous medium" under asynchronous evolution (Section 3.2),
- one using *cellular complexes* in 2D, starting from an empty space (Section 3.3).

In all models, we assume that the T-shapes start developing from one or a few entities in two successive phases: in the first growth phase (FGP), the process follows a vertical direction to form the stem of the T. In the second growth phase (SGP), the two horizontal segments at the top of the T grow in parallel.

We will not elaborate here on the preliminary acquisition of "vertical" and "horizontal" directions, as this type of positional information is not the focus of our example. Therefore, in the cellular automata model, we will use an anisotropic neighborhood that makes these directions explicit; in the amorphous medium model, we will rely on the coordinates of each node; and in the cellular complex model, some cell walls will receive labels (which will be explicitly propagated) to guide the asymmetric growth. Obviously, acquiring positional information by local means in an initial symmetric medium is a problem in itself (see for instance [62, 44, 2, 14, 37]), but the implementation of the various algorithms proposed in the literature is relatively straightforward. All examples presented here are actual MGS programs (the MGS interpreter and documentation are accessible at http://mgs.spatial-computing.org).

Genetic Control

This part, shared by all three example models, corresponds to the "genetic control" of the growth. It describes the local state of an entity, which contains here two counters, cpt_V and cpt_H : the first counter regulates the duration of FGP (the stem of

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the T) and the second counter regulates the duration of SGP (the hat of the T). Thus a cell is simply a record with two counters:

record Cell = { cpt_V , cpt_H }

We define a constant called seed to represent the initial state at time t = 0:

let seed = { $cpt_V = 5$, $cpt_H = 3$ }

The FGP subtype is a cell with the additional constraint that the counter cpt_V be different from zero:

record FGP = Cell + { $cpt_V \neq 0$ }

Note that MGS types are highly expressive: although they can be dependent on certain values, they are neither inferred nor statically type-checked.

Then, a cell finds itself in the second growing phase SGP iff the first counter has reached zero but not the second counter:

record SGP = Cell + { $cpt_V = 0$, $cpt_H \neq 0$ }

We also need a value to represent an empty location in the cells' spatial organization. For this, we define both a symbol `Empty and a record Empty representing entities that do not possess any of the counter fields:

record Empty = { $\sim cpt_V$, $\sim cpt_H$ }

To manage the two counters, we rely on the functions NextFGP and NextSGP:

fun NextFGP (c:FGP) = c + { $cpt_V = c.cpt_V - 1$ } fun NextSGP (c:SGP) = c + { $cpt_H = c.cpt_H - 1$ }

The c:FGP group following the function name declares an argument c of type FGP (same for SGP). The + operator in the body of the functions denotes an asymmetric merge of records. The expression $r_1 + r_2$ computes a new record r with the slots of both r_1 and r_2 : r.a has the value of $r_2.a$ if the slot a is present in r_2 , else it has the value of $r_1.a$. The asymmetric merge enables updating a slot knowing only the slot to update: this makes it possible to further refine the record by adding new slots without changing the code that was already written.

3.1 Cellular Automaton Implementation

Spatial Specification

The model based on cellular automata (CA) starts by specifying the underlying lattice. In MGS, we use the GBF defining a NEWS grid:

gbf NEWS = < north, east >

To define an initial population, we use the function create_NEWS generated by the previous type definition. The arguments of this function are an initialization function and the range of the generators used to iterate over a set of nodes. More precisely, the expression

```
create_NEWS(f, p, q)
```

creates an instance of the GBF NEWS in which the node north^x + east^y is labeled⁶ by the value f(x,y) for $0 \le x < p$ and $0 \le y < q$. Hence, the initial state state0 is computed by

```
fun init (x, y) = if (x=5 and y=3) then seed else 'Empty let state0 = create_NEWS(11, 11, init)
```

The initial state is a 11×11 grid, where all nodes except one at position (5,3) are labeled by `Empty.

Evolution Rules

The evolution of the CA is specified by two rules, one for each phase FGP and SGP. According the first rule, a cell in the FGP state extends to a north neighbor if this neighbor is empty:

```
trans Rules = {
    c:FGP |north> 'Empty ⇒ c, NextFGP(c);
    c:SGP <east> 'Empty ⇒ c, NextSGP(c);
}
```

In the second rule, a cell invades its neighbor to the east or west if this neighbor is empty. The syntax <east> refers either to the |east> or to the <east| direction (where <east| = |-east>).

The two elements matched in the left-hand side of a rule are replaced by the two elements computed in the right-hand side. In this case, the first element c remains untouched and the second element changes from `Empty to a cell with a counter that has decreased with respect to c.

By default, a transformation applies as much as possible (in space) the rules of a transformation. Thus, one application of a transformation corresponds to one elementary synchronous evolution step of a CA. The application is iterated to compute the successive states of the system: Rules[fixpoint](state0) (a possible trajectory is illustrated in Fig. 10).

3.2 Proximal Collection Implementation

Spatial Specification

A proximal collection contains elements whose neighborhood is defined by a predicate. Here, the elements are located in a 2D plane and two points P and Q may interact if their relative distance is below 100:

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⁶ Note that node labels are not necessarily unique because two different sums may produce the same node (for instance in the hexagonal lattice). However, MGS ensures that each node is visited only once in the specified domain, even if the "coordinates" of the node are not unique.



Fig. 10 The first 9 steps of the CA evolution. During the transition between states 6 and 7 the same rule finds two mutually exclusive matches: dividing a cell to the right or dividing it to the left. They are concurrent because the central cell is "consumed" and cannot be used in another rule application during the same time step. Because of that, horizontal growth is asymmetric (one branch is always one step farther than the other). Which branch grows first is randomly chosen during rule matching. The final step (not displayed here) adds a cell to the left branch.

proximal AMORPH = fun n \rightarrow 100 > (n.x * n.x + n.y * n.y)

(the right-hand side is an anonymous function, a lambda expression in MGS notation). By sampling the point randomly, we obtain the usual amorphous medium [1]:

```
fun init (i, acc) = { x = random(100), y = random(100) }::acc
let state0 = (seed+{x=50, y=25}) :: fold(init, AMORPH:(), 999)
```

The fold applies to the integer 999. When an integer p is used where a collection is expected, it corresponds to a cardinal, i.e., a set of p elements from zero to p-1. Thus the above fold iterates 999 times. The accumulator is initialized with the value AMORPH:(), which denotes the empty collection of type AMORPH. During the iterations, a record with two random slots x and y is added to the accumulator acc. The insertion of a new element in the collection is denoted by :: (such operation exists

only for monoidal collections: this is the case of proximal collections, which are multisets of elements with a dedicated neighborhood function).

Evolution Rules

Two auxilliary predicates are used for the evolution function. The predicate north is true if its second argument is lower than the first (following the y direction) and if the distance following x is less than 2. The definition of $east_west$ is similar but we restrict the variation to the y axis:

```
fun north (n1, n2) = (n2.y < n1.y) & 2 > abs(n2.x-n1.x)
fun east_west (n1, n2) = 2 > abs(n2.y-n1.y)
```

The transformation implementing the evolution function contains two rules similar to the CA rules:

```
trans Rules = {
    n1:FGP, n2:Empty / north(n1, n2) ⇒ n1, n2+NextFGP(n1)
    n1:SGP, n2:Empty / east_west(n1, n2) ⇒ n1, n2+NextSGP(n1)
}
```

Two elements n1 and n2 match one of these rules iff

- they are neighbors (via the comma operator),
- the first element n1 satisfies a phase predicate,
- the second element n2 is an empty place (i.e., an Empty record with no cpt_V or cpt_H slots),
- n2 is to the north of n1 in the first rule, or to the east_west of n1 in the second rule (constraints achieved by specifying a "guard" using the "/" operator).

In the right-hand side of the rule, the elements that replace the elements matched in the left-hand side are computed by asymmetric merge of records: here, the counter of n2 is updated with the counter of n1 decreased by one (Fig. 11).

By default, the maximal parallel application strategy is used in the application of the rules. However, it is easy to trigger only one rule at each transformation, achieving a fully asynchronous evolution:

Rules[fixpoint, strategy=`asynchronous] (state0)

The MGS pattern matching engine randomizes the matching in order to achieve a non-deterministic evolution.



Fig. 11 Proximal collection evolution: (left) initial step, (center) two intermediate steps, (right) final step. FGP cells (stem growth) are shown in blue, SGP cells (hat growth) in black.

3.3 Cellular Complex Implementation

In the two previous examples (cellular automata and proximal collections), the T-shape grew in a preexisting medium. There was no actual "development", but rather a *patterning* process during which the building of the shape required the representation of "empty" places "to invade".

In contrast, the approach presented here builds the shape intrinsically, without relying on the organization of a predefined space. The spatial structure underlying this object is an ACC (see Section 2.1.1) using 2-cells to represent the basic entities.

Spatial Specification

We start from an initial state made of one rectangular face:

```
let state0 =
   letcell v1 = new_vertex()
   and
          v2 = new_vertex()
          v3 = new_vertex()
   and
   and
           v4 = new_vertex()
           e12 = new_edge(v1, v2)
   and
   and
           e23 = new_edge(v2, v3)
           e34 = new_edge(v3, v4)
   and
           e41 = new_edge(v4, v1)
   and
          f = new_acell(2, (e12, e23, e34, e41))
   and
in
     \{x = \dots, y = \dots \} * v1
   + { x = ..., y = ... } \star v2
   + \{ x = ..., y = ... \} * v3
   + { x = ..., y = ... } * v4
   + 'Basal * e12 + 'Apical * e34
   + 'Lateral * e23 + 'Lateral * e41
   + seed * f
```

The letcell construct introduces a recursive definition of related cells. The definition is recursive because if a cell c is the face of c', then c' is a coface of c. letcell takes care of completing the necessary information, e.g., in the previous statement, we specify only the face of f, implicitly adding f to the coface of the other cells. The new_vertex and new_edge operations are a shortcut for the general primitive

new_acell(dimension [, faces list [, cofaces list]])

where the lists of faces or cofaces are optional and can be partial. In summary, the whole statement takes the form:

```
letcell ...cell creation and bonding...
in collection-specification
```

where the collection specification builds a collection using the cells introduced by the let command (and other cells, if needed). Finally, the ACC is built using the notation v*c, which associates value v to cell c, and the addition + to amalgamate all labeled cells.



Fig. 12 (a) The initial state is a 2-cell and its faces. (b) A face and its corresponding edges exert forces on the vertices at their boundaries.

In the above expression, a record of positions x and y is associated to the vertices, and the edges are labeled by symbols distinguishing among three types of edges (Fig. 12a). The idea is that growth takes place on the `Apical side during FGP and along the `Lateral sides during SGP.

Evolution Rules

We first specify the transformation used to compute the "mechanics" of the system. For the sake of simplicity, we resort to mass-spring systems and Aristotelian mechanics (i.e., force proportional to speed, not acceleration). This avoids the burden of double integration and does not change the results, because we are only interested in the final steady state. Every edge is a spring with resting length L0 and coefficient k. The transformation

```
let sum (acc, v) = { x=acc.x+v.x, y=acc.y+v.y }
trans<2> MecaFace[k, L0, dt] = {
    f ⇒ let n = cardinal(icells(f̂, 0)) in
        let g = icellsfold(sum, {x=0.0, y=0.0}, f̂, 0)
        in f + { x = g.x/n, y = g.y/n }
}
```

only matches the 2-cells (this is specified by <2> after the trans keyword). Parameters k, L0 and dt are additional arguments of the transformation. For each cell f the number of 0-cells in its border is computed: \hat{f} refers to the cell matched by the pattern variable f, and the expression icells (\hat{f} , 0) returns the set of faces of \hat{f} of dimension 0 ("i" stands for "incident"). Operator cardinal returns the number of elements in the set, while primitive icellsfold serves to iterate over the 0-cells in the border of \hat{f} . The reduction function is used to compute the center of mass of the corners of parallelogram f.

The next snippet of code integrates the forces and updates accordingly the position of the vertices (Fig. 12b):

```
let dist (v, v') =
    let d1 = v'.x - v.x and d2 = v'.y - v.y
    in sqrt(d1*d1 + d2*d2)
```

```
let suml (v, acc, v') =
    let d = dist(v, v') in
    let f = k * (d - L0) / d
    in { x=acc.x+f*(v'.x-v.x), y=acc.y+f*(v'.y-v.y) }
let sum2(k, v, acc, f') =
    let d = dist(f', v) in
    let f = k * (d - sqrt(2.0)*L0) / d
    in { x=acc.x+f*(f'.x-v.x), y=acc.y+f*(f'.y-v.y) }
trans<0,1> MecaVertex[k, L0, dt] = {
    v ⇒ let Fspring= neighborsfold(sum1(v), {x=0.0, y=0.0}, v) in
        let Ftot = icellsfold(sum2(k, v),Fspring, v̂, 2)
        in v + { x=v.x+dt*Ftot.x, y=v.y+dt*Ftot.y }
}
```

The qualifier <0,1> means that we focus on 0-cells and that the neighborsfold operation relies on a notion of neighborhood such that two 0-cells are neighbors iff they are in the border of a common 1-cell (i.e., linked by an edge). The variable Fspring corresponds to the summation of the spring forces, while Ftot iterates on the cofaces of dimension 2 of \hat{v} (there can be several such faces, for instance at the junction of the lines forming the T). The idea is that each 2-cell exerts an internal pressure from the inside to the outside, constraining the parallelogram to be convex. The initial value of the fold is given by the forces computed with Fspring. The "in" expression, simply integrates the total forces over a time step *dt*.

The reduction functions sum1 and sum2 used in the folds are only partially invoked: for example, the last two arguments of functions sum1 and sum2 are in common (here: acc, v') and provided by default by neighborsfold, so only sum1(v) and sum2(k, v) are called.

The full mechanical evolution is simply given by computing one evolution step of the face and one evolution step of the vertices:

fun Meca(ch) = MecaVertex(MecaFace(ch))

There is one additional transformation to compute the cell division:

```
trans Extrude = {
   \simv1 < e12 < \simf:FGP > e12 > \simv2
   /(2 = \dim(f)) \& (e12 = `Apical)
   \Rightarrow letcell v3 = new_vertex ()
      and v4 = new_vertex ()
      and e23 = new_edge(v2, v3)
      and e34 = new_edge(v3, v4)
      and e41 = new_edge(v4, v1)
      and e12' = new_edge(v1, v2)
      and f' = new_acell(2, (e12,e23,e34,e41))
      in
           (v_2 + \{ x = v_2.x + (v_2.x - f.x) * random(0.1), \}
                    y = v2.y + (v2.y-f.y) * random(0.1)  * v3
          + (v1 + \{ x = v1.x + (v1.x-f.x) * random(0.1) \}
                    y=v1.y + (v1.y-f.y) * random(0.1) }) * v4
          + 'Internal * e12'
          + 'Lateral * e23 + 'Lateral * e41
         + 'Apical * e34
          + (NextFGP f) * f'
```

In this code, a pattern $\sim v$ matches one element but this element can also be matched by another pattern (in the same transformation but not necessarily the same rule). Contrary to the classical pattern v, such elements are not removed from the result. The first pattern

~v1 < e12 < ~f:FGP > e12 > ~v2 / (2=dim(f)) & (e12= 'Apical)

matches one face f, which must be FGP, one edge e12 labeled by the symbol 'Apical, and the two vertices bounding e12. The vertices and the face remain in the result but the edge is removed. The right-hand side builds several new cells that replace e12 (and updates the neighborhood relationships of the remaining cells).

What is built on the right-hand side is a parallelogram (new face f'). The edge e12' replaces edge e12 and is now labeled by the symbol `Internal to prevent further development. The "opposite" edge e23 is labeled by `Apical in the first growth phase FGP and `Lateral in the second growth phase SGP.

The labels of v3 and v4 are the labels of v2 and v1, respectively, but updated to have new positions. These positions are computed from the previous positions shifted by a small random noise. The parallelogram will soon unfold by mechanical evolution in accordance with the internal pressure and the spring force.



Fig. 13 Growth of the T-shape using cellular complexes. (Top left) initial state, (bottom right) final state. Times flows from left to right and from top to bottom. In the center row, the images in the middle and the right show the mechanical relaxation after a cell division.

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}

The complete evolution of the system is obtained by composing an extended period of mechanical iteration (here, we arbitrarily chose 200 steps) with a single growth step:

fun Step(ch) = Extrude(Meca[iter=200](ch))

Snapshots of the trajectory are given in Fig. 13.

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References

- Abelson, H., Allen, D., Coore, D., Hanson, C., Homsy, G., Knight Jr, T., Nagpal, R., Rauch, E., Sussman, G., Weiss, R.: Amorphous computing. Communications of the ACM 43(5), 74–82 (2000)
- Beal, J., Bachrach, J., Vickery, D., Tobenkin, M.: Fast self-healing gradients. In: Proceedings of the 2008 ACM symposium on Applied computing, pp. 1969–1975. ACM (2008)
- Beal, J., Dulman, S., Usbeck, K., Viroli, M., Correll, N.: Organizing the aggregate: Languages for spatial computing. CoRR abs/1202.5509 (2012)
- Berti, G.: Generic programming for mesh algorithms: Towards universally usable geometric components. In: H.A. Mang, F.G. Rammerstorfer, J. Eberhardsteiner (eds.) Proceedings of the Fifth World Congress on Computational Mechanics (WCCMV. IACM (2002)
- Bigo, L., Giavitto, J.L., Spicher, A.: Building topological spaces for musical objects. In: Mathematics and Computation in Music, *LNCS*, vol. 6726. Springer, Paris, France (2011)
- Branin, F.: The algebraic-topological basis for network analogies and the vector calculus. In: Symposium on generalized networks, pp. 453–491 (1966)
- Buneman, P., Naqvi, S., Tannen, V., Wong, L.: Principles of programming with complex objects and collection types. Theoretical Computer Science 149(1), 3–48 (1995)
- Chard, J.A., Shapiro, V.: A multivector data structure for differential forms and equations. Math. Comput. Simul. 54(1-3), 33–64 (2000). DOI http://dx.doi.org/10.1016/S0378-4754(00) 00198-1
- Chopard, B., Droz, M., Press, C.U.: Cellular automata modeling of physical systems, vol. 122. Cambridge University Press Cambridge (1998)
- Dershowitz, N., Hsiang, J., Josephson, N., Plaisted, D.: Associative-commutative rewriting. In: Proceedings of the Eighth international joint conference on Artificial intelligence-Volume 2, pp. 940–944. Morgan Kaufmann Publishers Inc. (1983)
- Desbrun, M., Kanso, E., Tong, Y.: Discrete differential forms for computational modeling. In: Discrete differential geometry: an applied introduction, pp. 39–54. Schroder, P (2006). SIGGRAPH'06 course notes
- DiCarlo, A., Milicchio, F., Paoluzzi, A., Shapiro, V.: Solid and physical modeling with chain complexes. In: Proceedings of the 2007 ACM symposium on Solid and physical modeling, pp. 73–84. ACM (2007)

- DiCarlo, A., Milicchio, F., Paoluzzi, A., Shapiro, V.: Discrete physics using metrized chains. In: 2009 SIAM/ACM Joint Conference on Geometric and Physical Modeling, pp. 135–145. ACM (2009)
- Doursat, R.: Programmable architectures that are complex and self-organized: From morphogenesis to engineering. In: Artificial Life XI: Proceedings of the 11th International Conference on the Simulation and Synthesis of Living Systems (Alife XI), pp. 181–188. MIT Press (2008)
- Egli, R., Stewart, N.F.: Chain models in computer simulation. Math. Comput. Simul. 66(6), 449–468 (2004). DOI http://dx.doi.org/10.1016/j.matcom.2004.02.017
- Ermentrout, G., Edelstein-Keshet, L.: Cellular autornata approaches to biological modeling. J. theor. Biol 160, 97–133 (1993)
- Giavitto, J., Michel, O.: Declarative definition of group indexed data structures and approximation of their domains. In: Proceedings of the 3rd ACM SIGPLAN international conference on Principles and practice of declarative programming, pp. 150–161. ACM (2001)
- Giavitto, J.L.: Topological collections, transformations and their application to the modeling and the simulation of dynamical systems. In: 14th International Conference on Rewriting Technics and Applications (RTA'03), *LNCS*, vol. 2706, pp. 208–233. Springer, Valencia (2003)
- Giavitto, J.L.: The modeling and the simulation of the fluid machines of synthetic biology. In: M. Gheorghe, G. Paun, G. Rozenberg, A. Salomaa, S. Verlan (eds.) Membrane Computing - 12th International Conference, CMC 2011, Fontainebleau, France, August 23-26, 2011, Revised Selected Papers, *LNCS*, vol. 7184, pp. 19–34. Springer (2012)
- Giavitto, J.L., De Vito, D., Sansonnet, J.P.: A data parallel Java client-server architecture for data field computations over Zⁿ. In: EuroPar'98 Parallel Processing, *Lecture Notes in Computer Science*, vol. 1470, pp. 742–745 (1998)
- Giavitto, J.L., Malcolm, G., Michel, O.: Rewriting systems and the modelling of biological systems. Comparative and Functional Genomics 5, 95–99 (2004)
- Giavitto, J.L., Michel, O.: Mgs: a rule-based programming language for complex objects and collections. In: M. van den Brand, R. Verma (eds.) Electronic Notes in Theoretical Computer Science, vol. 59. Elsevier Science Publishers (2001)
- Giavitto, J.L., Michel, O.: Data structure as topological spaces. In: Proceedings of the 3nd International Conference on Unconventional Models of Computation UMC02, vol. 2509, pp. 137–150. Himeji, Japan (2002). LNCS
- Giavitto, J.L., Michel, O.: The topological structures of membrane computing. Fundamenta Informaticae 49, 107–129 (2002)
- Giavitto, J.L., Michel, O.: Modeling the topological organization of cellular processes. BioSystems 70(2), 149–163 (2003)
- Giavitto, J.L., Michel, O., Cohen, J., Spicher, A.: Computation in space and space in computation. In: Unconventional Programming Paradigms (UPP'04), *LNCS*, vol. 3566, pp. 137–152. Spinger, Le Mont Saint-Michel (2005)
- 27. Giavitto, J.L., Michel, O., Spicher, A.: Interaction based simulation of dynamical system with a dynamical structure. In: P. Kropf (ed.) proc. of the Summer Computer Simulation Conference (SCSC 2011), vol. Track: Modeling and Simulation of Dynamic Structure Systems. The Society for Modeling and Simulation International (SCS) & ACM, Curran assoc. inc. (2011)
- Giavitto, J.L., Spicher, A.: Simulation of self-assembly processes using abstract reduction systems. In: N. Krasnogor, S. Gustafson, D. Pelta, J.L. Verdegay (eds.) Systems Self-Assembly: multidisciplinary snapshots, pp. 199–223. Elsevier (2008). Doi:10.1016/S1571-0831(07)00009-3
- Giavitto, J.L., Spicher, A.: Topological rewriting and the geometrization of programming. Physica D 237(9), 1302–1314 (2008). DOI http://dx.doi.org/10.1016/j.physd.2008.03.039
- Giavitto, J.L., Spicher, A.: Morphogenesis: Origins of Patterns and Shapes, chap. Computer Morphogeneis, pp. 315–340. Springer (2011)
- Grady, L., Polimeni, J.: Discrete Calculus: Applied Analysis on Graphs for Computational Science. Springer (2010)

- Hammarlund, P., Lisper, B.: On the relation between functional and data parallel programming languages. In: Proceedings of the conference on Functional programming languages and computer architecture, pp. 210–219. ACM (1993)
- 33. Hocking, J.G., Young, G.: Topology. Dover publications, New-York (1988)
- Kubera, Y., Mathieu, P., Picault, S.: Interaction-oriented agent simulations: From theory to implementation. In: Proceeding of the 2008 conference on ECAI 2008: 18th European Conference on Artificial Intelligence, pp. 383–387. IOS Press (2008)
- Leavens, G.T.: Fields in physics are like curried functions or physics for functional programmers. Tech. Rep. TR94-06b, Iowa State University, Department of Computer Science (1994)
- Lindenmayer, A.: Mathematical models for cellular interaction in development, Parts I and II. Journal of Theoretical Biology 18, 280–315 (1968)
- Maignan, L., Gruau, F.: Integer gradient for cellular automata: Principle and examples. In: Second IEEE International Conference on Self-Adaptive and Self-Organizing Systems, SASO 2008., pp. 321–325. IEEE (2008)
- Mamei, M., Zambonelli, F.: Field-based coordination for pervasive multiagent systems. Springer-Verlag New York Inc (2006)
- Mamei, M., Zambonelli, F., Leonardi, L.: Co-fields: Towards a unifying approach to the engineering of swarm intelligent systems. Engineering Societies in the Agents World III pp. 77–98 (2003)
- Mattiussi, C.: The finite volume, finite element, and finite difference methods as numerical methods for physical field problems. Advances in Imaging and Electron Physics 113, 1–146 (2000)
- Mernik, M., Heering, J., Sloane, A.: When and how to develop domain-specific languages. ACM computing surveys (CSUR) 37(4), 316–344 (2005)
- 42. Michel, O., Spicher, A., Giavitto, J.L.: Rule-based programming for integrative biological modeling application to the modeling of the λ phage genetic switch. Natural Computing **8**(4), 865–889 (2009)
- 43. Munkres, J.: Elements of Algebraic Topology. Addison-Wesley (1984)
- Nagpal, R., Shrobe, H., Bachrach, J.: Organizing a global coordinate system from local information on an ad hoc sensor network. In: Proceedings of the 2nd international conference on Information processing in sensor networks, *IPSN'03*, vol. LNCS 2634, pp. 333–348. Springer-Verlag (2003)
- Palmer, R.S., Shapiro, V.: Chain models of physical behavior for engineering analysis and design. Research in Engineering Design 5, 161–184 (1993). Springer International
- 46. Păun, G.: Membrane Computing. An Introduction. Springer-Verlag, Berlin (2002)
- Prusinkiewicz, P., Hanan, J.: Visualization of botanical structures and processes using parametric L-systems. In: D. Thalmann (ed.) Scientific visualization and graphics simulation, pp. 183–201. J. Wiley & Sons, Chichester (1990)
- Barbier de Reuille, P., Bohn-Courseau, I., Ljung, K., Morin, H., Carraro, N., Godin, C., Traas, J.: Computer simulations reveal properties of the cell-cell signaling network at the shoot apex in Arabidopsis. PNAS **103**(5), 1627–1632 (2006). DOI 10.1073/pnas.0510130103
- Rozenberg G. an Schürr, A., Winter, A.J., Zündorf, A., Ehrig, H., Kreowski, H.J., Montanari, U. (eds.): Handbook of graph grammars and computing by graph transformation, vol. 1: Foundations, vol. 2: Applications, vol. 3: Concurrency, Parallelism, and Distribution. World Scientific (1997)
- Spicher, A., Michel, O.: Using rewriting techniques in the simulation of dynamical systems: Application to the modeling of sperm crawling. In: Fifth International Conference on Computational Science (ICCS'05), part I, *LNCS*, vol. 3514, pp. 820–827. Springer, Atlanta, GA, USA (2005)
- Spicher, A., Michel, O.: Declarative modeling of a neurulation-like process. BioSystems 87(2-3), 281–288 (2007)
- Spicher, A., Michel, O., Cieslak, M., Giavitto, J.L., Prusinkiewicz, P.: Stochastic p systems and the simulation of biochemical processes with dynamic compartments. BioSystems 91(3), 458–472 (2008)

- Spicher, A., Michel, O., Giavitto, J.L.: Algorithmic self-assembly by accretion and by carving in MGS. In: Proc. of the 7th International Conference on Artificial Evolution (EA'05), *LNCS*, vol. 3871, pp. 189–200. Springer-Verlag (2005)
- Spicher, A., Michel, O., Giavitto, J.L.: Interaction-based simulations for integrative spatial systems biology. In: W. Dubitzky, J. Southgate, H. Fuss (eds.) Understanding the Dynamics of Biological Systems: Lessons Learned from Integrative Systems Biology. Springer Verlag (2011)
- Toffoli, T., Margolus, N.: Cellular automata machines: a new environment for modeling. MIT Press, Cambridge (1987)
- 56. Tonti, E.: On the mathematical structure of a large class of physicial theories. Rendidiconti della Academia Nazionale dei Lincei 52(fasc. 1), 48–56 (1972). Scienze fisiche, matematiche et naturali, Serie VIII
- 57. Tonti, E.: The reason for analogies between physical theories. Appl. Math. Modelling 1, 37–50 (1976)
- Tonti, E.: A direct discrete formulation of field laws: The cell method. Computer Modeling in Engineering & Sciences 2(2), 237–258 (2001)
- 59. Tucker, A.: An abstract approach to manifolds. The Annals of Mathematics **34**(2), 191–243 (1933)
- Turing, A.M.: The chemical basis of morphogenesis. Phil. Trans. Roy. Soc. of London Series B: Biological Sciences(237), 37–72 (1952)
- Van Deursen, A., Klint, P., Visser, J.: Domain-specific languages: An annotated bibliography. ACM Sigplan Notices 35(6), 26–36 (2000)
- 62. Wolpert, L.: Positional information and the spatial pattern of cellular differentiation. Journal of theoretical biology **25**(1), 1–47 (1969)