Algebraic structures generating reaction-diffusion models: the activator-substrate system

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Abstract
We shall construct a class of nonlinear reaction-diffusion equations starting from an infinitesimal algebraic skeleton. Our aim is to explore the possibility of an algebraic foundation of integrability properties and of stability of equilibrium states associated with nonlinear models describing patterns formation.

Key words: reaction-diffusion; activator-substrate; integrability; algebraic structure; nonlinear model; skeleton; tower.

1 Introduction
In his famous paper, Turing suggested that a system of chemical substances reacting together and diffusing through a tissue, could describe the main phenomena of morphogenesis [13]. In particular, in his work it was emphasized that patterns could appear if one of the substances diffuses much faster than the other. Nonlinear reaction-diffusion systems have been then proposed to answer the question about how do cells, under the influence of their common genes, could produce spatial patterns, see e.g. [3] and references therein. They consist in models describing generation of patterns from an initially homogeneous state taking into account the relevance of chemical gradient in biological systems, in particular nonlinear interaction of two chemicals and their diffusion. Patterns formation turns out then to be the output of local self-enhancement such as local autocatalysis and long range inhibition. A simple model proposed by Koch & Meinhardt is the activator-substrate systems (constituted by a self-enhanced reactant and a depleted reactant which plays the role of the antagonist). In the simplest mathematical form, only few relevant parameters characterize the model: the normalized diffusion constant and the normalized cross-reaction coefficient. In particular, the inhibition due to the substrate reactant can be effective if the normalized diffusion constant is << 1 (that means the diffusion constant of the activator should be much lesser than the diffusion constant of the substrate), a necessary condition for the generation of stable patterns.
The scope of this work is to propose an algebraic form of the local mechanisms expressed by reaction-diffusion partial differential equations. Our results are based on the observation that two fundamental aspects are involved in pattern formations: symmetries on the one side (algebraic content) and changes in time and space on the other side (differential content).

Our considerations are based on the well known duality between linear differential forms and tangent vector fields on manifolds, and make use of algebraic and geometric techniques developed within a theoretical physics framework, see e.g. [2, 12, 9, 10, 11], in particular suitable generalization of the structure equations of a Lie group. In the present note, we show that parameters in a model can be introduced algebraically within an algebraic-geometric formulation in terms of integrable towers with infinitesimal algebraic skeletons.

2 Algebraic structures

Let us first recall a few mathematical tools constituting the background for a detailed treatment of which we refer to [9, 10, 11] and [7, 12]; the use of the concept of tower with skeleton has been inspired by (and is a mathematical generalization of) the procedure outlined in [4].

In particular, on the side of symmetry (algebraic content), we need to introduce, a notion which generalizes the concept of a homogeneous space, i.e. that of an algebraic skeleton on a finite-dimensional vector space $V$ as a triple $(E, G, \rho)$, with $G$ a (possibly infinite-dimensional) Lie group, $E = g \oplus V$ is a (possibly infinite-dimensional) vector space not necessarily equipped with a Lie algebra structure, $g$ is the Lie algebra of $G$, and $\rho$ is a representation of $g$ on $E$ such that it reduces to the adjoint representation of $g$ on itself. The fact that $E$ is not a direct sum of Lie algebras, but an open algebraic structure is fundamental in order to be able to generate whole families of nonlinear differential systems, starting from it.

We now consider a suitably constructed differentiable structure which is somehow modelled on the skeleton above. Let us introduce a differentiable manifold $P$ on which a Lie group $G$, with Lie algebra $g$, acts on the right; $P$ is a principal bundle $P \to Z \simeq P/G$. By construction, we have that $Z$ is a manifold of type $V$, i.e. $\forall z \in Z, T_z Z \simeq V$. Suppose we have a way to define a representation $\rho$ of the Lie algebra $g$ on $T_z Z$, in such a way that it could be possible under certain conditions to find an homomorphism between the open infinite dimensional Lie algebra, that we can construct in such a way, and a quotient Lie algebra (we can think the direct sum of the quotient Lie algebra so obtained with $g$ as a (possibly infinite dimensional) Lie algebra, let us call it $\mathfrak{k}$. From the differentiable side, a tower $P(Z, G)$ on $Z$ with skeleton $(E, G, \rho)$ is an absolute parallelism $\omega$ on $P$ valued in $E$, invariant with respect to $\rho$ and reproducing elements of $g$ from the fundamental vector fields induced on $P$. Let then $\mathfrak{k}$ be a Lie algebra and $\mathfrak{g}$ a Lie subalgebra of $\mathfrak{k}$. Let $G$ be a Lie group with Lie algebra $g$ and $P(Z, G)$ be a principal fiber bundle with structure group $G$ over a manifold $Z$ as above. A Cartan connection in $P$ of type $(\mathfrak{k}, G)$ is a
1–form \( \omega \) on \( P \) with values in \( \mathfrak{t} \) such that \( \omega|_{T_pP} : T_pP \to \mathfrak{t} \) is an isomorphism \( \forall p \in P, R^g_\ast \omega = Ad(g)^{-1} \omega \) for \( g \in G \) and reproducing elements of \( \mathfrak{g} \) from the fundamental vector fields induced on \( P \). It is clear that a Cartan connection \((P, Z, G, \omega)\) of type \((\mathfrak{t}, \mathfrak{g})\) is a special case of a tower on \( Z \). In the following, we shall be interested in the case when from a tower one can construct a Cartan connection by a quotienting.

### 2.1 The underlying skeleton

Consider the following infinite dimensional vector space \( E = \mathfrak{g} \oplus V \)

\[
\begin{align*}
[\psi_1, \psi_2] &= 0, [\psi_1, \psi_3] = 0, [\psi_1, \psi_4] = 0, [\psi_1, \psi_5] = 0, \\
[\psi_1, \psi_6] &= 0, [\psi_1, \psi_7] = 0, [\psi_1, \psi_8] = 0, \\
[\psi_2, \psi_3] &= -2D\psi_6, [\psi_2, \psi_4] = 2D\psi_7, [\psi_2, \psi_5] = 0, [\psi_2, \psi_6] = -2D\psi_2, \\
[\psi_2, \psi_7] &= 0, [\psi_2, \psi_8] = [\psi_4, \psi_6] + [\psi_3, \psi_7] \\
[\psi_3, \psi_4] &= 2D\psi_8, [\psi_3, \psi_5] = 0, [\psi_3, \psi_6] = 2\kappa D\psi_3, \\
[\psi_3, \psi_7] &= [\psi_2, \psi_8] - [\psi_4, \psi_6], [\psi_3, \psi_8] = 0, \\
[\psi_4, \psi_5] &= 0, [\psi_4, \psi_6] = D[\psi_1, \psi_5], [\psi_4, \psi_7] = [\psi_2, \psi_5] - 2D\psi_2, \\
[\psi_4, \psi_8] &= D[\psi_3, \psi_5] \\
[\psi_5, \psi_6] &= [\psi_2, [\psi_3, \psi_5]], [\psi_5, \psi_7] = [\psi_4, [\psi_3, \psi_5]], \\
[\psi_5, \psi_8] &= [\psi_4, [\psi_3, \psi_5]] \\
[\psi_6, \psi_7] &= 2D\psi_7 - [\psi_1, [\psi_2, \psi_5]], [\psi_6, \psi_8] = -2\kappa D\psi_8 - D[\psi_3, [\psi_1, \psi_5]] \\
[\psi_7, \psi_8] &= [\psi_4, [\psi_3, \psi_7]] - [\psi_3, [\psi_4, \psi_7]].
\end{align*}
\]

Notice that the commutators \([\psi_1, \psi_5], [\psi_2, \psi_5], [\psi_3, \psi_5] \) are not defined and in particular that even introducing new generators \( \psi_9, \psi_{10}, \psi_{11} \), the algebra anyway does not close as a Lie algebra. It is also important to stress that many other commutators between elements of the above vector space \( E \) are not defined as Lie algebra commutators since they are given in terms of \([\psi_1, \psi_5], [\psi_2, \psi_5], [\psi_3, \psi_5] \).

The vector space \( V \) is finite dimensional and generated by \([\psi_1, \psi_5], [\psi_2, \psi_5], [\psi_3, \psi_5], \psi_5 \). It has the property that each commutator of \([\psi_1, \psi_2], [\psi_1, \psi_3], [\psi_1, \psi_4], [\psi_1, \psi_6], [\psi_1, \psi_7], [\psi_1, \psi_8] \) (freely generating an infinite dimensional Lie algebra) with its generators is again in \( V \). We also notice that the commutator relations \([\psi_3, \psi_7] - [\psi_2, \psi_8] = D[\psi_1, \psi_5], [\psi_6, \psi_7] - 2D\psi_7 = [\psi_1, [\psi_2, \psi_5]], [\psi_6, \psi_8] + 2\kappa D\psi_8 = D[\psi_3, [\psi_1, \psi_5]], [\psi_4, \psi_7] + 2D\psi_2 = [\psi_2, \psi_5] \) and the related \([\psi_7, \psi_8] = [\psi_4, [\psi_3, \psi_7]] - [\psi_3, [\psi_4, \psi_7]] \) say that unknown commutators in the freely generated Lie algebra are related in such a way that their assigned relations are elements of \( V \). Therefore the algebraic relations above define an infinitesimal skeleton.

We define an homomorphism of the infinite dimensional freely generated Lie algebra with a quotient Lie algebra by fixing unknown commutators; we can do this either by fixing the value of \([\psi_1, \psi_5], [\psi_2, \psi_5], [\psi_3, \psi_5] \) as generated by elements in the freely generated Lie algebra, or by fixing the value of the unknown commutators \([\psi_2, \psi_5], [\psi_3, \psi_7], [\psi_4, \psi_7], [\psi_6, \psi_7], [\psi_6, \psi_8], \).
2.2 Homomorphisms with finite dimensional Lie algebras

We can find an homomorphism of the infinite dimensional open Lie algebra constructed starting from $E$ with a finite dimensional Lie algebra by taking the following quotient, with $\lambda$ a real parameter.

$$[\psi_3, \psi_7] = -\lambda \psi_4, \quad [\psi_3, \psi_4] = \lambda \psi_7, \quad [\psi_4, \psi_7] = \lambda \psi_3.$$  

We get then $\lambda \psi_7 = 2D\psi_8$, $[\psi_4, \psi_6] = \lambda \psi_4$, and, provided that $D \neq 0$,

$$[\psi_1, \psi_5] = \frac{\lambda}{D} \psi_4, \quad [\psi_2, \psi_5] = 2D\psi_2 + \lambda \psi_3, \quad [\psi_3, \psi_5] = \frac{\lambda}{D} \psi_3.$$  

Since we also have that $[\psi_4, \psi_8] = D[\psi_3, \psi_5]$ (see the skeleton), for the consistency of the relations, we get in particular $\lambda = 2D$; thus we can write

$$[\psi_7, \psi_3] = 2D\psi_4, \quad [\psi_3, \psi_4] = 2D\psi_7, \quad [\psi_4, \psi_7] = 2D\psi_3.$$  

It is easy to see that in this case the algebra closes as a Lie algebra

$$[\psi_1, \psi_5] = 2\psi_4, \quad [\psi_2, \psi_5] = 2D(\psi_2 + \psi_3), \quad [\psi_3, \psi_5] = 2\psi_3.$$  

Furthermore, since $\psi_7 = \psi_8$, then $[\psi_6, \psi_8] = -2\kappa D\psi_8 - D[\psi_3, [\psi_1, \psi_5]] = [\psi_6, \psi_7] = 0$ provides, by an iterated application of the Jacobi identity, the condition $-2\kappa D + 2D = 0$, then, if $D \neq 0$, we must have $\kappa = 1$, corresponding to activator and substrate having the same cross-reaction coefficients. Therefore we get

$$[\psi_2, \psi_3] = -2D\psi_6, \quad [\psi_3, \psi_6] = 2D\psi_3, \quad [\psi_2, \psi_6] = -2D\psi_2;$$  

however the consistency of $[\psi_5, \psi_7] = [\psi_4, [\psi_2, \psi_5]]$ and $[\psi_5, \psi_8] = [\psi_4, [\psi_3, \psi_5]]$ implies $D = \frac{1}{2}$, which corresponds to a closed Lie algebra (without a spectral parameter).

Let us then consider a different closing homomorphism by posing $\psi_8 = 0$ and $[\psi_3, \psi_7] = -\lambda \psi_4, [\psi_4, \psi_7] = \lambda \psi_3$. We get $[\psi_3, \psi_5] = 0$, $[\psi_4, \psi_6] = \lambda \psi_4$, and, in particular, provided that $D \neq 0$,

$$[\psi_1, \psi_5] = \frac{\lambda}{D} \psi_4, \quad [\psi_2, \psi_5] = 2D\psi_2 + \lambda \psi_3, \quad [\psi_3, \psi_5] = 0.$$  

By the Jacobi identity, from $[\psi_5, \psi_7] = -4D^2\psi_7$, and $[\psi_1, \psi_7] = 0$, we get $[\psi_4, \psi_7] = 0$ which implies $\lambda \psi_3 = 0$. We exclude the trivial case $\psi_3 = 0$; therefore let be $\lambda = 0$. In this case the commutation relations become $[\psi_3, \psi_7] = 0$, $[\psi_4, \psi_7] = 0$, $[\psi_1, \psi_5] = 0$, $[\psi_2, \psi_5] = 2D\psi_2$, $[\psi_3, \psi_5] = 0$; the remaining commutators are

$$[\psi_5, \psi_7] = -4D^2\psi_7, \quad [\psi_5, \psi_6] = -4D^2\psi_6, \quad [\psi_6, \psi_7] = 2D\psi_7.$$  

$$[\psi_2, \psi_3] = -2D\psi_6, \quad [\psi_3, \psi_6] = 2\kappa D\psi_3, \quad [\psi_2, \psi_6] = -2D\psi_2,$$

while we do not get a constraint on $\kappa$. Putting now $\psi_7 = 0$ and $\psi_6 = 0$ (since $\psi_3 \neq 0$ and $D \neq 0$ this implies $\kappa = 0$, i.e. the case where one of the
reaction coefficient is null) we obtain an homomorphism with the Lie algebra corresponding to a group of Euclidean movements in the plane

\[ [\psi_1, \psi_2] = 0, [\psi_1, \psi_5] = 0, [\psi_2, \psi_5] = 2D\psi_2. \]

The above results seem to be in accordance with what announced concerning the case \( D \geq 0 \) in [5], whereby, instead, integrability of reaction-diffusion type equations with \( D < 0 \), i.e. diffusion constants of opposite sign, have been studied (such systems play play a role in gauge theory of gravity [5]; similarities with coupled nonlinear Schroedinger equations describing the waves propagation in optical fibres can be recognized, see e.g. [11]; both cases are integrable and homomorphisms with infinite dimensional loop Lie algebras have been determined).

However, let us stress that alternatively we can choose \([\psi_1, \psi_5] = \lambda \psi_1, [\psi_2, \psi_5] = \lambda \psi_3, [\psi_3, \psi_5] = 0\) which define an homomorphism with a finite dimensional Lie algebra with spectral parameter. This case implies \( D = 0 \), i.e. the diffusion constant of the activator is null; the system would be integrable and would admit a Lax pair. In fact, the case \( D = 0 \) has been related with existence of travelling waves; it appears in a model for pattern formation on the shells of molluscs [6] and it is perhaps important to notice that it is a limit case of \( D << 1 \). In the following we shall consider the case \( 0 < D << 1 \) and we shall obtain the Koch & Meinhardt activator-substrate system from an integrability condition for a tower.

3 Reaction-diffusion models from integrable towers with skeleton \( E \)

For the purpose of this work, in fact, it is now a very remarkable feature that it is possible to obtain reaction-diffusion type models directly from the skeleton by using a generalization (a truncated version) of the structure equations. Indeed we need to introduce a way to produce (exterior) differential equations. Let us then construct a tower with the above skeleton \( E \) and its absolute parallelism forms; the corresponding integrability conditions, given by

\[ \omega^k = d\xi^k - \psi_j^k \theta^j, \quad d\omega^k = \psi_j^k d\theta^j - \frac{1}{2} [\psi_j, \psi_i]^k \theta^j \wedge \theta^i = 0, \quad (\text{mod } \omega^k). \]

where \( \theta^k \) are horizontal 1-forms on \( P \to Z \), provide us with the differentiable content we are looking for. In fact, the forms \( \omega^k \) can be recognized as tower forms of Cartan type (i.e. as a pull-back of contact forms by a Bäcklund map.
if the following exterior differential contraints are satisfied by the $\theta^k$:

\[
\begin{align*}
    d\theta^1 &= 0, \quad d\theta^4 = 0, \quad d\theta^5 = 0, \\
    d\theta^2 - 2D\theta^2 \wedge \theta^6 - 2D\theta^4 \wedge \theta^7 &= 0, \quad d\theta^3 + 2\kappa D\theta^3 \wedge \theta^6 = 0, \\
    d\theta^6 - D\theta^2 \wedge \theta^3 &= 0, \quad d\theta^7 + D\theta^2 \wedge \theta^4 + 2\theta^6 \wedge \theta^7 = 0, \\
    d\theta^8 + D\theta^3 \wedge \theta^4 + 2\kappa D\theta^6 \wedge \theta^8 &= 0, \\
    \theta^1 \wedge \theta^5 + D\theta^2 \wedge \theta^8 + D\theta^4 \wedge \theta^6 &= 0, \quad \theta^2 \wedge \theta^5 + \theta^4 \wedge \theta^7 = 0, \\
    \theta^2 \wedge \theta^6 + \theta^3 \wedge \theta^7 = 0, \quad d\theta^3 \wedge \theta^5 - \theta^4 \wedge \theta^8 = 0, \\
    \theta^5 \wedge \theta^6 = 0, \quad \theta^5 \wedge \theta^7 = 0, \quad \theta^5 \wedge \theta^8 = 0, \quad \theta^6 \wedge \theta^8 = 0, \quad \theta^7 \wedge \theta^8 = 0.
\end{align*}
\]

A solution is given by:

\[
\begin{align*}
    \theta^1 &= dt, \quad \theta^5 = \frac{1}{D} dt, \quad \theta^6 = -\frac{1}{D} \mu dt, \quad \theta^7 = \frac{1}{D} \mu dt, \\
    \theta^8 &= -\frac{1}{D} \nu dt, \quad \theta^4 = \frac{1}{D} dx, \quad \theta^2 = \frac{1}{D} (\mu dx + \mu_x dt), \quad \theta^3 = -\frac{1}{D} (\nu dx + \nu_x dt),
\end{align*}
\]

where $\mu$ and $\nu$ are 0-forms, depending on $x$ and $t$, which must satisfy the following reaction-diffusion equations (with a null basic production term)

\[
\begin{align*}
    \mu_t - D\mu_{xx} - 2\mu^2 \nu - 2\mu &= 0, \\
    \nu_t - \nu_{xx} - 2\kappa \mu \nu^2 &= 0.
\end{align*}
\]

### 3.1 The activator-substrate reaction-diffusion model

As we already explained the differentiable structure (i.e. the absolute parallelism) is of absolutely general nature, while the somehow ‘true’ content of a specific model comes from the algebraic structures we insert in the structure equations. This fact suggest the possibility of characterizing different models by their algebraic content.

Let us now, in fact, consider a slight change in the algebraic skeleton, such as

\[
[\psi_2, \psi_6] = 2\kappa D\psi_3 - 2D\psi_2, \quad [\psi_3, \psi_6] = 0, \quad [\psi_4, \psi_5] = 2\kappa D\psi_3.
\]

Such a change would provide the exterior differential equation

\[
d\theta^3 - 2\kappa D\theta^2 \wedge \theta^6 - 2\kappa D\theta^4 \wedge \theta^5 = 0,
\]

and therefore originate the system:

\[
\begin{align*}
    \mu_t - D\mu_{xx} - 2(\nu^2 \mu - \mu) &= 0, \\
    \nu_t - \nu_{xx} - 2\kappa (1 - \nu^2) &= 0.
\end{align*}
\]

i.e. the activator-substrate reaction-diffusion model proposed by Koch & Meinhardt, where $D$ is the diffusion constant and $\kappa$ the cross reaction coefficient.
Remark 1 We stress that a completely different system has been obtained by operating a slight change in the algebraic skeleton. This fact suggests that the parameters appearing in a given model can be somehow ‘controlled’ already at an algebraic level.

Moreover, suppose a metric could be defined on $E$, so that one can reasonable think of a condition of closeness, which we write for simplicity as $[\psi_4, \psi_7] \simeq [\psi_2, \psi_5]$. Having a glance at the skeleton structure, it is evident that such a condition would be equivalent to the request that $D << 1$, i.e. the diffusion constant of the activator much lesser than the diffusion constant of the substrate; therefore, we can characterize a condition for the appearance of patterns by means of properties of vectors in $E$.

4 Conclusions

Our results are of general nature and in principle could be applied to other mathematical models proposed in various branches of biology and ecology, see e.g. [8] and, for a review and further developments, [14]; of particular interest would be the possible application to models with delay. In fact, spatio-temporal pattern formation can be caused by time delay factors. The study of algebraic structures generating models with delay would be therefore of particular interest in comparing at an algebraic level the various approaches in modeling pattern formation.

In particular our result, see the Remark above, suggests the possibility of an algebraic-geometric study of stability of equilibrium states, depending on the parameters range and their mutual relations in a given model. Such characters could be formalized already at the algebraic level in terms of the representation of $g$ on $V$.

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