Process algebras
for epidemiological and ecological modelling

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Multi-scale Modelling of Biological Systems
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Outline

Introduction

Bio-PEPA for epidemiological systems

The BlenX language for ecological systems

Conclusions
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Process algebras

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2. they support a compositional way to model construction,
3. the individuals in the population can be described as distinct components with precise specifications of the interactions,
4. they can be seen as an intermediate language from which various kinds of analysis can be considered.
Which kind of analysis?

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Access to a variety of analysis techniques can help develop a better understanding of the behaviour of the system.
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Access to a variety of analysis techniques can help develop a better understanding of the behaviour of the system.

Furthermore, it can help discover possible errors.

Finally, it allows the modeller to select the most appropriate approach for the study of the model considered.
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The main aim is to explore the expressive and analysis power of these two languages in this field and discuss the possible drawbacks/benefits.
Related work

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The WSCCS (Weighted Synchronous Calculus of Communicating Systems) process algebra was used for modelling various ecological and epidemiological systems [Sumpter (2000), McCaig et al. (2008)].
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Epidemiological systems

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The population can be divided into classes: susceptibles (S), those who are infective (I) and those who have recovered and are immune (R). In addition to these, we can have other classes, describing, for instance, symptomatic or asymptomatic infectives, treated, untreated or immune individuals.
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Various models differ from each others in terms of the dynamics of the single species and the assumptions about the interspecific interactions.

In ecological modelling space is particularly relevant.
Abstract spatial structure

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- Generally an **abstract view** of space is sufficient to describe the spatial evolution of the epidemic/species.

- The term **metapopulation** is used to indicate a population distributed over a number of **patches** or **subpopulations**, i.e. groups of individuals in the model.

- Individuals can migrate from one patch to another and this can be described by a **migration matrix** $M(i, j)$, that determines the topology and the strength of the connections between the patches.
Population structures
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- There is a notion of **location** within models intended to capture the compartments and membranes.
- **Events** are used to present experiments such as the introduction of a species at a given time or a change in the system.
Using Bio-PEPA for epidemiological models

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- Interactions such as $I + S \rightarrow 2I$ are possible, where an entity is present on both sides of the interaction with different multiplicity.
- **Spatial structures** are often present in epidemiological models, but it is meaningless to distinguish membranes and compartments.
Modifying Bio-PEPA for epidemiology

A Bio-PEPA model for epidemiological system is described by the following syntax:

\[
S ::= (\alpha, \kappa) \downarrow S \mid (\alpha, \kappa) \uparrow S \mid (\alpha, (\kappa_1, \kappa_2)) \circ S \mid S + S \mid C \mid S@L
\]

\[
P ::= P \bowtie L \mid S(x)
\]
Bio-PEPA as an intermediate language

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- a system of differential equations for simulation and other kinds of analysis;
- a continuous time markov chains (CTMC with levels);
- a PRISM model (based on the CTMC with levels) for model checking.
Models of H5N1 Avian Influenza

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- Additionally in some cases we generated PRISM models and verified properties using stochastic model checking.
- Results were validated against previously published results of hand-crafted ODEs and stochastic simulations [Debarre et al, Ecology 2007].
Schema of the species involved

- $I_s$, $t_r$, $I_s, r$, $t_r$
- $I_r, t_r$
- $I_s, r, t_r$
- $S_{p_r}$
- $I$, $I_r$
- $S$

Symptoms, treatment, resistance
Quantities of interest

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▶ Epidemic’s peak value and time; i.e. the maximum number of infectives with respect to time and the time when this occurs.

▶ Instantaneous number of total infectives at a time $t$.

▶ Cumulative number of total infectives generated during epidemic within a time $t$. 
Simple model: single location, no drug treatment

The simple model is a $S / l_s R$. Infectives are distinguished between asymptomatic ($l$) and symptomatic ($l_s$) individuals:

\[
S \overset{\text{def}}{=} (\text{contact}1, 1) \downarrow S + (\text{contact}2, 1) \downarrow S
\]
\[
l \overset{\text{def}}{=} (\text{contact}1, (1, 2)) \odot l + (\text{contact}2, 1) \uparrow l
\]
\[
+ (\text{recovery}1, 1) \downarrow l + (\text{symp}, 1) \downarrow l
\]
\[
l_s \overset{\text{def}}{=} (\text{contact}2, (1, 1)) \odot l_s + (\text{recovery}2, 1) \downarrow l_s + (\text{symp}, 1) \uparrow l_s
\]
\[
R \overset{\text{def}}{=} (\text{recovery}1, 1) \uparrow R + (\text{recovery}2, 1) \uparrow R
\]

\[
S(450) \bowtie l(10) \bowtie l_s(40) \bowtie R(0)
\]
ODEs and Gillespie’s simulation

SIIsR model – ODE

SIIsR model – Gillespie

Time (days)

S
I
Is
R

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S
I
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Process algebras for epidemiological and ecological modelling
ODEs and Gillespie’s simulation
Total/cumulative number of infectives
PRISM properties

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- Probability of coexistence of the species at a given time $t$
- Probability of extinction of the disease at a given time $t$
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In the context of epidemiological systems some properties of interest are:

- Probability of coexistence of the species at a given time $t$
- Probability of extinction of the disease at a given time $t$
- Long run probabilities (steady states) of coexistence of the species and extinction of infection
PRISM properties

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In the context of epidemiological systems some properties of interest are:

- Probability of coexistence of the species at a given time $t$
- Probability of extinction of the disease at a given time $t$
- Long run probabilities (steady states) of coexistence of the species and extinction of infection
- Expected time until extinction of the disease.
PRISM Results (coexistence) — Varying contact rates

SIISR model: prob. Coexistence of all species

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Process algebras for epidemiological and ecological modelling
Models with multiple locations

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Five locations are used and the initial population of 500 is split evenly. Initially only one patch contains infected individuals.

Interactions between individuals are as in the previous model but constrained to only occur when they are in the same location.
Population structures
Island and necklace structures
Island and necklace structures
Island and necklace structures

Necklace–type – ODE

Necklace–type – Gillespie

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Process algebras for epidemiological and ecological modelling
Island and necklace structures
Total/cumulative number of infectives

Island−type − Infectives

Island−type − Infective cases

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Process algebras for epidemiological and ecological modelling
Total/cumulative number of infectives

Necklace-type – Infectives

Necklace-type – Infective cases
Treatment, prophylaxis and resistance to the virus

In the general model there are:

- Treatment. Treatment is for all the symptomatic individuals; it works with a certain delay.
- Prophylaxis is added at one day after the beginning of the study (represented by events).
- Drug resistance. Infectives that are treated and non-resistant to drugs can become resistant to them.

Only one third of susceptibles and asymptomatic infectives is subjected to prophylaxis. Furthermore, the transmission rates for individuals with prophylaxis is just 30 per cent of the usual one.
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The effect of prophylaxis/treatment

Island–type, treatment – ODE

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Process algebras for epidemiological and ecological modelling
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Process algebras for epidemiological and ecological modelling
Observations

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- Whilst developed for modelling biochemical pathways Bio-PEPA does seem capable of expressing a wide variety of epidemiological models.
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Ecological systems

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2. a food web of species describing a local community;
3. a social network of individuals characterizing a species.
Schema of the network
Landscape network

A landscape model describes a mosaic of habitat patches and corridors.
Landscape network

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The former ones are the place where the population can survive for a long time, whereas the latter are links connecting patches.
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Here landscape systems have an abstract spatial structure: the patches may have no explicit area and can be static (i.e. the patch/corridor topology is fixed) and homogeneous (i.e. its internal structure is not relevant).
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Species can migrate from one patch to the other.
Food webs

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In a food web a species can be classified as:

- **Top predator**: it can catch other species but cannot be captured by any other.

- **Intermediate species**: it can both be captured by or capture other species.

- **Basal species**: the species can be captured by other species but cannot capture any other.

Interspecific interactions are feeding (capture of the prey) and feeding-reproduction (capture of the prey and reproduction of the predator).

Here we consider one top predator, two intermediate species and two basal species.
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In a food web a species can be classified as:

- **Top predator**: it can catch other species but cannot be captured by any other.
- **Intermediate species**: it can both be captured by or capture other species.
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Here we consider one top predator, two intermediate species and two basal species.
Social networks

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Connected individuals changer their interspecific interactions, for instance, it is easier for them to capture the prey more with respect to unconnected individuals.
Questions

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▶ How do spatial dynamics (spatial structure, rates of migration from one patch to the other) of the ecosystem influence extinction risk of species?

▶ Do the initial distribution of individuals over all the habitat patches have effect on the temporal evolution of species?
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- How do spatial dynamics (spatial structure, rates of migration from one patch to the other) of the ecosystem influence extinction risk of species?
- Do the initial distribution of individuals over all the habitat patches have effect on the temporal evolution of species?
- How do changes in social network topology (connectivity) impact the temporal behaviour of species?
The BlenX language

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![Box diagram]

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**Federica Ciocchetta, CoSBi**  
*Process algebras for epidemiological and ecological modelling*
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![Diagram of a box with interfaces and process]

Interfaces (e.g. $x$, $y$ and $z$) have associated types (e.g. $S$, $T$, $V$) and represent the interaction capabilities of a box; the internal program ($P$) codifies for the mechanism of the transformation of an interaction into a conformational change.
The BlenX language: actions

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Alternatively, it is possible to *hide* or *unhide* a site, to *change* the type, to *expose* a new site or *die*.

Two boxes can interact by composing/decomposing or communicating (*inter-communication*) only if they have *compatible interfaces*.
The BlenX language: events

**Events** specify statements, or **verbs**, to be executed with a specified rate and/or when some **conditions** are satisfied.
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Simple examples of event are the following:

\[
\text{when } (A, B : (|A| > 2 \text{ and } |B| > 2) : r) \text{ join}(C)
\]

\[
\text{when } (A :: f) \text{ new}(1)
\]

\[
\text{when } (A :: f) \text{ die}(1)
\]
The BlenX language: stochastic simulation

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BlenX supports also immediate actions (using the keyword $\text{inf}$ as rate value), i.e. actions that have precedence with respect to actions with finite rates.
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A BlenX program can be executed within the Beta Workbench, a set of tools to design, simulate and analyze models written in BlenX.
The BlenX model

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1. Habitat patches are abstracted by names. Each box has a location interface with a specific type representing the patch.

2. Each species $i$ is represented by a box.

\[
\begin{align*}
& \text{B}_{\text{intra}_i,l,h} \quad \text{B}_{\text{inter}_i,l,h} \\
& \text{zih, Norep} \\
& \text{P}_{i,l,h} \mid \text{P}_{\text{aux},i} \quad \text{y, Loc}\end{align*}
\]
Single patch network vs four-patch network (island-type)

Mean and sd for A: no patches vs patches

Mean and sd for B: no patches vs patches

Mean and sd for C: no patches vs patches

Mean and sd for D: no patches vs patches

Mean and sd for E: no patches vs patches
Results

In an homogeneous population the species $D$ goes extinct, whereas the species $B$ grows up infinitely. Indeed the species $B$ is just regulated by $D$ and when $D$ disappears $B$ grows.
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The standard deviation shows a great variability between the various runs, especially for $B$.

When the island-type network is introduced, all the species with the exception of $B$ reach a higher level than before. In particular $D$ does not go extinct. The effect of the landscape structure is a better regulation and the survival for all the species.
Different spatial structure

Mean and sd for E: loop, island type

Mean and sd for E: necklace, island type

Mean and sd for E: spider, island type

Mean and sd for D: loop, island type

Mean and sd for D: necklace, island type

Mean and sd for D: spider, island type

Federica Ciocchetta, CoSBi
Figures

Mean and sd for B: loop, island type
Mean and sd for B: necklace, island type
Mean and sd for B: spider, island type
Mean and sd for A: loop, island type
Mean and sd for A: necklace, island type
Mean and sd for A: spider, island type

Federica Ciocchetta, CoSBi

Process algebras for epidemiological and ecological modelling
Analysis results

We consider the various spatial structures; in particular we compare the island-type structure with loop-type, necklace-type and spider-type structures.

The qualitative behaviour of each species is the same in all the cases. However, there are a few discrepancies between the networks with the island-type and the loop-type structures, whereas both the networks with necklace and the spider-type structures are similar to the one with island-type structure.
Radiation - initially equidistributed species (island type)

We compare the case of radiation from a single patch to the others and the case of species equally present in all the patches.
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The sum of individuals of a given species over all the patches is the same in both the situations. The graphs show that, after short initial time, we obtain the same temporal evolution for all the species.

For our specific choice of parameters, the initial state does not influence the behaviour of species.
Absence of connectivity vs connectivity

Mean and sd for A: with and without cooperation

Mean and sd for B: with and without cooperation

Mean and sd for C: with and without cooperation

Mean and sd for D: with and without cooperation

Mean and sd for E: with and without cooperation
Results

Connectivity increases the quantity of individuals of the top predator and intermediate species whereas the individuals of the basal species decrease.
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In particular, $A$ is quite close to zero and $B$, after a rapid increment in the first time interval, decreases close to zero too. However they do not go extinct but are very low as consumed by their predator quite rapidly.
Observations

We showed that:

1. In a fragmented population there is an increase of the number of individuals;
2. Connectivity among individuals of the same species (top predator and intermediate species) has the effect to increase the total number of individuals of that species preventing extinction.

These behaviours are in agreement with the behaviour of this kind of ecosystems in nature.
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Outline

Introduction

Bio-PEPA for epidemiological systems

The BlenX language for ecological systems

Conclusions
Summary

Two case studies concerning the application of two process algebras were showed.
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Two case studies concerning the application of two process algebras were showed.

The former was about some epidemiological models described in Bio-PEPA, the latter was about a complex ecological network in the BlenX language.

Both process algebras were suitable to describe the two systems and the analyses were useful to understand their behaviour.

In these examples stochastic simulation resulted appropriate as the systems are characterized by a certain variability, especially when the spatial structure was considered.
Future work

For the future, we are planning to extend our models in order to consider more complex assumptions.
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Furthermore, we would like to investigate the possibility to extend the languages in order to consider more complexes definition of space and a more compact definition of species with similar behaviour.
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Furthermore, we would like to investigate the possibility to extend the languages in order to consider more complexes definition of space and a more compact definition of species with similar behaviour.

Finally, we would like to apply sensitivity analysis to find out the parameters that have most impact on our models.