# On the Relationship between ODE, Simulation and Stochastic Process Algebras

Luca Bortolussi[1]

[1] Dipartimento di Matematica ed Informatica
Università degli studi di Trieste
luca@dmi.units.it

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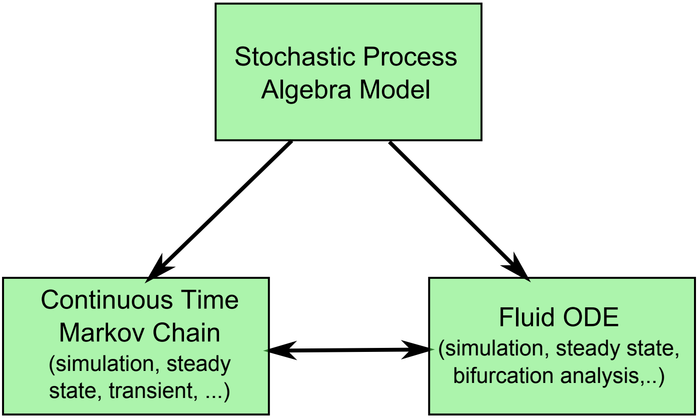
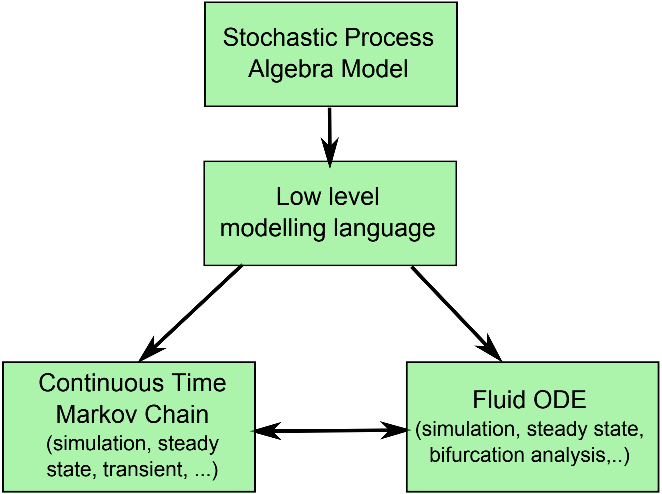
# Outline

# Overview


Stochastic Process
Algebra Model
Continuous Time
Markov Chain
(simulation, steady
state, transient, ...)
Fluid ODE
(simulation, steady state,
bifurcation analysis,..)

# Overview


Stochastic Process
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Low level
modelling language
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# Outline

# LOW LEVEL MODELLING LANGUAGE

## GLOBAL VIEW OF A SYSTEM

A (low-level) model is a tuple $\mathcal{X} = (\mathbf{X}, \mathcal{D}, \mathcal{T}, \mathbf{x_0})$, where:

1. $\mathbf{X} = \{X_1, \ldots, X_n\}$ — *variables*.
2. $\mathcal{D} = \prod_{i=1}^{n} \mathcal{D}_i$ — (usually countable) state space.
3. $\mathbf{x_0} \in \mathcal{D}$ —*initial state*.
4. $\tau_i \in \mathcal{T}$ — *transitions*, $\tau_i = (n, \varphi(\mathbf{X}), \mathbf{v}, r(\mathbf{X}))$
   1. $n$ — name (optional).
   2. $\varphi(\mathbf{X})$ — guard.
   3. $\mathbf{v} \in \mathbb{R}^n$ — *update vector* (from $\mathbf{X}$ to $\mathbf{X} + \mathbf{v}$)
   4. $r : \mathcal{D} \to \mathbb{R}_{\geq 0}$ — rate function (Lipschitz continuous and bounded).

# FROM SPA TO LOW LEVEL LANGUAGE

## RESOURCE MODEL IN PEPA

$$P_1 := (task_1, k_1).P_2$$
$$P_2 := (task_2, k_2).P_1$$
$$R_1 := (task_1, h_1).R_2$$
$$R_2 := (reset, h_2).R_1$$

$$P_1[n] \underset{task_1}{\bowtie} R_1[m]$$

## RESOURCE LOW LEVEL MODEL

- variables: $\{X_{P1}, X_{P2}, X_{R1}, X_{R2}\}$;
- state space: $[0, N]^4$, $N = m + n$;
- initial state $\mathbf{x_0} = (n, 0, m, 0)$
- transitions:
  $(task_2, \top, (1, -1, 0, 0), k_2 X_{P2})$
  $(reset, \top, (0, 0, 1, -1), h_2 X_{R2})$
  $(task_1, \top, (-1, 1, -1, 1),$
  $\min\{k_1 X_{P1}, h_1 X_{R1}\})$

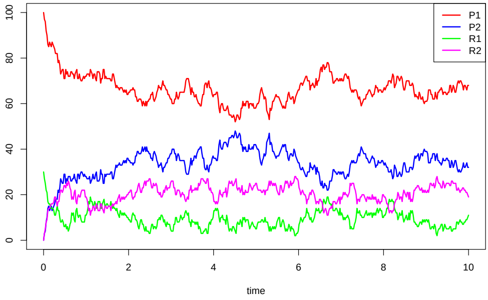
Mapping from SPA to Low Level language can be formalized and automated.

# CTMC SEMANTICS

## CTMC $\mathbf{X}(t)$ ASSOCIATED WITH A MODEL

- State space is $\mathcal{D}$.
- Infinitesimal generator matrix $Q = (q_{\mathbf{xy}})$:

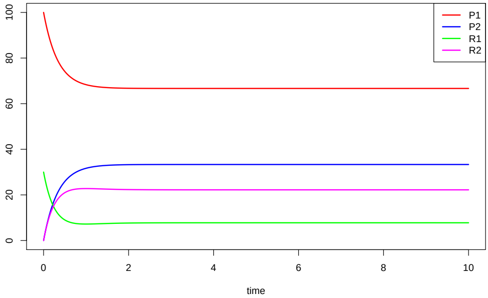
$$q_{\mathbf{xy}} = \sum \{ r_\tau(\mathbf{x}) \mid \mathbf{v}_\tau = \mathbf{y} - \mathbf{x} \wedge \varphi_\tau(\mathbf{x}) \ true \}.$$



# FLUID SEMANTICS

## ODE $\mathbf{x}(t)$ ASSOCIATED WITH A MODEL

- Assume all guards to be trivial.
- State space is $\mathbb{R}^n$.
- Drift function: $F(\mathbf{X}) = \sum_{\tau \in \mathcal{T}} \mathbf{v}_\tau r_\tau(\mathbf{X})$.
- $\mathbf{x}(t)$ is the solution of $\frac{d\mathbf{x}(t)}{dt} = F(\mathbf{x}(t))$.



# Outline

# MAIN IDEAS

## STATE SPACE EXPLOSION

- Models depend on a parameter $N$, which intuitively is the size of the system. In many cases, this is the total population $N$, but it can be the initial population, or the volume (for biochemical reactions).
- The larger $N$, the more severe the state space explosion for CTMC semantics.

- We look at the behaviour of the sequence of models $\mathcal{X}^{(N)}$, for different values of $N$.
- We want to understand what happens in the limit $N \rightarrow \infty$.
- To compare models of different sizes, we normalize then w.r.t. system size.

# Scaling assumptions

A normalized model $\bar{\mathcal{X}}^{(N)}$ is obtained from $\mathcal{X}^{(N)}$:

- Normalized variables (and domains): $\bar{\mathbf{X}} = \frac{\mathbf{X}}{N}$
- Normalized transitions: $(\bar{\varphi}^{(N)}(\bar{\mathbf{X}}), \frac{\mathbf{v}}{N}, \bar{r}^{(N)}(\bar{\mathbf{X}}))$
- Guards: $\bar{\varphi}^{(N)}(\frac{\mathbf{X}}{N}) = \varphi(\mathbf{X})$
- Update vectors: $\bar{\mathbf{v}} = \frac{\mathbf{v}}{N}$
- Density dependence condition for rates: exists $f$ such that

$$r^{(N)}(\mathbf{X}) = Nf\left(\frac{\mathbf{X}}{N}\right) = \bar{r}^{(N)}\left(\frac{\mathbf{X}}{N}\right) = \bar{r}^{(N)}(\bar{\mathbf{X}})$$

# Drift and limit ODE

## Fluid ODE

The drift of the normalized model $\bar{\mathcal{X}}^{(N)}$ is independent of $N$:

$$F(\mathbf{x}) = \sum_{\tau \in \mathcal{T}} \mathbf{v}_\tau f_\tau(\mathbf{x}).$$

The fluid ODE is therefore $\frac{d\mathbf{x}(t)}{dt} = F(\mathbf{x}(t))$.

## Drift of non-normalized models

The drift $F^{(N)}(\mathbf{X})$ of the non-normalized model is $F^{(N)}(\mathbf{X}) = NF(\frac{\mathbf{X}}{N})$, hence the ODE of the normalized model are just the rescaled version of the ODE for the normalized one.

# Deterministic Approximation: hypothesis

- $\overline{\mathbf{X}}^{(N)}(t)$: sequence of Markov processes satisfy conditions above.
- $E \subset \mathbb{R}^n$: open set containing the state space of each $\overline{\mathbf{X}}^{(N)}(t)$.
- $S \subseteq E$, open in $E$. $F$ Lipschitz continuous in $S$.
- $\exists \mathbf{x_0} \in S$ such that $\overline{\mathbf{X}}^{(N)}(0) \to \mathbf{x_0}$ in probability
- $\mathbf{x}(t)$: solution of $\dot{\mathbf{x}} = F(\mathbf{x})$, $\mathbf{x}(0) = \mathbf{x_0}$, living in $E$.
- $\zeta(S)$: exit time of $\mathbf{x}(t)$ from $S$.
- $\zeta^{(N)}(S)$: exit time of $\overline{\mathbf{X}}^{(N)}(t)$ from $S$.

# Deterministic Approximation

**Theorem**

*For any finite time horizon $T < \zeta(S)$, it holds that:*

1. $\mathbb{P}(\sup_{0 \leq t \leq T} ||\overline{\mathbf{X}}^{(N)}(t) - \mathbf{x}(t)|| > \varepsilon) \to 0;$
2. $\mathbb{P}(\zeta^{(N)}(S) < T) \to 0.$

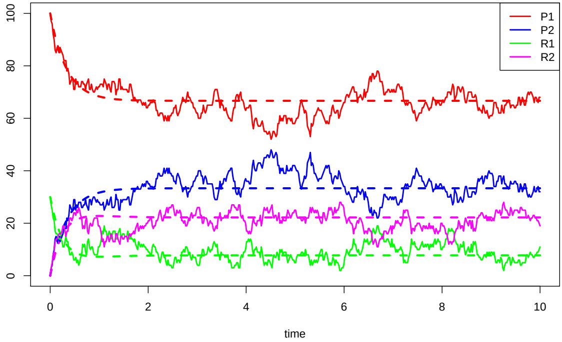
*Furthermore, if $\zeta(S) < \infty$, it holds that:*

3. $\mathbb{P}(\sup_{0 \leq t \leq \zeta(S)} ||\overline{\mathbf{X}}^{(N)}(\min\{t, \zeta^{(N)}(S)\}) - \mathbf{x}(t)|| > \varepsilon) \to 0;$
4. $\mathbb{P}(||\zeta^{(N)}(S) - \zeta(S)|| > \varepsilon) \to 0.$ □

# THE MEANING OF DETERMINISTIC APPROXIMATION

$T < \zeta(S)$: $\mathbb{P}(\sup_{0\leq t\leq T} ||\overline{\mathbf{X}}^{(N)}(t) - \mathbf{x}(t)|| > \varepsilon) \to 0$

For large $N$, simulated trajectories of the CTMC are essentially indistinguishable from the solution of the fluid ODE



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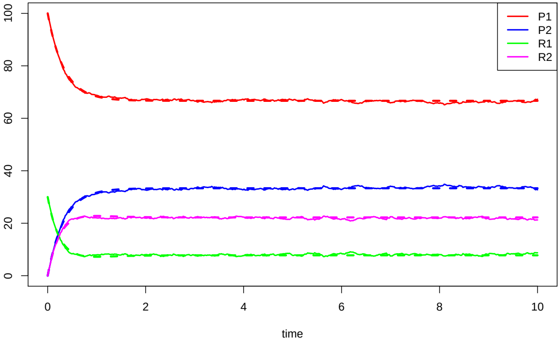

# The Meaning of Deterministic Approximation

$T < \zeta(S)$: $\mathbb{P}(\sup_{0 \le t \le T} ||\overline{\mathbf{X}}^{(N)}(t) - \mathbf{x}(t)|| > \varepsilon) \to 0$

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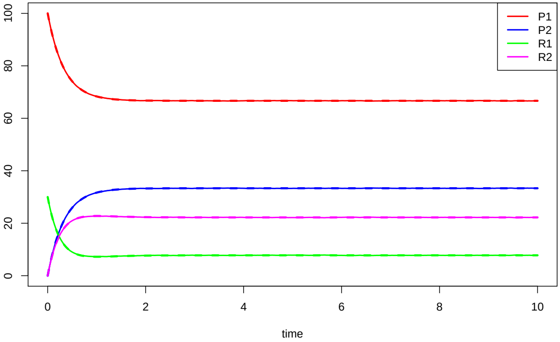

# Exit times

## $\mathbb{P}(||\zeta^{(N)}(S) - \zeta(S)|| > \varepsilon) \to 0$

For large $N$, the exit time of the CTMC from the set $S$ converges to the exit time of the solution of the fluid ODE.

## Why localize the theorem to $S \subseteq E$?

- Because the drift may not always be Lipschitz in $E$.
- Because one can reason about exit times.

## WARNING!!!

The theorem holds for finite time horizons $T < \infty$, i.e. it tells nothing about steady state behaviour of the CTMC. To do this additional properties on the fluid ODE phase space are required (globally attracting steady state).

# SPA and Scaling Assumptions

## Why do we care about SPA?

- Modelling with SPA is usually simpler than modelling with the low level language.
- SPA may generate a restricted class of low level models. This restrictions may automatically guarantee the validity of limit theorem hypothesis (PEPA).

# Outline

# AVERAGE OF CTMC MODEL

## ODE FOR THE AVERAGE

Sometimes we are interested only in the (transient) average behaviour of the CTMC.
From Kolmogorov equations, we can derive an ODE for the average state $\mathbb{E}_t[\mathbf{X}]$ of the CTMC:

$$\frac{d\mathbb{E}_t[\mathbf{X}]}{dt} = \mathbb{E}_t[F(\mathbf{X})] = \sum_{\tau \in \mathcal{T}} \mathbf{v}_\tau \mathbb{E}_t[f_\tau(\mathbf{X})].$$

## APPROXIMATIONS

If it holds that $\mathbb{E}_t[F(\mathbf{X})] = F(\mathbb{E}_t[\mathbf{X}])$, i.e. $\mathbb{E}_t[f_\tau(\mathbf{X})] = f_\tau(\mathbb{E}_t[\mathbf{X}])$ for all $\tau$, then the previous equation boils down to the fluid ODE.
But this can be done exactly only if $F(\mathbf{X})$ is a linear function.
Otherwise, the fluid ODE can be seen as a (first-order) approximation of the ODE for the true average.

# ODE for the average

## Simple shared resource model

$$\frac{d\mathbb{E}_t[X_{P1}]}{dt} = k_2\mathbb{E}_t[X_{P2}] - \mathbb{E}_t[\min\{k_1 X_{P1}, h_1 X_{R1}\}]$$

$$\frac{d\mathbb{E}_t[X_{P1}]}{dt} \approx k_2\mathbb{E}_t[X_{P2}] - \min\{k_1\mathbb{E}_t[X_{P1}], h_1\mathbb{E}_t[X_{R1}]\}$$

## Synchronization by rate product

$$\frac{d\mathbb{E}_t[X_{P1}]}{dt} = k_2\mathbb{E}_t[X_{P2}] - k_1 h_1\mathbb{E}_t[X_{P1}X_{R1}].$$

$$\frac{d\mathbb{E}_t[X_{P1}]}{dt} \approx k_2\mathbb{E}_t[X_{P2}] - k_1 h_1\mathbb{E}_t[X_{P1}]\mathbb{E}_t[X_{R1}].$$

In this case, the equation for the true average depends on higher order moments.

J. Bradley, R. Hayden. *A Fluid analysis framework for a Markovian Process Algebra*, Theor. Comp. Science, 2010.

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# MOMENT CLOSURE

## DINKIN'S FORMULA FOR NON-CENTRED MOMENTS

$$\frac{d\mathbb{E}_t[X_1^{m_1}\cdots X_n^{m_n}]}{dt} = \sum_{\tau\in\mathcal{T}} \mathbb{E}_t\left[ f_\tau(\mathbf{X}) \left( \prod_{j=1}^{n} (X_j + \mathbf{v}_{\tau,j})^{m_j} - X_1^{m_1}\cdots X_n^{m_n} \right) \right].$$

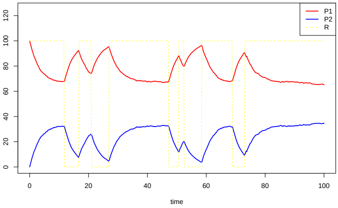
This equation provides a way to define a set of ODE for moments of any order.
If rate functions $f_\tau$ are polynomial (e.g. after a Taylor expansion), the previous equation depends only on non-centred moments. However, equations for moments of order $k$ may depend on moments of higher order: the system of ODE is not closed (infinite dimensional).
Equations can be closed by replacing higher order moment with non-linear functions of lower order moments.

A. Singh, J.P. Hespanha. *Lognormal moment closures for bio-chemical reactions*, Proc. of IEEE CDC 2006.

# HYBRID LIMITS

## UNBOUNDED RESOURCE WITH FAILURE

- variables: $\{X_{P1}, X_{P2}, X_R\}$;
- state space: $[0, N]^2 \times [0, 1]$;
- initial state $\mathbf{x_0} = (N, 0, 1)$
- transitions:
  $(failure, X_R = 1, (0, 0, -1), k_b)$
  $(repair, X_R = 0, (0, 0, 1), k_r)$
  $(task_2, \top, (1, -1, 0), k_2 X_{P2})$
  $(task_1, \top, (-1, 1, 0),$
  $\min\{k_1 X_{P1}, N h_1 X_R\}$




We cannot apply fluid theorem, because there is one single resource that can fail and be unavailable.

L. Bortolussi. *Limit Behavior of the Hybrid Approximation of Stochastic Process Algebras*. Proc. of ASMTA 2010.

# Hybrid Limits

**Unbounded Resource with Failure**

- variables: $\{X_{P1}, X_{P2}, X_R\}$;
- state space: $[0, N]^2 \times [0, 1]$;
- initial state $\mathbf{x_0} = (N, 0, 1)$
- transitions:
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  $(\mathit{task}_1, \top, (-1, 1, 0),$
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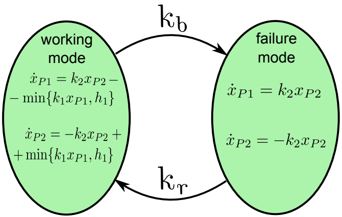
Keep some variables discrete and approximate the other as continuous. We obtain a stochastic hybrid system, and sequences of CTMC converge to it.

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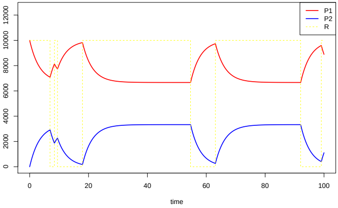


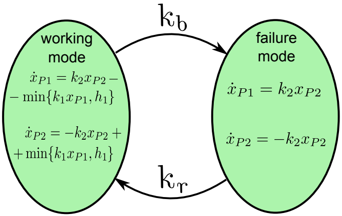

# DISCONTINUOUS RATES

- Deterministic approximation theorems require rate functions to be Lipschitz continuous.
- Therefore, cannot be used, as they can introduce discontinuities in rates.
- However, models with discontinuous rates generate discontinuous fluid ODE. If these ODE are piecewise-smooth, they can still have unique solutions, and a limit result still holds.

L. Bortolussi. *Hybrid Limits of Continuous Time Markov Chains*. Proc. of QEST 2011.

# CONCLUSIONS

- Fluid approximation is a powerful tools for analysis of models with large state spaces, when state space explosion is originated by the interaction of many simple agents (with few internal states).
- SPA are a powerful modelling framework, and restrictions on the language may provide the automatic satisfiability of conditions of limit theorems.
- Different extensions of limit results can be considered, further enhancing the scope of fluid analysis.

# Thanks for the attention. Questions?