On the Approximation of Stochastic Concurrent Constraint Programming by Master Equation

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INTRODUCTION

BASICS ON sCCP

APPROXIMATIONS AND MASTER EQUATION

EXAMPLES

SEMANTICS FOR SPA

SPA formalism
sCCP

CTMC

ODE

Hybrid Automata
**STOCHASTIC CONCURRENT CONSTRAINT PROGRAMMING**

**CCP = Constraints + Agents**

- **Constraints** are *formulae over an interpreted first order language* (i.e. \( X = 10, \ Y > X - 3 \)); they can be added to a "container", the **constraint store**, but can never be removed.

- Agents can perform two basic operations on this store (asynchronously): **tell** or **ask** a constraint.

\[
p :\!-\! A; \ \pi = [g \rightarrow u]_\lambda; \ M = \pi.A \mid M + M \\]
\[
A = 0 \mid M \mid p; \ N = A \mid A \parallel N
\]

\[
\text{rw}(X) :\!-\! [X > 0 \rightarrow X' = X - 1]_\lambda(X).\text{rw}(X)
\]
\[
+ [true \rightarrow X' = X + 1]_\lambda(X).\text{rw}(X)
\]

**STOCHASTIC CCP**

Each **ask** and **tell** instruction has a rate (function) attached to it:

\[
\lambda : C \longrightarrow \mathbb{R}^+.\]

The semantics of the language is given in terms of a **Continuous Time Markov Chain**.

**MODELING IN sCCP**

**MODELING BIOCHEMICAL REACTIONS**

\[ R_1 + \ldots + R_n \rightarrow_{f(R,X;K)} P_1 + \ldots + P_m \]

\[ f\text{-reaction}(R, X, P, k) :- \]
\[ \text{tell}_{f(R,X;K)}(R' = R - 1 \wedge P' = P + 1). \]

\[ f\text{-reaction}(R, X, P, k) \]

**ANALYSIS TOOLS**

- Stochastic simulation (Gillespie algorithm)
- Stochastic model checking and CTMC analysis
- Approximation with ODE’s and Hybrid Automata

**OREGONATOR**

\begin{align*}
B & \rightarrow_{k_1} A \\
A + B & \rightarrow_{k_2} \emptyset \\
A & \rightarrow_{k_3} 2A + C \\
2A & \rightarrow_{k_4} \emptyset \\
C & \rightarrow_{k_5} B
\end{align*}

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**Introduction**

**Basics on SCCP**

**Approximations and Master Equation**

**Examples**

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**From SCCP to ODE**

\[
\nu = \begin{pmatrix}
X \\
G_1 \\
G_0
\end{pmatrix} = \begin{pmatrix}
1 & 0 & 0 & -1 \\
0 & -1 & +1 & 0 \\
0 & +1 & -1 & 0
\end{pmatrix}
\]

\[
\phi = \begin{pmatrix}
k_p G_1 \\
k_b X G_1 \\
k_u G_0 \\
k_d X
\end{pmatrix}
\]

\[
\Phi^1 = \nu \cdot \phi : \begin{align*}
\dot{X} &= k_p G_1 - k_d X \\
\dot{G}_1 &= k_u G_0 - k_b X G_1 \\
\dot{G}_0 &= k_b X G_1 - k_u G_0
\end{align*}
\]
Circadian Clock
**Circadian Clock**

\[
p_{\text{gate}}(\alpha_A, \alpha'_A, \gamma_A, \theta_A, M_A, A) \parallel \\
p_{\text{gate}}(\alpha_R, \alpha'_R, \gamma_R, \theta_R, M_R, A) \parallel \\
\text{reaction}(\beta_A, [M_A], [A]) \parallel \\
\text{reaction}(\delta_{MA}, [M_A], []) \parallel \\
\text{reaction}(\beta_R, [M_R], [R]) \parallel \\
\text{reaction}(\delta_{MR}, [M_R], []) \parallel \\
\text{reaction}(\gamma_C, [A], [R]) \parallel \\
\text{reaction}(\delta_A, [AR], [R]) \parallel \\
\text{reaction}(\delta_A, [A], []) \parallel \\
\text{reaction}(\delta_R, [R], [])
\]
**Circadian Clock**

```
p_gate(\alpha_A, \alpha_A', \gamma_A, \theta_A, M_A, A) \parallel 
p_gate(\alpha_R, \alpha_R', \gamma_R, \theta_R, M_R, A) \parallel 
reaction(\beta_A, [M_A], [A]) \parallel 
reaction(\delta_{MA}, [M_A], []) \parallel 
reaction(\beta_R, [M_R], [R]) \parallel 
reaction(\delta_{MR}, [M_R], []) \parallel 
reaction(\gamma_C, [A, R], [AR]) \parallel 
reaction(\delta_A, [AR], [R]) \parallel 
reaction(\delta_A, [A], []) \parallel 
reaction(\delta_R, [R], []).
```
The master equation is equivalent to the Kolmogorov Forward Equation: it is a PDE for the time-evolution of the probability density function $P(X, t)$.

\[
\frac{\partial P(Y, t)}{\partial t} = \sum_j \left( \phi_j(Y - \nu_j)P(Y - \nu_j, t) - \phi_j(Y)P(Y, t) \right)
\]
**FIRST-ORDER APPROXIMATION**

**DIFFERENTIAL EQUATION FOR THE AVERAGE OF sCCP**

\[
\frac{d \langle Y_i \rangle_t}{dt} = \langle \Phi^1_i(Y) \rangle_t
\]

**TAYLOR EXPANSION OF \( \langle \Phi^1_i(Y) \rangle_t \)**

\[
\langle \Phi^1(Y) \rangle_t \approx \Phi^1(\langle Y \rangle_t) + \frac{1}{2} \sum_{h,k=1}^{\vert Y \vert} \partial^2_{hk} \Phi^1(\langle Y \rangle_t) \langle \langle Y_h Y_k \rangle \rangle_t
\]

**FIRST-ORDER EQUATION FOR THE AVERAGE**

\[
\frac{d \langle Y_i \rangle_t}{dt} = \Phi^1_i(\langle Y \rangle_t)
\]
**Second-Order Approximation**

**Exact Equation for Covariance**

\[
\frac{d \langle \langle Y_i Y_k \rangle \rangle_t}{dt} = \langle \Phi^2_{ik}(Y) \rangle_t + \langle (Y_i - \langle Y_i \rangle_t) \Phi^1_k(Y) \rangle_t + \langle (Y_k - \langle Y_k \rangle_t) \Phi^1_i(Y) \rangle_t
\]

**Second-Order Equations for Average and Covariance**

\[
\frac{d \langle Y_i \rangle_t}{dt} = \Phi^1(\langle Y \rangle_t) + \frac{1}{2} \sum_{h,k=1}^{\lvert T(N) \rvert} \partial^2_{hk} \Phi^1(\langle Y \rangle_t) \langle \langle Y_h Y_k \rangle \rangle_t
\]

\[
\frac{d \langle \langle Y_i Y_k \rangle \rangle_t}{dt} = \Phi^2_{ik}(\langle Y \rangle_t) + \sum_{h=1}^{\lvert Y \rvert} \partial_h \Phi^1_k(\langle Y \rangle_t) \langle \langle Y_i Y_h \rangle \rangle_t
\]

\[+ \sum_{h=1}^{\lvert Y \rvert} \partial_h \Phi^1_i(\langle Y \rangle_t) \langle \langle Y_k Y_h \rangle \rangle_t\]
**RANDOM WALK**

\[ \text{RW}_X \ni [\ast \rightarrow X' = X + 1]_k \cdot \text{RW}_X + [\ast \rightarrow X' = X - 1]_k \cdot \text{RW}_X, \]

\[ \Phi^1(X) = 0 \]
\[ \Phi^2(X) = 2k \]

\[
\begin{align*}
\langle X \rangle_t &= X_0 \\
\langle \langle X^2 \rangle \rangle_t &= 2kt + \langle \langle X_0^2 \rangle \rangle
\end{align*}
\]

\[
\begin{aligned}
\langle \dot{X} \rangle &= \Phi^1(\langle X \rangle) + \frac{1}{2} \langle \langle X^2 \rangle \rangle \partial_{xx}^2 \Phi^1(\langle X \rangle) = 0 \\
\langle \langle X^2 \rangle \rangle &= \Phi^2(\langle X \rangle) + 2 \langle \langle X^2 \rangle \rangle \partial_x \Phi^1(\langle X \rangle) = 2k
\end{aligned}
\]
**Effects of Variance**

\[
R_1 : [\star \rightarrow X' = X + 1]_k \cdot R_1; \quad R_2 : [\star \rightarrow Y' = Y + 1]_k \cdot R_2; \quad R_3 : [X > 0 \rightarrow X' = X - 1]_{\alpha_1} \cdot X \cdot R_3
\]

\[
R_4 : [Y > 0 \rightarrow Y' = Y - 1]_{\alpha_2} \cdot Y \cdot R_4; \quad R_5 : [X > 0 \land Y > 0 \rightarrow X' = X - 1 \land Y' = Y + 1]_{k_2} \cdot X \cdot Y \cdot R_5
\]

\[
R_1 \parallel R_2 \parallel R_3 \parallel R_4 \parallel R_5
\]
CIRCADIAN CLOCK
Circadian Clock

Stochastic

FO approximation
**Circadian Clock**

**Stochastic average**

**FO approximation**
**Circadian Clock**

Stochastic average

SO approximation
Robustness of the system: increase translation rate of $R$ from $\beta_R = 5$ to $\beta_R = 50$. 

Stochastic, $\beta_R = 50$

FO approximation, $\beta_R = 50$
Robustness of the system: increase translation rate of $R$ from $\beta_R = 5$ to $\beta_R = 50$.

Stochastic average, $\beta_R = 50$

FO approximation, $\beta_R = 50$
Robustness of the system: increase translation rate of $R$ from $\beta_R = 5$ to $\beta_R = 50$. 

Stochastic average, $\beta_R = 50$

SO approximation, $\beta_R = 50$
Many works in statistical mechanics deal with the relation between stochastic and deterministic description of systems. The Master Equation for a SPA is the key to use these methods also for the analysis of quantitative programming languages.

SPA introduce many new challenges: the main one is synchronization, which introduces discontinuities in the expression of rates.

Synchronization is discrete in nature: hybrid schemes of approximation should work better.