

A Logic of Behaviour in Context

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- \mathcal{LBC} – a logic for behaviour in context.
- \mathcal{LBC} is a tractable approach to combining temporal and spatial logics
- with application to continuous biochemical processes.

- \mathcal{LBC} was created as a logic for continuous π -calculus ($c\pi$)
- a continuous time, continuous space process algebra for biochemical systems.

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- Express useful things about biochemical systems.
- Guarantee operator from Cardelli and Gordon's spatial logic
 - $\phi \triangleright \psi$
 - $P \models \phi \triangleright \psi \iff \forall Q. Q \models \phi \implies P || Q \models \psi$
- Context introduction modality:
 - $Q \triangleright \psi$
 - $P \models Q \triangleright \psi \iff Q || P \models \psi$
- Context introduction is a more tractable interpretation of guarantee.

- $Q \triangleright \mathbf{F}_{[0,3]}([A] \geq c)$
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- we can make succinct statements about causality:
- $(Q \triangleright \mathbf{F}([A] \geq c)) \wedge \mathbf{G}([A] < c)$
 - If we introduce Q then eventually $[A] \geq c$, whereas without Q it won't.

- Nesting within temporal modalities gives increased expressive power:
- $\mathbf{F}(Q \triangleright \mathbf{F}([A] < c))$
 - *There exists some point in time such that if we introduce Q then $[A] < c$.*

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- and bounded modalities allow quite precise quantitative statements:
- $\mathbf{G}_{[3,5]}(Q \triangleright \mathbf{F}_{[0,10]}([A] \geq c))$
 - *For all points in time from 3 to 5 if we introduce Q then within 10 then $[A] \geq c$.*

For P , a process:

$$P \models \phi \mathbf{U}_I \psi \iff \exists t' \in I. ((P^{t'} \models \psi) \wedge (\forall t'' \in I < t'. P^{t''} \models \phi))$$

$$P \models Q \triangleright \phi \iff (Q \parallel P) \models \phi$$

- I is an interval in $[0, \infty)$
- P^t is the process reached from process P after time t .
- Q is a new process.

$$\mathbf{F}_t \phi \equiv \top \mathbf{U}_t \phi$$

$$\mathbf{G}_t \phi \equiv \neg \mathbf{F}_t \neg \phi$$

- We build a model using $c\pi$.
- This gives us some ODEs representing the dynamics of the system.
- We can take a discrete numerical simulation trace of the continuous system.
- A numerical ODE solver gives us a *Trace* of the form:

$$(t_0, \vec{c}_0), (t_1, \vec{c}_1), \dots$$

- A naive model checking algorithm is then easily expressed as a functional program:

Naive recursive model checking

check :: Trace \mapsto Formula \mapsto Bool

check (t:ts) (atom) = valid atom t

check (t:ts) ($\phi \wedge \psi$) = ...

check (t:ts) ($\phi \vee \psi$) = ...

check (t:ts) ($\neg\phi$) = ...

check (t:ts) ($\phi \mathbf{U}_{[t_0, t_n]} \psi$) = if (t < t₀) then check ts $\phi \mathbf{U}_{[t_0, t_n]} \psi$
else (t \leq t_n) AND ((check (t:ts) ψ) OR
(check (t:ts) ϕ) AND (check (ts) ($\phi \mathbf{U}_{[t_0, t_n]} \psi$)))

check (t:ts) ($Q \triangleright \phi$) = check (solve (compose Q (proc (t:ts)))) ϕ

solve :: Process \mapsto Trace

compose :: Process \mapsto Process \mapsto Process

proc :: Trace \mapsto Process

Improved model checking

- The naive algorithm has complexity $O(n^f)$ for trace length n and depth f of nested temporal operators.
 - We repeatedly re-compute sub-formulae along the trace,
 - e.g. in $\mathbf{G}(\mathbf{F}\phi)$ if ϕ isn't true until the end of the trace we have cost n^2 .
- To improve on this we can make use of the dynamic programming approach used in:



Calzone, L., Chabrier-Rivier, N., Fages, F., Soliman, S.

Machine learning biochemical networks from temporal logic properties.

Transactions on Computational Systems Biology VI, 2006, pp. 68–94.

- where we traverse the trace only once, evaluating all sub-formulae simultaneously.




Hybrid algorithm

- The dynamic programming algorithm avoids unnecessary re-computation.
- However we lose the ability to *short-circuit* the checking, e.g. stop when we find a witness for $\mathbf{F}\phi$.
- By using a hybrid of the two algorithms we can have the best of both.
- The naive algorithm can be restructured as:
 - an outer recursion over the trace
 - and an inner recursion over the sub-formulae.
- Implementation in Haskell exploits any potential laziness and only computes over as much of the trace as we need.

Calls to the solver

- By far the greatest computational cost comes from solving ODEs.
- The key to efficient model checking is reducing the number of calls we have to make to the solver.
- Consider $\mathbf{G}(Q \triangleright \phi)$ – we must compute a new trace introducing Q at every time point.
 - This is *embarrassingly parallel*.
- Context introduction itself doesn't increase complexity, as we can re-write, e.g.:
 - $(Q \triangleright \phi) \wedge (Q \triangleright \psi) \rightarrow Q \triangleright (\phi \wedge \psi)$
 - $Q \triangleright (Q' \triangleright \phi) \rightarrow (Q \parallel Q') \triangleright \phi$
- We have $O(n^d)$ where d is the depth of temporal operators separated by context introductions – $\mathbf{G}(Q \triangleright (\mathbf{G}\phi))$ has $O(n^2)$

- $c\pi$ workbench – implementation in Haskell
 - $c\pi$ interactive interpreter
 - species transition system exploration
 - ODE output
 - ODE solvers
 - internal GSL solvers: explicit (RKf45) / implicit (BSimp)
 - external: interface to GNU Octave for LSODE
 - Jacobian computed symbolically by the tool.
 - graph plotting
 - logic and model checker (various algorithms)

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 -  Kwiatkowski, M., & Stark, I.
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