pre-kappa expander for κ language

Héctor Urbina

October 17, 2011

What is κ

κ is a formal language for defining agents as sets of sites.

Sites hold an internal state as well as a binding state.

κ also enables the expression of rules of interaction between agents.

These rules are executable, inducing a stochastic dynamics on a mixture of agents.

A κ model is a collection of rules (with rate constants) and an initial mixture of agents on which such rules begin to act.

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κ Syntax short introduction

Rule in English:

"Unphosphorilated Site1 of A binds to Site1 of B."

κ Rule:

A(Site1~u),B(Site1) $\rightarrow$ A(Site1~u!1),B(Site1!1)

- Agent Names : an identifier.
- Agent Sites : an identifier.
- Internal States : ~$\langle$value$\rangle$.
- Binding States : !$\langle$n$\rangle$, !_ or !?.

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Kappa file structure

```
#### Signatures
%agent:  A(x,c) # Declaration of agent A
%agent:  B(x) # Declaration of B
%agent:  C(x1~u~p,x2~u~p) # Declaration of C with 2 modifiable sites
#### Rules
‘a.b’ A(x),B(x) -> A(x!1),B(x!1) @ ‘on_rate’ #A binds B
‘a..b’ A(x!1),B(x!1) -> A(x),B(x) @ ‘off_rate’ #AB dissociation
’ab.c’ A(x!_,c),C(x1~u) ->A(x!_,c!2),C(x1~u!2) @ ‘on_rate’ #AB binds C
’mod x1’ C(x1~u!1),A(c!1) ->C(x1~p),A(c) @ ‘mod_rate’ #AB modifies x1
’a.c’ A(x,c),C(x1~p,x2~u) -> A(x,c!1),C(x1~p,x2~u!1) @ ‘on_rate’ #A binds C on x2
’mod x2’ A(x,c!1),C(x1~p,x2~u!1) -> A(x,c),C(x1~p,x2~p) @ ‘mod_rate’ #A modifies x2
#### Variables
%var:  ‘on_rate’ 1.0E-4 # per molecule per second
%var:  ‘off_rate’ 0.1 # per second
%var:  ‘mod_rate’ 1 # per second
%obs:  ‘AB’ A(x!x.B)
%obs:  ‘Cuu’ C(x1~u,x2~u)
%obs:  ‘Cpu’ C(x1~p,x2~u)
%obs:  ‘Cpp’ C(x1~p,x2~p)
#### Initial conditions
%init:  1000 A,B
%init:  10000 C
```

KaSim reference manual v1.06

DLab's current work

DLab members study complex dynamical systems.

Currently, Cesar Ravello is modeling muscle contration and Felipe Nuñez is simulating massive responses to zombie attacks on human populations, whereas Ricardo Honorato is adapting Model Checking techniques to be used with systems expressed in κ language.

Without intervening the κ language, we have reached some interesting levels of abstraction!

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DLab's current work

- Space-related simulations.
  - Compartmentalization.
  - Diffusion events.
- Timing control.
  - Polymer-driven rules to manipulate latency.

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Compartmentalization

#Signatures
%agent: A(x,c,loc~i~j~k)
%agent: B(x,loc~i~j~k)

#Rules

#A binds B

A(x,loc~i),B(x,loc~i) $\rightarrow$ A(x!1,loc~i),B(x!1,loc~i) @ 'on_rate'

A(x,loc~j),B(x,loc~j) $\rightarrow$ A(x!1,loc~j),B(x!1,loc~j) @ 'on_rate'

A(x,loc~k),B(x,loc~k) $\rightarrow$ A(x!1,loc~k),B(x!1,loc~k) @ 'on_rate'

Compartmentalization

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%agent: A(x,c,loc~i~j~k)
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#Rules

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A(x,loc~j),B(x,loc~j) → A(x!1,loc~j),B(x!1,loc~j) @ 'on_rate'

A(x,loc~k),B(x,loc~k) → A(x!1,loc~k),B(x!1,loc~k) @ 'on_rate'

Compartmentalization

#Locations i, j and k have different volumen/area!

```
#Signatures
%agent: A(x,c,loc~i~j~k)
%agent: B(x,loc~i~j~k)

#Rules

#A binds B

A(x,loc~i),B(x,loc~i) -> A(x!1,loc~i),B(x!1,loc~i) @ 'on_rate_loc(i)'

A(x,loc~j),B(x,loc~j) -> A(x!1,loc~j),B(X!1,loc~j) @ 'on_rate_loc(j)'

A(x,loc~k),B(x,loc~k) -> A(x!1,loc~k),B(X!1,loc~k) @ 'on_rate_loc(k)'

#AB dissociation

A(x!1,loc~i),B(x!1,loc~i) -> A(x,loc~i),B(x,loc~i) @ 'off_rate'

A(x!1,loc~j),B(x!1,loc~j) -> A(x,loc~j),B(x,loc~j) @ 'off_rate'

A(x!1,loc~k),B(x!1,loc~k) -> A(x,loc~k),B(x,loc~k) @ 'off_rate'
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%agent: A(x,c,loc~i~j~k)
%agent: B(x,loc~i~j~k)

#Rules

#A binds B

A(x,loc~i),B(x,loc~i) → A(x!1,loc~i),B(x!1,loc~i) @ 'on_rate_loc(i)'

A(x,loc~j),B(x,loc~j) → A(x!1,loc~j),B(X!1,loc~j) @ 'on_rate_loc(j)'

A(x,loc~k),B(x,loc~k) → A(x!1,loc~k),B(X!1,loc~k) @ 'on_rate_loc(k)'

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A(x!1,loc~i),B(x!1,loc~i) → A(x,loc~i),B(x,loc~i) @ 'off_rate'

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A(x,loc~j),B(x,loc~j) $\rightarrow$ A(x!1,loc~j),B(X!1,loc~j) @ 'on_rate_loc(j)'

A(x,loc~k),B(x,loc~k) $\rightarrow$ A(x!1,loc~k),B(X!1,loc~k) @ 'on_rate_loc(k)'

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A(x!1,loc~k),B(x!1,loc~k) $\rightarrow$ A(x,loc~k),B(x,loc~k) @ 'off_rate'

Diffusion events


```
#Signatures
%agent: A(x,c,loc~i~j~k)
%agent: B(x,loc~i~j~k)
%agent: T(s,org~i~j~k,dst~i~j~k)
```

Diffusion events

#Rules

#A diffusions

A(loc~i,x,c),T(org~i,dst~j) → A(loc~j,x,c),T(org~i,dst~j) @ 'Adiff_ij'

A(loc~i,x,c),T(org~i,dst~k) → A(loc~k,x,c),T(org~i,dst~k) @ 'Adiff_ik'

A(loc~j,x,c),T(org~j,dst~i) → A(loc~i,x,c),T(org~j,dst~i) @ 'Adiff_ji'

A(loc~j,x,c),T(org~j,dst~k) → A(loc~k,x,c),T(org~j,dst~k) @ 'Adiff_jk'

A(loc~k,x,c),T(org~k,dst~i) → A(loc~i,x,c),T(org~k,dst~i) @ 'Adiff_ki'

A(loc~k,x,c),T(org~k,dst~j) → A(loc~j,x,c),T(org~k,dst~j) @ 'Adiff_kj'

polymer-driven rules

#Signatures
%agent: S(x)
%agent: Z()
%agent: V(p,n)

#Rules
'Infection' Z(),S(x) → Z(),S(x!1),V(p!1,n) @ 'infection_rate'
'Polymerization' V(n) → V(n!1),V(p!1,n) @ 'polymer_rate'
'Expression' S(x!1),V(p!1,n!2),V(p!2,n!3),V(p!3,n!4), \
V(p!4,n!5),V(p!5,n!6),V(p!6,n!7),V(p!7,n!8),V(p!8,n!9), \
V(p!9,n!10),V(p!10,n) → Z() @ [inf]

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pre-Kappa expander

A Python (V2) script that takes as input a (built in-house) pre-κ file and outputs a kappa file which can subsequently be used with KaSim.

This is done using Lexer & Parser techniques, available in Python through ply library.

It facilitates κ abstraction while reducing error-proneness.

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pre-Kappa syntax: Locations

```
#Locations
%loc: i 100 10000 1201
%loc: j 1000 20000 3902
%loc: k 500 30000 2890
#Location list
%locl: all i j k
#Signatures

%expand-agent: all A(x,c)
%expand-agent: all B(x)

gives:
%agent: A(x,c,loc~i~j~k)
%agent: B(x,loc~i~j~k)
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pre-Kappa syntax: Locations

A bimolecular stochastic rate constant γ, expressed in $s^{-1}molecule^{-1}$, is related to its deterministic counterpart k, expressed in $s^{-1}M^{-1}$ as

$$\gamma = \frac{k}{AV}, \tag{1}$$

where A is Avogadro's number.

Krivine et. al. Programs as models: Execution. Unpublished work.

pre-Kappa syntax: Locations


```
#Locations
%loc: i 100 10000 1.201
%loc: j 1000 20000 3.902
%loc: k 500 30000 2.89
#Location list
%locl: all i j k
#A binds B
%expand-rule: all A(x),B(x) → A(x!1),B(x!1) @ %loc[2]
```

gives:

```
A(x,loc~i),B(x,loc~i) → A(x!1,loc~i),B(x!1,loc~i) @ 1.201
A(x,loc~j),B(x,loc~j) → A(x!1,loc~j),B(x!1,loc~j) @ 3.902
A(x,loc~k),B(x,loc~k) → A(x!1,loc~k),B(x!1,loc~k) @ 2.89
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A(x,loc~k),B(x,loc~k) → A(x!1,loc~k),B(x!1,loc~k) @ 2.89

pre-Kappa syntax: Location Matrices

...
#Location matrices
%locm:

TM	i	j	k
i	0	0.5	1.5
j	2.0	0	1.8
k	1.0	1.1	0

#A diffusions
%expand-rule: TM A(x,c),T() → A(%,x,c),T() @ %cell

gives:

A(loc~i,x,c),T(org~i,dst~j) → A(loc~j,x,c),T(org~i,dst~j) @ 0.5

A(loc~i,x,c),T(org~i,dst~k) → A(loc~k,x,c),T(org~i,dst~k) @ 1.5

A(loc~j,x,c),T(org~j,dst~i) → A(loc~i,x,c),T(org~j,dst~i) @ 2.0

A(loc~j,x,c),T(org~j,dst~k) → A(loc~k,x,c),T(org~j,dst~k) @ 1.8

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A(loc~i,x,c),T(org~i,dst~k) → A(loc~k,x,c),T(org~i,dst~k) @ 1.5

A(loc~j,x,c),T(org~j,dst~i) → A(loc~i,x,c),T(org~j,dst~i) @ 2.0

A(loc~j,x,c),T(org~j,dst~k) → A(loc~k,x,c),T(org~j,dst~k) @ 1.8

A(loc~k,x,c),T(org~k,dst~i) → A(loc~i,x,c),T(org~k,dst~i) @ 1.0

A(loc~k,x,c),T(org~k,dst~j) → A(loc~j,x,c),T(org~k,dst~j) @ 1.1

pre-Kappa syntax: Location Matrices

...
#Location matrices
%locm:

TM	i	j	k
i	0	0.5	1.5
j	2.0	0	1.8
k	1.0	1.1	0

#A diffusions
%expand-rule: TM A(x,c),T() → A(%,x,c),T() @ %cell

gives:

A(loc~i,x,c),T(org~i,dst~j) → A(loc~j,x,c),T(org~i,dst~j) @ 0.5

A(loc~i,x,c),T(org~i,dst~k) → A(loc~k,x,c),T(org~i,dst~k) @ 1.5

A(loc~j,x,c),T(org~j,dst~i) → A(loc~i,x,c),T(org~j,dst~i) @ 2.0

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pre-Kappa syntax: Location Matrices


```
...
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  TM     i     j     k
  i      0     0.5   1.5
  j      2.0   0     1.8
  k      1.0   1.1   0

#Observing transporters
%expand-obs: TM 'Transporter(%org,%dst)' T()
```

gives:

```
%obs: 'Transporter(i,j)' T(org~i,dst~j)
%obs: 'Transporter(i,k)' T(org~i,dst~k)
%obs: 'Transporter(j,i)' T(org~j,dst~i)
%obs: 'Transporter(j,k)' T(org~j,dst~k)
%obs: 'Transporter(k,i)' T(org~k,dst~i)
%obs: 'Transporter(k,j)' T(org~k,dst~j)
```

pre-Kappa syntax: Location Matrices

...

#Location matrices

%locm:

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i	0	0.5	1.5
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%obs: 'Transporter(i,k)' T(org~i,dst~k)

%obs: 'Transporter(j,i)' T(org~j,dst~i)

%obs: 'Transporter(j,k)' T(org~j,dst~k)

%obs: 'Transporter(k,i)' T(org~k,dst~i)

%obs: 'Transporter(k,j)' T(org~k,dst~j)

pre-Kappa syntax: Chains

#Rules

'Expression' S(x!1),V(p!1,n!2),V(p!2,n!3),...,V(p!10,n) $\rightarrow$ Z() @ [inf]

gives:

'Expression' S(x!1),V(p!1,n!2),V(p!2,n!3),V(p!3,n!4), \
V(p!4,n!5),V(p!5,n!6),V(p!6,n!7),V(p!7,n!8),V(p!8,n!9), \
V(p!9,n!10),V(p!10,n) $\rightarrow$ Z() @ [inf]

pre-Kappa syntax: Chains

#Rules
'Expression' S(x!1),V(p!1,n!2),V(p!2,n!3),...,V(p!10,n) $\rightarrow$ Z() @ [inf]

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'Expression' S(x!1),V(p!1,n!2),V(p!2,n!3),V(p!3,n!4), \
V(p!4,n!5),V(p!5,n!6),V(p!6,n!7),V(p!7,n!8),V(p!8,n!9), \
V(p!9,n!10),V(p!10,n) $\rightarrow$ Z() @ [inf]