PISKa: Parallel Implementation of Spatial Kappa

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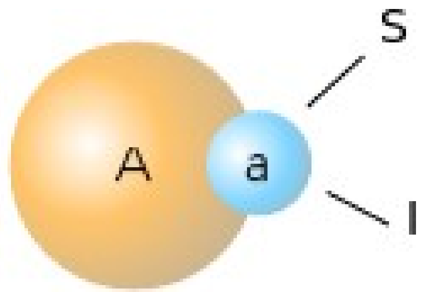
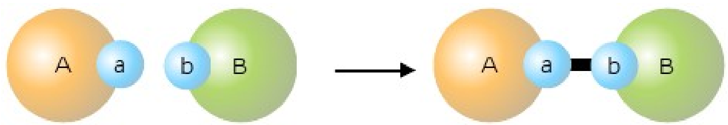
Kappa Language

- Modelling language based on rules-agents and rates
  - Agents:
    - AgentName(site~state1~state2)
    - Ex: A(a~S~I)

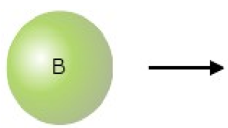


Kappa Language

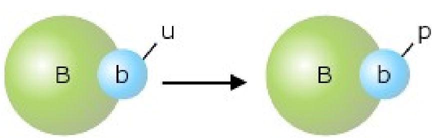
- Modelling language based on rules-agents and rates
  - Rules:
    - “bind / unbind”



    - “create / remove”



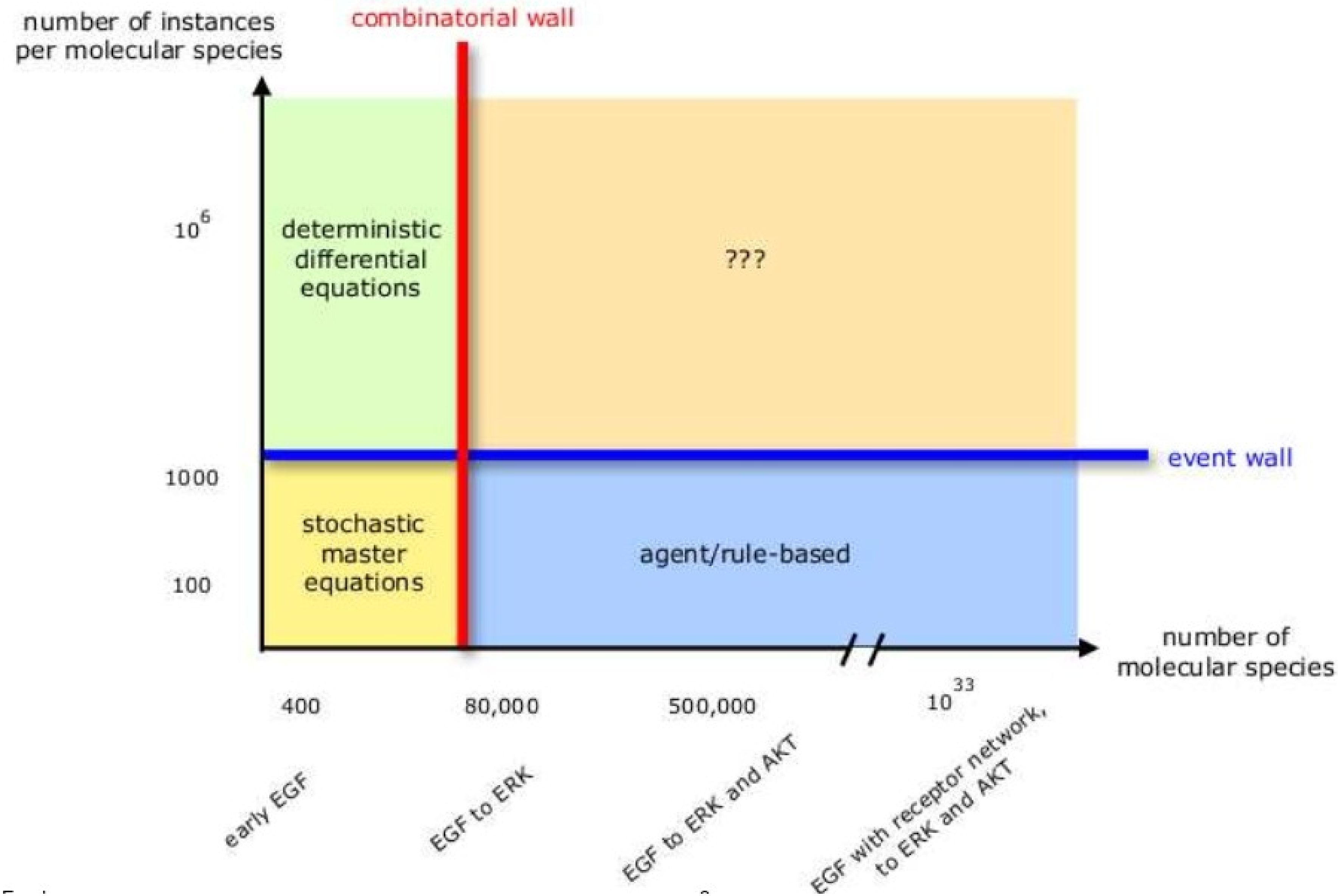
    - “change state”



KaSim Software

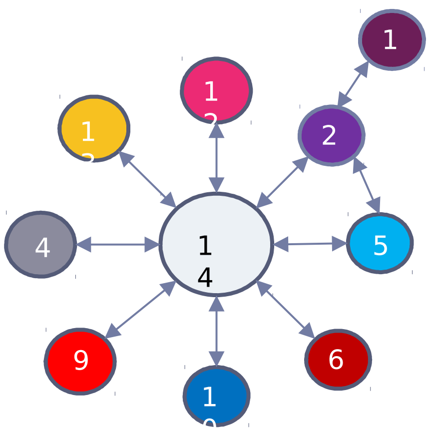
- Simulation tool for kappa models.
- Performs adapted Gillespie.
- Open Source.

Motivation
agent/rule based



Motivation
PISKa

SSA Volume



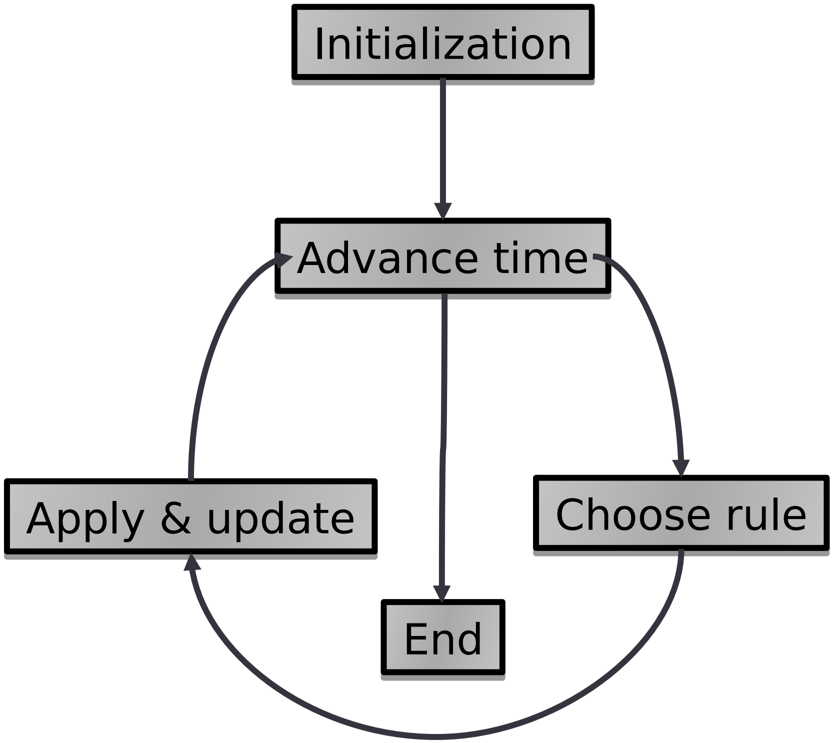
Cell Network

The cell

Stochastic Simulation Algorithm

- Stochastic Simulation Algorithm (SSA)
  - Proposed by Gillespie in 1976.
  - As a method to describe the behavior of particle-based systems along time.
  - SSA average trajectory approximate the solution of the implicit diferential equation system.
  - SSA is a state algorithm that works only in well-mixed systems.
  - KaSim algorithm adapts SSA to agent-rule models

Stochastic Simulation Algorithm



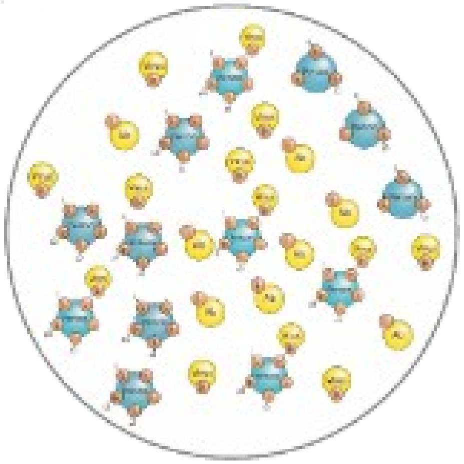
Get final state and trajectory of the system

Rule-Based Model
- Initial State (S_0)
- Rules (R)

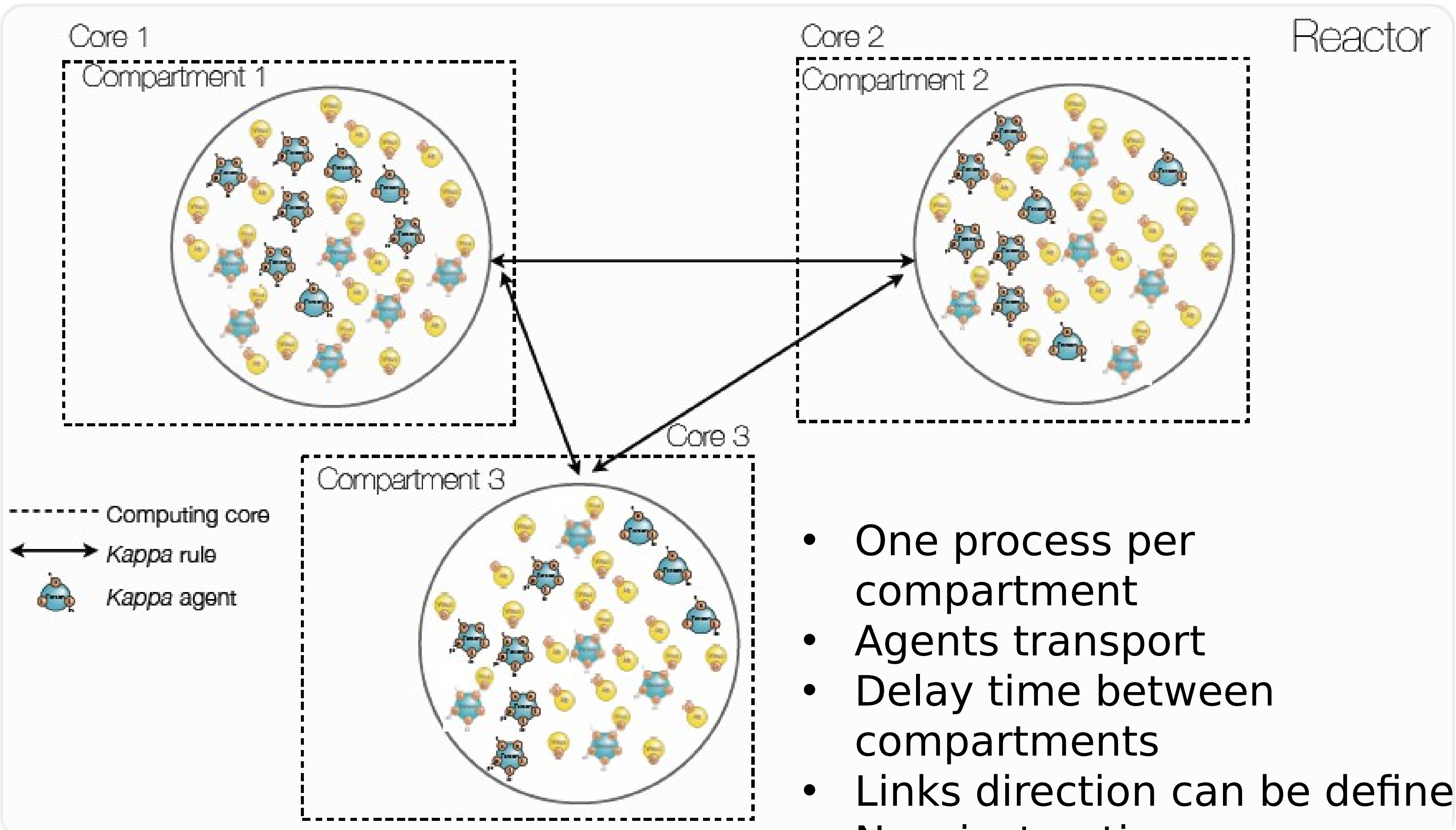
$$p(t) = \alpha e^{-\alpha t}$$

Where alpha is the total reactivity of R

$$p(r \in R) = \frac{reactivity(r)}{\alpha}$$



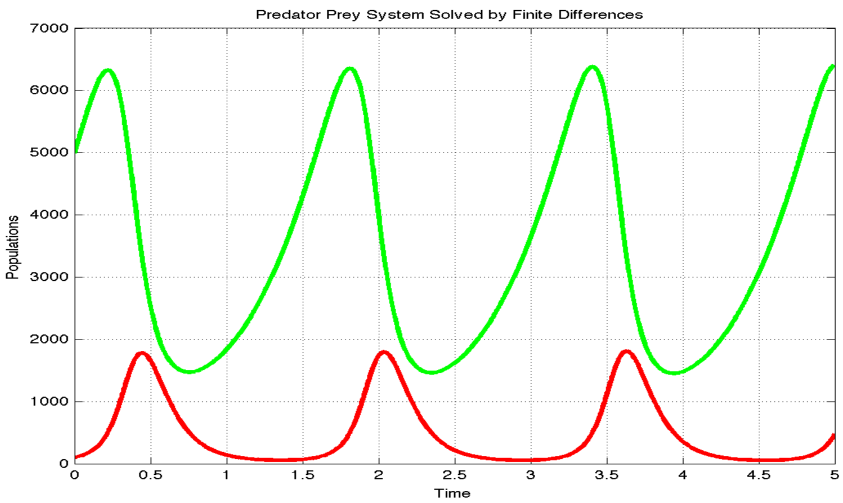
PISKa: Algorithm

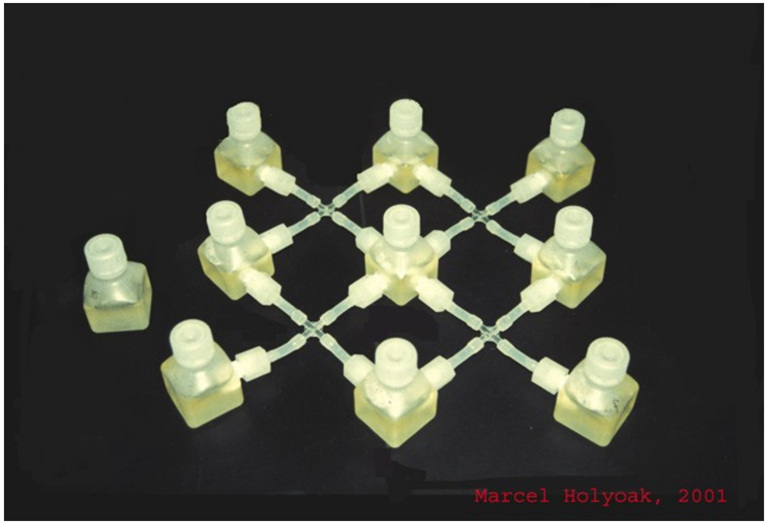


- One process per compartment
- Agents transport
- Delay time between compartments
- Links direction can be defined
- New instructions

Results
Example model predator - prey

- Simple predator-prey behavior
- Logistic growth, predation
- Extinction is prone on simple volumes.



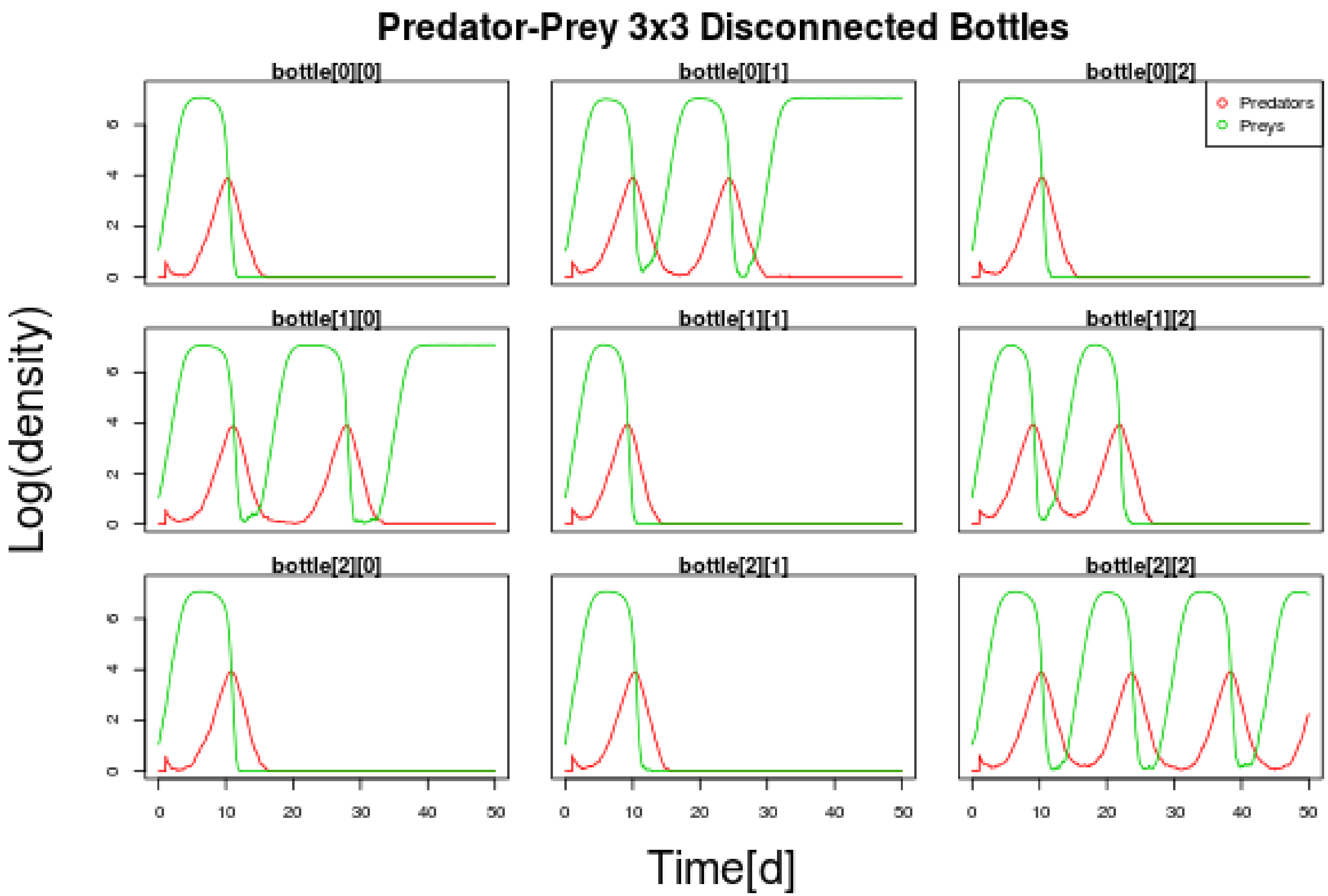


- Based on a real experiment(2)
  - Isolated bottles drive to extinction
  - Interconnected bottles avoid extinction

(2) *Holyoak et al. (1996). Persistence of an extinction-prone predator-prey interaction through metapopulation dynamics. Ecology, 77(6):1867–1879.*

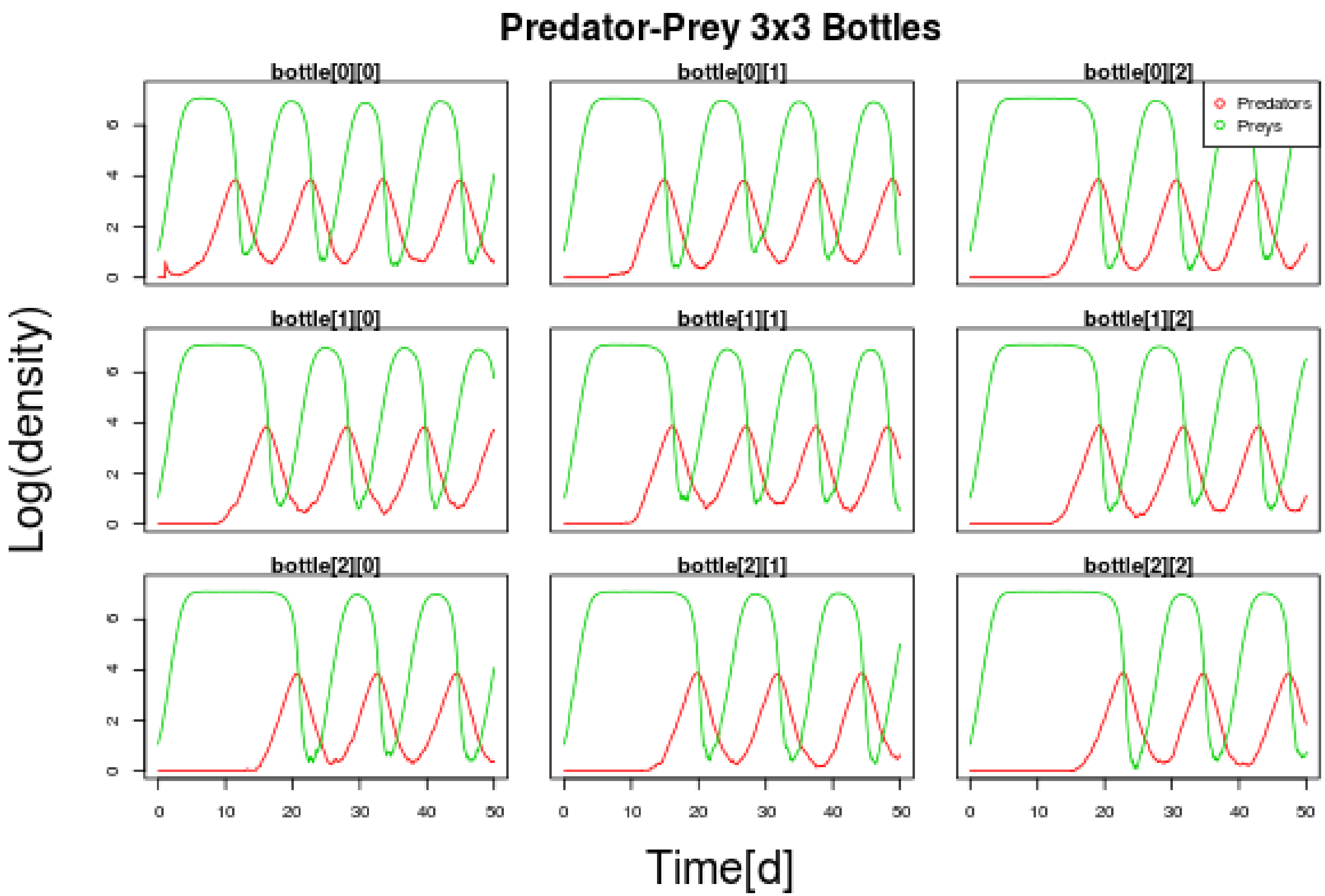
Results
Example model predator - prey

- Results with isolated bottles:



Results
Example model predator - prey

- Results with connected bottles:



PISKa Features

- Pros
  - Language statements allow declaration of compartments explicitly.
  - Improved execution time performance on similar models.
  - The distributed paradigm increases available resources.
- Cons
  - PISKa is not a good option for all spatial simulations.
  - Speed-Up is strongly restricted by the model.
  - Until now, there is no way to estimate or limit the error.

Acknowledgments

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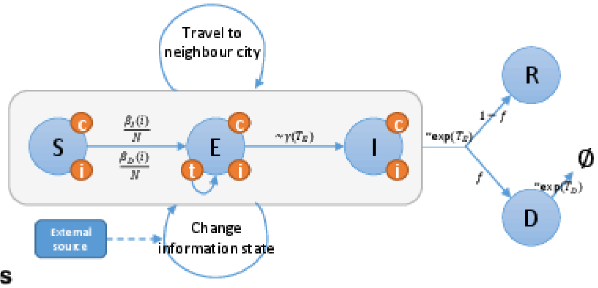
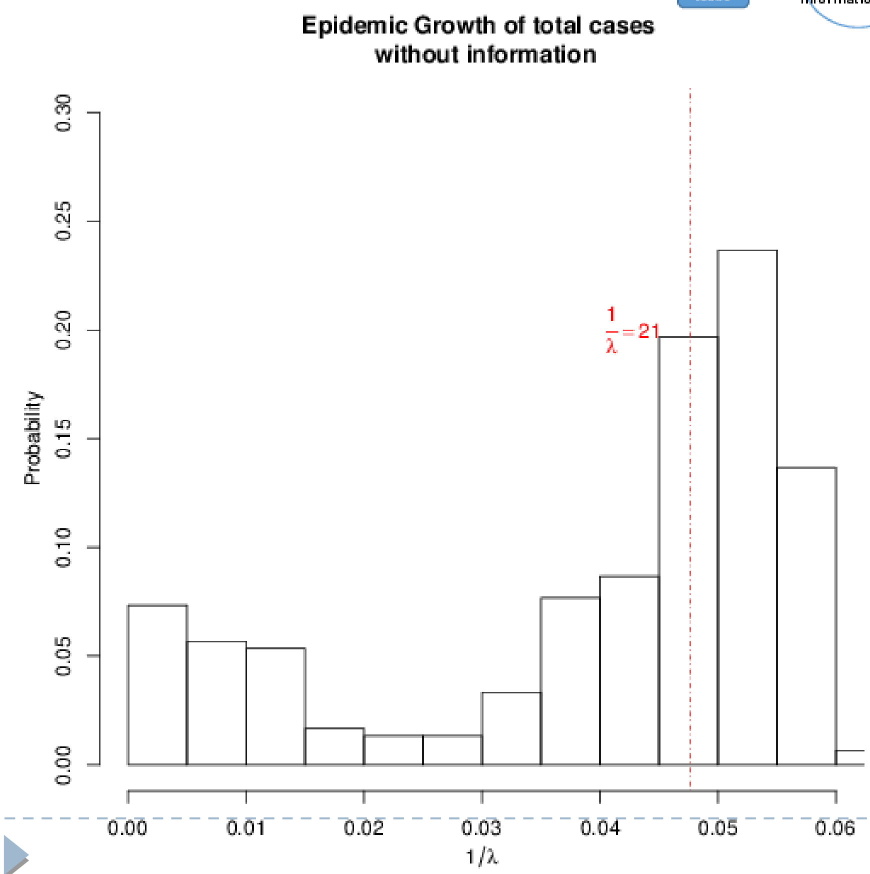
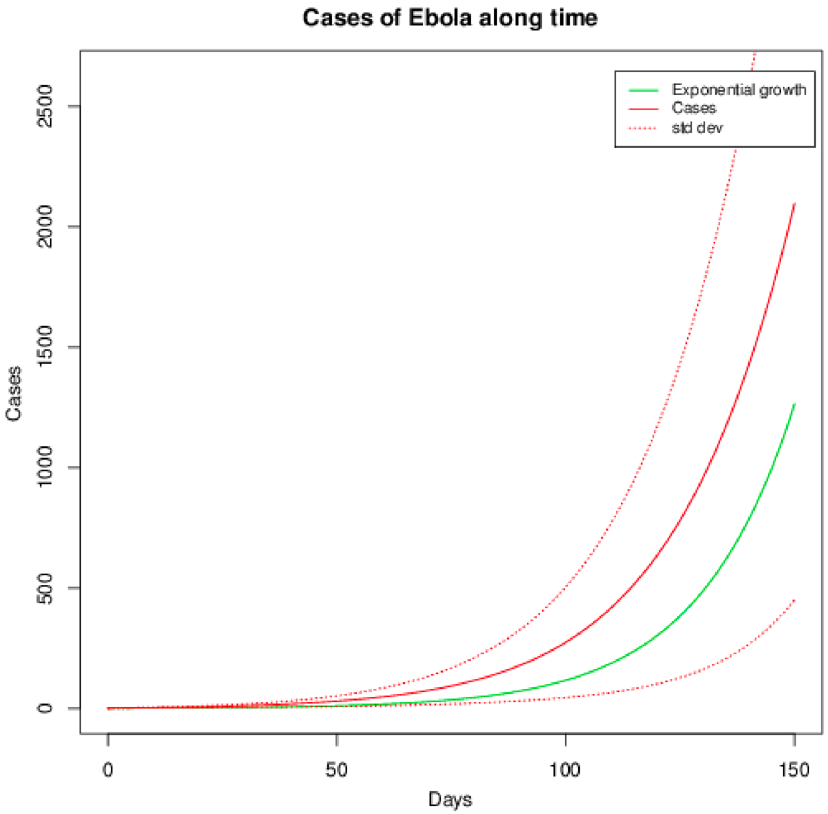
- Access to supercomputing time from NLHPC ECM-02

Results
Ebola approach

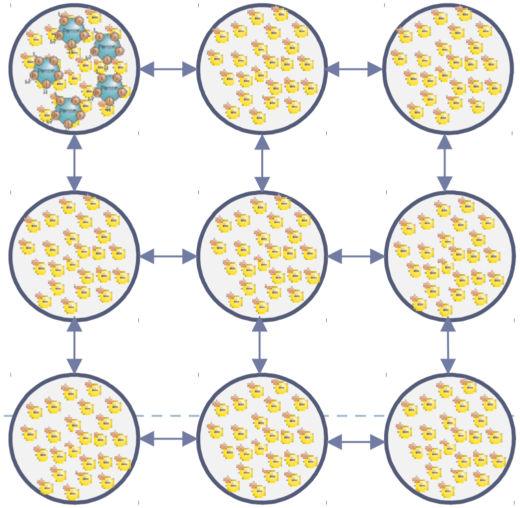






Results
Example model predator - prey

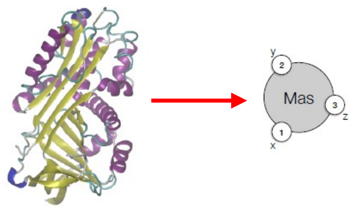
- New syntax:
  - %compartment: ‘Bottles’[3][3] 1.0 #Only Constants
  - %link: ‘tubes’ ‘Bottles’[x][y] <->‘Bottles’[x+1][y] $0.0
  - %link: ‘tubes’ ‘Bottles’[x][y] <->‘Bottles’[x][y+1] $0.0
  - %transport: ‘tubes’ Predator() @ 1.0
  - %init: 100 Prey()
  - %use: ‘Bottle’[0][0]
  - %init: 5 Predator()

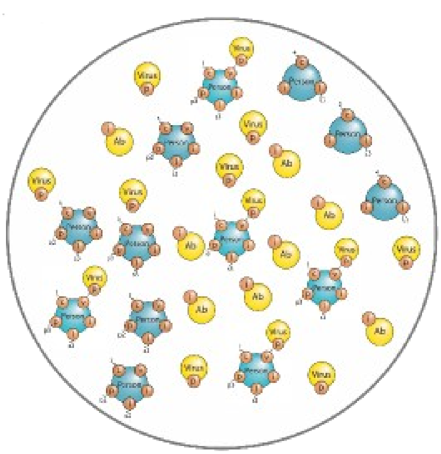


Kappa Syntax Extensions

Common declarations

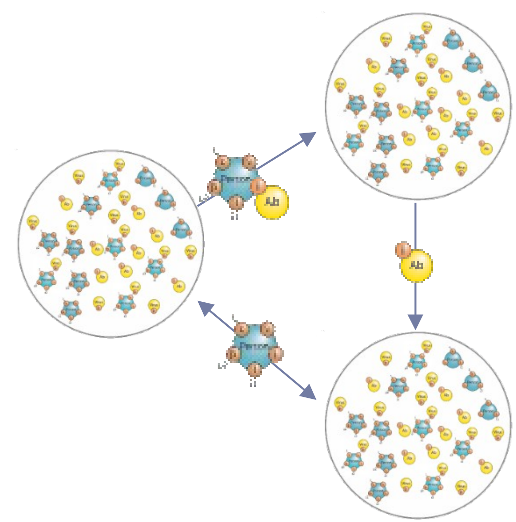
- Agents
- Rules
- Initializations
- Perturbations
- Variables and Observables





New declarations

- Compartments
- Links
- Transports
- Compartment context



Code example

```
%compartment: 'cityA' 1 # compartments declaration
%compartment: 'cityB' 2

%link: 'highway' 'cityA' <-> 'cityB' $1 # links between compartments

%transport: 'highway' person() @ 0.01 # delay time between compartments, agents
                                      # allowed to travel.

%agent: person(s~S~I) #agents of the simulation, with its sites and states.

#Rules
'contact1' person(s~S), person(s~I) -> person(s~I), person(s~I) @ 0.001

%use: 'cityA'             #initialization of first compartment
%init: 1000 person(s~S)
%init: 1 person(s~I)

%use: 'cityB'             #initialization of second compartment
%init: 1500 person(s~S)

%use:                     #output
%obs: 'person_S' person(s~S)
%obs: 'person_I' person(s~I)
```

Results: Validity

Model	Synch. Step	R	τ	MIC
Mammalian Circadian Clock (2)	0.5	0.39	0.15	0.49
	0.1	0.48	0.42	0.73
	0.02	0.93	0.90	0.99
Mammalian Circadian Clock(3x3x3)	0.5	0.53	0.16	0.32
	0.1	0.50	0.46	0.75
	0.02	0.98	0.94	0.99
Predator / Prey	1.0	0.48	0.23	0.71
	0.2	0.75	0.76	0.96
	0.05	0.91	0.89	0.99

Where *R* is Pearson coefficient, τ is Kendall coefficient and MIC is the Maximal Information Coefficient[(3)]

(3) Reshef, David N. et al - Detecting Novel Associations in Large Data Sets