IMT SCHOOL FOR ADVANCED STUDIES LUCCA

Quantitative Abstractions For Collective Adaptive Systems

Mirco Tribastone and Andrea Vandin

SFM'16 – Bertinoro

24 June 2016

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Outline

- ERODE: A tool for the Evaluation and Reduction of ODEs
  - Frontend
  - Core
  - Reduction Techniques
- Case Studies
  - Large case studies
    - Continuous time Markov chains from MRMC distribution
    - Chemical Reaction Networks from the literature
  - Spatial dynamics
    - Crowd Dynamics
    - Multi-community Epidemiology

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ERODE: Evaluation and Reduction of ODEs

IDOL: Intermediate Drift-oriented Language **[POPL'16]**

$$p ::= \varepsilon \mid \dot{x}_i = f,\ p$$

$$f ::= n \mid x_i \mid f + f \mid f \cdot f \mid f^{\frac{1}{m}}$$

Reaction Networks **[CONCUR'15, TACAS'16]**

$$x_i + x_j \xrightarrow{k_1} x_i + x_j + x_k$$

$$x_i \xrightarrow{k_2} x_i + x_j$$

$$\emptyset \xrightarrow{k_3} x_i$$

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- Forward Equivalence
- Backward Equivalence

Reaction Networks **[CONCUR'15, TACAS'16]**

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- Forward Bisimulation
- Backward Bisimulation

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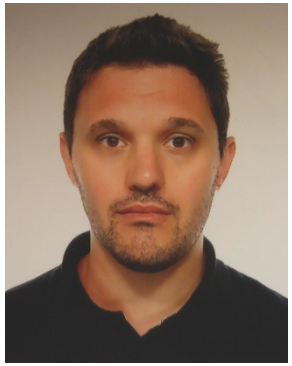
Luca Cardelli[1]

Mirco Tribastone[2]

Max Tschaikowski[2]



Andrea Vandin[2]

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[2] IMT School for Advanced Studies Lucca, Italy

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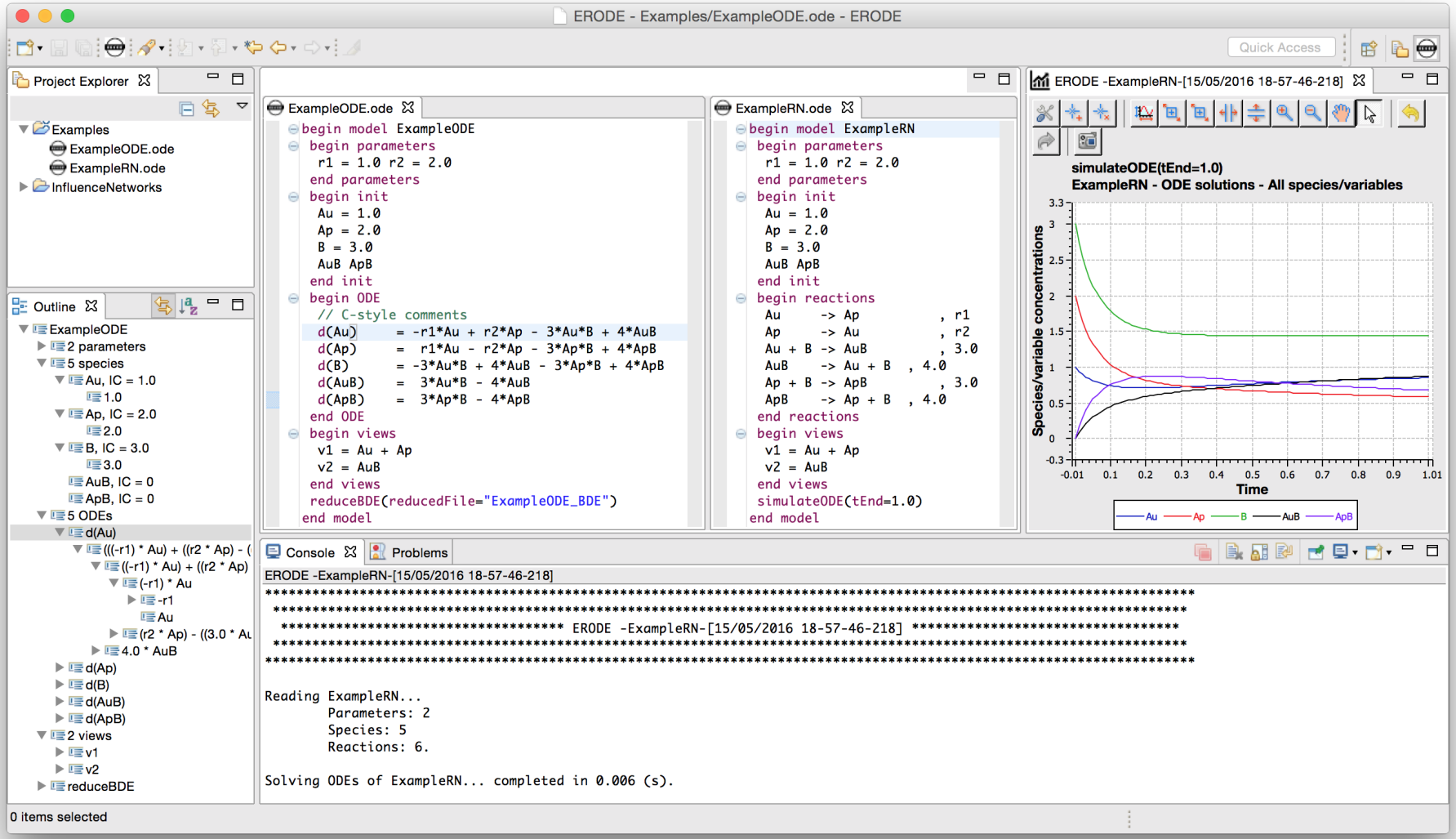
ERODE: Evaluation and Reduction of ODEs



http://sysma.imtlucca.it/tools/erode/

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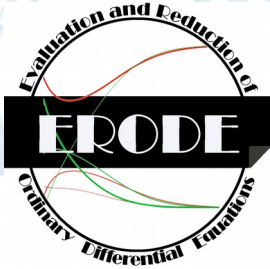
ERODE: Evaluation and Reduction of ODEs



FRONTEND

- **ODE and RN Editor**
  - Auto-completion
  - Error detection
  - Fix suggestion
- **ERODE Views**
  - Project explorer
  - Outline & Problems
  - Console & Plots
- **ERODE Wizards**
  - Update manager
  - New ERODE Project & File
  - Import BNG, Matlab, LBS

CORE

- ODE Simulator
- BDE/FDE Reducer
- ODE ⟷ RN Encoder
- Stochastic Simulator (RN)
- Statistical Model Checker (RN)
- BB/FB Reducer (RN)
- Importer/Exporter (BNG,Matlab,LBS,SBML)

APIs

- Apache Commons Math
- FERN
- MultiVeStA
- Microsoft Z3

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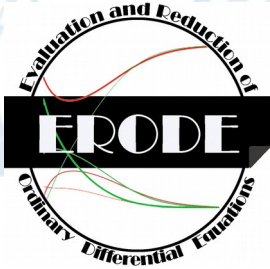
ERODE: Frontend



FRONTEND

ODE and RN Editor
Auto-completion
Error detection
Fix suggestion

ERODE Views
Project explorer
Outline & Problems
Console & Plots

ERODE Wizards
Update manager
New ERODE Project & File
Import BNG, Matlab, LBS

CORE

ODE Simulator

BDE/FDE Reducer

ODE ⟷ RN Encoder

Stochastic Simulator (RN)

Statistical Model Checker (RN)

BB/FB Reducer (RN)

Importer/Exporter (BNG,Matlab,LBS,SBML)

APIs

Apache Commons Math

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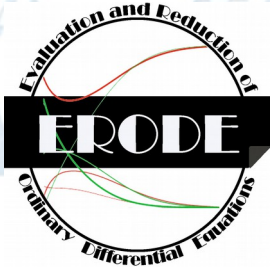
Microsoft Z3

IMT SCHOOL FOR ADVANCED STUDIES LUCCA

ERODE: Frontend



Highlights:

- The Project explorer
- Project and file creation
- Parts composing an ERODE file
- The Outline
- Auto completion, error detection and fix suggestion
- Importer wizards
- Updates manager

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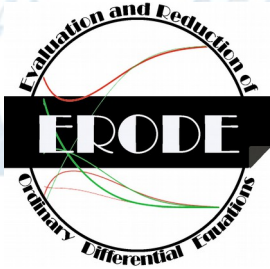
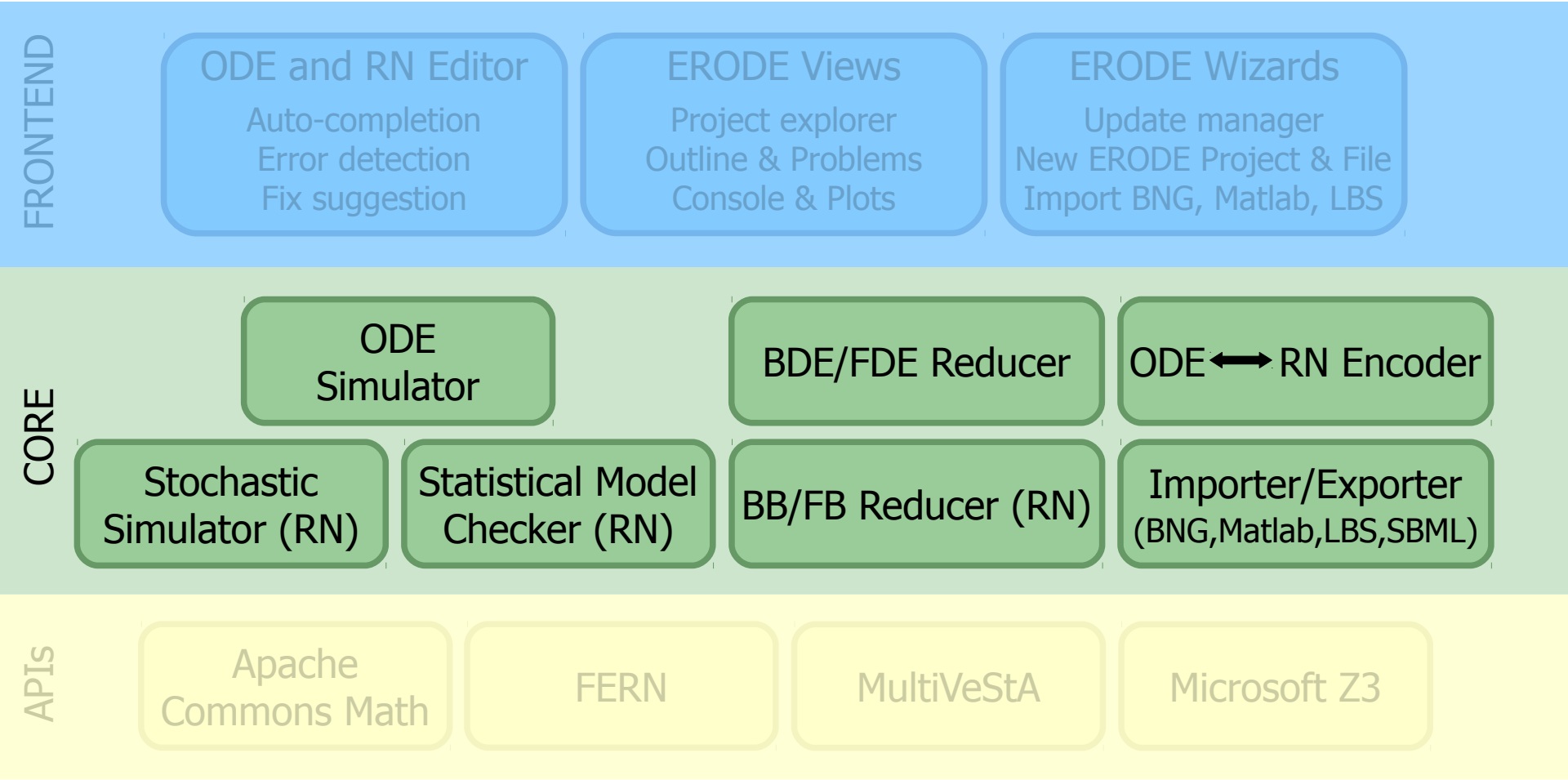
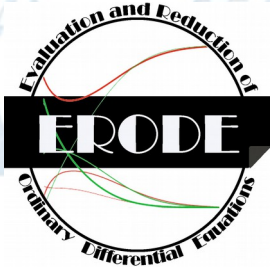
ERODE: Core





ERODE: Core



Highlights

- SimulateODE
- setIC/setParam,
- Plots and CSV files
- Views in plots
- RN to ODE encoding
- Specific features of ODE editor
- Matlab export/import
- Stochastic simulation

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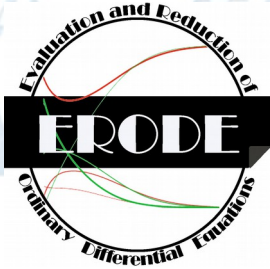
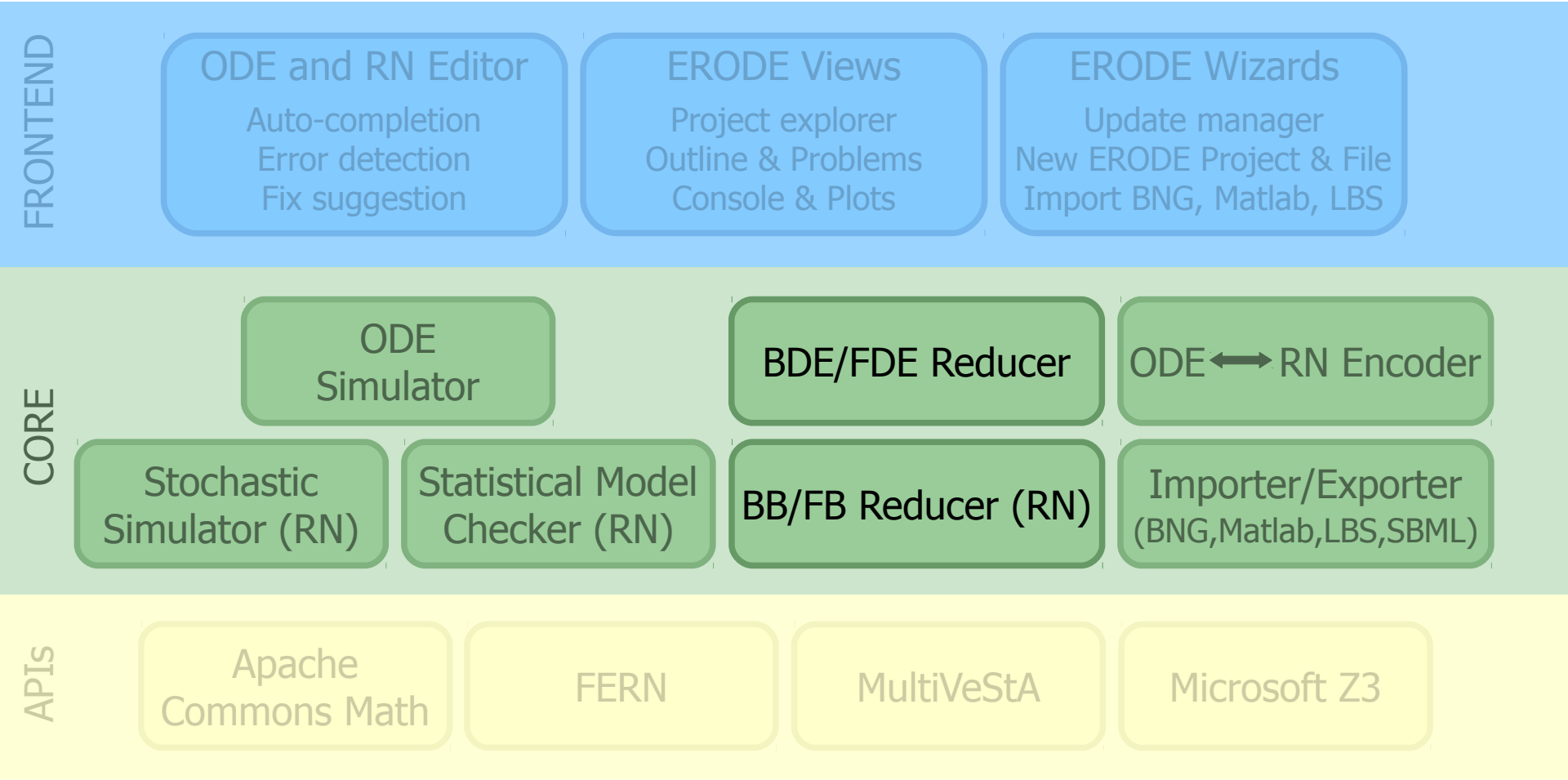
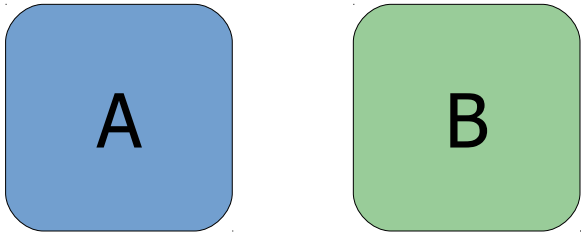
ERODE: Core – Reduction techniques





ERODE: Core – Reduction techniques

A simple binding/unbinding model



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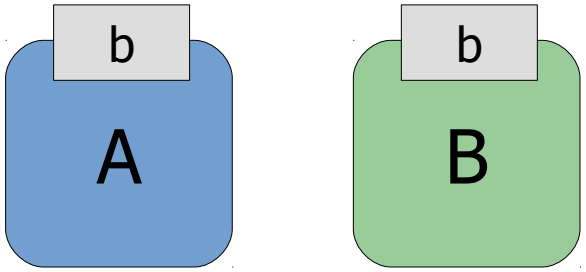

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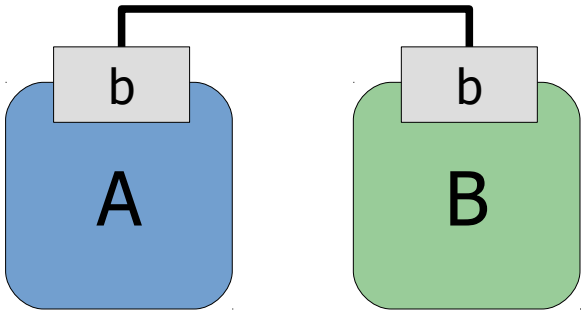

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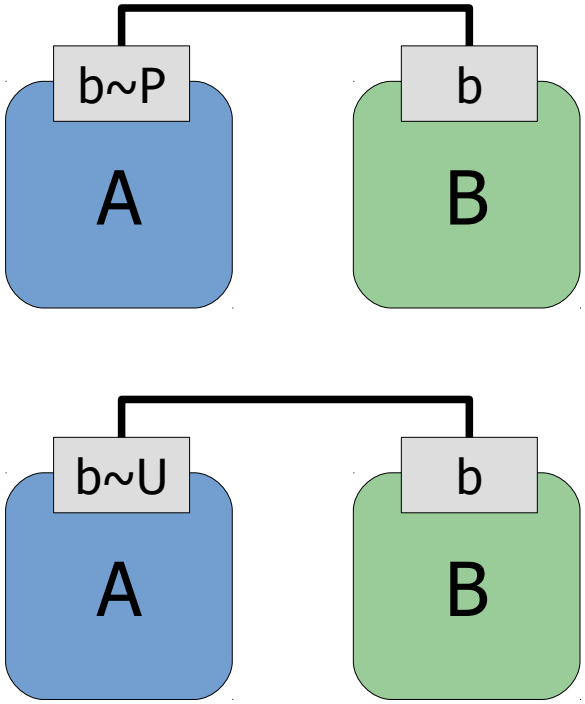

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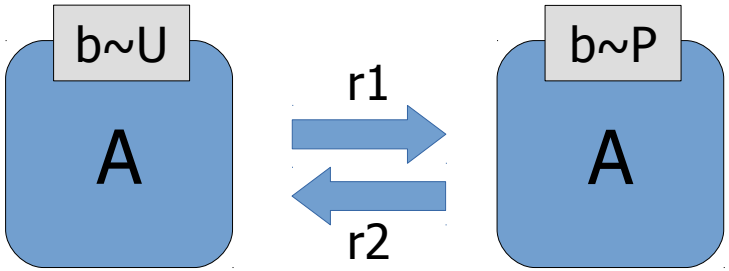
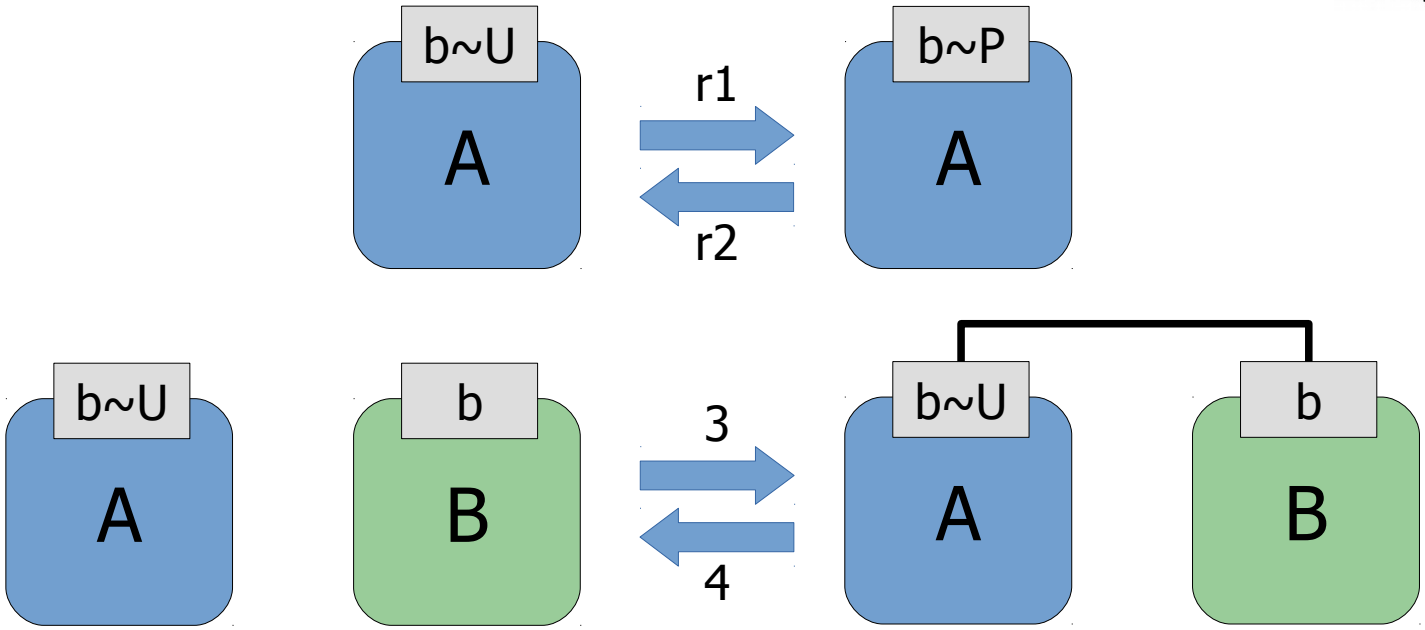


ERODE: Core – Reduction techniques



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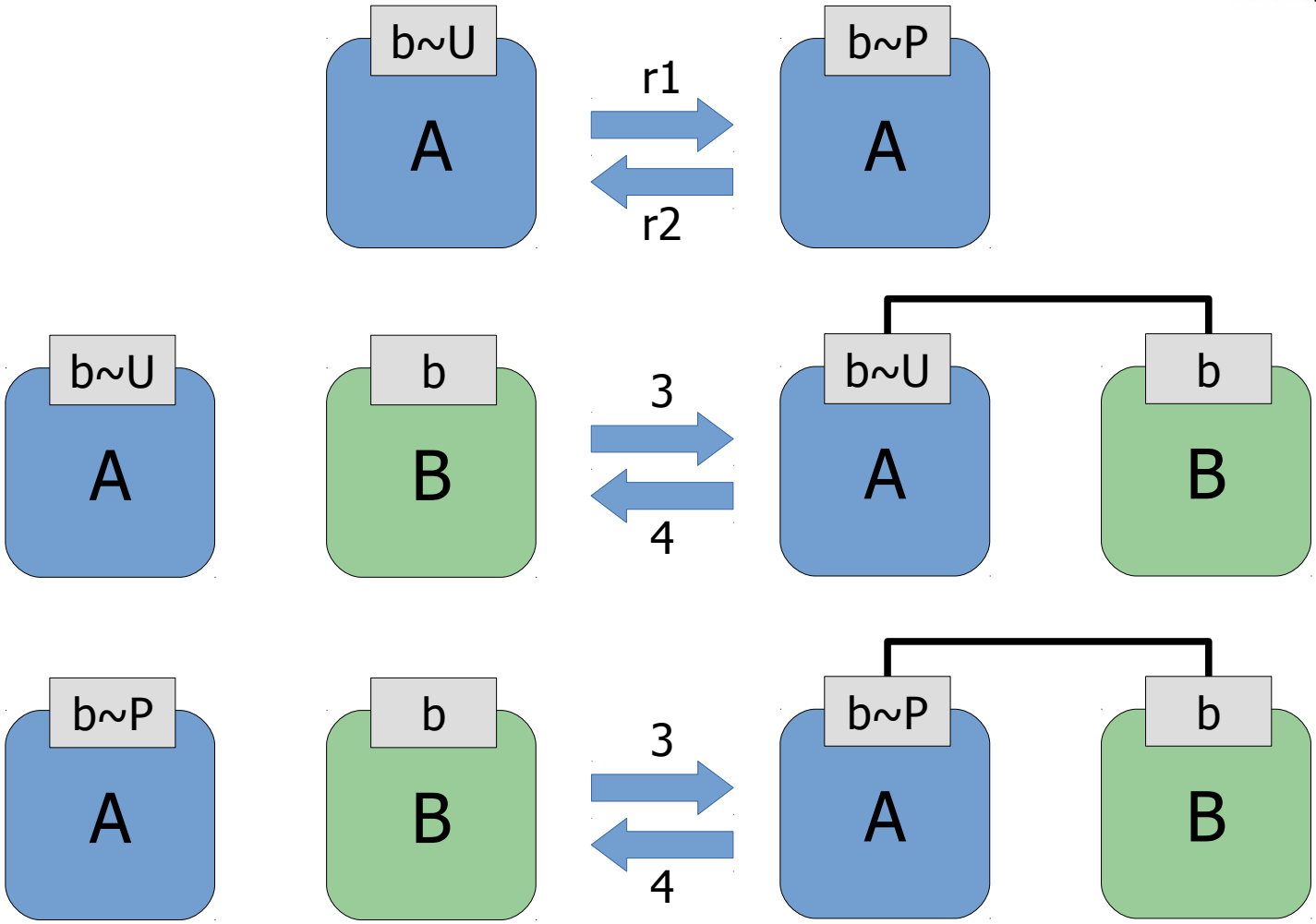
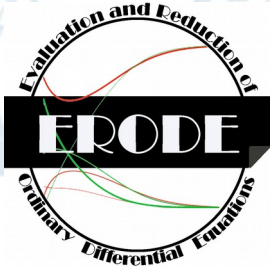
ERODE: Core – Reduction techniques



ERODE: FDE/BDE



Highlights

- RN specification
- ODE simulation
- ODE specification (via encoding)
- FDE reduction
  - With & without pre-partitioning
  - Explanation of reduction via plots
- BDE reduction
  - For r1=r2 and not
  - With & without IC pre-partitioning
  - Explanation of reduction via plots

ERODE: Core – Reduction techniques

Model

$$\dot{x}_1 = -x_1$$
$$\dot{x}_2 = k_1 \cdot x_1 - x_2$$
$$\dot{x}_3 = k_2 \cdot x_1 - x_3$$

Candidate partition

$$\{\{x_1\}, \{x_2, x_3\}\}$$

ERODE: Core – Reduction techniques

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$$\dot{x}_1 = -x_1$$
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Candidate partition

$$\{\{x_1\}, \{x_2, x_3\}\}$$

Equivalence condition (quantifier free)

$$\phi \equiv (x_2 = x_3) \implies k_1 \cdot x_1 - x_2 = k_2 \cdot x_1 - x_3$$

ERODE: Core – Reduction techniques

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$$\dot{x}_1 = -x_1$$
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$$\phi \equiv k_1 \cdot x_1 - x_2 = k_2 \cdot x_1 - x_2$$

SMT check

$$\mathrm{sat}(\neg\phi) = \mathbf{false}$$

ERODE: Core – Reduction techniques

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$$\dot{x}_1 = -x_1$$
$$\dot{x}_2 = k_1 \cdot x_1 - x_2$$
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Candidate partition

$$\{\{x_1\}, \{x_2, x_3\}\}$$

Equivalence condition (quantifier free)

$$\neg\phi \equiv k_1 \cdot x_1 - x_2 \neq k_2 \cdot x_1 - x_2$$

SMT check

$$\mathrm{sat}(\neg\phi) = \mathbf{false}$$

ERODE: Core – Reduction techniques

Algorithm. Compute the largest equivalence that refines a given partition of variables:

$$k_1 = k_2 = 3$$

$$\begin{aligned}\dot{x}_1 &= -x_1\\ \dot{x}_2 &= 3 \cdot x_1 - x_2\\ \dot{x}_3 &= 3 \cdot x_1 - x_3\end{aligned}$$

$$\{\{x_1, x_2, x_3\}\}$$

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Algorithm. Compute the largest equivalence that refines a given partition of variables:

$$\{\{x_1, x_2, x_3\}\}$$

1. SMT check of negation of

$$x_1 = x_2 = x_3 \implies$$
$$-x_1 = 3 \cdot x_1 - x_2 = 3 \cdot x_1 - x_3$$

ERODE: Core – Reduction techniques

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$x_1 = x_2 = x_3 = 1$

$$\begin{aligned}\dot{x}_1 &= -1\\ \dot{x}_2 &= 3 \cdot 1 - 1\\ \dot{x}_3 &= 3 \cdot 1 - 1\end{aligned}$$

sat

ERODE: Core – Reduction techniques

Algorithm. Compute the largest equivalence that refines a given partition of variables:

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   $x_1 = x_2 = x_3 \implies$
   $-x_1 = 3 \cdot x_1 - x_2 = 3 \cdot x_1 - x_3$
2. If **sat** get witness and split partition preserving its uniformity. Goto 1.

$k_1 = k_2 = 3$

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$\{\{x_1, x_2, x_3\}\}$

$x_1 = x_2 = x_3 = 1$

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$$\dot{x}_2 = 3 \cdot 1 - 1$$ **sat**
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ERODE: Core – Reduction techniques

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   $-x_1 = 3 \cdot x_1 - x_2 = 3 \cdot x_1 - x_3$
2. If **sat** get witness and split partition preserving its uniformity. Goto 1.
3. If **unsat** the current partition is the coarsest refinement. End.

$k_1 = k_2 = 3$

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$\{\{x_1, x_2, x_3\}\}$

$x_1 = x_2 = x_3 = 1$

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http://rise4fun.com/Z3/lW7d1

ERODE: FB/BB

Highlights

- RN Encoding
- FDE & FB reduction
  - Same FDE reductions as for ODE
  - FB is stricter than FDE
- BDE & BB reduction
  - Same BDE reductions as for ODE
  - The two reductions coincide
  - Comparison of the BDE/BB reduced RNs

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  - Reduction Techniques
- Case Studies
  - Large case studies
    - Continuous time Markov chains from MRMC distribution
    - Chemical Reaction Networks from the literature
  - Spatial dynamics
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    - Multi-community Epidemiology

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Some considered large case studies

Original model		*FB reduction*			*BB reduction*		
$\|R\|$	$\|S\|$	*Red.(s)*	$\|R\|$	$\|S\|$	*Red.(s)*	$\|R\|$	$\|S\|$
Continuous-time Markov chains							
22 871 849	3 101 445	2.01E+3	1 069 777	135 752	1.34E+3	1 166 931	148 092
11 583 520	2 373 652	9.78E+1	5 792 531	1 187 597	3.07E+2	5 814 622	1 187 597
10 485 761	1 048 576	1.76E+1	3301	792	1.23E+1	5083	792
Biochemical reaction networks							
3 538 944	262 146	7.49E+0	990	222	1.21E+1	2 614	222
786 432	65 538	1.58E+0	720	167	2.51E+0	1 873	167
172 032	16 386	2.89E–1	504	122	6.03E–1	1 305	122
194 054	14 531	3.88E–1	142 165	10 855	6.00E–1	91 001	6 634
187 468	10 734	6.09E–1	57 508	3 744	1.40E+0	145 650	5 575
32 776	2 506	1.19E–1	16 481	1 281	2.14E–1	*32 776*	*2 506*
41 233	2 562	2.69E–1	33 075	1 897	3.97E–1	*41 233*	*2 562*

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Largest models from MRMC distribution

Comparison with state-of-the-art model checker to assess scalability and correctness

Original model		*FB reduction*			*BB reduction*		
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J.P. Katoen, T. Kemna, I.S. Zapreev, and D.N. Jansen.
Bisimulation minimisation mostly speeds up probabilistic model checking. TACAS, 2007

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Continuous-time Markov chains							
22 871 849	3 101 445	2.01E+3	1 069 777	135 752	1.34E+3	1 166 931	148 092
11 583 520	2 373 652	9.78E+1	5 792 531	1 187 597	3.07E+2	5 814 622	1 187 597
10 485 761	1 048 576	1.76E+1	3301	792	1.23E+1	5083	792
Biochemical reaction networks							
3 538 944	262 146	7.49E+0	990	222	1.21E+1	2 614	222
786 432	65 538	1.58E+0	720	167	2.51E+0	1 873	167
172 032	16					05	122
194 054	14					01	6 634
187 468	10 734	6.09E–1	57 508	3 744	1.40E+0	145 650	5 575
32 776	2 506	1.19E–1	16 481	1 281	2.14E–1	*32 776*	*2 506*
41 233	2 562	2.69E–1	33 075	1 897	3.97E–1	*41 233*	*2 562*

$$R_Q = \{ s_i \xrightarrow{Q_{i,j}} s_j \mid Q_{i,j} \neq 0 \}$$

J.P. Katoen, T. Kemna, I.S. Zapreev, and D.N. Jansen.
Bisimulation minimisation mostly speeds up probabilistic model checking. TACAS, 2007

IMT SCHOOL FOR ADVANCED STUDIES LUCCA

Largest models from MRMC distribution

Comparison with state-of-the-art model checker to assess scalability and correctness

Original model		*FB reduction*			*BB reduction*		
$\|R\|$	$\|S\|$	*Red.(s)*	$\|R\|$	$\|S\|$	*Red.(s)*	$\|R\|$	$\|S\|$
Continuous-time Markov chains							
22 871 849	3 101 445	2.01E+3	1 069 777	135 752	1.34E+3	1 166 931	148 092
11 583 520	2 373 652	9.78E+1	5 792 531	1 187 597	3.07E+2	5 814 622	1 187 597
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41 233	2 562	2.69E–1	33 075	1 897	3.97E–1	*41 233*	*2 562*

$$R_Q = \{ s_i \xrightarrow{Q_{i,j}} s_j \mid Q_{i,j} \neq 0 \}$$

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Biochemical models from BioNetGen repository

Support for state-of-the-art tool for the analysis of biological networks

Original model		*FB reduction*			*BB reduction*		
$\|R\|$	$\|S\|$	*Red.(s)*	$\|R\|$	$\|S\|$	*Red.(s)*	$\|R\|$	$\|S\|$
Continuous-time Markov chains							
22 871 849	3 101 445	2.01E+3	1 069 777	135 752	1.34E+3	1 166 931	148 092
11 583 520	2 373 652	9.78E+1	5 792 531	1 187 597	3.07E+2	5 814 622	1 187 597
10 485 761	1 048 576	1.76E+1	3301	792	1.23E+1	5083	792
Biochemical reaction networks							
3 538 944	262 146	7.49E+0	990	222	1.21E+1	2 614	222
786 432	65 538	1.58E+0	720	167	2.51E+0	1 873	167
172 032	16 386	2.89E–1	504	122	6.03E–1	1 305	122
194 054	14 531	3.88E–1	142 165	10 855	6.00E–1	91 001	6 634
187 468	10 734	6.09E–1	57 508	3 744	1.40E+0	145 650	5 575
32 776	2 506	1.19E–1	16 481	1 281	2.14E–1	*32 776*	*2 506*
41 233	2 562	2.69E–1	33 075	1 897	3.97E–1	*41 233*	*2 562*

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Observable-preserving FB reduction

Original model		*FB reduction*			*FB reduction with prep.*			
$\|R\|$	$\|S\|$	*Red.(s)*	$\|R\|$	$\|S\|$	$\|Prep.\|$	*Red.(s)*	$\|R\|$	$\|S\|$
194 054	14 531	3.88E–1	142 165	10 855	1 345	3.28E–1	147 797	12 037
5 797	796	1.90E–2	4 210	503	18	4.10E–2	4 210	503
487	85	2.00E–3	264	56	4	2.00E–3	362	69

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Observable-preserving FB reduction

Original model		*FB reduction*			*FB reduction with prep.*			
$\|R\|$	$\|S\|$	*Red.(s)*	$\|R\|$	$\|S\|$	$\|Prep.\|$	*Red.(s)*	$\|R\|$	$\|S\|$
194 054	14 531	3.88E–1	142 165	10 855	1 345	3.28E–1	147 797	12 037
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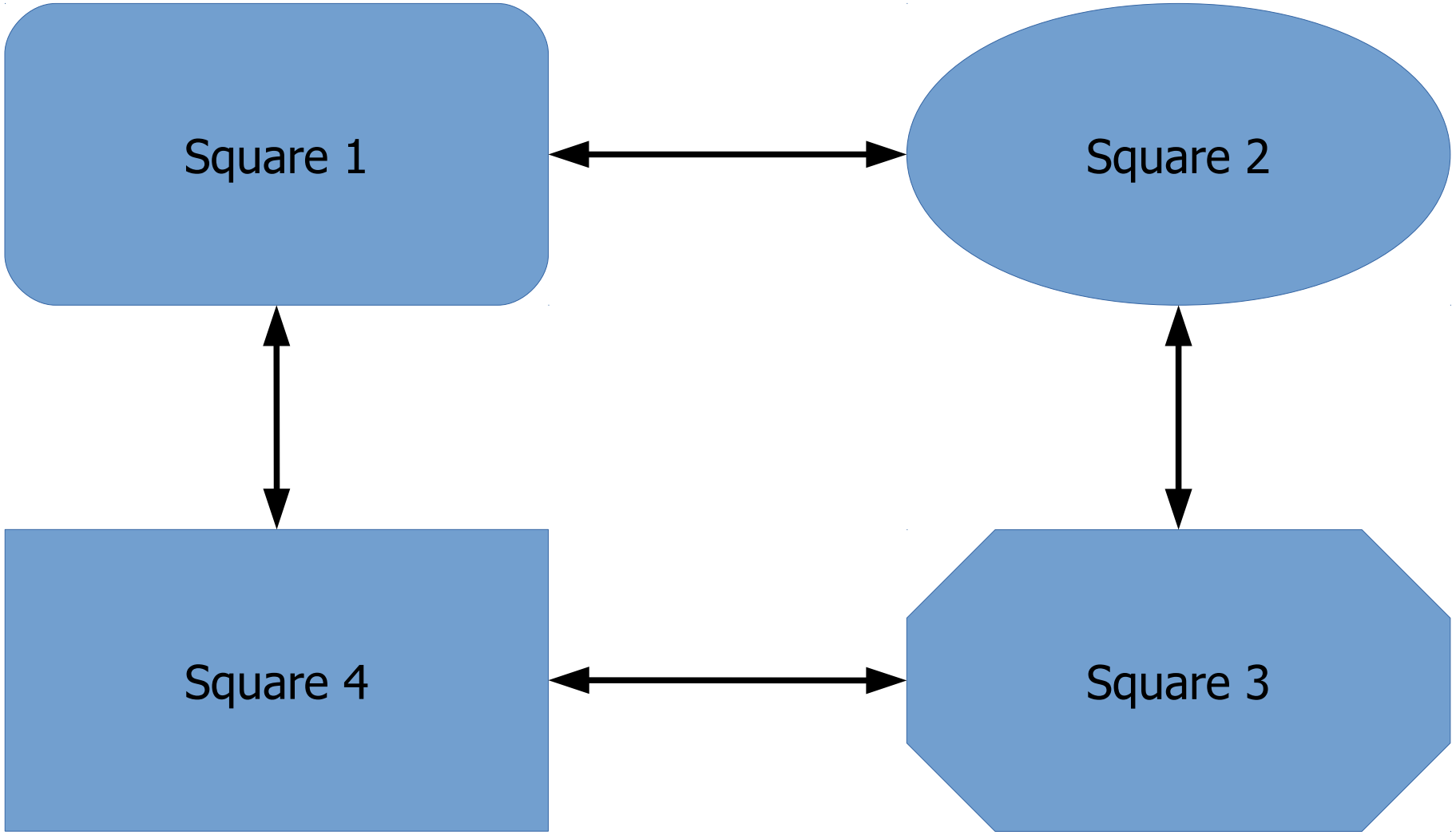
Outline

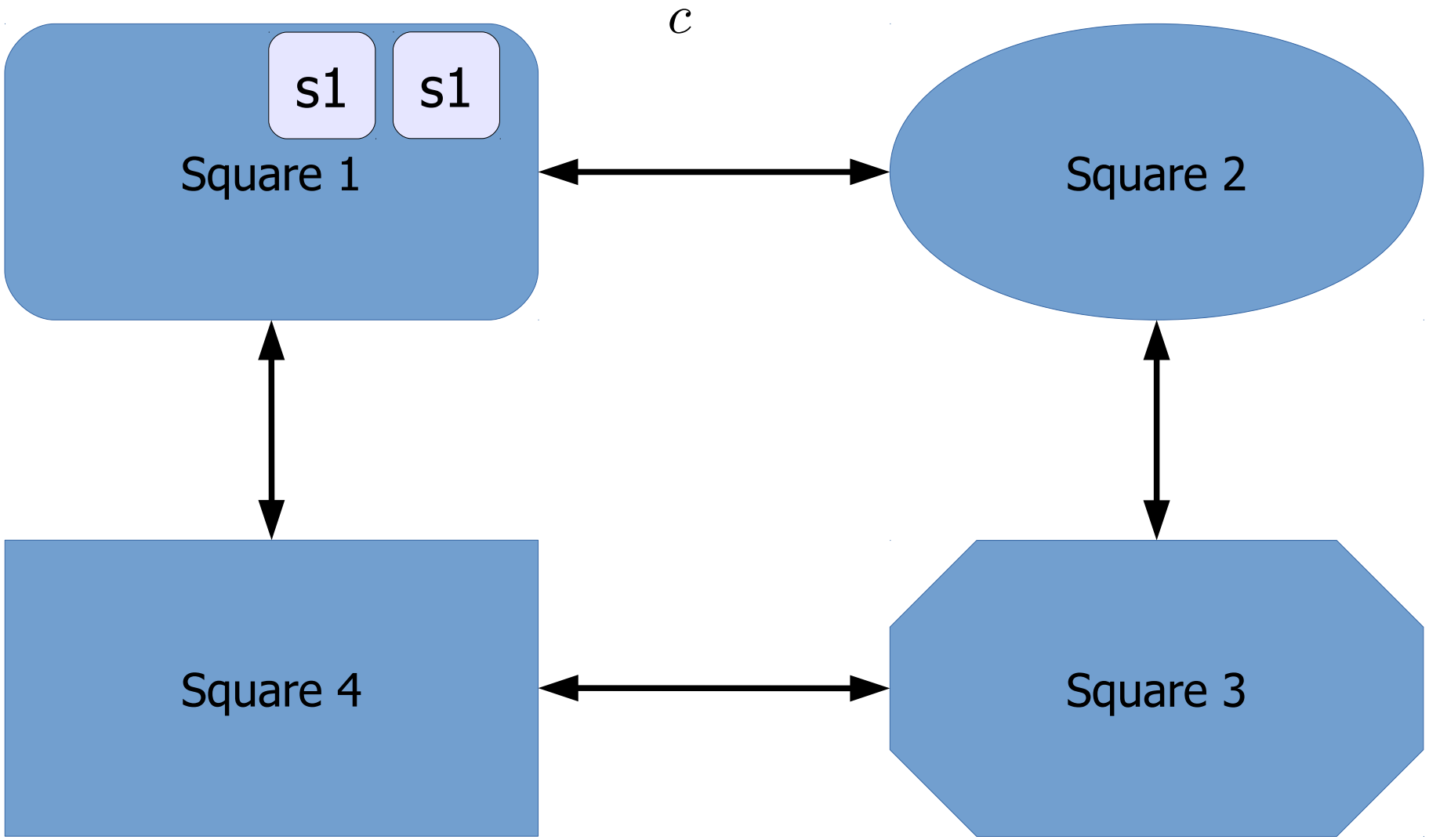
- ERODE: A tool for the Evaluation and Reduction of ODEs
  - Frontend
  - Core
  - Reduction Techniques
- Case Studies
  - Large case studies
    - Continuous time Markov chains from MRMC distribution
    - Chemical Reaction Networks from the literature
  - Spatial dynamics
    - Crowd Dynamics
    - Multi-community Epidemiology

Crowd Dynamics



J.E. Rowe, R.L. Gomez. El Botellon: Modeling the movement of crowds in a city. Complex Systems 14, 2003
L. Bortolussi, D. Latella, M. Massink. Stochastic process algebra and stability analysis of collective systems. Coordination 2013

Crowd Dynamics



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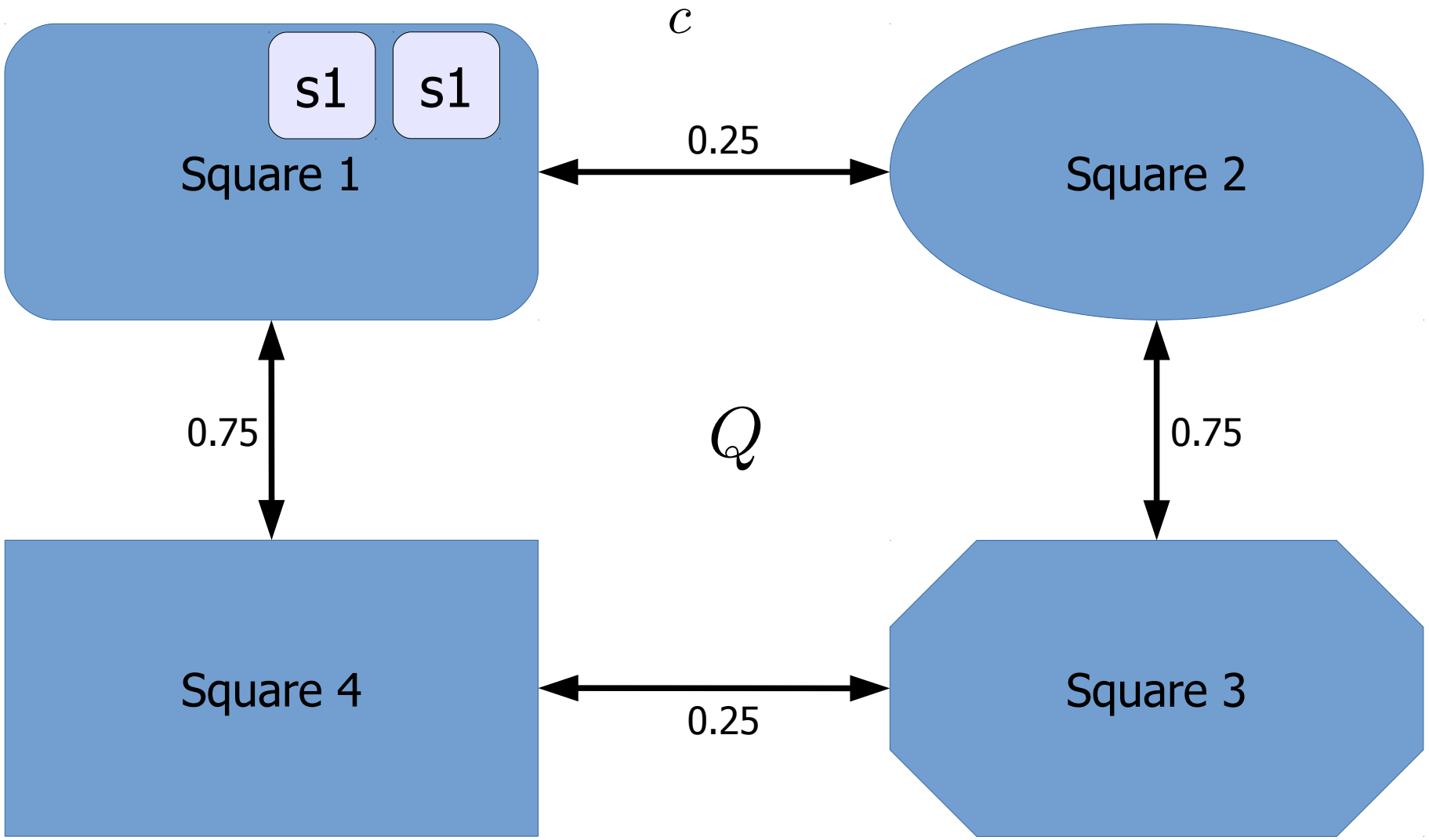
Crowd Dynamics



J.E. Rowe, R.L. Gomez. El Botellon: Modeling the movement of crowds in a city. Complex Systems 14, 2003
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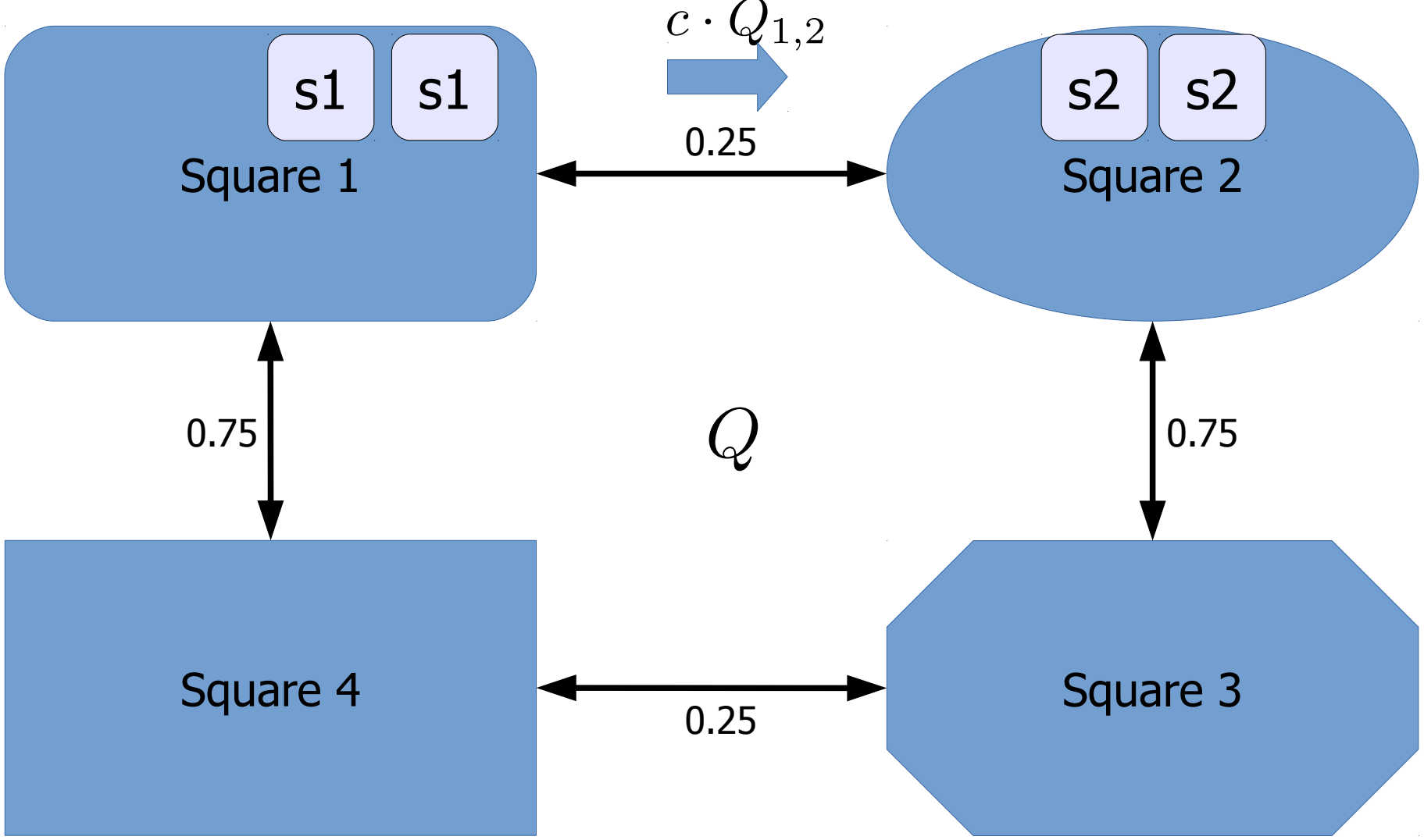
Crowd Dynamics



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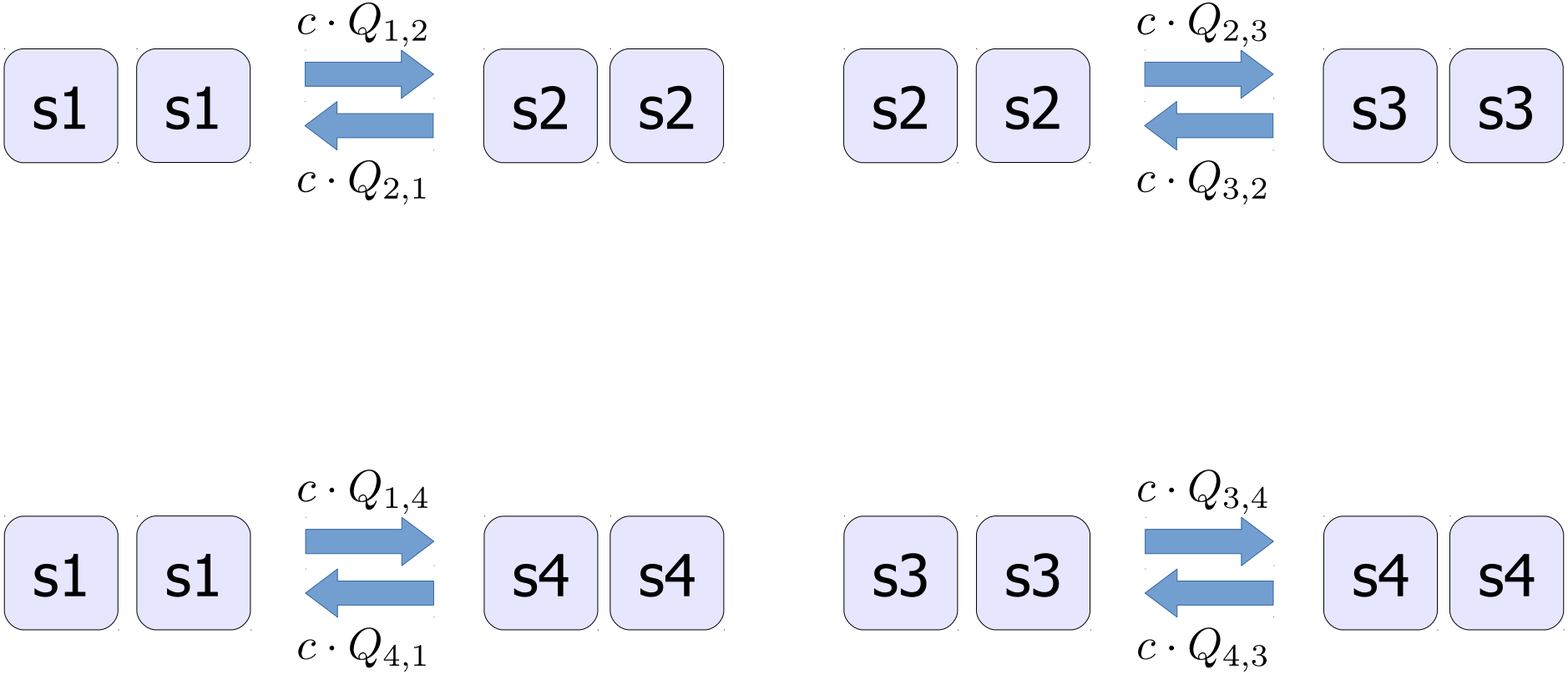
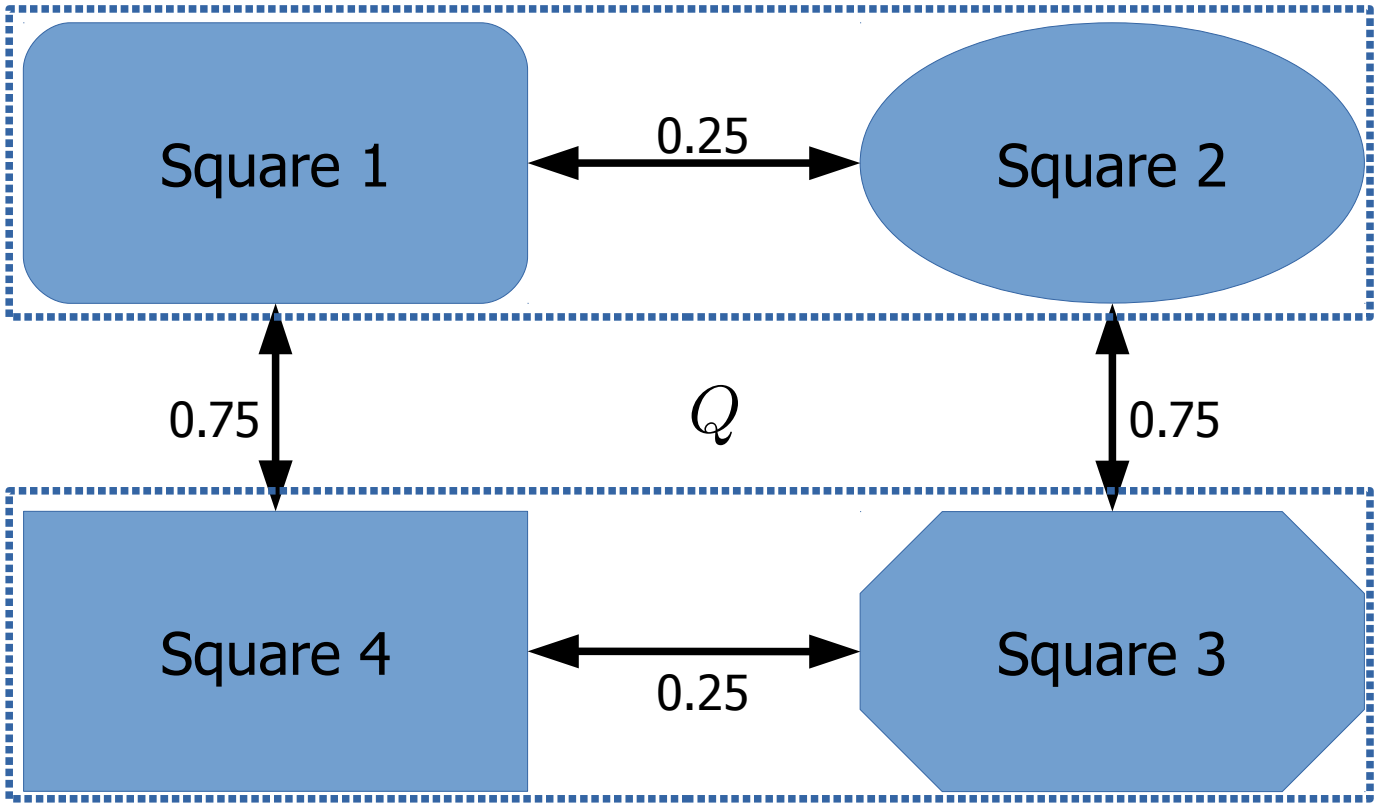
Crowd Dynamics



Highlights

- Plots for different IC
- BDE/BB formally proves the presence of "symmetric squares"



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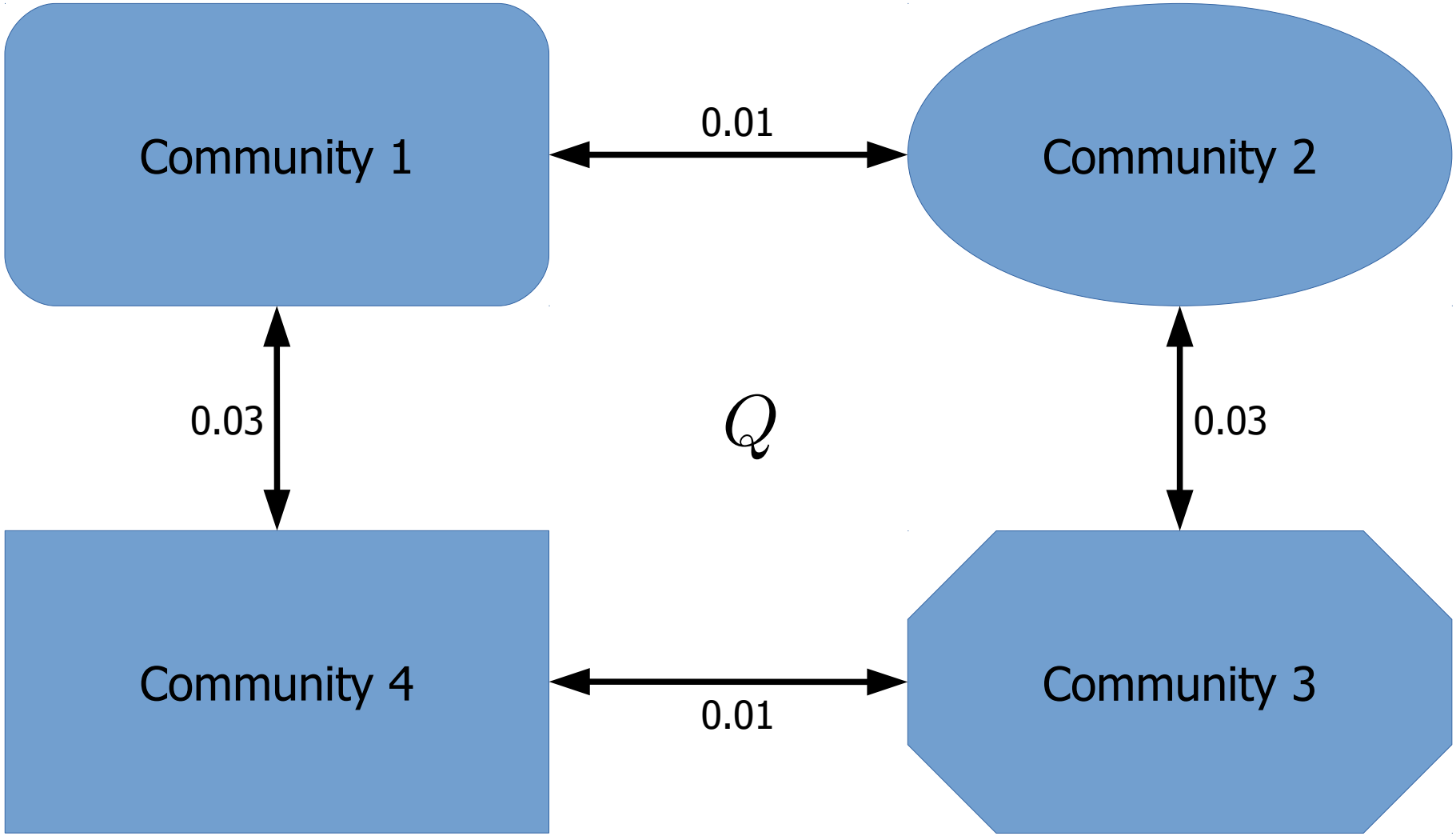
Multi-community Epidemiology



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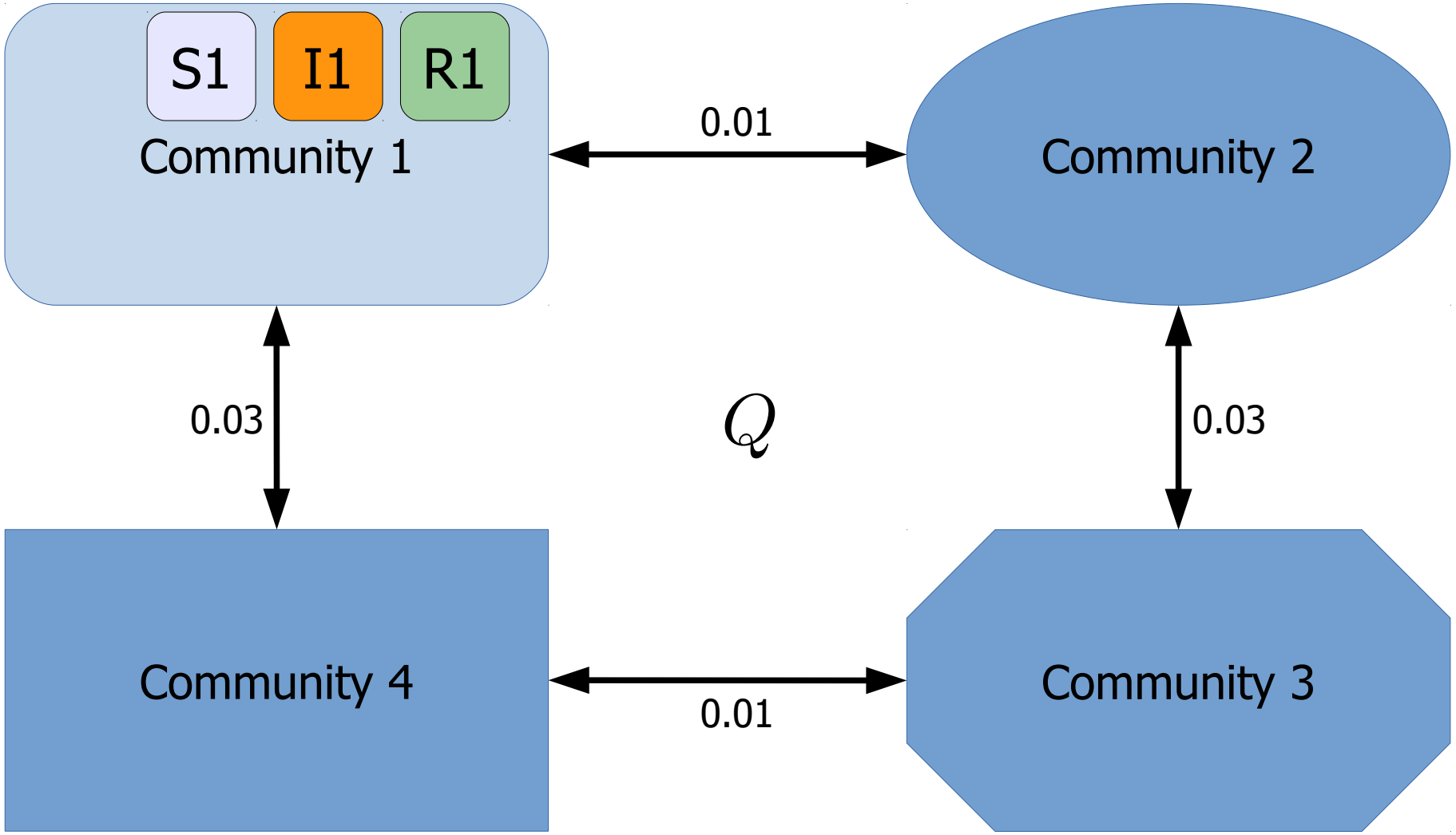
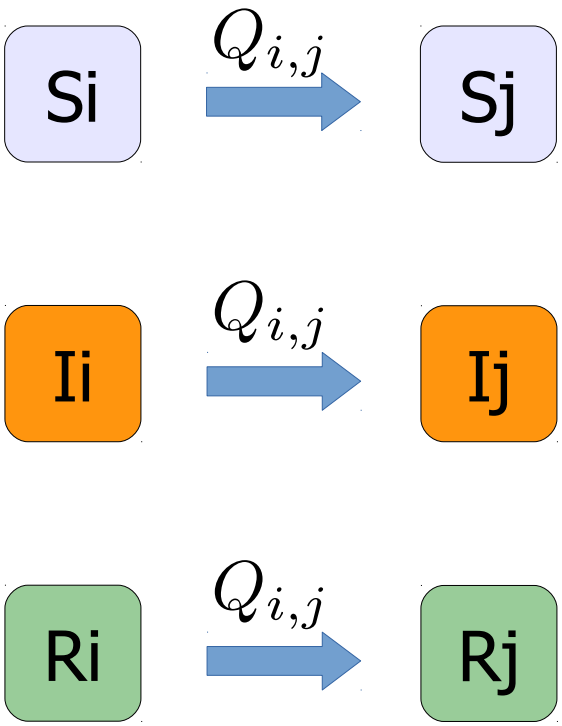
Multi-community Epidemiology



Multi-community Epidemiology

Movements



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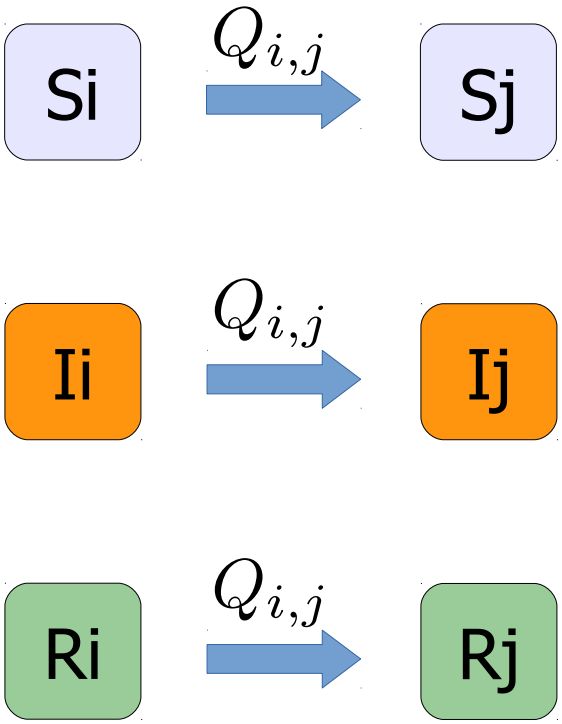
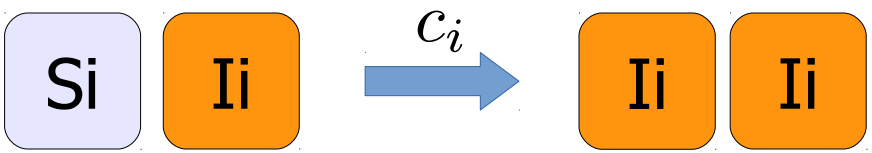
Multi-community Epidemiology

ERODE Evaluation and Reduction of Ordinary Differential Equations

Movements



Local interactions



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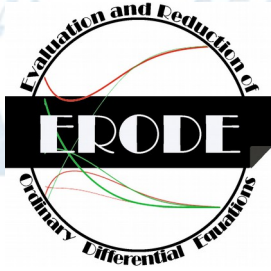
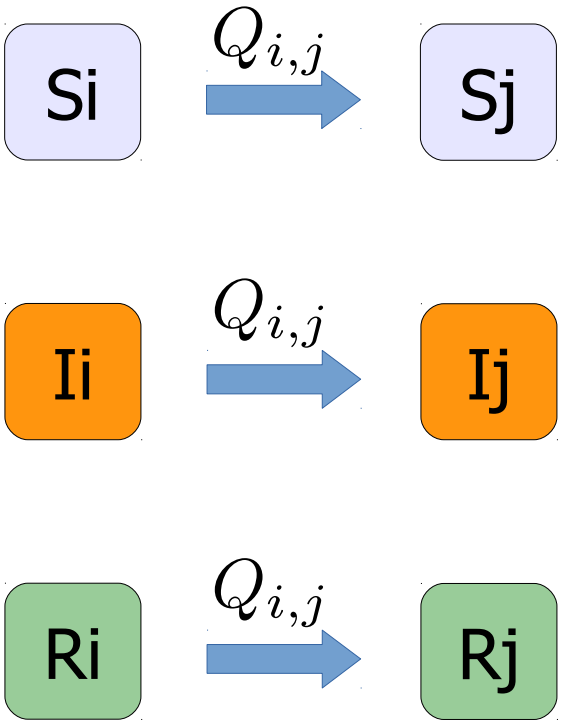
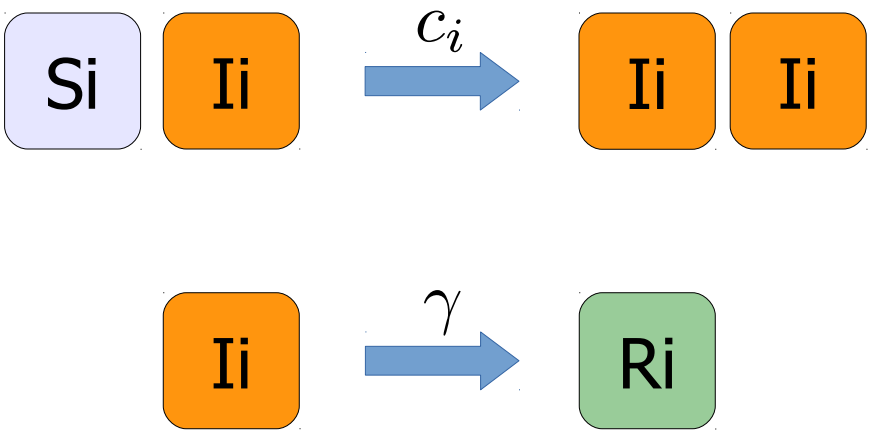
Multi-community Epidemiology



Movements



Local interactions



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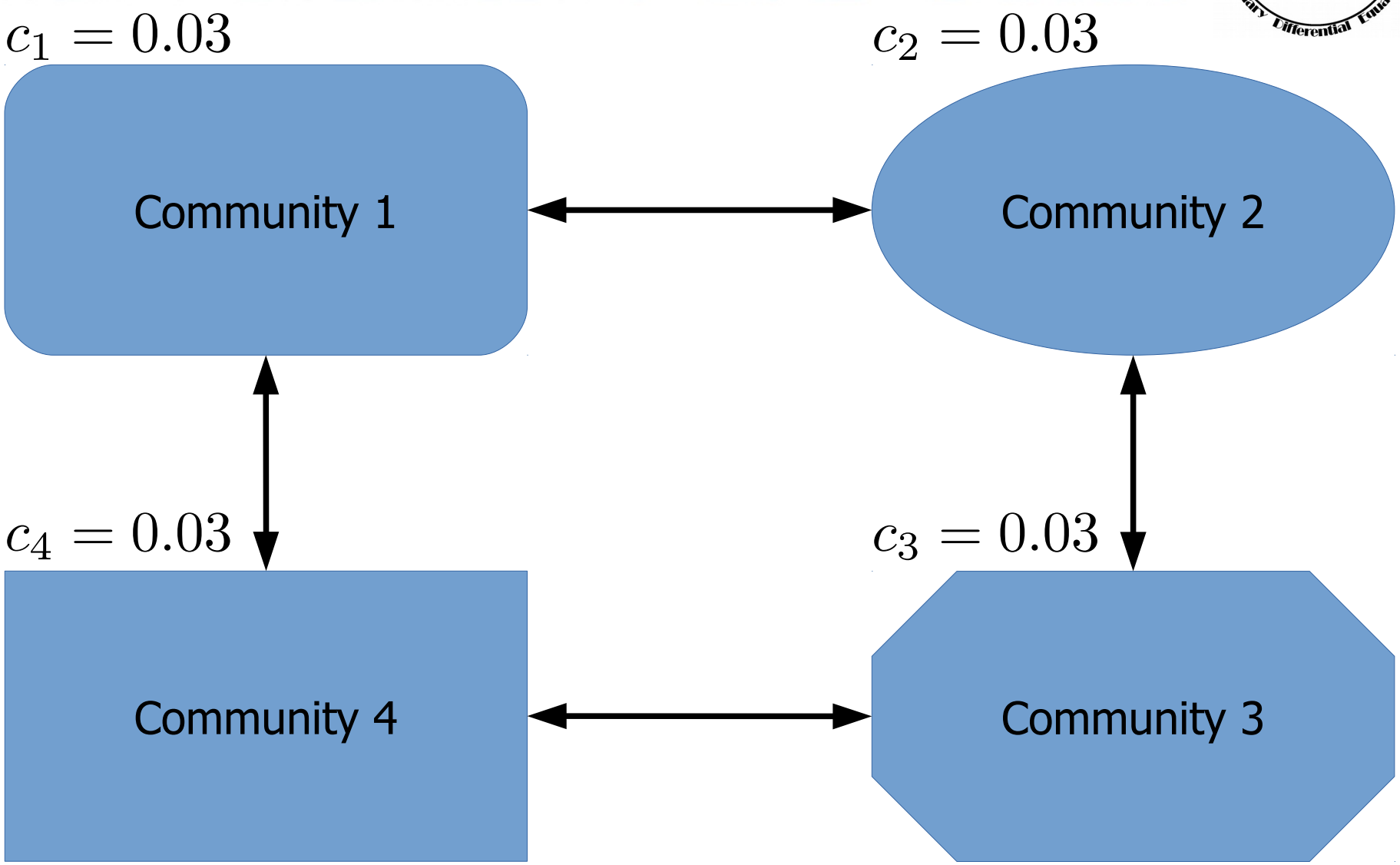
Multi-community Epidemiology



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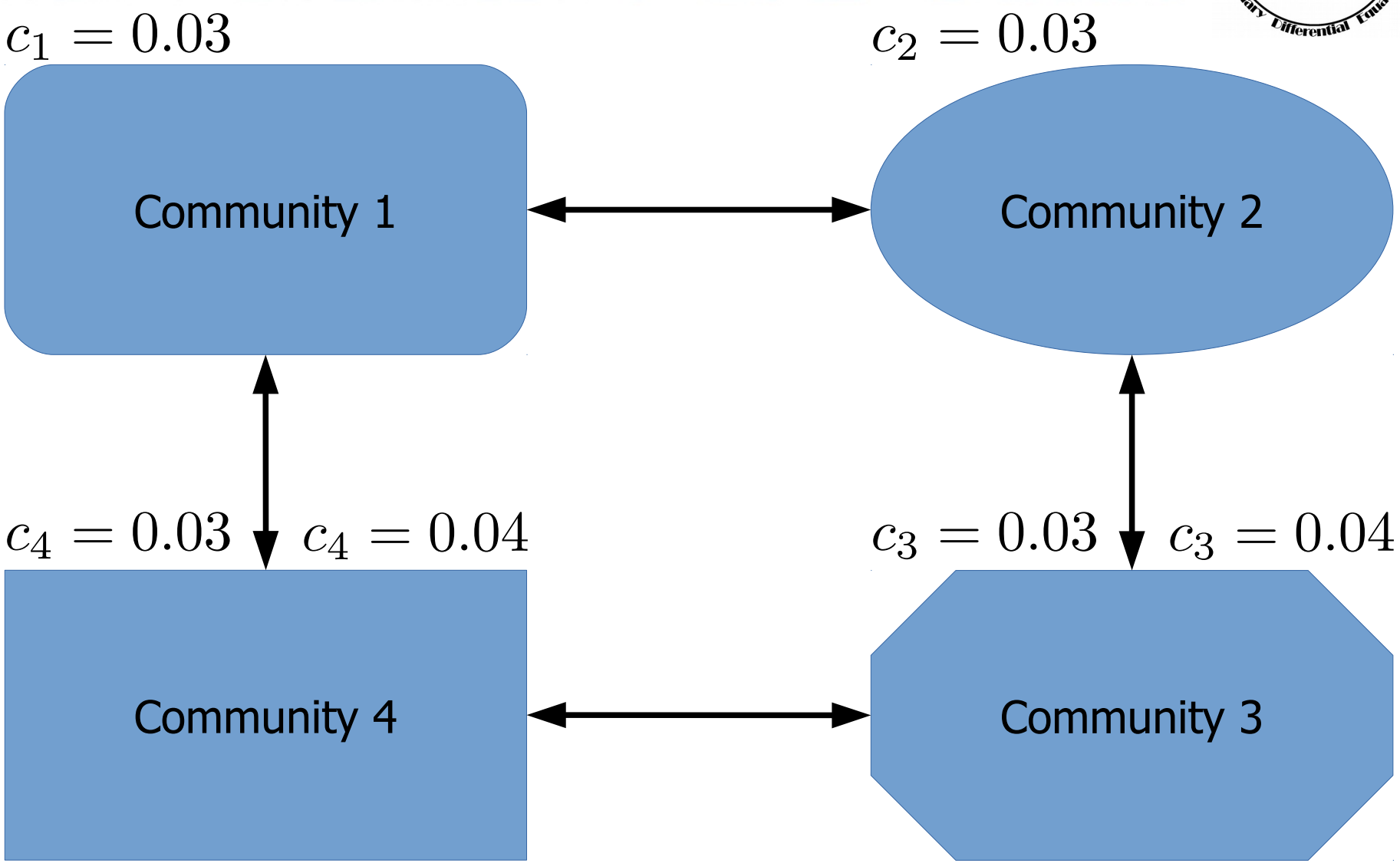
Multi-community Epidemiology



IMT SCHOOL FOR ADVANCED STUDIES LUCCA

Multi-community Epidemiology

Evaluation and Reduction of Ordinary Differential Equations — ERODE

http://groups.inf.ed.ac.uk/paloma/SIR.paloma

```
#params
param p =0.5;

#states
//an agent in state "S" can receive a "contact" msg and become infected, or move to another location.
S(0,0):= ?(contact,p)@Pr{1/(|S(0,0)|+|I(0,0)|+|R(0,0)|)}.I(0,0)+(move_0_1,0.01).S(0,1)+(move_0_2,0.01).S(1,0);
S(0,1):= ?(contact,p)@Pr{1/(|S(0,1)|+|I(0,1)|+|R(0,1)|)}.I(0,1)+(move_1_0,0.01).S(0,0)+(move_1_3,0.01).S(1,1);
S(1,0):= ?(contact,p)@Pr{1/(|S(1,0)|+|I(1,0)|+|R(1,0)|)}.I(1,0)+(move_2_0,0.01).S(0,0)+(move_2_3,0.01).S(1,1);
S(1,1):= ?(contact,p)@Pr{1/(|S(1,1)|+|I(1,1)|+|R(1,1)|)}.I(1,1)+(move_3_1,0.01).S(0,1)+(move_3_2,0.01).S(1,0);

//an agent in state "I" can send out "contact" broadcast msg to its current location, or move to another location.
I(0,0):= !(contact,0.03)@IR{local}.I(0,0)+(recover,0.2).R(0,0)+(move_0_1,0.01).I(0,1)+(move_0_2,0.01).I(1,0);
I(0,1):= !(contact,0.03)@IR{local}.I(0,1)+(recover,0.2).R(0,1)+(move_1_0,0.01).I(0,0)+(move_1_3,0.01).I(1,1);
I(1,0):= !(contact,0.03)@IR{local}.I(1,0)+(recover,0.2).R(1,0)+(move_2_0,0.01).I(0,0)+(move_2_3,0.01).I(1,1);
I(1,1):= !(contact,0.03)@IR{local}.I(1,1)+(recover,0.2).R(1,1)+(move_3_1,0.01).I(0,1)+(move_3_2,0.01).I(1,0);

//an agent in state "R" can only move to another location.
R(0,0):= (move_0_1,0.01).R(0,1)+(move_0_2,0.01).R(1,0);
R(0,1):= (move_1_0,0.01).R(0,0)+(move_1_3,0.01).R(1,1);
R(1,0):= (move_2_0,0.01).R(0,0)+(move_2_3,0.01).R(1,1);
R(1,1):= (move_3_1,0.01).R(0,1)+(move_3_2,0.01).R(1,0);

#agents
S(0,0)[150] || I(0,0)[11] || R(0,0)[12] ||
S(0,1)[150] || I(0,1)[11] || R(0,1)[12] ||
S(1,0)[150] || I(1,0)[11] || R(1,0)[12] ||
S(1,1)[150] || I(1,1)[11] || R(1,1)[12]
```

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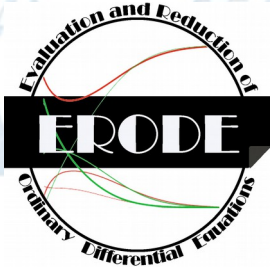
Multi-community Epidemiology



fluidflow.m

```
1   function dy =  fluidflow(y)
2   dy=zeros(90,1);
3
4   %First-order moments (12 ODEs)
5   dy(1)=0-1*0.03*y(1)-1*0.01*y(1)+1*0.01*y(2)+1*0.03*y(9)+1*0.2*y(10);
6   ...
7   dy(12)=0+1*0.03*0.5*1/(y(5)+y(12)+y(2))*y(69)+1*0.01*y(10)+1*0.03*y(1
8
9   %Second-order moments (12 ODEs)
10  dy(13)=0+0.03*(1)^2*y(1)-2*y(13)*0.03*1+0.01*(1)^2*y(1)-2*y(13)*0.01*
11  ...
12  dy(24)=0+0.03*(0.5*1/(y(5)+y(12)+y(2)))^2*(y(17)*((y(69))^2)/(y(12)+e
13
14  %Further 66 auxiliary ODEs
15  dy(25)=0-0.03*1*y(25)-0.01*1*y(25)+0.01*1*y(13)-0.01*(1)^2*y(1)-0.03*
16  ...
17  dy(90)=0+0.03*0.5*1/(y(5)+y(12)+y(2))*(y(69)*y(90)*y(68)/(y(12)+eps),
18
19  end
```

C. Feng, J. Hillston, V. Galpin.
Automatic Moment-Closure Approximation of Spatially Distributed Collective Adaptive Systems. ACM Trans. Mod. Comp. Sim. 26, 2016

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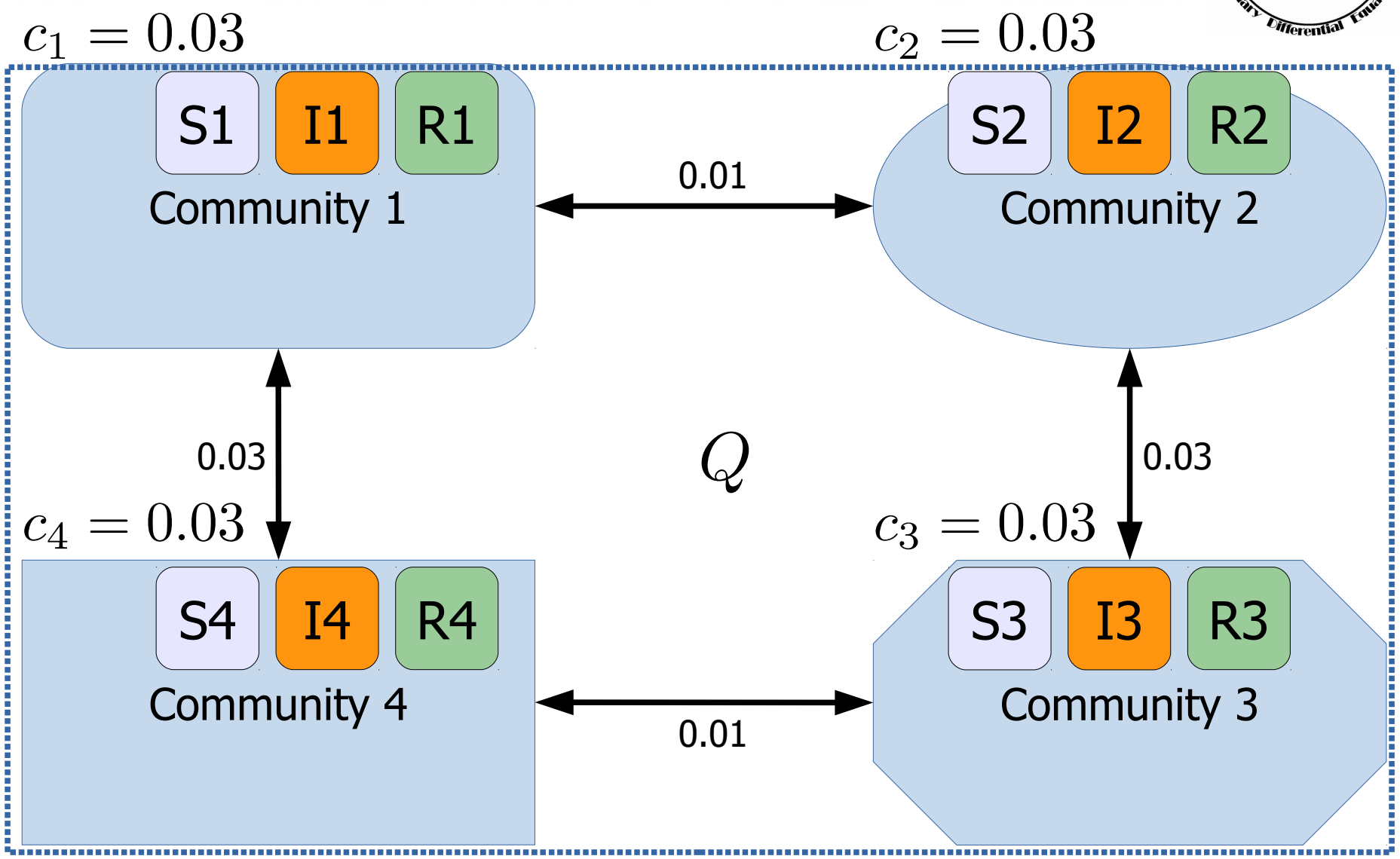
Multi-community Epidemiology



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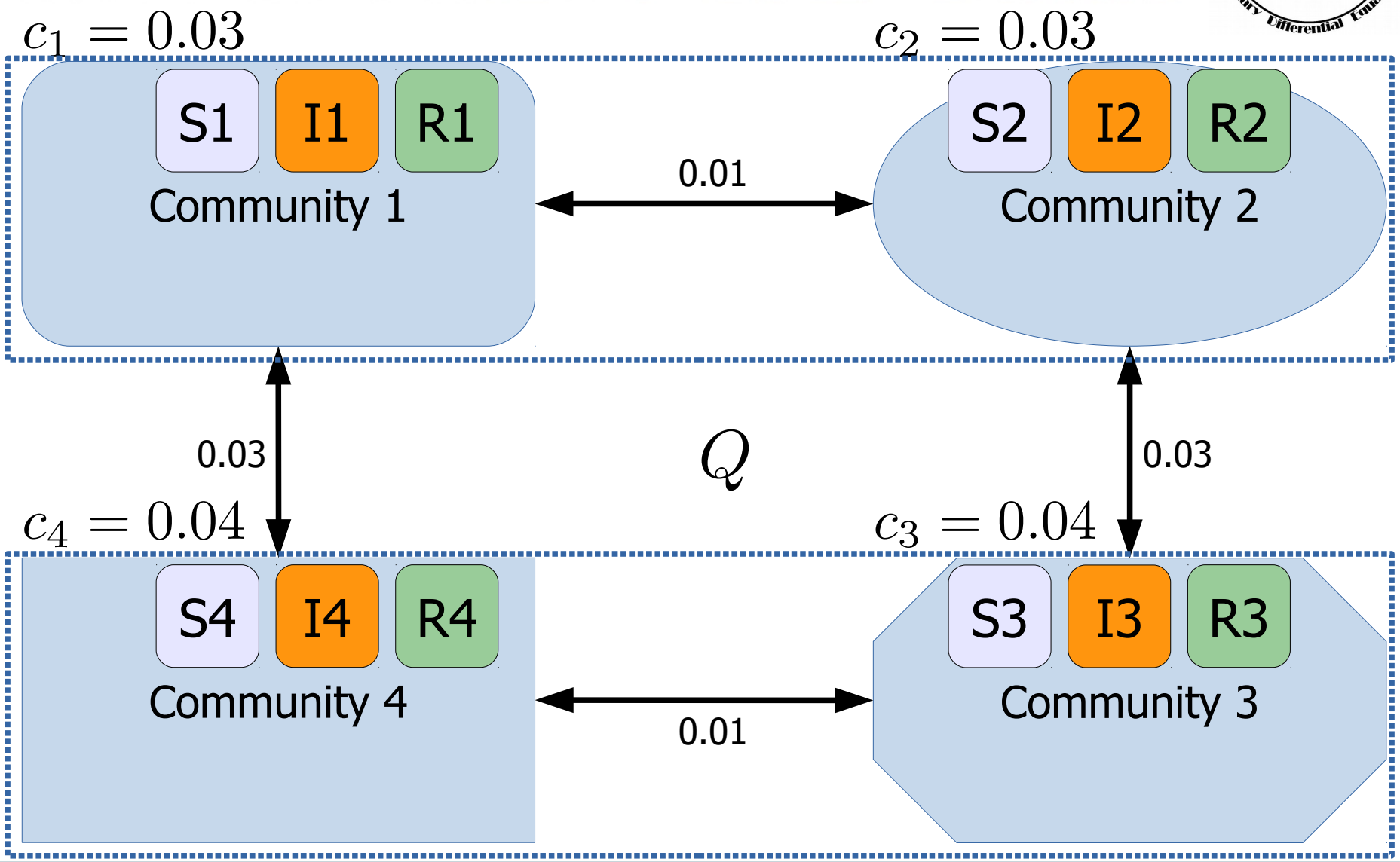
Multi-community Epidemiology



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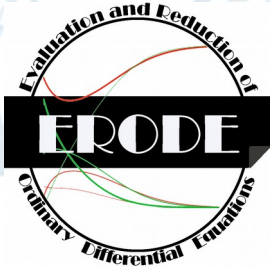
ERODE: Evaluation and Reduction of ODEs



FRONTEND

- **ODE and RN Editor**
  - Auto-completion
  - Error detection
  - Fix suggestion
- **ERODE Views**
  - Project explorer
  - Outline & Problems
  - Console & Plots
- **ERODE Wizards**
  - Update manager
  - New ERODE Project & File
  - Import BNG, Matlab, LBS

CORE

- ODE Simulator
- BDE/FDE Reducer
- ODE ⟷ RN Encoder
- Stochastic Simulator (RN)
- Statistical Model Checker (RN)
- BB/FB Reducer (RN)
- Importer/Exporter (BNG,Matlab,LBS,SBML)

APIs

- Apache Commons Math
- FERN
- MultiVeStA
- Microsoft Z3

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