Spatial Computing with Chemistry

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Forewords

A research direction in Computer Science

- Chemical-inspired concurrent models are a tradition[a]
- Spatial computing is gaining momentum in large-scale systems[b]

$\Rightarrow$ Since few years we are working at combining the two

$\Rightarrow$ Context: SAPERE FP7 project (`http://www.sapere-project.eu`)

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[a] Jean-Pierre Banâtre and Daniel Le Métayer. "Programming by multiset transformation". In: *Commun. ACM* 36.1 (1993), pages 98–111. ISSN: 0001-0782. DOI: `http://doi.acm.org/10.1145/151233.151242`.

[b] Jacob Beal, Stefan Dulman, Kyle Usbeck, Mirko Viroli, and Nikolaus Correll. "Organizing the Aggregate: Languages for Spatial Computing". In: *CoRR* abs/1202.5509 (2012).

Idea of this talk

Pave the way towards a convergence with researches studying biochemical mechanisms to achieve given spatial structures in vitro

Disclaimers

- The gap to fill is seemingly rather wide now, technically and culturally
- Our background is very different, not sure I'll be effective

$\Rightarrow$ .. it is worth discussing the issue anyway..

Outline

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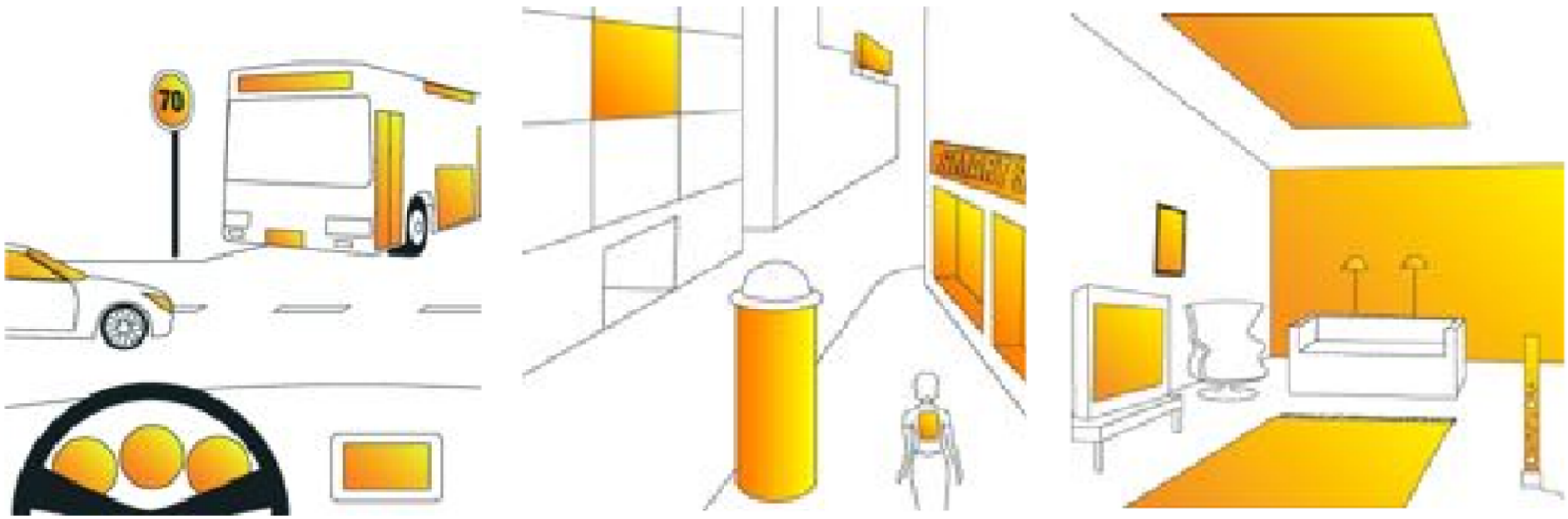
Our starting point: Tomorrow pervasive environments



(Pict. by A. Ferscha, JKU)

Impact on the network model

Features ($\Rightarrow$ resembling biochemical systems in a way)

- Highest density of devices/nodes (almost a continuum)
- Physical Mobility: devices continuously relocate (smartphones, cars)
- Logical Mobility: processes and data float around

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New computing applications

- Sensor networks (dynamically aggregating/diffusing data)[a]
- Swarm and modular robotics (cooperative team work)[b]
- Pervasive computing (crowd steering, coordinated visualisation)[c]

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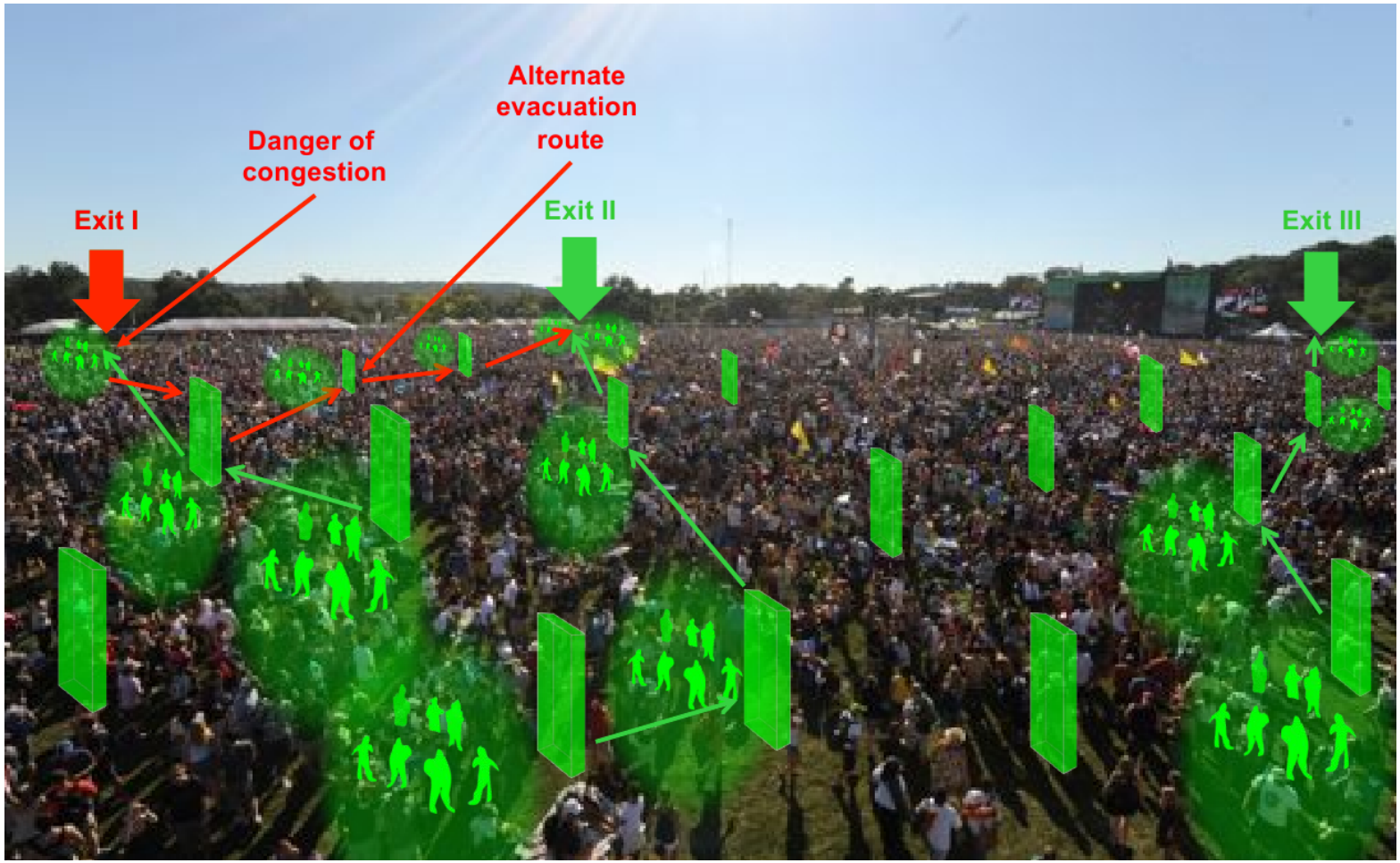
[a] Jacob Beal and Jonathan Bachrach. "Infrastructure for Engineered Emergence on Sensor/Actuator Networks". In: *IEEE Intelligent Systems* 21.2 (2006).

[b] Jonathan Bachrach, Jacob Beal, and James McLurkin. "Composable continuous-space programs for robotic swarms". In: *Neural Computing and Applications* 19.6 (2010).

[c] Mirko Viroli, Matteo Casadei, Sara Montagna, and Franco Zambonelli. "Spatial Coordination of Pervasive Services through Chemical-inspired Tuple Spaces". In: *ACM Transactions on Autonomous and Adaptive Systems* 6.2 (2011).

The case of *Crowd Engineering* – see SAPERE project



(Pict. by A. Ferscha, JKU)

Data-space computing model

Approach

- Each device holds a "space of data", and interacts with neighbours
- Data items comes equipped with diffusion/aggregation rules
- Each injection of a data item possibly results in a diff/aggr process

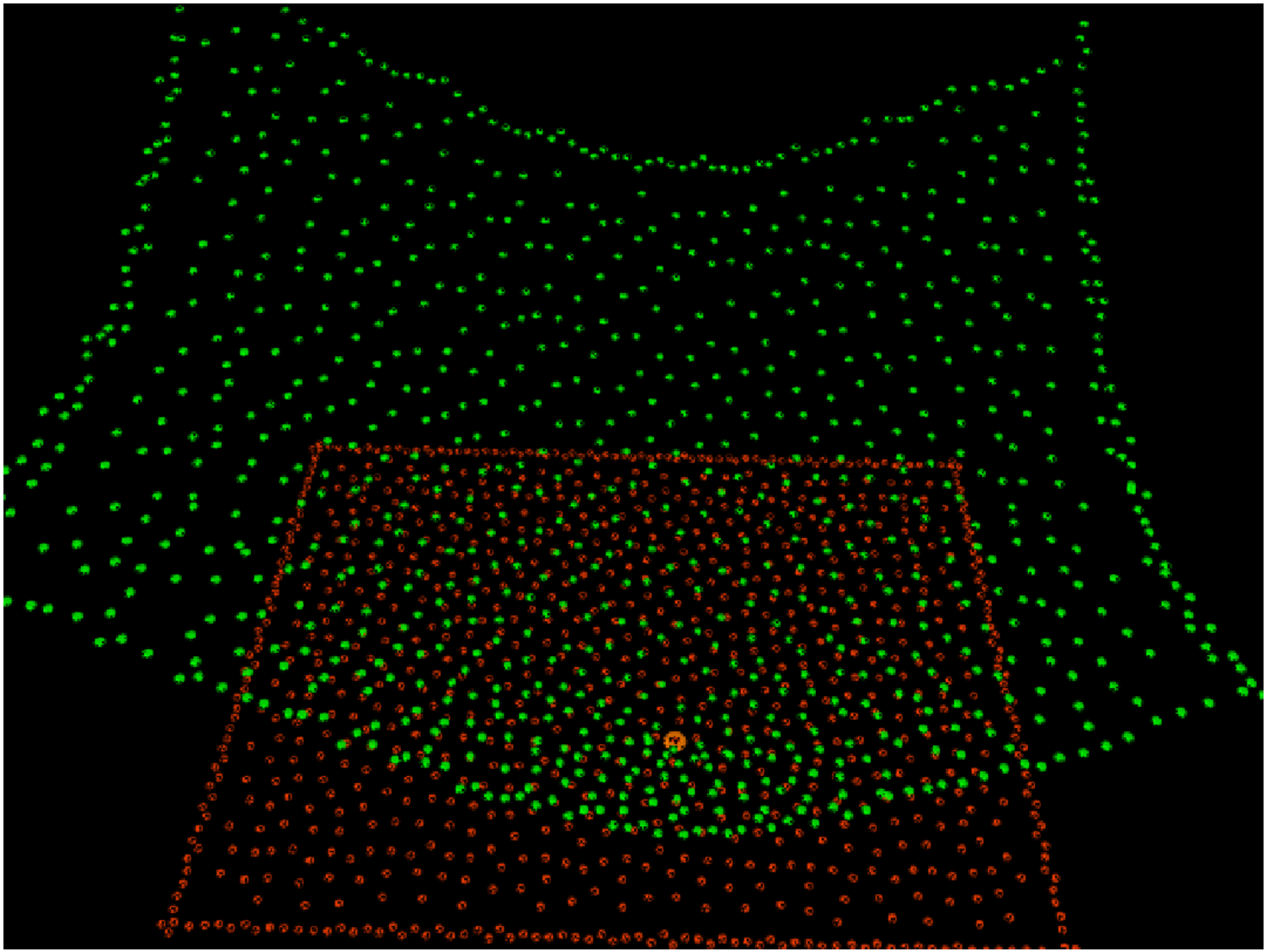
$\Rightarrow$ .. a *field* (a "spatial structure") might self-stabilise

The gradient case, informally

- Diffuse and re-aggregate such that in farther nodes we have a higher number of data-items (could be done also in decreasing fashion)
- The resulting spatial structure known as a *gradient*

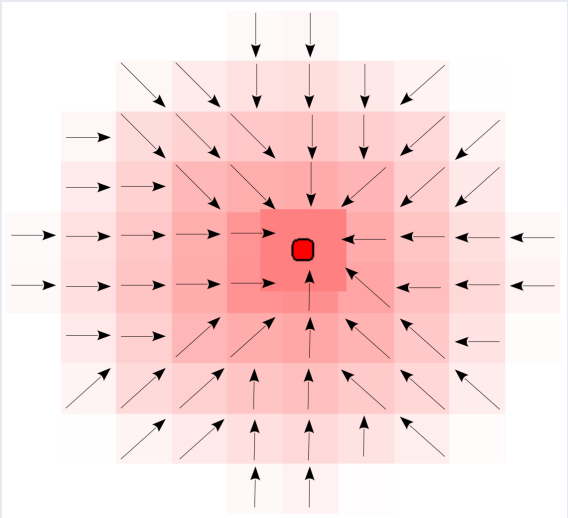
$\Rightarrow$ Can be used to reach a target, by chemotaxis

A 3D rendering of a uniform increasing gradient structure



A call for useful space-time abstractions

Attracting ball (discrete, flat continuous, structured continuous)



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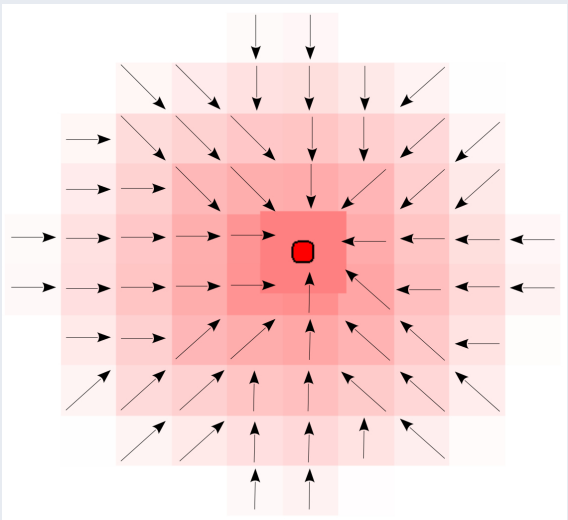

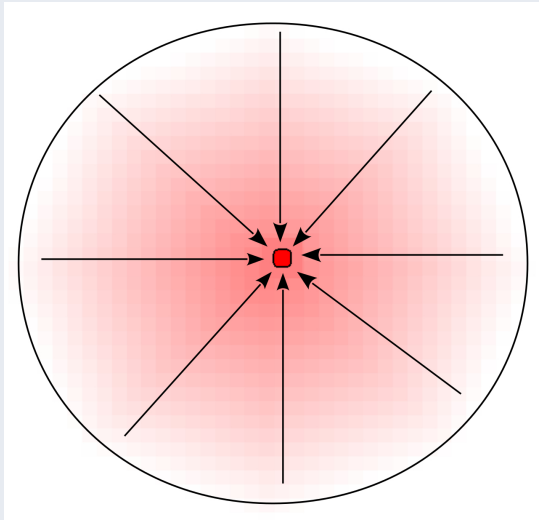

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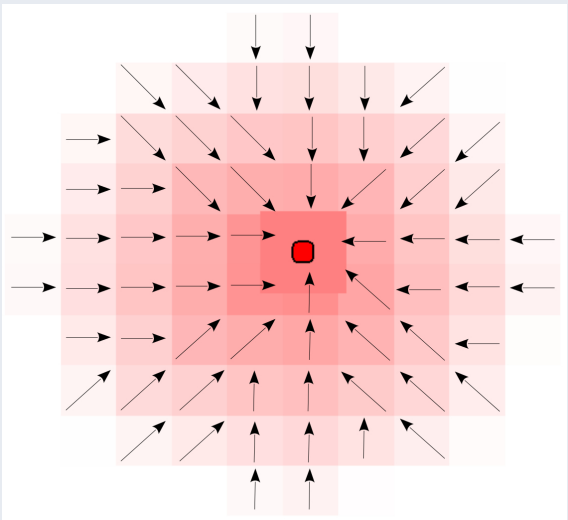

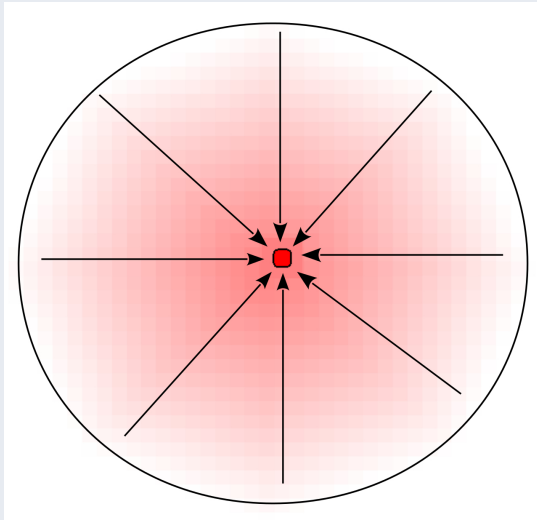

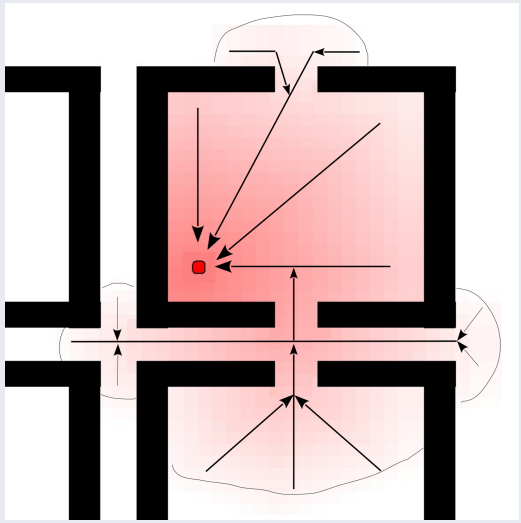

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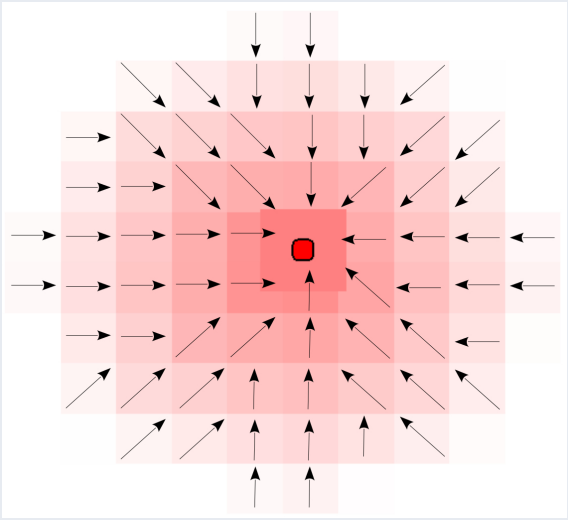
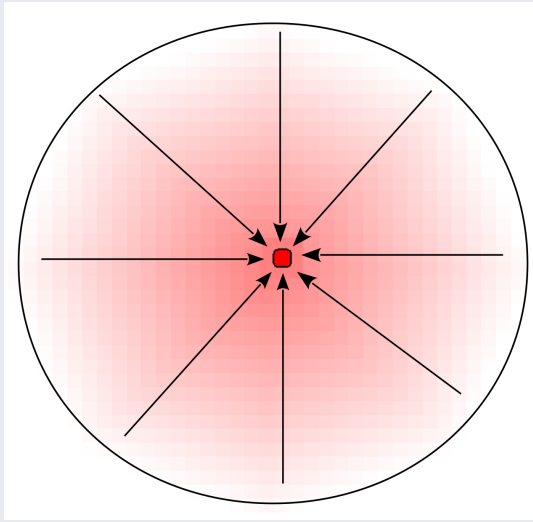
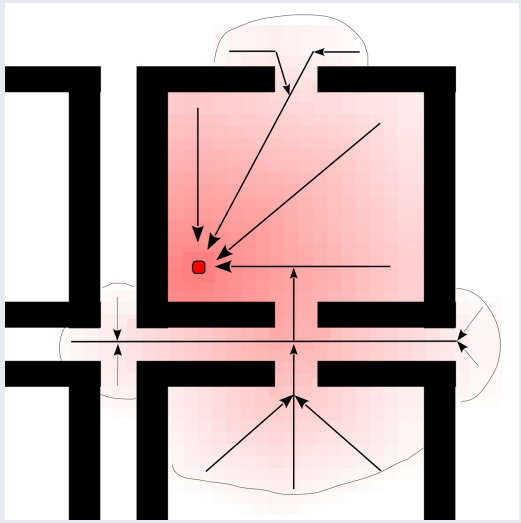
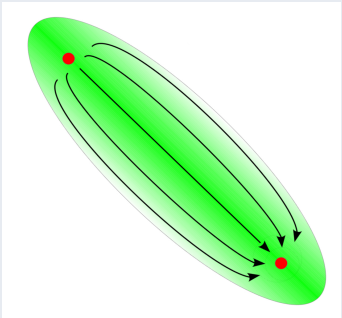
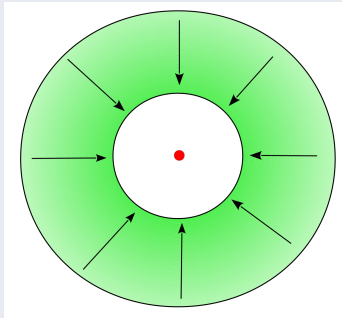
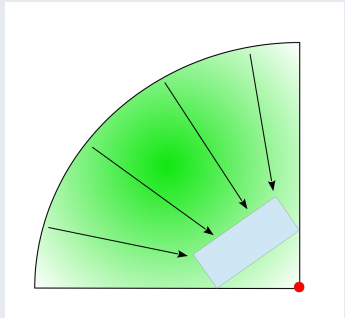
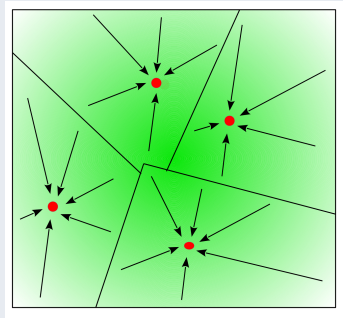
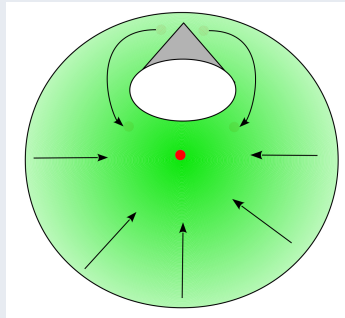
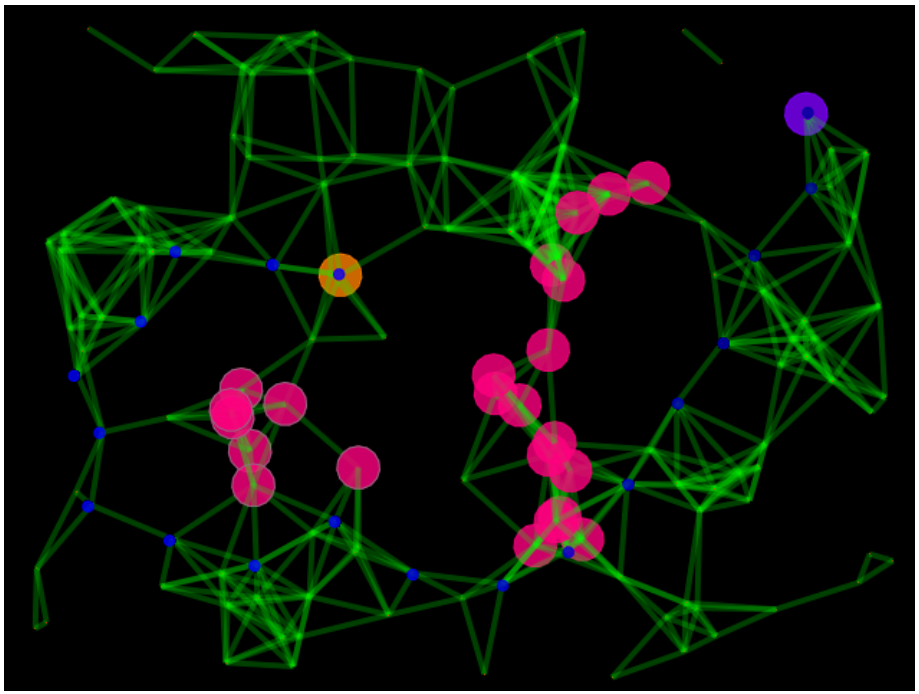




Other structures (channel, shrinking crown, sector, partition, shadow, . . .)

On the shift from discrete to continuous computations..



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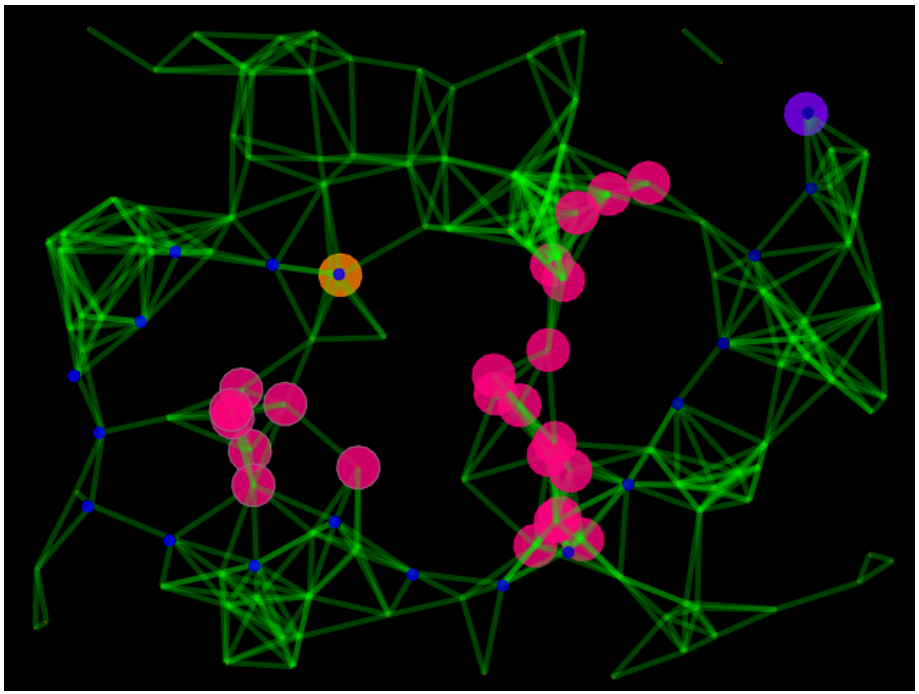
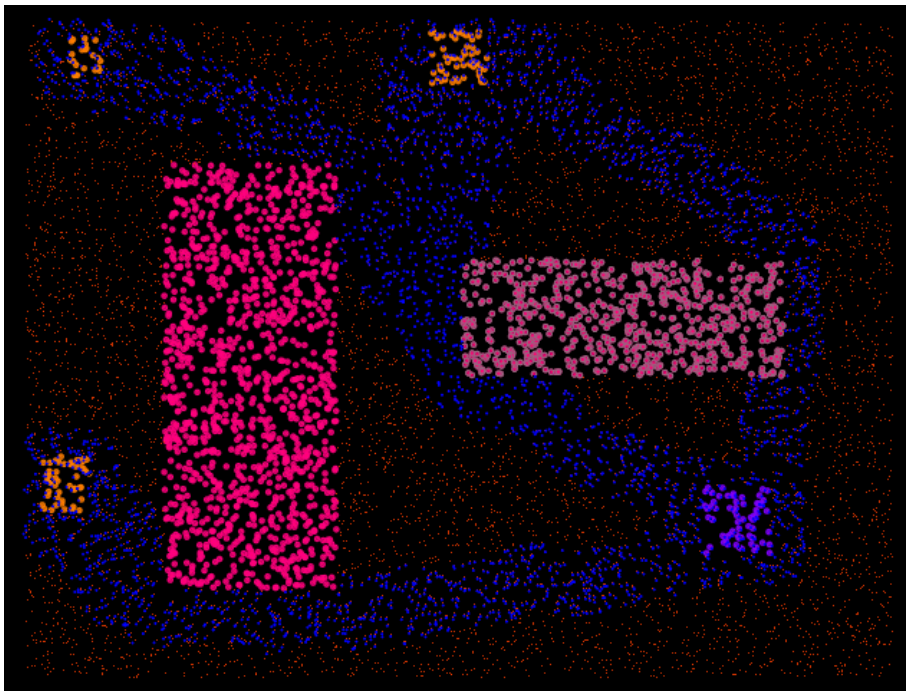




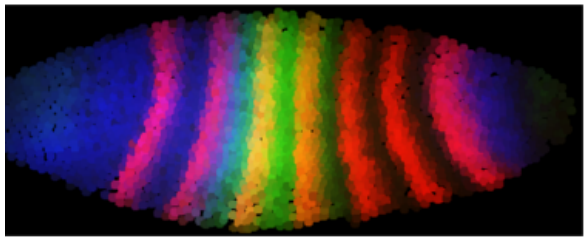
The shadow pattern in action

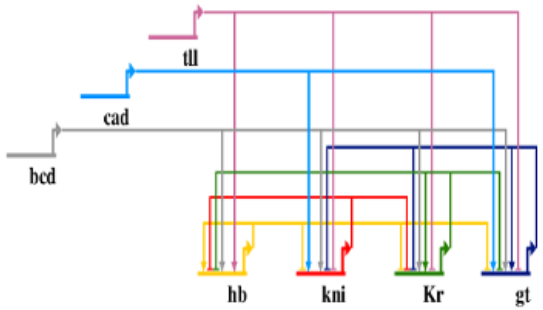
Application to crowd steering

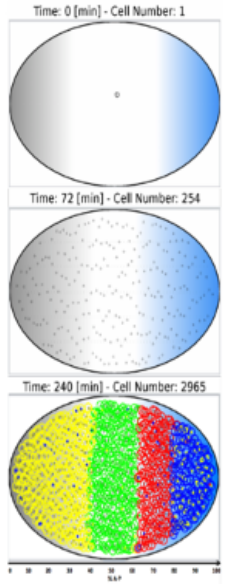
Application to morphogenesis[1]

Finding the biochemistry of stripe pattern formation in Drosophila

- Start from available data (until Cleavage Cycle 14 temporal class 8)
- Create a model of diffusion, movement and mitotic division
- Stochastic (event-based) simulation + euristic evolution of parameters







[1] Sara Montagna, Danilo Pianini, and Mirko Viroli. "A Model for Drosophila Melanogaster Development from a Single Cell to Stripe Pattern Formation". In: *Proceedings of the 27th Annual ACM Symposium on Applied Computing (SAC 2012)*. (SAC). ACM, 2012, pages 1406–1412. ISBN: 978-1-4503-0857-1.

Outline

Our first exploration of chemistry for spatial structures[2]

Ideas

- A network of nodes as a set of communicating compartments
- Compartments do not move, interact due to proximity
- Handle data-items "exactly" as molecules of a bio-chemical system
- Concentration in one node is the value of the spatial structure there
- Intra-node behaviour realised by "synthetic" chemical rules
- Node-to-node interaction by "firing molecules" ($\mathtt{X}^{\rightsquigarrow}$)

Method

- Using the event-based simulator Alchemist (`http://alchemist.apice.unibo.it`)

[2] Viroli, Casadei, Montagna, and Zambonelli, "Spatial Coordination of Pervasive Services through Chemical-inspired Tuple Spaces".

A (decreasing) gradient – exponential slope

Chemical laws: a single PUMP token generates a FIELD

$$\begin{aligned}
&\text{(PUMP)} && \texttt{PUMP} \xmapsto{r_pump} \texttt{PUMP} + \texttt{FIELD} \\
&\text{(DECAY)} && \texttt{FIELD} \xmapsto{r_decay} 0 \\
&\text{(DIFFUSE)} && \texttt{FIELD} \xmapsto{r_diff} \texttt{FIELD} + \texttt{FIELD}^{\rightsquigarrow}
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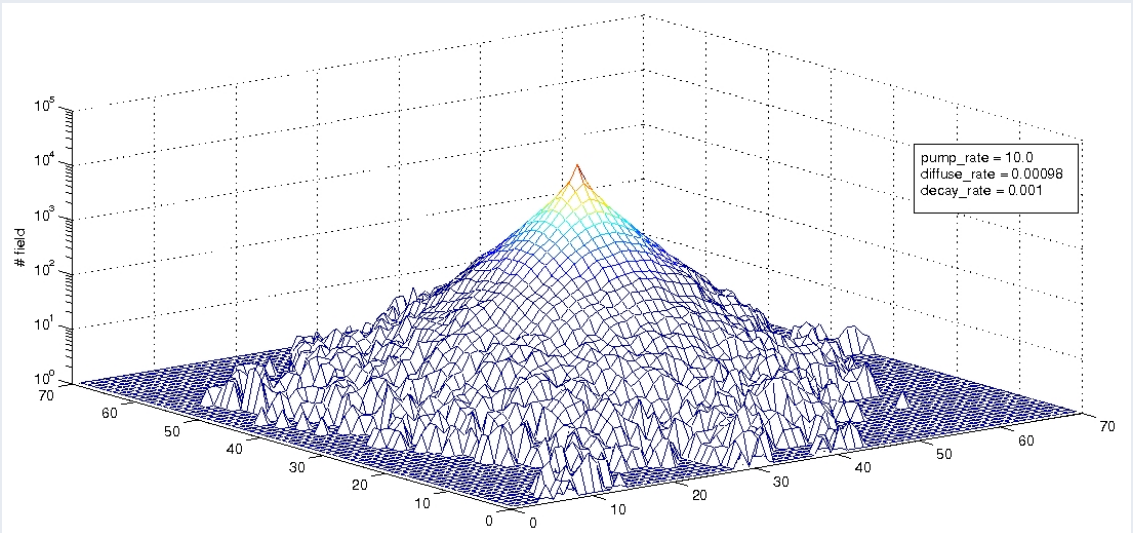
Chart



Field ascent: chemotaxis

Ascent rule: $\mathtt{X}^{\rightsquigarrow}(\uparrow \mathtt{Y})$ moves $\mathtt{X}$ where $\mathtt{Y}$'s concentration is higher

$$(\mathtt{ASCENT}) \qquad \mathtt{REQ} \xmapsto{r\_asc} \mathtt{REQ}^{\rightsquigarrow}(\uparrow \mathtt{FIELD})$$

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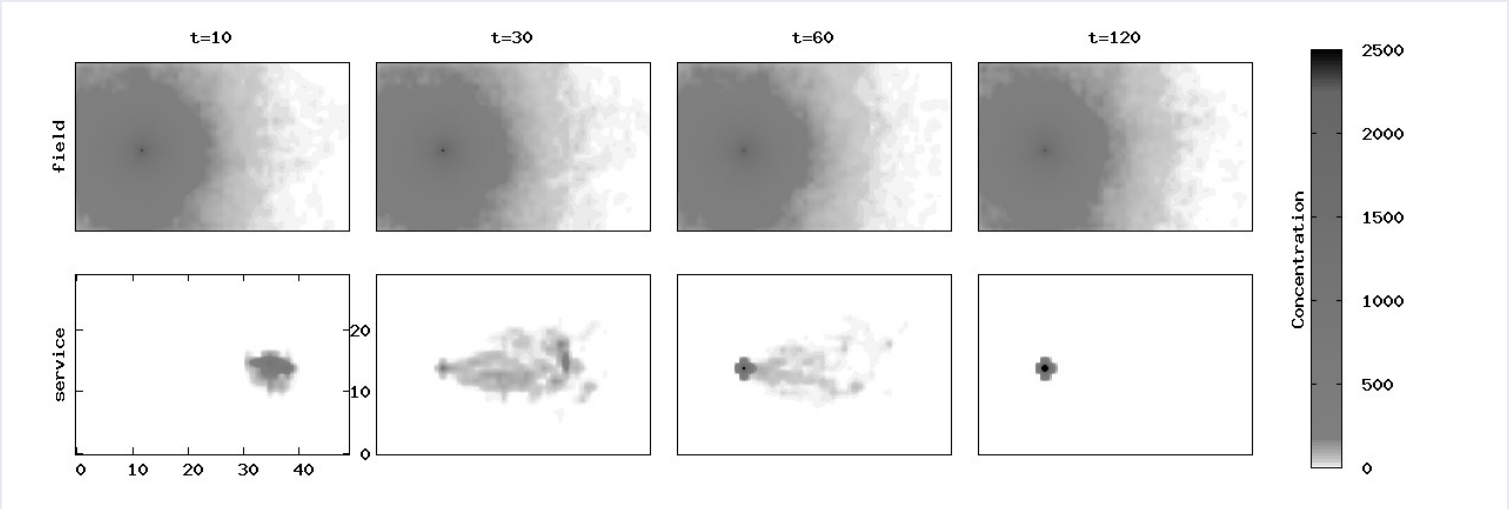
Simulation parameters

- Field: pump=10, decay=0.01, diffuse=0.0098
- Ascending item: initial conc=10′000, ascent rate=1.0

Charts



Path creation: a region for information transferring

Path diffusion

$$\text{(DIFFUSE-P)} \qquad \texttt{PATH} \xmapsto{r\_diff} \texttt{PATH} + \texttt{PATH}^{\rightsquigarrow}(\uparrow \texttt{FIELD})$$

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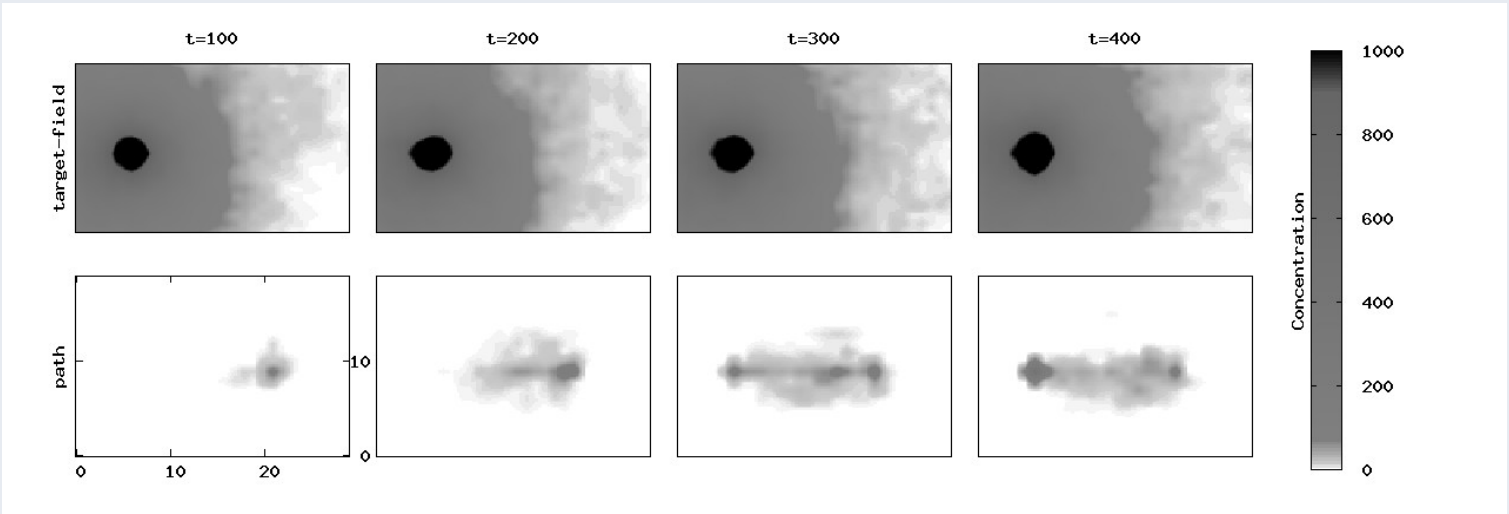
Simulation parameters

- Field: pump=10, decay=0.01, diffuse=0.0098
- Path: pump=10, decay=0.01, diffuse=0.0095

Charts

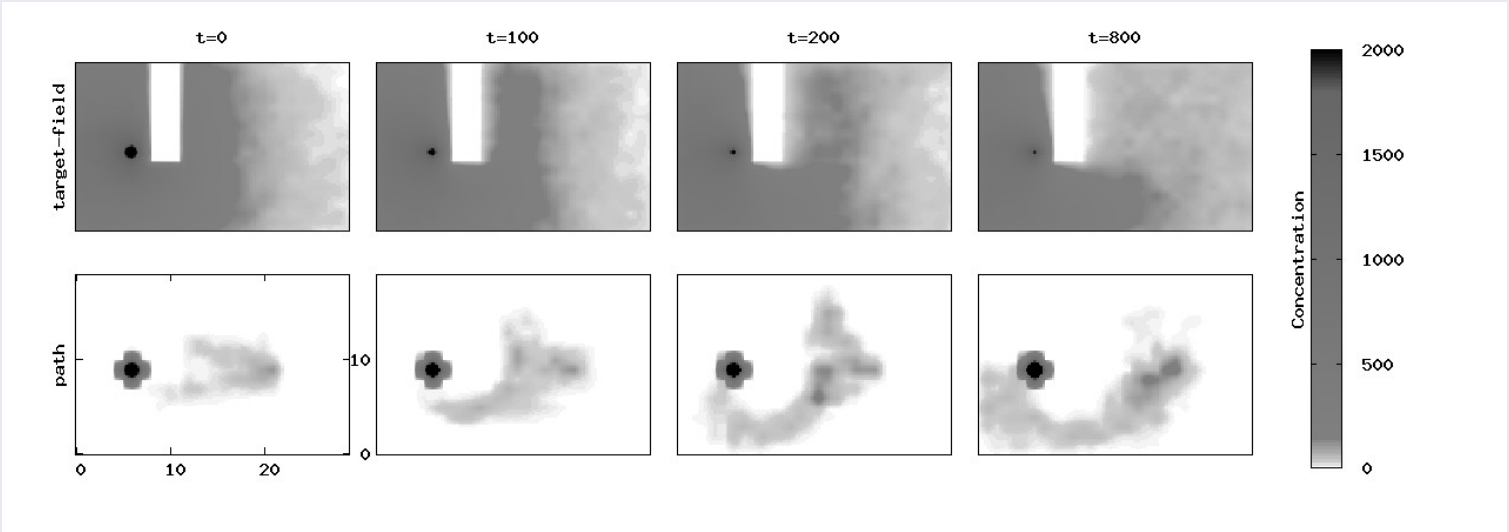


Self-adapting to topology and their changes

Dealing with obstacles

- A network failure
- The context suddenly inhibits fields

Charts



Segregation: splitting the network in contextual areas

Rule for segregated diffusion

$$\texttt{(SEGREGATE)} \quad \texttt{REGION} \xrightarrow{r\_seg} \texttt{REGION} + \texttt{REGION}^{\rightsquigarrow}(\downarrow \texttt{OTHER\_REGIONS})$$

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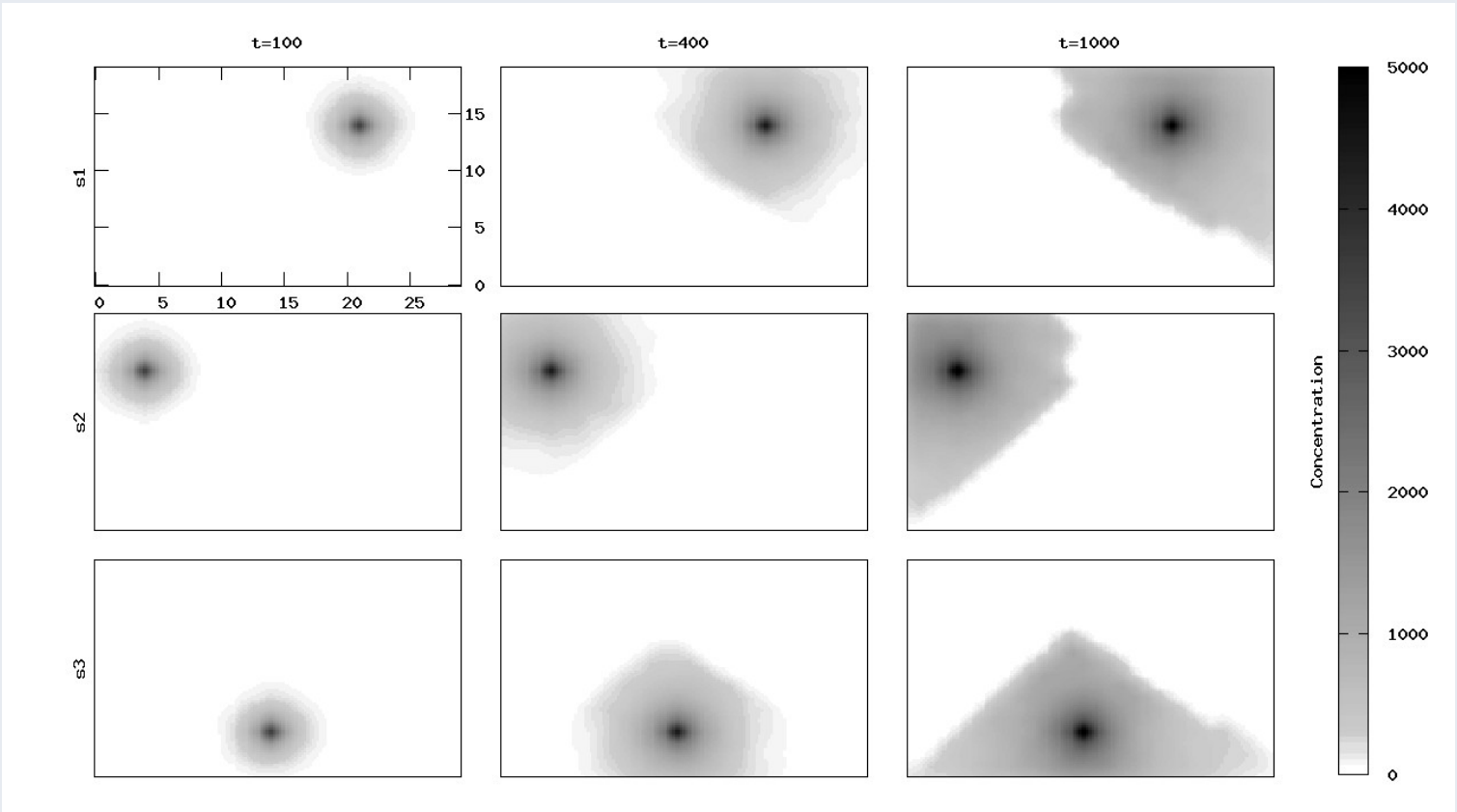

Wrap-up of this experience

Elements

- Using the natural chemical stochastic engine
- Diffusion is still a "synthetic" one
- Can support basic spatial structures

Limits

- The whole approach is somehow computationally "rigid"
- Cannot flexibly express the slope of gradients
- Cannot flexibly combine fields (e.g. by mathematical operators)

$\Rightarrow$ need chemical bricks of computation

Outline

Departing from natural chemistry

A more suitable computational model

- Do not use concentration level to construct the field's value
- Each data-item (molecule) carries a value used to construct the field
- Aggregation laws guarantee one data-item locally exists per field
- Keep using a chemical-like format of rules

$\Rightarrow$ rules now also mathematically affect those values

Case 1 – The linear gradient

Chemical-like laws

$$
\begin{array}{rrcl}
(PUMP) & \langle \texttt{source} \rangle & \rightarrow & \langle \texttt{source} \rangle + \langle \texttt{grad}, 0 \rangle \\
(DIFF) & \langle \texttt{grad}, n \rangle & \rightarrow & \langle \texttt{grad}, n \rangle + \langle \texttt{grad}, n+1 \rangle^{\rightsquigarrow} \\
(AGR) & \langle \texttt{grad}, n \rangle + \langle \texttt{grad}, m \rangle & \rightarrow & \langle \texttt{grad}, n \rangle \quad (n \leq m)
\end{array}
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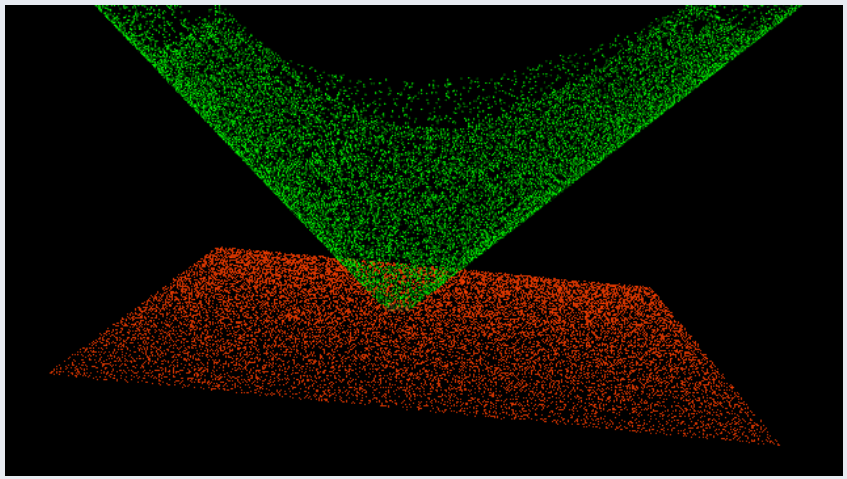
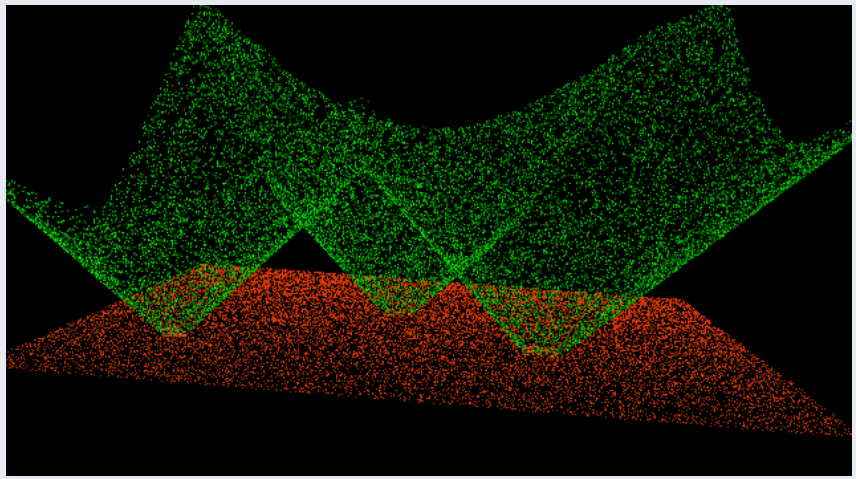
Shape: a cone in 3D, multiple ones with more sources





Case 2 – Filtering by amplitude

Chemical-like laws

$$(FILT) \quad \langle \texttt{grad}, n \rangle \quad \rightarrow \quad \langle \texttt{grad}, n \rangle + \langle \texttt{filt} \rangle \quad (n_0 \leq n \leq n_1)$$

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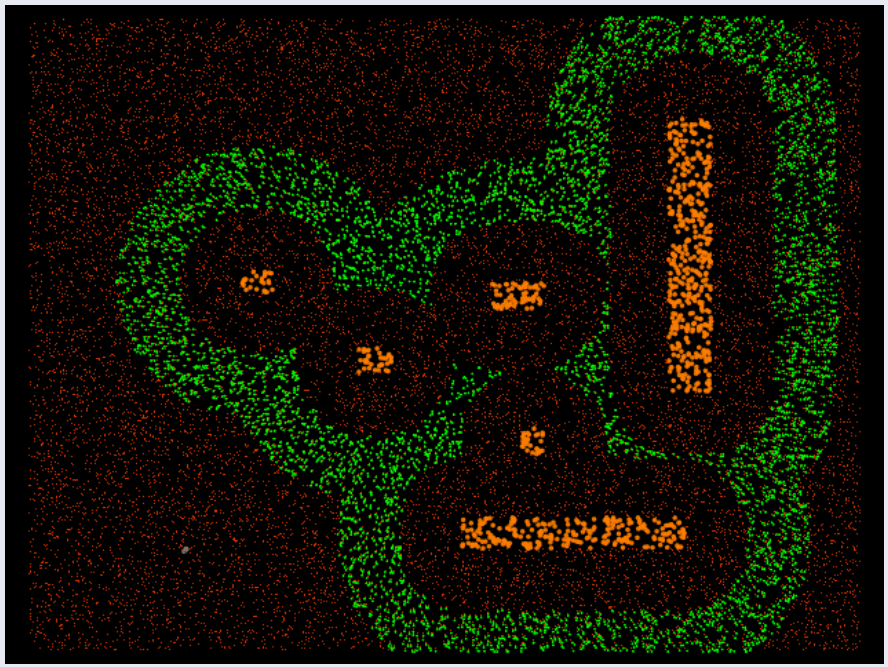
Shape: filtered value in green, sources in yellow



Case 3 – Denying diffusion

Chemical-like laws

$$(DENY) \quad \langle \texttt{grad}, n \rangle + \langle \texttt{deny} \rangle \quad \rightarrow \quad \langle \texttt{deny} \rangle$$

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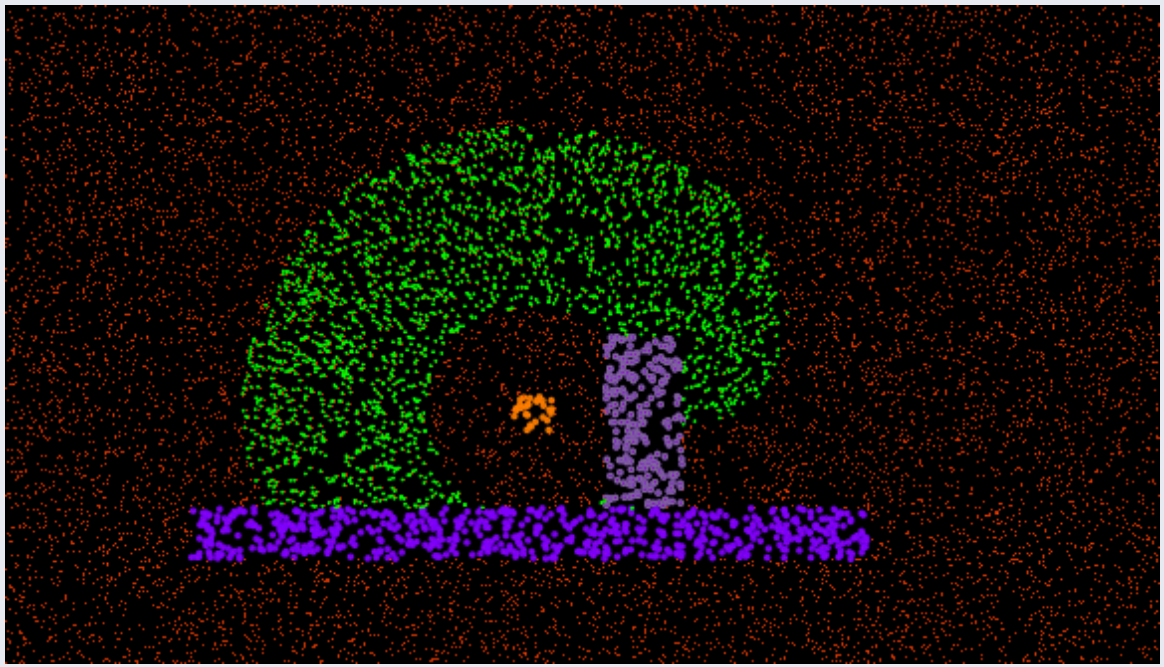
$$(DENY) \quad \langle \texttt{grad}, n \rangle + \langle \texttt{deny} \rangle \quad \rightarrow \quad \langle \texttt{deny} \rangle$$

Shape: filtered value in green, denyal zone in violet



Case 4 – Mathematical Combination

Laws: assume two gradients (source,grad) and (source',grad')

$$
\begin{array}{rl}
(DIST) & \langle \texttt{source} \rangle + \langle \texttt{grad}', d \rangle \rightarrow \langle \texttt{source} \rangle + \langle \texttt{grad}', d \rangle + \langle \texttt{dist}, d \rangle \\
(GSP) & \langle \texttt{dist}, d \rangle \rightarrow \langle \texttt{dist}, d \rangle + \langle \texttt{dist}, d \rangle^{\rightsquigarrow} \\
(CHN) & \langle \texttt{dist}, d \rangle + \langle \texttt{grad}, g \rangle + \langle \texttt{grad}', g' \rangle \rightarrow \\
 & \langle \texttt{dist}, d \rangle + \langle \texttt{grad}, g \rangle + \langle \texttt{grad}', g' \rangle + \langle \texttt{path} \rangle \quad (g + g' - d \leq w)
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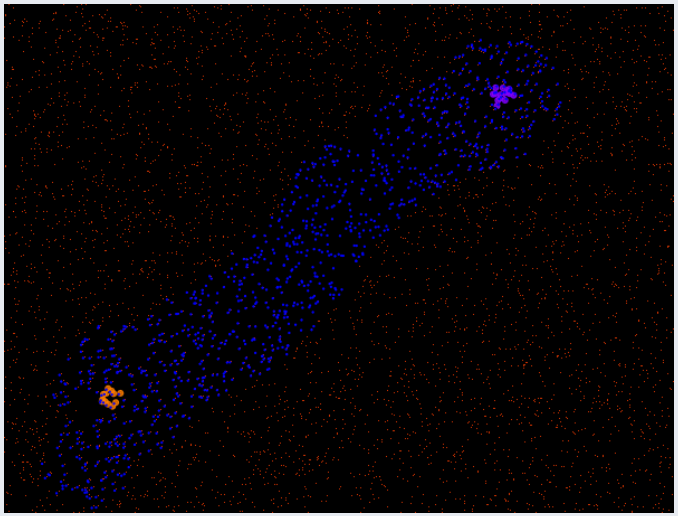
\end{array}
$$

Shape: source in yellow, target in violet, denyal in magenta, path in blue



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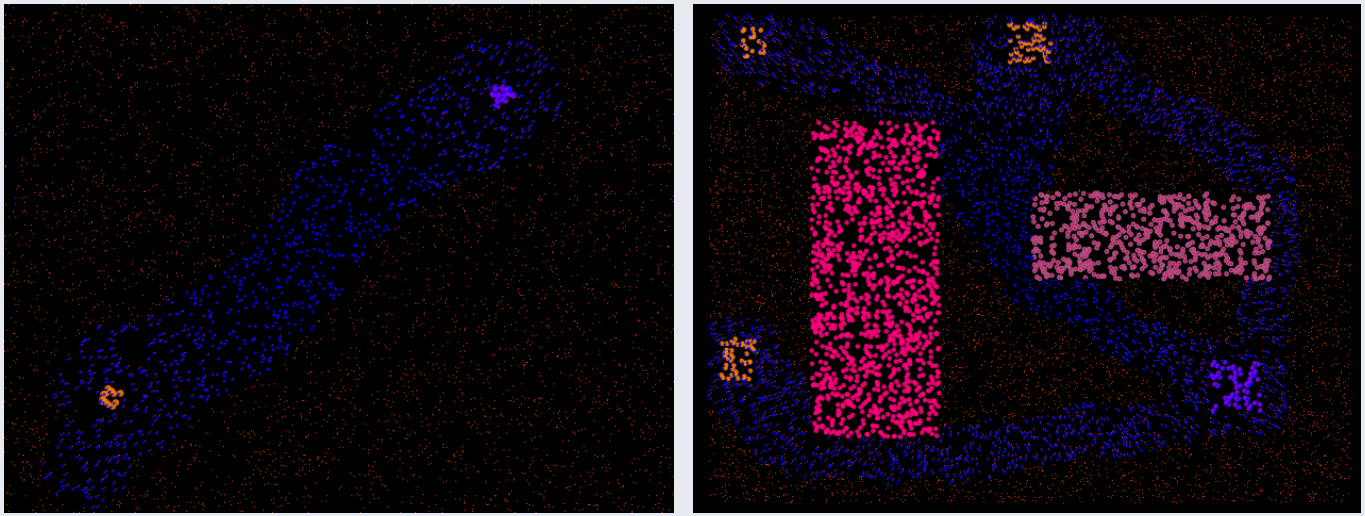
$$
\begin{array}{rl}
(DIST) & \langle \mathtt{source} \rangle + \langle \mathtt{grad}', d \rangle \rightarrow \langle \mathtt{source} \rangle + \langle \mathtt{grad}', d \rangle + \langle \mathtt{dist}, d \rangle \\
(GSP) & \langle \mathtt{dist}, d \rangle \rightarrow \langle \mathtt{dist}, d \rangle + \langle \mathtt{dist}, d \rangle^{\rightsquigarrow} \\
(CHN) & \langle \mathtt{dist}, d \rangle + \langle \mathtt{grad}, g \rangle + \langle \mathtt{grad}', g' \rangle \rightarrow \\
 & \langle \mathtt{dist}, d \rangle + \langle \mathtt{grad}, g \rangle + \langle \mathtt{grad}', g' \rangle + \langle \mathtt{path} \rangle \quad (g + g' - d \leq w)
\end{array}
$$

Shape: source in yellow, target in violet, denyal in magenta, path in blue

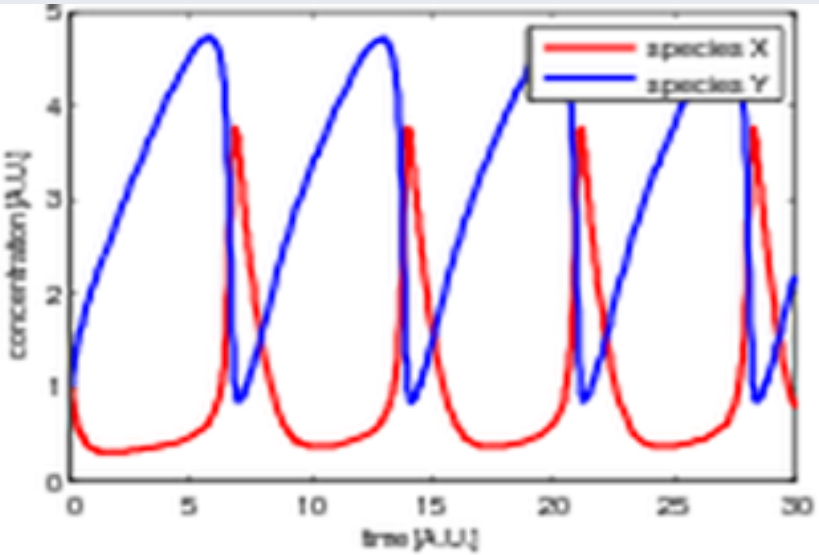


Outline

The Brussellator Case

A theoretical model: implemented by BZ reaction

$$A \rightarrow X$$
$$2X + Y \rightarrow 3X$$
$$B + X \rightarrow Y + D$$
$$X \rightarrow E$$



Intuition

- It is possible to design artificial chemical models exposing "strange" behaviours $\Rightarrow$ possible in vitro realisation at some point
- Brussellator seems to include some of the features we need

A methodology

Identify theoretical models that simulate the required functions

1. Linear gradient (ascending or descending)
   - a diffusion process making concentration decrease quasi-linearly
2. Filtering
   - making a reactant "activate" only if in a given range of concentration
3. Denyal
   - making a substance be consumed by a "denying" molecule
4. Mathematical combination
   - being able to create a substance c whose concentration is (approximately) sum or difference of those of substances a, b

Techniques

- Good inspiration
- Euristics to guide us towards the right rates

Conclusion

Final questions

- What spatial patterns might be of interest in your community?
- Are some of the problems I'm posing already solved?
- Do we care if possibility of actual realisation seems remote?

Spatial Computing with Chemistry

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