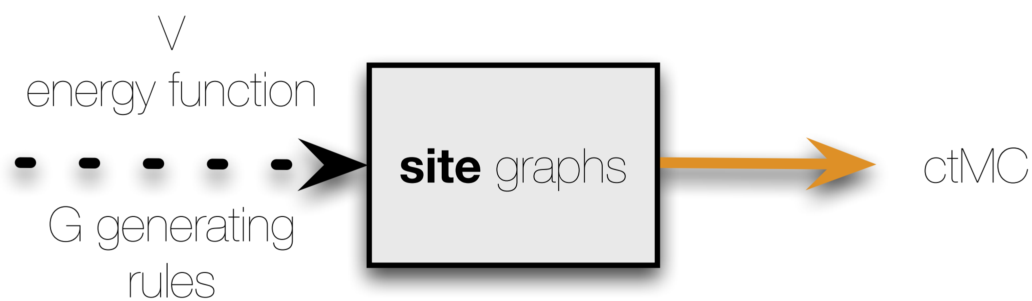
Thermodynamic graph rewriting

joint work with
Russ Harmer and
Ricardo Honorato-Zimmer

the idea is to not write the rules directly
but just the
energy landscape

then,only, do we generate the rules



Kappa language (with Laneve)
compiler to KaSim (Krivine, Feret)

Why?

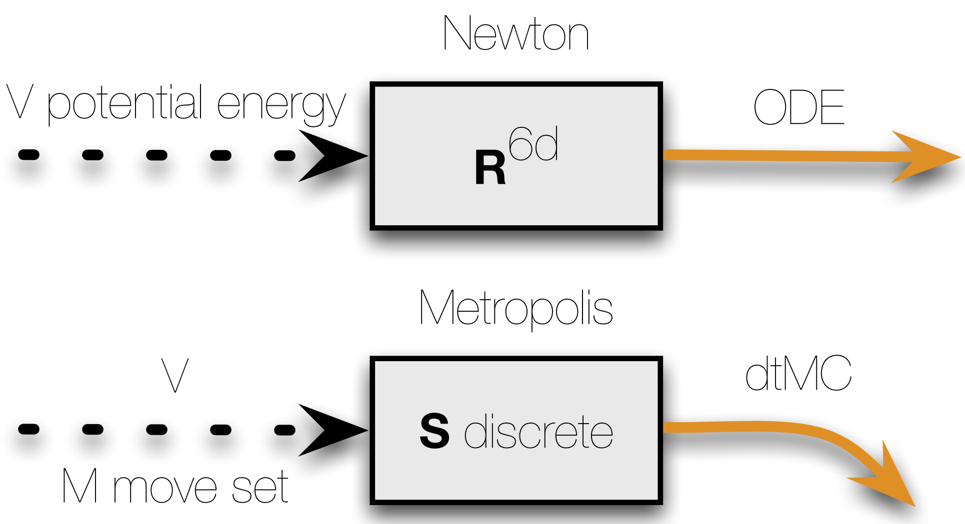
super-concise way of building models
in applications

captures a certain physicky way to do things
in a syntax

thermodynamic consistency guaranteed
(whereas undecidable in general)

natural parsimonious parameterizations

From statics to dynamics



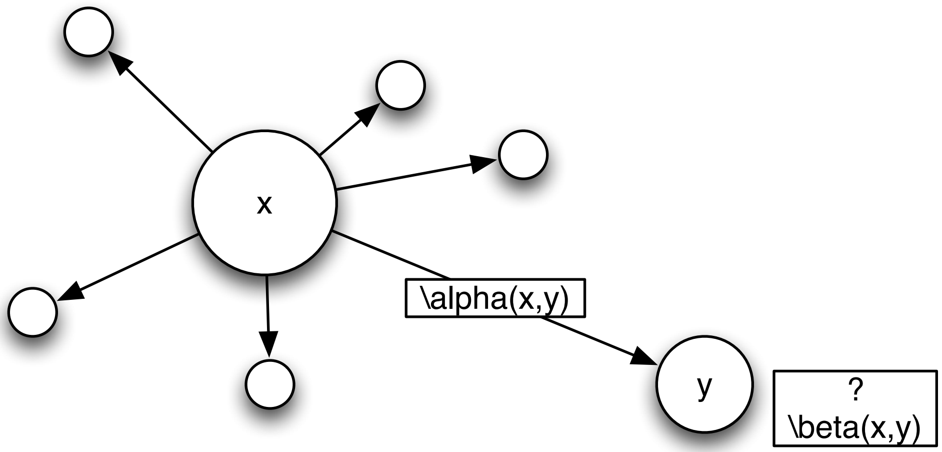
$$x \to x + v\,dt$$
$$v \to v - c\,\partial_x V$$

$$x \to y \quad \textit{with prob 1 when } \Delta V \leq 0$$
$$x \to y \quad \textit{with prob exp}(-\Delta V)$$
$$\textit{when } \Delta V \geq 0$$

Metropolis-Hastings

From statics to dynamics

discrete transition graph

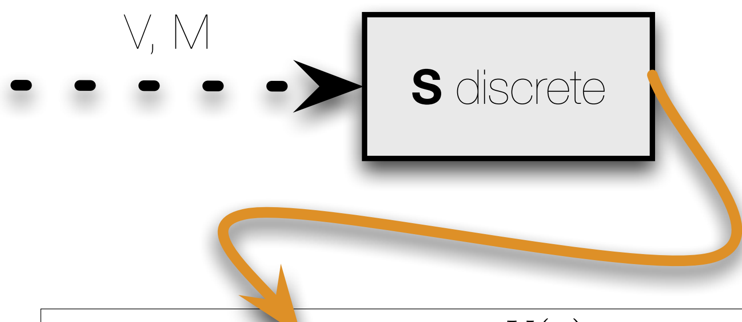


$$x \to y \quad \textit{with prob 1 when } \Delta V \leq 0$$
$$x \to y \quad \textit{with prob } exp(-\Delta V) \textit{ when } \Delta V \geq 0$$

$$\beta(x,y) = \min(1, e^{V(x)}\alpha(x,y)^{-1} \cdot e^{-V(y)}\alpha(y,x)) \quad \text{acceptance probability}$$
$$p(x,y) = \alpha(x,y)\beta(x,y) \quad \text{total motion probability}$$

$$p(x,x) = 1 - \sum_{y \neq x} \alpha(x,y)\beta(x,y) \quad \text{null event probability}$$

dt detailed balance

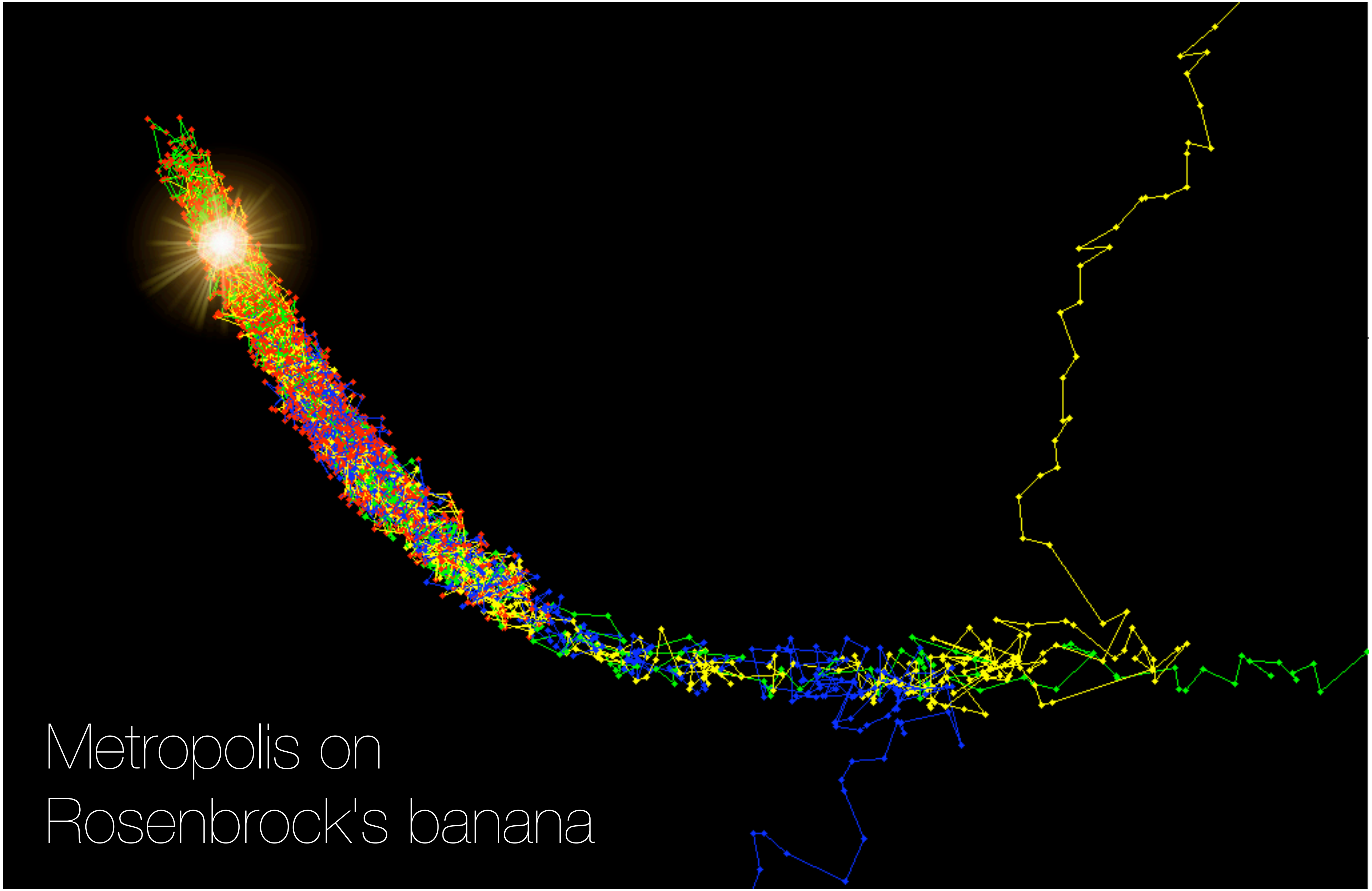


$$\begin{aligned} \beta(x,y) &= \min(1, e^{V(x)}\alpha(x,y)^{-1} \cdot e^{-V(y)}\alpha(y,x)) && \text{acceptance probability} \\ p(x,y) &= \alpha(x,y)\beta(x,y) && \text{total motion probability} \end{aligned}$$

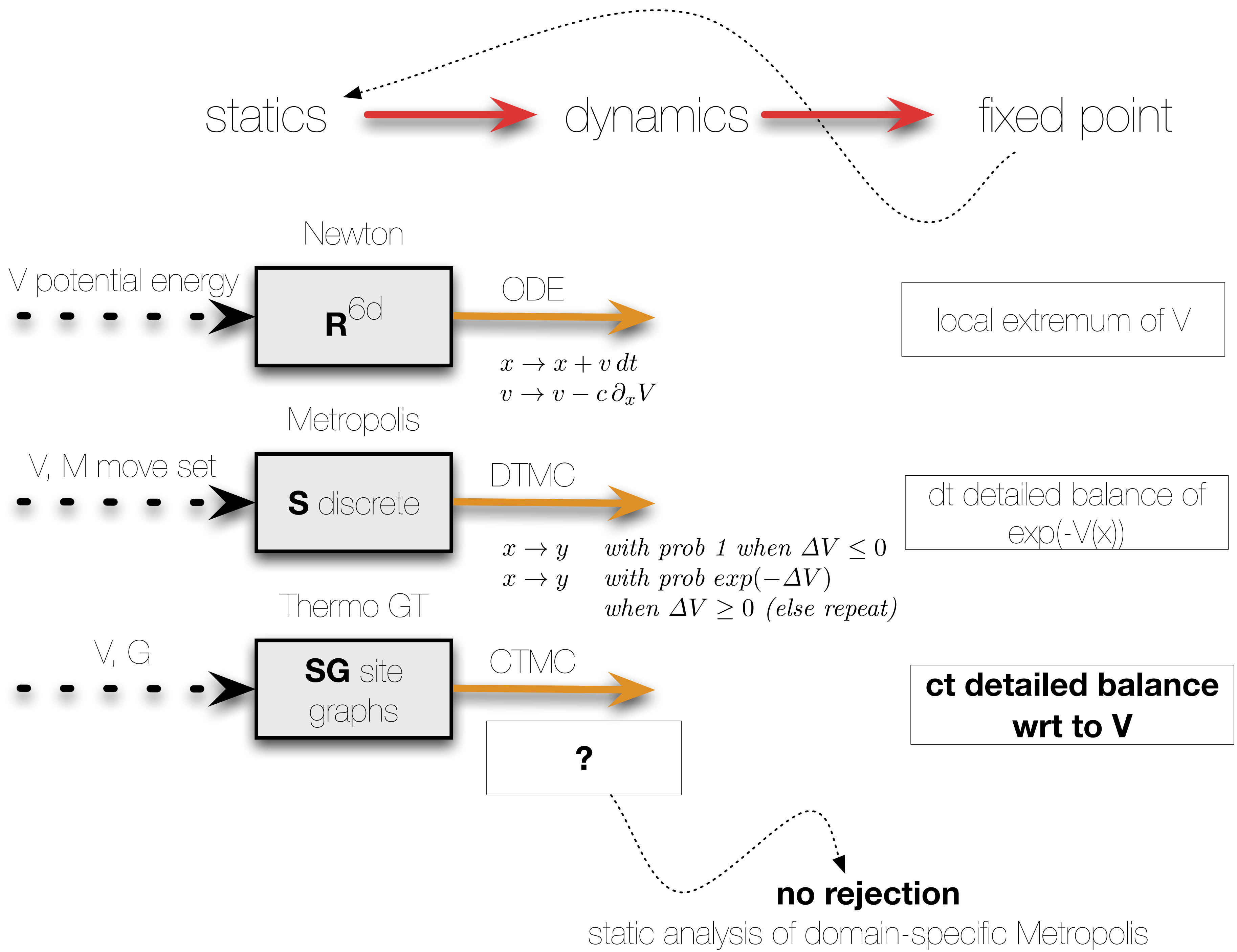
$$\begin{aligned} p(y,x)/p(x,y) &= \alpha(y,x)/\alpha(x,y) \cdot \beta(y,x)/\beta(x,y) \\ &= \alpha(y,x)/\alpha(x,y) \cdot e^{-V(x)}\alpha(x,y) \cdot e^{V(y)}\alpha(y,x)^{-1} \\ &= e^{V(y)} \cdot e^{-V(x)} \end{aligned}$$

$$p(y,x)e^{-V(y)} = p(x,y)e^{-V(x)}$$

under suitable conditions: the dynamics converges to the probabilistic fixed point



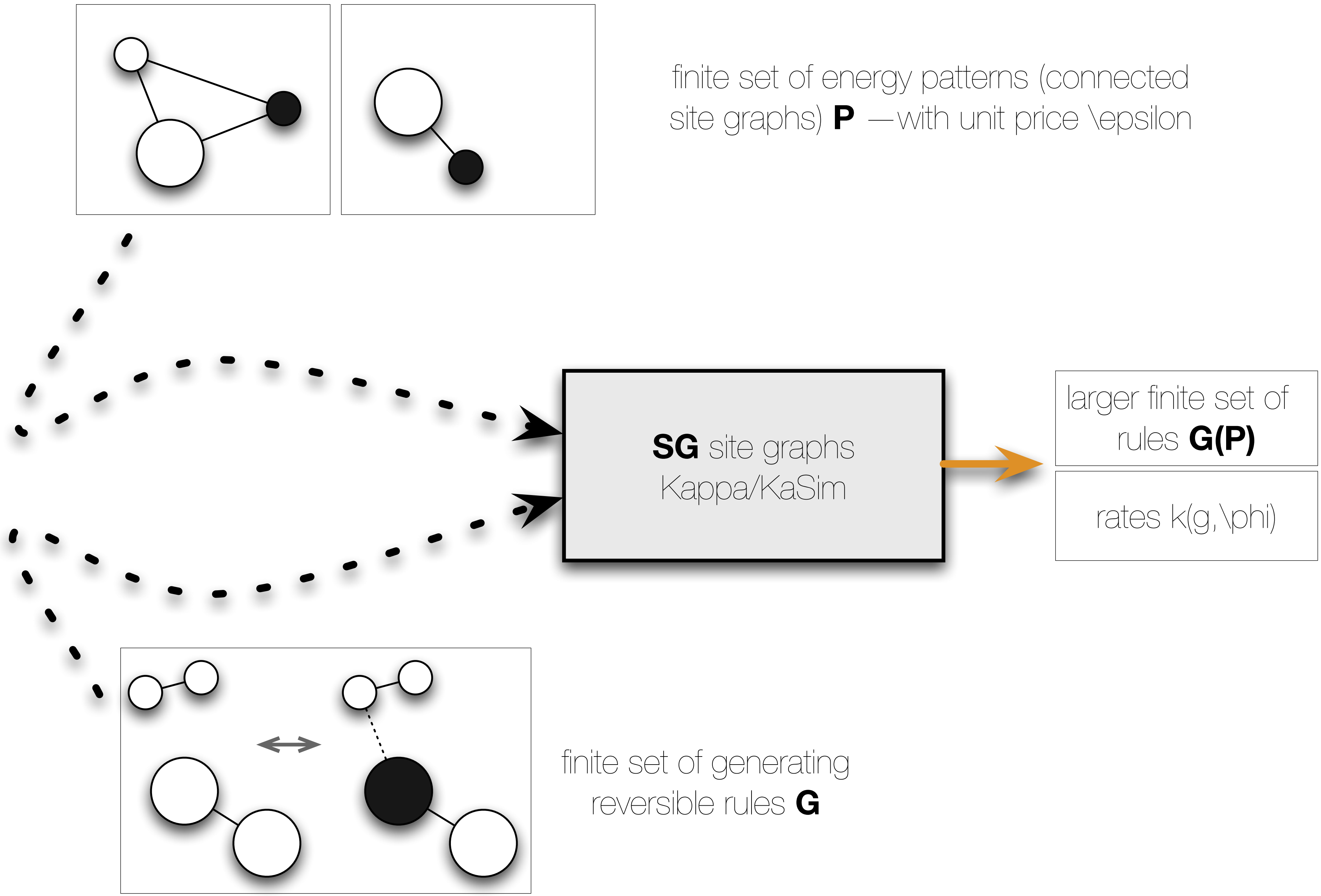
source: wikipedia


statics
dynamics
fixed point
Newton
V potential energy
R6d
ODE
$x \to x + v\,dt$
$v \to v - c\,\partial_x V$
local extremum of V
Metropolis
V, M move set
S discrete
DTMC
$x \to y$ with prob 1 when $\Delta V \leq 0$
$x \to y$ with prob $exp(-\Delta V)$ when $\Delta V \geq 0$ (else repeat)
dt detailed balance of exp(-V(x))
Thermo GT
V, G
SG site graphs
CTMC
?
ct detailed balance wrt to V
no rejection
static analysis of domain-specific Metropolis

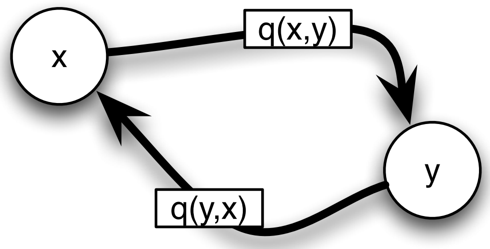
Thermodynamic graph rewriting

intuitions

Thermodynamic graph rewriting



instance independence of energy delta



total energy V(x) of x

$$q(y,x)\, e^{-\epsilon\cdot\mathcal{P}(y)} = q(x,y)\, e^{-\epsilon\cdot\mathcal{P}(x)}$$

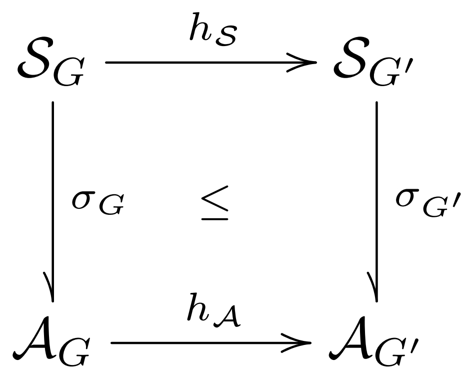
instances of a rule should have constant V(y)-V(x)
equivalently constant P(y)-P(x)

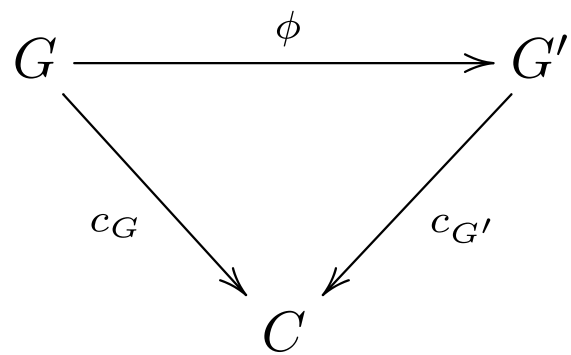
G(P) obtained by partitioning **G** so as to reveal enough context for each rule **g** to have a well-defined P-balance

Thermodynamic graph rewriting

the algebra

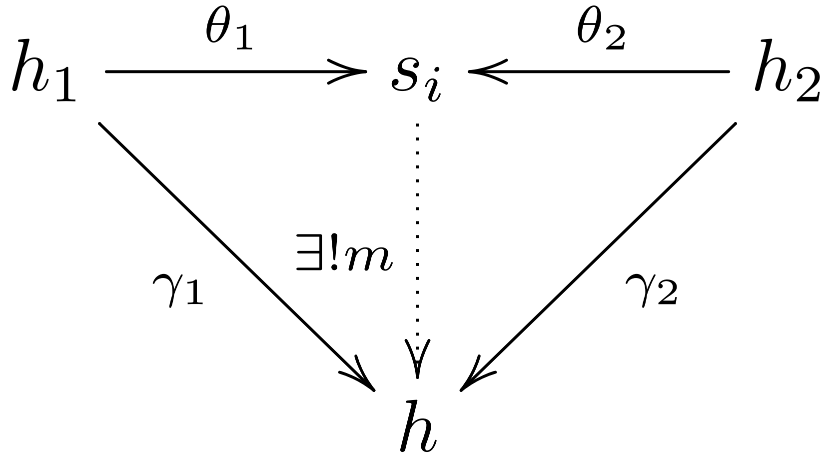
$rSGe_C$ realizable site graphs over C





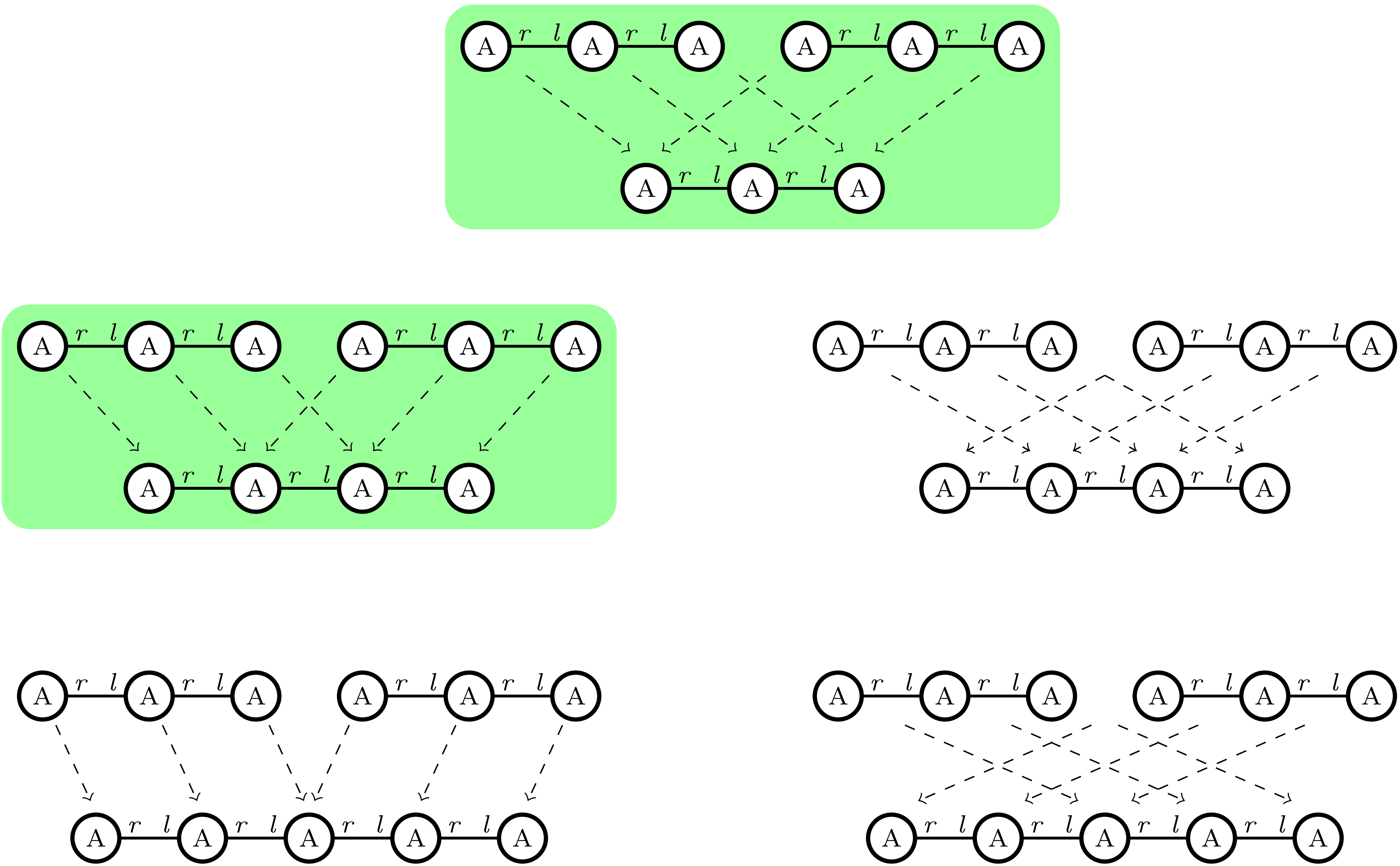
category of realizable site graphs typed by C
with embeddings (mono reflecting edges)

rSGe$_C$ has multi-sums

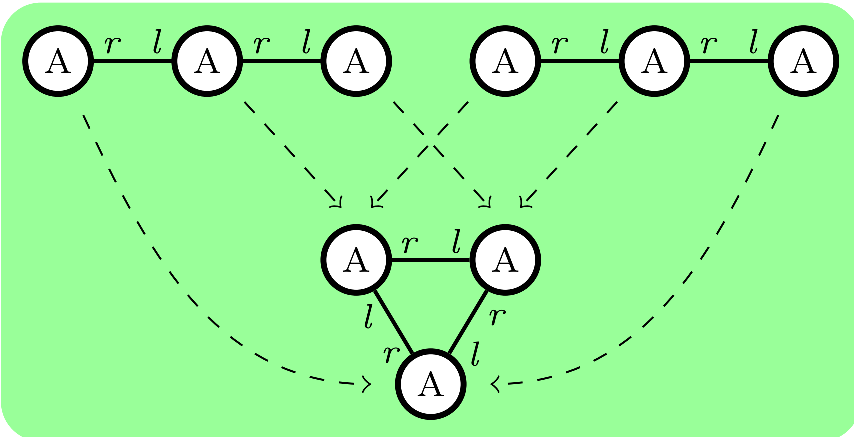


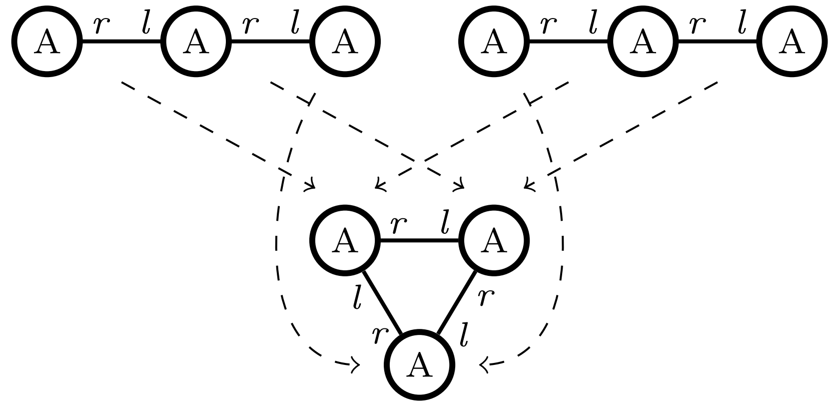
we do not have a sum—but finitely many minimal ones; we call them **minimal glueings**

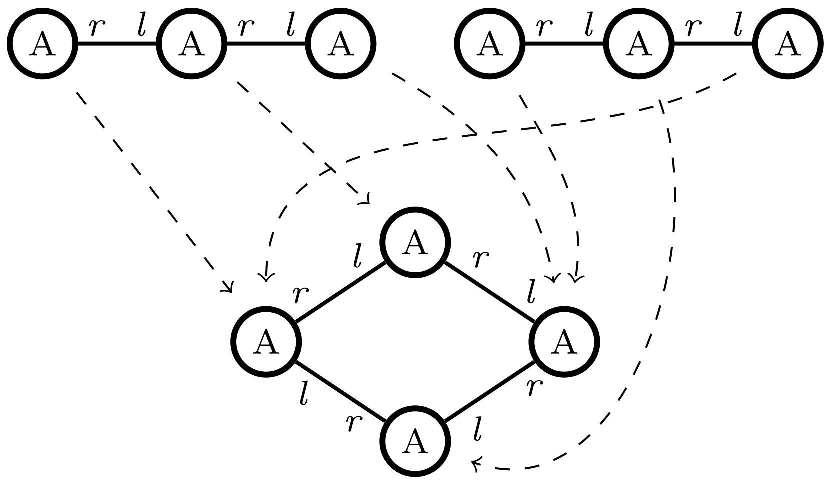
multi-sums example



multi-sums example

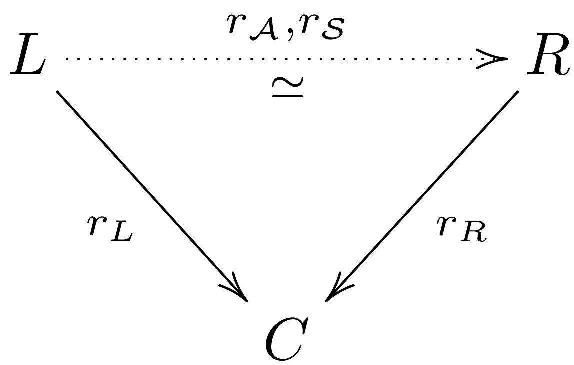




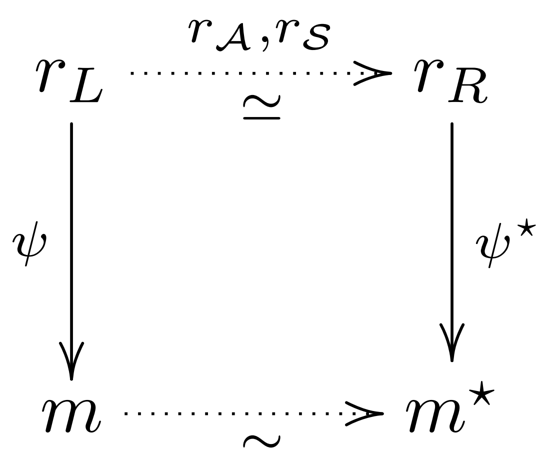


+ disjoint sum not shown

rules and rule application

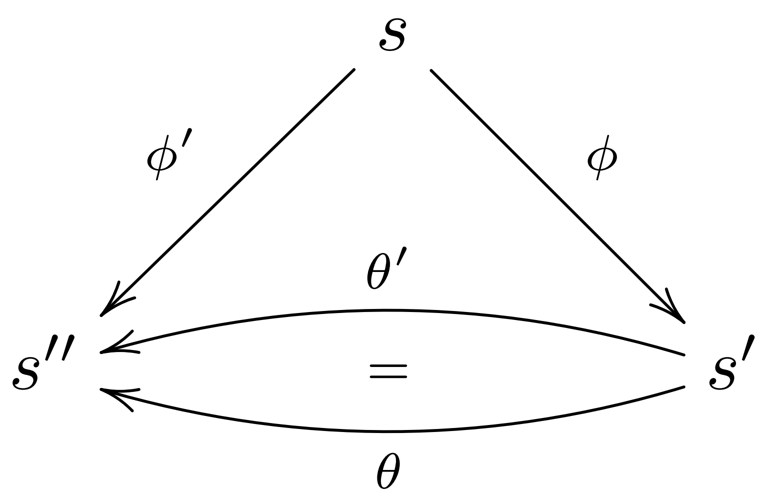


top arrow is a pair of set bijections



rules are node-preserving and hence reversible

extensions of a pattern, of a rule

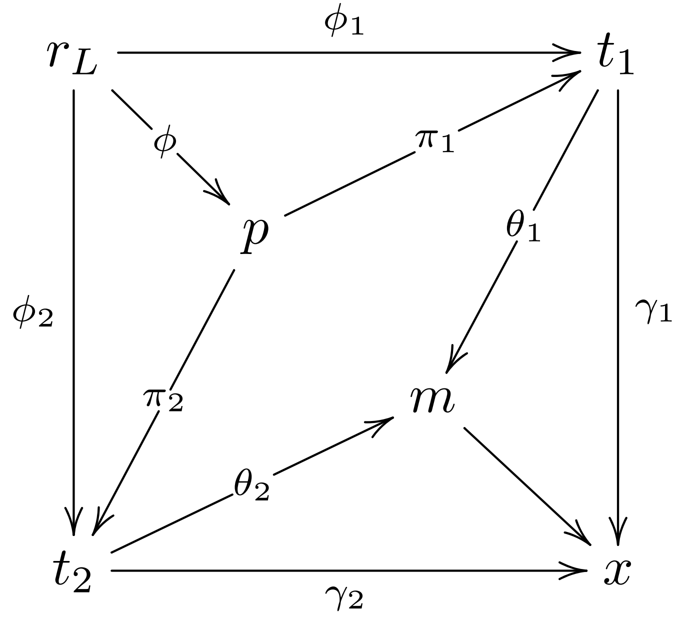


sub-category of epis below s: every connected component of s' has a preimage in s

growth policies and rule partitioning

growth policy \Gamma(\phi) maps every node of the image of \phi to a set of sites (of C)

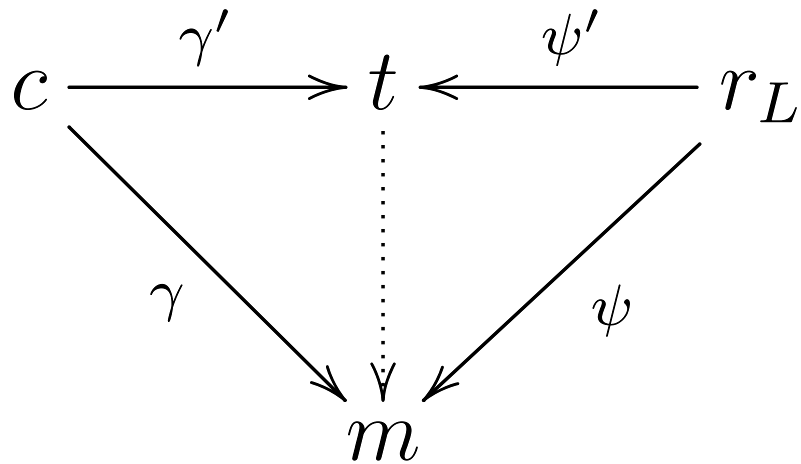
\phi has to be **faithful:** site requests are invariant under further extension



\phi is mature if all all nodes in the image of \phi have exactly the set of sites requested by \Gamma

the set of mature extensions of a pattern form a partition of the instances of the pattern (up to isomorphisms of extensions)

relevant minimal glueings



c is in P
rL the left hand
side of r in G
\psi is a match for r in m

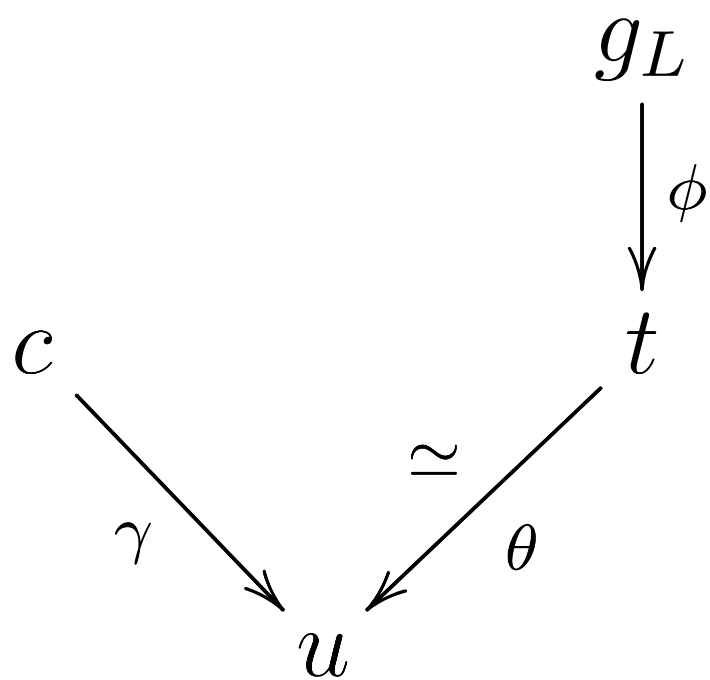
only if *the* minimal glueing of the cospan
\psi,\gamma defines an overlap modified by r is
the rule instance consuming \gamma— we call it relevant

balanced rules wrt to **P**

\phi is **left**-**P-balanced** if no proper relevant minimal glueing of c with t

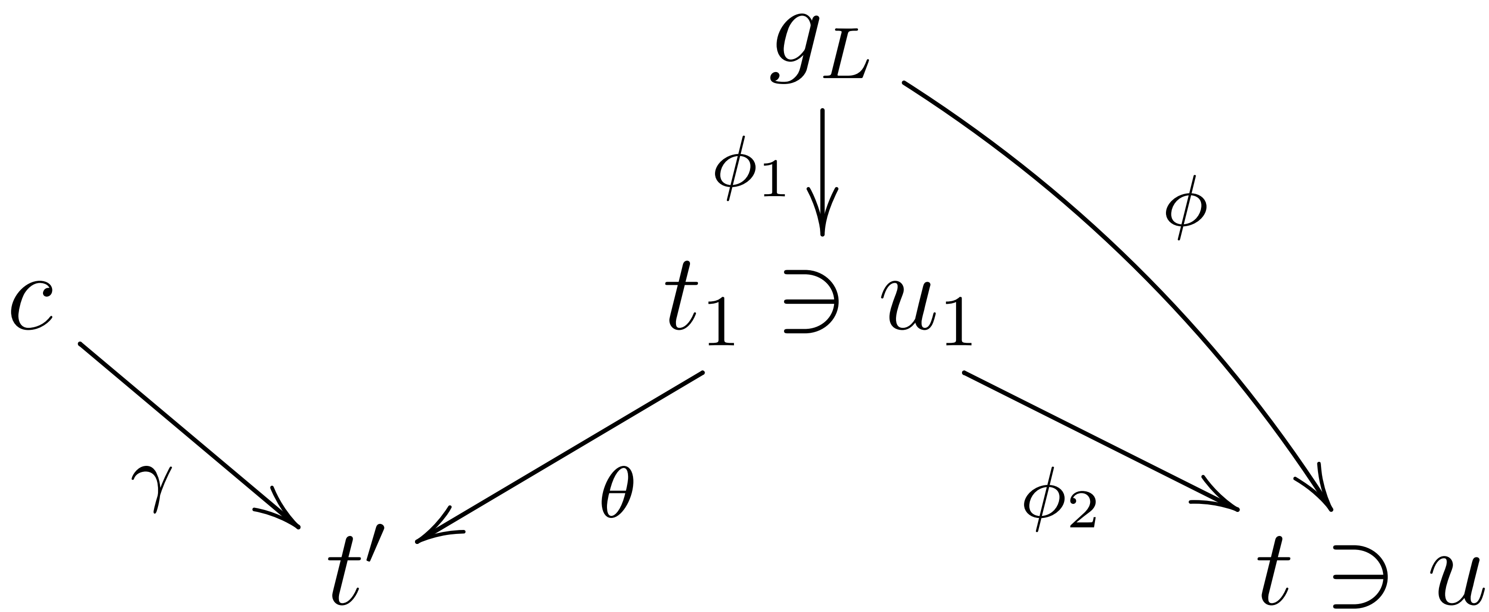
\phi is **P-balanced** if also symmetric condition on \phi*

equivalent to P-instance independence



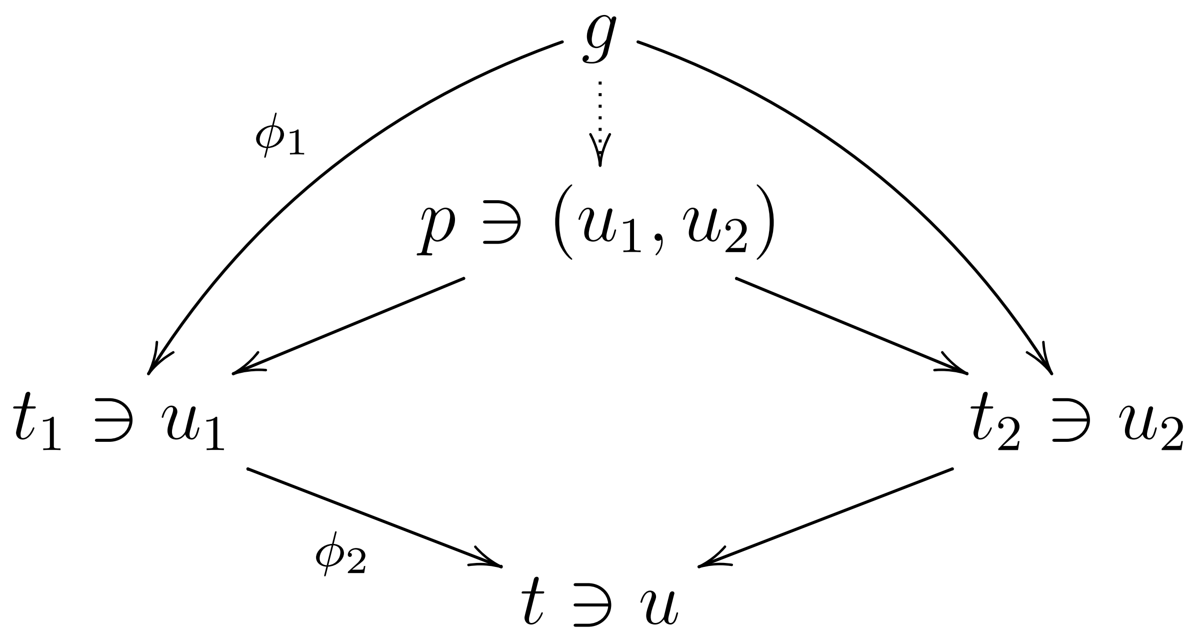
all we need is to define a growth policy which guarantees P-balance …

add by relevant glueing



\Gamma requests site s to u in \phi if —in the past of \phi— one energy pattern c in P glues relevantly to (the ancestor of) u and adds site s on its image via \theta

a growth policy indeed
and a surjective finite one



suppose u is requested to show site s along
another rewind of \phi …

… this defines G(P) as the union of the refined rules

The Result

$$\log k(g^{\star}_{\phi^\star}) - \log k(g_\phi) = \epsilon \cdot \Delta\phi$$

$$\pi_x(y) := e^{-\epsilon\cdot\mathcal{P}(y)} / \sum_{y\in\mathcal{L}_{\mathcal{G}}(x)} e^{-\epsilon\cdot\mathcal{P}(y)}$$

Theorem *Let $\mathcal{G}$, $\mathcal{P}$, $\mathcal{G}_{\mathcal{P}}$, k, and π_x be as above. We have that: $\mathcal{L}_{\mathcal{G}_{\mathcal{P}}}$ and $\mathcal{L}_{\mathcal{G}}$ are isomorphic as symmetric LTSs; and, furthermore, for any mixture x, the irreducible continuous-time Markov chain $\mathcal{L}^k_{\mathcal{G}_{\mathcal{P}}}$ has detailed balance for, and converges to π_x, on $\mathcal{L}_{\mathcal{G}_{\mathcal{P}}}(x) = \mathcal{L}_{\mathcal{G}}(x)$ the strongly connected component of x.*

parsimonious parameterization

$$\log(k_g(\phi)) \quad := \quad c_g - A_g(\epsilon) \cdot \Delta\phi$$

$$c_{g^\star} = c_g \quad \text{and} \quad A_{g^\star} + A_g = I$$

$$c_{g^\star} - A_{g^\star}(\epsilon) \cdot \Delta\phi^\star = c_g - A_g(\epsilon) \cdot \Delta\phi + \epsilon \cdot \Delta\phi$$

A remarkable particular case is obtained when $c_{g^\star} = c_g = 0$, $A_{g^\star} = 0$, $A_g = I$:

$$\begin{aligned} k_g(\phi) &= e^{-\epsilon \cdot \Delta\phi} \\ k_{g^\star}(\phi^\star) &= 1 \end{aligned}$$

Thermodynamic graph rewriting

an example