On Sequential Monte Carlo (SMC) strategies for Target Distributions

M. Rousset [1,2]
F. Cérou, A. Guyader, B. Delyon, T. Lelièvre, G. Stoltz, C.E. Bréhier, L. Goudenège, P. Héas. (PhDs: F. Ernoult, K. Tit).

[1]Inria Rennes Bretagne Atlantique

[2]IRMAR, Université de Rennes 1

2021

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- **SMC = particle methods= Importance splitting**. As "opposed" to MCMC methods. Start with a sample of N replicas ('particles'). Algorithms output: sample of N particles (approx. indep.) with distribution the 'target' + estimator of normalisation.
- **Aim of the talk:** Overview on variants and adaptivity + app. to neutrons (cf. talk of Lelièvre and Del Moral).

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- $\mathrm{score} : \mathbb{R}^d \to \mathbb{R}$ a given computable function.
- Assume $\pi(\{\mathrm{score} > 0\}) = 1$. Problem for given s:

$$\begin{cases} \text{Estimate} \quad p_s := \pi(\{\mathrm{score} > s\}) \ll 1 \\ \text{Simulate according to } \underline{\text{'target'}} \quad \eta_s(dx) := \pi(dx | \mathrm{score}(x) > s). \end{cases}$$

Idea (For high dimensions / low temperature)

Estimate/Simulate **"smoothly" and sequentially** *the path*

$$s \mapsto (p_s, \eta_s), \quad s \in [0, 1].$$

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- Previous rare event model is particular case for:

$$V_s(x) = \begin{cases} +\infty & \text{if } \mathrm{score}(x) \leqslant s \\ 0 & \text{if } \mathrm{score}(x) > s \end{cases}$$

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- Target : $\mathrm{e}^{-V_s} d\pi_s / z_s$.
- $s \mapsto \pi_s$ a path of mutually singular non-negative reference measures and a family of computable maps $i_{s,s'} : \mathbb{R}^d \to \mathbb{R}^d$ with $s, s' \in \mathbb{R}$ such that:

$$\pi_{s'} = i_{s,s'}[\pi_s] \quad \text{(push-forward)}$$

Example

$\pi_s := 2d' < 2d$-dimensional phase-space volume of a parametric family of co-tangent spaces $s \mapsto T^*\Sigma_s \subset \mathbb{R}^{2d}$. $i_{s,s'}$ is a simulable symplectic projection.

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Motivated by pbs where:

$$\text{Relative Entropy}(\text{target} \mid \text{educated proposal}) \to +\infty.$$

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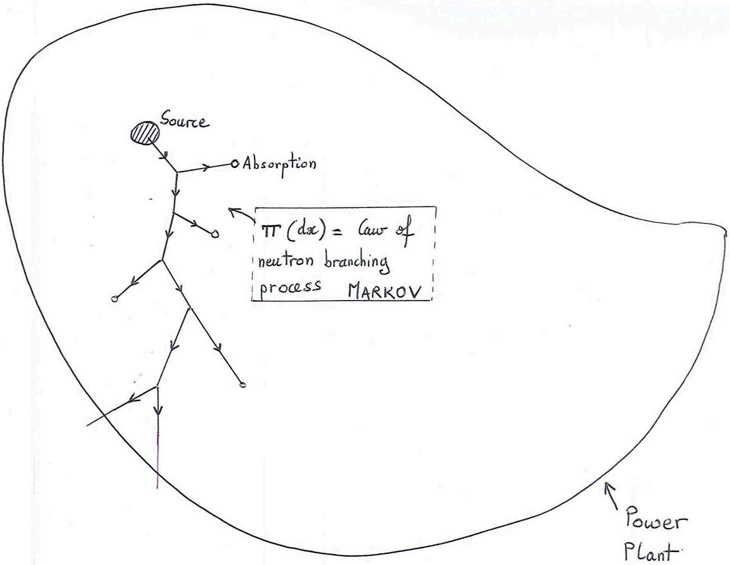
- Rare event.

Branching Neutron Transport Application



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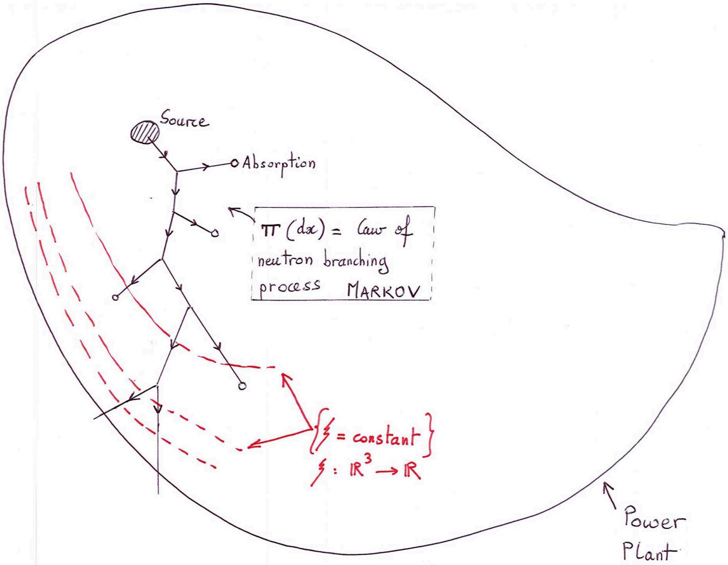

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- Exemple of choice of score function, e_0 given critical energy:

$$\mathrm{score}(X) := \max_{t \geqslant 0} \zeta(X_t)$$

$$= \max_{t \geqslant 0} \inf \Big\{ s \in \mathbb{R} \mid \text{total energy of neutrons at time } t \text{ in } \{\xi \geqslant s\} \leqslant e_0 \Big\}$$

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- Corresponding choice of rare event flow:

$$z_s = p_s := \pi(\{\mathrm{score} \geqslant s\}), \qquad \eta_s := \pi(\quad \mid \mathrm{score} \geqslant s)$$

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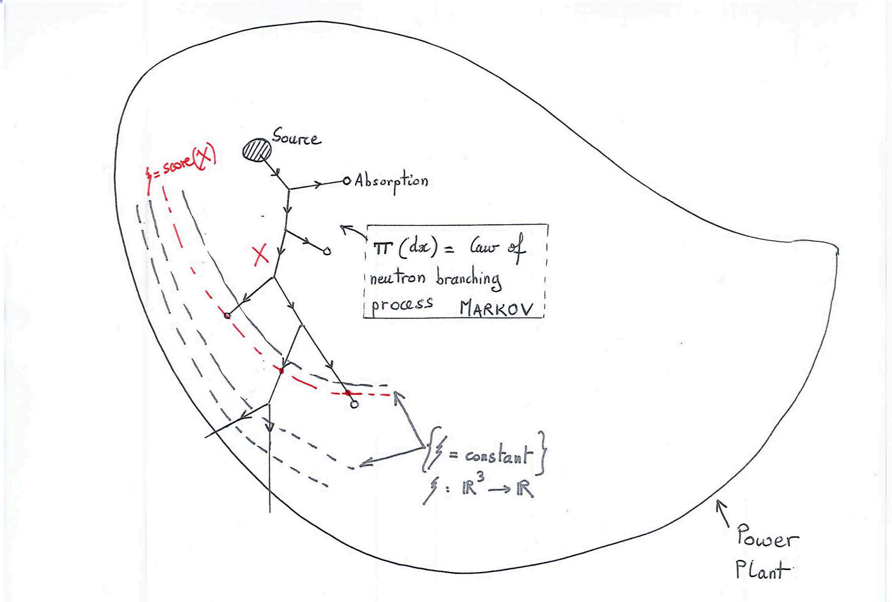

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- Define the stopping time for the natural filtration of the branching neutron transport process X

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- Using the strong Markov property, one can simulate new neutrons starting from $X_{\tau_s(X)}$. This yields a Markov kernel $M_s(x, dx')$ leaving π conditioned by $\{\mathrm{score} \geqslant s\}$ invariant.

$$\int M_s(x, dx')\eta_s(dx) = \eta_s(dx').$$

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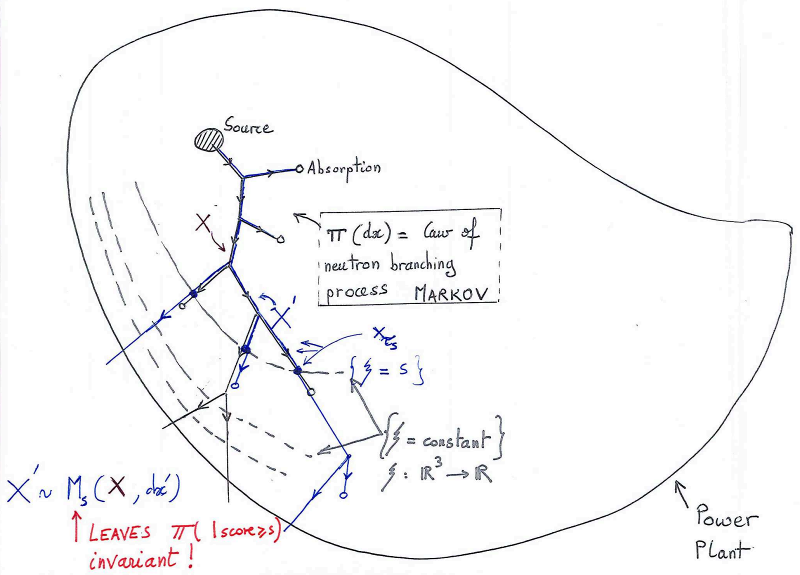

Sequential Monte-Carlo a.k.a. Importance Splitting

Define: $0 = s_{(0)} < \ldots < s_{(i_{\max})} = 1$ a given, finite ladder of scores.

$X^n_{s_{(i)}}$ state of replica n at iteration i.

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- (i) **Weights:** update the 'importance weight' of each replica $n \in (1, N)$ by $\mathrm{e}^{-V_{s_{(i)}}(X^n_{s_{(i-1)}})+V_{s_{(i-1)}}(X^n_{s_{(i-1)}})}$ (target: $\mathrm{e}^{-V_{s_{(i)}}}\pi$).

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- (ii) **Selection (optional)** kill and/or split replicas and update weights. E.g.: triggered if weights are too degenerate.
- (iii) **Mutation (optional)**: modify ('mutate') (all or some or none) replicas with Markov Chain Monte Carlo transition $M_{s_{(i)}}(x, dx')$ that leaves invariant the target $\eta_{s_{(i)}}(dx)$.

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- Target measures $\eta_s = \frac{1}{z_s} \mathrm{e}^{-V(x,s)} \pi(dx)$ are estimated by weighted empirical measures with normalization

$$\eta^N_{s_{(i)}} := \sum_{n=1}^{N} \mathrm{Weight}^n_{s_{(i)}} \delta_{X^n_{s_{(i)}}} \Big/ \sum_{n=1}^{N} \mathrm{Weight}^n_{s_{(i)}} .$$

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- Normalizations are estimated by the average weights over replicas

$$z^N_{s_{(i)}} := \frac{1}{N} \sum_{n=1}^{N} \mathrm{Weight}^n_{s_{(i)}}$$

Selection schemes

Definition

A selection or re-sampling scheme draw branching numbers $B_n \in \mathbb{N}$ splitting or killing each replica $n = 1 \dots N$. New weights are defined accordingly:

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- $B^n \geqslant 1$ *and* $\mathbb{E}(B_n)$ *is independent on* n*:* **neutral bearing**.

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- In this talk I propose a different 'mindset':

Idea

Scores are always deterministic -> continuous ladder.

Interpret **'Adaptivity'** $=$ **'Mutations Only If Selection'**.

Nothing happens for most scores ('weighting $=$ waiting') because of the triggering of mutations by selection.

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- **Mutations-On-Child**: The mutation kernel M_s applied only to children when selction is such that the sample of children $\simeq$ target.

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- *Triggered mutations are applied on children ONLY.*

Adaptive/Triggered Mutation variant

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- *The goal of triggered Mutations (If-Selection, On-Child) is to save computational power by avoiding mutations (hence evaluation of V or ∇V) if simple weighting is sufficient.*

Adaptive/Triggered Mutation variant

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- *Well-known rare event case: Adaptive Multilevel Splitting (AMS) algorithm (see after).*
- *AMS in the dynamical setting has a hidden non-adaptive Feynman-Kac-Del Moral structure (see below).*

Remark on Adaptive Mutations

Additional Intrinsic Adaptivity on Mutations: The mutation kernel M_s is random and depends on the past replica empirical distribution. E.g.: if M_s is based on accept/reject, proposal is adaptively tuned to target an average acceptance rate $r_0 \in (0, 1)$.

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- Nota Bene: in Del Moral, re-sampling/selection is put in a (very slightly restrictive) 'mean-field' form.

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- *Exists experimentally !!*

The Feynman-Kac-Del Moral structure

Proposition (Unbiasedness)

Un-normalized estimators are unbiased for algorithms following the Feynman-Kac-Del Moral structure.

Proof.

First remark that $\int \varphi \, \mathrm{e}^{-V_{s(i)}} \, d\pi = \mathbb{E}[\varphi(X_{s_{(i)}})\mathrm{e}^{-V_{s(i)}(X_{s_{(i-1)}})+V_{s(i-1)}(X_{s_{(i-1)}})} \times \ldots \times \mathrm{e}^{-V_{s(1)}(X_{s(0)})+V_{s(0)}(X_{s(0)})}] =: \mathbb{E}[Q^{0\to i}(\varphi)(X_0)]$ where $i \mapsto X_{(i)}$ is the MCMC chain used in the mutation step. Then check that for $i \leqslant i_0$

$$i \mapsto z^N_{s(i)} \int Q^{i\to i^0}(\varphi) \, d\eta^N_{s(i)}$$ is a martingale.

$\square$

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In $\mathbb{R}^d$, if coordinates of X are i.i.d. and V has a sum form over coordinates and is smooth w.r.t. s, by CLT, non-degeneracy of weights requires:

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- Idea: switch to a continuum of scores:

$$s \in \left\{ s^{(0)}, \dots, s^{(I)} \right\} \quad \text{becomes} \quad s \in [0,1].$$

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Example

Piecewise constant Markov jump process

$$L_s(\varphi)(x) = \lambda_s(M_s(\varphi)(x) - \varphi(x)), \quad \eta_s M_s = \eta_s$$

can be simulated: i) mutations occur at random score (higher than s_0 with proba $\mathrm{e}^{-\int_0^{s_0} \lambda_s ds}$), ii) mutations with M_s.

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- Other examples: discretization of a Stochastic Differential Equation, or Piecewise Deterministic Markov Process.

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- (Exit) Stop if $S^{(j)} = 1$ else $j \to j+1$.

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- *AMS in 'dynamic setting' is an example with PSEUDO-triggered Mutation-On-Child: they are in fact preset mutations given by the model itself !, (see after).*

[a] See also Brehier Gazeau Goudenege Lelievre Rousset GAMS 2016

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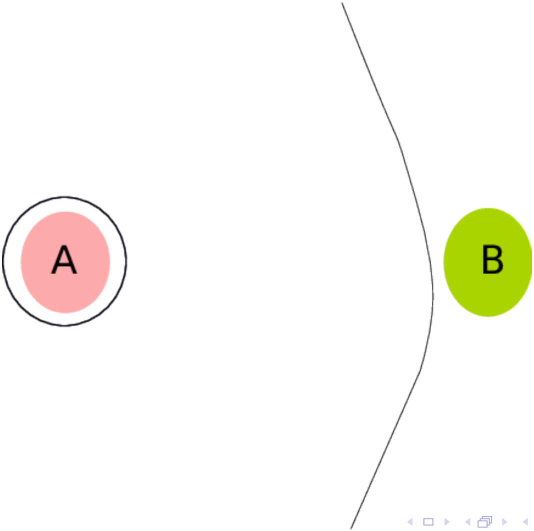
Adaptive Multilevel Splitting

– Black line: $\{\xi = constant\}$.



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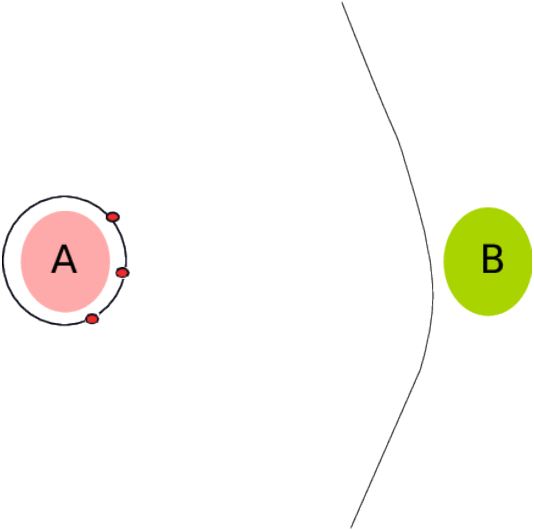

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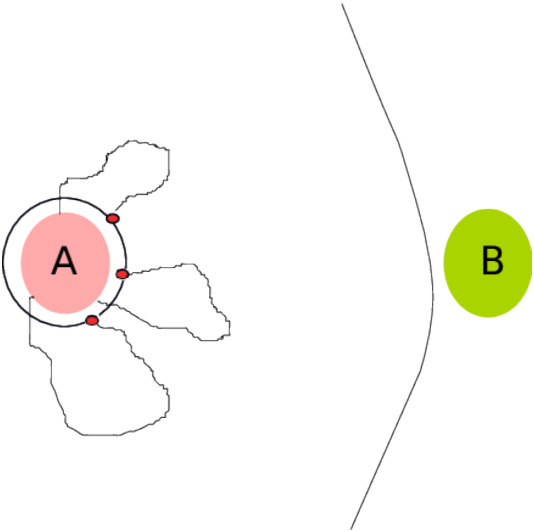

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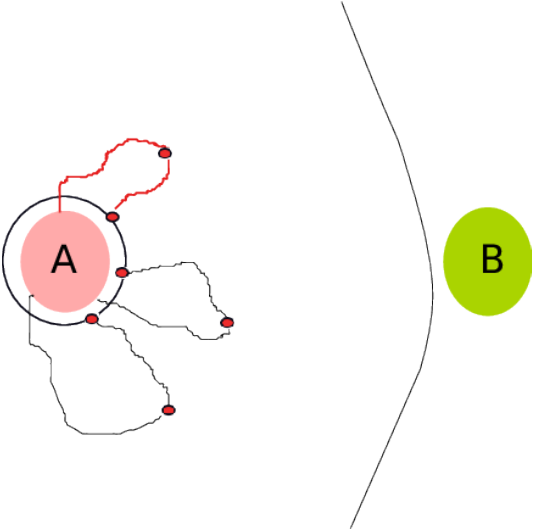

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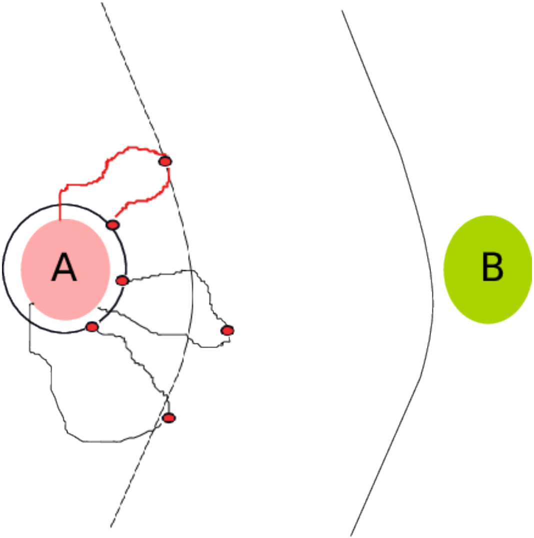

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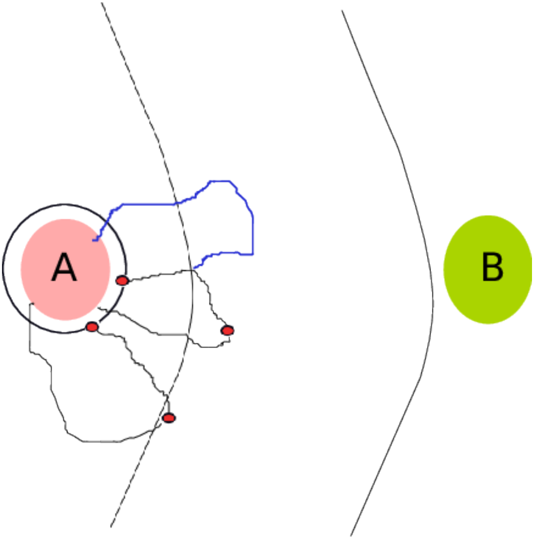

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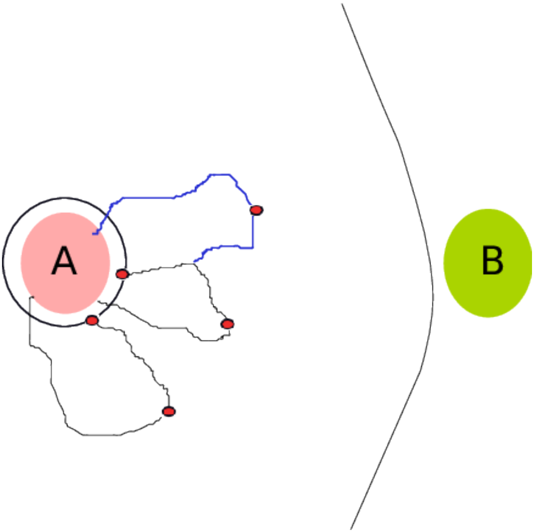

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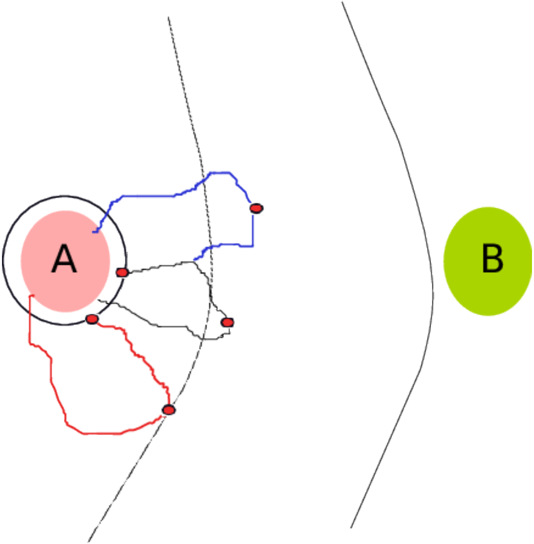

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- Ref: Cérou, (Delyon), Guyader , Rousset: series of paper.