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# Branching Stochastic Processes for Feynman-Kac Representations of Drift-involving Non-linearities

Daniel Yaacoub, Jérémie Dauchet, Thomas Vourc'h and Jean-François Cornet  
*Université Clermont Auvergne, Clermont Auvergne INP,  
 CNRS, Institut Pascal, F-63000 Clermont-Ferrand, France*

Stéphane Blanco and Richard Fournier  
*UPS, CNRS, INPT, LAPLACE UMR CNRS 5213, Université de Toulouse,  
 118 route de Narbonne, F-31065 Toulouse, Cedex 9, France*

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Many drift-diffusion transport models rely on a coupling with a sub-model of the drift velocity. In this letter we extend Feynman-Kac's theory to provide probabilistic representations of such velocity-coupled models, so far remained out of reach. Hence a single embedded stochastic process is built, enabling such representations in a single branching path-space. To address this, we propose renewed physical insights in terms of propagative pictures to non-linear physics such as Navier-Stokes, Keller-Segel and Poisson-Nernst-Planck equations in confined and complex geometries.

Keywords: Feynman-Kac, Path-space, Branching stochastic processes, Drift-diffusion, Non-linear coupling

Probabilistic representations of non-linear Partial Differential Equations (PDEs) have been enabled - until recent advances - by step forward approaches extending Feynman-Kac theory, initially based on superposition and linearity, to a first class non-linear physics, and thus bringing renewed insights in terms of path-space propagative pictures. This has resulted in reactive nonlinearities, such as Boltzmann kinetic equation [1–5], Kolmogorov-Petrovsky-Piskunov (KPP) reaction-diffusion equations [6–8] or non-linear Fredholm equations [9] benefiting from a conceptual framework with a unique process propagating toward sources, so-called branching stochastic process. Such non-linear PDEs are represented in a single path-space instead of an infinity of inlaid ones.

For non-linearities involving drift-velocity, such a feat has not yet been achieved. Yet large and diverse theoretical and applicative communities are concerned: drift-diffusion transport models for unmagnetized collisional plasma, incompressible fluids, globular clusters [10], semiconducting crystals, bacterial colonies [11, 12], extraneuronal ions [13, 14] and biological microswimmers, including Navier-Stokes, Poisson-Nernst-Planck or Keller-Segel equations, rely on a coupling with a sub-model of the drift velocity. Drift modeling with a prescribed velocity is intrinsically linear but as soon as a drift-velocity model is involved, the resulting coupled physics is non-linear. Drift-velocities are as diverse as gravitational field for self-gravitating globular clusters, chemical gradients for the chemotactic aggregation of bacterial colonies, or electrical field for ions surrounding neurons, electrons/holes within semiconducting crystals and electrotactic microswimmers. In terms of physical insights, the resulting non-linearity class is today a crucial question uniting these communities.

As an illustration, let us consider a density field submitted to only advection, at a stationary regime, in a confined domain. In the linear case of Fig. 1 a), *i.e.* when

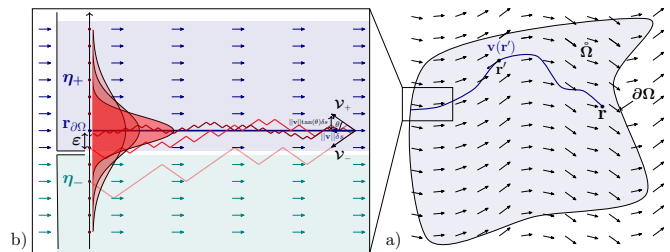


FIG. 1. Illustration in the stationary and purely advective regime. a) Canonical Feynman-Kac ballistic path traced using the local knowledge of a prescribed drift velocity field  $\mathbf{v}$ . b) Zoom close to the boundary, where  $\eta(y > -\varepsilon) = \eta_+$  or  $\eta(y < -\varepsilon) = \eta_-$  and  $\mathbf{v}$  is uniform. [blue]  $\delta\mathcal{R}_s = \mathbf{v}\delta s$  straight-backwardly propagates up to the boundary wall where the encountered value is  $\eta = \eta_+$ . [red]  $\delta\mathcal{R}_s = \mathbf{V}\delta s$  sample paths are broken lines since  $\mathbf{V}$  is a random vector. Spurious intuition: hitting positions on the wall are spatially distributed, preventing to reconstruct  $\eta = \eta_+$ . Counterintuitive solution: the hitting-position distribution for three values of  $\delta s$  is shown in red curves. There follows a normal distribution whose standard deviation decreases as  $\delta s$  vanishes (see End Matter A).

the drift-velocity field  $\mathbf{v}$  is known, the purely advective stochastic process  $\delta\mathcal{R}_s = \mathbf{v}(\mathcal{R}_s)\delta s$  leads to the density solution  $\eta(\mathbf{r}) = \eta(\mathbf{r}_{\partial\Omega})$ , where for any  $\mathbf{r}$  we note  $\mathbf{r}_{\partial\Omega}$  the boundary location backwardly ending the stream. Now assume that the drift of this main process is only known as the expectation  $\mathbf{v} = \mathbb{E}[\mathbf{V}]$  of a secondary process  $\mathbf{V}$ . If in place of a drift velocity we were dealing with a reactive term, in the vein of Skorokhod, McKean or Dimov [6, 7, 9], we could replace  $\mathbf{v}$  by  $\mathbf{V}$  in the main process. This would be perfectly correct and the non-linearity would be treated exactly. However, doing so in the case of a drift velocity would lead to a spurious situation.

Consider indeed, close to the boundary as in Fig. 1 b), that  $\mathbf{v}$  is now uniform and perpendicular to the boundary. The stream is a straight line. How would it be pos-

sible to reconstruct such a ballistic path with an advective stochastic process that uses a random drift-velocity  $\mathbf{V}$  that never equals the uniform value of  $\mathbf{v}$ ? Naively, the first hitting locations to the left-sided boundary wall would be spatially distributed around  $\mathbf{r}_{\partial\Omega}$ . In Fig 1 b) the boundary density is discontinuous ( $\eta_+$  or  $\eta_-$ ). Trivially,  $\eta(\mathbf{r}) = \eta_+$  as  $\mathbf{r}$  and  $\mathbf{r}_{\partial\Omega}$  are  $\varepsilon$  above the discontinuity. Meanwhile, how could the exact solution  $\eta_+$  be physically pictured as an average of  $\eta_+$  and  $\eta_-$ ?

This *a priori* spurious intuition has prevented the use of branching stochastic processes for drift-diffusion transport, but the present letter intends to show that this intuition comes from an improper limit inversion and that the two processes (drifting along the expectation or drifting along the velocity random process) are rigorously similar. With this view, an extension of Feynman-Kac path-integral formalism to velocity-coupled PDEs is hereafter proposed by means of embedded Continuous Branching Stochastic Processes (CBSP). We show that by using such processes it is possible to provide a generic framework allowing breakthrough physical insights in terms of propagative pictures of such non-linearly coupled PDEs and to handle subsequent statistical estimations in both confined and complex geometries, as shown in Fig. 3.

*a. State of the art* In 1947, [15] first introduced the term "Branching Process", although Discrete Branching Stochastic Processes were first conceptually formulated by [16, 17] and used by [18] to unravel probabilistic insights to one-dimensional diffusion equations such as the limit of a Bienaymé-Galton-Watson process. Between late 40's and late 60's, [15, 19] and subsequent developments such as those of [20] in the field of superprocesses laid the theoretical foundations for branching Markov processes and especially CBSP [21, 22], of which branching brownian motion is a particular case. The first use of these CBSP was finally made by [6, 7] to provide probabilistic Feynman-Kac representations of solutions to KPP reaction-diffusion equations [23]  $\partial_t \eta(\mathbf{r}, t) = D \nabla^2 \eta(\mathbf{r}, t) + f[\eta(\mathbf{r}, t)]$  in which the non-linearity occurs within the source term  $f[\eta]$  (e.g. Fisher-KPP:  $f[\eta] = \eta(1 - \eta)$  [24]). As mentioned above, the present paper deals with another wide class: PDEs non-linearly coupled to a model of the drift velocity. As a formal illustration of this coupling we can mention Poisson-Nernst-Planck equations

$$\begin{cases} \partial_t c(\mathbf{r}, t) &= -\nabla \cdot (-D \nabla c(\mathbf{r}, t) - \mu c(\mathbf{r}, t) \mathbf{E}(\mathbf{r}, t)) \\ \nabla \cdot \mathbf{E}(\mathbf{r}, t) &= -e c(\mathbf{r}, t) / \epsilon \end{cases} \quad (1)$$

describing the dynamics of charged particles with concentration  $c(\mathbf{r}, t)$  submitted to the electrical field  $\mathbf{E}(\mathbf{r}, t)$ . This system is analogous to Keller-Segel's [11, 12] describing the chemotactic aggregation of bacterial colonies ( $\mathbf{E}$  standing then for chemical gradients) or even self-gravitating systems such as globular clusters ( $\mathbf{E}$  standing then for the gravitational field) [10]. A second formal illustration of such a coupling can be seen in the vorticity rephrasing of incompressible Navier-Stokes equations

$$\begin{cases} \partial_t \omega(\mathbf{r}, t) &= \nu \nabla^2 \omega(\mathbf{r}, t) - (\mathbf{v}(\mathbf{r}, t) \cdot \nabla) \omega(\mathbf{r}, t) \\ \nabla \times \mathbf{v}(\mathbf{r}, t) &= \omega(\mathbf{r}, t) \end{cases} \quad (2)$$

where  $\mathbf{v}$  is the fluid velocity and  $\omega$  its vorticity.

Until now, many probabilistic representations for free-space Navier-Stokes have treated the non-linear terms involving drift velocity as sources [25–27], rather than considering it as part of the stochastic process. These studies were thus able to make use of CBSPs previously developed for KPP's reactive non-linearities, in a similar vein as [7]. This approach relies on the probabilistic representation of spatial derivatives using Malliavin stochastic calculus [28, 29]. Another approach is to study Navier-Stokes in Fourier space. The terms involving velocity become reactive non-linearities, which also benefit from previous developments for KPP equations [30–32]. We should also mention the use of such Fourier spaces in the study of Poisson-Vlasov equations [33, 34] which also benefit from KPP's branching path-space - stochastic cascades - in a similar vein as [9]. Although these strategies have achieved a huge step forward in being able to provide probabilistic representations and propagative insights of such non-linearly coupled PDEs, they remain incompatible with confined domains (especially due to the use of Malliavin calculus). This is a major issue for many applications, such as those shown in Fig. 3.

In contrast, some probabilistic representations compatible with confined domains - but at what cost? - have been advanced by considering velocity-involving terms as being fully part of the process itself. They can be conceptualized as an infinity of inlaid path-spaces [35, 36]. In the context of our introductory illustration, such a *McKean inlaid representation* is obtained by replacing  $\mathbf{v}$  with  $\mathbb{E}[\mathbf{V}]$  in the main process, as shown in Fig. 2 a). This approach has been applied to Keller-Segel [37], Stokes-Burger [38], or Navier-Stokes [39] equations. Statistical estimations based on these representations have been investigated either by pointwise [40, 41] or particle-systems approaches [42]. The cost is huge, since in comparison with KPP's branching trees, the coupling in terms of a single stochastic process is lost: a full  $\mathbf{V}$  path-space is inlaid at each location  $\mathcal{R}_s$  of the main path.

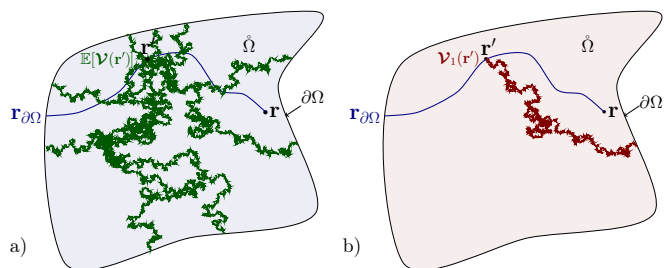


FIG. 2. a) McKean inlaid representation in the situation of Fig. 1:  $d\mathcal{R}_s = \mathbb{E}[\mathbf{V}|\mathcal{R}_s, s]ds$  requiring the estimation of  $\mathbf{v} = \mathbb{E}[\mathbf{V}] = \lim_{N \rightarrow \infty} (1/N) \sum_{i=1}^N (\mathbf{V}_i)$  with an infinite-size sample mean at each main-path location  $\mathbf{r}'$  (only nine realizations  $\mathbf{V}_i$  of  $\mathbf{V}$  are here represented at  $\mathbf{r}'$ ). b) Our proposition  $d\tilde{\mathcal{R}}_s = (\mathbf{V}|\tilde{\mathcal{R}}_s, s)ds$ : a unique realization  $\mathbf{V}_1$  of  $\mathbf{V}$  is required at  $\mathbf{r}'$ .

Although large impacts could be expected, no attempt

has yet been reported to encompass this non-linearity in a single branching path-space to provide probabilistic representations of velocity-coupled PDEs in confined geometries. We address such a generic framework with the same intents as those of applied mathematics communities - providing probabilistic representations [32] - but by resorting to embedded stochastic processes and their connections with the path-integral formalism of field equations (Fokker-Planck PDEs) [43]. Thus the coupling in a single path-space as illustrated in Fig. 2 b) is achieved, in contrast with the hitherto available inlaid McKean representation in Fig. 2 a). As a major outcome, we recover branching tree representations which enabled the previously-mentioned achievements for reactive non-linearities.

*b. Feynman-Kac canonical framework.* The Feynman-Kac framework aims at providing probabilistic insights into the solution of a field physics parabolic PDE, by resorting to brownian motion. Such insights were first introduced by [44, 45] to allow representations of the Dirichlet problem's harmonic measure. It was then extended to a wide class of differential operators by [46–48] with breakthrough insights in terms of propagative pictures for quantum mechanics. [49] finally achieved the connections between probability theory and Green functions. Here, the scope of (1)-(2) is extended to include an additive source  $+k(\mathbf{r})\eta^*(\mathbf{r}, t)$  and a killing term  $-k(\mathbf{r})\eta(\mathbf{r}, t)$  in addition to drift-diffusion, leading to the class of advection-reaction-diffusion equations

$$\partial_t \eta(\mathbf{r}, t) = D\nabla^2 \eta(\mathbf{r}, t) + \mathbf{v}(\mathbf{r}, t) \cdot \nabla \eta(\mathbf{r}, t) - k(\eta - \eta^*) \quad (3)$$

for all  $\mathbf{r} \in \mathring{\Omega}$  and  $t \in ]t_0; +\infty[$ . We focus on prescribed Initial Boundary Value (IBV)  $\eta_{\text{IBV}}(\mathbf{r}, t) \equiv \mathbb{1}_{\{\mathbf{r} \in \partial\Omega\}} \eta^{\partial\Omega}(\mathbf{r}, t) + \mathbb{1}_{\{t=t_0\}} \eta_0(\mathbf{r})$ , where  $\eta^{\partial\Omega}$  stands for the boundary value and  $\eta_0$  the initial one. The Feynman-Kac probabilistic representation of  $\eta$  is [50]

$$\eta(\mathbf{r}, t) = \mathbb{E}_{\mathcal{R}_s} \left[ \mathcal{F}(\mathcal{R}_{\mathcal{T}}, t - \mathcal{T}) \middle| \mathcal{R}_0 = \mathbf{r} \right] \quad (4)$$

given the stochastic functional  $\mathcal{F}$

$$\begin{aligned} \mathcal{F}(\mathcal{R}_{\mathcal{T}}, t - \mathcal{T}) &\equiv \eta_{\text{IBV}}(\mathcal{R}_{\mathcal{T}}, t - \mathcal{T}) e^{-\int_0^{\mathcal{T}} ds' k(\mathcal{R}_{s'})} \\ &+ \int_0^{\mathcal{T}} ds k(\mathcal{R}_s) \eta^*(\mathcal{R}_s, t - s) e^{-\int_0^s ds' k(\mathcal{R}_{s'})} \end{aligned} \quad (5)$$

$\mathcal{R}_{\mathcal{T}}$  is an Itô integral [51] defined as the continuous limit of the sum of stochastic increments  $\sum_i \delta \mathcal{R}_{i\delta s}$  as  $\delta s \rightarrow 0$  (see End Matter B). In such a limit, the stochastic process  $\mathcal{R}_{s \in ]s; t-t_0[}$  can be defined by the stochastic differential equation

$$d\mathcal{R}_s = \mathbf{v}(\mathcal{R}_s, s) ds + \sqrt{2D} d\mathfrak{W}_s \quad (6)$$

with  $\mathcal{R}_0 = \mathbf{r}$  and  $d\mathfrak{W}_s$  the Gaussian Wiener process. Realizations of  $\{\mathcal{R}_s\}_{s \in [0; t-t_0]}$  describe a non-standard continuous brownian path  $\{\mathbf{r}_s\}_{s \in [0; t-t_0]}$  starting from  $\mathbf{r}$  and backwardly propagating until a boundary/initial/volume

source is found (within the meaning of Green). According to (4)-(5),  $\eta$  results in the expected value of exponentially attenuated initial/boundary/volumic sources encountered along each path. The first passage time of this stochastic process to the boundary  $\partial\Omega$  is a random variable defined as  $\mathcal{T}_{\partial\Omega} := \inf\{s | \mathcal{R}_s \notin \Omega\}$ . The stopping time  $\mathcal{T} := \min\{\mathcal{T}_{\partial\Omega}, t-t_0\}$  is either  $\mathcal{T}_{\partial\Omega}$ , in which case the Dirichlet boundary condition  $\eta^{\partial\Omega}(\mathcal{R}_{\mathcal{T}_{\partial\Omega}}, t - \mathcal{T}_{\partial\Omega})$  is taken for  $\eta_{\text{IBV}}$ , or  $\mathcal{T} = t - t_0$  if the initial instant is reached before the process exits the domain  $\Omega$ , in which case the initial condition  $\eta_0(\mathcal{R}_{t-t_0})$  is taken. The ensuing set of paths draws a path-space and the Feynman-Kac representation (4) is understood as a path-integral over this Wiener-measurable functional domain [47, 52–54].

*c. Coupling Feynman-Kac representations through drift-velocities* In the earlier framework, the velocity field  $\mathbf{v}$  was prescribed, as it was for the source term  $\eta^*$ . Now, we address the rephrasing of the Feynman-Kac representation for  $\eta$  without having a prescribed velocity field, but given instead a probabilistic formulation  $\mathbf{v}(\mathbf{r}, t) = \mathbb{E}_{\mathcal{V}}[\mathcal{V} | \mathbf{r}, t]$  which can itself be a Feynman-Kac representation of an IBV problem. With this view, the Feynman-Kac representation of  $\eta$  writes

$$\begin{cases} \eta(\mathbf{r}, t) = \mathbb{E}_{\mathcal{R}_s} [\mathcal{F}(\mathcal{R}_{\mathcal{T}}, t - \mathcal{T}) | \mathcal{R}_0 = \mathbf{r}] \\ d\mathcal{R}_s = \mathbb{E}_{\mathcal{V}} [\mathcal{V} | \mathcal{R}_s, s] ds + \sqrt{2D} d\mathfrak{W}_s \end{cases} \quad (7)$$

Such a representation is available even when  $\mathcal{V}$  is a functional of  $\eta$  [4]. At each time  $s \in [0, t - t_0]$  the knowledge of this McKean stochastic process  $\{\mathcal{R}_s\}_s$  implies  $\mathbb{E}_{\mathcal{V}}[\mathcal{V} | \mathcal{R}_{s'}, s']$  for all  $s' < s$ , *i.e.* the whole velocity field. A path  $\{\mathbf{r}_s\}_s$  is constructed by inlaying a full velocity path-space centered at each  $\mathbf{r}_{s'}$ , as illustrated in Fig. 2 a). In the context of Fig. 1 it reconstructs strictly the ballistic path.

The question of handling the coupling in a single branching path-space is now addressed using an embedded CBSP  $\{\tilde{\mathcal{R}}_s\}_s$  that enables us to write (7) as

$$\begin{cases} \eta(\mathbf{r}, t) = \mathbb{E}_{\tilde{\mathcal{R}}_s} [\mathcal{F}(\tilde{\mathcal{R}}_{\mathcal{T}}, t - \mathcal{T}) | \tilde{\mathcal{R}}_0 = \mathbf{r}] \\ d\tilde{\mathcal{R}}_s = (\mathcal{V} | \tilde{\mathcal{R}}_s, s) ds + \sqrt{2D} d\mathfrak{W}_s \end{cases} \quad (8)$$

At each time  $s \in [0, t - t_0]$  the knowledge of the process  $\{\tilde{\mathcal{R}}_s\}_s$  is now entirely determined by  $\mathcal{V} | \tilde{\mathcal{R}}_{s'}, s'$  for all  $s' < s$ , that is the statistics of  $\mathcal{V}$  only, in contrast with the full velocity field that was required above. A path  $\{\tilde{\mathbf{r}}_s\}_s$  is constructed by embedding a unique path of  $\mathcal{V}$  centered at each  $\mathbf{r}_{s'}$ , as illustrated in Fig. 2 b). In other words, sub-paths ( $\mathcal{V}$ -paths) pass on all the information about the coupled velocity model to the main path ( $\eta$ -path), without inlaying a full sub-path-space but drawing instead a unique branch [55].  $\{\tilde{\mathcal{R}}_s\}_s$  can therefore be understood as an embedded process that includes the statistics of  $\mathcal{V}$ . As mentioned in the introduction and shown in Fig. 1 b), this counterintuitive viewpoint is constructed as the continuous limit of a branching process, which is studied hereafter.

The theoretical argument leading to (8) lies in a limit inversion. Instead of trying to handle the coupling on

the basis of (7), that is after taking the continuous limit of stochastic increments building  $\mathcal{R}_{\mathcal{T}}$ , we seek to handle it before taking the continuous limit. For this purpose, a finite-size time interval  $\delta s$  is introduced, during which neither an initial value nor a boundary value are encountered by the main path. The corresponding stochastic increment is  $\delta\mathcal{R}_o = \mathbb{E}_{\mathcal{V}}[\mathcal{V}|\mathcal{R}_o, 0] \delta s + \sqrt{2D}\delta\mathcal{W}_o$ . We can then write  $\eta(\mathbf{r}, t) = \mathbb{E}_{\mathcal{R}_s}[\mathcal{F}(\mathcal{R}_o + \delta\mathcal{R}_o, t - \delta s)|\mathcal{R}_o = \mathbf{r}]$  by substituting  $\eta_{IBV}$  with  $\eta$  itself into the stochastic functional  $\mathcal{F}$ . When  $\delta s$  approaches zero, the leading terms are linear with respect to  $\delta\mathcal{R}_o$  (see End Matter B), hence  $\mathcal{F}$  can be treated as a linear functional between  $\mathcal{R}_o = \mathbf{r}$  and  $\mathcal{R}_o + \delta\mathcal{R}_o$ . Thus, the linearity property of the expectation operator  $\mathbb{E}[\mathcal{F}(\mathbb{E}[\cdot])] = \mathbb{E}[\mathcal{F}(\cdot)]$  leads us to

$$\eta(\mathbf{r}, t) = \mathbb{E}_{\mathcal{R}_s, \mathcal{V}} \left[ \mathcal{F} \left( \begin{array}{c} \mathcal{R}_o \\ + (\mathcal{V}|\mathcal{R}_o, 0) \delta s, t - \delta s \\ + \sqrt{2D}\delta\mathcal{W}_o \end{array} \right) \right] \quad (9)$$

We can therefore define an embedded increment  $\delta\tilde{\mathcal{R}}_o = (\mathcal{V}|\tilde{\mathcal{R}}_o, 0)\delta s + \sqrt{2D}\delta\mathcal{W}_o$  such that  $\eta(\mathbf{r}, t) = \mathbb{E}_{\mathcal{R}_s}[\mathcal{F}(\tilde{\mathcal{R}}_o + \delta\tilde{\mathcal{R}}_o, t - \delta s)|\tilde{\mathcal{R}}_o = \mathbf{r}]$ . Then the whole  $\eta$ -path can be recursively constructed before taking the continuous limit as  $\delta s \rightarrow 0$ , thus defining the proper Itô integral  $\tilde{\mathcal{R}}_{\mathcal{T}}$  (see End Matter B) and making  $\{\tilde{\mathcal{R}}_s\}_s$  an embedded continuous process. Thus the Feynman-Kac path-space representation of  $\eta$  coupled to a model of the drift velocity now reads as in (8).

Therefore, the similitude is strict between  $\eta$ -paths re-

sulting from the McKean process (7) - drifting along the expectation - and our embedded CBSP (8) - drifting along the velocity associated with a single  $\mathcal{V}$ -path - as illustrated by the blue path in Fig. 2, and in accordance with Fig. 1 b). This equivalence enables us to provide profound physical insights into non-linear physics. Such physical insights benefit from propagative pictures that have been a major and powerful breakthrough for reactive non-linearities.

*d. Can we also expect benefits in numerical terms?*  
We implemented (8) using Monte Carlo Maruyama path sampling in confined and complex geometries without any need for additional numerical work. As mentioned with Fig. 1 b), one could predict the numerical impracticability of such representations because of limit inversions occurring when discretizing. However, we were able to prove the well-foundedness of such an implementation. Indeed, collaborating with photoconversion engineering communities working on solar fuels production using artificial photosynthesis, we put this representation to the test in Fig. 3 with the concrete problem of estimating electron concentration at a given location inside a porous photo-anode. Interactions with the computer graphics community have allowed us to advance a numerical implementation which not only behaves well, but also takes advantage of the most advanced techniques handling complexity [56–58], and is thus of major interest for computational physicists communities. A noteworthy aspect is that computation times are insensitive to the refinement in the geometric description of the system.

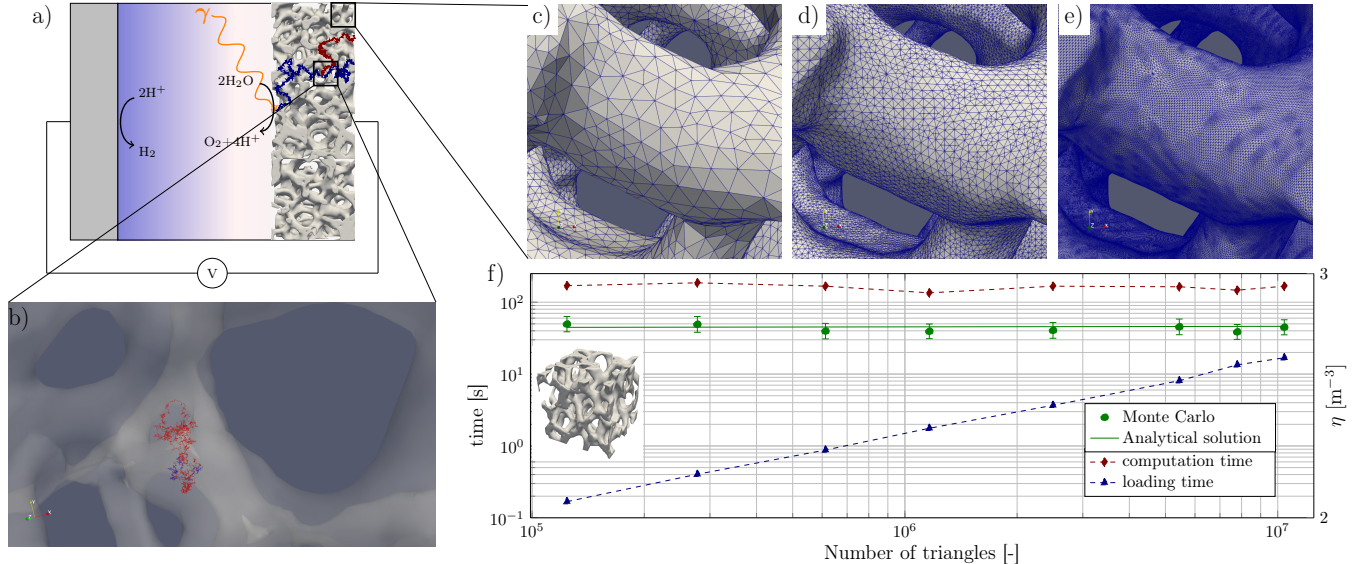


FIG. 3. a) Photocatalytic water splitting device involving charge carrier drift-diffusion transport. Sampled paths: main path in blue, velocity sub-path in red. b) Zoom of the porous photoanode. c-e) Three different levels of refinement (*i.e.* number of triangles) in the geometric description of the porous semiconducting crystal composing the photoanode, whose morphology is a key issue in attaining optimal efficiency. f) (green/right y-axis) Maruyama Monte-Carlo estimation using our Embedded CBSP, compared to the analytical solution (see End Matter C). (red) Computation time. (blue) Geometry loading time.

*e. Conclusions and perspectives* In the present letter, a generic theoretical framework dedicated to the probabilistic representation of drift-diffusion transport equations coupled to a sub-model of the drift velocity was proposed for confined domains. This coupling, being of prime interest for both applicative and theoretical communities, results in a non-linearity class. A single embedded CBSP was constructed, enabling such a representation in a single branching path-space and giving access to renewed physical insights in terms of propagative pictures for non-linear physics such as Navier-Stokes, Keller-Segel and Poisson-Nernst-Planck. Finally, we performed the numerical implementation in both confined and complex geometries.

Therefore, we believe that our formal extension of the Feynman-Kac framework opens a series of new research avenues. To begin with, it would be interesting to apply this proposition to models in which the sub-model of the drift velocity is not explicit as in (1) and (2), but concerns directional derivatives of a diffusive observable such as an electrical/gravitational potential or a stream potential (e.g.  $\mathbf{E} = -\nabla\Phi$  or  $\mathbf{v} = \nabla \times \Psi$ ) in confined geometries, avoiding any use of Malliavin stochastic calculus. Then, even if no conceptual progress is to be expected, it would certainly be useful to apply our approach to other appli-

cations such fluidics, for instance. It would also be useful to compare various path-sampling strategies and to examine their behavior when the regime tends towards pure advection. In this regard, it would be useful to explore how to handle such - by now allowed - coupling through other numerical schemes using first passage distributions of stochastic processes instead of Maruyama discretization, in order to produce unbiased estimators, even in the case of non-Dirichlet boundary conditions [59, 60]. Finally, the extension of our branching tree representations to velocity non-linearities such as in Navier-Stokes equations could lead to new insights for stochastic cascade descriptions of Kolmogorov turbulence, initially introduced and conjectured by Mandelbrot [61].

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- [1] Y. Nyffenegger-Péré, R. Armante, M. Bati, S. Blanco, J.-L. Dufresne, M. E. Hafi, V. Eymet, V. Forest, R. Fournier, J. Gautrais, R. Lebrun, N. Melado, N. Mourta day, and M. Paulin, Spectrally refined unbiased monte carlo estimate of the earth's global radiative cooling, *Proceedings of the National Academy of Sciences* **121**, e2315492121 (2024), <https://www.pnas.org/doi/pdf/10.1073/pnas.2315492121>.
  - [2] G. Terrée, M. El Hafi, S. Blanco, R. Fournier, J. Dauchet, and J. Gautrais, Addressing the gas kinetics boltzmann equation with branching-path statistics, *Phys. Rev. E* **105**, 025305 (2022).
  - [3] M. Kac, Foundations of kinetic theory, in *Volume 3 Proceedings of the Third Berkeley Symposium on Mathematical Statistics and Probability, Volume III*, edited by J. Neyman (University of California Press, Berkeley, 1956) pp. 173–200.
  - [4] H. McKean, A class of markov processes associated with nonlinear parabolic equations, *Proceedings of the National Academy of Sciences of the United States of America* **56**, 1907 (1966).
  - [5] H. McKean, An exponential formula for solving boltzmann's equation for a maxwellian gas, *Journal of Combinatorial Theory* **2**, 358 (1967).
  - [6] A. V. Skorokhod, Branching diffusion processes, *Theory of Probability & Its Applications* **9**, 445 (1964), <https://doi.org/10.1137/1109059>.
  - [7] H. P. McKean, Application of brownian motion to the equation of kolmogorov-petrovskii-piskunov, *Communications on Pure and Applied Mathematics* **28**, 323 (1975), <https://onlinelibrary.wiley.com/doi/pdf/10.1002/cpa.3160280302>.
  - [8] S. Ermakov, V. Nekrutkin, and A. Sipin, *Random Processes for Classical Equations of Mathematical Physics* (Springer Dordrecht, 1989).
  - [9] I. T. Dimov and T. V. Gurov, Monte Carlo algorithm for solving integral equations with polynomial non-linearity. Parallel implementation, *Pliska Studia Mathematica Bulgarica* **13**, 117 (2000).
  - [10] P. H. Chavanis, On the analogy between two-dimensional vortices and stellar systems, in *IUTAM Symposium on Geometry and Statistics of Turbulence*, edited by T. Kambe, T. Nakano, and T. Miyauchi (Springer Netherlands, Dordrecht, 2001) pp. 47–53.
  - [11] E. F. Keller and L. A. Segel, Initiation of slime mold aggregation viewed as an instability, *Journal of Theoretical Biology* **26**, 399 (1970).
  - [12] W. Jager and S. Luckhaus, On explosions of solutions to a system of partial differential equations modelling chemotaxis, *Transactions of the American Mathematical Society* **329**, 819 (1992).
  - [13] A. Solbrå, A. W. Bergersen, J. van den Brink, A. Malthe-Sørensen, G. T. Einevoll, and G. Hanes, A kirchhoff-nernst-planck framework for modeling large scale extracellular electrodiffusion surrounding morphologically detailed neurons, *PLOS Computational Biology* **14**, 1 (2018).
  - [14] M. Léonetti and E. Dubois-Violette, Theory of electrodynamic instabilities in biological cells, *Physical Review Letters* **81**, 1977 (1998).
  - [15] N. A. Dmitriev, Branching random processes, in *Selected Works of A. N. Kolmogorov: Volume II Probabil-*

- ity Theory and Mathematical Statistics*, edited by A. N. Shiryaev (Springer Netherlands, Dordrecht, 1992) pp. 309–314.
- [16] I. Bienaymé, De la loi de multiplication et de la durée des familles, *L'institut*, 131 (1845).
- [17] H. W. Watson and F. Galton, On the probability of the extinction of families, *The Journal of the Anthropological Institute of Great Britain and Ireland* **4**, 138 (1875).
- [18] W. Feller, Diffusion processes in genetics, *Second Berkeley Symp. Math. Stat. Prob.*, 227 (1951).
- [19] N. Ikeda, M. Nagasawa, and S. Watanabe, On branching markov processes (1965).
- [20] D. Dawson, Geostochastic calculus, *Canadian Journal of Statistics* **6**, 143 (1978), <https://onlinelibrary.wiley.com/doi/pdf/10.2307/3315044>.
- [21] M. Jiřina, Stochastic branching processes with continuous state space, *Czechoslovak Mathematical Journal* **08**, 292 (1958).
- [22] J. Lamperti, The Limit of a Sequence of Branching Processes, *Zeitschrift für Wahrscheinlichkeitstheorie und Verwandte Gebiete* **7**, 271 (1967).
- [23] A. Kolmogorov, I. Petrovskii, and N. Piscunov, A study of the equation of diffusion with increase in the quantity of matter, and its application to a biological problem, *Byul. Moskovskogo Gos. Univ.* **1**, 1 (1937).
- [24] R. A. FISHER, The wave of advance of advantageous genes, *Annals of Eugenics* **7**, 355 (1937), <https://onlinelibrary.wiley.com/doi/pdf/10.1111/j.1469-1809.1937.tb02153.x>.
- [25] P. Henry-Labordère, N. Oudjane, X. Tan, N. Touzi, and X. Warin, Branching diffusion representation of semilinear PDEs and Monte Carlo approximation, *Annales de l'Institut Henri Poincaré, Probabilités et Statistiques* **55**, 184 (2019).
- [26] J. Y. Nguwi, G. Penent, and N. Privault, *A fully non-linear feynman-kac formula with derivatives of arbitrary orders* (2023).
- [27] B. Busnello, A probabilistic approach to the two-dimensional navier-stokes equations, *The Annals of Probability* **27**, 1750 (1999).
- [28] E. Fournié, J.-M. Lasry, J. Lebuchoux, P.-L. Lions, and N. Touzi, Applications of Malliavin calculus to Monte Carlo methods in finance, *Finance and Stochastics* **3**, 391 (1999).
- [29] P. Warren and R. Allen, Malliavin weight sampling for computing sensitivity coefficients in brownian dynamics simulations, *Phys. Rev. Lett.* **109**, 250601 (2012).
- [30] R. N. Bhattacharya, L. Chen, S. Dobson, R. B. Guenther, C. Orum, M. Ossiander, E. Thomann, and E. C. Waymire, Majorizing kernels and stochastic cascades with applications to incompressible navier-stokes equations, *Transactions of the American Mathematical Society* **355**, 5003 (2003).
- [31] M. Ossiander, A probabilistic representation of solutions of the incompressible Navier-Stokes equations in  $\mathbb{R}^3$ , *Probability Theory and Related Fields* **133**, 267 (2005).
- [32] Y. Le Jan and A. S. Sznitman, Stochastic cascades and 3-dimensional Navier-Stokes equations, *Probability Theory and Related Fields* **109**, 343 (1997).
- [33] J. A. Acebrón and Ángel Rodríguez-Rozas, Highly efficient numerical algorithm based on random trees for accelerating parallel vlasov–poisson simulations, *Journal of Computational Physics* **250**, 224 (2013).
- [34] E. Floriani, R. Lima, and R. Vilela Mendes, Erratum: Poisson-Vlasov: Stochastic representation and numerical codes (*European Physical Journal D*), *European Physical Journal D* **46**, 407 (2008).
- [35] H. P. McKean, A class of markov processes associated with nonlinear parabolic equations, *Proceedings of the National Academy of Sciences of the United States of America* **56**, 1907 (1966).
- [36] L. Izydorczyk, N. Oudjane, and F. Russo, Mckean feynman-kac probabilistic representations of non-linear partial differential equations, *Geometry and Invariance in Stochastic Dynamics*. Eds. S. Ugolini et al. **378**, 187 (2021).
- [37] D. Talay and M. Tomašević, A new McKean-Vlasov stochastic interpretation of the parabolic-parabolic Keller-Segel model: The one-dimensional case, *Bernoulli* **26**, 1323 (2020), [arXiv:1712.10254](https://arxiv.org/abs/1712.10254).
- [38] P. Calderoni and M. Pulvirenti, Propagation of chaos for burgerséquation, *Annales de l'I.H.P. Physique théorique* **39**, 85 (1983).
- [39] A. Lejay and H. Mardones González, A forward-backward probabilistic algorithm for the incompressible navier-stokes equations, *Journal of Computational Physics* **420**, 109689 (2020).
- [40] D. Rioux-Lavoie, R. Sugimoto, T. Özdemir, N. H. Shimada, C. Batty, D. Nowrouzezahrai, and T. Hachisuka, A monte carlo method for fluid simulation, *ACM Trans. Graph.* **41**, 10.1145/3550454.3555450 (2022).
- [41] R. Sugimoto, C. Batty, and T. Hachisuka, Velocity-based monte carlo fluids, in *ACM SIGGRAPH 2024 Conference Papers*, SIGGRAPH '24 (Association for Computing Machinery, New York, NY, USA, 2024).
- [42] M. Tomasevic, *On a probabilistic interpretation of the Keller-Segel parabolic-parabolic equations*, *Theses*, COMUE Université Côte d'Azur (2015 - 2019) (2018).
- [43] E. Woillez, Y. Zhao, Y. Kafri, V. Lecomte, and J. Tailleur, Activated escape of a self-propelled particle from a metastable state, *Phys. Rev. Lett.* **122**, 258001 (2019).
- [44] S. Kakutani, Two-dimensional Brownian motion and harmonic functions, *Proceedings of the Imperial Academy* **20**, 706 (1944).
- [45] S. Kakutani, Markoff process and the Dirichlet problem, *Proceedings of the Japan Academy* **21**, 227 (1945).
- [46] M. Kac, Random walk and the theory of brownian motion, *American Mathematical Monthly* **54**, 369 (1947).
- [47] R. P. Feynman, Space-time approach to non-relativistic quantum mechanics, *Rev. Mod. Phys.* **20**, 367 (1948).
- [48] M. Kac, On distributions of certain wiener functionals, *Transactions of the American Mathematical Society* **65**, 1 (1949).
- [49] M. Kac, On some connections between probability theory and differential and integral equations, *Proceedings of the Second Berkeley Symposium on Mathematical Statistics and Probability*, 189 (1951).
- [50] I. Karatzas and S. E. Shreve, *Brownian Motion and Stochastic Calculus*, Graduate Texts in Mathematics, Vol. 113 (Springer New York, New York, NY, 1998).
- [51] K. Itô, Stochastic integral, *Proceedings of the Japan Academy, Series A, Mathematical Sciences* **20**, 45 (1944).
- [52] L. Onsager and S. Machlup, Fluctuations and irreversible processes, *Phys. Rev.* **91**, 1505 (1953).
- [53] M. Freidlin, *Functional Integration and Partial Differ-*

*ential Equations. (AM-109)* (Princeton University Press, 1985).

- [54] N. Wiener, The average of an analytic functional, *Proceedings of the National Academy of Sciences of the United States of America* **7**, 253 (1921).
- [55] J. M. Tregan, J. L. Amestoy, M. Bati, J.-J. Beziau, S. Blanco, L. Brunel, C. Caliot, J. Charon, J.-F. Cornet, C. Coustet, L. d'Alençon, J. Dauchet, S. Dutoir, S. Eibner, M. El Hafi, V. Eymet, O. Farges, V. Forest, R. Fournier, M. Galtier, V. Gattepaille, J. Gautrais, Z. He, F. Hourdin, L. Ibarrart, J.-L. Joly, P. Lapeyre, P. Lavieille, M.-H. Lecureux, J. Lluc, M. Miscevic, N. Mourtaday, Y. Nyffenegger-Péré, L. Pelissier, L. Penazzi, B. Piaud, C. Rodrigues-Viguier, G. Roques, M. Roger, T. Saez, G. Terrée, N. Villefranque, T. Vourc'h, and D. Yaacoub, Coupling radiative, conductive and convective heat-transfers in a single monte carlo algorithm: A general theoretical framework for linear situations, *PLOS ONE* **18**, 1 (2023).
- [56] N. Villefranque, F. Hourdin, L. d'Alençon, S. Blanco, O. Boucher, C. Caliot, C. Coustet, J. Dauchet, M. E. Hafi, V. Eymet, O. Farges, V. Forest, R. Fournier, J. Gautrais, V. Masson, B. Piaud, and R. Schoetter, The “teapot in a city”: A paradigm shift in urban climate modeling, *Science Advances* **8**, eabp8934 (2022), <https://www.science.org/doi/pdf/10.1126/sciadv.abp8934>.
- [57] R. Sawhney, D. Seyb, W. Jarosz, and K. Crane, Grid-free monte carlo for pdes with spatially varying coefficients, *ACM Trans. Graph.* **41**, 10.1145/3528223.3530134 (2022).
- [58] R. Sawhney and K. Crane, Monte carlo geometry processing: a grid-free approach to pde-based methods on volumetric domains, *ACM Trans. Graph.* **39**, 10.1145/3386569.3392374 (2020).
- [59] R. Sawhney, D. Seyb, W. Jarosz, and K. Crane, Walk on stars: A grid-free monte carlo method for pdes with neumann boundary conditions, *ACM Trans. Graph.* (2023).
- [60] B. Miller, R. Sawhney, K. Crane, and I. Gkioulekas, Walkin' robin: Walk on stars with robin boundary conditions, *ACM Trans. Graph.* **43**, 10.1145/3658153 (2024).
- [61] B. Mandelbrot, Intermittent turbulence in self-similar cascades: divergence of high moments and dimension of the carrier, *Journal of Fluid Mechanics* **62**, 331–358 (1974).

## Appendix A: Statistics for Fig. 1

*a. The problem.* Random drift  $\mathbf{V}$  is defined as  $\mathbf{V} = \|\mathbf{v}\|(-1, (1 - 2\mathcal{B}(1/2))\tan(\theta))^\dagger$ , where  $\mathcal{B}(1/2)$  is the Bernoulli variable of probability 1/2.  $\mathbf{V}$  outcomes are  $\mathbf{V}_+ = \|\mathbf{v}\|(-1, \tan(\theta))^\dagger$  or  $\mathbf{V}_- = (-1, -\tan(\theta))^\dagger$  with equal probability, and its expectation  $\mathbb{E}_{\mathbf{V}}[\mathbf{V}] = \|\mathbf{v}\|(-1, 0)^\dagger$  is equal to  $\mathbf{v}$ .

Starting from  $\mathbf{r} := (l, y)^\dagger$ , the first hitting locations of the purely advective stochastic embedded process  $\{\tilde{\mathcal{R}}_s\}_s$  to the left-sided boundary wall are given by

$$\tilde{\mathcal{R}}_{N\delta s} = \mathbf{r} + \sum_{i \in [0; N-1]} \mathbf{v}_i \delta s$$

with  $N := l/(\|\mathbf{v}\|\delta s)$ . Its horizontal component is null by

construction:  $\tilde{\mathcal{X}}_{N\delta s} = l - N\|\mathbf{v}\|\delta s = 0$ . Thus, only first passage heights  $\tilde{\mathcal{Y}}_{N\delta s}$  are distributed and their realizations can take values within the lattice  $\mathbb{Z}\|\mathbf{v}\|\delta s \tan(\theta) := \{k\|\mathbf{v}\|\delta s \tan(\theta) | k \in \mathbb{Z}\}$ .

*b. Distribution of first passage heights.* As the result of successive Bernoulli trials, the first passage height distribution follows the binomial law

$$\mathbb{P}\{\tilde{\mathcal{Y}}_{N\delta s} = y + k \|\mathbf{v}\|\delta s \tan(\theta)\} = \binom{N}{\frac{N-k}{2}} \left(\frac{1}{2}\right)^N$$

When  $N \rightarrow \infty$ , that is  $\delta s \rightarrow 0$ ; this discrete probability law behaves as the gaussian distribution

$$d\mathbb{P}\{\tilde{\mathcal{Y}}_{l/\|\mathbf{v}\|\delta s} = \tilde{y}_{\partial\Omega}\}_{\delta s \rightarrow 0} = \frac{\exp\left\{\frac{-(\tilde{y}_{\partial\Omega} - y)^2}{2l\|\mathbf{v}\|\delta s \tan^2(\theta)}\right\}}{\sqrt{2\pi l\|\mathbf{v}\|\delta s \tan^2(\theta)}} d\tilde{y}_{\partial\Omega}$$

with mean  $\mathbb{E}\left[\tilde{\mathcal{Y}}_{l/\|\mathbf{v}\|\delta s}\right] = y$  and variance  $\mathbb{V}\left[\tilde{\mathcal{Y}}_{l/\|\mathbf{v}\|\delta s}\right] = l\|\mathbf{v}\|\delta s \tan^2(\theta)$ . The variance vanishes as  $\delta s \rightarrow 0$ .

*c. Unbiased Feynman-Kac representation.* In the situation depicted in Fig. 1 the exact analytical solution of  $\eta$  is  $\eta(l, y) = \eta^{\partial\Omega}(y) = \mathbb{1}_{\{y > -\varepsilon\}}\eta_+ + \mathbb{1}_{\{y \leq -\varepsilon\}}\eta_-$ . As  $\delta s \rightarrow 0$ , the embedded process  $\{\tilde{\mathcal{R}}_s\}_s$  becomes a continuous branching stochastic process allowing us to write the strict probabilistic representation

$$\eta(\mathbf{r}) = \mathbb{E}_{\tilde{\mathcal{R}}_s} \left[ \eta^{\partial\Omega}(\tilde{\mathcal{R}}_{\mathcal{T}_{\partial\Omega}}) \mid \tilde{\mathcal{R}}_0 = \mathbf{r} \right]$$

Indeed,

$$\begin{aligned} & \lim_{\delta s \rightarrow 0} \mathbb{E}_{\tilde{\mathcal{Y}}_{l/\|\mathbf{v}\|\delta s}} \left[ \mathbb{1}_{\{\tilde{\mathcal{Y}}_{l/\|\mathbf{v}\|\delta s} > -\varepsilon\}}\eta_+ + \mathbb{1}_{\{\tilde{\mathcal{Y}}_{l/\|\mathbf{v}\|\delta s} \leq -\varepsilon\}}\eta_- \right] \\ &= \int_{\mathbb{R}} \lim_{\delta s \rightarrow 0} d\mathbb{P}\{\tilde{\mathcal{Y}}_{l/\|\mathbf{v}\|\delta s}\} \times \\ & \quad \left[ \mathbb{1}_{\{\tilde{\mathcal{Y}}_{l/\|\mathbf{v}\|\delta s} > -\varepsilon\}}\eta_+ + \mathbb{1}_{\{\tilde{\mathcal{Y}}_{l/\|\mathbf{v}\|\delta s} \leq -\varepsilon\}}\eta_- \right] \\ &= \int_{\mathbb{R}} \delta(\tilde{y}_{\partial\Omega} - y) d\tilde{y}_{\partial\Omega} \left[ \mathbb{1}_{\{\tilde{y}_{\partial\Omega} > -\varepsilon\}}\eta_+ + \mathbb{1}_{\{\tilde{y}_{\partial\Omega} \leq -\varepsilon\}}\eta_- \right] \\ &= \mathbb{1}_{\{y > -\varepsilon\}}\eta_+ + \mathbb{1}_{\{y \leq -\varepsilon\}}\eta_- \equiv \eta(\mathbf{r}) \end{aligned}$$

and

$$\begin{aligned} & \lim_{\delta s \rightarrow 0} \mathbb{V}_{\tilde{\mathcal{Y}}_{l/\|\mathbf{v}\|\delta s}} \left[ \mathbb{1}_{\{\tilde{\mathcal{Y}}_{l/\|\mathbf{v}\|\delta s} > -\varepsilon\}}\eta_+ + \mathbb{1}_{\{\tilde{\mathcal{Y}}_{l/\|\mathbf{v}\|\delta s} \leq -\varepsilon\}}\eta_- \right] \\ &= \int_{\mathbb{R}} \left[ \mathbb{1}_{\{\tilde{y}_{\partial\Omega} > -\varepsilon\}}\eta_+ + \mathbb{1}_{\{\tilde{y}_{\partial\Omega} \leq -\varepsilon\}}\eta_- \right]^2 \delta(\tilde{y}_{\partial\Omega} - y) d\tilde{y}_{\partial\Omega} \\ & \quad - \left( \int_{\mathbb{R}} \left[ \mathbb{1}_{\{\tilde{y}_{\partial\Omega} > -\varepsilon\}}\eta_+ + \mathbb{1}_{\{\tilde{y}_{\partial\Omega} \leq -\varepsilon\}}\eta_- \right] \delta(\tilde{y}_{\partial\Omega} - y) d\tilde{y}_{\partial\Omega} \right)^2 \\ &= \eta^2(\mathbf{r}) - \eta^2(\mathbf{r}) = 0 \end{aligned}$$

where  $\delta(\cdot)$  is the delta Dirac distribution.

## Appendix B: Itô integral representation

*a. Canonical/McKean framework.* Knowing the drift field  $\mathbf{v}$ ,  $\{\mathcal{R}_s\}_s$  is a stochastic process such that



$\mathcal{R}_T$  appearing in Feynman-Kac representations (4) and (7) is constructed as the continuous limit of the sum of stochastic increments

$$\mathcal{R}_{N\delta s} = \mathcal{R}_o + \sum_{i \in \llbracket 0; N-1 \rrbracket} \delta \mathcal{R}_{i\delta s} \quad (\text{B1})$$

Defining  $N$  such that  $T = N\delta s$  and providing us with a regular subdivision  $\{i\delta s | i \in \llbracket 0; N-1 \rrbracket\}$  of  $[0; T]$ , these increments write

$$\delta \mathcal{R}_{i\delta s} = \mathcal{R}_{(i+1)\delta s} - \mathcal{R}_{i\delta s} = \mathbf{v}(\mathcal{R}_{i\delta s}, i\delta s)\delta s + \sqrt{2D}\delta \mathbf{W}_{i\delta s}$$

The fundamental Wiener increment  $\delta \mathbf{W}_{i\delta s}$  is a gaussian vector with mean  $\mathbb{E}[\delta \mathbf{W}_{i\delta s}] = \mathbf{0}$  and variance  $\mathbb{V}[\delta \mathbf{W}_{i\delta s}] = 2D\delta s\delta_{m,n}$  ( $(m, n)$  standing for component labels). The continuous limit is obtained when  $N \rightarrow \infty$ , that is  $\delta s \rightarrow 0$ , and has to be understood as convergence in probability (rather than almost-surely). Thus (B1) becomes the following Itô stochastic integral

$$\mathcal{R}_T = \mathcal{R}_o + \int_0^T ds \mathbf{v}(\mathcal{R}_s, s) ds + \sqrt{2D} \int_0^T d\mathbf{W}_s \quad (\text{B2})$$

This construction is the same when the drift velocity  $\mathbf{v}$  is itself obtained from a sub-model, that is  $\mathbf{v}(\mathbf{r}, t) = \mathbb{E}_{\mathcal{V}}[\mathcal{V}|\mathbf{r}, t]$ , as in the inlaid McKean picture. Such an Itô integral (B2) may be represented as the stochastic differential equation (6).

*b. Coupled framework.* Treating the reactive term  $-k(\eta - \eta^*)$  is (3) as a volume source along main paths, in the same vein as for KPP representations, and the Feynman-Kac representation (4) becomes a second kind Fredholm equation in which the stochastic functional is

$$\begin{aligned} \mathcal{F}(\mathcal{R}_T, t - T) &= \eta_{\text{IBV}}(\mathcal{R}_T, t - T) \\ &+ \int_0^T ds k(\mathcal{R}_s) (\eta^*(\mathcal{R}_s, t - s) - \eta(\mathcal{R}_s, t - s)) \end{aligned} \quad (\text{B3})$$

Between  $\mathcal{R}_o$  and the first stochastic increment  $\delta \mathcal{R}_o = \mathbb{E}_{\mathcal{V}}[\mathcal{V}|\mathcal{R}_o, 0] \delta s + \sqrt{2D}\delta \mathbf{W}_o$ , this functional leads us to

$$\begin{aligned} \mathcal{F}(\mathcal{R}_o + \delta \mathcal{R}_o, t - \delta s) &= \eta(\mathcal{R}_o + \delta \mathcal{R}_o, t - \delta s) \\ &+ \delta s k(\mathcal{R}_o) (\eta^*(\mathcal{R}_o, t) - \eta(\mathcal{R}_o, t)) \end{aligned} \quad (\text{B4})$$

where  $\eta_{\text{IBV}}$  has been substituted by  $\eta$  itself since neither an initial value nor a boundary value are encountered during  $\delta s$ . The last term in (B4) is totally independent of  $\delta \mathcal{R}_o$ . Concerning the term  $\eta(\mathcal{R}_o + \delta \mathcal{R}_o, t - \delta s)$ , second-order expansion around  $\mathcal{R}_o$  (as  $\delta s$  approaches zero)

$$\begin{aligned} \eta(\mathcal{R}_o + \delta \mathcal{R}_o, t - \delta s) &= \eta(\mathcal{R}_o, t) + \delta \mathcal{R}_o \cdot \nabla \eta(\mathcal{R}_o, t) \\ &- \delta s \partial_t \eta(\mathcal{R}_o, t) + \frac{1}{2} \delta \mathcal{R}_o^\dagger \text{Hess}[\eta](\mathcal{R}_o, t) \delta \mathcal{R}_o + \dots \end{aligned}$$

is required in accordance with Itô stochastic calculus. Indeed

$$\frac{1}{2} \delta \mathcal{R}_o^\dagger \text{Hess}[\eta](\mathcal{R}_o, t) \delta \mathcal{R}_o = \delta s D \nabla^2 \eta(\mathcal{R}_o, t) + \dots$$

and higher-order terms are of the order  $\mathcal{O}(\delta s \|\delta \mathbf{W}_o\|)$ ,  $\mathcal{O}(\delta s^2)$ . Thus we can establish that leading terms in  $\eta$  are at most linear with respect to the stochastic increment  $\delta \mathcal{R}_o$ . Hence,  $\mathcal{F}$  is a linear functional of  $\delta \mathcal{R}_o$  as  $\delta s$  vanishes. According to the above definition of  $\delta \mathcal{R}_o$ ,  $\mathcal{F}$  is also linear with respect to  $\mathbb{E}_{\mathcal{V}}[\mathcal{V}|\mathcal{R}_o, 0]$ , enabling us to commute  $\mathcal{F}(\cdot)$  and  $\mathbb{E}_{\mathcal{V}}[\cdot]$  in (9) and to define the embedded increment  $\delta \tilde{\mathcal{R}}_o$ .

For the next increment, *i.e.* between  $\mathcal{R}_{\delta s}$  and  $\mathcal{R}_{\delta s} + \delta \mathcal{R}_{\delta s}$ , the stochastic functional is

$$\begin{aligned} \mathcal{F}(\mathcal{R}_{\delta s} + \delta \mathcal{R}_{\delta s}, t - 2\delta s) &= \eta(\mathcal{R}_{\delta s} + \delta \mathcal{R}_{\delta s}, t - 2\delta s) \\ &+ \delta s k(\mathcal{R}_o) (\eta^*(\mathcal{R}_o, t) - \eta(\mathcal{R}_o, t)) + \delta s k(\mathcal{R}_o + \delta \mathcal{R}_o) \\ &\times (\eta^*(\mathcal{R}_o + \delta \mathcal{R}_o, t - \delta s) - \eta(\mathcal{R}_o + \delta \mathcal{R}_o, t - \delta s)) \end{aligned}$$

Here too,  $\eta$  is linear with respect to  $\delta \mathcal{R}_{\delta s}$  and the leading order in the last terms  $\delta s k \eta^*$  and  $-\delta s k \eta$  is independent of  $\delta \mathcal{R}_{\delta s}$ . Hence,  $\mathcal{F}$  is linear with respect to  $\mathbb{E}_{\mathcal{V}}[\mathcal{V}|\mathcal{R}_o, 0]$ , allowing us to commute  $\mathcal{F}(\cdot)$  and  $\mathbb{E}_{\mathcal{V}}[\cdot]$  and to define the embedded increment  $\delta \tilde{\mathcal{R}}_{\delta s}$ . This construction then has to be repeated until a boundary/initial condition is encountered, after  $N$  steps. Then, as  $N \rightarrow \infty$ , that is  $\delta s \rightarrow 0$ , the sum  $\tilde{\mathcal{R}}_{N\delta s}$  of these embedded stochastic increments defines the following Itô integral

$$\tilde{\mathcal{R}}_T = \tilde{\mathcal{R}}_o + \int_0^T ds (\mathcal{V}|\tilde{\mathcal{R}}_s, s) ds + \sqrt{2D} \int_0^T d\mathbf{W}_s \quad (\text{B5})$$

which may be represented as the stochastic differential equation (8).

### Appendix C: Statistical estimation within Fig. 3

In Fig. 3, we solve the electron concentration  $c$  submitted to the stationary drift-diffusion transport  $0 = -\nabla \cdot (-D\nabla c(\mathbf{r}) - \mu \mathbf{E}(\mathbf{r})c(\mathbf{r}))$  coupled to Gauss equation  $\nabla \cdot \mathbf{E}(\mathbf{r}) = 0$  describing the electrostatic field in the solid. In order to compare statistical estimations to an analytic solution of the coupled confined system, the porous geometry is here embedded within a particular solution

$$\begin{cases} c^\infty(\mathbf{r}) = \sqrt{D/\mu} \left( \text{erf}\left(r_x \sqrt{\mu/2D}\right) + \text{erf}\left(r_y \sqrt{\mu/2D}\right) \right) \\ \quad + \sqrt{D/\mu} \text{erfi}\left(r_z \sqrt{\mu/D}\right) \\ \mathbf{E}^\infty(\mathbf{r}) = r_x \hat{\mathbf{x}} + r_y \hat{\mathbf{y}} - 2r_z \hat{\mathbf{z}} \end{cases}$$

of the free space coupled system

$$\begin{cases} 0 &= -\nabla \cdot (-\nabla c^\infty(\mathbf{r}) - \mu \mathbf{E}^\infty(\mathbf{r})c^\infty(\mathbf{r})) & ; \mathbf{r} \in \mathbb{R}^3 \\ \nabla \cdot \mathbf{E}^\infty(\mathbf{r}) = 0 & & ; \mathbf{r} \in \mathbb{R}^3 \end{cases}$$

In other words, boundary conditions are chosen to be  $c(\mathbf{r} \in \partial\Omega) = c^\infty(\mathbf{r})$  and  $\mathbf{E}(\mathbf{r} \in \partial\Omega) = \mathbf{E}^\infty(\mathbf{r})$  at the porous surface.

Maruyama-Monte-Carlo numerical estimation of the concentration  $c$  is evaluated at location  $(r_x = 1.05, r_y = 1.05, r_z = 0.9)$  within the porous semiconductor by sampling  $10^3$  main paths of  $c$  and considering

Maruyama-discretized stochastic paths ( $\delta s = 4.10^{-4}$  s,  $\mu = 1 \text{ m}^2 \cdot \text{V}^{-1} \cdot \text{s}^{-1}$  and  $D = 1 \text{ m}^2 \cdot \text{s}^{-1}$ ). Results are plot-

ted against the analytic solution for several geometric refinements (*i.e* increasing number of triangles describing the porous geometry).