Post-doctoral appointment at CEA/Paris-Saclay

TRANSPAREMS (Particle Transport in Stochastic Media with Memory Effects)

Short summary

In order to model the **transport of particles in multi-scale disordered media**, which often occur in several applications in nuclear engineering, two approaches are possible. The first is based on the generation of a very large number of random geometries, in order to estimate the averages of the quantities of interest. This "reference" approach requires extremely long calculation times. The second is based on the derivation of so-called “effective” transport equations, taking into account in a condensed way the effects of disorder during a single calculation. The reliability of these models, which are fast but approximate, must be established with respect to the reference solutions. In a previous project (GEOSTOH, 2021 – a collaboration between CEA/DES and CEA/DAM) we have been able to compute for the first time the "reference" solutions for the case of random media with spatial gradients, essential in the modeling of realistic disordered structures. The TRANSPAREMS project (Particle Transport in Stochastic Media with Memory Effects) aims at extending the advances of GEOSTOH by designing a new class of "effective" transport models. This project will involve **developing innovative Monte Carlo methods** to take into account simultaneously, within a single calculation, the spatial memory effects induced by the disorder on the trajectories of the particles as well as the presence of spatial gradients. The qualification of the predictive power of these “effective” models will be done in relation to the “reference” solutions.

To achieve these objectives, the TRANSPAREMS project will hire a 12-month (renewable) **post-doc at CEA/Paris-Saclay**, to start in **January 2023**. **Applications are now open**.

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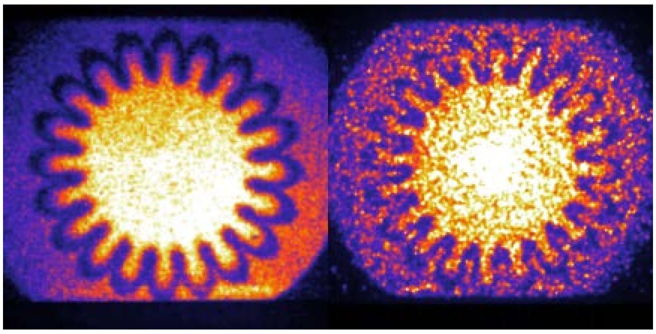
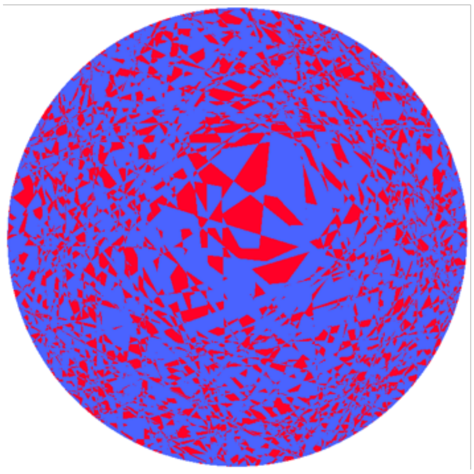


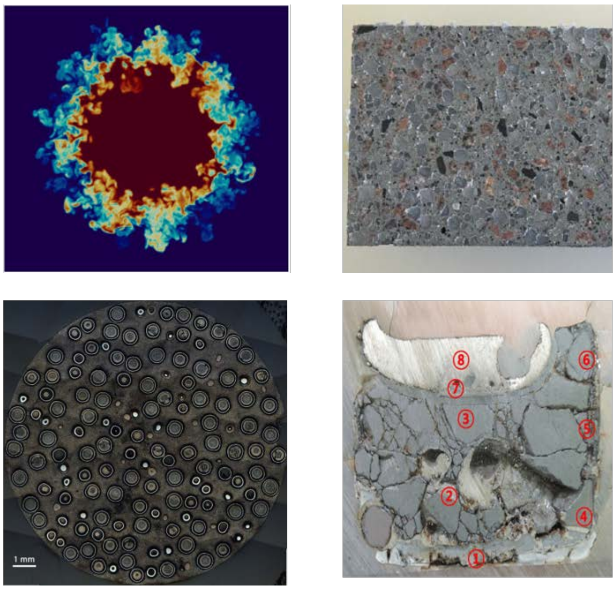
Example of random media encountered in applications: Rayleigh-Taylor instabilities in turbulent layers generated by inertial confinement fusion. The statistical disorder of the media is coupled with spatial gradients due to gravity-induced stratification effects. Figure taken from reference J. P. Sauppe et al., Phys. Rev. Lett. 124, 185003 (2020).



Modeling of a three-dimensional Markovian random geometry (here, two-dimensional cut) with spatial gradient, obtained by Poisson tessellation. Taken from reference [6].

Scientific project

Several applications emerging in nuclear science and engineering, such as the evaluation of the safety margins related to re-criticality accidents with fuel assemblies in a degraded configuration (uranium/moderator mixtures), or the study of the propagation of photons in turbulent layers for inertial confinement, require the modeling of particle transport in disordered multi-scale media (Fig. 1). In this context, the propagation of particles is often described using the theory of linear transport in stochastic media [1, 2], and two approaches to modeling are then possible.


Inertial confinement fusion (ICF) Rayleigh-Taylor instabilities at the interface between fuel and ablator.

Neutron shields Inclusions of polyethylene and Boron carbide in concrete.

TRISO Fuel UOX particle coated in SiC and dispersed in a graphite matrix.

Corium Re-solidified mixture of UOX, Zr and BC_4.

Figure 1. Examples of random media emerging in nuclear engineering applications.

The first approach is based on the generation of a large number of random geometries describing the medium through which the particles are transported, using a statistical model such as Poisson tessellations (Markovian media). For each geometric realization sampled from the model, the Boltzmann equation is then solved, typically by Monte Carlo methods, and the observables of interest for particle transport are calculated. Finally, we determine the distributions of the observables on all the realizations, in order to characterize the impact of the disorder of the environment on the physical properties of the transport (Fig. 2). This approach, in principle exact, yields so-called **"reference"** results [1], at the cost of extremely high computing times, demanding HPC resources for massively parallel simulations: parallelization with respect to random realizations of and parallelization with respect to particle transport in each realization [1, 3].

The second approach is based on the derivation of so-called **“effective”** transport equations, taking into account in a condensed way the effects of disorder during a single transport calculation (Fig. 2). In the context of Markovian stochastic media, a particularly well-known effective model is the Levermore-Pomraning system of equations, with its Monte Carlo counterpart called Chord Length Sampling (CLS) [1]. In CLS, the impact of spatial correlations induced by the disorder of the medium is partially reproduced by sampling on the fly random pseudo-interfaces between the different material components during the tracking of the trajectories of the particles. As the pseudo-interfaces are regenerated after each displacement of the particles in the medium, this treatment is not exact, in all generality. The reliability of these models, much faster to solve by simulation but approximate, must therefore be established on the basis of comparisons with the "reference" solutions [1, 4].

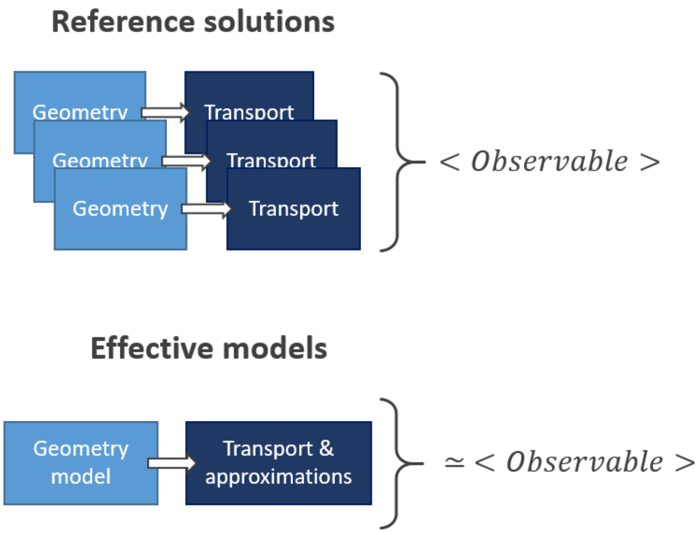


Figure 2. The two approaches to modeling random media. Top: “reference” solutions on a set of configurations. Bottom: “effective” models of condensed disorder.

Within the framework of the GEOSTOH project (2021), a scientific collaboration between CEA/DES and CEA/DAM has made it possible to achieve a major breakthrough in the "reference" approach for the case of Markovian random media. Based on the theory of stochastic Poisson tessellations, we were able to first establish a rigorous mathematical framework and then develop the simulation tools necessary to sample a set of three-dimensional Markovian media with spatial gradients. This allowed calculating for the first time “reference” solutions for this very important class of random media [5, 6]. Until now, for reasons of algorithmic complexity and computational cost, these simulations were almost exclusively limited to the dimension d=1 [7, 8]. Recent results have made it possible to access the dimension d=3 for the case of Markovian random media, subject to a hypothesis of spatial homogeneity (i.e., the characteristic scale of the disorder being the same at any point in space) [9]. In the GEOSTOH project, the homogeneity hypothesis was relaxed for three-dimensional media (Fig. 3): the ability to take into account non-homogeneous statistical properties, and in particular spatial gradients, turns out to be essential in the modeling of realistic disordered structures, such as the stratification of materials due to gravity or the complex interfaces of multiphase mixtures (Rayleigh-Taylor instabilities) [5, 6].

Figure 3. Example of a three-dimensional Markovian medium with spatial gradients (less dense in the center and denser on the periphery, following a linear radial gradient). Taken from reference [6].

In the TRANSPAREMS project, we propose to extend the advances of GEOSTOH to "effective" transport models: we will develop new Monte Carlo methods, inspired by the CLS type approach, in order to treat the effects disorder on the trajectories of the particles in a condensed way, within a single transport calculation.

In the case of spatially homogeneous Markovian media, the CLS method has recently been developed and tested in dimension d=3: its statistical properties and its predictive power have been characterized with respect to reference solutions [4]. In general, the CLS method shows deviations from the reference solutions, due to its inability to take into account spatial correlations. However, it has been shown that it is possible to significantly improve the precision of the CLS method by introducing spatial memory effects: instead of regenerating the material pseudo-interfaces each time the particles move, the particles will remember the position of the last interfaces crossed, and this during several consecutive movements [10]. Several models with memory have been proposed, including Poisson-Box Sampling (PBS) developed at CEA/DES, or Local Realization Preserving (LRP) developed at LLNL (United States). By increasing the number of interfaces that each particle remembers, the accuracy of these “effective” methods with spatial memory increases considerably (at the expense of computation time).

Initial attempts carried out within the framework of the GEOSTOH project have shown that the classical CLS method (without memory and spatially homogeneous) can be adapted in order to take into account spatially non-homogeneous media [6]. However, as for the homogeneous case, the preliminary comparisons between the CLS and the reference solutions reveal discrepancies that can be mainly attributed to the absence of memory in the processing of the effects of the disorder (Fig. 4).

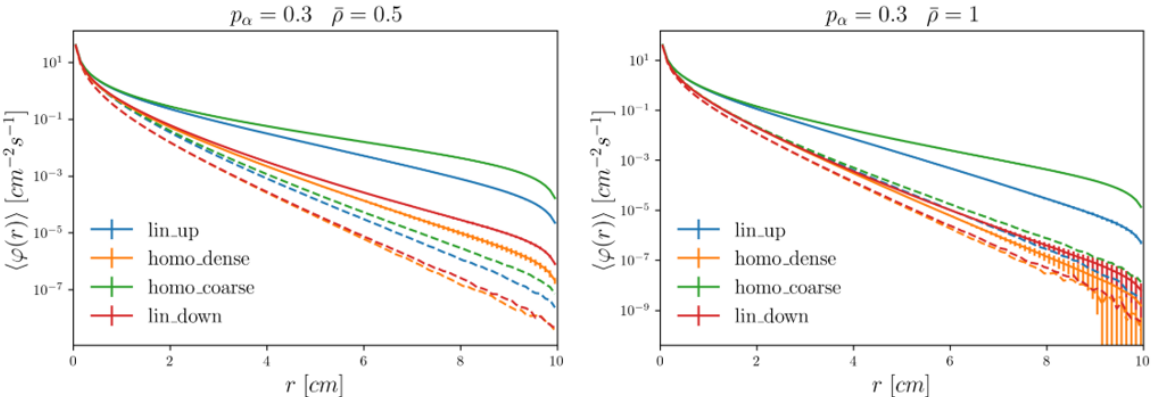


Figure 4. Comparison between “reference” solutions (solid lines) and “effective” CLS model without memory (dotted lines). The calculated observable is the flux of particles inside a sphere, in the direction of the radial gradient, for different types of gradients (linearly increasing and decreasing), two limiting homogeneous cases, and two material densities rho. Taken from reference [6].

In view of these results, the central idea of the TRANSPAREMS project is to generalize “effective” models of the PBS or LRP type (with memory) to the case of inhomogeneous Markovian media, with spatial gradients. This would allow having effective methods (condensed disorder) fast, offering more fidelity with respect to applications thanks to the possibility of taking into account the spatial heterogeneities, and with an increased precision thanks to the inclusion of the memory of the pseudo-interfaces material. Verification of the level of precision will be carried out using "reference" solutions, according to the approach deployed during the GEOSTOH project. This subject is very innovative and not explored in the literature.

The main scientific obstacles are both theoretical, concerning the derivation of transport algorithms that simultaneously take into account particle memory and spatial gradients, and computational, due to the HPC efforts required to perform the simulations.

The work plan will be as follows:

1 – Investigation of the state of the art concerning the “effective” models CLS, PBS and LRP, in particular in relation to random Markovian media. Familiarization with recent work carried out at CEA as part of the GEOSTOH project (modeling random media with spatial gradients): these results will constitute the starting point for the analysis of effective models with memory;

2 – Development of algorithms for “effective” models with memory and spatial heterogeneity in dimension d=3, by generalizing PBS and LRP type models. Preliminary comparisons of the results obtained by these new models with respect to the "reference" solutions, in a few simplified benchmark configurations;

3 – Porting of the developed models on the CEA computing clusters, so to perform massively parallel simulations for the “reference” solutions in realistic configurations and interpretation of the obtained results: comparison with the case of spatially homogeneous geometries and effective models without memory.

Contacts and applications

For the TRANSPAREMS project, CEA will hire a **post-doc for a period of 12 months (renewable)**. The post-doc will be hosted at the **CEA/Paris-Saclay center** (located south of Paris), and co-supervised between the CEA/DES and CEA/DAM research teams.

The tentative **starting date** for the post-doc is **January 2nd, 2023.**

Applications are now open: to apply, send an email to

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including your curriculum and a motivation letter.

References

[1] G. C. Pomraning, Linear Kinetic Theory and Particle Transport in Stochastic Mixtures, World Scientific, Singapore (1991).

[2] S. Torquato, Random Heterogeneous Materials: Microstructure and Macroscopic Properties, Springer-Verlag (2013).

[3] C. Larmier, F.-X. Hugot, F. Malvagi, A. Mazzolo, and A. Zoia, Benchmark solutions for transport in d-dimensional Markov binary mixtures, J. Quant. Spectrosc. Radiat. Transf. 189, 133–148 (2017).

[4] C. Larmier et al., Monte Carlo Chord Length Sampling for d-dimensional Markov binary mixtures, J. Quant. Spectrosc. Radiat. Transf. 204, 256-271 (2018).

[5] M. A. Kowalski, C. Larmier, F. Madiot, J. Durand, S. Lemaire, A. Zoia, Particle Transport in Markov Stochastic Mixtures with Spatial Gradients, in Proceedings of Physor22, Pittsburgh, PA, May 15-20 (2022).

[6] M. A. Kowalski, C. Larmier, F. Madiot, J. Durand, S. Lemaire, A. Zoia, Transport in Markov media with spatial gradients: comparison between reference solutions and Chord Length Sampling, J. Quant. Spectrosc. Radiat. Transf. 286, 108185 (2022).

[7] C. Deutsch, D. Vanderhaegen, Radiative transfer in statistically heterogeneous mixtures, J. Quant. Spectrosc. Radiat. Transf. 44, 163-169 (1990).

[8] P. Brantley at al., Verification of a Monte Carlo Levermore-Pomraning algorithm for spatially inhomogeneous binary stochastic media, in Proceedings of M&C2019, Portland, OR, August 25-29 (2019).

[9] C. Larmier, Stochastic particle transport in disordered media: beyond the Boltzmann equation, Thèse de doctorat de l'Université Paris-Saclay (2018).

[10] C. Larmier, A. Zoia, F. Malvagi, E. Dumonteil, A. Mazzolo, Poisson-Box Sampling algorithms for three-dimensional Markov binary mixtures, J. Quant. Spectrosc. Radiat. Transf. 206, 70–82 (2018).