Post-doc GEOSTOH : GEOmétries STOchastiques Hétérogènes

Short summary

The GEOSTOH project (Heterogeneous STOchastic GEOmetries) at ***CEA, Saclay center****, aims at implementing new numerical simulation tools allowing a more faithful description of* ***particle transport*** *in* ***disordered media*** *with* ***multi-scale heterogeneities*** *and* ***spatial gradients****. The targeted applications relate, for example, to radiative transfer in turbulent mixtures or re-criticality risk in fissile systems. The geometric structure of these media can be described using* ***random tessellations*** *stemming from various probabilistic models. Until now, for reasons of algorithmic complexity and computational cost, the simulations were almost exclusively limited to the dimension d = 1, with an assumption of spatial homogeneity (the characteristic scale of the disorder being the same at all points of space). Recent works have made it possible to access the dimension d = 3. In this project, we propose to relax the homogeneity hypothesis and investigate the impact of spatial gradients on particle transport in random media. To achieve these objectives, within the framework of the GEOSTOH project, CEA intends to recruit a* ***post-doc over a period of 12 months****, in order to develop the tools required for generating spatially heterogeneous three-dimensional random tessellations. CEA will provide the HPC resources necessary to carry out these simulations, which are extremely demanding in terms of computation time.* ***Recruitment*** *will take place* ***from September 2020*** *(and no later than April 2021).*

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Context

The propagation of particles in multiscale materials is often described using linear transport theory in stochastic media [1, 2]. For this purpose, the CEA has recently developed new simulation tools for the generation of random geometries from probabilistic models, such as stochastic Poisson or Voronoi tessellations (Fig. 1 and 2), dealing in particular with three-dimensional configurations [3, 4]. In the GEOSTOH project (Heterogeneous STOchastic GEOmetries), we propose to develop new algorithms enabling to handle the case of spatially heterogeneous random geometries, which are key to the modeling of realistic disordered structures [5, 6]. The main scientific obstacles are both theoretical, concerning the development of a coherent probabilistic formulation for non-homogeneous random tessellations, and numerical, due to the computational cost required in order to determine the distributions of the desired observables. For this purpose, the GEOSTOH project intends to develop the theory and algorithms of random tessellations in a context of high-performance computing. The computer clusters necessary for the project will be made available by the CEA.

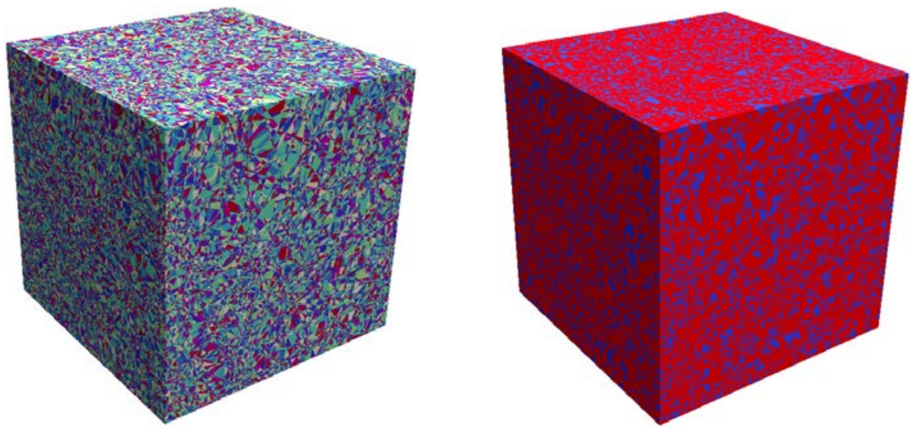

Fig. 1 et 2. Left: Example of realization of a homogeneous and isotropic random Poisson tessellation, in three dimensions, created by using the generator of random geometries developed at CEA [3]. Right: The same realization after applying a binary coloring procedure for the polyhedra (probability of red 75% and blue 25%). These tessellations are spatially homogeneous, their statistical properties being the same at any point in space.

Scientific approach and goals pf the project

The modeling of particle transport in disordered environments presenting multiscale heterogeneities is of prime interest for many applications, such as radiative transport in turbulent mixtures, the determination of the probability of re-criticality with diffusion and multiplication of neutrons in fuel configurations under degraded conditions, or the simulation of the transport of radiation in the cement matrices of radioactive waste containers [1, 2]. In this context, particle propagation is often described using linear transport theory in stochastic media [1]. For this purpose, the CEA has recently developed a new simulation tool for the generation of random geometries from probabilistic models, such as stochastic Poisson or Voronoi tessellations, dealing in particular with three-dimensional configurations [3, 4].

Poisson geometries are arguably the best known and most often used class of random tessellations [1, 3, 4]. A domain is partitioned into polyhedra as follows: a number of hyperplanes are sampled according to a Poisson law, the intensity of which depends on the dimension d and on a parameter which corresponds to the density of the tessellation; then, each hyperplane is drawn at random in order to guarantee the spatial homogeneity of the tessellation, and its intersections with the polyhedra making up the tessellation are calculated (Fig. 3). An arbitrary line will then be cut by the polyhedra into segments (chords) distributed exponentially. The average length of the chords defines the characteristic scale of the disorder of the geometry (to be compared with the mean free path, i.e., the typical size of the particle displacements in the modeled medium) and is inversely proportional to the density of the tessellation.

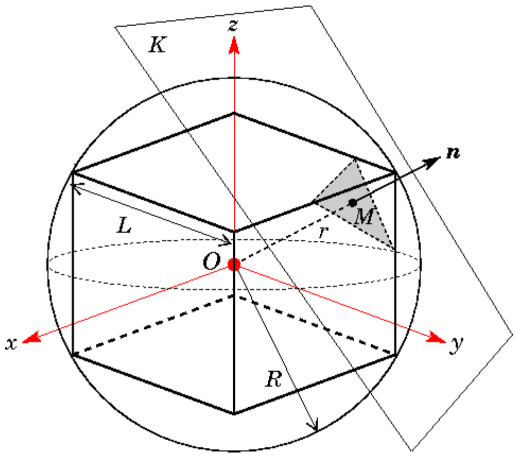

Fig. 3. Poisson tessellation of a cube of side L in dimension d = 3: drawing a random plane K. The circumscribed sphere has a radius R = sqrt (3) L / 2. The point M is defined by OM = r n, where r is drawn uniformly over the interval [-R; R] and the normal vector n of each hyperplane is drawn from an arbitrary distribution H (n). The plane orthogonal to the vector n and passing through OM is the desired random plane K [3].

Voronoi tessellations are also a very common model, especially in the description of the microstructure of materials [2]. Their construction is based on the following principles: points (germs) are drawn randomly from a homogeneous Poisson process in the domain to be partitioned. For each germ, Voronoi cells are then constructed, defined as the regions of points in space being closer to the germ under consideration than to any other germ (Fig. 4).

Once the tessellations are generated, we proceed to the so-called coloring step, in which each polyhedron is assigned a material composition, such as water or fuel, respecting the volume proportions. Coloring potentially induces preferential paths for the particles, which can be investigated using percolation theory [3].

So-called reference results for observables linked to particle transport can be obtained by generating a large number of geometries describing the medium through which the particles pass. For each geometric realization we solve the linear transport equation (Boltzmann), for example using a Monte-Carlo code, and we calculate the observables of interest, such as the concentration of the particles inside the middle. Finally, we determine the distributions of the observables over the set of realizations. This approach, which is in principle exact, generates extremely high computation times, requiring HPC resources for massively parallel simulations [3, 4]. The use of these reference results is essential for the validation of homogenized models, such as the Levermore-Pomraning model, much faster but approximate [1, 7, 8].

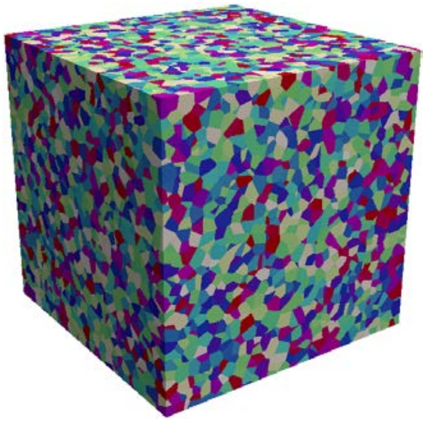

Fig. 4. Example of realization of a homogeneous and isotropic random Voronoi tessellation, in three dimensions, created from the generator of random geometries developed at CEA [3].

Due to the algorithmic complexity and the computational cost, until very recently the application of random geometries to particle transport was restricted to problems in dimension d = 1 or d = 2 [1]. The passage to the dimension d = 3 has recently been acquired [3, 4].

With rare exceptions, almost all the random tessellation models proposed in the literature introduce the simplifying hypothesis of spatial homogeneity: their statistical properties must be the same at any point in space [1, 2]. In the GEOSTOH project (Heterogeneous STOchastic GEOmetries), we propose to develop new breakthrough algorithms making it possible to deal with the case of **spatially heterogeneous** three-dimensional random geometries, which prove to be essential in the modeling of realistic disordered structures, including for example the effects stratification of materials due to gravity or complex interfaces due to Rayleigh-Taylor instabilities in multiphase mixtures [5, 6, 9].

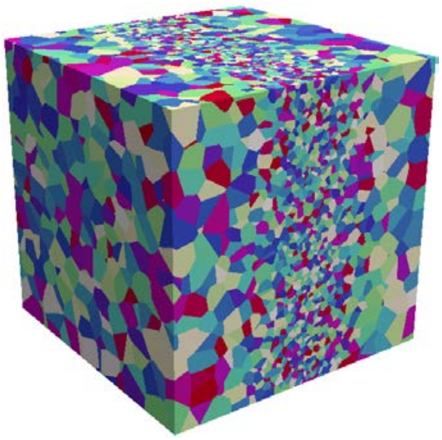

Fig. 5. Example of realization of a three-dimensional non-homogeneous random Voronoi tessellation, with spatial gradient along an axis (the density of the tessellation is smaller at the edges and larger at the center of the volume), created from recent developments in the random geometry generator developed at CEA [10].

The main scientific challenges are both theoretical and numerical. To begin with, it will be necessary to develop a coherent probabilistic formulation for non-homogeneous random tessellations: this is an innovative subject and little explored in the literature; nevertheless, preliminary results for the case of Voronoi geometries with spatial gradient (ie, statistical properties which vary along an axis following a given law, as illustrated in Fig. 5) have shown the feasibility of this approach and will thus constitute the starting point for the work to be done [10], in particular for the generalization to the case of Poisson geometries. Then, after having developed algorithms for the construction of tessellations with spatial gradients, it will be necessary to implement the computational resources required for the simulation of transport in these structures, in order to determine the distributions of the desired observables: it will be a question of port and optimize geometry generation algorithms and transport codes for massively parallel computing clusters.

To carry out this work, the GEOSTOH project intends to bring together the skills of two CEA teams in a complementary manner, within the framework of a new collaboration. In particular, the first is actively working on the theory and algorithms of random tessellations and since 2016 has been developing software for the "construction" of geometries adapted to transport codes. This team is also in charge of the development of the TRIPOLI-4® Monte-Carlo code for particle transport, recently optimized for geometrical pursuit in random tessellations, which are potentially composed of several tens of millions of polyhedra. The second team has a lot of experience in the physical modeling of structures with spatial gradients (especially in the context of turbulent mixtures) and will thus be able to guide the choice of the most suitable algorithms to describe the problems of interest. In addition, this second team will provide the TERA supercomputer necessary to estimate the distributions of physical observables via massively parallel reference simulations and will contribute to the portability of the codes to ensure high performance calculations on this cluster.

Post-doctoral work planning

For the GEOSTOH project, the CEA would like to recruit a **post-doc** for a period of **12 months**, who would be hosted at the **CEA (Saclay center)**. Recruitment will take place from **September 2020** and no later than April 2021.

The post-doc **work program** is as follows:

1 - study of the state of the art on random tessellations (in particular for the heterogeneous case). Getting to grips with recent work on three-dimensional Voronoi geometries with spatial gradients and the existing mathematical literature on heterogeneous Poisson geometries: these results will constitute the starting point for the analysis of the algorithms to be developed;

2 - improvement of methods for heterogeneous Voronoi geometries and development of algorithms for heterogeneous Poisson geometries in dimension $d = 3$ (if the three-dimensional case proved to be too complicated to achieve, we would switch to lower-dimensional geometries , which are easier to process);

3 - porting the geometry generator and the particle transport code to the computation clusters, carrying out simulations and interpreting the results obtained (distributions of the physical observables of interest and comparison in the case of spatially homogeneous geometries).

Impact of the projet

The goal of the GEOSTOH project is to implement new numerical simulation tools allowing a more faithful description of the transport of particles in disordered media with multi-scale heterogeneities and spatial gradients. The envisaged applications concern, among other things, the estimation of safety margins for re-criticality accidents with degraded fuel, the transport of radiation in porous media, or the radiative transfer in turbulent mixtures for fusion by inertial confinement. The results acquired during the project will be promoted through publications in peer-reviewed journals and / or presentations at international conferences. In addition, the algorithms and simulation methods developed will be industrialized and incorporated into existing software, in order to make them available to the user community.

References

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