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Complementary Finite Element and Monte-Carlo Methods to Solve Industrial Thermal Problems

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Abstract. This paper presents the integration of a Monte-Carlo solver inside SYRTHES, an open-source thermal code, originally based on finite elements method. Insensitive to both the geometric complexity of the model and the fineness of its discretization, this stochastic method is a good complementary option to simulate large configurations with specific locations of interest. Radiation, conduction and convection can be combined to solve thermal problems in complex geometries. The Monte-Carlo method is described before showing its integration in the code SYRTHES. Comparisons against results obtained thanks to finite elements and Monte-Carlo approaches or analytical solutions are presented. Finally, industrial cases illustrate the advantages of using these two complementary approaches.

1 Introduction

In the field of electricity generation (nuclear, renewable) or energy efficiency, EDF studies numerous configurations where thermal aspects are present. To carry out these analyses, EDF R&D has developed the numerical tool SYRTHES [1], an open-source thermal code for industrial and/or research studies. SYRTHES is a well validated code which tackles a very wide range of thermal problems caracterized by a large range of sizes, from micrometer to several kilometers and from a fraction of a second up to thousands of years like in deep repository for nuclear waste. The classical Finite Element Method (FEM) is used for conduction while thermal radiation relies on a radiosity approach. Large size problems (meshes above billion of elements) can be handled thanks to distributed parallelism through MPI on several hundreds of processors. Recently a need has been identified for problems when users are mainly interested by the temperature at specific locations. For these cases, calculating the entire field seems costly in terms of CPU but also regarding the production of a well adapted mesh, the postprocessing step or storage requirements. A second resolution method based on an innovative Monte-Carlo approach seems adequate to meet this demand. Even if the Monte-Carlo approach has been proposed more than 70 years ago, the method suffered from high CPU costs. Recently, the world of image synthesis in the film industry

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has made the transition from the deterministic to the statistical and proposes open-source librairies. This leads to the possibility of using statistical methods to solve thermal problems.

Considering that, on the one hand, EDF is developing an industrial code using finite element method (SYRTHES) and on the other, Meso-Star/Laplace laboratory are developing a thermal simulation framework (*stardis_solver* [2]), based on Monte-Carlo algorithms, a joint work has been started for the integration of Monte-Carlo solvers into SYRTHES.

This article presents the Monte-Carlo method for thermal problems, its potential and its computer implementation within open-source libraries, and the possibility to use the same set of geometric and physical data as those used by SYRTHES. Several industrial cases and some perspectives are presented.

2 Monte-Carlo approach : *stardis_solver*

The company MESO-STAR is developping *stardis_solver*, a thermal simulation framework for complex 2D and 3D environments, based on new Monte-Carlo algorithms built from reformulations of the main heat transfer phenomena: conduction, convection and radiation. A set of cross-recursive algorithms have then been derived, and result in the simulation of "thermal paths" that explore space and time until a boundary condition or an initial condition is found. The key concept here is that heat transfer phenomena are not considered separately but are naturally coupled via the cross-recursion of the various Monte-Carlo algorithms.

Regarding the physical model, opaque solids with homogeneous thermophysical properties; perfectly transparent fluids, with homogeneous thermophysical properties and also temperature (perfectly mixed fluids); thermal resistances can be taken into account at the interface between solids. Boundary conditions may be: Dirichlet (prescribed temperature), or a composition of Neumann and Robin conditions (i.e. convective exchange and also possibly a prescribed net flux). Homogeneous volumic source terms can also be prescribed within solid domains, and the radiative temperature of the ambiance surrounding a given system can be provided.

Finally, the initial state has to be provided at each position in the system, since we are interested in transient heat transfer solutions.

2.1 Coupled transient linear heat transfer

Following the notations of the work of Tregan et al. [3] where the technique is presented in full details, the quantity of interest is the temperature $\theta(\vec{x}, t)$ at any position in the system and at any time, or any surfacic or volumic average thereof. Four main concepts are introduced: the temperature $\theta_S(\vec{x}, t)$ in a solid domain, the temperature $\theta_{F,i}(t)$ in the i-th fluid domain, the temperature $\theta_B(\vec{x}, t)$ at a boundary (either between two solids, or between a solid and a fluid domain) and the radiative temperature $\theta_R(\vec{x}, t)$.

The main idea is to formulate each one of these temperatures as a sum; this makes possible to consider each quantity as the expectancy of a random variable, and therefore its estimation using the Monte-Carlo method.

Consider the local energy budget in a opaque solid domain that is assigned a volumic heat source term $p(\vec{x}, t)$ $[W.m^{-3}]$ and a known initial temperature profile $\theta_{S,I}(\vec{x})$:

$$\rho_S C_S \partial_t \theta_S(\vec{x}, t) = \lambda_S \Delta\theta_s(\vec{x}, t) + p(\vec{x}, t) \tag{1}$$

The solution of which can be formulated using Green functions (see [3] for details):

$$\begin{aligned}\theta_S(\vec{x},t) = &\int_{\Omega_S} g_{S,I}(\vec{x},t|\vec{x}_I,t_I)\theta_{S,I}(\vec{x}_I)d\vec{x}_I \\ &+ \int_{t_I}^{t}\int_{\partial\Omega_S} g_{S,\partial\Omega_S}(\vec{x},t|\vec{x}_B,t_B)\theta_B(\vec{x}_B,t_B)d\vec{x}_B dt_B \\ &+ \int_{t_I}^{t}\int_{\Omega_S} g_{S,\Omega_S}(\vec{x},t|\vec{x}_S,t_S)p(\vec{x}_S,t_S)d\vec{x}_S\,dt_S\end{aligned} \tag{2}$$

with $g_{S,I}$, $g_{S,\partial\Omega_S}$ and g_{S,Ω_S} the Green functions (propagators) for, respectively, the initial temperature profile, the boundary temperature and the volumic source term. The Monte-Carlo algorithm associated with this formulation consists in sampling positions $\vec{x}_I$ where the initial condition $\theta_{S,I}(\vec{x}_I)$ is evaluated, positions and times $(\vec{x}_B, t_B)$ on the boundary $\partial\Omega_S$ of the solid and over the $[t_I, t]$ interval, where the temperature $\theta_B(\vec{x}_B, t_B)$ is evaluated, and positions and times $(\vec{x}_S, t_S)$ within the solid domain Ω_S and over the $[t_I, t]$ interval, where the source term $p(\vec{x}_S, t_S)$ is computed. The various sampling have to be performed according to their respective propagator.

In pratice, all three samplings are combined in a procedure named *walk on δ-sphere*: a single realization for the evaluation of the probe temperature $\theta_S(\vec{x}_0 = \vec{x}, t_0 = t)$ consists in first sampling uniformly a position $\vec{x}_1$ over a sphere of prescribed radius δ, centered on the $\vec{x}_0$ probe position, and sampling a time interval τ_1 according to the appropriate probability density (see [3]). The Monte-Carlo weight is $\theta_S(\vec{x}_1, t_0 - \tau_1)$, i.e. the temperature in the solid domain, for position $\vec{x}_1$ and time $t_1 = t_0 - \tau_1$, a constant term $\frac{p\delta^2}{6\lambda_S}$ being accumulated. But in all generality, temperature $\theta_S(\vec{x}_1, t_1)$ is not known. Using the principle of the double randomization (in short: the expectancy of a expectancy is also a expectancy), it is evaluated by the same recursive procedure. This produces a random walk of prescribed step length δ within the solid domain, and that goes backward in time, that stops in two cases: first, when $t_i = t_{i-1} - \tau_i < t_I$, in which case the initial temperature $\theta_{S,I}(\vec{x}_i)$ is retained; and next, when the random walk crosses the boundary of the solid domain at a position and time $(\vec{x}_B, t_B)$: the weight of the Monte-Carlo realization is then $\theta_B(\vec{x}_B, t_B)$. When the temperature is prescribed at this position (Dirichlet limit condition), this quantity is known and the realization stops; it is otherwise unknown, and we shall see later what comes next.

Let us see now what happens when evaluating the temperature $\theta_{F,i}(t)$ of the i-th fluid domain; the energy budget again makes possible to derive a Monte-Carlo algorithm for the evaluation of the expectancy of its associated random variable; a single realization consists in sampling a position $\vec{x}_B$ over the boundary of the fluid domain, and a time interval τ. If $t - \tau < t_I$, the initial temperature of the fluid domain is retained, and the realization stops; otherwise, the Monte-Carlo weight is $\theta_B(\vec{x}_B, t - \tau)$, that may be unknown.

Within the limits of a linearized radiative transfer, a realization of the Monte-Carlo algorithm associated with the radiative temperature $\theta_R(\vec{x}, t)$ consists in sampling a radiative path from position $\vec{x}$; this path consists in straight lines between successive impact positions $\vec{x}_B$ over solid/fluid interfaces. At each impact, an absorption or reflection event is sampled according to the appropriate probabilities. The path ends when an absorption is selected, with a weight equal to $\theta_B(\vec{x}_B, t)$, the temperature at the final (boundary) temperature, and time t. Which is, of course, unknown, except in the case of a Dirichlet condition. In the case when the optical path fails to hit a surface, the (known) ambiant radiative temperature is retained, and the realization stops.

Let us finally examine what happens when a boundary temperature $\theta_B(\vec{x}, t)$ has to be evaluated. In the case of the boundary between two solids, the flux conservation translates to a

simple Monte-Carlo algorithm, that consists in retaining the temperature $\theta_S(\vec{x}+\delta\vec{n},t)$ within one of the two solids (with $\vec{n}$ the incoming normal for each solid), with probabilities that involve their respective conductivities. The evaluation of this temperature requires the previously described algorithm for solving the diffusion equation. In the case of the boundary between a solid domain and the i-th fluid domain, the flux conservation makes possible to express $\theta_B(\vec{x},t)$ as a ponderated sum of $\theta_S(\vec{x}+\delta\vec{n},t)$, $\theta_{F,i}(t)$ and $\theta_R(\vec{x},t)$. One of these quantities is sampled according to the associated probability set, which requires the corresponding previously described algorithm. Also, when a net flux density ϕ is prescribed for this interface, a quantity $\frac{\phi}{h_c+h_r+\lambda_S/\delta}$ must be accumulated (with h_c and h_r respectively the local exchange coefficients associated with convection and radiation).

The theoretical construct is now complete: the evaluation of a given probe temperature requires using various algorithms that will recursively interrogate each other; the associated image is of a thermal path that explores space and time (backwards), and that also switches between heat transfer processes, until a known temperature is reached: the initial temperature for a solid or a fluid domain, a prescribed (Dirichlet) temperature, or the ambiant radiative temperature. Each algorithm may also provide a accumulated weight (in the unit of a temperature) that accounts for volumic source terms or boundary net flux densities; this quantity is added to the (known) temperature reached at the end of the thermal path.

2.2 The non-linearity of radiation

Thermal conduction and convection are modeled as linear processes, but radiative transfer, integrated over the whole spectrum, may only be expressed as a difference of temperatures to the power 4. The algorithm described in the previous section for solving the radiative temperature is based on a linearization of this difference of temperatures to the power 4. This linearization requires the a-priori knowledge of a reference radiative temperature, refered as $\theta_{R,ref}$, which is another numerical parameter (the first being the value of the δ parameter used for the solid random walk, in each solid domain) that should definitely be provided by the enlightened user.

The algorithm used for radiative processes in *stardis_solver* has been generalized thanks to the PhD work of J.M. Tregan [4]. The so-called *Picard scheme* now needs to sample boundary and radiative temperatures recursively, for a prescribed maximum order n: special case n=1 reverts to the usual linear situation that was previously described. The scheme theoretically converges to the correct representation of a radiative exchange proportional to a difference of temperatures to the power 4, for $n \to \infty$; however, since computation times become impractical at high orders, the user now has to provide the maximum recursion order allowed to the radiation algorithm. The method also requires the a-priori knowledge of the maximum temperature that will ever be encountered in the system.

2.3 Green functions

In section 2.1, the Green functions associated with each boundary condition have been introduced. The global Monte-Carlo algorithm that makes possible to compute any temperature $\theta_{S/F/R/B}(\vec{x},t)$ may actually be seen as a practical way to evaluate the propagator for each source (known temperatures, initial temperatures, source terms, net flux densities) that stops a realization whenever evaluated by the thermal path. The probe temperature of interest can be seen as nothing more than a linear combination of these sources. The coefficients involved in the corresponding polynom are the propagators for each source over the required probe temperature.

Of course, *stardis_solver* will compute and store these propagators. This makes possible to obtain the value of a probe temperature when the values of sources are modified: when the physical configuration remains identical, the values of the various propagators are preserved. It is then easy to evaluate the value of the probe temperature for new values of each source. This is of course only true in the limit of linear physics, which means the Picard scheme must be used with recursion order n=1 for computing propagators.

3 Thermal code SYRTHES

SYRTHES [1] is an open source software dedicated to transient thermal simulations in 2D and 3D solids and wall to wall radiation heat transfer thanks to radiosity and view factors. To solve conduction, the geometrical description is done through a mesh composed exclusively of triangles (2D) or tetraedra (3D). To perform a calculation, this geometric data is supplemented by an ASCII file (generated by the GUI of the code) describing material properties, boundary conditions and numerical options. Figure 1 shows a traditional SYRTHES workflow for a conduction/radiation study with finite element solver (example of a schematic furnace) and how the calculation progresses.

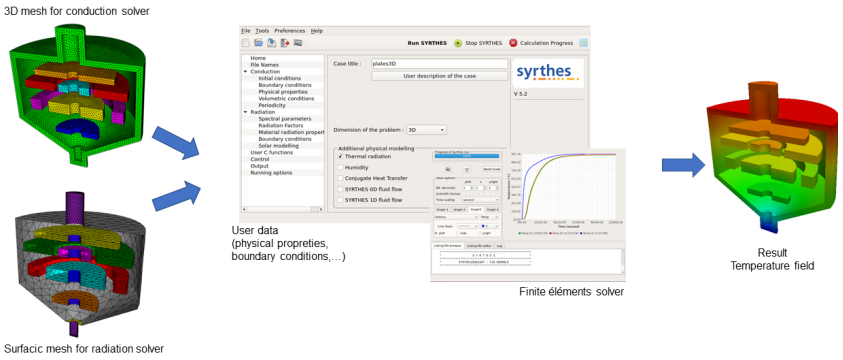


Figure 1. Workflow of SYRTHES calculation – Finite element solver

Although the databases required for a finite element calculation and a Monte-Carlo calculation differ greatly, we have chosen to retain the original SYRTHES operation in its entirety. Thus, during a Monte-Carlo calculation, the two meshes (3D conduction and surface radiation) and the data file (physical properties, boundary conditions,...) are supplied to the code in an identical fashion. A SYRTHES-integrated automatic interfacing module then reconditions the input data to the required database for the Monte-Carlo resolution libraries. Monte-Carlo resolution is not based on a 3D volume mesh, but only on the surfacic mesh of the geometry (figure 2).

This strategy has several advantages:

- A regular user of SYRTHES can easily carry out a Monte-Carlo thermal calculation,
- Input data are given thanks the same Graphical User Interface,
- It is possible to quickly switch from a finite element simulation to a Monte-Carlo simulation (and vice versa), with a very limited risk of error in the input data,
- Both methods can be used simultaneously in the same calculation, which allows to compare and validate results at particular points of interest in the calculation.

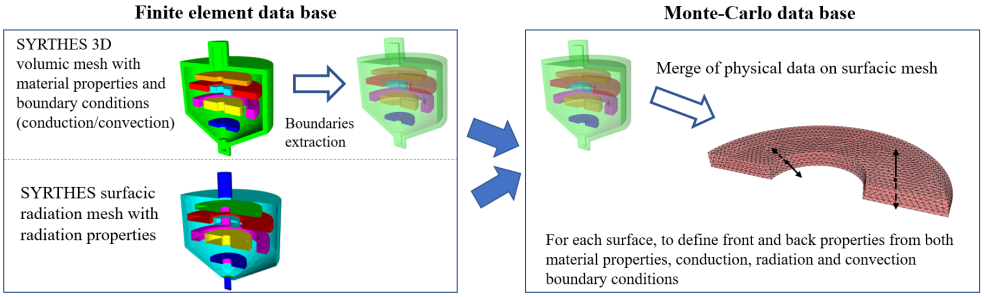
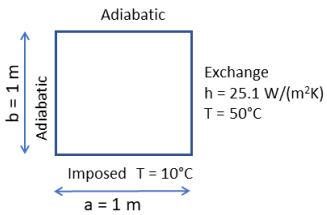


Figure 2. Data extraction from finite element database for the Monte-Carlo solver

Validation of Finite Elements and Monte-Carlo methods

The SYRTHES validation database includes many test-cases, some of which have an analytical solution. Figure 3 shows the case of a steel plate with one side subjected to an imposed temperature and a second side subjected to an exchange condition. This configuration (conduction only) has an analytical solution. We run calculation both with finite element method and Monte-Carlo method (for points on x=0.5 and y=0.5 profiles). Figure 4 shows the temperature field (finite element result) and comparisons of temperature (finite element calculation, Monte-Carlo calculation and analytical values) along two profiles. It shows very good agreement between the calculated and the analytical values.



$$T(x,y) = T_{ext} + 2h(T_{imp} - T_{ext}) \sum_{n=1}^{\infty} \frac{cos\ \alpha_n x\ \ cosh\ \alpha_n(1-y)}{[\ (\alpha_n{}^2 + h^2) + h]\ cos\ \alpha_n\ \ cosh\ \alpha_n}$$

where α_n are roots of following transcendental equation :

$$\alpha_n\ tan\ \alpha_n = 1$$

Figure 3. Steel plate, boundary conditions and analytical solution

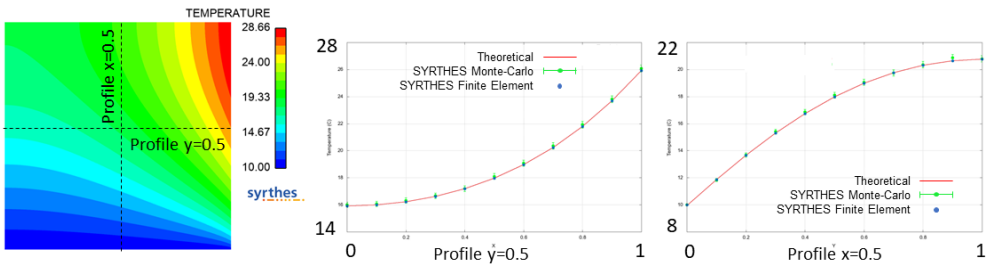


Figure 4. Temperature field calculated by SYRTHES-Finite elements and comparison between finite element values, Monte-Carlo values and analytical values for x and y profiles

4 Long-Lived High-Level nuclear Waste disposal

The handling of Long Lived High Level radioactive Waste (LL-HLW) is a topic that the nuclear industry must address. The possibility of a deep geological disposal is under study. The underground disposal facility consists of disposals cells excavated in an argillite formation at a depth of about –500 m and containing the waste packages (vitrified glass canisters).

The design of the repository results from an optimization between storing a maximum number of packages while respecting thermal and mechanical criteria. The repository consists of galleries connected to several parallel horizontal cells about 150 meters long, dead end, caracterized by an excavated diameter of around 0.7 meter. Each waste package has a metallic sleeve which supports the argillite and enables package handling during the introduction and positioning phase, as well as a possible retrieval (figure 5). Radioactive wastes have a residual power that decreases slowly over time (figure 5).

The aim of the thermal study is to assess the temperature reached in the geological massif during very long transients. To take into account slow diffusion in the massif without disturbing the field by inappropriate boundary conditions, the calculation domain must extend from the surface of the ground to a great depth. But, in fact, only few locations are points of interest: points in the vicinity of the packages, where the massif will see the highest temperatures, and points located between two consecutive cells (due to mechanical constraint consideration). Figure 5 shows the calculation domain. Due to symmetrical reasons, only half of a cell and its surrounding need to be considered. Figure 6 shows the temperature field calculated by SYRTHES-Finite Element after 970 years.

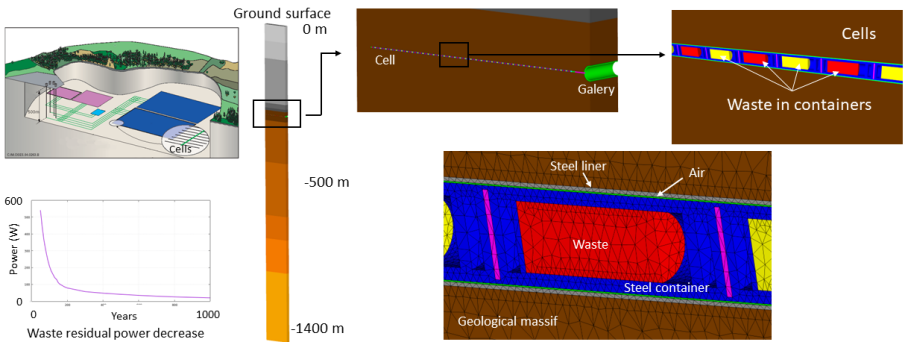


Figure 5. Schematic sketch of a deep geological disposal and numerical model for half a cell

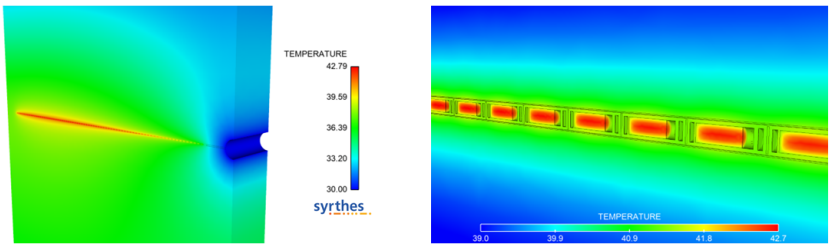


Figure 6. Temperature near the cell (left) and zoom around the waste packages (right) after 970 years

Instead of calculating the entire field, Monte-Carlo algorithms allow the temperature to be calculated only at some strategic points of interest and only at defined times. For a given location, the average temperature is calculated as an average of the temperatures found at the end of each statistical path. Figure 7 gives an example of one particular path among the 10000 calculated. A comparison between the two approaches for the same points (in space and time) shows reasonnable agreement. A reduction of the uncertainty provided by the Monte-Carlo approach can be obtained if the number of statistical paths used is increased, but of course at a higher CPU cost.

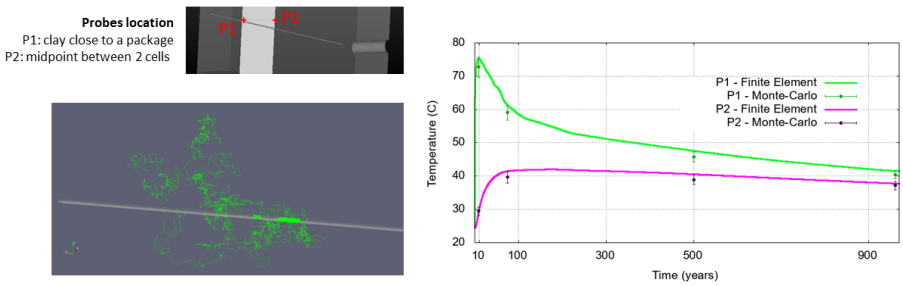


Figure 7. Probes positions (top left) - Heat path for 1 probe (bottom left) - Comparison of probes temperatures over time, finite element and Monte-Carlo methods (right)

5 Long-lived intermediate-level nuclear waste storage

Activated Long-Lived Intermediate-Level metallic radioactive Waste (LL-ILW) from dismantled or in operation nuclear power plants are conditioned in concrete packages and then transferred to large halls to be stored during decades before being disposed in an ultimate 500 m underground geological disposal. To control the risk of Delayed Ettringite Formation (DEF) in the packages, core temperature of the packages must stay below temperature criteria under normal storage conditions. A storage hall has a capacity of around 1100 packages stacked on three levels (Figure 8). In penalizing cases, the nuclear waste occupies only a small part of the package, the rest being filled only with grout (figure 8, middle). For a fully packed hall, different residual powers (from 41 W to 170 W) are considered for each package, depending on the activity of the waste. Conduction, radiation and convection, must be evaluated and coupled together to obtain the thermal field in the packages. For this simulation, a theoretical constant outside temperature of $10°C$ and a heat exchange coefficient of $10W/(m^2K)$ are considered. Initial temperature of hall, packages and air is set at $10°C$.

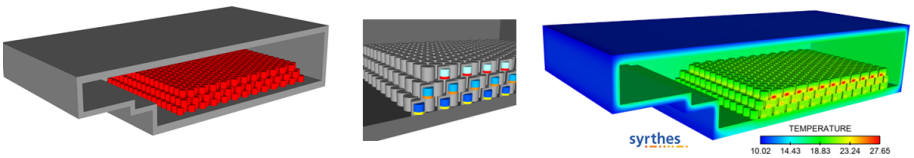


Figure 8. Storage hall with packages (left) - Waste and grout inside packages (middle) - Temperature field after 1 month, calculated by SYRTHES finite element method (right)

Temperatures at three locations (one for each level) are presented on figure 9 and show a good agreement between both methods. The statistical path shown on figure 9 exhibits the fact that, according the probabilities, this specific statistical path follows alternatively conduction, convection and radiation modes. The radiation mode is caraterized by long rays starting from the wall surface at one location, and following a random direction up to location where the ray impacts a new wall. There, according probabilistic weight (depending on the local emissivity, the conductive properties and the exchange coefficient), either the radiation path is reflected or enters a conduction or convection mode.

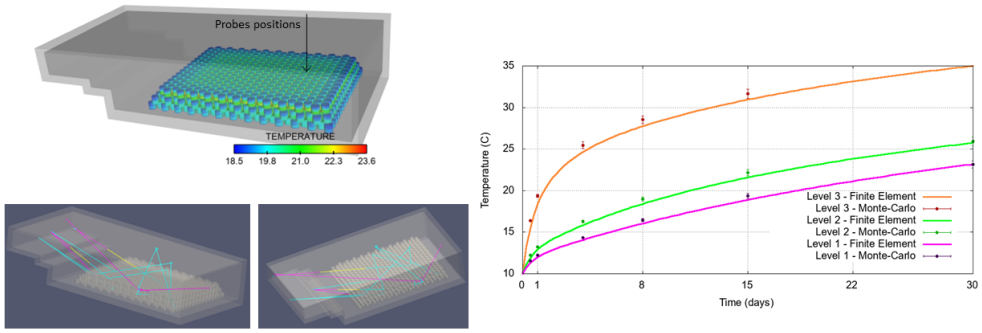


Figure 9. Probes positions (top left) - Heat path for 1 probe (bottom left) - Comparison of probes temperatures over time, finite element and Monte-Carlo methods (right)

6 Thermal study of electrical cannes

Another example illustrating the interest of the dual approach described in this paper is related to the thermal aspect of electrical cannes (here for solar industry). Users are interested by the temperature reached by an electrical canne in which heat is deposited thanks to Joule effect in two helicoidal wires. Indeed above a given temperature mechanical dammage could result. The wires are sourrounded by a MgO layer and a protecting cladding and cooled by the medium that the canne is supposed to heat. The geometry is complex and does not exhibit any possiblity to reduce the domain, so this implies to simulate a sufficient number of helix (10). The wire diameter being small, this leads to relatively large meshes (around 30 million elements).

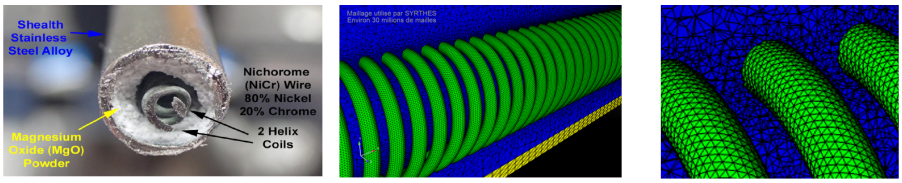


Figure 10. Mesh used both for the finite element and the Monte-Carlo approaches

For a power deposit of 100 MW/m^3, calculations find a wire temperature of 150°C. This result is found both by the finite element approach and the statistical approach. The latter method has the advantage to provide not only the value but the uncertainty associated. This particular example illustrates also the Green function procedure. At the end of the statistical computation for a deposit of 100 MW/m^3, the 10000 coefficients (propagators of each source for a specific probe temperature, corresponding to the end of the 10000 statistical paths) are stored in a file. Then it is possible to calculate a new temperature using just a linear combination for a new value of the source (for example here a new power deposit value). Since the computation is limited to a simple polynomial expression, it is instantaneous even if all the complexity of the problem is kept. The graph (figure 11) shows that the estimated temperatures for several power deposit obtained at just a fraction of the CPU-cost show a good agreement with results requiring a complete finite element computation.

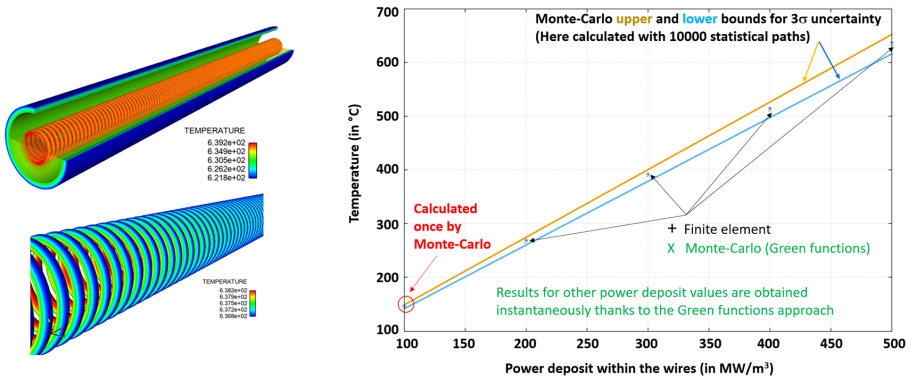


Figure 11. Overview of thermal field and zoom on the wire temperature field with an adapted scale and plot of the temperature at the center of wire using finite element, Monte-Carlo and Green functions

7 Conclusion and perpectives

This paper describes the possibility and the advantages of studying a same thermal problem by two complementary approaches. The finite element method provides a complete temperature field that generally helps to understand the phenomenology. On the other hand it requires an adequate space discretization, and this meshing step often turns out to be a bottleneck in studies. Moreover this dual approach answers the need of validated solutions. The Monte-Carlo approach allows to focus on specific locations or quantities, help to validate a field approach especially at locations of interest. For example, it can constitute an alternative to mesh convergence studies. In parameters identification studies, where solutions are compared to a limited set of data, solutions need to be calculated only at these locations. The strategy consisting in having in the same framework, field and Monte-Carlo approaches, allows users to calculate a complete field at the end of this identification process. Likewise shape optimisation studies could take advantage of this dual approach because the Monte-Carlo method is based upon the surface enclosing each material, which is much simpler to deform or modify (provided the topology of the domain stay identical). Finally one underlines that the statistical approach can be seen as well adapted to recent computers counting more and more cores due to the fact that the many statistical paths can be calculated independently. However it should be noted that the Monte-Carlo approach is still at an early stage of development and that many works [5][6][7] [8] are in progress to tackle in the future thermal problems similar as those presently handled by finite element method. Typically, adressing non-linearities turns out to be very challenging, even if major progresses have recently been made regarding the coupling between conduction and radiation.

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