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Probabilistic modeling of coupled heat transfer: A step towards optimization based on multiphysics Monte Carlo simulations

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ABSTRACT

This article presents a modular framework allowing to construct probabilistic models of coupled heat transfer problems in complex systems. First, a substructuring approach has been applied to formalize the problem. This process allowed for the coupling of physical field submodels, in our case temperature and radiative intensity. Each physical model was established according to the conservation law inside of its domain (solid and fluid) and the continuity laws at interfaces. Then, these models have been rewritten from the deterministic point of view to a probabilistic one. This enables a recursive Monte Carlo algorithm to estimate the desired values. After a validation stage, against academic cases, this framework is applied to examples emulating heat transfer in buildings. This approach presents a major beneficial behavior for complex systems optimization: only the influential parts of the problem have an effect on the computational time. These regions are automatically identified in a self-adaptive way, even in intricate or extensive geometries.

1. Introduction

For decades, the optimization processes have enabled engineers and designers to improve systems during their design stages. Taking advantage of the increasing computational power, they now wish to optimize more and more complex systems (complicated geometry, multivariate and/or multi-objective design, multi-scale phenomena, multiphysics problems). Simulation-based optimization methods are aiming at finding, by an iterative process, an extremum of a function, known as the objective function, which is evaluated thanks to the simulation results [1–3]. To perform these simulations, the most spread methods are the grid-based quadratures. Yet their use usually requires to describe complex systems by a great number of mesh elements owing to tortuosity, extensive geometry and/or multi-scale problems. Furthermore a vast grid implies a proportional need of computing power and memory to run a simulation. This limitation becomes all the more important when the complexity of systems is increasing.

Another kind of quadrature exists: the stochastic grid-free quadratures among which the Monte Carlo method is found. This method was first formalized by Metropolis and Ulam, in 1949, in the neutron diffusion field of science [4]. Fifteen years later, Hammersley and Handscomb highlighted the opportunity to use this method in a large variety of other domains among which the solution of linear operator equations, statistical mechanics or polymer science [5]. This approach allows for a stochastic estimation of a quantity of interest. The estimation is the mean value and the standard error of a great number of independent evaluations of a probabilistic model. Its two main characteristics are being a meshless quadrature and presenting a convergence rate independent of the problem dimension. Consequently, the higher the number of problem dimensions and the more competitive the Monte Carlo method is, compared to grid-based quadratures. Indeed, the laters follow a decreasing convergence rate when the problem dimension increase [6,7]. That is why even today the Monte Carlo method is mostly restricted to problems described by more than 3 dimensions such as radiative transfer, finance, particle physics, acoustics, cosmological models [8,9]. The drawback of a meshless approach is that the result is a single value (and its standard error), which can be a function evaluated locally or integrated over a domain. This could be a considerable disadvantage if you are looking to the whole unknown field. But, when using an optimization process, only the objective function needs to be assessed, not the whole field. Hence, that main drawback of the Monte Carlo grid-free approach can easily be overcome for an optimization process. Indeed, using the Monte Carlo method to estimate directly the objective function will only cost a single

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Nomenclature

$c_{p\,\Omega}$ Specific heat capacity of the Ω domain $[J.\ kg^{-1}.\ K^{-1}]$
$\boldsymbol{d}_{i,j}$ Direction vector defined at the $\boldsymbol{r}_{i,j}$ point $[m]$
δ Thermal dissipation coefficient $[W.\ m^{-2}.\ K^{-1}]$
$\mathbf{H}^{\Omega+}(\boldsymbol{x})$ Hemisphere of the directions incident from the Ω domain at the $\boldsymbol{x}$ point (identifying name)
$\mathbf{H}^{\Omega-}(\boldsymbol{x})$ Hemisphere of the directions leaving the $\boldsymbol{x}$ point towards the Ω domain (identifying name)
$h^{\Omega}_{\partial\Omega}$ Convection coefficient at the interface ∂Ω, on the Ω fluid domain side $[W.\ m^{-2}.\ K^{-1}]$
$I(\boldsymbol{x}, \boldsymbol{\omega})$ Total directional intensity field at the $\boldsymbol{x}$ point towards the $\boldsymbol{\omega}$ direction $[W.\ m_{\perp}^{-2}.\ sr^{-1}]$
$\langle i+j \rangle$ Mean length of the exploration paths used to compute the estimation (calculated in number of interaction points)
$\dot{m}_{\Omega+}$ Total mass flow rate leaving the Ω fluid domain (positively defined) $[kg.\ s^{-1}]$
$\dot{m}_{\Omega-}(\Omega_e)$ Mass flow rate coming from the Ω_e fluid domain into the Ω domain (positively defined) $[kg.\ s^{-1}]$
$\boldsymbol{n}^{\Omega+}_{\partial\Omega}$ Normal direction vector at the boundary ∂Ω leaving the Ω domain $[m]$
$\boldsymbol{n}_{cond}$ Direction vector along which the conductive heat transfer takes place (1D plane model) $[m]$
$P(\text{event})$ Probability that the event occurs
p_{RV} Probability density function associated with the RV random variable
$\dot{q}^{\Omega+}$ Total net flux density leaving the Ω domain $[W.\ m^{-2}]$
$\dot{Q}^{\Omega+}_{mode}$ Net flux leaving the Ω domain by the *mode* of heat transfer (*cond*uction, *conv*ection, *rad*iation or *enth*alpy) $[W]$
$\dot{q}^{\Omega+}_{mode}$ Net flux density leaving the Ω domain by the *mode* of heat transfer (*cond*uction, *conv*ection, *rad*iation or *enth*alpy) $[W.\ m^{-2}]$
$\dot{q}^{2D}_{src}$ Flux density of surfacic heat source at an interface $[W.\ m^{-2}]$
$\boldsymbol{r}_{i,j}$ Vector of the j-th position of the total directional intensity exploration path/series starting at the $\boldsymbol{x}_i$ point $[m]$
$s^{\Omega}_{\partial\Omega}$ Specularity ratio for the reflection at the interface ∂Ω, on the Ω domain side
$T(\boldsymbol{x})$ Temperature field at the $\boldsymbol{x}$ point $[K]$
T_{ref} Reference temperature used for the radiative transfer linearization $[K]$
$\hat{w}_{\text{event}}$ Monte Carlo weight associated to the event occurrence
$\boldsymbol{X}_i$ Random variable of the i-th position vector $\boldsymbol{x}_i$ $[m]$
$\boldsymbol{x}_i$ Vector of the i-th position of the exploration path/series $[m]$
$\boldsymbol{x}_i^{\in\Omega}$ $:=\boldsymbol{x}_i \in \Omega$ $[m]$
$\boldsymbol{x}_i^{\in\partial\Omega}$ $:=\boldsymbol{x}_i \in \partial\Omega$ $[m]$

Greek symbols

$\alpha^{\Omega}_{\partial\Omega}$ Total hemispherical absorpivity of ∂Ω boundary, on the Ω domain side
$\varepsilon^{\Omega}_{\partial\Omega}$ Total hemispherical emissivity of ∂Ω boundary, on the Ω domain side
λ_{Ω} Thermal conductivity of the Ω domain $[W.\ m^{-1}.\ K^{-1}]$
Ω Volumetric domain (identifying name)
$\partial\Omega$ Domain boundary (identifying name)
$\rho^{\Omega}_{\partial\Omega}$ Total hemispherical reflectivity at the interface ∂Ω, on the Ω domain side
σ Stefan-Boltzmann constant: $5.67 \times 10^{-8} [W.\ m^{-2}.\ K^{-4}]$
σ_t Standard error of the computational time estimation (t) $[s]$
σ_T Standard error of the temperature estimation (T) $[K]$
$\tau_{\partial\Omega}$ Total hemispherical transmittivity for the interface ∂Ω

estimation.

According to the Los Alamos National Laboratory [10], two of the main limitations to the Monte Carlo method spreading in simulation-based optimization are: the ability to evaluate nonlinear functions of integrals and the coupling issue because complex systems are generally multiphysic. Recent works [11–13] are bringing perspectives in order to alleviate the first challenge. We will focus on the second one, which is also a current concern for the grid-based methods and is shared by a wide variety of fields from astrophysics to biochemistry passing by nuclear reactor engineering or rarefied gas [14–18]. When dealing with multiphysic problems, the most spread approach consists in trying to couple several models or even simulation codes, one for each physical phenomenon, in a iterative converging process. The main difficulty is to keep coherent results from different tools, which rely on their own assumptions and have sometimes radically different solving strategies.

Regarding more specifically coupled heat transfer, and by instance the coupling of conduction and radiative transfer, we can find in the litterature different examples. Originally motivated by reducing computational time within a context of lesser available computational power, numerous attempts to couple grid-based methods for both radiative and conductive heat transfer can be found [19–26]. That approach has the advantage of coupling two similar methods but suffers twice of the drawbacks of grid-based quadratures as the systems become more and more complex. Furthermore, examples of coupling a grid-free method with a finite volumes or elements method can be found in literature [27–31]. Usually, in these cases, the Monte Carlo method is used to model the radiative transfer. These attempts have spread thanks to the increasing availability of computational power but are especially difficult to implement owing to the heterogeneity of the techniques which have to cooperate together. Finally, the third possibility is to use the Monte Carlo method to solve the whole problem. That approach allows to take advantage from both model characteristics homogeneity and the aforementioned attractive features of the Monte Carlo method. This goal was announced by the presentation of a first draft, in collaboration with the Meso-Star start-up, during the CTRPM-V conference [32]. Nevertheless, according to the best of authors' knowledge, this way of coupling has not been investigated yet. Although, Vignoles proposed very recently a method dedicated to simulation inside of porous media by coupling two Monte Carlo Random Walks, one for each phenomenon, in Ref. [33]. The idea is to follow the spreading of a "walker" population into the porous medium by both a radiative random walk and a conductive one. Each "walker" carrying a "quantum of excess enthalpy". At the end of a simulation, the temperature perturbation field is approximated by counting the number of "walker" in each discretized volume element. Even if this technique is also named "Monte Carlo", it features important differences with the Monte Carlo method used in the present article which is using neither a volume discretization nor following an energy quantum carrier population.

In order to solve the whole problem, i.e. coupled condution, convection and radiative heat transfer, using a single Monte Carlo algorithm, the prerequisite is to get a probabilistic model of the system. However, the more complex the system, the more difficult its modeling step. Therefore, to face this challenge, we have created a framework easing the construction stages, by using a systemic substructuring approach. This tool allows to assemble components, which have been already independently modeled. This approach provides several benefits: modularity, versatility and ease to upgrade. The aim of this article is to show how such an approach can be applied to fully coupled heat transfer problems. First we describe the substructuring approach and how the Monte Carlo algorithm can be used to solve modular models. Next, each submodel is detailed. Then the reliability of this approach is assessed by validating the framework results against academic cases. Finally, an application to heat transfer in a building will show the practical advantages of this strategy.