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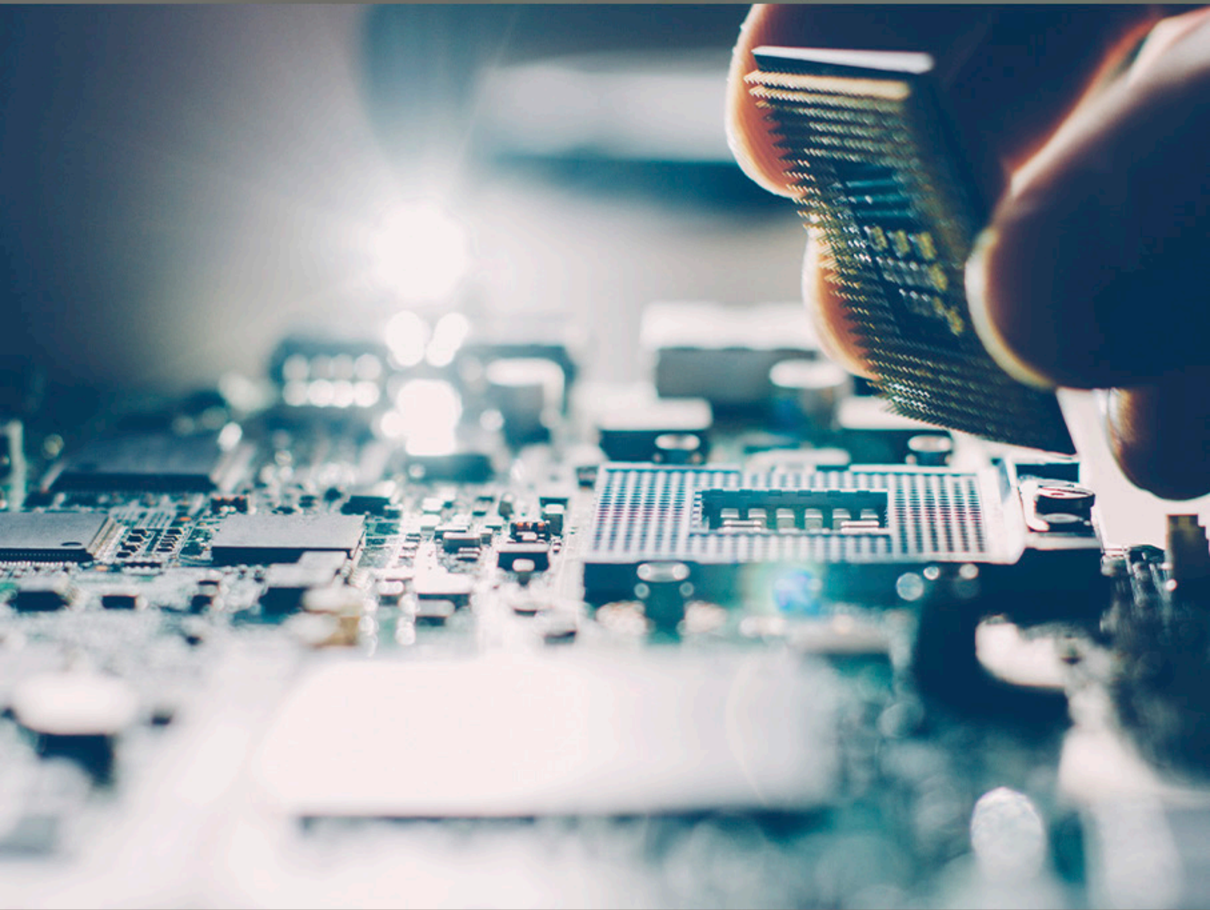
ENGENHARIA DE COMPUTAÇÃO 2



ERNANE ROSA MARTINS
(ORGANIZADOR)

Atena Editora
Ano 2021

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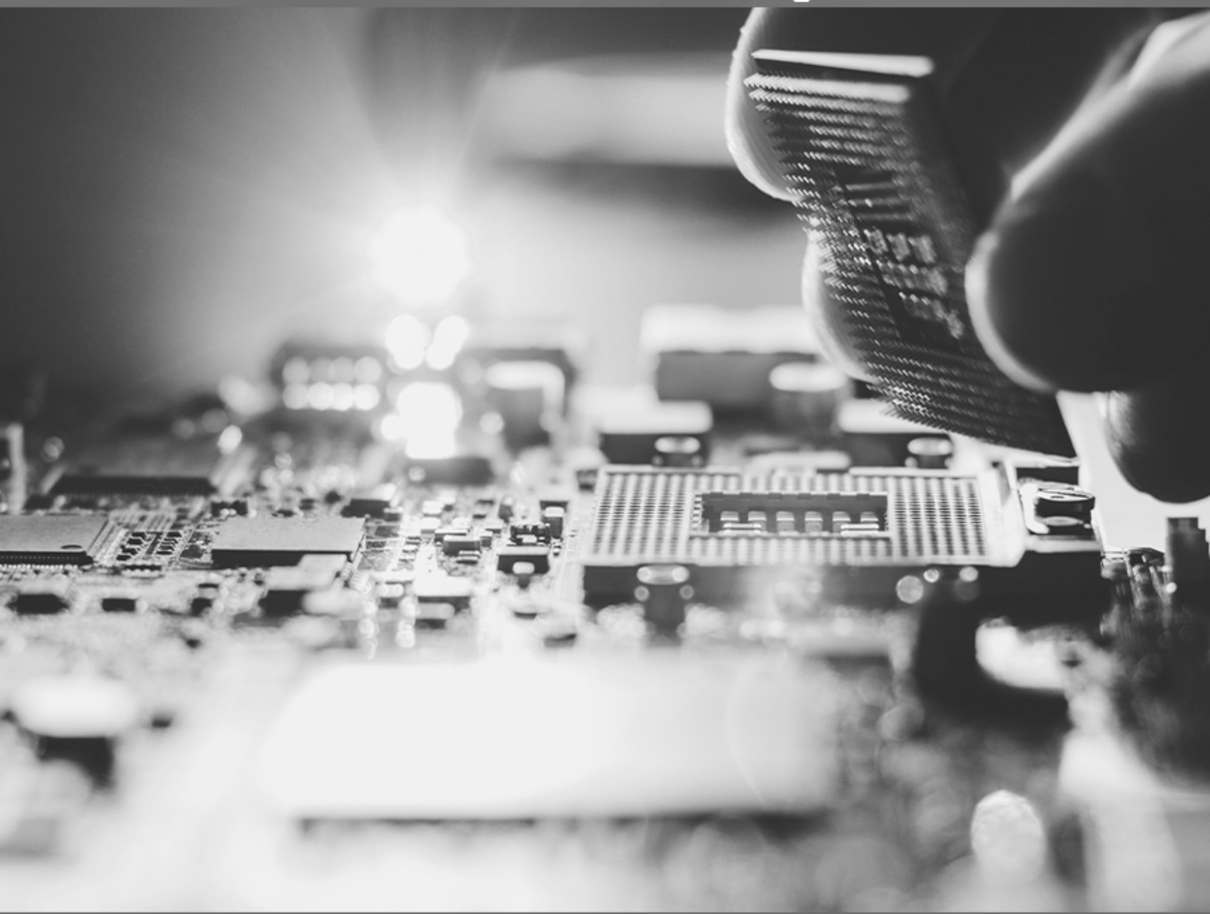

ERNANE ROSA MARTINS
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APRESENTAÇÃO

A Engenharia de Computação é a área que estuda as técnicas, métodos e ferramentas matemáticas, físicas e computacionais para o desenvolvimento de circuitos, dispositivos e sistemas. Esta área tem a matemática e a computação como seus principais pilares. O foco está no desenvolvimento de soluções que envolvam tanto aspectos relacionados ao software, quanto à elétrica/eletrônica. Os profissionais desta área são capazes de atuar principalmente na integração entre software e hardware, tais como: automação industrial e residencial, sistemas embarcados, sistemas paralelos e distribuídos, arquitetura de computadores, robótica, comunicação de dados e processamento digital de sinais.

Dentro deste contexto, esta obra aborda diversos aspectos tecnológicos computacionais, tais como: implementação e modificações numéricas a serem feitas no algorítmo de Anderson (2010) para simular o escoamento sobre uma asa finita submetida a ângulos de ataque próximos ao estol; modelo distribuído para analisar a influência da formação e do adensamento de geada sobre o desempenho de evaporadores do tipo tubo-aletado, comumente usados em refrigeradores frost-free; um algoritmo de Redes Neurais Convolucionais(CNN) que identifica se a pessoa está ou não utilizando a máscara; potencialidades do M-Learning e Virtual Reality no curso técnico em Agropecuária; avaliação da qualidade da energia elétrica em um sistema de geração de energia fotovoltaica; uma abordagem para a segmentação de imagens cerebrais, utilizando o método baseado em algoritmos genéticos pelo método de múltiplos limiares; estudo numérico de uma âncora torpedo sem aletas cravada em solo isotrópico puramente coesivo, utilizando um modelo axissimétrico não-linear em elementos finitos; estudo acerca da análise numérica de placas retangulares por meio do método das diferenças finitas, obtendo soluções aproximadas para o campo de deslocamentos transversais bem como os correspondentes momentos fletores, para problemas envolvendo uma série de condições de contorno, utilizando-se o software Matlab® para simulação; desenvolvimento e aplicação da Realidade Virtual (RV) como Tecnologia de Informação e Comunicação (TIC) para auxiliar no processo de ensino-aprendizado de disciplinas do Ensino Médio; avaliação dos resultados obtidos em campanhas de medição de qualidade da energia elétrica (QEE) na rede básica em 500 kV; examinar o comportamento mecânico-estático de uma longarina compósita projetada para uma aeronave esportiva leve através de investigações numéricas, empreendidas em software (ANSYS Release 19.2) comercial de elementos finitos; construção de um sistema para monitoramento de ativos públicos; a relação da Sociedade 5.0 envolvida no contexto da Indústria 4.0 e a Transformação Digital; algoritmos de seleção e de classificação de atributos, identificando as vinte principais características que contribuem para o desempenho alto ou baixo dos estudantes; a Mask R-CNN, utilizada para a segmentação de produtos automotivos (parabrisas, faróis, lanternas, parachoques e retrovisores) em uma empresa do ramo de reposição automotiva; o nível de usabilidade do aplicativo protótipo para dispositivo móvel na área da saúde voltado ao auxílio do monitoramento móvel no uso de medicamentos em seres humanos.

Sendo assim, está obra é significativa por ser composta por uma gama de trabalhos pertinentes, que permitem aos seus leitores, analisar e discutir diversos assuntos importantes desta área. Por fim, desejamos aos autores, nossos mais sinceros agradecimentos pelas significativas contribuições, e aos nossos leitores, desejamos uma proveitosa leitura, repleta de boas reflexões.

Ernane Rosa Martins

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CAPÍTULO 4

INFORMATION THEORY BASED STOCHASTIC HETEROGENEOS MULSTISCALE

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ABSTRACT. This work brings together theoretical formulation and computational strategies for upscaling in random heterogeneous mediums. The approach uses a mixing of information theory and statistical mechanics to extract relevant probabilistic information from microscale and adaptively control the stochastic distance between two scale responses. A goal-oriented upscaling procedure is defined to guarantee equivalence between micro and macroscale target to specific output, and its generalization to a mathematical sound multi-goal-oriented response where users control distinct accuracies of specific target responses. Preliminary applications in one-dimension domain for elliptic and hyperbolic equations are presented. Applications use realizations from microscale parameters distributions producing a reduced number of equivalent macroscale realizations, as required by to satisfy user desired accuracy. The full formulation requires solving an optimization problem for an extended Lagrangian formulation that is solved with a Parallel Deterministic Annealing. Mathematical formulation is such that parallelization is done over realizations so that the overall computation cost of the stochastic scale transposition is on the same order of a deterministic one.

KEYWORDS: Reservoir, Stochastic, Multiscale, Multiphysics, Goal-oriented

MULTIESCALA HETEROGENEA E ESTOCÁSTICA BASEADA NA TEORIA DA INFORMAÇÃO

RESUMO: Este trabalho reúne formulação teórica e estratégias computacionais para upscaling em meios heterogêneos aleatórios. A abordagem usa uma mistura de teoria da informação e mecânica estatística para extrair informações probabilísticas relevantes de microescala e controlar de forma adaptativa a distância estocástica entre respostas de duas escalas. Um procedimento de upscaling orientado a objetivos é definido para garantir a equivalência entre o alvo micro e macroescala para saída específica, e sua generalização para uma resposta matemática orientada a múltiplos objetivos onde os usuários controlam precisões distintas de respostas alvo específicas. Aplicações preliminares no domínio unidimensional para equações elípticas e hiperbólicas são apresentadas. As aplicações usam realizações das distribuições

dos parâmetros em microescala, produzindo um número reduzido de realizações em macroescala equivalentes, conforme exigido por para satisfazer a precisão desejada pelo usuário. A formulação completa requer a resolução de um problema de otimização para uma formulação Lagrangiana estendida que é resolvida com um Recozimento Determinístico Paralelo. A formulação matemática é tal que a paralelização é feita sobre as realizações de modo que o custo total de computação da transposição da escala estocástica seja da mesma ordem de um determinístico.
PALAVRAS - CHAVE: Reservatório, estocástico, multiescala, multifísica, orientado a objetivos.

INTRODUCTION

This text describes some mathematical and computational aspects of a formulation for transposing scales governed by different stochastically physics, of a microscale whose equations are discretized by a dense mesh, or *micromesh*, that adequately captures the uncertain heterogeneities of the parameters, for macroscales (*generative upscaling*), represented by sparse meshes, or *macromesh*, appropriate to the execution of hundreds or thousands of probabilistic sample simulations (realizations) of these uncertain parameters. Consequently, it is assumed that the system of equations resulting from discretization at the microscale is prohibitively large for the capacity of the computers available, particularly when resolved repeatedly, in response sampling procedures (optimization, stochastic control). Former applications on elliptic equations are done in Costa et. al. (2017).

Although the formulation is quite general (in the sense that it applies to the solution of systems of elliptical, parabolic and hyperbolic differential equations), the greatest interest is in the simulation of hydrocarbon reservoirs. It is realized that the reservoir is described by a finite number of *geostatistical realizations* of different distributions (variograms) used for description of the lithofacies of a given geological scenario. Also, and especially important, the techniques of discretization in space and time (finite elements or volumes, finite differences, etc.) are immaterial, as well as the characteristics of the solution and the algorithms used to find them. The formulation is non-invasive.

The formulation imitates Koutsourelakis (2007). It adds new elements: the possibility of to use different physics at different scales; a generalization of the principles presented in Weinan and Engquist (2003); fruitful mesh ideas oriented to the objectives, as used in the technology of the finite element method (goal-oriented FEM); and extended to finite elements for multiple scales in Nonnenmacher (2011). The transposition of the micro to the macroscale brings inevitable losses of resolution or accuracy of the answers. However, these losses can be substantially reduced if transitions are made to different macroscales with different objectives and accuracy, hence the notion proposed here of *upscaling oriented to the objectives* of the analysis.

In the technique presented here, at least two measures are used to quantify the quality of the transposition of scales and physics. With a first measure, similarly to the spectral decompositions of covariance (KKL expansions, for example), the retention in the macroscale of probabilistic information relevant to the problem is evaluated. The importance of the information retained, being dependent on the problem - the source terms, the objective of the problem, etc. - requires a measure or a set of them that judges the accuracy of the desired response compared to the response on the microscale. The use of more than one measure contrasts with the usual techniques of *upscaling* and, equivalently, of the basis reduction techniques (e.g., KKL, PCA, POD decompositions).

A final problem of conditional extremity is solved with an Augmented Lagrangian formulation, and with the elaboration of a parallel algorithm, PDA – *Parallel Deterministic Annealing*, a parallel and extended version of DA- *Deterministic Annealing*, described in Koutsourelakis (2007), that originated in Rose (1991, 1994, 1998). PDA is naturally parallelized over geostatistical realizations. These variants of the probabilistic *Simulating Annealing* are the natural ones for this class of problems given the spontaneous occurrence of possible exponential distributions in their solution. Clearly, other algorithms can be used efficiently.

METHODOLOGY

Let the reservoir be described by a set of N_R geostatistical realizations collectively aggregated in the ensemble ***X***, each with a number of cells.

We identify ***X*** with the random field it represents (discrete random fields). It is recognized that field ***X*** may contain more information than it is necessary for the solution of a given reservoir simulation problem. The objective is to describe this field by random vectors ***Y*** with $n < N$ cells and, possibly, $n_R < N_R$ realizations of the macroscale, in such a way that the answer to the specific problem can be found with less computational effort, within pre-established approximations. It is thought that can be as detailed as a *geocellular mesh*, and that it contains information on the *microscale* that can be compressed into a desired *macroscale* for the *specific objective*.

If the properties described by ***X*** can be compressed into ***Y*** for the solution of a specific problem, what needs to be determined is what information in ***X*** must be *statistically* preserved, in such a way that the distortion in the statistics of the desired response can be controlled. At least two measures need to be established in this way. The first is the fidelity of the representation of ***X*** by ***Y***, and another of the statistical accuracy of the desired response. Notoriously, physics at the *microscale* and the *macroscale* do not need, or should not, in many cases, be the same.

Traditional spectral techniques, such as *KKL expansions*, the analysis of the main components (PCA), (same as *KKL decompositions*), multidimensional scaling (MDS), and its variants that are not linear, seek to preserve the covariance structure using a hierarchy of approximations given by a sequence of eigenvalues and eigenvectors. This does not maximize the compression of the information, since both preserve unnecessary modes and omit, by the early truncation of the series or succession, eigenmodes that may be important for a specific response, they do not consider the characteristics of external excitations. For covariance functions that are not smooth and for long and weakly correlated processes, high order eigenmodes cannot be neglected without causing a significant loss of accuracy. The Galerkin-wavelet approaches, although they improve the accuracy of high-order eigenmodes, they do not solve the problem mentioned above, namely, the indeterminacy of the relevant eigenmodes for a specific response, since they recognize only the covariance and never the excitation.

The idea behind the described methodology is that it is not possible to choose representative elements of volume (REV) or to make use of periodicity of information in the microscale, given the essentially stochastic character in all scales of heterogeneities and that, probably, some separation of scales cannot be guaranteed. In this way, the change of scales must be made based on approximation measures, which may not be as approximate as desired.

The usual deterministic *upscaling* techniques are extended here (Weinan and Engquist, 2003). for stochastic transposition of scales (see Appendix). An adjacent set of cells is replaced by an equivalent cell (macrocell, macroelement), to be stochastically homogenized. One that ensures that the statistical description of the response has the desired accuracy. Such procedures are usually referred to as semi-local to local. It is evident that a global-local procedure can also be employed at the expense of greater computational effort in the generation of the macro mesh.

The scale change is made by assimilation of previous data from the models, from observed data, or both, making the technique also suitable for stochastic control, as for example, in closed loop control with prediction and assimilation of production data, at any scale of time. One of the main problems of stochastic control is the computational effort in the two phases, prediction, and assimilation. In this case, the parameterization techniques, such as spectral decompositions, can be conveniently replaced by macro meshes, which are stochastically equivalent. Both Bayesian methods, such as MCMC and RML, as classical estimators, such as those of maximum likelihood, regularized (maximum *a posteriori*, for example), benefit from the computational economy of the scale change, from the use of a macro mesh. This summarizes the importance of the present study.

Indicator of mutual information between random fields

The main aspect of the methodology follows Koutsourelakis (2007) and is generalized for multiple physics and multiple algorithms. It is based on models of statistical mechanics (Hill, 1956), and of information theory originating mainly in Shannon (1948), with specific algorithms developed in Rose (1991, 1994, 1998).

The substitution of the ***X*** field for smaller ***Y***, implies the possibility of assigning the same value to large regions of the domain. The concept of the indicator of mutual information is introduced by Shannon (1948) as a measure of the average information that the knowledge of ***Y*** can provide of ***X*** and vice versa.

The hypothesis that the large regions of the heterogeneous domain of interest can be assigned the same values allows the description of the random field ***X*** by the field of smaller dimension ***Y***. A measure of the ability of ***Y*** to approach ***X*** can be given by the *mutual information indicator* (Shannon, 1948),

$$I(\mathbf{X},\mathbf{Y}) = \iint p_{XY}(x,y)\log\frac{p_{XY}(x,y)}{p_X(x)p_Y(y)}dxdy, \tag{1}$$

where $p_{XY}(x,y)$ is the joint density of (X and $p_X(x)$, $p_Y(y)$ are the respective marginal distributions. Its *minimum value* is zero when the two fields are independent, in other words, $p(\mathbf{X},\mathbf{Y}) = p_X(\mathbf{X})p_Y(\mathbf{Y})$. Its *maximum value* is known as the *entropy* of $\mathbf{X}$, that occurs when the two fields are identical ***X*** ≡ ***Y***. Defining *joint entropy* as the indicator itself, and developing,

$$H(\mathbf{X},\mathbf{Y}) = -\int p_X(x)\log p_X(x)dx + \iint p_{XY}(x,y)\log\frac{p_{XY}(x,y)}{p_Y(y)}dxdy, \tag{2}$$

using the fact that $\iint p_{XY}(x,y)\log p_X(x)dxdy = \int p_X(x)\log p_X(x)dx$. The first term in the second member of eq. (2) is the entropy (Planck (1948)) of **X,**

$$H(\mathbf{X}) = -\int p_X(x)\log p_X(x)dx, \tag{3}$$

while the second is *conditional entropy* or *equivocation*, or, preferably, *ambiguity*,

$$H_Y(\mathbf{X}) = -\iint p_{XY}(x,y)\log\frac{p_{XY}(x,y)}{p_Y(y)}dxdy, \tag{4}$$

which is zero when ***X*** = ***Y***. Then we have that $I(X,Y) = H(X) - H_y(X)$ and $I(\mathbf{X}) = H(\mathbf{X})$. In information theory, $I(X,Y)$ it is also known as the rate of transmission of information from a continuous channel (Shannon, 1948).

The convenience of using logarithmic measures, usually based on information theory, is justified by practicality, intuitive property, and mathematical convenience. However, entropy and the mutual information indicator, although they can measure uncertainty, are not probabilistic measures. Apparently, a probabilistic measure can be obtained by dividing the indicator by the entropy of ***X***. Se the entropy of ***Y*** is less than that of ***X***, compression can be done at higher rates. The authors, based on the concept of relative entropy or Kullback-Leibner divergence, are currently developing other appropriate non-probabilistic measures of proximity of the two fields.

Fidelity of the macroscale to the microscale

It seems evident that, apart from some atypical pathologies, the quality of representation in the macroscale should be evaluated, for greater accuracy, with measures that compare specific responses, and not all possible responses. As, for example, the ability of the macroscale to approximate the history matching of a certain quantity produced by the microscale, is of great interest in reservoir geoengineering. It is difficult to imagine that a single macroscale can, in general, satisfactorily replace the microscale in the solution of all the problems of interest. So, it makes sense to imagine that, optimally, you can have specific models on the macro scale to reproduce specific responses, or classes of them.

The measure of fidelity is known as the *measure of distortion* of the response provided by the two fields. This measure can be a scalar, a vector or a matrix. Without loss of generality, it will be assumed that the measure is scalar, since the other measures should always be transformed into one or a set of scalar measures. To exemplify, be the distance given by,

$$d(\mathbf{X},\mathbf{Y}) = (r(\mathbf{X}) - r(\mathbf{Y}))^2, \tag{5}$$

where $r(\mathbf{X})$ is the response due to the microscale and $r(\mathbf{Y})$ to the macroscale, usually functions implicitly defined by one *or different numerical simulators*.

There are no statistics in the eq. (5), that is, the random functions $r(\mathbf{X}):\Re^N \to \Re$, and $r(\mathbf{Y}):\Re^n \to \Re$ should be understood as an ensemble, or set, of samples, or realizations, $r(X_i), i=1,\ldots,N_R$, e $r(Y_i), i=1,\ldots,n_R$. In addition, it will be admitted, without loss of generality, that the microscale is represented only by a random variable Y. This means that the macro mesh has a single element, cell, or block, with a single property that, essentially, is its best stochastic representation. The distance, in this case, will be an application $d(\mathbf{X},Y):\Re^N \times \Re \to \Re^+$.

It is important to note, at this stage, that there is no reference to the physics that prevail in the geometric domain. It is possible, for example, to evaluate $r(\mathbf{X})$ in a complex physics of carbonates, using *Darcy-Stokes* or *Stokes-Brinkman* with *Darcyan* fractures, or even in compositional models, and $r(\mathbf{Y})$ in the physics of the *Black-Oil* model. The role of admitting heterogeneity in the physics involved is evident here.

In addition, some, or all the domain in the microscale may have been transformed into a spectral representation, such as the KKL decomposition or some of its variants. This is always unnecessary, but if it is done, it will possibly have significant and unknown loss of accuracy, as previously mentioned. It does not in any way replace the natural option of decreasing the accuracy in the calculation of the distortion.

The goal is twofold. First, a compression scheme of $\mathbf{X}$ to $\mathbf{Y}$ that leads to minimal distortion of the desired response and then determine its value. Determining the optimal transformation involves assessing the *a posteriori* distribution of $Y, p_Y(y)$.

Importantly, from a practical point of view, is that once the desired distortion is specified, the scheme will allow the determination of several suboptimal transformations and their respective distortions. In practice, suboptimal transformation could be preferable.

For the stochastic scheme to be complete, it is necessary to evaluate the distortion in a probabilistic way. One possibility is that distortion is the mathematical expectation of distance, but more significant functions for certain applications, such as percentiles and risk measures on probability density tails, can be chosen,

$$D = E[d(\mathbf{X}, Y)]. \tag{6a}$$

In cases, such as those described above, it is convenient to use expressions that represent *sample arithmetic means*, of the type,

$$d(x,y) = \frac{1}{M}\sum_{i=1}^{M}\left(R_i(y) - r_i(x)\right)^2, \tag{5b}$$

where index i can indicate, for example, each of the *M* components of the answers at a certain point, or at different points, in the domain.

The mathematical expectation of the distortion remains the same as in equation (6a), for example,

$$D(X;Y) = E_{p(x,y)}[d(x,y)] \tag{6b}$$

By hypothesis, the field that describes the microscale is given by the ensemble of N_R geostatistical realizations. Thus, the evaluation of the distortion, its mathematical expectation, or any other convenient stochastic measure, can be done using some Monte Carlo technique, or some simplifying variant. Schemes that avoid Monte Carlo can be imagined. Since ***X*** is already sampled it is possible to write, using the relationship between joint density and conditional density,

$$D = E[d(\mathbf{X},Y)] = \sum_{\mathbf{X},Y} p_{\mathbf{X}Y}(\mathbf{X},Y)d(\mathbf{X},Y) = \sum_{\mathbf{X},Y} p_{\mathbf{X}}(\mathbf{X})p_{\mathbf{X}Y}(Y/\mathbf{X})d(\mathbf{X},Y), \tag{7}$$

where $p_{\mathbf{X}Y}(Y/\mathbf{X})$ is the conditional density of Y. Its minimum with respect to $p_{\mathbf{X}Y}(Y/\mathbf{X})$, will be a *Dirac's delta* function that assigns to each x of X the Y that minimizes *d* (X,Y).

This optimization problem requires more computational effort than desired. Instead, we try to solve the *Augmented Lagrangean* with the restriction that indicator $I\,(X,Y)$ is less than or equal to a pre-specified value $I(\mathbf{X},Y) \le R$.

With this objective, we can develop eq. (1),

$$I(\mathbf{X},Y) = \sum_{\mathbf{X},Y} p_{\mathbf{X}}(\mathbf{X})p_{\mathbf{X}Y}(Y/\mathbf{X})\log\frac{p_{\mathbf{X}}(\mathbf{X})p_{\mathbf{X}Y}(Y/\mathbf{X})}{p_{\mathbf{X}}(\mathbf{X})\sum_{\mathbf{X}} p_{\mathbf{X}}(\mathbf{X})p_{\mathbf{X}Y}(Y/\mathbf{X})}, \tag{8}$$

obtaining, after cancellation of $p_{\mathbf{X}}(\mathbf{X})$,

$$I(\mathbf{X},Y)=\sum_{\mathbf{X},Y}p_{\mathbf{X}}(\mathbf{X})p_{\mathbf{X}Y}(Y/\mathbf{X})\log\frac{p_{\mathbf{X}Y}(Y/\mathbf{X})}{q_Y(Y)}, \tag{9}$$

where,

$$q_Y(Y)=\sum_{\mathbf{X}}p_{\mathbf{X}}(\mathbf{X})p_{\mathbf{X}Y}(Y/\mathbf{X}), \tag{10}$$

is the marginal of Y.The augmented Lagrangean function to be minimized will then give by,

$$F=D+T(I(\mathbf{X},Y)-R), \tag{11}$$

where $T\geq 0$ is the Lagrange multiplier. The minimum will be given for derivative of F, with respect to $p_{XY}(Y/X)$ equal to zero, and $T(I(X,Y)$ - $R)$ = 0 better known as Kuhn-Tucker conditions. In this way, keeping T greater than zero and gradually increasing R, realizations of will be obtained that are more informative of the realizations of $\mathbf{X}$. This minimization problem is equivalent to minimizing the complementary Lagrangian function,

$$F^c=I(\mathbf{X},Y)+\beta(D-D_0), \tag{12}$$

for a specified D_0 distortion. Both functions are simultaneously minimized for $T=\beta^{-1}$

The Lagrange multiplier T can be attributed the same meaning as the temperature in the method known as *Simulating Annealing*, originating in Statistical Mechanics. The algorithm described below takes advantage of this similarity.

The optimal conditional distribution is that of Gibbs, obtained by canceling the gradient of F,,

$$p^*_{XY}(Y/\mathbf{X})=\frac{q_Y(Y)\exp(-\frac{d(\mathbf{X},Y)}{T})}{Z(\mathbf{X})}, \tag{13}$$

where,

$$Z(\mathbf{X})=\sum_{\mathbf{X}}q_Y(Y)\exp(-\frac{d(\mathbf{X},Y)}{T}) \tag{13a}$$

is a normalizing constant. It converges to the Dirac delta when T goes to zero. The corresponding minimum of F will be,

$$F^*=-T\sum_{\mathbf{X}}p(\mathbf{X})\log Z(\mathbf{X})+TR=-T\sum_{\mathbf{X}}p(\mathbf{X})\log\sum_{\mathbf{X}}q_Y(Y)\exp(-\frac{d(\mathbf{X},Y)}{T})+TR. \tag{14}$$

We can eliminate the product TR from the above expression without any loss, since only the values of the variables that minimize it are relevant, namely, the Y realizations and their probabilities of occurrence given by the marginal $q_Y(Y)$ Achievements $\mathbf{X}$, in turn, are supposed to be provided associated with your probabilities. Geostatistical achievements, in general, are not ranked. In this case, it is usual to assume the same probability $1/N_R$ for each.

The problem posed is to minimize F^* in relation to the random variable Y submitted to the constraint that $\sum_i q_i = 1$, that is, to minimize the increased Lagrangean $F^{**}(y_i, q_i, \lambda)$ given by,

$$F^{**}(y_i, q_i, \lambda) = F^{*}(y_i, q_i) - \lambda(\sum_i q_i - 1), \tag{15}$$

where $y_i \in Y$ are the achievements on the macroscale, λ the Lagrange multiplier, and q_i the marginal of y_i Taking the gradient in q_i,

$$\frac{\partial F^{**}}{\partial q_i} = T \sum \frac{1}{Z(\mathbf{X})} \exp(\frac{d(\mathbf{X}, y_i)}{T}) = 0, \tag{16}$$

and, considering eq. (3) and eq. (10), results in that

$$\sum_X p_{\mathbf{X}}(\mathbf{X}) \frac{p_{\mathbf{X}Y}(Y / \mathbf{X})}{q_Y(Y)} = \frac{\lambda}{T} = 1. \tag{17}$$

Now taking the gradient in y_i,

$$\frac{\partial F^{**}}{\partial y_i} = \sum p_{\mathbf{X}}(\mathbf{X}) p^{*}_{\mathbf{X}Y}(y_i / \mathbf{X}) \frac{\partial d(\mathbf{X}, y_i)}{\partial y_i} = 0, \tag{18}$$

by which one obtains

$$r(y_i) = \frac{\sum_{\mathbf{X}} p_{\mathbf{X}}(\mathbf{X}) p_{\mathbf{X}Y}(y_i / \mathbf{X}) r(\mathbf{X})}{q_Y(y_i)}. \tag{19}$$

We are now able to formulate algorithms to determine *Y* and its associated marginal $q_Y(Y)$.

PDA Algorithm

The algorithm below is a version of the so-called *Deterministic Simulated Annealing*, or DA, elaborated and discussed in Koutsourelakis (2007) and Rose (1991, 1994, 1998). It finds Y and his associated marginal $q_Y(Y)$ It is considered a deterministic version of the classic *Stochastic Simulated Annealing*.

The details given are greater than those normally provided in the literature, allowing their immediate programming. In addition, the computations are ordered in such a way that the calculations for each microscale realization are done in parallel. Thus, the use of the geocellular mesh is encouraged because it is the description on a smaller available stochastic scale.

Algorithm PDA: *Parallel Deterministic Annealing*

(1)Start with K = 1 a sufficient higher value of $T = T_{\max}$ a factor $a < 1$,y_1 arbitrary, q_1 = 1, ε_1, ε_2 tolerances for convergences, and T_f a final value close to zero,

(2)Para k = 1, 2, ..., K do in parallel for each microscale realization.

a. Calculate the N_R distances to y_k, $d(X_i, Y_k) = (r(X_i) - r(y_k))^2$ eq. (5),

b. Calculate the N_R denominators, $Z(X_j) = \sum_{i=1}^{K} q_i \exp(-\frac{d(X_j, y_i)}{T})$,

c. Calculate the N_R conditional densities, $p(y_k/X_j)=\frac{q_k\exp(\frac{-d(X_j,y_k)}{T})}{Z(X_j)}$, eq. (13),

d. Estimate (Monte Carlo) the marginal of y_k, $q_k=\sum_{j=1}^{N_R}p(X_j)p(y_k/X_j)$, see eq. (10),

e. Estimate (Monte Carlo), $G_k=\sum_{j=1}^{N_R}p(X_j)p(y_k/X_j)r(X_j)$, see eq. (19),

f. Solve the unidimensional problem $y_k=r^{-1}(\frac{G_k}{q_k})$ see eq. (19).

(3)Check with ε_1 the convergence of Y_k and q_k If not satisfied, repeat step (2). Otherwise, continue to step (4),

(4)Estimate, using Monte Carlo, the average distortion, and the indicator, (in parallel),

a. The average distortion, $D=\sum_{k=1}^{K}\sum_{j=1}^{N_R}p(X_j)p(y_k/X_j)d(X_j,y_k)$,

b. The indicator, $I=\sum_{k=1}^{K}\sum_{j=1}^{N_R}p(X_j)p(y_k/X_j)\log\frac{p(y_k/X_j)}{q_k}$,

(5) Reduce the temperature T, $T\leftarrow aT\geq T_f$.

(6) Double the number of realizations y_k in other words, do $K\leftarrow 2K$ and initialize y_{K+k}= y_k, $q_{K+k}=q_k$, $k=1,\dots,K$.

(7) Eliminate redundancies with ε_2 in Y determine $n_R\leq K$ and consolidate q_k, k = 1, ..., n_R.

There are more current sequential versions of this algorithm, which will be studied later. Usually the cooling should be slow, as, for example, reducing the temperature by its thousandths, that is, a = 1/1.001. Modern Homotopy or Continuation methods can be used in an equivalent way.

What distinguishes this algorithm from *Simulated Annealing* is the introduction of a deterministic algorithm (*steepest descent*) at each temperature level. For some distances d and answers r to eq. (18) does not have a single fixed point, therefore, it does not offer a single answer. In these cases, one should choose the one with the lowest average distortion D.

The *Machine Learning* literature reports that, although with different algorithms and different objectives, suboptimal solutions obtained with a specific value for $\beta=T^{-1}$, dependent on the class of problems, are sufficient. This needs to be studied in the present context.

APLICATIONS

Example 1

In order to evaluate the quality of the formulation and the accuracy of its results, consider (Koutsourelakis, 2007) the second order differential equation with a variable stochastic coefficient, where $\omega\in\Omega$, Ω the sample space,

$$\frac{d}{dx}\left[a(x,\omega)\frac{dp}{dx}\right]=0,\ x\in[0,1], \tag{20}$$

with mixed boundary conditions, $p(0)=0$ and $v(1)=a(1)\left.\frac{dp}{dx}\right|_{x=1}$ =1.

This equation corresponds both to a problem of steady state monophasic flow in a porous medium with prescribed pressure and velocity, known as pressure equation; as for an elastic bar with prescribed displacements and force; Fig. 1.1.

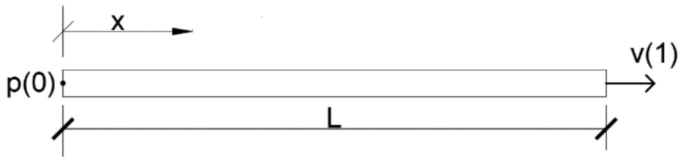

Figure 1.1 – Elastic bar or one dimensional, one phase, steady state flow in reservoir

Source: The Author.

The variability of the parameter $a(x,w)$, is given by,

$$a(x,\omega) = 1 + 0{,}5cos\left(2\pi\frac{x}{x_0} + \emptyset(\omega)\right) \qquad (21)$$

where the phase angle $\emptyset(w)$ is uniformly distributed over the interval $[0,2\pi]$, and the constant x_0 characterizes the length or scale of correlation of spatial heterogeneity. For each realization, there is an equivalent, or effective parameter, given by the harmonic mean of its values in the domain. For small values of the correlation length the variance is small, and the distribution of the effective parameter can be given by its harmonic mean.

The problem is to find the equivalent distribution for the determination of $p(1)$ when the correlation length is large, typically larger than the domain. The chosen microscale has 1000 elements, and the macroscale only one element. The scheme used is of the local-global type. Two exercises are performed, one with a correlation length less than the length of the domain, and the other with a correlation length ten times its length. Note that the learning takes place for fixed boundary conditions, unlike Example 2, where the learning will take place for a given range of variation of the boundary condition.

For x_0 =1/100, the stochastic field was described by 100 microscale realizations, and the 100 solutions were calculated for estimating $p(1)$, one for each realization. The macro-scale realizations are then estimated, *oriented* towards the estimate of $p(1)$.The problem is essentially deterministic and the result is a single realization with the parameter given by the harmonic mean. The mathematical expectation of distortion is null.

Taking x_0 =10 >> 1, greater than the extension of the geometric domain, and simulating 1000 microscale realizations, the macro realizations were recalculated, with the same objective of determining $p(1)$. Fig. 1.2 shows the Distortion-Rate graph. To avoid that the algorithm remains trapped in a local minimum, only N_R = 500 realizations were used by means of random selections, during the annealing, of the $v(1)$'s values in the microscale.

The initial temperature used was T =100 with a slow annealing given by a = 1/1.001. Fig. 1.3 shows the *optimal density* of the effective properties calculated for the macroscale. The distributions on the two scales are shown in the Fig. 1.4.

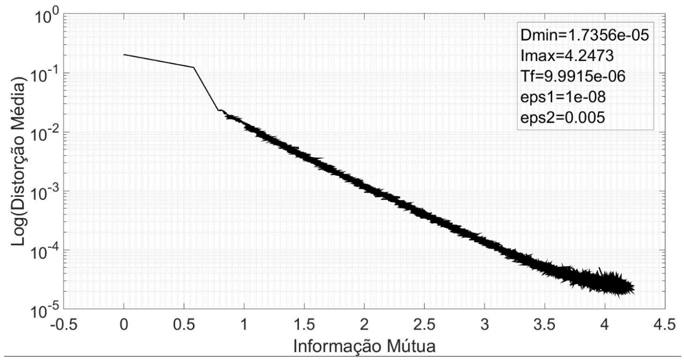

Figure 1.2 - Average Distortion × Mutual Information, Example 1, showing its minimum (Dmin) and maximum (Imáx) values, respectively, the final temperature value Tf and the PDA convergence tolerances.

Source: The Author.

Fig. 1.4 shows the exact distribution of $p(1)$ obtained using the effective parameters, a_{efi}, i = 1, ..., 1000, given by the harmonic means of the parameters of the elements in each realization i. The solution for each realization is given by,

$$p_i(1) = v(1)/a_{ef_i} = 1/a_{ef_i}, \tag{22}$$

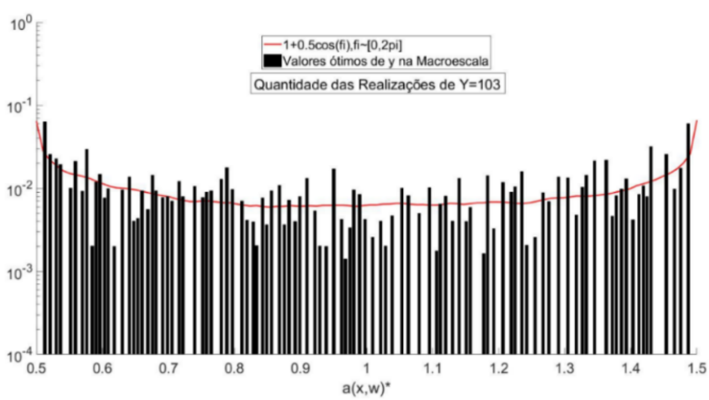

Figure 1.3 - Density and distribution of realizations on the two scales, Example 1, only 1 macro element.

Source: The Author.

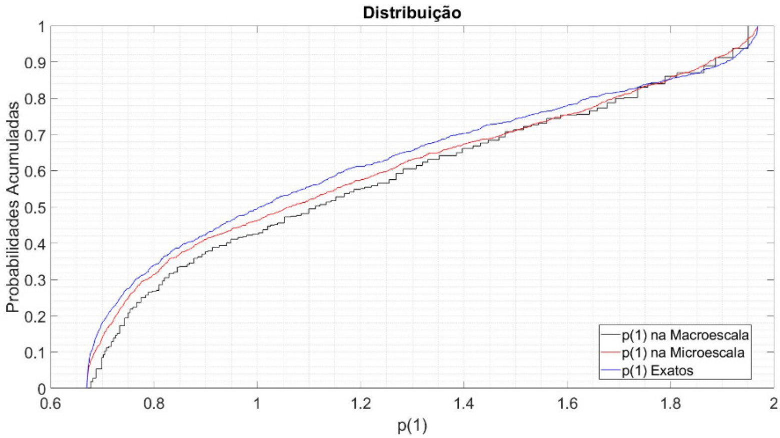

Figure 1.4 - Distribution of realizations of displacement (pressures) on the macroscale, microscale and exact. Example 1, only 1 macro element.

Source: The Author.

while the probabilities $q_i[pi(1)]$ of the 1000 realizations of the solution $pi(1)$, i = 1, ..., 1000, are uniformly distributed,

$$q_i[(p_i(1)] = {}^1/_{1000}. \tag{23}$$

The distributions of $p(1)$ on the microscale and on the macroscale are also shown in Fig. 1.4. The sampling in the microscale, for each of the realizations, was obtained from the solution of the linear system resulting from the discretization of eq. (20). The probabilities of N_R realizations in the micromesh are uniformly distributed with 1/ N_R, where N_R = 1000.

The optimal distribution of the solution on the macro scale was obtained with n_R = 103 realizations y_i and their respective probabilities q_i, arising from the PDA, as Fig. (1.3). The q_i [p_i(1)] probabilities of the optimal p_i(1) are obtained as,

$$p_i(1) = \frac{v(1)}{y_i} \tag{24}$$

$$q_i[p_i(1)] = \frac{q[v(1)]}{q(y_i)}\frac{1}{Z_i} = \frac{q(y_i)^{-1}}{Z_i} \tag{25}$$

where, $Z_i = \sum_{i=1}^{n_R} \frac{1}{p(y_i)}$ is a normalization constant.

In Fig. 1.4, there is a difference between the values obtained of $p(1)$ in the microscale and the exact solution, due to the processes used in the calculations; in the microscale through linear systems and in the exact one using effective parameters. As it is a stochastic problem, small variations can be found for different methods of solution.

The number of realizations used in the macroscale, n_R = 103, can be considered large. This is an extreme example with a long correlation length and great variability, completely inappropriate for KKL expansions and decompositions (PCA, POD).

Example 2

In this example, the proposed methodology is applied to a one-dimensional reservoir with two-phase flow, of oil and water, and depletion by water injection, studied by Emerick and Reynolds (2013). This reservoir was also used to study strategies and algorithms in stochastic control by Fonseca (2015).

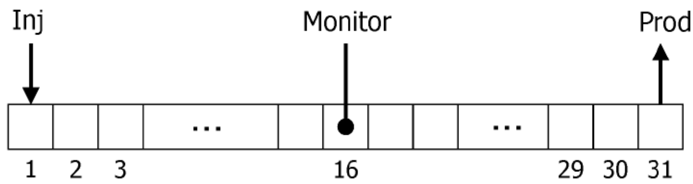

Figure 2.1 - Reservoir micromesh. Emerick, A, Reynolds, A, (2013)

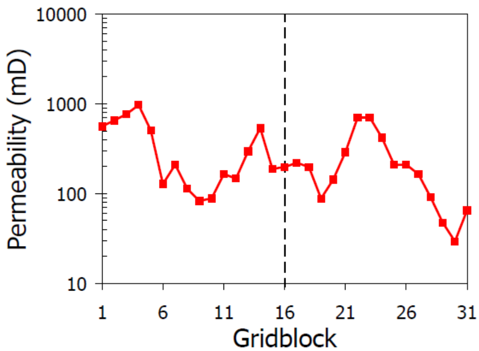

Figure 2.2 - Permeability of the true model represented by its 100 realizations in the micromesh. Emerick, A, Reynolds, A, (2013).

The reservoir is described in Fig. 2.1 and has 31 blocks of dimensions 50ft x 50ft x 50ft. The natural logarithm of permeabilities, $In(k)$, has an exponential autocorrelation function with a correlation length of 10 blocks, with a mean of 5 and variance 1. The porosity is constant and equal to 0.25, the water viscosity is 1.0cP and oil, 2.0cP. The initial pressure in the reservoir is 3500psi and the compressibility of oil, water and rock are $10^{-5}psi^{-1}$, 10^{-6} psi^{-1} e 5 x 10^{-6} psi^{-1}, respectively. There is a water injector well in the first block that operates with a 4000 psi downhole pressure. In the last block there is a producing well that operates at a bottom pressure of 3000 psi. There is a pressure observation well in the center of the reservoir. The production period is 360$days$, with monthly measurements. The production period was defined such that there is water production in the observation well, but not in the producing well.

Authors generated a permeability field described by 100 equally probable realizations, based on the scenario shown in Fig.2.2. All the problem data were provided by the authors through digital files, as well as the executable code of the simulator used by them. The problem was originally devised to compare methods for solving inverse problems for permeability fields.

The exercise here consists in determining the new field of absolute permeabilities for the macro mesh given in Fig.2.3. Original micromesh dimensions of the three blocks with wells were maintained. The remaining blocks were scaled two by two, resulting in a macro mesh of 1 blocks. It is known that, in multiphase problems, there is also a need to change the scale of the relative permeabilities, and that the reservoirs are more sensitive to this change in scale if the reduction in cardinality is high. The reduction in geometric cardinality in this exercise is the lowest possible uniform reduction. Therefore, it is expected that the absence of a change in the scale of relative permeabilities will have little influence.

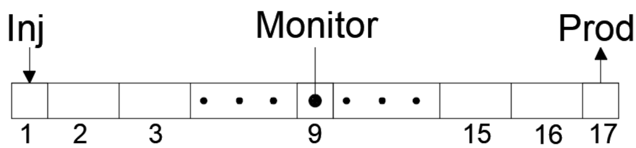

Figure 2.3 – Reservoir macromesh.

Source: The Author.

Reservoir simulations used in this example were made with MRST-2017b, Lie (2016), and the scale transposition was done with the values taken from the simulations, in a single-phase problem (water), when reservoir were in steady state flow.

The procedure starts with the simulation of the 100 realizations in the micro mesh. These are the only simulations performed on the micro mesh. 14 scale changes were made, one for each macro element, with Dirichlet boundary conditions in the simulation of each macro element, and with the distortion measure given by Eq. (5b).

Boundary conditions for each macroelement were calculated with the stationary values of the micro mesh, where the pressure on the left (right) is the pressure of the microelement on its left (right).

The responses, $r\,(x_j)$, used in Eq. (5b) were the speeds at the interface of each two microelements; while the answers, $R(y_k)$, are the velocities at the center of each macro element.

For the solution of the one variable inverse problem, given by,

$$y_k = R^{-1}\left[\frac{E_{p(x,y_k)}[r(x)]}{p(y_k)}\right] = R^{-1}\left[\frac{G(X;y_k)}{p(y_k)}\right]. \quad (27)$$

Among the three options given by Zujl and Trykozko (2001), the first option was used, which corresponds to the conservation of the driving force. With this option,

$$y_k = k_k^* = \frac{-\mathrm{u}}{\nabla \mathrm{p}} = \frac{G(X;y_k)l}{p(y_k)(p_o - p_i)} \tag{28}$$

where $\bar{u}$ is the average speed at the center of the macro element, l = 100ft is its length, and p_i and p_o are the pressures on the left and right sides of the macro element, respectively.

Table 2.1 summarizes the data and results for this example. Fig. 2.4 shows the Average Distortion by Mutual Information graph for two macro element. Figs. 2.5 shows the quantization of the probability densities of the absolute permeabilities obtained during the application of the PDA for two macroelement. Fig. 2.6 shows the speeds obtained for two element of the macro mesh and micro mesh. In order to verify the results obtained by the PDA, a comparison between the model obtained by the macro mesh and the original model in the micro mesh, both biphasic, was carried out. Figs. 2.7 and 2.8 show the water and oil saturations and the reservoir pressures in 750 days in both the macro mesh and the micromesh.

Example 2 - Results obtained by PDA				
$Tf = 0.5 \times 10^{-7}$ $\epsilon 1 = 1 \times 10^{-5}$ $\epsilon 2 = 5$				
Macroelements	$\overline{\nabla p} \times 10^5$	D_{min}	$I_{máx}$	$\mathbf{n_R}$
2	7,32	4.45×10^{-9}	10.83	12
3	6,56	1.25×10^{-12}	5.79	10
4	5,81	3.01×10^{-10}	24.21	11
5	5,40	4.25×10^{-12}	17.63	8
6	5,19	1.94×10^{-10}	13.02	9
7	5,98	8.32×10^{-9}	12.16	16
8	6,03	8.98×10^{-10}	49.08	12
10	6,15	5.27×10^{-12}	12.02	8
11	5,99	8.76×10^{-9}	19.75	11
12	5,72	5.34×10^{-10}	12.30	7
13	6,55	2.07×10^{-10}	11.01	10
14	6,02	3.64×10^{-10}	14.38	12
15	6,28	7.59×10^{-9}	16.92	8
16	7,27	9.06×10^{-9}	2.74	15

Table 2.1: Summary of the results obtained in Example 2, showing the values of the pressure gradient (force), the minimum value of the mean distortion (Dmin), the maximum value of the mutual information (Imax) and the temperature (Tf), the amount of achievements of the macro mesh and the tolerances used in the PDA algorithm.

Source: The Author.

From the results obtained in Table 2.1, it can be seen that the distortions, D_{min}, were very small, with an order of magnitude from 10^{-9} a 10^{-12}, a fact that results from the application of the PDA algorithm in just two blocks (in the other applications they ranged from 100 to 1000). Mutual Information continues to demonstrate good results, for non-linear time dependent problems.

The number of realizations, n_R, varied between 7 and 16, which shows a significant reduction in the probability dimension of the micro mesh, in the order of 90%.

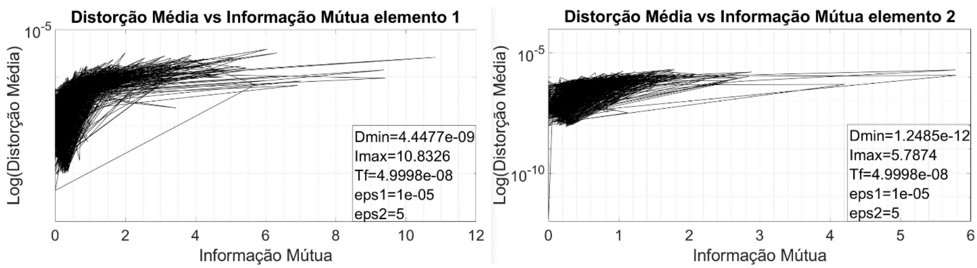

Figure 2.4: Average distortion and mutual information of macroelements 1 and 2.

Source: The Author.

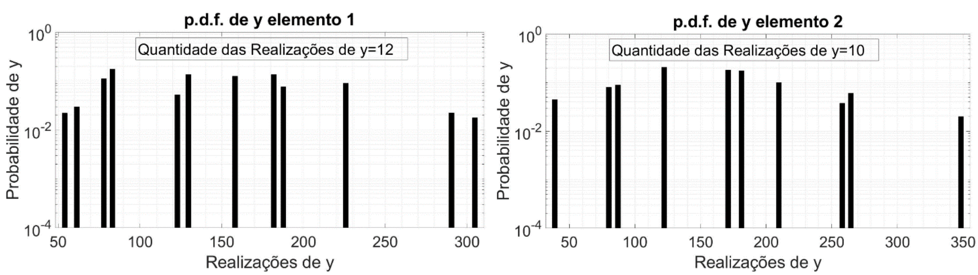

Figure 2.5: Quantization of the densities of the properties of macroelements 1 and 2.

Source: The Author.

From the analysis of the saturation and pressure graphs, Fig. 2.6 and Fig. 2.7 of the two-phase reservoir it is possible to say that the results obtained with 100 micro meshes and 10 macro meshes realizations are very close, in particular that of the pressures, showing that, with the application of the PDA in two phases reservoir problems, it is possible to reduce both the probabilistic dimension and the cardinality of the meshes in a controlled and goal-oriented manner.

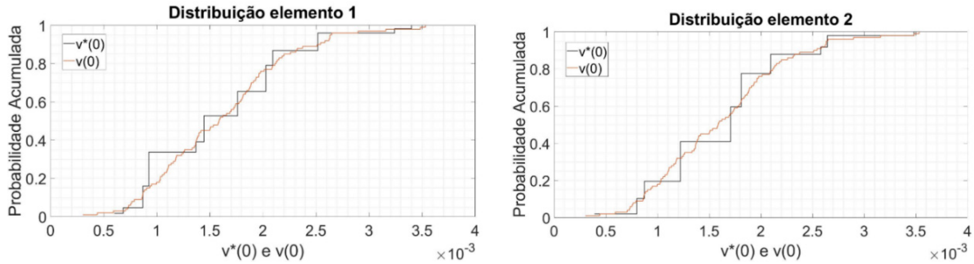

Figure 2.6: Velocity distribution of macroelements 1 and 2.

Source: The Author.

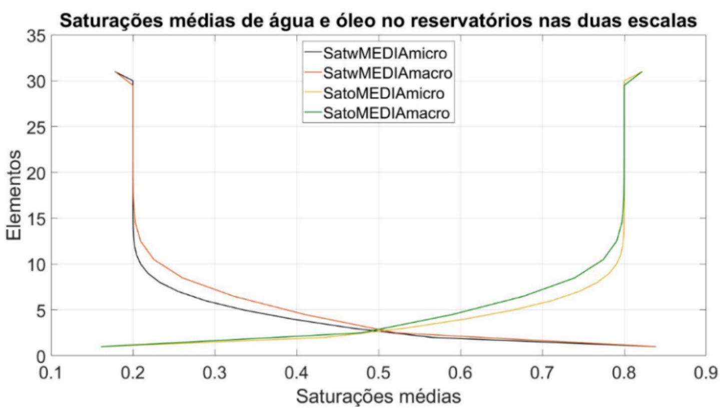

Figure 2.7 – Average saturation of water and oil in the reservoir in both scales, at 750 days, showing the average saturation of water and oil in the micro mesh and the macro mesh

Source: The Author.

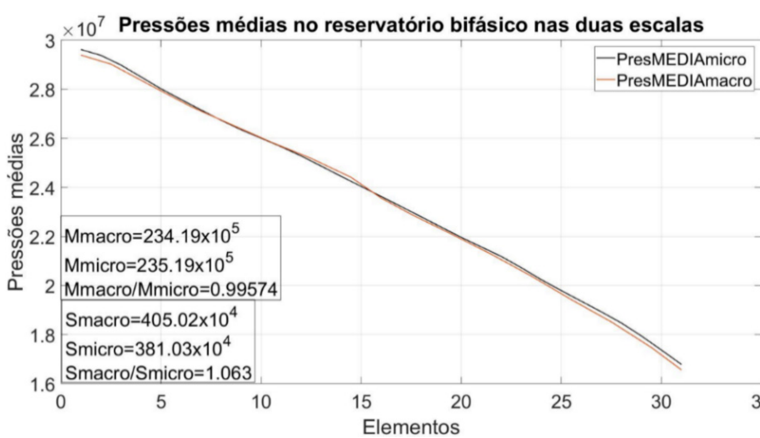

Figure 2.8 – Average reservoir pressures at both scales, at 750 days.

Source: The Author.

CONCLUSIONS

The main conclusion to be drawn from this work is that the development of a computer program for the end user is fully justified. This program would use calls to a commercial program, as a black box, for control and optimization of reservoir management. In addition, other relevant conclusions can be highlighted, which may be:

Determining the succession of distributions from a given temperature to the optimal distribution has an extremely high computational cost.

The scale change process studied is quite adequate to produce models that estimate characteristic values of a solution distribution. The proposed technique can then be classified as goal oriented. It is thought that it must be especially important in the problems of stochastic control (closed loop control) and stochastic optimization.

Proposed techniques should obtain more expressive computational gains in problems with three-dimensional geometric domain.

Application of Monte Carlo methods for Multiple Scales (MSMC) in reservoirs with heterogeneous (or physical) permeabilities requires that there are at least three meshes embedded, physically and probabilistically consistent. The author does not know any method of scale change in the literature that simultaneously meets these three requirements, in addition to what is proposed in this work.

The mathematical and computational experience acquired in the development of this work suggests that the continuity of the investigative process may be in the direction of some points.

Given an ensemble with N_R realizations, it is not possible to know a priori what the number of realizations is to be used to analyze the microscale, unless after the numerical simulation of each realization, and, perhaps, after the analysis of the statistics. In other words, which realizations are of interest, a priori, in each problem? This question stems from the fact that, for realistic problems, the viable number of simulations, n_s, must be much less than the amount N_R of geocellular realizations, typically between a dozen and a hundred, $n_S \in [10{,}100] \ll N_R$. Procedures that avoid the numerical simulation of all geocellular realizations must be investigated. Some possibilities that merit systematic investigation can easily be glimpsed.

A possible alternative procedure to PDA is to establish a priori, (and, perhaps, adaptively) a specific amount of macro realizations, and to use a stochastic-deterministic algorithm (e.g. SPSA) to directly minimize the functional $F[p(y|x)]$, or its complement, $F^c[p(y|x)]$, or some variant of them. One possibility is to use Stochastic Variational Inference to maximize a lower dimension of one of these functionalities. These changes may allow for some semi-local-global schemes that are not easily treatable by the techniques of this work.

Finally, the future seems to point to the use of ideas recently exposed in the literature that is dedicated to the construction of a mathematical analysis of *Deep Learning*, until then non-existent - see Tishby, Pereira and Bialek (1999), for the origins of their origins. The idea is to extend the Distortion Rates Theory by conditioning the solution to similarity with a third distribution. Variational Principles are established and as a consequence, the distortion measure becomes a Kullback-Leibler distance - a metric distance between two distributions.

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APPENDIX

Scale Transposition Schemes

The large dimensions of the real reservoirs justify schemes that avoid the simulation of the micro mesh in the PDA algorithm. Weinan and Engquist, 2003, suggest some schemes that today are widely used in the deterministic *upscaling* literature, which can, with great advantages, also be used in the scale transposition methodology proposed in this work.

Fig. A1 shows the scheme called local-local (LL), by which only the region to be homogenized (hatched) is simulated, instead of the simulation of the entire micro mesh. Good results are expected with this scheme when the correlation length of the geostatistical realization is sufficiently small. Strictly, in the order of the diameter of the region to be homogenized.

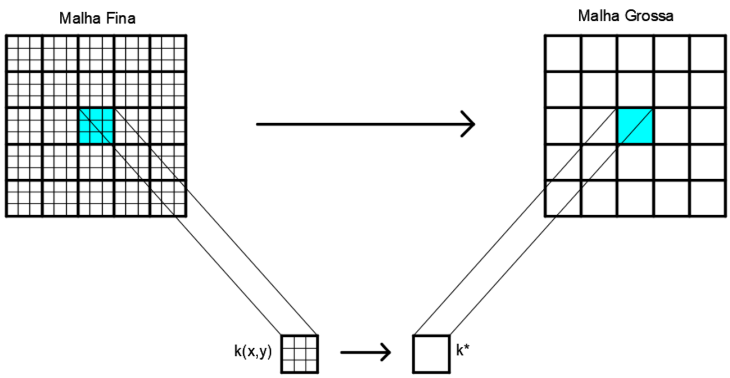

Figure A1 – Local-local scheme (LL), Weinan and Engquist, 2003.

Fig. A2 shows a semilocal-local (SL) scheme to be considered when the correlation length is greater than the region to be homogenized. For correlation lengths of the order of magnitude of the reservoir, or greater, a global-local (GL) scheme may be convenient. The decision on the scheme to be used depends on the acceptable balance between cost and accuracy.

The choice of the type of scheme should be adaptive, that is, the choice should be made as the PDA algorithm develops. With the intention of balancing the cost-accuracy ratio, the schemes should vary from region to region of the reservoir. The geometric dimensions of the region to be homogenized is also subject to the decision to balance the cost-accuracy ratio.

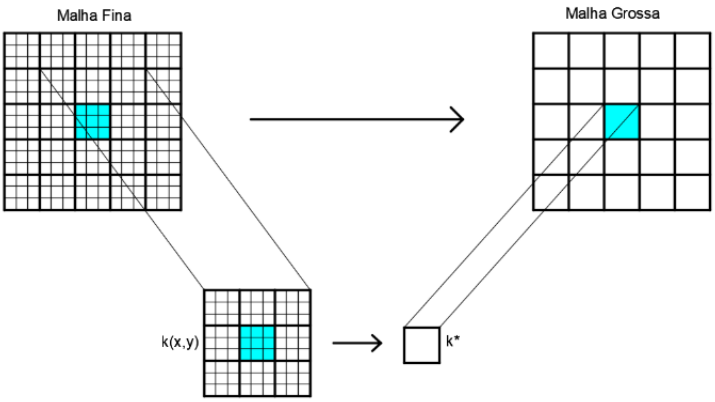

Figure A2 - Semilocal-local scheme (SL), Weinan and Engquist, 2003, with the global-local scheme (GL) as a limit.

At the geometric limit of the SL schemes is the global-local scheme (GL), when the entire micro mesh is simulated in the PDA.

In choosing these alternative schemes, a strong influence of the type of reservoir problem is also expected. Less demanding schemes can be used when dealing with problems that involve the entire reservoir and that depend a lot on the average behavior of the reservoir, such as, for example, in the stochastic control and optimization under uncertainty of the field NPV in the sweeping water. In some problems, the intensity of discretization around the wells can be decisive. This seems to be the case for thermal recoveries with parallel wells close to vapor injection and fluid intake, as well as around smart wells with multiple flow outlets.

The example used in this work were developed with the global-local scheme, GL.

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