ACCELERATION OF GENETIC ALGORITHMS FOR THE DESIGN OF RANDOM MICRO-HETEROGENEOUS MATERIALS

Federico Carlos Buroni
GMAp Group of Applied Mechanics – Universidade Federal do Rio Grande do Sul - CNPq
Rua Sarmento Leite 425, 90050-150, Porto Alegre, Brasil
fedeburoni@mecanica.ufrgs.br

Herbert Martins Gomes
GMAp Group of Applied Mechanics – Universidade Federal do Rio Grande do Sul
Rua Sarmento Leite 425, 90050-150, Porto Alegre, Brasil
herbert@mecanica.ufrgs.br

Adrián Pablo Cisilino
Welding and Fracture Division, INTEMA, CONICET – Universidad Nacional de Mar del Plata
Av. Juan B. Justo 4302 (7600), Mar del Plata, Argentina
cisilino@fi.mdp.edu.ar

Abstract. *A key of success of many modern structural components is the tailored behavior of the material. A relatively inexpensive way to obtain macroscopically desired responses is to enhance the base matrix properties by the addition of microscopic matter (particles), i.e. to manipulate the microstructure. It is presented in this work a general procedure for the design of random micro-heterogeneous materials in order to deliver a specified linearly elastic response. The devised procedure makes use of genetic algorithm (GA) with approximate fitness evaluation. The design variables are the Young modulus and the Poisson ratio of the particles and the particle volume fraction. When compared with standard GA's, the proposed algorithm results in important savings in computing time with only minor losses in accuracy.*

Keywords: *Genetic algorithms, effective mechanical properties, random micro-heterogeneous materials, acceleration of algorithms*

1. Introduction

A key of success of many modern structural components is the tailored behavior of the material. A relatively inexpensive way to obtain macroscopically desired responses is to enhance the base matrix properties by the addition of microscopic matter, *i.e.* to manipulate the microstructure. Accordingly, in many modern engineering designs, materials with highly complex microstructures are now in use. The macroscopic characteristics of modified base materials are the aggregate response of an assemblage of different "pure" components, for example several particles or fibers suspended in a binding matrix material. Thus, microscale inhomogeneities are encountered in metal matrix composites, concrete, etc. In the construction of such materials, the basic philosophy is to select material combinations to produce desired aggregate responses. For example, in structural engineering applications, the classical choice is a harder particulate phase that serves as a stiffening agent for a ductile, easy to form, base matrix material.

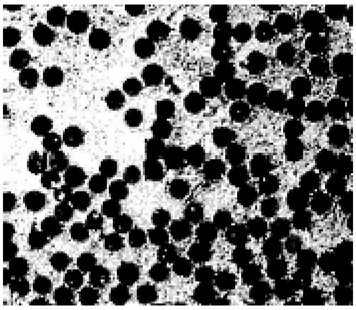
If one were to attempt to perform a direct numerical simulation of the mechanical response of a macroscopic engineering structure composed of a microheterogeneous material incorporating all the microscale details, an extremely fine spatial discretization mesh would be needed. Furthermore, the exact subsurface geometry is virtually impossible to ascertain throughout the structure. In short, complete solutions are virtually impossible. Because of these facts, regularized or homogenized material models are used. The usual approach is the compute a constitutive "relation between averages", relating volume averaged field variables. The volume averaging takes place over a statistically representative sample of material, referred in the literature as a representative volume element (RVE). The internal fields to be volumetrically averaged must be computed by solving series of boundary value problems with test loadings (see Zohdi, 2002).

There are a variety of difficulties in the computational design of macroscopic solid material properties formed by doping a base matrix material with randomly distributed particles of different phases. There are three primary problems are: (1) the wide array of free microdesign variables, such as particle topology, volume fraction and mechanical property phase contrasts, which force the associated objective functions to be highly nonconvex, (2) the associated objective functions are not continuously differentiable with respect to design space, primarily due to microscale design constraints, such as limits on the desired local stress field intensities, and (3) the effective responses of various finite sized samples, of equal volume but of different random distributions of the particulate matter, exhibit mutual fluctuations, leading to amplified noise in optimization strategies where objective function sensitivities or comparisons are needed. The lack of robustness of classical gradient based deterministic optimization processes to solve this kind of problems can be rectified by application of a family of methods, usually termed "genetic" algorithms. Genetic algorithms (GA) are search methods based on the principles of natural selection and, as such, they are highly probabilistic. There are a variety of such methods, which employ concepts of species evolution, such as reproduction, mutation and crossover (Goldberg, 1999). At the same time, it is worth to mention that GA's could result very expensive in terms of computing costs as they could require the objective function to be evaluated hundreds (if not thousands) of times.

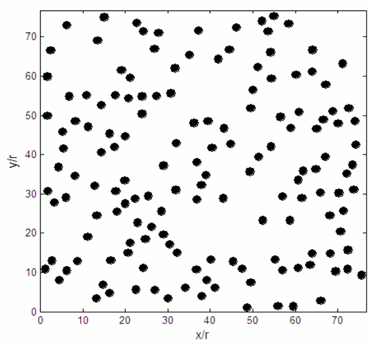
This work presents a general procedure to determine possible microstructures that can deliver a specified linearly elastic response. The devised procedure makes use of a GA with approximate evaluation of the objective function. When compared with standard GA's, the approximate objective function evaluation results in important savings in computing time with only minor losses in accuracy.

2. Computational testing methods

A variety of materials are characterized by particulate inhomogeneities embedded in an otherwise homogeneous base matrix, for example aluminum-boron alloy (Figure 1-a). The simplified microstructure considered is this work consists in an isotropic and homogeneous matrix with spherical inclusions randomly distributed (see Figure 1-b). The problem was assumed two-dimensional in order to be solved using the available computer resources (desktop PC).



(a)



(b)

Figure 1. (a) Microstructure of 6061 aluminum alloy reinforced with pitch-55 boron (x250) (b) Microstructure considered in this work.

The objective function for the GA was selected as the difference between the desired effective mechanical properties and those resulting for the optimized microstructure. As the isotropic behavior of a material is completely represented by two independent constant, the expression for the objective function is:

$$\Pi = \left| \omega_\kappa \frac{\left(\kappa^* - \kappa_D^*\right)}{\kappa_D^*} \right| + \left| \omega_\mu \frac{\left(\mu^* - \mu_D^*\right)}{\mu_D^*} \right| \tag{1}$$

where κ^* and μ^* are the effective bulk modulus and the effective shear modulus, respectively. The subscript *D* denotes the "desired" elastic constants. The coefficients ω_κ and ω_μ stand for weighting factors that are set by the user in order to make the two terms in the RHS of expression (1) of the same magnitude.

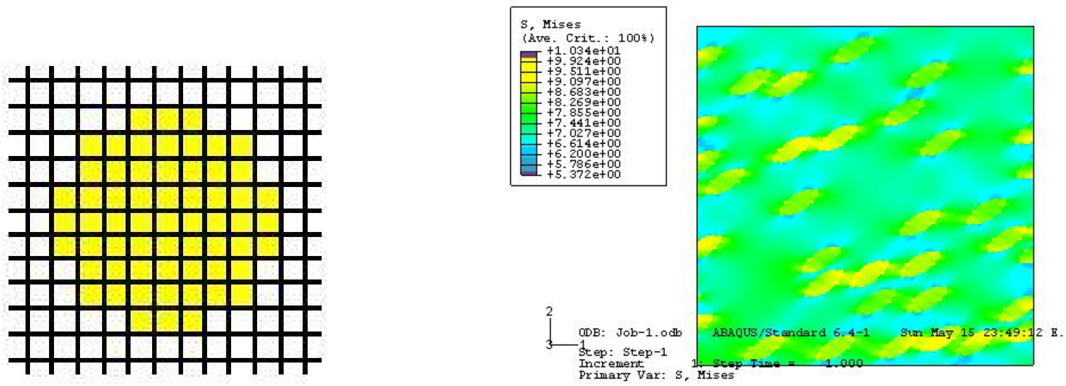
The effective elastic constants κ^* and μ^* are evaluated using expressions (2) and (3):

$$3\kappa^* = \frac{\left\langle \frac{tr\sigma}{3} \right\rangle_\Omega}{\left\langle \frac{tr\varepsilon}{3} \right\rangle_\Omega} \tag{2}$$

$$2\mu^* = \sqrt{\frac{\left\langle \sigma - \frac{tr\sigma}{3} I \right\rangle_\Omega : \left\langle \sigma - \frac{tr\sigma}{3} I \right\rangle_\Omega}{\left\langle \varepsilon - \frac{tr\varepsilon}{3} I \right\rangle_\Omega : \left\langle \varepsilon - \frac{tr\varepsilon}{3} I \right\rangle_\Omega}} \quad (3)$$

where the domain Ω must be defined large enough to be a statistically representative of the microstructure (the representative volume element or RVE). The operator $\left\langle \cdot \right\rangle_\Omega \overset{def}{=} \frac{1}{|\Omega|} \int_\Omega \cdot \, d\Omega$, the symbol ":" denotes the operation defined $\mathbf{A} : \mathbf{B} \overset{def}{=} \mathrm{A}_{ij} \mathrm{B}_{ij} = tr\left(\mathbf{A}^T \mathbf{B}\right)$ where Einstein index summation notation is used, and σ and ε are the stress and strain tensor fields within a microscopic sample of material, with volume $|\Omega|$. The boundary conditions must be of linear displacement for the fulfillment of the Hill's energy condition (Zohdi, 2002; Nemat-Nasser and Hori, 1999). Also the material must be perfectly bonded (without interface separation) and in absence of body forces. For isotropic effective response only one load case containing non-zero spherical and deviatoric components is sufficient to determine the effective bulk and shear moduli.

The elastic problems were solved by means of FEA using Abaqus Standard 6.4 (Hibbitt, Karlsson & Sorensen, R.I. USA, 2004). In order to facilitate the automatic mesh generation for the microstructures an aligned mesh strategy was employed. This approach imposes that the element boundaries coincide with material interfaces and therefore the elements have no material discontinuities within them. Following the results of the convergence study performed in a previous work (Buroni, 2004), each particle was discretized using 9 elements in the diameter (see Figure 2-a). The model discretization is performed using 4-node bilinear elements in plane stress condition (CPS4R). Figure 2-b illustrates a typical result for the stress field.



(a) (b)

Figure 2. (a) One particle scheme discretization of one particle. (b) A typical result for the von Mises stress field.

The size of RVE is selected based on the results of previous works by the authors (Buroni, 2004 and Batista et al., 2003). In these works the size of the RVE was computed by using the strategy proposed by Zohdi (2003), which is based in the statistical analysis of the macroscopic response of a set of samples containing an increasing number of inclusions. The RVE is given by the size of the sample containing the lowest number of inclusions for which the macroscopic response results invariant. Based on this criterion the RVE was chosen to have 30 inclusions for the example presented in this work.

The Young modulus E_p and the Poisson ratio ν_p of the particles and the particle volume fraction ϕ were selected as design variables. On the other hand, the mechanical properties of the matrix were prescribed and kept constant during the optimization process. The particle volume fraction ϕ was allowed to vary within the range $0.05 \leq \phi \leq 0.2$. The fulfillment of the Drucker stability conditions (Malvern, 1968) for the inclusion material was enforced by penalization. In this way, an arbitrarily high value was assigned to the objective function of those individuals with design variables not fulfilling the Drucker stability conditions.

3. Genetic Algorithm with approximate evaluation of the objective function

GA's popularity is partially due to the facts that (i) they do not require continuity and/or differentiability of the functions involved, (ii) do not require extensive problem (re-)formulation, (iii) are not very sensitive to the initialization procedure, (iv) are less prone converge to entrapment in local optima, and (v) are naturally parallel (Goldberg 1999).

The approximate models for the objective function serve to speed up GA's. The incorporation of approximate models in evolutionary computation should ensure that the evolutionary algorithm converges to the global optimum (or close to it) and that the computational cost is reduced as much as possible. When the approximate model is used together with the original function a model management or evolution control is required. Thus, an individual that is evaluated with the original objective function is called a *controlled individual* and a generation evaluated with the original function is called a *controlled generation*. As far as model management is concerned one has (Fonseca et al. 2004):

- *No Evolution Control*: The approximate model is high-fidelity and the original objective function is not used in evaluations.
- *Fixed Evolution Control*: Two approaches can be used: individual-based and generation-based. In individual-based control some of the individuals are evaluated with the approximated model and others are evaluated with the original fitness function. In generation-based control the whole generation is either evaluated with the approximate model or with the exact fitness function.
- *Adaptive Evolution Control:* The frequency of evolution control depends on the observed fidelity of the approximate model.

In this work, *Fixed Evolution Control* is employed. The proposed strategy uses both individual-based and generation-based controls. Controlled and approximated generations are processed alternatively (i.e. an approximated generation is always followed by a controlled generation). At the same time, a small fraction of the individuals in the approximated generations have their fitness evaluated using the original fitness function (controlled individuals). The number of controlled individuals is specified via the *Fraction of control*, which it is defined as the ratio between the number of controlled individuals and the population size.

Individuals evaluated using the approximate model inherit their fitness value from their parents. This scheme is similar to that proposed by Fonseca et al. (2004). It is proposed in this work that the fitness value results from the weighted average of the fitness value of the parents, with the weights given by the crossover point. Thus, the resulting fitness function depends of the number of genes that each individual inherits from each parent. The diagram in Figure 3 illustrates the proposed procedure which makes use of a *single point* strategy.

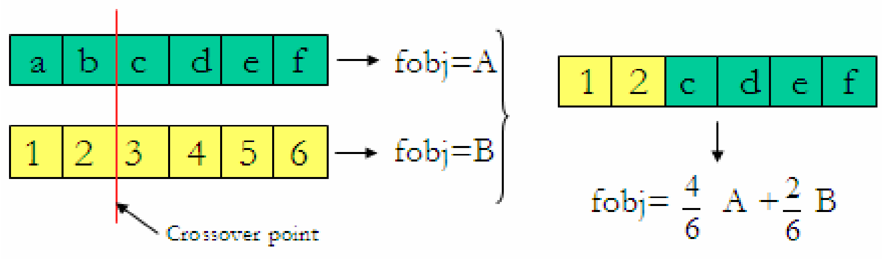


Figure 3. Diagram of fitness inheritance procedure.

The above described procedure was implemented in MATLAB by adapting the *Genetic Algorithm* toolbox. The function *ga.m* was modified in order to include the new variable *Fraction of Control* as it is showed in the figure 4.

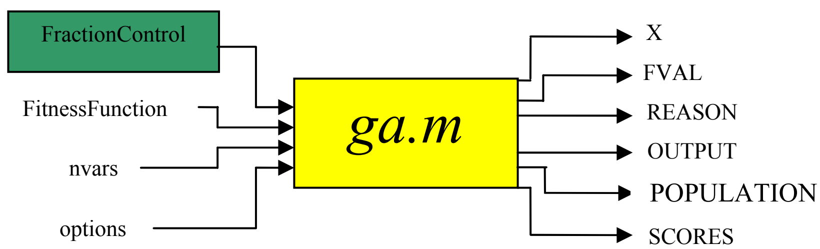


Figure 4. Diagram of variables for the *ga.m* function.

Then, the input variables for the modified *ga.m* function are: the fraction of control (*FractionControl*), the objective function (*FitnessFunction*), the number of variables (*nvars*) and some optional parameters (*options*). The output variables are: the fittest individual *(X)*, the objective function value for the fittest individual (*FVAL*) and some other information. During the optimization procedure the first generation is always a controlled one. The second generation is an approximated one, with the number of controlled individuals specified by *FractionControl*. The process continues by alternating controlled and approximated generations.

The function *stepGA.m* of the MATLAB toolbox computes the objective function value of the new individuals. This function (which is called by *ga.m*) was also adapted to include the approximate model for the objective function. Thus, two new input variables have been included: *FractionControl* and *Control*. The later serve to indicate whether a generation is controlled or approximated. The function *stepGA.m* computes the objective function of the new individuals using the function *fval.m* and *crossoversinglepoint.m*. The later has been also adapted to include the computation of the weights for the approximated model. The computed weights are stored in the vector *pesosPonder*. Figure 6 illustrates a diagram with the changes introduced to *stepGA.m*.

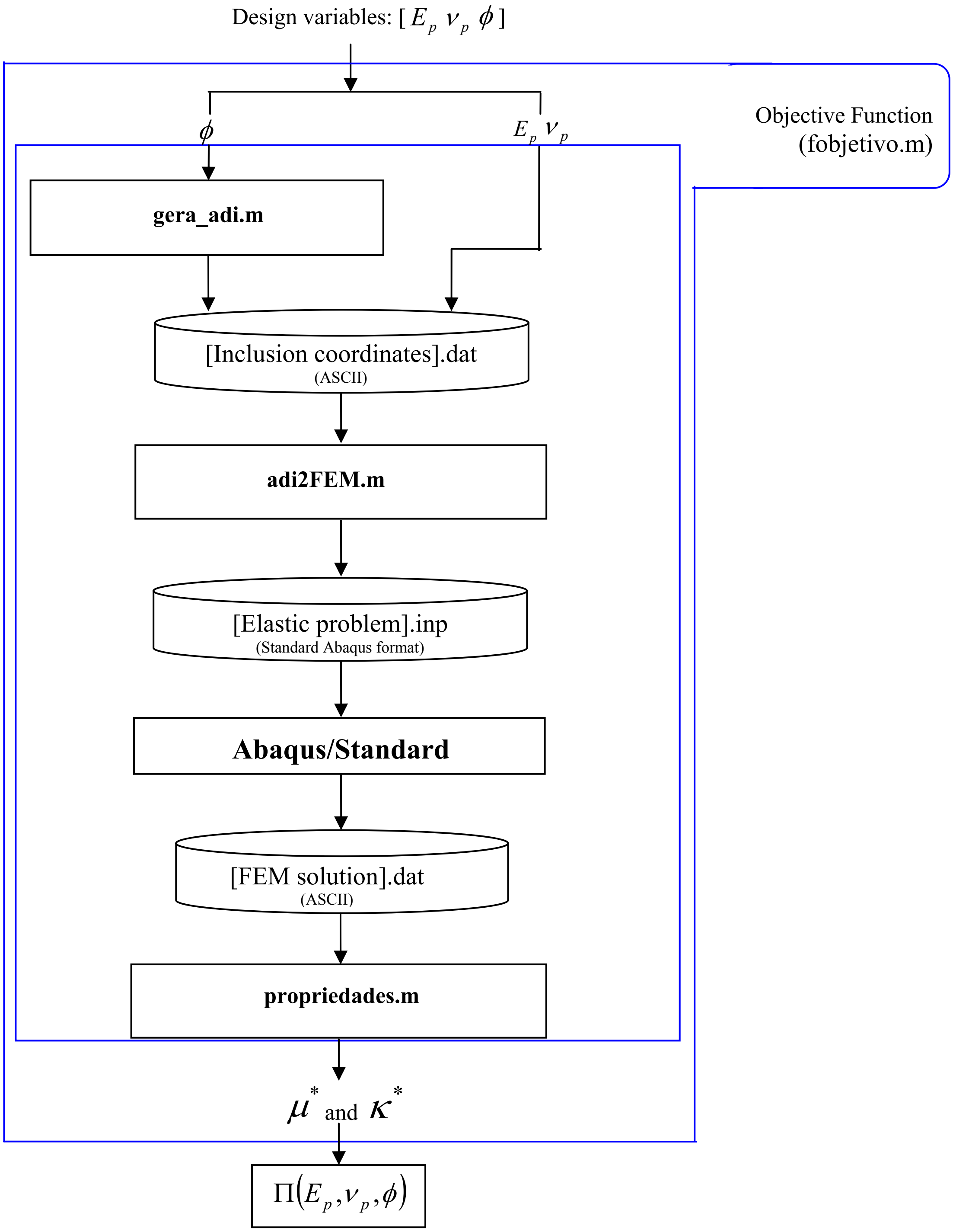


Figure 5. Schematic of the function *fobjetivo.m*

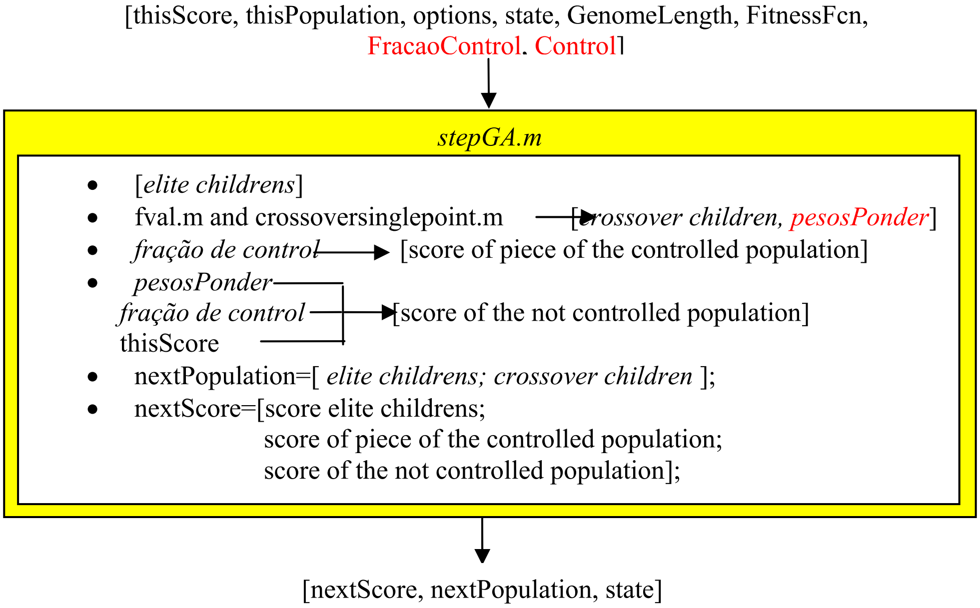


Figure 6. Schematic of the function *stepGA.m.*

The evaluation of the objective function is done by means of the function *fobjetivo.m*. A schematic of this function is illustrated in the Figure 5. The design variables are the input variables for this function. The subroutine *gera_adi.m* serves to randomly generate the coordinates with the positions the particles, which are stored in the file *inclusion_coordinates.dat*. The number of particles is 30 in all cases (irrespective of the particle volume fraction ϕ). At the same time the radius of the particles is always taken as unity and used to normalize the dimensions the sample. The subroutine *adi2FEM.m* constructs the input file for ABAQUS, which results in the file *elastic_problem.inp*. In this file the elastic constants assigned to each element depending on whether its position coincides with the matrix or a particle (see Figure 2-a). Afterwards the problem is solved using ABAQUS in shell mode, and the solution (stresses and strains) tabulated in *FEM_solution.dat*. Using these data the subroutine *propiedades.m* computes the effective elastic properties following the procedure outlined in Section 2. Finally the objective function (1) is evaluated.

4. Application example

The performance and capabilities of the devised algorithm is illustrated in this section by solving an application example. It consists in the design of a aluminium-matrix composite with macroscopic elastic constants $E_D^* = 67.5GPa$ and $\nu_D^* = 0.2$. The Young modulus and the Poisson ratio can be related to the effective bulk modulus and the effective shear modulus κ^* and μ^* using the well known expressions:

$$\kappa_D^* = \frac{E_D^*}{3\left(1-2\nu_D^*\right)} = 37500 \text{ MPa} \tag{4a}$$

$$\mu_D^* = \frac{E_D^*}{2\left(1+\nu_D^*\right)} = 28125 \text{ MPa} \tag{4b}$$

Since the values of κ^* and μ^* are of the same order, the factors ω_κ and ω_μ are both set equal to one. Then, the objective function (1) results

$$\Pi = \left|\frac{\left(\kappa^* - 37500\text{MPa}\right)}{37500\text{MPa}}\right| + \left|\frac{\left(\mu^* - 28125\text{MPa}\right)}{28125\text{MPa}}\right| \tag{5}$$

The parameters for the genetic algorithm are summarized in Table 1. The population size was chosen equal to 30 individuals, with a *fraction control* of 20% (5 individuals) for the approximated generations. The *Number of elite children* stands for the number of individuals of each generation (the fittest ones) that are automatically transferred to the next generation without any change. This parameter was set equal 3 (10% of the population). The crossover was performed using a *single point strategy* (see Section 3). Mutation was not allowed. As mentioned in Section 3, the Young modulus E_p and the Poisson ratio ν_p of the particles and the particle volume fraction ϕ were selected as design variables (3 design variables). The elastic properties of the aluminium matrix were given: $E_m = 70GPa$ and $\nu_m = 0.3503$ kept constant during the optimization procedure.

Parameter	Value
Population size	30
Fraction of control	0.2 (5 individuals)
Stopping criterion	8 generations
Number of elite children	3
Number of mutated children	no individual
Number of design variables	3
Crossover	Simple point

Table 1. Input parameters for the GA

The problem was solved using three different configurations of the GA. One run was made using a standard GA without any approximation. This result was used as a reference for comparison to the approximated results. The other two configurations corresponded to approximated evaluations of the fitness function: the weighted scheme proposed in this work (see Section 3) and the scheme proposed by Fonseca et al (2004). In the work by Fonseca et al. the inherited (approximated) fitness is simply evaluated as the average parents' fitness. Two runs were made in each case. The stopping criterion was arbitrarily set to 8 generations for in every case. This value was selected after performing preliminary tests which showed that 8 generations were enough to achieve results with an error less than 1% in κ^* and μ^*.

Obtained results are presented in Figure 7 and Table 2. For the sake of simplicity only the best results are included in Figure 7. It can be observed that the two approximate algorithms perform very similar, producing a result with less than 0,5% error. The worst result corresponds to the test #1 with the average approximation (not plotted) with an error of around 1%. Surprisingly, the standard GA provides results worse than those of the approximate GA. However, it is worth note that this result corresponds to only one test. Savings in computing time for the approximate algorithms are around 50%.

AG	Young's modulus particle [MPa]	Poisson's coefficient Particle	Fraction of volume	Objective function	Young's modulus effective [MPa]	Poisson's coefficient effective	Time [seg]
Standard	151700	0.3454	0.0496	0.0062	67114	0.2001	123091
Average test 1	99179	0.3449	0.15014	0.0109	68085	0.1996	94505
Average test 2	129530	0.3384	0.072484	0.0015334	67473	0.1998	63521
Weight test 1	129530	0.3384	0.072484	0.001283	67481	0.1998	59861
Weight test 2	129530	0.3384	0.072484	0.0015162	67466	0.1998	65616

Table 2. GA results

Finally it is worth to note that in a practical situation the feasibility of the composite will depend on the availability of inclusions with elastic properties (design variables) coincident to those resulting from the analysis. Note that in the case that the inclusions have to be chosen from a given collection of materials, extra restrictions could be incorporated to the GA in order to select the best option.

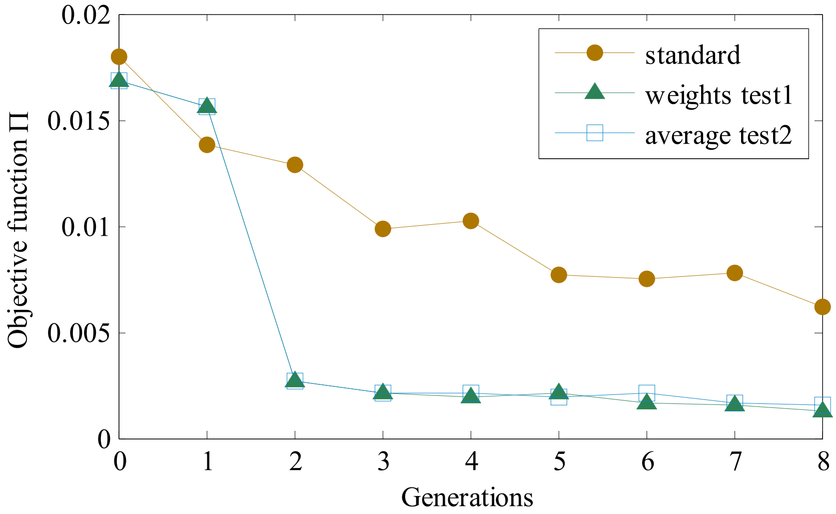


Figure 7. Convergence plots for the GA´s.

5. Conclusions

A general procedure for the design of random micro-heterogeneous materials in order to deliver a specified linearly elastic response has been presented in this work. The devised procedure makes use of genetic algorithm with approximate fitness evaluation. The Young modulus and the Poisson ratio of the particles and the particle volume fraction were selected as design variables, while the objective function was constructed in terms of the effective bulk modulus and the effective shear modulus of the resulting material.

In order to accelerate the GA a strategy for the approximate evaluation of the fitness function has been proposed. This strategy combines individual-based and generation-based controls. Individuals evaluated using the approximate model inherit their fitness from their parents by means of a weighted average which depends on the crossover point.

The performance and capabilities of the devised algorithm were illustrated by solving an application example. Obtained results demonstrate important savings in computing time with only minor losses in accuracy.

6. Acknowledgements

One of the authors (FCB) wishes to express his thanks for the financial support of CNPq. This work has been supported by PROMEC (Programa de Pós-graduação em Engenharia Mecânica) of the UFRGS and the ANPCYT (Agencia Nacional de Promoción Científica y Tecnológica de la República Argentina) under grant PICT 12-12528.

7. References

Batista R. G., Cisilino A. P. and Iturrioz I. 2003. *Aplicación del método de los elementos discretos a la homogenización de las propiedades mecánicas de materiales microporosos*. Mecánica Computacional XXII. ENIEF 2003. Bahia Blanca. Argentina.

Buroni, F. C. 2004. *Projeto de materiais compostos micro-heterogêneos.* Trabalho Final da disciplina Otimização de Processos. Programa Pós-Graduação em Engenheria Mecânica. PROMEC. UFRGS.

Fonseca, L. G., Barbosa, H. J. C., Lemonge, A. C. C. 2004. *A genetic algorithm with aproximate fitness evaluation for structural optimization.* In XXV CILAMCE Iberian Latin-American Congress on Computational Methods in Engeneering.

Goldberg, D. E. 1999, *Genetic algorithms in search optimization & machine learning.* Addison Wesley Longman.

Malvern, L. 1968. *Introduction to the mechanics of a continuous medium*, Prentice Hall.

Nemat-Nasser S. and Hori M., 1999. *Micromechanics: overall properties of heterogeneous solids.* 2nd Edition, Elsevier.

Zohdi, T. I. 2002. *Computational modeling and design of new random microheterogeneous materials.* CISM Course notes.

Zohdi T. I. 2003. *Genetic design of solids possessing a random-particulate microstructure.* The Royal Society. Phil. Trans. R. Soc. Lond. A 361, 1021–1043.

8. Responsibility notice

The authors are the only responsible for the printed material included in this paper.