Computer Science • Vol. 9 • 2008

S. Kluska-Nawarecka*, A. Smolarek-Grzyb**, A. Byrski***,
D. Wilk-Kołodziejczyk****

OPTIMIZATION OF SIMULATION MODEL PARAMETERS FOR SOLIDIFICATION OF METALS WITH USE OF AGENT-BASED EVOLUTIONARY ALGORITHM

The finite elements method (FEM) is currently widely used for simulation of thermal processes. However, one of still unresolved problems remains proper selection of mathematical model parameters for these processes. As far as modelling of cooling casts in forms is concerned, particular difficulties appear while estimating values of numerous coefficients such as: heat transport coefficient between metal and form, specific heat, metal and form heat conduction coefficient, metal and form density. Coefficients mentioned above depend not only on materials properties but also on temperature. In the paper the idea of optimalization of simulation method parameters based on adaptive adjustment of curve representing simulation result and result obtained in physical experiment is presented along with the idea of evolutionary and agent-based evolutionary optimization system designed to conduct such optimizations. Preliminary results obtained with use of ABAQUS system available in ACK CYFRONET and software developed at AGH-UST conclude the paper.

Keywords: *numerical simulation, evolutionary algorithm, agent systems, solidification casting process, casting*

OPTYMALIZACJA PARAMETRÓW MODELU SYMULACYJNEGO PROCESU KRZEPNIĘCIA METALI Z ZASTOSOWANIEM AGENTOWEGO ALGORYTMU EWOLUCYJNEGO

Metoda elementów skończonych (MES) znajduje obecnie liczne zastosowania w symulacji procesów cieplnych. Wciąż jednak nierozwiązalny pozostaje problem doboru niektórych współczynników modeli matematycznych tych procesów. Przy modelowaniu stygnięcia odlewów w formie, szczególne trudności powstają przy wyznaczeniu wartości licznych parametrów, np.: współczynnika transportu ciepła pomiędzy metalem a formą, ciepła właściwego, współczynnika przewodnictwa cieplnego metalu i formy, gęstości metalu i formy. Współczynniki te zależą nie tylko od właściwości materiałów, lecz również od temperatury. W artykule zaproponowano metodę optymalizacji wartości parametrów modelu

* The Foundry Research Institute, Krakow, nawar@iod.krakow.pl
** Department of Metals Engineering and Industrial Computer Science, AGH University of Science and Technology, Krakow, asg@tempus.metal.agh.edu.pl
*** Department of Computer Science, AGH University of Science and Technology, Krakow, olekb@agh.edu.pl
**** The Andrzej Frycz Modrzewski Krakow University College, Krakow, dwk@tempus.metal.agh.edu.pl

opartą na adaptacyjnym dostosowaniu krzywej stanowiącej wynik symulacji do przebiegu uzyskanego w eksperymencie fizycznym z zastosowaniem algorytmu ewolucyjnego w wersji agentowej. Wstępne wyniki obliczeń zostały zrealizowane przy wykorzystaniu systemu ABAQUS dostępnego w ACK CYFRONET oraz oprogramowania opracowanego przez AGH-UST.

Słowa kluczowe: *numeryczna symulacja, algorytmy ewolucyjne, system agentowy, proces krzepnięcia odlewów, odlew*

1. Introduction

Striving for increasing the competitiveness of metal goods requires taking some modernization activities aimed for raising their quality with simultaneous lowering of production costs. As far as cast industry is concerned, a matter of fundamental importance is providing required physical properties of materials and limiting casts faults creation. Even when norms and procedures are followed the fulfillment of requirements is fairly difficult. These difficulties are connected with wide variety of used technologies and materials and specification of some casts. Physical experiments in their complexity are fairly expensive and time-consuming. Therefore, they cannot be used in real production conditions on a large scale. As a result, there are constructed some mathematical models of thermophysical processes occurring in casts based on the finite elements method. Designing process of cast production technology might be significantly widened, modernized and improved by taking opportunities created by numerical method introduction into calculations of solidification and cooling metal in forms.

Still, the problem of providing required conformity of simulation results remains. Complex physical processes occurring in joint of metal and form cause discrepancy between tabular coefficients values and the real values. The shortage of exact data connected with definite values makes it difficult or even impossible to use mathematical models of metal solidification and cooling process effectively. Consequently, obtaining the cast with required properties becomes hardly feasible [1].

Numerical modelling of physical phenomena occurring in the processes is connected with making simplifying assumptions (because of the problem complexity), often significantly modifying basic parameters of examined problem. Therefore, a vital criterion of numerical model usefulness becomes its experimental verification. Also, verification is necessary while taking empirical adjustment of parameters required in model calculations into consideration. Especially, when it comes to determining material characteristics or thermal boundary conditions in a manner that guarantees maximal conformity of numerical results with experimental results.

In the face of shortage of effective algorithms for numerous essential calculation and decision problems, more and more attention is paid to systems modelled on the rules of biological evolution processes so-called evolutionary algorithm. These systems might be used for searching and parametrical optimization of the model of simulative solidification and cooling process on the basis of data obtained from physical experiments.

This paper presents the concept of using of evolutionary algorithm in agent-based version in parameter identification of FEM simulation model. A short intruduction to evolutionary multi-agent systems, and some selected experimental results which confirm practical possibility of application of this method were also given.

2. Simulation with the usage of the finite elements method

One of the most often used technique of numerical methods simulation is the finite elements method. Popularity of this method is reflected in the number of tools supporting a preparation of simulation models. Commercial simulation systems such as MAGMA have closed character and they do not give the opportunity to introduce any modifications. Therefore, the only available information tool enabling realization of planned research intentions is the ABAQUS system.

Simulation of cooling and solidification processes with the usage of the finite element methodusing ABAQUS simulation package made accessible by ACK–Cyfronet in Cracow with allowance of ABAQUS/CAE graphical user interface possibilities. Simple ball model has been designed in conformity with physical experiment assumptions and with omission of some form construction elements connected with practical cast realization, for example ingoting system and the riser have been ignored (see Fig. 2). In the Figure 1 presented model with ingoting system and the riser.

Presented below mathematical model of cast solidification and cooling process is the basis of our research based on computer simulation. The majority of available simulation packages enable modelling of phenomena occurring during cast solidification by means of the Fourier-Kirchhoff equation [3]:

$$X \in \Omega : c(T)\rho(T)\frac{\delta T(X,t)}{\delta t} = div\ [\lambda(T)\ grad\ T(X,t)] + Q(X,t) \tag{1}$$

where:

- X – point of cast area,
- T – temperature [K],
- t – time [s],
- $c(T)$ – specific heat [J/kgK],
- ρ – density [kg/m^3],
- $\lambda(T)$ – thermal conductivity [W/mK],
- $Q(X,t)$ – source of heat – amount of heat generated in volume unit in particular time unit [W/m^3].

Gradient and divergence in spherical coordinate system while λ is constant:

$$\lambda\ \mathrm{div}(\mathrm{grad}\ T) = \lambda \left[\frac{1}{r^2}\frac{\delta}{\delta r}\left(r^2\frac{\delta T}{\delta r}\right) + \frac{1}{r^2\ sin^2\vartheta}\frac{\delta^2 T}{\delta \varphi^2} + \frac{1}{r^2\ sin\theta}\frac{\delta}{\delta\vartheta}\left(sin\vartheta\frac{\delta T}{\delta\vartheta}\right)\right] \tag{2}$$

while λ is variable:

$$\operatorname{div}(\lambda \text{ grad } T) = \left[\frac{1}{r^2}\frac{\delta}{\delta r}\left(\lambda r^2 \frac{\delta T}{\delta r}\right) + \frac{1}{r^2 sin^2\vartheta}\left(\lambda \frac{\delta^2 T}{\delta \varphi^2}\right) + \frac{1}{r^2 sin\vartheta}\frac{\delta}{\delta \vartheta}\left(\lambda \; sin\vartheta \frac{\delta T}{\delta \vartheta}\right)\right] \tag{3}$$

where:

r – coordinate in radius direction,

ϑ – angle in meridional direction,

φ – azimuth angle.

Therefore, it has been decided to define thermophysical coefficients according to the above equation. Searched values are density, heat capacity coefficient and conduction of heat coefficient, the last two values are defined as functions of temperature and a source of heat has been omitted.

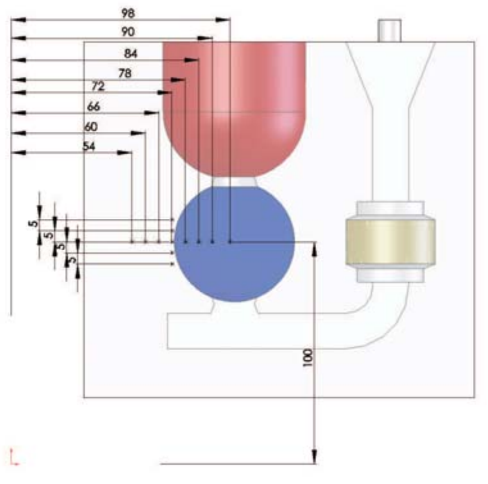

Fig. 1. Ball model with ingoting system and the riser

One significant parameter of cast cooling process is temperature. Value and speed of temperature changes have influence on cast microstructure and on thermal stress. In the Figure 3 the course of temperature changes in an indicated form and cast points are presented. Analysis of the presented graphs allows to state, that the simulation fulfilled required conditions. The conformity of simulation results with real results depends on proper selection of particular parameters values and assumed simplifications. The selection of some parameters for example conduction of heat coefficient between cast and form requires verification [1].

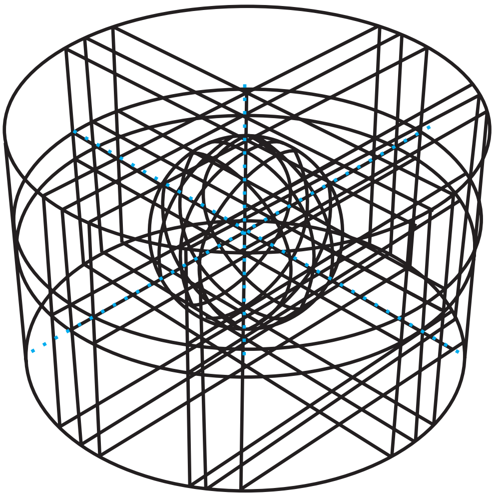

Fig. 2. Numerical model designed in ABAQUS

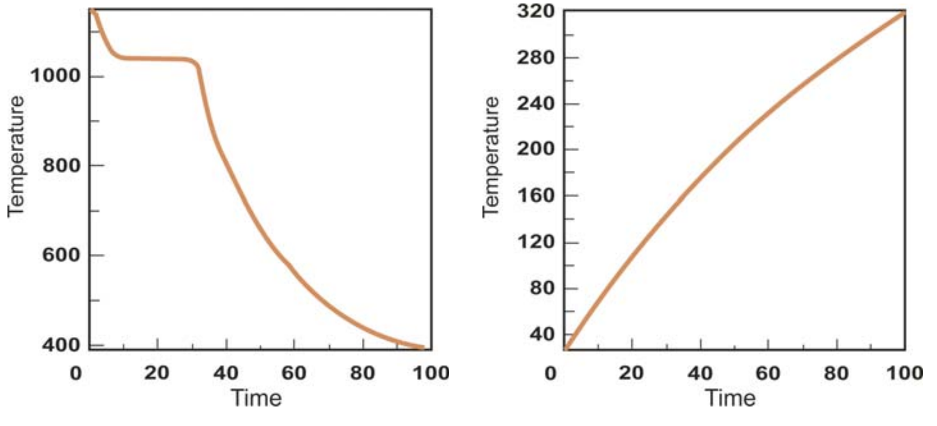

Fig. 3. The course of temperature changes in an indicated form point and in an indicated cast point

3. Optimization of simulation model parameters for solidification process

In the case of simulation of cast solidification and cooling processes the usage of expanded calculation algorithms based on the finite elements method does not guarantee obtaining satisfactory simulation results. The usage of the finite elements method assumes complete knowledge connected with the simulated process as well as parameters describing the phenomena such as: model geometry, boundary conditions, physical parameters and mathematical model describing the phenomena. However, comparison between the results obtained from physical experiments and from the simulation indicates inaccuracy which might be the result of improperly selected elements shape or mesh geometry. In many cases the knowledge about simulated process is not sufficient. Unknown parameters might be obtained only by means of experiments, this requires conducting numerous physical experiments though. As it has been mentioned before physical experiments are quite expensive and sometimes difficult to conduct. Therefore, an alternative solution might be searching for values of simulation parameters with the usage of artificial intelligence methods through adjustment of simulation results with obtained real results. The comparison between experiment and simulation results allows to define "the quality" of matched set of parameters of cast solidification simulation. Evolutionary algorithm are the example of optimization method. They do not require the knowledge of analytical model of the task therefore they might be used for solution of that kind of problems (see Fig. 4).

The correctness of obtained simulation model will depend on the number of model degrees of freedom (parameters which are subject of optimization) and the number of components of such a criterion (available experiment results). The more degrees of freedom and criterion components, the better results might be obtained, though with increased amount of calculations [1].

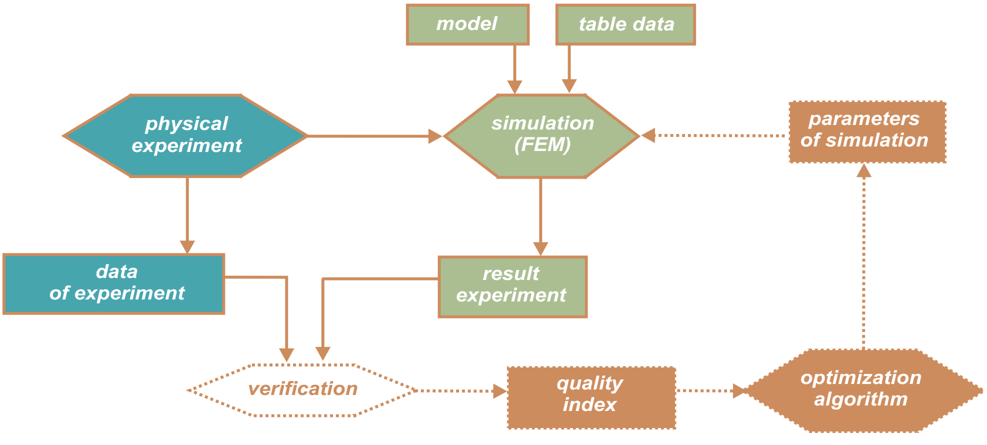

Fig. 4. The course of MES simulation experiment with the simulation parameters optimization [2]

4. Evolutionary optimization of FEM solidification model

Evolutionary algorithms are general optimization technique often called population–based technique, because they deal with the population of the individuals (containing solutions of the given problem), which are assigned with a certain quality measure called fitness. Population is transformed with use of so-called variation operators (such as mutation and crossover) which are applied to the individuals chosen by the means of selection algorithm. In this way subsequent generations are created. The process finishes usually after defined number of such transformations [4].

Evolution is a parallel process, therefore specific algorithms of parallel evolution were created. Standard approach called "global parallelization" is parallel implementation of selected algorithm steps taken for different individuals using many calculation units. In this case selection as well as individual selection are carried out globally (in the whole population). Therefore, these operations with a view to relatively slight calculation complexity in relation to communication costs or synchronization in access to particular individuals of the population are rarely subject of parallelization (generational synchronization). Most often the subject of parallelization is value calculation of individuals fitness, sometimes also operators of variation. In master-slave (see Fig. 5) architecture called sometimes farming model, the whole population is managed by supreme calculation unit (master). It carries out sequential algorithm steps and is responsible for assignment paralleled tasks (sending individuals or individuals groups) between remaining calculation units (slaves), calculation coordination and results receiving. Between inferior units the communication does not exist. The advantages of global parallelization are conformity with classic schema of evolutionary algorithm and easiness of implementation. Significant acceleration in case of expensive fitness functions is usually obtained. Master process realizes evolutionary algorithm [4]. For value calculation of fitness function of each individual it sends uncode individuals to slave processes [5].

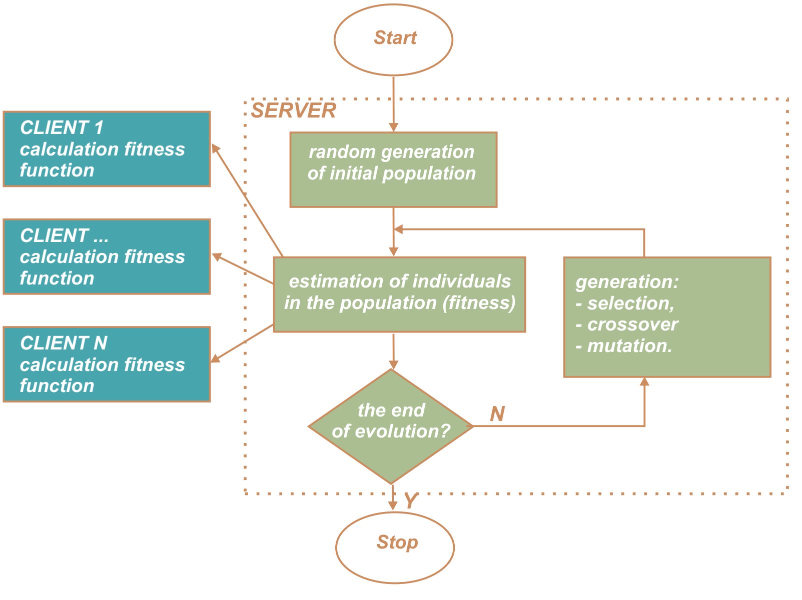

Fig. 5. Schema of distributed evolutionary algorithm

5. Evolutionary multi-agent systems

While different forms of classical evolutionary computation use specific representation, variation operators, and selection scheme, they all employ a similar model of evolution – they work on a given number of data structures (population) and repeat the same cycle of processing (generation) consisting of the selection of parents and production of offspring using variation operators. Yet this model of evolution is much simplified and lacks many important features observed in organic evolution, e.g.:

- dynamically changing environmental conditions,
- many criteria in consideration,
- neither global knowledge nor generational synchronization assumed,
- co-evolution of species,
- evolving genotype-fenotype mapping.

At least some of these shortcomings may be avoided utilizing the idea of decentralised evolutionary computation, which may be realised as an evolutionary multi-agent system (EMAS) as described below [6] (see Fig. 6).

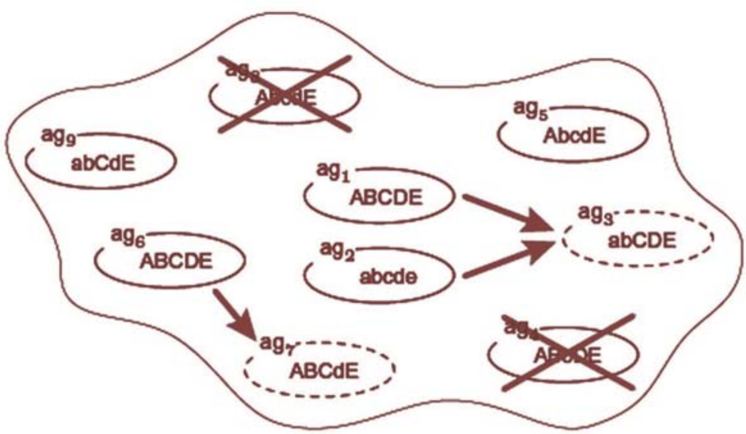

Fig. 6. Evolutionary multi-agent system

Following neodarwinian paradigms, two main components of the process of evolution are inheritance (with random changes of genetic information by means of mutation and recombination) and selection. They are realized by the phenomena of death and reproduction, which may be easily modelled as actions executed by agents:

- action of death results in the elimination of the agent from the system,
- action of reproduction is simply the production of a new agent from its parent(s).

Inheritance is to be accomplished by an appropriate definition of reproduction, which is similar to classical evolutionary algorithms. The set of parameters describing core properties of the agent (genotype) is inherited from its parent(s) – with the use of mutation and recombination. Besides, the agentmay possess some knowledge acquired during its life, which is not inherited. Both the inherited and acquired information determines the behaviour of the agent in the system (phenotype) [6].

Selection is the most important and most difficult element of the model of evolution employed in EMAS. This is due to an assumed lack of global knowledge (which makes it impossible to evaluate all individuals at the same time) and autonomy of agents (which causes that reproduction is achieved asynchronously). In such a situation selection mechanisms known from classical evolutionary computation cannot be used. The proposed principle of selection corresponds to its natural prototype and is based on the existence of non-renewable resource, called life energy. The energy is gained and lost when the agent executes actions in the environment. Increase in energy is a reward for "good" behaviour of the agent, decrease – a penalty for "bad" behaviour (which behaviour is considered "good" or "bad" depends on the particular problem to be solved). At the same time the level of energy determines actions the agent is able to execute. In particular, low energy level should increase possibility of death and high energy level should increase possibility of reproduction [7].

In short, EMAS should enable the following:

- local selection allows for an intensive exploration of the search space, which is similar to parallel evolutionary algorithms,
- the way phenotype (behaviour of the agent) is developed from genotype (inherited information) depends on its interaction with the environment,
- self-adaptation of the population size is possible when appropriate selection mechanisms are used.

What is more, explicitly defined living space facilitates an implementation in a distributed computational environment. Proposed EMAS should be a good metaphor for parallelization and simulation of presented evolutionary FEM model optimization.

6. Evolution model of solidification parameters

Possibilities of evolutionary algorithms usage have been presented on the example of the problem of searching thermal conductivity coefficient value for the sphere model. For the remaining data: density, specific heat table values have been assumed. Classic genetic algorithm has been used and in it the particular individuals represent different interdependences of thermal conductivity coefficient on temperature:

$$x = [x_1 = \lambda(T_1), \dots, x_5 = \lambda(T_5)] \tag{4}$$

where:

T – temperature indicating interpolation point of dependence of thermal conductivity coefficient on temperature,

$\lambda(T_i)$ – $i \in [1, 5]$, discrete values of thermal conductivity coefficient from the $(0, 1]$ range with 0.05 step.

Fitness function is based on simulated values. Fitness function might be convergent with the point in the particular time, area, the chart of assigned function in the time and it has been assumed according to the pattern:

$$target(\nu_1, \nu_2, \ldots, \nu_n) = \sum_{i=1}^{n} importance_i \cdot delta(\nu_i, exp_i) \tag{5}$$

$$delta(\nu_i, exp_i) = \begin{cases} (\nu_i - exp_i)^2 & \text{where Fit to point} \\ \sum_{t=t_{start}}^{t_{stop}} delta_{area}(\nu_i(t), exp_{i\ min,max}) & \text{where Fit to area} \\ \sum_{t=t_{start}}^{t_{stop}} (\nu(t) - exp_i(t))^2 & \text{where Fit to function} \end{cases} \tag{6}$$

$$delta_{area}(\nu_i, exp_{i\ min,max}) = \begin{cases} (\nu_i(t) - exp_{imin})^2 & \text{where } \nu_i < exp_{i\ min} \\ (\nu_i(t) - exp_{imax})^2 & \text{where } \nu_i > exp_{i\ max} \\ else\ 0 \end{cases} \tag{7}$$

where:

ν_i – simulated value,

$importance$ – importance of simulated value,

exp_i – expected result of simulated value (point, area or function).

7. Evolutionary optimization of FEM simulation in Master-Slave model

Before realization of EMAS for FEM simulation classical Master-Slave evolutionary algorithm was implemented. In this specific implementation after receiving the data system generates entry file for ABAQUS program. After simulation is finished, temperature courses which have been obtained are compared with pattern temperature courses in order to specify the quality of individual.

The application consists of: evolutionary algorithm (Master), workers (Slaves) running ABAQUS, parser for dealing with configuration files, and simple Graphical User Interface.

The sequence (Fig. 7) presents the overall structure of the distributed evolutionary algorithm performed in the discussed system.

Fig. 7. Sequence diagram

Due to the fact that each iteration requires procedure repetition of simulation of temperature course in a cast, what is a time consuming procedure the usage of evolutionary algorithm in agent version has been suggested. Thanks to employing new algorithms (e.g. agent-based evolutionary and immunological), time complexity of the process might be lowered in certain cases [7].

Using the implemented system, the course of temperature during cast cooling for assigned dependence of thermal conductivity coefficient value on temperature was monitored. In the Figure 8 the values of the fitness of individuals (the best, the worst, average) in the succeeding algorithm generations were presented. The best solution improves at least as long as the variety of population is maintained [2].

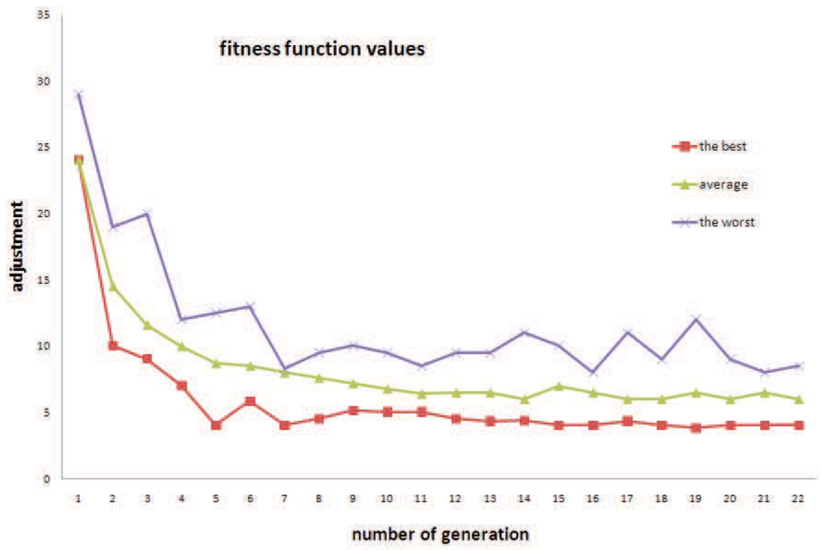

Fig. 8. Fitness in consecutive generations of the algorithm

8. Conclusions

The usage of intelligent methods with the combination of knowledge in the field of metal products producing allows to select parameters of simulation models properly. Therefore, it enables more efficient impact on the course of cast solidification and cooling process in order to provide its required quality. Thanks to the fact that the designed system has been built on the existing ABAQUS simulating environments, significant simplification of preparation process and realization of that kind of calculations is possible. What is more, the usage of distributed model significantly decreases time complexity of the calculations requiring parameters. The aim of the conducted studies is preparing of dispersed calculation platform with specified characteristics as well as the set of algorithms ready to use in discussed class of optimization problems.

The system will be based on agent-based biologically-inspired algorithms (e.g. evolutionary and immunological ones) what may lead to lowering the time complexity of the calculation.

Acknowledgments

The Commissioned Research Project
No. PBZ – KBN 114/T08/2004
No. 3 T08B 072 29

References

[1] Górny Z., Kluska-Nawarecka S., Kisiel-Dorohinicki M.: *Mathematical and simulation models in studies of copper and aluminium alloys.* The Foundry Research Institute, Kraków, 2003

[2] Byrski A., Kisiel-Dorohinicki M., Kluska-Nawarecka S.: *Evolutionary optimization of FEM simulation parameters of cooling and solidification process.* KomPlasTech 2004, Kraków, 2004

[3] Suchy J., Mochnacki B.: *Modelling and simulation solidification process.* PWN, Warszawa, 1993

[4] Goldberg D. E.: *Genetic Algorithms in Search, Optimization and Machine Learning.* Kluwer Academic Publishers, Boston, 1989

[5] Handzlik P., Trębacz L., Byrski A., Kisiel-Dorohinicki M.: *Application of distributed genetic algorithm to optimisation of FEMsimulation parameters of solidification process.* KomPlasTech 2005, Kraków, 2005

[6] Byrski A., Kisiel-Dorohinicki M., Nawarecki E.: *Agent-based evolution of neural network architecture, Applied informatics: International Symposium on Artificial Intelligence and Applications.* Proceedings of the IASTED Conference, Austria, 2002

[7] Byrski A., Kisiel-Dorohinicki M.: *Agent-based evolutionary and immunological optimization.* Computational Science ICCS 2007, Springer Verlag LNCS 4487-4490, Beijing, 2007