

Cellular Automaton–Finite Volume model for the simulation of grain evolution during solidification

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A model based on Cellular Automaton - Finite Volume (CAFV) for simulating grain nucleation and anisotropic growth during the solidification of alloys has been implemented in commercial software. This model operates on a sub-grid scale, capturing heterogeneous nucleation and competitive dendritic growth while incorporating orientation-dependent growth kinetics, thereby providing a physically consistent representation of grain selection mechanisms in directional solidification. Validation against cases reported in the literature confirms the model's accuracy, offering a robust tool for optimizing process parameters in single-crystal castings and other advanced castings, with potential extensions to welding and additive manufacturing processes.

KEYWORDS: GRAIN EVOLUTION; DIRECTIONAL SOLIDIFICATION; SIMULATION.

INTRODUCTION

The numerical simulation of dendritic grain structures formed during solidification becomes important to reduce the risk of microstructural defects that negatively impact mechanical properties of the casting.

New methodologies including more detailed physics have been developed in last decades to support this analysis better than the traditional predictive criteria based solely on the thermal field and generally limited.

CAFV is one of these methodologies: it is based on the 3D Cellular Automaton (CA) model solved on a microscopic computational grid to reproduce nucleation and growth of grains at large scales (cm). This CA grid is superimposed to a coarser finite volume (FV) mesh where the solution of the heat flow equation is computed; the coupling of these models constitutes the CAFV model.

This work presents its implementation in the commercial software *FLOW-3D® CAST*. Modelling and results are described in the following sections.

MODELLING

The CA modelling through simple local laws was first proposed in [1]. The model was coupled to the thermal solution obtained from a finite element (FE) mesh, leading to the first versions of the Cellular Automaton-Finite Element (CAFE) model [1,2]. Similarly, the CAFV (Cellular

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Automaton – Finite Volumes) model couples the CA model with the solution of the heat transfer equation based on an FV mesh, and includes the representation of grain envelope through an octahedral form, the heterogeneous nucleation based on nucleation sites and the growth kinetics along preferential directions of the dendrites.

At the initial time of the simulation, the uniform CA grid is generated: it requires a structured block of cubic cells and the unique cell size l_{ca} has to be of the order of the secondary dendrite arm spacing; this way, this grid may be much finer than FV mesh. The CA cells are grouped into CA blocks (a block contains the centre of its associated cells), and these blocks are grouped into CA windows, that are user-defined parallelepipeds identifying the zones of interest where the CA grid overlaps the FV mesh: the nucleation and growth can occur only inside them.

The use of blocks and windows allows to limit the computational domain and to deactivate dynamically the parts of the domain which are still fully liquid or have completely solidified. This leads to save computational time [2] and is essential because without such constraints a large num-

ber of cells in CA grid may require significant memory. Minimizing data storage is, therefore, a priority.

A state index represents the state of a cell: -1 means the cell is passive, 0 means the cell is liquid; otherwise, it coincides with the grain index; the cells having the same grain index belong to the same grain.

Then, the nucleation sites are identified. The heterogeneous nucleation is a phenomenon of instantaneous formation of a solid grain occurring in the liquid bulk or at the surface of the mold, when a critical undercooling is reached. Nucleation is based on the stochastic instantaneous nucleation model described in [2], which is based on the definition of nucleation sites. They can be defined in different ways: as points, surfaces or volumes. In the first case, the properties of the nuclei are assigned deterministically. In the other cases, the number of nucleation sites is calculated as $n_{max}V^{\nu}$, where n_{max} is the maximum grain density and V is a given volume (or area, for surfaces), then they are randomly distributed among the CA cells. The grain density depends on the undercooling ΔT , which is defined as:

$$\Delta T = T_L - T \quad (1)$$

where T_L is the liquidus temperature and T is the temperature of the nucleation site at the cell-centre.

This dependency is modelled through a Gaussian dis-

tribution described by the following probability density function [1,5]:

$$f(\Delta T) = \frac{n_{max}}{\Delta T_{\sigma} \sqrt{2\pi}} e^{-\left(\frac{(\Delta T - \Delta T_a)^2}{2\Delta T_{\sigma}^2}\right)} \quad (2)$$

where ΔT_a is the mean undercooling and ΔT_{σ} the standard deviation. For a given alloy, these parameters are determined experimentally.

A critical nucleation undercooling is attributed to each cell containing a nucleation site, according to the pre-

scribed Gaussian distribution. If a cell contains more than one nucleation site, only the smaller critical nucleation undercooling is used.

The method of Box-Muller [4] is used for this operation:

$$\Delta T_{nucI} = \sqrt{-2 \ln u_1} \cos(2\pi u_2) \Delta T_{\sigma} + \Delta T_N \quad (3)$$

where $\Delta T_{nucI} = T_L - T_{nucI}$ is the critical undercooling, T_{nucI} is the critical nucleation temperature, and u_1 and u_2 are two random numbers in (0,1).

A new grain forms when the undercooling ΔT of a liquid cell containing nucleation sites exceeds a prescribed critical nucleation undercooling:

$$\Delta T > \Delta T_{nucI} \quad (4)$$

At this instant, a crystallographic orientation is given by a set of 3 Euler angles.

After the initialization of the nucleation sites, the resolution in time and space starts. Typically, the time step used for the FV mesh is too big for CA grid: the CA advancement requires an inner loop over sub-time-steps, where at each iteration the FV temperature is interpolated to

the CA grid at nucleation sites and at the locations of the growing grains. This allows to update the grain growth velocity and increase their size, computing the growth and capture dynamics; at the end of the iteration the nucleation of new sites is checked.

Figure 1 shows the structure of the CA algorithm, reproducing the grain evolution, during one FV time step.

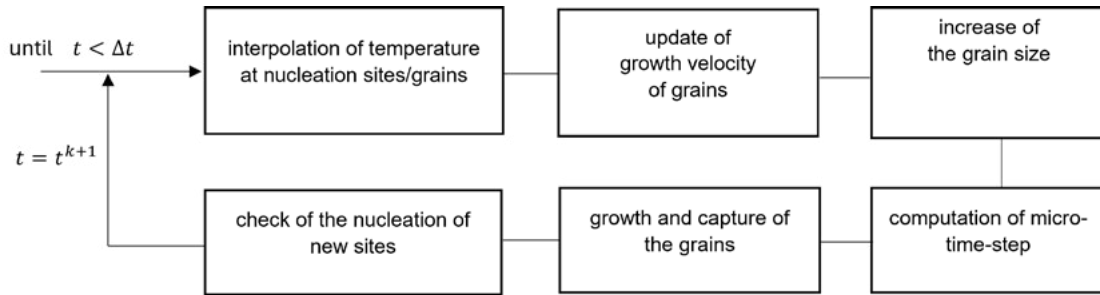


Fig.1 - Scheme of the CA algorithm. t and Δt are micro-time-step and time-step, respectively / *Schema dell'algoritmo CA. t e Δt sono rispettivamente il micro-time-step e il time-step.*

The grain evolution modelling is now described in more detail. The growth of the dendritic network during a time-step cannot exceed the cell spacing. Consequently, the time-step is subdivided into several sub-time-steps,

called micro-time-steps, used for the integration of the growth kinetics velocity v and computed in the following way [2]:

$$\delta t = \alpha \frac{l_{CA}}{v_{max}} \quad (5)$$

where α is a security coefficient to avoid having a growth of the envelope that exceeds the cell without being able to capture it and to manage multiple captures at the same instant, and $v_{max} = v(\Delta T_{max})$ is the velocity at maximum undercooling of all the growth cells in the domain. The value of α is in $[0,1]$. A grain is supposed to have an envelope of octahedral shape, which is modified locally in order to reflect the growth of the grain itself. Every involved cell has

its own octahedron. Its growth is reproduced through a kinetics law, guaranteeing the preferential growth directions $\langle 100 \rangle$ and the irrelevance of the grid on the orientation. The kinetics law, which represents the velocity of the dendrite tips, is a function of the undercooling ΔT of the cell, and is usually fitted (in order to speed up the calculations) with a polynomial approximation, for instance:

$$v(\Delta T) = a \Delta T^n \quad (6)$$

where a is a coefficient and n is the exponent.

Within a micro-time-step δt , the increment L of the radii,

$$L = v(\Delta T) \delta t \quad (7)$$

The evolution of the octahedron involves the neighbouring cells and, through the dynamic of capture the growth of the grain, proceeds inside the CA domain. When the

i.e. the diagonals of the octahedron, is obtained by integrating the kinetics velocity of the dendritic tips [2]:

octahedron envelope encloses the centre of a neighbouring liquid cell, this cell is captured by the grain. The de-centred octahedron growth algorithm described in [3] is

used to avoid a strong anisotropy effect due to the cubic cell lattice.

When a liquid cell starts to solidify, it becomes mushy. A grain is then associated with the cell, and the mushy zone fraction is defined as in [5].

The modelling is completed taking into consideration the type of coupling CA-FV: in weak coupling, CA scheme is used just as "output", without affecting the temperature field and solid fraction in the FV mesh; in full coupling, instead, a two-way transfer of the computed variables is executed between the two computational domains.

VERIFICATION RESULTS

The CAFV model has been verified against some analytical/experimental/numerical cases described in [1], [3], [4]. A couple of them are reported briefly here.

The first test case presents a validation of the growth of 2D multigrain, measuring the competition between the grains [4]. It involves a 2D domain (mm^2): $0 \leq x \leq 4.14$ and $0 \leq y \leq 8.31$. 3 nuclei are placed at the boundary $y=0$, the properties are described in table 1.

Tab. 2 - Properties of grains for test 1 / *Proprietà dei grani nel test 1.*

Alloy	succinonitrile-1.3%wt acetone
Nucleation undercooling	$\Delta T_{nucl} = 0 \text{ K}$
Growth kinetics	$v(\Delta T) = 8.26e^{-6}\Delta T^2 + 8.18e^{-5}\Delta T^3 \text{ m/s}$
Orientation for $x \leq 0.71 \text{ mm}$	4°
Orientation for $0.71 \leq x \leq 3.43 \text{ mm}$	30°
Orientation for $3.43 \leq x \leq 4.14 \text{ mm}$	11°

The thermal conditions are imposed thermal gradient of 1900 K/m along the vertical direction and imposed cooling rate of -0.1634 K/s. The aim is to measure the angle θ_d between the central and right grains (see image on the left in

figure 2); its theoretical value is 19° . The predicted results using $l_{ca}=25\mu\text{m}$ (cell density of 1600 mm^{-2}) are presented in figure 2 (on the right), compared with the reference ones (on the left).

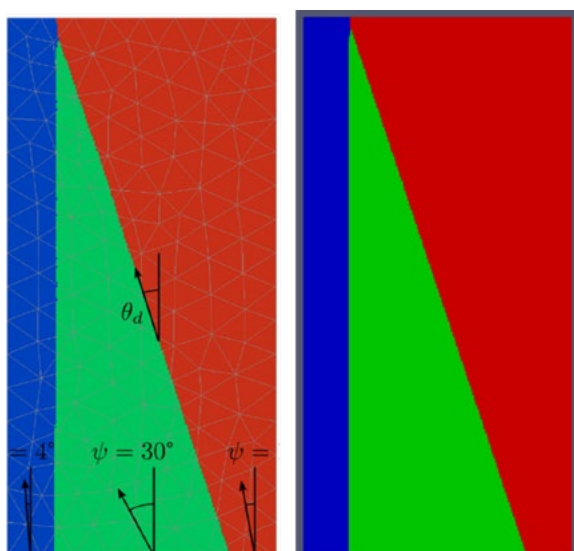


Fig.2 - Reference (left) and numerical (right) results / *Risultato di riferimento (sinistra) e numerico (destra).*

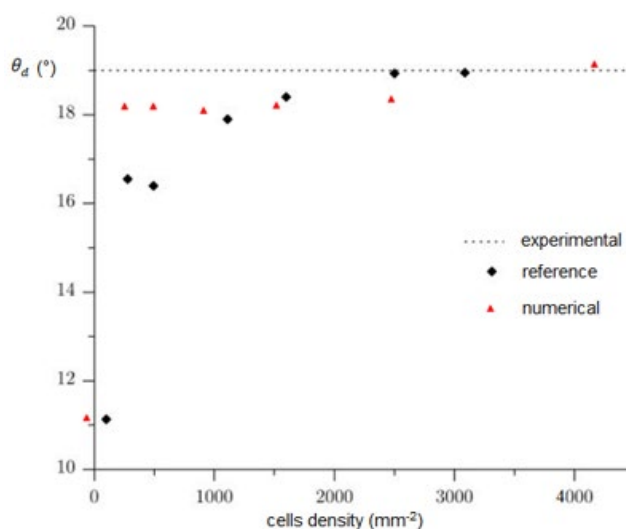


Fig.3 - θ_d in function of the cell density / θ_d in funzione della densità di celle.

Figure 3 shows the convergence analysis, where different cell sizes l_{CA} (reported in function of the cell density) are used to study the evolution of θ_d . The results confirm that the numerical solution is very close to the experimental one; the predicted angle θ_d matches the theoretical value even using a low cells density. The second test case presents the growth of 3D multigrain and the measurement of the temperature [4].

In a 3D cylindrical domain with radius of 35 mm and height of 173 mm the surface nucleation at $x=0$ and the volumetric nucleation occur, under an imposed profile temperature at $z=0$ and an imposed heat flux at $z=173$ mm. The alloy is AlSi7. Properties and parameters are reported in tables in [4].

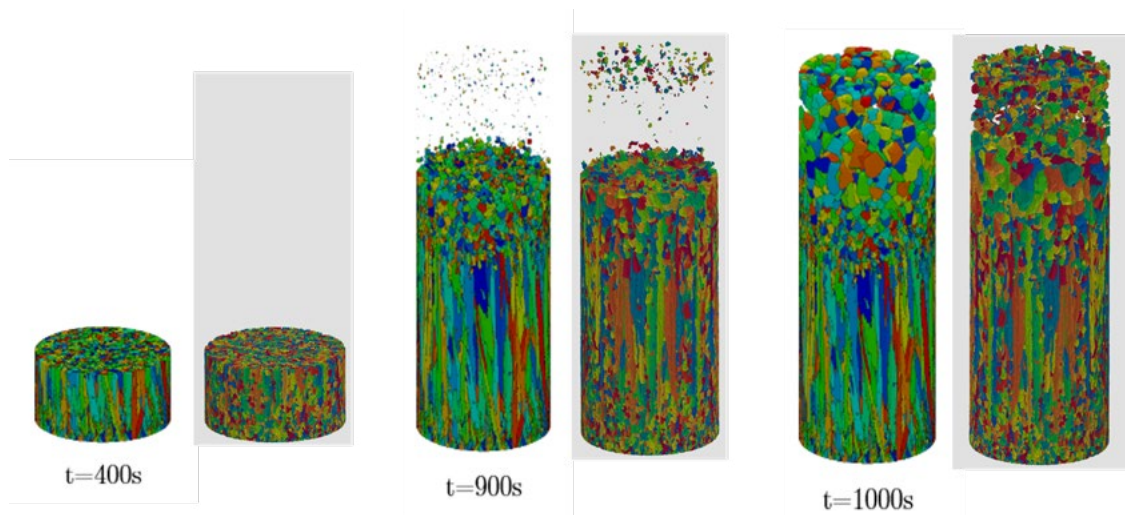


Fig.4 - Grains evolution (reference on the left, numerical on the right) / *Evoluzione dei grani (riferimento sulla sinistra, numerico sulla destra).*

Figure 4 shows the grain evolution in 3 instants, comparing the results (right) against the reference ones (left), while figure 5 reports the good agreement between ex-

perimental (grey) and numerical (colored) temperature evolution measured at 6 equidistant probes along the vertical axis.

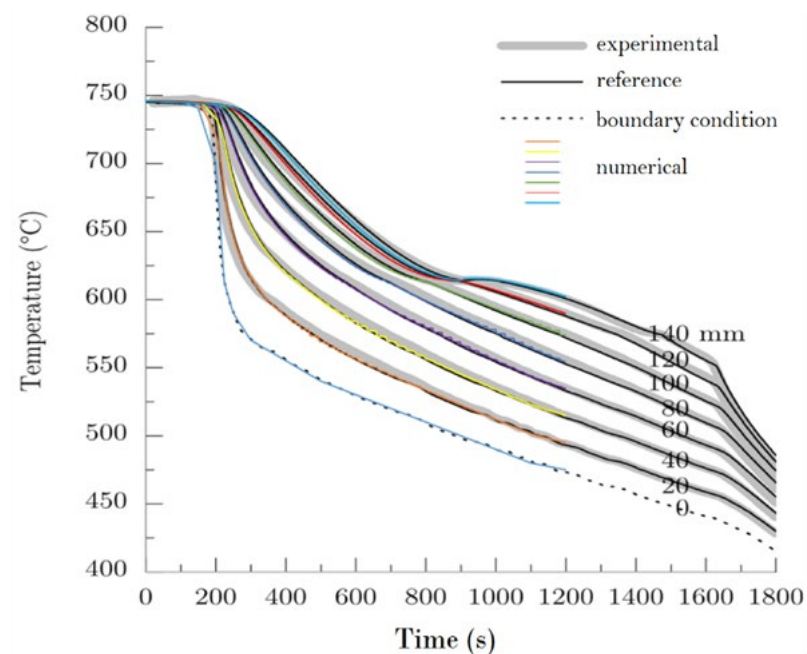


Fig. 5 - Comparison between experimental (grey) and numerical (coloured) temperature profiles at 6 probes / *Confronto tra profilo di temperature sperimentale (grigio) e numerico (colorato) in 6 punti di campionamento.*

Finally, a qualitative industrial case is mentioned. A tensile test manufactured was conducted at Safran Aircraft Engines laboratory, following a Bridgman process to achieve a controlled solidification. The alloy of the casting

is AM1, while its geometry, created ad hoc to study parasitic grains that prevent the production of a single-crystal piece, is shown in figure 6.

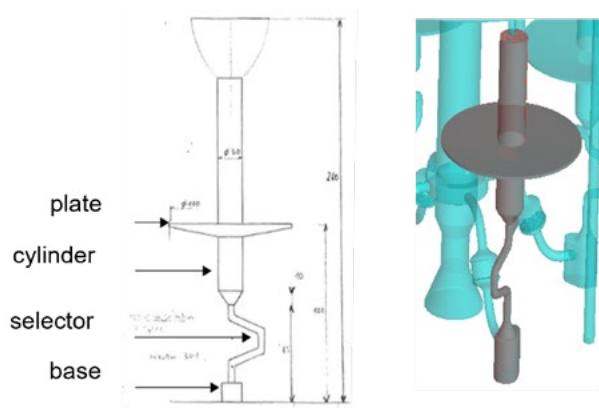


Fig. 6 - Geometry of industrial case / *Geometria del caso industriale.*

Solidification starts at the base: many grains form and grow, undergoing strong competition. In the selector only a few grains remain, reaching the cylinder where a

single grain prevails. The solidification continues in the plate, where parasitic grains form can be identified by observing the surface of the plate.



Fig. 7 - Details of the base, the selector and the plate with parasitic grains (compared to experimental case) / *Dettagli della base, del selettore e del piatto con i grani parassiti (paragonato ad un caso sperimentale).*

The comparison of the grain distribution between the experimental result and the simulation shows a reasonable agreement, as in figure 7; surely, exact correspondence is not possible, due to the random nature of the solidification. The shape, size and number of the parasitic grains are influenced by the alloy-dependent and hard-to-measure properties as well: the CAFV model is useful to predict their impact and calibrate them.

industrial scientists to study the process parameters in their casting applications. Furthermore, this model can be extended for other kinds of applications like welding. This version, implemented in commercial software, demonstrates very good performance, satisfying the theoretical features of the CAFV model through verification tests from literature. Finally, a realistic case in industrial conditions gave good agreement as well.

CONCLUSION

The CAFV model is a performing simulation tool that enables detailed predictions of microstructure, useful for

REFERENCES

- [1] Ch.-A. Gandin, M. Rappaz, A coupled finite element-cellular automaton model for the prediction of dendritic grain structures in solidification processes, *Acta Metall. Mater.* 42 2233, 1994.
- [2] Ch.-A. Gandin, J.-L. Desbiolles, M. Rappaz, Ph. Thevoz, A three-dimensional cellular automation-finite element model for the prediction of solidification grain structures. *Metallurgical and Materials Transactions A*, 30(12):3153–3165, 1999.
- [3] Ch.-A. Gandin, M. Rappaz, A 3d cellular automaton algorithm for the prediction of dendritic grain growth. *Acta Materialia*, 45(5):2187–2195, 1997.
- [4] T. Carozzani, Développement d'un modèle 3D Automate Cellulaire-Éléments Finis (CAFE) parallèle pour la prédiction de structures de grains lors de la solidification d'alliages métalliques. PhD thesis, 2012.
- [5] H. Ben Hamouda, Modelling and Simulation of solidification structure in nickel-based superalloys: application AM1. Thesis, Ecole Nationale Supérieure des Mines de Paris, September 2012.

Il modello Cellular Automaton per la simulazione diretta dei grani durante la solidificazione

Un modello basato su Cellular Automaton - Volumi Finiti (CAFV) per la simulazione della nucleazione dei grani e della crescita anisotropica durante la solidificazione delle leghe è stato implementato in un software commerciale. Tale modello opera su una scala sub-griglia, catturando la nucleazione eterogenea e la crescita dendritica competitiva e incorporando una cinetica di crescita dipendente dall'orientamento, fornendo così una rappresentazione fisicamente coerente dei meccanismi di selezione dei grani nella solidificazione direzionale.

La validazione rispetto a casi di letteratura conferma la bontà del modello, offrendo uno strumento robusto per l'ottimizzazione dei parametri di processo nei getti monocristallini e in altri getti avanzati, con possibili estensioni ai processi di saldatura e di produzione additiva.

PAROLE CHIAVE: EVOLUZIONE DEI GRANI; SOLIDIFICAZIONE DIREZIONALE; SIMULAZIONE.

TORNA ALL'INDICE >