Does MCWASP still follow Moore's law? 
Forty years of advances in microstructure modeling

M Rappaz
Ecole Polytechnique Fédérale de Lausanne, Institute of Materials, Station 12, CH-1015 Lausanne, Switzerland
E-mail: michel.rappaz@epfl.ch

Abstract. Over the past forty years, the series of MCWASP conferences has been the witness of the fantastic developments in the field of modeling of welding and solidification processes. This has been made possible thanks to the exponential increase in computing power but also to the emergence of new numerical methods and tools. While the "size" of computer simulations reported in MCWASP proceedings continues to follow Moore's law describing the evolution of computers power, the present contribution focuses on the evolution of microstructure modeling. In this respect, a major turning point is the introduction of the phase field (PF) method in the mid-90's. While PF is still the method of choice for the direct simulation of microstructure formation, it is also very CPU intensive. Therefore, it did not replace and rather complement other coarser methods such as analytical micro-macro models, Cellular Automata coupled with Finite Elements (so-called CAFE approach), modified-CAFE methods, mesoscopic model based on a dendrite envelope or Dendritic Needle Network (DNN) model. Some of these models as well as PF are coupled with fluid flow models based either on standard Navier-Stokes or Lattice-Boltzmann solutions. In parallel to these developments, wonderful experimental tools have become available to complement and validate numerical simulations: in situ X-ray radiography and tomography, EBSD, atom probe, FIB, etc. Besides a review of the past forty years, the present contribution will outline future directions of research in the area of microstructure modeling.

1. Introduction
In 1980 was held in New Hampshire the first "Modeling of Casting and Welding Processes" conference, with Harold Brody and Diran Apelian as chairmen [1]. If 1-Dimensional (1-D) simulations of heat flow involving melting or freezing date back to 1959 [2], the casting and welding community was clearly behind mechanical engineering, physics or meteorology in the field of numerical modeling. At the end of this first conference, the participants concluded that "...activity in the field [of solidification processes] would merit a second conference in 2-3 years.... the format of this conference contributed to its success and that future conferences should be limited to a group of about 100 individuals".

Over the past forty years, this first New Hampshire conference has been followed by fourteen more editions, including the present one in Stockholm, Sweden [3-16]. Section 2 traces back the initial developments of the conference series, from the first one held in 1980 up to the fifth one held in Davos ten years later, which was then renamed with the actual brand name "MCWASP". The period from MCWASP VI to VIII (section 3) has seen the emergence of two important methods in the field of microstructure modeling, namely Phase Field (PF) and Cellular Automata (CA). From the turn of the millennium, the MCWASP conference series has seen many applications of these two methods to
various problems, but also the development of other original meso-scale approaches (section 4). Finally, in section 5, it will be shown that the development of microstructure modeling is strongly linked with the evolution of the available computing power, but also the usage of adaptive meshing techniques and massively parallel computations on GPUs. For simplicity, papers published in MCWASP proceedings are only referenced with the volume number of the volume in which they appear ([1, 3-15]).

2. From the first Modelling of Casting and Welding Conference to the first MCWASP

At the time of the first Modelling of Casting and Welding Processes conference in 1980 [1], the focus of the conference was mainly on heat and fluid flow, with one session dedicated to stresses and deformation. However, M. Glicksman, in charge of organizing a half-day session on analytical and computer modeling of solidification kinetics and structure, contacted W. Kurz to present an invited talk. The title of Kurz and Fisher's presentation "Directional growth of eutectic and dendrites at the limit of stability" reminds us that the marginal stability criterion for the growth of a dendrite tip, which gives the right order of magnitude for the tip radius and undercooling (while missing the question of anisotropy), was proposed only a few years before by Langer and Müller-Krumhaar. While most of the presentations in this session were focused on experimental results and theoretical interpretations, Gilmer described an Ising model for the growth of a crystal-melt interface. A few talks were also concerned with microsegregation modeling. Interestingly, what is maybe missing nowadays in MCWASP conferences, a full session was dedicated to outline future directions and needs in the field.

The second conference, dedicated to Chvorinov for his 80th birthday, was essentially focused on the same topics [3]. Rapid solidification, a topic extensively studied in the 1980's which has seen a regain of interest nowadays with additive manufacturing processes, was the subject of an entire session. Flood and Hunt presented their first Columnar-to-Equiaxed Transition (CET) model, followed in 1984 by the publication of Hunt's CET analytical criterion [17]. This criterion was further extended to unsteady-state conditions in the third proceeding by the same authors in [4]. This conference could have already been renamed MCWASP since it focused on several advanced solidification processes.

Besides the first appearance of color maps grouped at the end of the proceeding, the IVth conference proceeding [5] has published the first micro-macroscopic models of equiaxed dendritic solidification for grain structure predictions. This approach, initially developed in Stefanescu's group and at EPFL, was able to produce grain structure or undercooling maps (see figure 1). It should be pointed out that Oldfield pioneered such micro-macro approaches for cast iron solidification more than twenty years earlier [18]. Interestingly, a steel hammer casting was used for a Round Robin session to test and validate several heat flow simulations performed by different groups. This test was certainly key to demonstrate the importance of materials properties, initial and boundary conditions for the accuracy of temperature predictions, a prerequisite for any accurate microstructure modeling.

![Figure 1](image_url)

**Figure 1.** Grain-radius map of equiaxed grains in a 2-Dimensional (2-D) section of an axisymmetric Al-Si brake cylinder, as calculated with a micro-macro approach. As there were no color printer at that time, this is a screen photograph taken with an argentie camera, thus explaining the distortion of the frame. (From the work of Desbiolles *et al.* presented in [5]).

In 1990, the Vth conference [6] certainly has set up a landmark in microstructure and defect modeling with a full session dedicated to this topic, with a keynote delivered by G. Lesoult from Nancy. Organized for the first time outside the USA in Davos, Switzerland, the conference was renamed with its present label: "Modeling of Casting, Welding and Advanced Solidification Processes", or MCWASP in short. It
was also the first reporting in MCWASP proceedings of the much more refined micro-macro models of Beckermann and co-workers, using a two-phase formalism approach, also developed at that time by Bennon and Incropera [19] and Voller and Prakash [20]. The cover page of this proceeding, reproduced from the communication of Brown and Spittle, shows four cross sections of Al-Cu sand castings demonstrating nicely the influence of the Cu-composition on the CET (figure 2(a)). These authors were developing a 2-D stochastic model of equiaxed and columnar grain growth based on a Monte-Carlo type approach (figure 2(b)). Although this method developed for grain growth in the solid state does not encapsulate the physics of solidification, it really paved the direction to go, i.e. produce simulated grain structures or microstructures which can be directly compared with metallographic cross sections or in-situ solidification observations.

Figure 2. (a) Sand-casting of Al-0.75wt.%Cu and (b) first 2-D stochastic model based on a Monte-Carlo method for grain structure predictions in a square ingot (from Brown and Spittle in [6]). (c) First 2-D Cellular Automaton (CA) prediction for a similar configuration (from Gandin et al. in [7]).

3. From MCWASP VI to MCWASP VIII
Clearly for the VIth MCWASP conference [7], the novelties in the field of microstructure modeling were the appearance for the first time of two new methods, namely Phase Field (PF) and Cellular Automata (CA), which have become now standard techniques in the field. The history of the PF method development can be found in the recent review of W. Kurz et al. [21], including the first 1978 notes of J. Langer outlining the bases of this technique. R. Kobayashi was the first to compute a full 3-D thermal dendrite (or seaweed when there is no anisotropy) using the PF method [22]. The method was introduced in the MCWASP community by W. Boettinger and co-workers in [7] (see figure 3). A few years later, Warren and Boettinger extended the PF method to solutal dendrites [23] (see also in [8]) and the number of PF contributions has risen sharply since then (e.g. a dozen publications related to PF in [15]).

Figure 3. First 2-D phase-field simulation reported in MCWASP proceedings [7] by Boettinger et al. The left and right figures show the temperature and the phase-field maps, respectively.
Cellular Automata, first developed for an isothermal volume (see figure 2(c)), was initially referred to as a "stochastic approach" of grain structure modeling, even though the only stochastic aspects are related to the location and crystallographic orientation of heterogeneous nuclei. Once this is known in a volume (or surface) of a casting, the capture of CA cells is deterministic, based on an analytical dendrite tip (and arms) growth kinetics law. The CA technique was then coupled with Finite Elements (FE) heat flow calculations, leading to the so-called CAFE model, the principle of which, like PF, was later applied to other materials science problems (e.g. [24] for fracture). Applications made with the 2-D and 3-D versions of CA can be found in [8] and [9], respectively. Although the CAFE model does not consider the solutal interactions at the detailed level of dendrite tips/arms (i.e. hard- instead of soft-impingement), it has become an industrial tool to predict grain structures in casting and welding processes.

In parallel to PF and CAFE, substantial progresses were made in analytical micro-macro modeling to predict mushy zone evolution and associated macrosegregation. For predicting freckles formation (e.g. Combeau and Lesoult, Poirier and Heinrich in [7]), the solid is assumed to be fixed while the Navier-Stokes equation for the liquid phase is modified to include a Darcy-type term describing the drag effect exerted by the solid already formed in the mushy zone. During this period, Beckerman, keynote speaker in [7], released the assumption of a fixed solid and developed two-phase approaches which account for different velocities of the liquid and solid phases, with proper interactions between the phases derived from averaging over a representative volume element. This allows to include the effect of grain sedimentation or floatation in macrosegregation predictions.

It should also be pointed out that inverse modeling, first appearing in [6] and introduced in the field by Beck and Zabaras, was applied by Dantzig and co-workers to the optimization of solidification conditions in [7], and of the shape of the Round Robin hammer casting in [8]. In the same MCWASP VII proceeding of the conference held in London, a benchmark for mold filling calculations was proposed by Campbell based on a comparison with in situ X-ray radiographies.

MCWASP VIII established a new, and yet today unsurpassed record: that of the thickest proceeding (1267 pages)! It was dedicated to K. Brimacombe, who passed away one year before in 1997. Thanks to the progresses made over past MCWASP conferences for cast iron modeling, a full session with a keynote by Svensson was organized on this topic. In the same way, a session focused on "Direct microstructure simulation" included a keynote by Steinbach, while most contributions were based on PF. Adaptative grids, massively parallel PF computations start to appear (e.g. Provatas et al.), together with multi-PF approaches in particular for eutectic simulation (e.g. Seesselberg and Tiaden) as well as the coupling between PF and fluid flow computations (e.g. Diepers et al., Tong et al., figure 4(a)).

![Figure 4](image_url)

**Figure 4.** (a) 2D PF simulation of an equiaxed dendrite in a forced flow [25]. (b) 14 equiaxed grains randomly distributed with a random orientation, as predicted from a mesoscopic model considering thermal interactions [26]. (c) Metallographic section of dendrites during e-beam remelting of Al-Si and modified-CA predictions (from Diltthey and Pavlik in [9]).
A new mesoscopic model based on PF was developed by Steinbach et al. for a thermal dendrite: it considers the dendrite envelope without the full details of the internal arms structure to speed up the computations, while a confocal envelope at some fixed distance is used to compute the undercooling (figure 4(b)). The CA model is modified by Dilthey and Pavlik to include solute diffusion around growing dendrites, with an estimation of the curvature based on the local fraction of solid distribution (figure 4(c)). Although these so-called “modified-CAFE” are usually not validated and are thus semi-quantitative, they provide an interesting view of the internal dendritic structure of the grains at a scale which, at that time, could hardly be reached with PF.

4. From MCWASP IX to MCWASP XIV

At the turn of the millennium, MCWASP IX [10] organized in Aachen is more oriented toward industry, with interesting keynotes setting one step out of the field: one on meteorology and climate research modeling by Kaas, and another one on discrete particle modeling by Tsuji. There is no major innovation in the field of microstructure modeling, except for the introduction of an orientation-parameter in PF by Warren et al. to predict the impingement of a family of grains and the extension of the method to multiphases and multicomponents, sometimes coupled with thermodynamic databases, by Nestler et al. or Steinbach et al.

A full session dedicated to PF is organized in 2003 at MCWASP X [11]. One of the key actors in this area, A. Karma, had developed quantitative methods with the introduction of an anti-trapping term to compensate for the artificially increased thickness of the diffuse interface [27]. A full session is devoted also to CA and modified-CA applications.

But more importantly in MCWASP X [11], the first in-situ radiographies of directional solidification of Al-Cu thin specimens are reported by Mathiesen and Arnberg, with unprecedented resolution thanks to the use of X-ray synchrotron radiation (figure 5(a)). In the same proceeding, Bernard et al. use X-ray tomography to deduce the 3-D morphology of eutectic regions in Al-Cu specimens, and calculate with this information and solving Stokes equation the permeability of these alloys just above the eutectic temperature.

![Figure 5](image1.png)

**Figure 5.** (a) First high-resolution X-ray radiography reported in MCWASP by Mathiesen and Arnberg for directionally solidified Al-30wt.%Cu in [11]. (b) X-ray radiography of nucleation and growth in Al-15%Cu inoculated with Al5Ti1B in a small gradient (Prasad et al. in [15]).

In situ X-ray observations (radiography, tomography, topography) see such a fantastic development that a full session devoted to this topic is organized in the following MCWASP conference organized in Opio-France [12]. Among the main contributions, one can mention the tomography observation of pores formation by Salvo et al., radiography of the CET in Al-Ni by Reinhart et al., dendrite fragmentation by Mathiesen et al., dendrite extension past a re-entrant corner by Yasuda et al. The PF method continues
to be more and more extensively used in 3-D situations (Puztai et al.), for eutectic growth (Parisi and Plapp, figure 6(a)), for ternary eutectics (Böttger et al., Nestler et al.) and for Mg alloys (Eiken et al.).

In MCWASP XII, held on a cruise boat leaving Vancouver for Alaska [13], and even more in MCWASP XIII, held in Schladming-Austria [14], in situ X-ray observation techniques are increasingly used. At the microscale, tomography is used to characterize the 3-D shape formation of pores and intermetallics by Lee et al. in [13], while Yasuda et al. in [14] use radiography to observe the γ-δ transition in Fe-C. In situ radiography is also used at a larger scale, e.g. for flow imaging by Reilly et al. in [13], for freckles formation in Ga-In by Shevchenko et al. or for particle pushing by Kareh et al. in [14]. This last group also presents a Discrete Element Method (DEM) to explain their observations.

Micro-macro modeling including the transport of grains in [13] and of (grains + inoculant particles) in [14] is further developed by the group of Založnik and Combeau. Using a granular approach, Phillion et al. in [13] have extended to 3-D the solidification model for randomly oriented globular grains previously reported in MCWASP XI [12] by Vernède et al. This granular approach was completed by Sistaninia et al. (in [14]) in order to ultimately model in situ hot tearing tomography observations performed by Terzi et al. [28, 29]. In the same proceeding, the same experiment was modelled by Zaragoci et al. using a level-set method.

**Figure 6.** (a) Stable zig-zag structure observed with a long-distance microscope in CBr$_4$-C$_2$Cl$_6$ (top) and 3-D PF simulations (bottom) by Parisi et al. in [12] (the top and bottom figures are taken from [30] and [31] respectively). (b) Comparison of DNN and PF calculations for an equiaxed dendrite showing the solutal field by Tourret and Karma in [14]. (c) Comparison of the solutal fields between PF (left) and mesoscopic model (right) predictions for columnar dendrites by Založnik et al. in [15].

While PF modeling continues to be applied to various situations, e.g. twinned dendrites by Salgado et al. in [13], Dendrite Orientation Transition (DOT) observed in Al-Zn alloys by Friedli et al. in [13] and [14], MCWASP XIII sees the first appearance of the Dendrite Needle Network model of Tourret and Karma (figure 6(b)), a model that, like the mesoscopic model, bridges the gap between PF and CAFE. As the name indicates, the DNN model replaces a dendritic network of primary, secondary and higher other branches by sharp needles that interact through solutal diffusion fields. The tip velocity of each needle is determined by combining a standard solvability condition and an additional solutal flux balance made over the dendrite tip region. During the same conference, Wu et al. present for the first time the coupling of a CA model with a fluid flow model based on the Lattice Boltzmann Method (LBM) for the prediction of dendrite and bubble formation during solidification. Figure 7 is a good illustration.
of the evolution of the CAFE model over the past twenty years (to be compared with figure 2(c)): the 3-D CA model is coupled with FE solution of heat, mass, momentum and solute transport in order to predict the evolution of the grain structure and macrosegregation for a benchmark experiment developed in Grenoble (from Carozzani et al. in [14]).

Figure 7. Simulation of a macrosegregation benchmark experiment for Sn - 3%Pb, using a 3-D CA coupled with FE solution of heat-and-mass transfers, (a) at $t = 3000$ s when the cavity is partially liquid and (b) $t = 5000$ s after the alloy has solidified. From Carozzani et al. in [14].

It is interesting to point out that the proceeding of MCWASP XIII [14] is for the first time published as an open source publication of IOP in a bundle format (paper and electronic version). The proceeding of the following MCWASP conference held in Awaji-Japan [15] was also published as an open source but only under an electronic format, demonstrating the evolution of the publication modes. This last conference honoured two key members of the MCWASP community: Itsuo Ohnaka, who very sadly died in 2016, only six months after giving an invited talk at Awaji "How to solve complex problems in foundry plants - future of casting simulation", and Jon Dantzig, who was chairman of the second conference with John Berry.

MCWASP XIV confirms the evolution seen over the two previous conferences, in particular large scale computations, and combined in situ X-ray observations and simulations [15]. Takaki’s group uses massively parallel PF computations on GPUs to simulate dendrite growth, without convection (figure 8) and with convection using LBM. Adaptive meshing techniques are used for PF simulations performed by Bollada et al. or by Guo and Xiong. The effect of Sr on the solidification of Al-Si is modelled in 3-D by Eiken and Apel, while Akamatsu et al. used both PF and the boundary-integral method to investigate the effect of the anisotropy of $\alpha$-$\beta$ interfaces during eutectic growth. The DNN model is extended to 3-D and compared with in situ experiments on Al-Cu by Tourret et al. The mesoscopic model is compared with PF by Založnik et al. (figure 6(c)), while Mondoux et al. analyze the percolation in 3-D of a family of smooth granular grains. No doubt that many of these contributions will be extended and included in the present MCWASP proceeding [16].
Figure 8. 3-D PF simulations showing the competition of dendrites at a converging grain boundary in directional solidification by Sakane et al. in [15]. The grain on the left has a \(\langle 100 \rangle\) direction well oriented with the vertical thermal gradient \(G\), while that on the right is misoriented by 30 deg and is slightly more undercooled due to a larger velocity.

5. Moore's law evolution of MCWASP conferences

The development of numerical models over the past forty years was only possible thanks to the fantastic evolution of computers' power. To show that, it is sufficient to consider the first workstation that we bought at EPFL in 1985 to develop the micro-macro model producing the result of figure 1. This Apollo DN 550 workstation had a performance of 0.3 Mips, with 1.5 Mbytes of central memory and 75 Mbytes of disc! Yet, its cost was 135'000 CHF (about the same amount in USS at present conversion rate). In 2020, the performance-over-price ratio of computers is about \(10^8\) to \(10^9\) better as compared with the DN 550, while Moore's law over 35 years gives a factor \(10^7\)!

In 2002, Voller and Porté-Agel [32] made an interesting count of the number of computation nodes reported in the proceedings of the MCWASP conference series since the first edition (see figure 9). They concluded that the mean number of nodes was evolving with an exponential law: \(1000 \times 2^{0.6667 \times \text{year-1980}}\), as a function of the year following the first conference (held in 1980, proceedings published in 1981 [1]). In other words, the number of nodes was doubled every 1.5 years, exactly like Moore's law for the computers power evolution.

Celebrating the 40th anniversary of the MCWASP conference series, we should see in 2020 computations with about 100 billion nodes if this law is correct! Taking the previous proceeding [15], the largest PF simulations reported by Takaki’s group are \(1.6 \times 10^9\) nodes (for figure 8), while the extrapolation of Voller and Porté-Agel predicts \(10.6 \times 10^9\) nodes. However, in their 2013 publication [33], the same group reports simulations involving \(4'000^3\) nodes, a value 16 times larger than the extrapolated Moore's law of figure 9. Therefore, without making further detailed accounting of the number of nodes, we can quite confidently conclude that the "size" of the microstructure simulations continues to follow the evolution of computers power, thanks in particular to the use of massively parallel calculations performed on GPUs.

Figure 9. Number of nodes reported in the first 10 MCWASP proceedings as a function of the years following the first conference. The figure has been redrawn from the original analysis made by Voller and Porté-Agel [32]. The linear fit in this log-lin scale shows that the "size" of the simulations follows Moore's law, i.e. the number of nodes in the largest simulations reported in MCWASP conferences doubles every 1.5 years.
6. Conclusion
The past forty years have been very exciting from the point of view of microstructure modeling, thanks to the development of new approaches and methods as well as to the fantastic evolution of computation power. However, the complexity of casting and welding processes are such that their modeling requires multiple approaches in order to address the ten orders of magnitude length scales involved. In between ab initio calculations at the atomistic scale and FE/FV solutions of average conservation equations at a component scale, PF, CAFE, DNN, granular models or mesoscopic approaches allow to predict microstructures, defects and grain structures at intermediate scales. In parallel to modeling, new experimental tools have become available, in particular in situ X-ray observations techniques, but also EBSD, EDX, atom probe, FIB, STEM, etc., sometimes used for 3-D characterizations.

Still, many materials properties and behaviors are key in obtaining valuable modeling results and/or understanding some of the microstructure/defects forming during solidification. Among those: solid-liquid interfacial properties, grain boundary energies, diffusion coefficients, thermal diffusivity, attachment kinetics contribution, high temperature behavior of the solid, partial ordering of the liquid phase, etc. Atomic calculations will probably contribute increasingly in the future to calculate some of these properties.

Finally, as stated by the mathematician S. Karlin (1924-2007), "The purpose of a [mathematical] model is not to fit the data, but to sharpen the questions". In 2020, year of the XVth MCWASP conference, well-controlled experiments, analysis tools and modeling at all scales can be used jointly to sharpen many remaining questions in the field of solidification.

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