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Accelerating Microstructural Evolution Simulations in DIGIMU® through a Front-Tracking Lagrangian Solver: Implementation and Validation in AISI 304L Stainless Steel

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Abstract. A new efficient numerical solver inspired by front-tracking concepts is implemented within the DIGIMU® framework to accelerate full-field simulations of microstructural evolution. The solver is applied to AISI 304L stainless steel and compared with the conventional level-set formulation under laboratory hot-torsion tests and industrial multi-pass hot rolling conditions. After a limited recalibration of grain boundary mobility and solute drag parameters, both solvers provide comparable predictions of recrystallization kinetics, grain size evolution and final microstructures. The new solver achieves a reduction in computational cost close to two orders of magnitude, while preserving the predictive capabilities of DIGIMU®, thereby enabling more efficient industrial-scale simulations. Simulated predictions will be compared to Ugitech experimental work on lab torsion tests and industrial extrusion processes.

Introduction

Metallic material properties are strongly governed by their microstructures, which are themselves inherited from the thermomechanical treatments applied during processing. As a consequence, understanding, predicting, and ultimately optimizing microstructural evolution remains a central challenge and a key driver for competitiveness in modern metallurgical industries. Within this context, huge advances have been made in the last decades in order to link processing parameters, microstructural evolution, and final material properties.

However, predicting microstructural evolution during complex thermomechanical treatments, particularly multi-pass hot forming processes, remains extremely challenging. Grain growth (GG), solid-state phase transformations (SSPT), discontinuous dynamic recrystallization (DDRX) and continuous (CDRX) mechanisms, as well as post-dynamic recrystallization (PDRX), can occur simultaneously and interact in a highly complex manner. Small variations in temperature, strain, strain rate, or inter-pass times can lead to significant differences in the resulting microstructure.

Classical phenomenological models, such as those based on Johnson–Mehl–Avrami–Kolmogorov (JMAK) kinetic[1]–[3], offer very low computational cost but are generally limited to narrow validity domains defined by the calibration conditions. To overcome these limitations, more advanced modeling strategies have been developed. Mean-field models extend the applicability range by introducing statistical descriptions of grains, precipitates, and dislocation densities, but they rapidly reach their limits when dealing with complex, non-monotonic, multi-pass industrial processes [4]–[6]. This has motivated the development of mesoscopic, full-field approaches, in which the polycrystalline microstructure is explicitly represented within representative volume elements and local thermomechanical fields provided by macroscopic simulations are used as boundary conditions. Among the full-field approaches, several numerical frameworks have been proposed and widely studied, including Monte Carlo Potts models [7],cellular automata [8]–[10], phase-field and

multi-phase-field methods [11]–[13], front-tracking or vertex models [14], [15] and level-set (LS) formulations [16]–[19]. Each of these methods presents specific advantages and limitations in terms of numerical robustness, physical fidelity, and computational efficiency. The DIGIMU® software has been developed within this mesoscopic, full-field paradigm, relying on a finite-element (FE) formulation coupled with a level-set description of grain boundaries [20]. DIGIMU® has demonstrated strong predictive capabilities for grain growth, recrystallization, precipitate evolution, and, more recently, solute drag effects, with successful applications to industrially relevant alloys such as AISI 304L stainless steel [21], [22].

Despite these achievements, the conventional DIGIMU® framework remains computationally demanding, especially for large-scale and multi-pass industrial simulations. A significant fraction of the total computation time is associated with mesh adaptation procedures required to accurately capture evolving grain boundary networks. To address this limitation, the present work focuses on the implementation and validation of a new, highly efficient numerical solver inspired by front-tracking concepts and previously proposed by Florez et al [23].

The primary ambition of this new solver is to achieve a substantial reduction in computational time while maintaining an accuracy level comparable to that of the conventional level-set DIGIMU® framework. In the present work, both approaches are systematically compared through simulations representative of laboratory and industrial thermomechanical processing of AISI 304L stainless steel, providing a clear assessment of the performance–accuracy trade-off offered by the new numerical model.

Numerical Models in DIGIMU®

Level-Set Model. The historical numerical core of DIGIMU® is based on a FE formulation combined with the LS method to describe evolving grain boundary networks. In this front-capturing approach, grain boundaries are implicitly defined as iso-surfaces of one or several level-set functions, whose evolution is governed by transport equations coupled with local driving forces such as grain boundary curvature, stored energy gradients, Zener pinning, and solute drag effects.

The FE–LS framework offers several important advantages. First, it naturally handles complex topological events such as grain disappearance, grain coalescence and junction evolution without requiring explicit tracking of interfaces. Second, it is particularly well suited for large deformations of the computational domain, which are typical of thermomechanical processing routes encountered in metal forming. These characteristics have made the LS approach a robust and versatile choice for industrially oriented full-field simulations.

Over the years, substantial developments have been carried out to improve the robustness and performance of the DIGIMU® LS solver, including advanced remeshing strategies and optimized algorithms for coupling microstructural evolution with thermomechanical fields [24]–[26]. Nevertheless, the computational cost remains high. In particular, a large proportion of the total simulation time is associated with remeshing operations and distance function reinitialization required to accurately resolve grain boundaries as the microstructure evolves. As a result, further performance improvements within the conventional FE–LS framework have become increasingly difficult to achieve.

Front-Tracking Lagrangian Model. To overcome the performance limitations of the level-set approach, a new numerical solver has been introduced into DIGIMU®, inspired by front-tracking and vertex-based methods. In contrast to front-capturing techniques, front-tracking approaches explicitly represent interfaces as sets of connected segments in two dimensions or surfaces in three dimensions. Geometrical quantities such as curvature and normal vectors are computed directly at the interfaces, and interface motion is described in a Lagrangian manner.

The new DIGIMU® solver adopts this philosophy while remaining compatible with a FE description of grain interiors. Geometrical and physical quantities are evaluated only at grain boundaries, and grain boundary migration is governed by an explicit Lagrangian scheme driven by local kinetic driving forces. This strategy allows to reduce the spatial discretization compared to the level-set

method and avoid some expensive steps such as the solving of the convection-diffusion equation and the distance reinitialization used in the level-set method. The cost of this approach is the burden of constant, complex remeshing to preserve the topological description during every event: grain growth or dissolution, grain collapse, grain nucleation, multiple junctions. For now, only 2D simulations are available. It is important to underline that both approaches are based on the same physical models and equations.

The new proposed solver in DIGIMU is strongly based on the Lagrangian model introduced by Florez et al. [14], called the ToRealMotion (TRM) code for "topological remeshing in Lagrangian framework for large interface motion". This solver was specifically designed to handle large interface motions, complex topological changes, and strong domain deformations. By combining explicit interface tracking with unstructured FE meshes for grain interiors, the model allows the incorporation of intragranular state variables, such as stored energy, which are essential for recrystallization modeling. A more detailed description of the TRM solver, including remeshing, repartition, grain computation at grain boundaries and multiple junction, could be found in [14, 23, 26].

Parameter Calibration and Comparison Methodology

In order to perform a meaningful comparison between the conventional DIGIMU® solver and the newly implemented numerical framework, a strict and controlled methodology was adopted. AISI 304L austenitic stainless steel was selected as the material. Microstructure evolution was studied under thermomechanical loading conditions representative of laboratory and industrial rolling processes. All the experimental tests were carried out by UGITECH. In depth analysis and presentation of the experimental work is presented in Sourisseau et al. [22].

The simulations were conducted using identical initial microstructures, thermomechanical paths (temperature, strain, strain rate, and inter-pass times), and physical descriptions of the governing mechanisms, including grain growth, dynamic and post-dynamic recrystallization, Zener pinning, and solute drag. The only difference between the two simulation frameworks lies in the numerical formulation used to describe grain boundary migration and interface evolution.

Due to the intrinsic differences between the LS formulation and the new front-tracking inspired Lagrangian approach (TRM), small discrepancies in the effective kinetics of interface migration may arise, even when identical physical parameters are employed. For this reason, a limited and physically motivated recalibration of selected kinetic parameters was performed for the new solver.

More specifically, only three parameters were adjusted: the grain boundary mobility and two parameters (α and β described in [21]) associated to the Cahn-Lücke-Stüwe solute drag model [27], [28]. All other material parameters, including grain boundary energy, nucleation parameters and recovery parameters were kept strictly identical between the two solvers. All other physical parameters were directly taken from previous DIGIMU® reported in [22].

The calibration procedure was carried out using reference conditions representative of laboratory-scale hot-torsion and hot-rolling tests, as described in the abstract, with the objective of matching the overall recrystallization kinetics and the order of magnitude of the resulting grain size. Once identified, the adjusted parameters were fixed and subsequently applied without modification to the industrial multi-pass hot rolling simulations.

It is important to emphasize that the computational performance of the two solvers is entirely independent of this parameter calibration. The observed differences in computation time arise solely from the numerical formulation of interface motion and mesh management strategies, and not from the choice of kinetic parameters.

Results

Following the comparison methodology and calibration strategy described in the previous section, the predictive capabilities of the conventional LS solver and TRM solver are assessed through a series of representative thermomechanical loading cases. The comparison is carried out at different levels, including laboratory condition and industrial processing conditions. For all cases, the same material

parameters are used. A further deep description of the experimental conditions is presented in Sourisseau et al. [22].

Hot-torsion laboratory tests. The first level of comparison focuses on the hot-torsion tests. In these tests three different strain rates and temperatures were studied covering a range of use between 1020°C-1220°C and $0.1s^{-1}$-$5s^{-1}$. The evolution of the recrystallized fraction as a function of strain was measured by interrupted tests followed by EBSD maps. In Fig. 1, the experimental evolution of the microstructure along with the simulations performed with the LS and TRM solver are shown. Both solvers exhibit very similar kinetics, with nearly overlapping curves over the full range of deformation. Furthermore, a good fitting with the experimental data all over the range of temperature and strain rate is achieved.

Fig. 2 presents the evolution of the average grain size predicted by both solvers under the same thermomechanical conditions. The results show a very close agreement throughout the processing path, both in terms of transient evolution and final grain size values. Minor discrepancies, when observed, remain within the expected numerical variability and do not affect the overall trends or the final microstructural state.

In addition to integral quantities, a direct comparison of the simulated microstructures provides valuable insight into the spatial fidelity of the two numerical formulations. Fig. 3 shows the final grain structures predicted by the LS based solver and the TRM solver for all the tests performed at a strain rate of $1s^{-1}$. Both approaches lead to comparable grain morphologies, grain size distributions, and recrystallized patterns. The similarities observed in terms of grain topology and heterogeneity further confirm that the new solver preserves the essential physical mechanisms governing microstructural evolution, despite the different numerical treatment of interfaces.

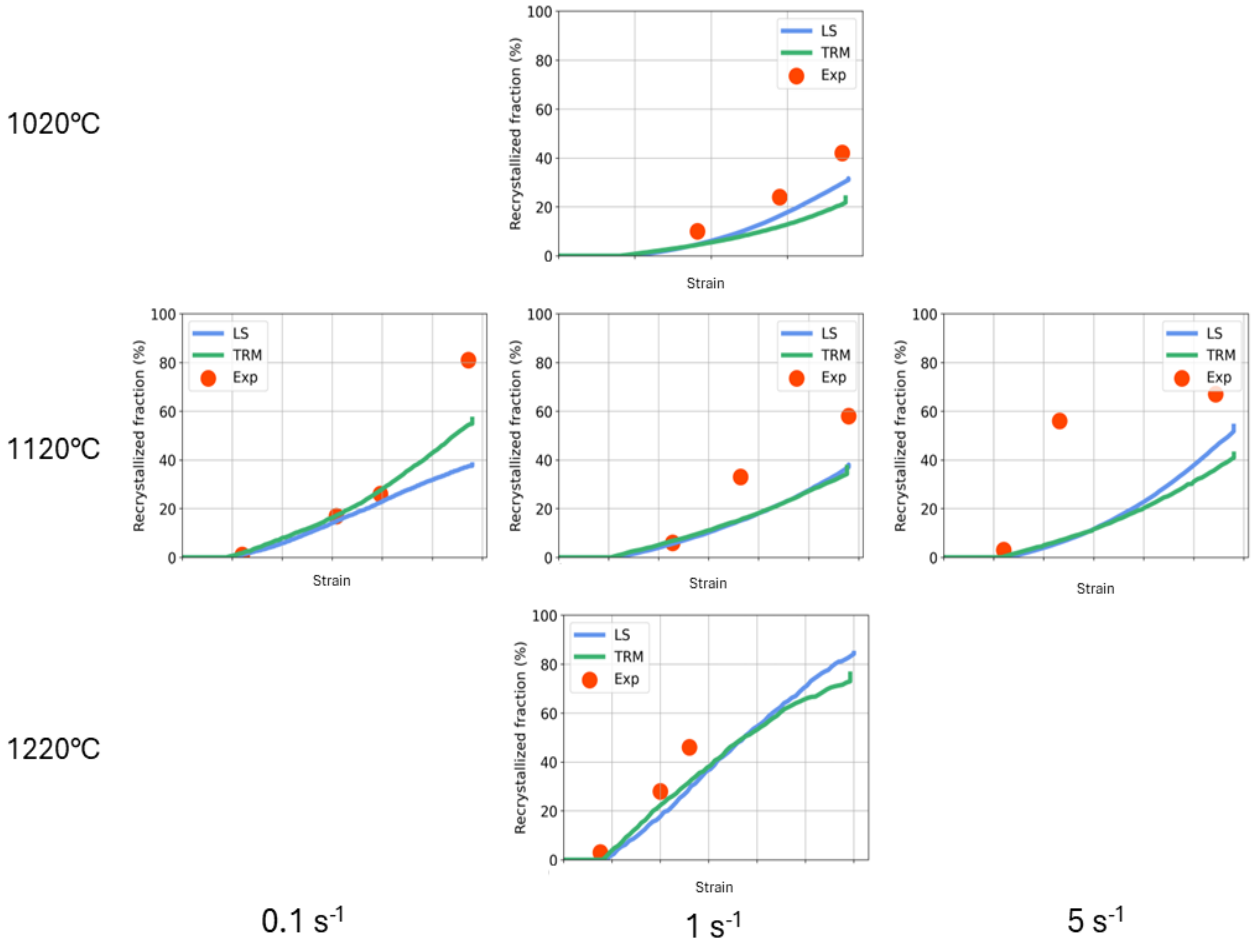

Fig. 1. Evolution of the recrystallized fraction measured experimentally, predicted by the conventional level-set solver and the TRM solver under representative hot-torsion and hot-rolling conditions for AISI 304L stainless steel.

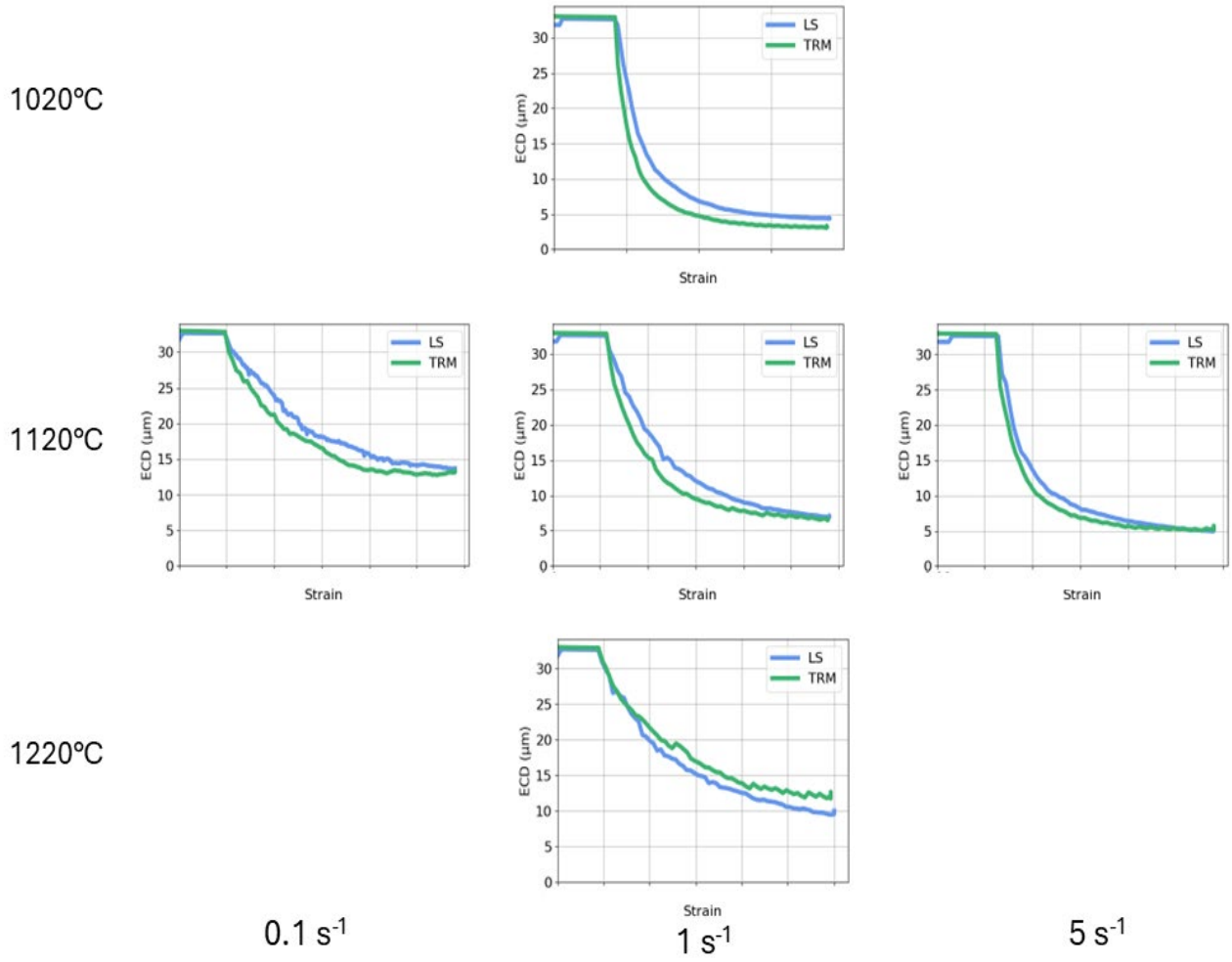

Fig. 2. Comparison of the mean grain size evolution predicted by the level-set-based solver and the new solver for identical thermomechanical loading paths.

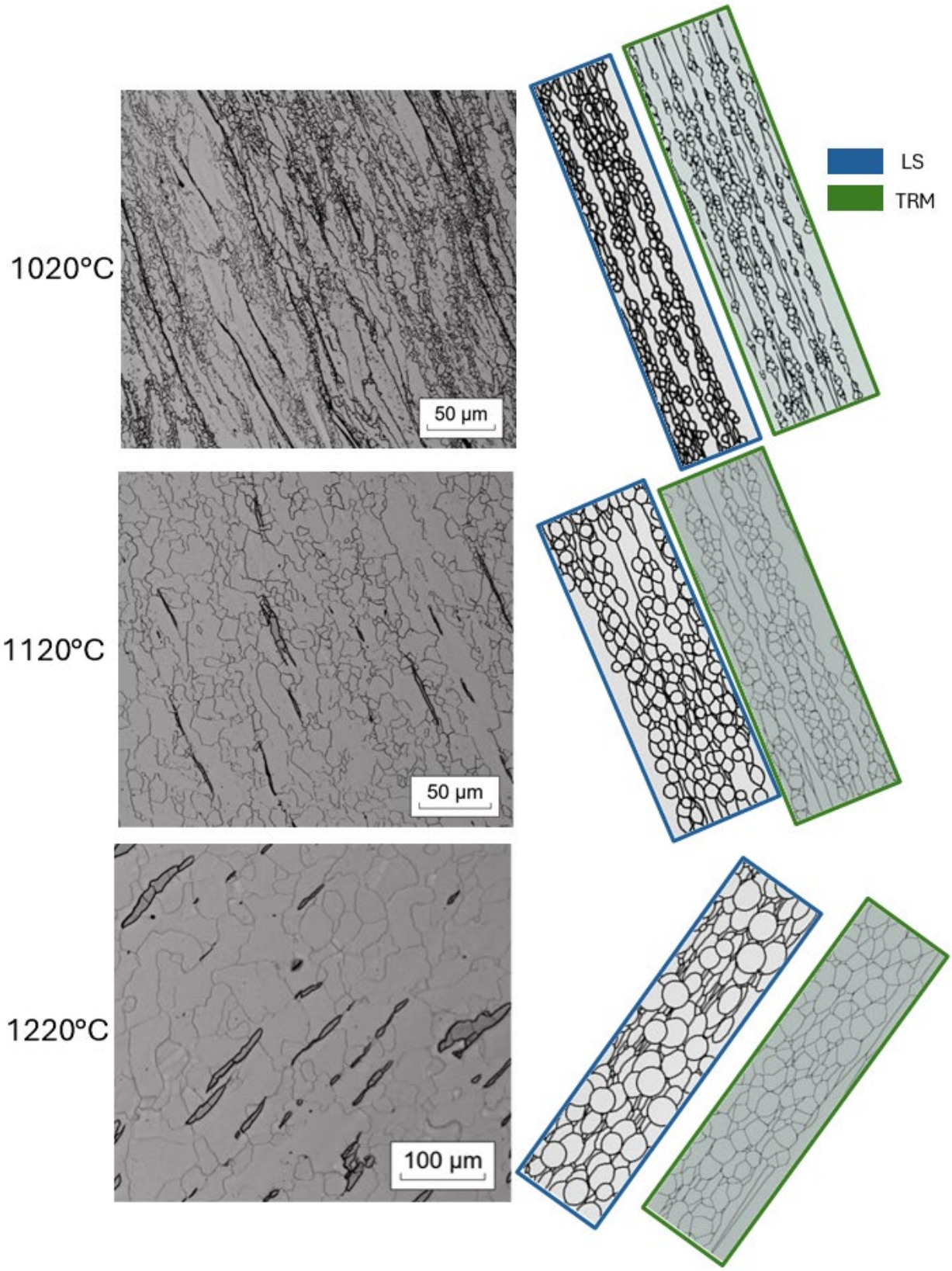

Fig. 3. Comparison between experimental microstructures and final grain structures predicted by the LS and (b) TRM solver for all the studied temperatures and a strain rate of $1s^{-1}$.

Industrial multi-pass case. In this section, the predictive capabilities of both solvers are evaluated through a real industrial application. The study focuses on the microstructural evolution during the multi-pass hot-rolling process at UGITECH.

The thermomechanical history of the product was obtained via FORGE® FE simulations. For this analysis, the study focuses on a representative point at the product surface. The process parameters involve a temperature range of 1000–1250°C and strain rates varying from 0.1 s^{-1} to 15s^{1}. The resulting thermomechanical path for the multi-pass sequence is illustrated in Fig. 4.

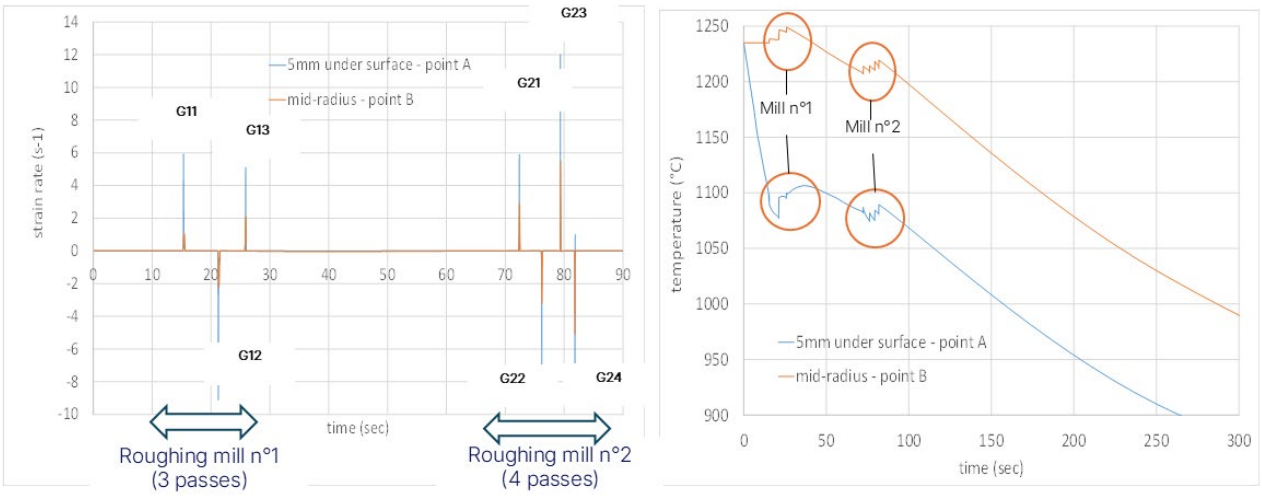

Fig.4. Thermomechanical path of the multi-pass hot rolling mill.

The evolution of the recrystallized fraction shows a good agreement between the two solvers (Fig. 5a). Regarding the mean grain size, both models yield acceptable results, with predictions falling within the range of experimental values (Fig. 5b).

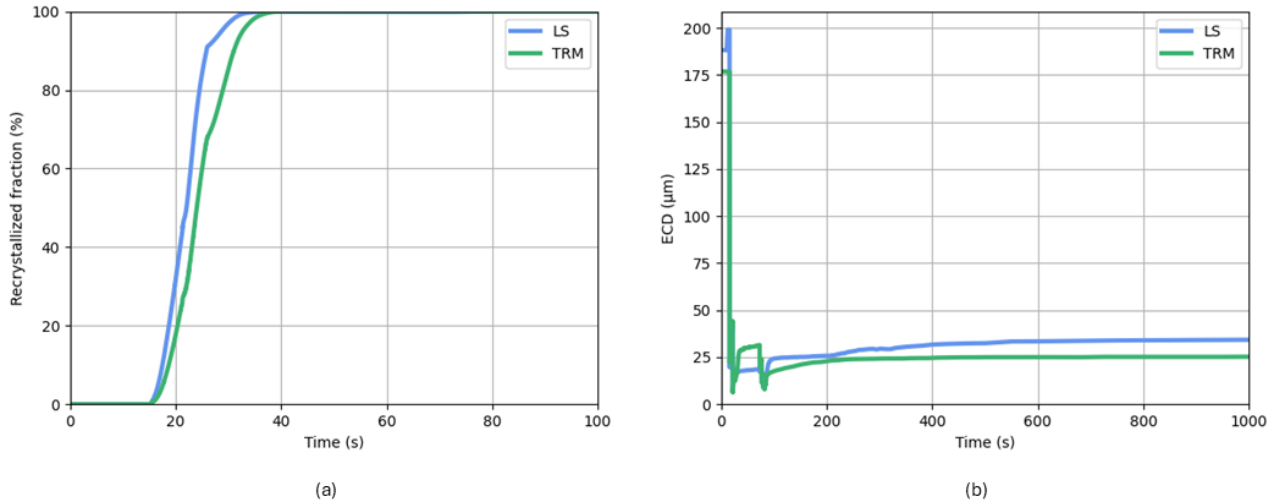

Fig.5. Comparison of the recrystallized fraction (a) and the mean grain size (b) evolution predicted by the LS solver and the TRM solver for the industrial multi pass case.

However, discrepancies arise when analyzing the grain size distribution and morphology. As shown in Fig. 6, neither LS nor the TRM solver is currently able to capture the largest grains observed in the experimental microstructure. This limitation suggests an area for further investigation to improve the solvers' sensitivity to grain size extremes. Furthermore, a comparison of the final grain structures reveals that the simulated microstructures are significantly more equiaxed than the experimental ones. The complex grain morphologies observed in the experimental images are not yet fully represented by the simulations, which tend to produce more regularized geometries.

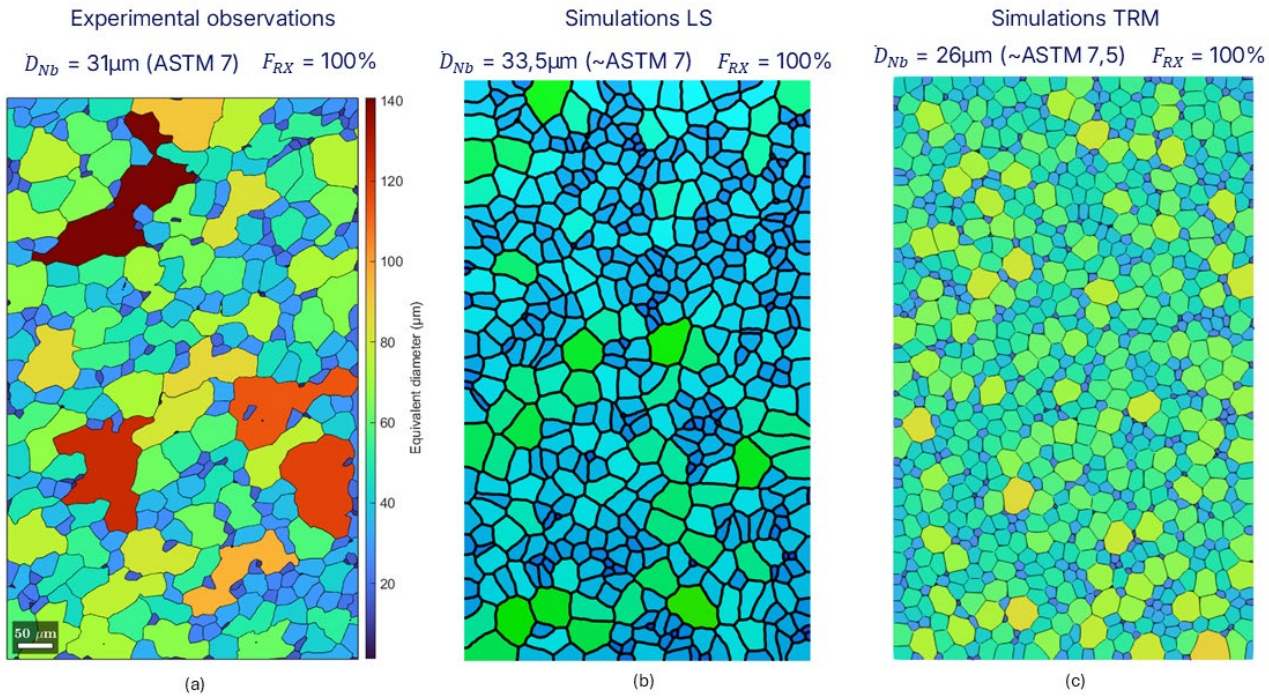

Fig. 6. Comparison between experimental microstructure (a) and final grain structures predicted by the LS and (b) TRM solver for all the studied temperatures and a strain rate of $1s^{-1}$.

Computational performance and efficiency. While the previous sections demonstrate the equivalence of the microstructural predictions obtained with both numerical approaches, the primary motivation for the development of the new solver is the improvement of computational efficiency. This section therefore focuses on a detailed comparison of the computational cost associated with each numerical framework.

As shown in Table 1, all simulations performed with the new TRM solver were carried out using a single CPU core, resulting in computation times ranging from a few seconds to several minutes, depending on the case considered. In contrast, all simulations performed with the conventional DIGIMU® level-set solver required 16 or 24 CPU cores and led to computation times on the order of several minutes to several hours.

Table 1 summarizes the computation times and hardware configurations used for the different simulation cases. For all investigated conditions, the new solver exhibits a significant reduction in computation time, confirming the substantial performance gain achieved by the new numerical formulation.

Discussion

The results presented in this study demonstrate that the newly implemented front-tracking-inspired solver within DIGIMU® is capable of reproducing the main microstructural features observed during the hot forming of AISI 304L stainless steel, with a level of accuracy comparable to that of the conventional level-set formulation. After a limited and physically motivated recalibration of selected kinetic parameters, both numerical approaches yield consistent predictions of recrystallization kinetics, grain size evolution, and overall microstructural morphology under laboratory and industrial processing conditions.

Table 1. Comparison of computational cost between the conventional level-set solver and the new solver for laboratory, semi-industrial, and industrial simulation cases.

Simulation		Cores		Computation time	
		LS	TRM	LS	TRM
Hot-torsion test	1020°C – $1s^{-1}$	16	1	2h 2min	16s
	1120°C – $0.1s^{-1}$	16	1	1h 4min	5s
	1120°C – $1s^{-1}$	16	1	30 min	6s
	1120°C – $5s^{-1}$	16	1	7 min	5s
	1220°C – $1s^{-1}$	16	1	7 min	4s
Industrial	Surface	24	1	3h 30min	19min 35s

The need for a minor recalibration of the grain boundary mobility and solute drag–related parameters arises from the intrinsic differences in the numerical treatment of interface motion between the two solvers. While the underlying physical models remain identical, the explicit Lagrangian representation of grain boundaries modifies the effective kinetics of interface migration compared to the implicit front-capturing strategy of the level-set approach. The adjusted parameters directly control interface mobility and solute drag effects and are therefore the most sensitive to the numerical formulation and numerical diffusion in the results of the level-set formulation. However, this is not surprising, as the grain boundary mobility is always a model parameter in full-field models.

The comparison under industrial rolling conditions highlights both the strengths and current limitations of the modeling approaches. Both solvers provide comparable predictions of recrystallized fraction and mean grain size in a very wide range of temperature and strain rates on real industrial processes. However, discrepancies remain when comparing very locally simulated and experimental grain morphologies and size distributions. In this case, neither solver fully captures the largest grains, nor the complex non-convex morphologies observed experimentally. These differences point to modeling challenges that are not specific to the way of solving the equation. Probably, some more advanced work on the parameters identification could allow us to optimize our results and make them even closer to reality. However, some missing elements in the modelling equation themselves still prevent us from obtaining all the complexity of the local grain topology formalism.

From a computational perspective, the new solver delivers a substantial performance improvement, with computation times reduced by approximately one order of magnitude despite being executed on significantly fewer computational cores, maintaining the same accuracy level than the older DIGIMU solver. This gain is primarily attributed to the elimination of frequent global remeshing operations and to the coarser meshes used in the TRM solver. By explicitly tracking grain boundaries in a Lagrangian framework, the numerical effort is focused on physically relevant regions of the microstructure, resulting in a more efficient use of computational resources.

Despite the coarsening of the mesh adopted in the TRM formulation, no significant loss of accuracy is observed, as demonstrated by the comparative results. This is primarily due to the intrinsic front-tracking nature of the TRM approach, which allows all interface-related calculations to be performed directly and exactly at the grain boundary position. As a consequence, highly refined meshes within the grain interiors are no longer required. Furthermore, the TRM formulation avoids the need for repeated reinitialization of the level-set function to preserve its distance function properties, as well as the extremely fine discretization typically required around the level-set 0 iso-value to accurately capture interface motion. This leads to a substantial reduction in computational cost without compromising predictive precision.

Conclusions

A new, highly efficient numerical solver inspired by front-tracking concepts has been implemented and validated within the DIGIMU® framework for the simulation of microstructural evolution in AISI 304L stainless steel. The solver was systematically compared with the conventional level-set formulation and to UGITECH experimental observations on laboratory hot-torsion tests and industrial multi-pass hot rolling conditions.

After a limited recalibration of the grain boundary mobility and solute drag–related parameters, the new solver was shown to reproduce the main microstructural features predicted by the reference formulation, including recrystallization kinetics, grain size evolution, and final microstructural morphology. This confirms that the change in numerical strategy does not compromise the physical consistency of the simulations. Although the level-set formulation is used as the reference numerical framework in this study, the predictions obtained with this solver are not expected to be perfectly accurate. For this reason, the comparison was not limited to the level-set formulation alone, but was also systematically carried out against experimental results, including recrystallized fraction, mean grain size evolution, and EBSD-based microstructural observations.

The main outcome of this work is the significant improvement in computational efficiency achieved with the new solver, with computation times reduced by a factor of 50 to 100. This performance gain is solely attributed to the numerical formulation of interface motion and mesh management and is independent of the parameter calibration. Enhanced efficiency substantially extends the applicability of full-field microstructural simulations in industrial environments, making reliable simulation of complex, multi-pass thermomechanical processes more accessible within realistic computation times.

The present study intentionally addresses a wide range of thermomechanical conditions, involving the simultaneous activation of several interacting mechanisms such as GG, DDRX, solute drag and post-dynamic recrystallization, over a broad domain of temperatures and strain rates representative of industrial hot-forming processes. The objective was not to achieve an extremely fine calibration for a single processing condition, but rather to demonstrate robustness and representativeness across an industrially relevant operating window. More extensive validation and further developments are currently in progress to refine the predictions for specific cases and to extend the applicability of the approach.

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