modelling

MDPI

Article

Developing a Framework for Using Molecular Dynamics in Additive Manufacturing Process Modelling

Panagiotis Stavropoulos * and Vasiliki Christina Panagiotopoulou

Laboratory for Manufacturing Systems and Automation, University of Patras, 26504 Patras, Greece; panagiotopoulou@lms.mech.upatras.gr

* Correspondence: pstavr@lms.mech.upatras.gr; Tel.: +30-2610-910160

Abstract: Additive Manufacturing (AM), or else Smart Manufacturing, has been an intrinsic concept in Industry 4.0, offering flexibility and material efficiency. Certain limitations prevent AM from being used in the industrial setting extensively, despite its advantages. Therefore, a literature review on the process modelling approaches, their advantages and limitations was performed. The most frequently used process modelling approaches were reviewed and summarized with respect to the process modelling approach, scale and limitations. The different categories of process modelling approaches were compared, with molecular dynamics being a promising modelling technique that can be used in software applications. A new framework for modelling additive manufacturing processes based on molecular dynamics was proposed in this work, combining previously published manufacturing methodologies for the AM process, such as manufacturability, design and planning of the AM. A validation plan followed, with the main parameters and details highlighted. The proposed framework is offering a unique approach for modelling the AM process, based on parameters from the manufacturing design, planning and process. This framework will be used in software platforms for predicting temperature distributions and for optimizing shape and AM process.

Keywords: molecular dynamics; additive manufacturing; multiscale modelling; 3D-printing

Citation: Stavropoulos, P.; Panagiotopoulou, V.C. Developing a Framework for Using Molecular Dynamics in Additive Manufacturing Process Modelling. *Modelling* **2022**, *3*, 189–200. https://doi.org/10.3390/modelling3010013

Academic Editor: Abílio M.P. De Jesus

Received: 18 December 2021
Accepted: 16 March 2022
Published: 18 March 2022

1. Introduction

In March 2016, a new initiative was launched by America Makes and the American National Standards Institute (ANSI), called America Makes and ANSI Additive Manufacturing Standardization Collaborative (AMSC), in order to coordinate and accelerated the standardization of industrial Additive Manufacturing (AM). According to AMSC, "AM, sometimes referred to as three-dimensional (3D) printing, encompasses a variety of processes wherein a 3D object is produced from a digital model by adding successive layers of material to create the object. In name, it stands in contrast to traditional or subtractive manufacturing where material is removed through machining or other means to create an object" [1]. In the same report [1], the need for standardization was highlighted, starting from the design of the object to the maintenance protocols for machines, parts and systems required for AM.

In general, AM allows the creation of products with complex and highly customized shapes, in the least amount of time required turnaround from design to product. It also allows for a zero-defect approach, with minimum waste produced during the production of the objects that can be used in various areas of applications, including biomedical and aeronautical applications [2]. AM is a relatively new manufacturing approach, with a promising future. It is considered less wasteful than traditional methods with potential to affect the environmental impact of manufacturing in a positive way, using zero defect principles [3]. In addition, other benefits include the ability to customize production, the easy sharing of the digital files of the models and the ability to produce novel and complex structures. However, there are certain limitations that prevent the application of AM in industrial sector, such as the current high cost of production, the need for new material

development, the gap in standardization approaches, the lack of mechanical and thermal properties being validated, the lack of automation approaches that would improve the efficiency and the need for post-processing steps that improve the surface of the additive manufactured products.

AM is based on layer-by-layer processing using powder, resin or filament as a starting material and heat to bond the materials together. The bonding is usually responsible for defects, such as pin hole voids, incomplete melting, or filling. The challenge is to reduce their occurrence, which could be done by modelling, optimization and standardization of the procedure. Modelling approaches can be used to improve the outcome, by simulating the steps involved, with key parameters being the scale of the approach, the aim, the use of discrete or continuous methods, the constraints and assumptions that will be used and the computational power and cost of the methods. There are three main approaches for the modelling and simulation of AM Processes: Finite Element Analysis (FEA), Lattice Boltzmann Method (LBM) and Molecular Dynamics (MD). The modelling methods can be used in software platforms and applications in industry, in the form of Digital Twins and Artificial Intelligence, to simulate the processes in real-time and provide tools for the digitalization and optimization of AM processes.

Certain challenges are associated with the different modelling approaches and will be listed later when comparing the different approaches. The aim of the current review is to propose a new framework for modelling the AM approaches, by compiling a detailed literature review of the modelling approaches used in AM, comparing the different approaches and highlighting the superiority of MD for industrial uses compared to the rest of computational approaches.

2. Literature Review on Modelling for AM

Several reviews were performed and published in literature, identifying and summarizing the types of AM processes and modelling approaches [4–9]. However, their focus was on simply describing the types or approaches in a research level, neither focusing on the industrial applications nor developing frameworks for AM modelling that could be used in software applications.

Using the following key words "modelling", "molecular dynamics", "metal" and "laser additive manufacturing" in Google Scholar, 148 papers were identified. Via title and abstract checking for their compatibility to the subject, 117 articles were not included in this review as irrelevant to the topic. The rest of the papers (n = 31) were categorized according to their modelling approaches and information was collected. Categorization of literature according to type of AM process and type of modelling approach used is found in Table 1 and Figure 1.

Table 1. Categorization of literature according to type of Additive Manufacturing and Modelling approach.

Type of AM	Modelling Approach	Literature
Selective Laser Sintering (SLS)	Discrete Element Method (DEM)	Averardi 2020 [10]
	Empirical	Panda 2016 [11]
	MD	Cheung 2014 [12], Hu 2017 [13], Zhang 2018 [14]
	Particle-scale numerical modelling	Maeshima 2020 [15]
Selective Laser Melting	MD	Babuska 2019 [16], Etesami 2020 [17], Guo 2017 [18], Kurian 2020 [19], Rahmani 2018 [20], Tan 2017 [21], Vo 2017 [22], Wang 2020 [23], Yao [24], Nandy 2019 [25], Nandy 2020 [26]
	Lattice Boltzmann Method	Cattenone 2019 [27]
	FE	Johnson 2019 [28]
	DEM	Cao 2019 [29], Steuben 2016 [30]
	Process energy demand model	Peng 2018 [31]
	Multiphysics simulation	Martin 2019 [32]
	FVM/DEM	Wang 2018 [33]
	MD/DEM/FEA	Zhang 2018 [34]
	Phase Field	Zhang 2018 [35]
	Computational Fluid Dynamics	Haley 2019 [36]

Table 1. *Cont.*

Type of AM	Modelling Approach	Literature
Wire Arc AM	MD/PF/FE	Geng 2021 [37]
Filament Material Extrusion-Fused Deposition Modelling	Analytical +Empirical	Komineas 2018 [38]
Hybrid AM	MD	Lin 2018 [39]

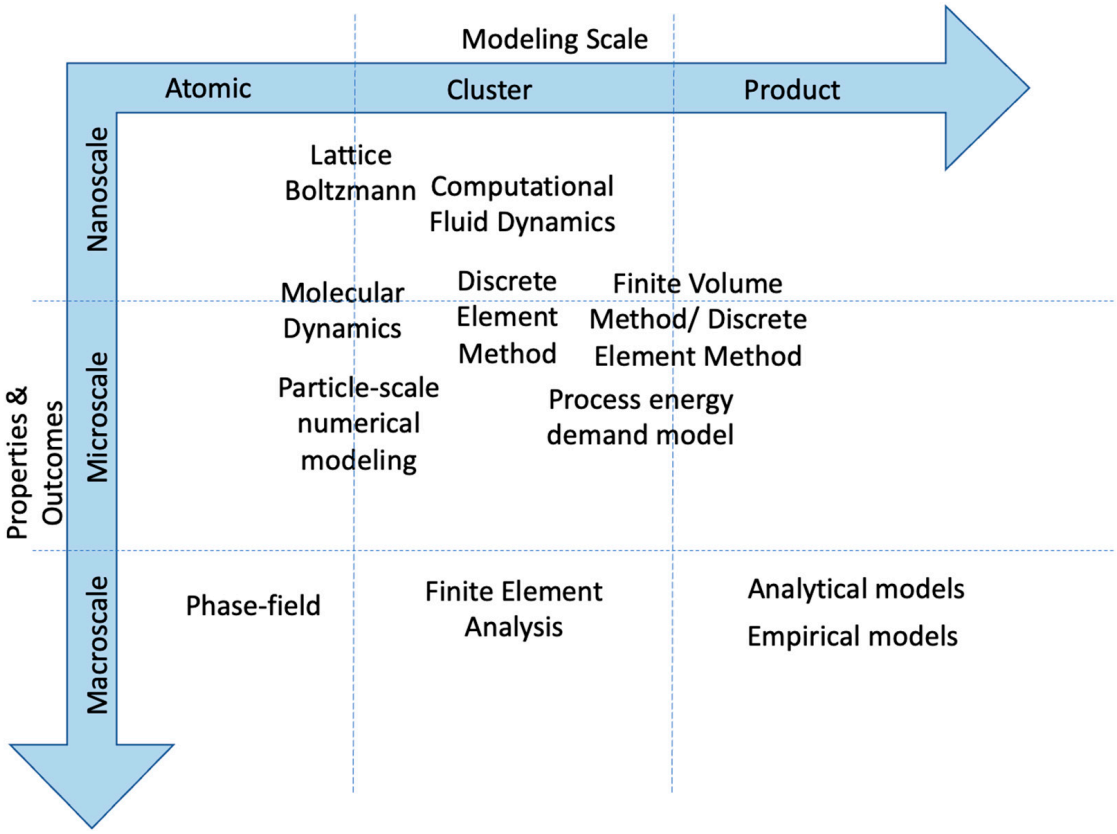

Figure 1. Distribution of models according to the selection of scale, e.g., atomic, particle or product scale, and the properties or outcomes scale, e.g., nanoscale, microscale or macroscale.

The mathematical approaches are mainly grouped into empirical, analytical, numerical or a combination of those methods. Empirical methods are based on the description of experimental values and the adaptation of commonly used mathematical equations to fit the experimental values. Analytical methods are used to fully describe the simulations using mathematical expressions, but when this is not possible, numerical estimations are used instead. Specific models used in AM simulations are: Phase-field models (PF), Molecular Dynamics, Lattice Boltzmann Method and Fluid Dynamics. Numerical methods include finite element analysis, finite volume methods and discrete element methods.

The different modelling approaches are modelling the AM at a different scale, ranging from nanoscale to macroscale, and from a different aspect of the AM process, from an atomic, cluster or product point of view (Figure 1). Starting from the nanoscale and inter-particle level, Lattice Boltzmann method [27] may offer an insight on the particle kinetics, but it requires significant computational efforts to simulate powder bed fusion processes, making the process impossible to simulate more than a microscopic part of the domain. Still on a nanoscale level, but after assuming a cluster of particles instead of individual particles, the use of computational fluid dynamics has been proposed [36]. The input parameters are the radius of the particle, the initial particle temperature, the initial melt pool temperature, the equilibrium contact angle, but also material properties (such

as density and viscosity), and thermophysical properties. The predictions resulted from the Computational Fluid Dynamics fall between ±50% of the respective numerical prediction, because of the assumptions made in the analytical model, therefore this approach does not provide accurate predictions that can address and fulfill the industrial demands and requirements.

When using a Discrete Element Method (DEM), the approach assumes clustering of atoms and addresses phenomena from a nano- to a microscale [10,29,30,33,34], with input parameters being laser properties (power, scan rate, scanning geometry), powder bed properties (layer thickness, working atmosphere, temperature, thickness) and particle properties (size distribution). The limitations are summarized as (1) being able to model only single pass formation [29], (2) loss of definition in the output model [30] and (3) impact of increased number of particles on the computational loop, as in slowdown of the modelling approach [31]. DEM can be combined with other modelling approaches, such as Finite Volume Method (FVM), to approach the AM from a cluster or product point of view [33].

The Particle-scale numerical modelling focuses on a microscale level and approach on atomic/cluster level, with input parameters being the laser properties (power, radius, velocity, absorptivity, penetration depth), material parameters and modelling aspects (grid space, nodes, material points). The disadvantage of this approach is the high computational cost, which is compensated though by the potential of the method to develop a sophisticated melting and crystallization simulation of the process [15].

Another approach at the microscale level is the process energy demand model, from a cluster/produce point of view, with input parameters being mainly the laser properties such as the laser power and diameter. The disadvantages of this technique are (1) the high number of simplifications required, for the scanning strategy, powder morphology and laser type and (2) the inability of the energy density to accurately reflect the material specifications [31].

Phase-field modelling has been used in modelling AM, from a macroscopic point of view on the atomic level [35]. The input parameters are laser parameters (laser power, surface reflectivity, effective laser spot radius, scanning speed), material parameters (powder bed porosity, reflectivity, surface emissivity), microstructure (porosity, mass density, surface energy, grain boundary energy). The main limitation is the inability of the method to simulate large domains.

Finite Element Analysis, a well-known technique, focuses on modelling macroscopic phenomena, from a cluster point of view. The input parameters vary from study to study, but throughout the approaches, the main disadvantage is the reduced sensitivity of the method [28,34,37].

When empirical approaches are used, the main input parameters are the absorptivity of the laser power system, laser power, the beam radius and the scan speed [11,38]. However, the empirical approaches, since they are developed based on specific examples, thus lacking the ability of providing a global modelling approach.

The Molecular Dynamics (MD) models phenomena on the nanoscale, such as the sintering and the crystallization. The main advantages of the approach, besides providing a better understanding on the complex physical phenomena governing the solidification and microstructural evolution [19], are the (1) revealing of the effects of asymmetric heating on the built part [12], (2) the potential of using coarse grain methods to scale up from the nanometer range [12], (3) description of complex and quantitatively accurate temperature distribution [19], (4) modelling of the interface of different materials at an atomic level [21] and (5) understanding the power behavior during the spreading core and the particle movement [24]. The disadvantages are summarized in (1) lack of experimental data for the non-equilibrium thermodynamics and (2) lack of sophisticated potentials [17]. Despite the limitations, MD is a powerful tool to study the physical and chemical phenomena during sintering [27] but also to quantify the mechanical and physical properties of the materials [25]. All modelling approaches have certain limitations that have been summarised and presented in Table 2.

Table 2. Identifying limitations in the most frequently used modelling approaches and how MD can address this.

Modelling Approach	Limitations	How MD Can Address This?	Relevant Reference
Lattice Boltzmann Method	• Significant computational effort • Impossible to simulate more than a microscopic part of the domain	• Clustering of atoms decreases the computational effort • Ability to simulate larger domains because of coarse grain method	[12]
Computational Fluid Dynamics	• Assumptions made in the analytical model result in poor predictions	• Good agreement between modelling and experimental results	[25]
Discrete Element Method	• Ability to model only single pass formation • Loss of definition in the output model • The more the particles, the slower the modelling approach	• Because of clustering, larger domains can be modeled • Good agreement between modelling and experimental data • Clustering allows increased number of particles without increasing the computational time	[12,17,25]
Particle-scale numerical modelling	• High computational cost	• Computational cost may vary based on clustering	[12,22]
Process Energy demand model	• High number of simplifications required • Inability of the energy density to accurately reflect the material specifications	• Small number of specifications, mainly driven by computational effort • Better understanding of complex physical phenomena	[19]
Phase field modelling	• Inability to simulate large domains	• Ability to simulate large domains	[12]
Finite Element Analysis	• Reduced sensitivity of the method	• High sensitivity at the nanoscale level	[12,24]
Empirical methods	• Lack of applicability in other scenarios	• Increased applicability	[11,38]

3. Proposing a Framework for Modelling and Optimizing AM Using MD

3.1. Description of MD and Literature Review on MD Approaches in AM

Molecular Dynamics is a computer simulation method for analyzing the physical movements of atoms and molecules. The atoms and molecules are allowed to interact for a fixed period of time, giving a view of the dynamic "evolution" of the system. Most commonly, the trajectories of atoms and molecules are determined by numerically solving Newton's equations of motion for a system of interacting particles where forces between the particles and their potential energies are often calculated using interatomic potentials or molecular mechanics force fields.

As already mentioned, MD approaches are focusing on the nanoscale level, modelling sintering and crystallization phenomena. For the calculation, it is important to select the potential that will be used for the modelling between the molecules. The majority of the papers (Table 1) are using embedded atom model (EAM) potential for the interatomic interactions and large atomic/ molecular massively parallel simulator (LAMMPS) for the simulation. In addition, it is vital to specify and determine boundary and initial conditions for the problem to be well defined. Some studies use periodic, some shrink-wrapped and some fixed boundary conditions. The aim of the papers using MD vary with most of the papers focused on the investigation of the melting and sintering processes, while few have used this approach to study the temperature gradient or the mechanical properties of the products.

3.2. Proposing a Framework for Modelling and Optimization of AM Using MD

The proposed framework focuses on defining a simulation approach for additive manufacturing based on molecular dynamics and on parameters derived from the additive manufacturing approach. As already determined by the literature review (Table 1), MD has been used in selective laser sintering, selective laser melting, wire arc AM and hybrid AM, so these processes will be used basis in this framework when any process details will be required. The overarching aim of this simulation is to be used as a basis for software platforms and digital tools, that will simulate the physical system using digital twins or artificial intelligence, predicting the outcomes by simulating what-if-scenarios, optimizing the operations and improving the quality of processes and products by enhancing and maintaining the repeatability and reproducibility of the AM process. Therefore, the proposed framework is based and aligned with a combination of frameworks and methodologies used for the manufacturability, the designing and the process of AM [40–42]. Figure 2 reflects this relationship between manufacturing frameworks and the current simulation methodology, via the link between manufacturing parameters and modelling parameters.

AM starts from conceptualizing the functional requirements of the product, starting from the conceptual design, identifying the basic properties and specifications of the 3D-printed product. Based on the desired properties, the material is selected, which also defines the selection of the AM process. Regarding the selection of the material, the most important parameters are the material that will be used for the object, the size of the object, the complexity of the structure and the desired properties of the product. These parameters will determine the type of AM process, the time that will be required for the production of the object and the parameters of the process, such as the melting temperature, power of laser etc. The AM process will be defined based on the object, along with the properties of the material, the laser beam properties and the process parameters.

Once material and process are selected, then the computer-aided design (CAD) is created which will be used for the printing of the product. The process is then planned, with the most important part being the identification of the best building strategy. The AM process then takes place, and the product is ready to be post-processed to obtain the optimal quality.

The parameters that control the manufacturing planning and process are presented in the second box of Figure 2 (green colour), starting from the properties of the material used in the AM process. It is important to know the chemical composition (pure metal vs alloy), the powder granulometry, the melting temperature, the latent heat of fusion, the thermal conductivity and the specific heat capacity density. These parameters offer an insight on the melting and solidification phase of the AM process and affect the mechanical properties of the product. The characteristics of the laser beam are also important, with main ones being the laser power, laser beam spot diameter, scanned head speed and laser offset. Last but not least, the building strategy is a result of the process planning and has an impact on the manufacturing process. Before the start of the process, the parameters are initial temperature (ambient temperature), powder layer thickness and powder bed dimension.

During the process, the main properties are scanning speed of the laser beam, the building orientation, heating phase, melting phase, equilibration phase and cooling phase.

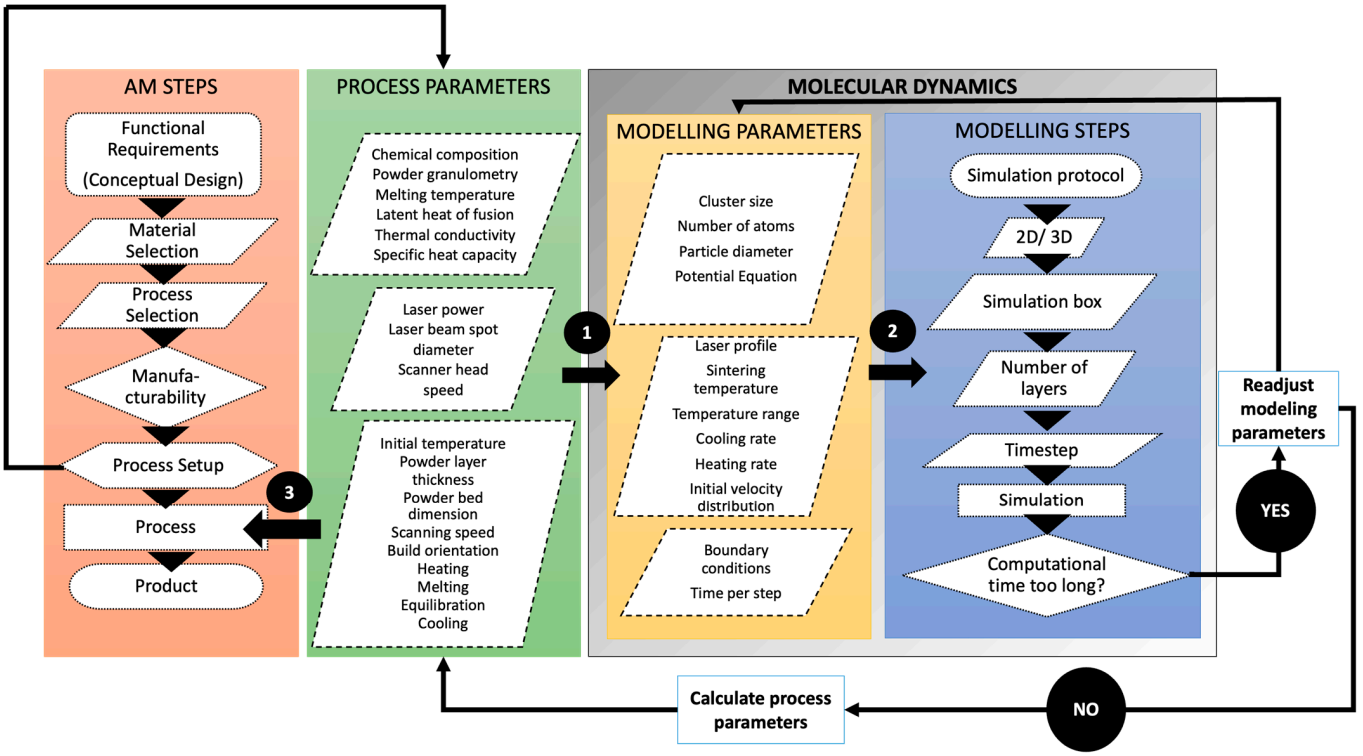

Figure 2. Flowchart of the framework, with process setup defining the process parameters, process parameters defining the modeling parameters (arrow number 1), modeling parameters defining the simulation protocol (arrow number 2), while final process parameters post-simulation defining the process (arrow number 3).

The simulation framework is strongly related to the selection of the modelling parameters. These parameters are derived or defined by the manufacturing properties, such as the material properties, laser beam properties and building strategy. More specifically, cluster size, number of atoms and diameter of the particles are strongly related the material selected for AM, while the selection of the potential equation depends on the atoms/molecules involved. The laser beam properties define the laser profile (Gaussian or not), the sintering temperature and the temperature range, but also the cooling and the heating rate. The building strategy defines the initial velocity distribution of the molecules, the boundary conditions and the time spent per step of the modelling procedure.

The simulation is then planned and performed by identifying and defining the following information:

- Simulation protocol
- Two- or three-dimensional structure
- Dimensions of the simulation box
- Number of layers
- Timestep

Before the simulation. The molecular dynamics approach will include details about the simulation, mostly about the size of the simulation box, the cluster size which is the number of molecules that consist the particle, the potential equation (Morse potential, Embedded Atom Method, Lennard-Jones) and the boundary conditions (periodic, fixed etc.). In addition, the timestep needs to be specified, to match the kinetics of the natural process. There are also four different ensembles which are listed as such:

(a) Microcanonical, an adiabatic- no heat exchange process
(b) Canonical with constant temperature
(c) Isothermal-isobaric
(d) Generalized with slow dynamics of disordered spin systems and parallel tempering.

If the computational time is longer than expected, a redefinition of the modelling parameters or adaptation of the simulation protocol will be required, until the simulation is completed in a time that is acceptable for an industrial software or digital platform. In order to decrease the time needed, one of the techniques used is the coarse-graining method, where a group of atoms or molecules defines one particle, decreasing thus the computational needs of the models (Figure 3).

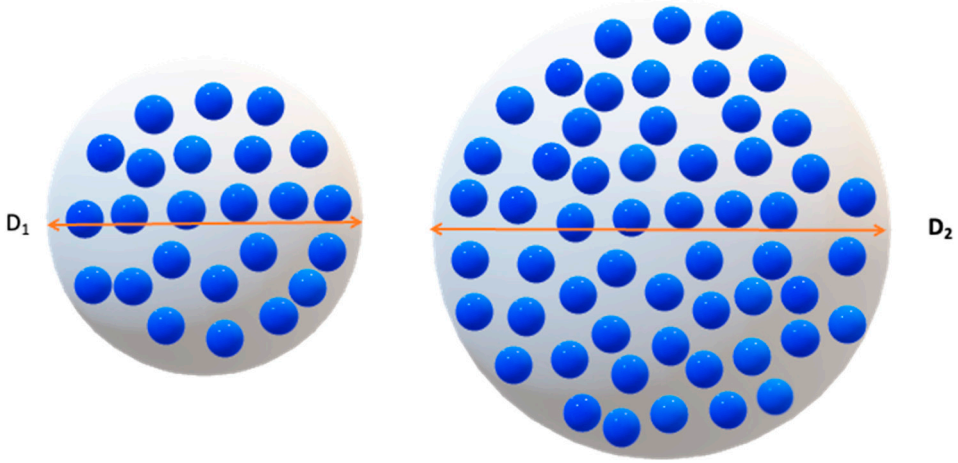

Figure 3. Increase of the particle size (white shape) with increase of the number of atoms included in the particle (blue circles), with $D_1 < D_2$.

3.3. Validation Plan of the Proposed Framework

Adapting a methodological approach for validation of computer models [43] for the specific application, the validation plan will include the following list of steps:

1. Specification of model parameters with specified range of values and associated uncertainties
2. Determination of criteria that will be used to evaluate the framework
3. Collection of data from the model
4. Analysis of the model output
5. Providing feedback and feedforward for the framework validation

Before starting the validation process, one must define whether the validation parameters will come from research or industrial AM process. Regarding the 1st step, the functional requirements of the product will be defined, starting with a simple, yet frequently used structure. The material selection will be based upon the functional requirements, with pure metal powder as a first approach, followed by an alloy powder once the simulation has been validated for pure metal powders. A selective laser melting approach will be used for the validation work, with the design of the process following a simple building strategy for validating the framework. Manufacturability of the product will be assessed based on the framework suggested by Lianos et al. [42], followed by the process planning and the final product. Based on the manufacturing framework, the main parameters of the material properties, laser beam properties and building strategy will be defined.

Moving towards the simulation model, the model parameters will be determined; initial values for the cluster size, number of atoms and particle diameters will be assumed, but modified later based on the evaluation criterion that will be described in the next paragraph. The equation for the potential relationship between the molecules will be selected based on the material that will be used for the AM process and on the available

literature. Laser profile, sintering temperature, temperature range and cooling/heating rates will be defined or calculated from the laser beam properties and material properties of the manufacturing process, with initial velocity distribution calculated from the ambient temperature. Simulation related parameters such as boundary conditions, time per step, dimensions of the simulation box and number of layers will be determined from the computational capabilities of the simulator.

The evaluation criterion for the validation of the framework is the time requested for the simulation completion. If the computational time is large, then new values for the modifiable parameters (cluster size, number of atoms and diameter of particles) will be assumed, and the new computational time will be evaluated.

Once the criterion is satisfied, the data from the model will be collected and analyzed, especially regarding the temperature distribution, the shape and the compositional characterization from the simulated scenario, in comparison to the 3D-printed product.

4. Discussion

AM processes in industrial settings are still in its infancy, mainly because of a need for more optimized, faster and more robust process against uncertainties. Therefore, frameworks for manufacturing are required to formulate the manufacturing process, but the biggest breakthrough will come from modelling and simulation tools that will provide a real-time insight into the AM processes and improve the quality of the products (geometrical, mechanical and physical characteristics) and the energy efficiency. In the current work, a framework was proposed for the simulation of processes using molecular dynamics and parameters deriving from the characteristics of the manufacturing aspect. The main parameters that need to de defined beforehand are the cluster size, number of atoms, diameter of particle, potential equation, laser profile, laser temperature, temperature range, cooling and heating rates, initial velocity distribution, boundary conditions and time per steps.

The modifiable parameters for the simulation are cluster size, number of atoms and diameter of particles, since they are related to the computational time required for the simulation. These parameters can be further modified if the computational time is longer than expected for a simulation fit for industrial settings. One of the parameters that can be optimized is the number of atoms per cluster with the higher the number of atoms per cluster, the smaller the number of clusters per simulation will be. On one hand, a high number of clusters (means a more complex structure and simulation, while a low number of clusters results in a longer computational time. Particle diameter is also an important parameter; small particle diameter means a more accurate description of the structural characterization, but with longer computational time. In contrast, large particle diameter leads to a less accurate structural characterization, in a much quicker time.

In literature, there are frameworks for the manufacturability of the AM products and the modelling of AM processes, but to the knowledge of the authors there is no framework for simulation of AM processes that is based on the manufacturing planning, process and parameters. The frameworks in literature are focusing on the design [43,44], the manufacturability and the optimization [42] of the processes, such as finding the optimal building strategy [45].

On the other hand, modelling of AM is focusing on describing a layer-by-layer simulation of research-based AM using either molecular dynamics or finite element method or physicochemical mathematical equations. Optimization of AM processes is limited due to limited modelling approaches [4], because the physical phenomena involved are complicated in their mathematical formulation. Applications for digital twins in AM have been described [46], where the authors described the resources required for the digital twin and included the material type, the laser light source, the controller synthesis, the sensing device and any extra technologies required for real-time simulation.

Another challenge faced for the integration of modelling approaches in AM is the lack of a monitoring software tool that will be able to monitor the process and provide feedback in real time to the process simulation model. For this, integration of selected

sensors is required and synchronization of robotic arm paths with the process execution via the simulation model and controllers installed [47].

The currently proposed framework focuses on parameters and characteristics derived from the manufacturing design, planning and process. In order to validate this theoretical approach, a validation approach has been described based on the parameters used for the AM design, planning and process. This way, the framework is validated using data from a real case study from either a research- or industrial-based AM process.

5. Conclusions

AM processes in industry are still lacking in terms of repeatability, performance and optimization. One way to address this is to develop a software tool that will provide a real-time insight in the AM process. A molecular dynamics-based approach offers many advantages such as increased accuracy in description of the melting and solidication phases, while clustering of atoms into larger particles offers the possibility for simulation time reduction without significant loss of accuracy. Therefore, in this paper, a framework for molecular dynamics approach is proposed, based on the manufacturing planning strategy and process via the use and translation of key parameters from the process itself to the simulation key characteristics.

Future work will focus on studying case studies of AM processes, in order to highlight the applicability of the process and its transferability in industrial case scenarios. In addition, the limitations for full use of the framework in industrial settings will be described and methodologies for overcoming this hurdle will be proposed. The development of a software platform will signify the applicability of the approach in industry.

Author Contributions: Conceptualization, P.S.; methodology, P.S. and V.C.P.; validation, P.S.; formal analysis, P.S. and V.C.P.; investigation, V.C.P.; resources, P.S.; writing—original draft preparation, V.C.P.; writing—review and editing, P.S. and V.C.P.; supervision, P.S.; project administration, P.S.; funding acquisition, P.S. All authors have read and agreed to the published version of the manuscript.

Funding: This research received no external funding.

Institutional Review Board Statement: Not applicable.

Informed Consent Statement: Not applicable.

Data Availability Statement: Not applicable.

Conflicts of Interest: The authors declare no conflict of interest.

References

1. America Makes, AMSC. *Standardization Roadmap for Additive Manufacturing—Version 2.0*; America Makes & ANSI Additive Manufacturing Standardization Collaborative (AMSC): American National Standards Institute: New York, NY, USA, 2018; Volume 2, pp. 1–269.
2. Herzog, D.; Seyda, V.; Wycisk, E.; Emmelmann, C. Additive manufacturing of metals. *Acta Mater.* **2016**, *117*, 371–392. [CrossRef]
3. Ford, S.; Despeisse, M. Additive manufacturing and sustainability: An exploratory study of the advantages and challenges. *J. Clean. Prod.* **2016**, *137*, 1573–1587. [CrossRef]
4. Bikas, H.; Stavropoulos, P.; Chryssolouris, G. Additive manufacturing methods and modelling approaches: A critical review. *Int. J. Adv. Manuf. Technol.* **2016**, *83*, 389–405. [CrossRef]
5. Foteinopoulos, P.; Papacharalampopoulos, A.; Stavropoulos, P. On thermal modeling of Additive Manufacturing processes. *CIRP J. Manuf. Sci. Technol.* **2018**, *20*, 66–83. [CrossRef]
6. Frazier, W.E. Metal Additive Manufacturing: A Review. *J. Mater. Eng. Perform.* **2014**, *23*, 1917–1928. [CrossRef]
7. Ghosh, S. Predictive modeling of solidification during laser additive manufacturing of nickel superalloys: Recent developments, future directions. *Mater. Res. Express* **2018**, *5*, 012001. [CrossRef]
8. Steuben, J.C.; Iliopoulos, A.P.; Michopoulos, J.G. Recent developments of the multiphysics discrete element method for additive manufacturing modeling and simulation. In Proceedings of the ASME Design Engineering Technical Conference; American Society of Mechanical Engineers (ASME), Cleveland, OH, USA, 6–9 August 2017; Volume 1. [CrossRef]
9. Hashemi, S.M.; Parvizi, S.; Baghbanijavid, H.; Tan, A.T.L.; Nematollahi, M.; Ramazani, A.; Fang, N.X.; Elahinia, M. Computational modelling of process–structure–property–performance relationships in metal additive manufacturing: A review. *Int. Mater. Rev.* **2021**, *67*, 1–46. [CrossRef]

10. Averardi, A.; Cola, C.; Zeltmann, S.E.; Gupta, N. Effect of particle size distribution on the packing of powder beds: A critical discussion relevant to additive manufacturing. *Mater. Today Commun.* **2020**, *24*, 100964. [CrossRef]
11. Panda, B.; Garg, A.; Shankhwar, K. Empirical investigation of environmental characteristic of 3-D additive manufacturing process based on slice thickness and part orientation. *Measurement* **2016**, *86*, 293–300. [CrossRef]
12. Cheung, S.L.; Chua, C.K.; Zhou, K.; Wei, J. Effects of temperature on particle coalescence in the selective laser sintering process. In Proceedings of the International Conference on Progress in Additive Manufacturing, Singapore, 14–17 May 2018; Pro-AM: Pebble Beach, CA, USA, 2014; Volume 24, p. 29. [CrossRef]
13. Hu, Z.; Mahadevan, S. Uncertainty quantification and management in additive manufacturing: Current status, needs, and opportunities. *Int. J. Adv. Manuf. Technol.* **2017**, *93*, 2855–2874. [CrossRef]
14. Zhang, Y.; Zhang, J. Sintering phenomena and mechanical strength of nickel based materials in direct metal laser sintering process—A molecular dynamics study. *J. Mater. Res.* **2016**, *31*, 2233–2243. [CrossRef]
15. Maeshima, T.; Kim, Y.; Zohdi, T.I. Particle-scale numerical modeling of thermo-mechanical phenomena for additive manufacturing using the material point method. *Comput. Part. Mech.* **2021**, *8*, 613–623. [CrossRef]
16. Zhang, X.; Liao, Y. A phase-field model for solid-state selective laser sintering of metallic materials. *Powder Technol.* **2018**, *339*, 677–685. [CrossRef]
17. Babuska, T.F.; Wilson, M.A.; Johnson, K.L.; Whetten, S.R.; Curry, J.F.; Rodelas, J.M.; Atkinson, C.; Lu, P.; Chandross, M.; Krick, B.A.; et al. Achieving high strength and ductility in tradi-tionally brittle soft magnetic intermetallics via additive manufacturing. *Acta Mater.* **2019**, *180*, 149–157. [CrossRef]
18. Etesami, S.A.; Laradji, M.; Asadi, E. Reliability of molecular dynamics interatomic potentials for modeling of titanium in additive manufacturing processes. *Comput. Mater. Sci.* **2020**, *184*, 109883. [CrossRef]
19. Guo, S.; Wang, M.; Zhao, Z.; Zhang, Y.; Lin, X.; Huang, W. Molecular dynamics simulation on the micro-structural evolution in heat-affected zone during the preparation of bulk metallic glasses with selective laser melting. *J. Alloys Compd.* **2016**, *697*, 443–449. [CrossRef]
20. Kurian, S.; Mirzaeifar, R. Selective laser melting of aluminum nano-powder particles, a molecular dynamics study. *Addit. Manuf.* **2020**, *35*, 101272. [CrossRef]
21. Rahmani, F.; Jeon, J.; Jiang, S.; Nouranian, S. Melting and solidification behavior of Cu/Al and Ti/Al bimetallic core/shell nanoparticles during additive manufacturing by molecular dynamics simulation. *J. Nanoparticle Res.* **2018**, *20*, 133. [CrossRef]
22. Sorkin, A.; Tan, J.; Wong, C. Multi-material modelling for selective laser melting. *Procedia Eng.* **2017**, *216*, 51–57. [CrossRef]
23. Vo, T.Q.; Kim, B.H. Molecular dynamics study of thermodynamic properties of nanoclusters for additive manufacturing. *Int. J. Precis. Eng. Manuf. Technol.* **2017**, *4*, 301–306. [CrossRef]
24. Wang, J.; Luo, Q.; Wang, H.; Wu, Y.; Cheng, X.; Tang, H. Microstructure characteristics and failure mechanisms of Ti-48Al-2Nb-2Cr titanium aluminide intermetallic alloy fabricated by directed energy deposition technique. *Addit. Manuf.* **2020**, *32*, 101007. [CrossRef]
25. Yao, D.; An, X.; Fu, H.; Zhang, H.; Yang, X.; Zou, Q.; Dong, K. Dynamic investigation on the powder spreading during selective laser melting additive manufacturing. *Addit. Manuf.* **2021**, *37*, 101707. [CrossRef]
26. Nandy, J.; Sahoo, S.; Sarangi, H. Study on shape dependency of Al-alloy nanoparticles during coalescence in direct metal laser sintering: A molecular dynamics approach. *Mater. Today Proc.* **2021**, *41*, 347–351. [CrossRef]
27. Nandy, J.; Yedla, N.; Gupta, P.; Sarangi, H.; Sahoo, S. Sintering of AlSi10Mg particles in direct metal laser sintering process: A molecular dynamics simulation study. *Mater. Chem. Phys.* **2019**, *236*, 121803. [CrossRef]
28. Cattenone, A.; Morganti, S.; Auricchio, F. Basis of the Lattice Boltzmann Method for Additive Manufacturing. *Arch. Comput. Methods Eng.* **2019**, *27*, 1109–1133. [CrossRef]
29. Johnson, L.; Mahmoudi, M.; Zhang, B.; Seede, R.; Huang, X.; Maier, J.T.; Maier, H.J.; Karaman, I.; Elwany, A.; Arróyave, R. Assessing printability maps in additive manufacturing of metal alloys. *Acta Mater.* **2019**, *176*, 199–210. [CrossRef]
30. Cao, L. Numerical simulation of the impact of laying powder on selective laser melting single-pass formation. *Int. J. Heat Mass Transf.* **2019**, *141*, 1036–1048. [CrossRef]
31. Steuben, J.C.; Iliopoulos, A.P.; Michopoulos, J.G. Discrete element modeling of particle-based additive manufacturing processes. *Comput. Methods Appl. Mech. Eng.* **2016**, *305*, 537–561. [CrossRef]
32. Peng, T.; Chen, C. Influence of energy density on energy demand and porosity of 316L stainless steel fabricated by selective laser melting. *Int. J. Precis. Eng. Manuf. Green Technol.* **2018**, *5*, 55–62. [CrossRef]
33. Martin, A.; Calta, N.; Hammons, J.A.; Khairallah, S.A.; Nielsen, M.H.; Shuttlesworth, R.M.; Sinclair, N.; Matthews, M.J.; Jeffries, J.R.; Willey, T.; et al. Ultrafast dynamics of laser-metal interactions in additive manufacturing alloys captured by in situ X-ray imaging. *Mater. Today Adv.* **2019**, *1*, 100002. [CrossRef]
34. Wang, Z.; Yan, W.; Liu, W.K.; Liu, M. Powder-scale multi-physics modeling of multi-layer multi-track selective laser melting with sharp interface capturing method. *Comput. Mech.* **2019**, *63*, 649–661. [CrossRef]
35. Zhang, J.; Zhang, Y.; Lee, W.H.; Wu, L.; Choi, H.-H.; Jung, Y.-G. A multi-scale multi-physics modeling framework of laser powder bed fusion additive manufacturing process. *Met. Powder Rep.* **2018**, *73*, 151–157. [CrossRef]
36. Haley, J.C.; Schoenung, J.M.; Lavernia, E.J. Modelling particle impact on the melt pool and wettability effects in laser directed energy deposition additive manufacturing. *Mater. Sci. Eng. A* **2019**, *761*, 138052. [CrossRef]

37. Geng, R.; Du, J.; Wei, Z.; Xu, S.; Ma, N. Modelling and experimental observation of the deposition geometry and microstructure evolution of aluminum alloy fabricated by wire-arc additive manufacturing. *J. Manuf. Process.* **2021**, *64*, 369–378. [CrossRef]
38. Komineas, G.; Foteinopoulos, P.; Papacharalampopoulos, A.; Stavropoulos, P. Build Time Estimation Models in Thermal Extrusion Additive Manufacturing Processes. *Procedia Manuf.* **2018**, *21*, 647–654. [CrossRef]
39. Lin, D.; Motlag, M.; Saei, M.; Jin, S.; Rahimi, R.M.; Bahr, D.; Cheng, G.J. Shock engineering the additive manufactured graphene-metal nanocomposite with high density nanotwins and dislocations for ultra-stable mechanical properties. *Acta Mater.* **2018**, *150*, 360–372. [CrossRef]
40. Lianos, A.K.; Bikas, H.; Stavropoulos, P. A Shape Optimization Method for Part Design Derived from the Buildability Restrictions of the Directed Energy Deposition Additive Manufacturing Process. *Designs* **2020**, *4*, 19. [CrossRef]
41. Bikas, H.; Lianos, A.K.; Stavropoulos, P. A design framework for additive manufacturing. *Int. J. Adv. Manuf. Technol.* **2019**, *103*, 3769–3783. [CrossRef]
42. Lianos, A.K.; Koutsoukos, S.; Bikas, H.; Stavropoulos, P. Manufacturability Assessment and Design for AM. *Procedia CIRP* **2020**, *91*, 290–294. [CrossRef]
43. Bayarri, M.J.; Berger, J.O.; Paulo, R.; Sacks, J.; Cafeo, J.A.; Cavendish, J.; Lin, C.-H.; Tu, J. A Framework for Validation of Computer Models. *Technometrics* **2007**, *49*, 138–154. [CrossRef]
44. Bikas, H.; Koutsoukos, S.; Stavropoulos, P. A decision support method for evaluation and process selection of Additive Manufacturing. *Procedia CIRP* **2019**, *81*, 1107–1112. [CrossRef]
45. Foteinopoulos, P.; Papacharalampopoulos, A.; Angelopoulos, K.; Stavropoulos, P. Development of a simulation approach for laser powder bed fusion based on scanning strategy selection. *Int. J. Adv. Manuf. Technol.* **2020**, *108*, 3085–3100. [CrossRef]
46. Stavropoulos, P.; Papacharalampopoulos, A.; Michail, C.K.; Chryssolouris, G. Robust Additive Manufacturing Performance through a Control Oriented Digital Twin. *Metals* **2021**, *11*, 708. [CrossRef]
47. Stavropoulos, P.; Foteinopoulos, P.; Papacharalampopoulos, A.; Bikas, H. Addressing the challenges for the industrial application of additive manufacturing: Towards a hybrid solution. *Int. J. Light. Mater. Manuf.* **2018**, *1*, 157–168. [CrossRef]