

**A Material Point Method Framework for the Simulation of Extrusion-Based
Additive Manufacturing Processes**

by

Mustafa Erden Yildizdag

A dissertation submitted in partial satisfaction of the

requirements for the degree of

Doctor of Philosophy

in

Engineering – Mechanical Engineering

in the

Graduate Division

of the

University of California, Berkeley

Committee in charge:

Professor Tarek I. Zohdi, Chair

Professor Hayden Taylor

Professor Per-Olof Persson

Fall 2018

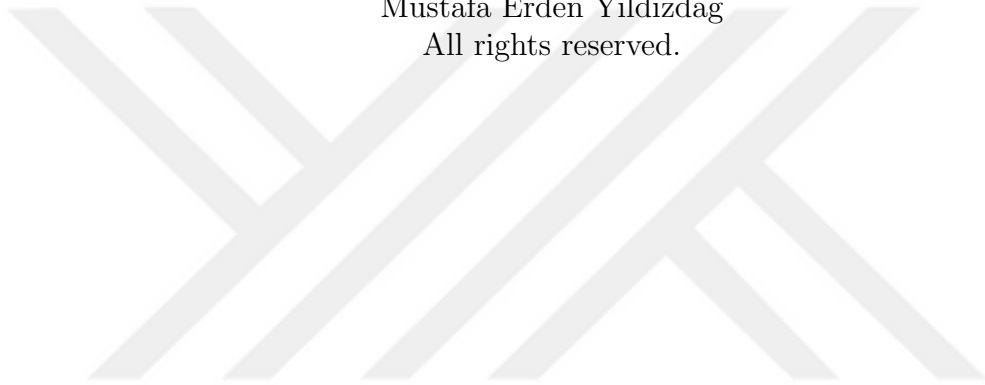
A Material Point Method Framework for the Simulation of Extrusion-Based Additive Manufacturing Processes

Copyright © 2018

by

Mustafa Erden Yildizdag

All rights reserved.



Abstract

A Material Point Method Framework for the Simulation of Extrusion-Based Additive Manufacturing Processes

by

Mustafa Erden Yildizdag

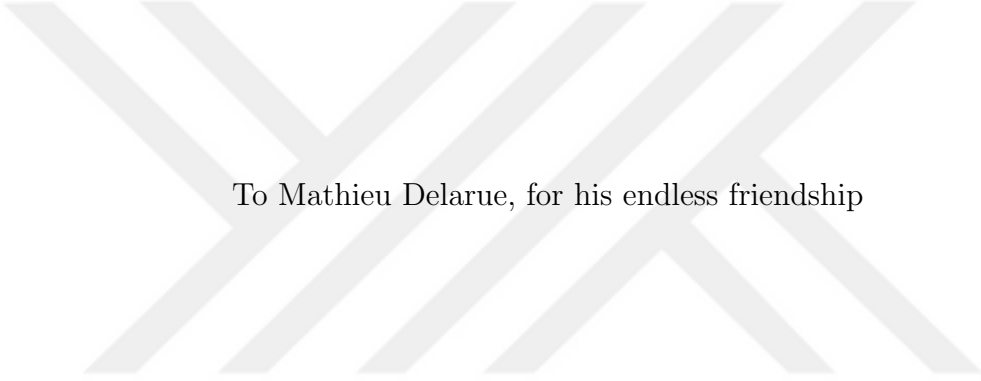
Doctor of Philosophy in Engineering – Mechanical Engineering

University of California, Berkeley

Professor Tarek I. Zohdi, Chair

Additive Manufacturing (AM), also known as 3D Printing (3DP) or rapid prototyping, is defined as building three-dimensional objects by adding materials in a layer-by-layer fashion. Although AM technologies have been developed since the late 1980's, they have garnered academic and industrial interest in the past ten years due to its wide application in different industrial fields such as automotive, aerospace, biomedical, architecture, and medicine. Currently, AM is seen as a clever solution in a more and more complex manufacturing environment, specifically in terms of customization, multifunctionality, innovative design, and geometry. Many industrial companies are now trying to improve their manufacturing capabilities by adopting different AM technologies to fabricate their products.

In this study, a computational framework is developed to optimize process parameters and simulate residual stresses in extrusion-based additive manufacturing processes. A particle-based method, namely the material point method (MPM) is adopted for simulations. The proposed numerical framework has two main parts. In the first part, the extrusion behavior of print material is simulated. Here, the fluid flow is modeled as an incompressible viscous fluid with the thermal changes due to cooling accounted for the simulations. Moreover, the main MPM code is coupled with the level set method and the ghost fluid method to track the free surface and apply the free surface boundary conditions. In the second part, a thermo-mechanical model is solved to investigate the cooling-induced residual stresses of extruded material. The applicability of the proposed numerical framework is first validated by solving select representative problems and comparing with other numerical methods. Then, it is applied to the extrusion-based manufacturing processes. The effects of different process parameters (nozzle velocity, extrusion velocity, nozzle temperature, etc.) are investigated by adopting a parametric study.



To Mathieu Delarue, for his endless friendship

Contents

Contents	ii
List of Figures	iv
List of Tables	vii
1 Introduction	1
1.1 Additive Manufacturing	1
1.2 Overview of AM technologies and literature review	4
1.3 Scope of this work	10
2 Numerical Model	12
2.1 Introduction to the material point method	12
2.2 MPM formulation for linear elasticity problems	14
2.3 MPM formulation for incompressible fluids	19
2.4 Surface tracking and applying free surface boundary conditions	23
2.4.1 Surface tracking with the level set method	24
2.4.2 Applying the free surface boundary conditions with the ghost fluid method	30
2.5 Thermal field and phase change	34
2.6 Simulation of cooling-induced residual stresses	36
2.7 Code outline	37
3 Extensions of the material point method	41
3.1 Generalized interpolation material point method	41
3.2 Convected particle domain interpolation method	43
3.2.1 1D linear convected particle domain	44
3.2.2 2D bilinear quadrilateral and constant triangular convected domains .	44
3.2.3 3D linear tetrahedron convected domains	45
3.3 B-spline material point method	46
3.3.1 Non-uniform rational B-splines (NURBS)	46
4 Numerical validation	49

4.1	Isothermal droplet impingement	49
4.2	Forced heat convection	56
4.3	Evolution of non-equilibrium droplet	58
5	Numerical Experiment	60
5.1	Problem definition and simulation parameters	60
5.2	Parameter study	62
5.2.1	Nozzle velocity variation study	62
5.2.2	Nozzle gap variation study	66
5.2.3	Cooling rate variation study	68
6	Conclusions and future work	71
6.1	Conclusions	71
6.2	Future work	72
	Bibliography	73
A	Parameter Study Results	85
A.1	Nozzle velocity variation study	85
A.2	Nozzle gap variation study	89
A.3	Cooling rate variation study	91

List of Figures

1.1	Fused deposition modeling technology [2]	4
1.2	Material jetting technology [2]	5
1.3	STL file of a vinyl record [1]	6
1.4	3D printed vinyl record [1]	7
1.5	Binding jetting technology [2]	8
1.6	Stereolithography technology [2]	8
1.7	Selective laser sintering technology [2]	9
1.8	Selective laser melting technology [2]	10
2.1	Discretization in MPM	13
2.2	Mapping from particles to nodes	17
2.3	Mapping from nodes to particles and position update	17
2.4	MPM schemes vs. FEM [128]	18
2.5	Background grid to solve pressure Poisson equation (2D view)	22
2.6	Calculation of the pressure gradient at nodes (2D view)	23
2.7	Level set function	24
2.8	Initial level set function	25
2.9	Reinitialization results with the upwind scheme proposed by Sussman et al. [96] (2D case)	27
2.10	Reinitialization with the modified upwind scheme proposed by Russo and Smereka et al. [79] (2D case)	28
2.11	Unit normal vectors (2D case)	30
2.12	Ghost fluid cells (2D case)	31
2.13	Ghost fluid cells (2D case)	31
2.14	Ghost fluid cells determined by using level set function (2D case)	32
3.1	1D linear convected domain	44
3.2	2D convected domains	44
3.3	3D linear tetrahedron convected domain	45
3.4	NURBS curve with knot vector $\Xi=[0, 0, 0, 0, \frac{1}{3}, \frac{2}{3}, 1, 1, 1, 1]$ and uniform weights	47
3.5	1-D B-Spline basis functions of knot vector $\Xi=[0, 0, 0, 0, \frac{1}{3}, \frac{2}{3}, 1, 1, 1, 1]$	48

4.1	Isothermal droplet impingement problem	50
4.2	Isothermal droplet impingement with viscosity $\mu = 0.02 \text{ Pa} \cdot \text{s}$	50
4.3	Isothermal droplet impingement with viscosity $\mu = 0.04 \text{ Pa} \cdot \text{s}$	51
4.4	Isothermal droplet impingement with viscosity $\mu = 0.1 \text{ Pa} \cdot \text{s}$	51
4.5	MPM vs 2-phase flow solver with viscosity $\mu = 0.02 \text{ Pa} \cdot \text{s}$	52
4.6	MPM vs 2-phase flow solver with viscosity $\mu = 0.04 \text{ Pa} \cdot \text{s}$	53
4.7	MPM vs 2-phase flow solver with viscosity $\mu = 0.1 \text{ Pa} \cdot \text{s}$	54
4.8	Mesh dependency study	55
4.9	Mesh dependency results with viscosity $\mu = 0.02 \text{ Pa} \cdot \text{s}$	55
4.10	Heat convection	56
4.11	MPM vs FEM results for forced convection problem	57
4.12	Evolution of non-equilibrium droplet with the MPM framework	58
4.13	Comparison with GIMP-CSF modeling	59
5.1	Nozzle geometry and extrusion velocity profile	61
5.2	Extrusion process for $v_N = 12 \text{ mm/s}$	63
5.3	Residual stress distribution for $v_N = 12 \text{ mm/s}$	63
5.4	Extruded material for different nozzle velocity (v_N) values	64
5.5	Residual stresses for different nozzle velocity (v_N) values	65
5.6	Extruded material for different h_N/D_N values	66
5.7	Residual stresses for different h_N/D_N values	67
5.8	Extrusion process for different cooling rates	68
5.9	Residual stress distributions for different cooling rates for $v_N = 18 \text{ mm/s}$	69
5.10	Extrusion process for different cooling rates for $v_N = 14 \text{ mm/s}$ and $h_N = 0.4 \text{ mm}$	70
5.11	Residual stress distributions for different cooling rates for $v_N = 14 \text{ mm/s}$ and $h_N = 0.4 \text{ mm}$	70
A.1	Extrusion process for $v_N = 12 \text{ mm/s}$	85
A.2	Extrusion process for $v_N = 14 \text{ mm/s}$	86
A.3	Extrusion process for $v_N = 16 \text{ mm/s}$	86
A.4	Extrusion process for $v_N = 18 \text{ mm/s}$	87
A.5	Extrusion process for $v_N = 20 \text{ mm/s}$	87
A.6	Extrusion process for $v_N = 22 \text{ mm/s}$	88
A.7	Extrusion process for $v_N = 24 \text{ mm/s}$	88
A.8	Extrusion process for $h_N/D_N = 0.9$	89
A.9	Extrusion process for $h_N/D_N = 0.8$	89
A.10	Extrusion process for $h_N/D_N = 0.7$	90
A.11	Extrusion process for $h_N/D_N = 0.6$	90
A.12	Extrusion process for $h_{air} = 100 \text{ W}/(\text{m}^2 \cdot \text{K})$	91
A.13	Extrusion process for $h_{air} = 200 \text{ W}/(\text{m}^2 \cdot \text{K})$	91
A.14	Extrusion process for $h_{air} = 400 \text{ W}/(\text{m}^2 \cdot \text{K})$	92
A.15	Extrusion process for $h_{air} = 1000 \text{ W}/(\text{m}^2 \cdot \text{K})$	92

A.16 Extrusion process for $h_{air} = 100 \text{ W}/(\text{m}^2 \cdot \text{K})$	93
A.17 Extrusion process for $h_{air} = 200 \text{ W}/(\text{m}^2 \cdot \text{K})$	93
A.18 Extrusion process for $h_{air} = 400 \text{ W}/(\text{m}^2 \cdot \text{K})$	94
A.19 Extrusion process for $h_{air} = 1000 \text{ W}/(\text{m}^2 \cdot \text{K})$	94



List of Tables

1.1	Additive manufacturing technologies and common materials (adopted from [2]) .	3
5.1	Process parameters for variation in v_N	62
5.2	Process parameters for variation in h_N	66
5.3	Process parameters for variation in h_{air}	68

Acknowledgments

This is the end of my troubled sleep. Now, it is the moment for killing the past and coming back to life.

I would like to express my deepest appreciation and thanks to my advisor Prof. Tarek Zohdi for his endless support throughout this work. I would also thank to my other dissertation committee members Prof. Hayden Taylor and Prof. Per-Olof Persson for their valuable feedback.

I would like to thank everybody that I had nice time during my PhD life. I thank to my former and current labmates: Donghoon Kim, Maxwell Micali, Nicolas Castrillon, Youngkyu Kim, Chang Yoon Park, Zeyad Zaky, and Marc Russell. I would like to thank the members of our mechanics group: Rubens Salsa, Brett Hendrickson, Milad Shirani, Magda Ntetsika, Evan Hemingway, Zacharias Vangelatos, Haris Sheikh, and Nate Goldberg. I also appreciate my friends Dilara Semerci, Tugce Gurek, Kamil Nar, David Alpert, and Elizabeth Luebben. My PhD life at UC Berkeley could have been so boring without my friends.

I would like to express my special thanks to my friend Orhan Ocal for helping and motivating me all the time with his sincere friendship and endless energy.

I must thank to Prof. David Steigmann, Prof. Oliver O'Reilly, Prof. James Casey and Prof. Panos Papadopoulos for teaching amazing mechanics courses during this 4.5 years. I also owe a very important debt to my colleagues Prof. Ahmet Ergin and Ibrahim Tugrul Ardic for taking care of my former studies on isogeometric analysis during this period.

I really appreciate my friends Alican Askun, Onur Yildiz, Adem Ozturk, and Kaan Tinaz for their long-distance support from Turkey.

I gratefully acknowledge The Scientific and Technological Research Council of Turkey (TUBITAK) for supporting my PhD education with the scholarship program BIDEB 2213.

Last but not least, I would like to thank to my mother Hatice Koroglu and my grandmothers Emine Koroglu and Hatice Erden Ergil who always supported and motivated me during this period.

Chapter 1

Introduction

1.1 Additive Manufacturing

Additive Manufacturing (AM), also known as 3D Printing (3DP) or rapid prototyping, is defined as building three-dimensional objects by adding materials in a layer-by-layer fashion. Historically, the roots of AM technology can be traced back to the two manufacturing techniques; photo sculpture and topography arose in the late 19th century. they have garnered academic and industrial interest in the past ten years due to its wide application in different industrial fields such as automotive, aerospace, biomedical, architecture, and medicine. Currently, AM is seen as a clever solution in a more and more complex manufacturing environment, specifically in terms of customization, creativity, multifunctionality, innovative design, and geometry. Many industrial companies are now trying to improve their manufacturing capabilities by adopting different AM technologies to fabricate their products. AM is also referred to as “the third industrial revolution” in many different media platforms, and this has inspired the “maker movement” and “do it yourself” (DIY) culture all over the world.

In AM processes, three-dimensional objects are built by using the data provided from virtual solid models. A typical AM process has five main steps:

1. 3D virtual model.
2. Tool planning.
3. Printing.
4. Removal of prints.
5. Post processing.

The product is first prepared as a 3D virtual model, computer aided design (CAD) tools are commonly used to create the virtual model at this stage. Although it sounds like AM can deal with any geometric complexity easily, some important design rules has to be considered

at this stage to avoid printing fails. In general, these rules are applied for the design of supported/unsupported walls, overhangs, holes, connecting/moving parts, and engravings, and they may vary for different AM technologies [2]. Then, the CAD model is exported as the standard AM file format, standard tessellation language (STL). In STL file format, the surface of the virtual model is represented with a set of triangles. Next, tool planning, also referred to as “slicing” is carried out by using a tool planning software. At this stage, 3D virtual model is divided into layers considering the geometry of the internal structure, and each layer is formed by following the tool planning. Also, process parameters such as speed, pressure and temperature are specified at this stage, and then all the input (tool planning and process parameters) is converted into a G-code (a numerical control programming language) file to sent to the target AM machine to build the final product. When the product is built, it is removed from build platform and post processing operations (removing support structures, surface finishing, etc.) are applied if necessary.

Due to its distinct properties, AM processes have significant advantages in comparison with the conventional manufacturing techniques. The AM technology can easily build complex 3D objects with its layer-wise approach and eliminates the dependency on many additional design constraints such as fixtures and tooling. Importantly, increasing geometric complexity and design flexibility do not require extra cost and extra process time. Therefore, topologically optimized complex geometries can be designed and fabricated with AM, and products can easily be customized to satisfy user’s specific needs. In addition, AM technologies enable manufacturing of complex multiple-material parts optimizing and tuning the overall material properties. In this way, functionalized materials with complex microstructure can be printed with AM. Moreover, AM minimizes the amount of waste compared to subtractive manufacturing methods, print materials can be re-cycled and used for another print. For further details, we refer readers to recent review papers of the state of the art by Guo and Leu [38], Gao et al. [32], Huang et al. [41], and Bikas et al. [10]. One can also find review papers on different aspects of AM such as polymer matrix composites [107], micro-additive manufacturing applications [105], material issues [11, 88], multiple material additive manufacturing [104], 3D printing of biomaterials [18], metal additive manufacturing [29], 3D printing of ceramic-based materials [103], laser additive manufacturing [37], thermal modeling in AM processes [28], powder-based AM for tissue engineering [84], and societal impact [40].

According to American Society for Testing and Materials (ASTM) [89], AM technology is classified into seven categories: material extrusion, power bed fusion, vat photopolymerization, material jetting, binder jetting, sheet lamination, and directed energy deposition. In Table 1.1, these categories are summarized with their technologies and common print materials used in the applications.

Category	Technology	Material
Material Extrusion	Fused Deposition Modeling (FDM)	ABS, PLA, Nylon, PC, fiber-reinforced Nylon, ULTEM, composite filaments (wood-filled, metal-filled, etc.)
Powder Bed Fusion	Selective Laser Sintering (SLS) Direct Metal Laser Sintering (DMLS) Selective Laser Melting (SLM) Electron Beam Melting (EBM) Multi Jet Fusion (MJF)	Nylon, alumide, carbon-fiber filled nylon, PEEK, TPU Aluminum, titanium, stainless steel, nickel alloys, cobalt-chrome Titanium, cobalt-chrome Nylon
VAT Polymerization	Stereolithography (SLA) Direct Light Processing (DLP) Continuous Direct Light Processing (CDLP)	Photopolymer, Ceramics (alumina, zirconia, PZT) Standard castable resins Standard, tough, flexible, transparent, castable resins
Material Jetting	Material Jetting (MJ) Nano particle jetting (NPJ) Drop-On-Demand (DOD)	Rigid , transparent, multi-color, rubber-like, ABS-like Stainless steel, ceramics Wax
Binder Jetting	Binder Jetting (BJ)	Silica sand, PMMA particle material, gypsum, stainless steel, ceramics, cobalt-chrome, tungsten-carbide
Sheet Lamination	Laminated Object Manufacturing (LOM)	Plastic Film, metallic sheet, ceramic tape
Directed Energy Deposition	Laser Engineered Net Shaping (LENS) Electron Beam Additive Manufacturing (EBAM)	Titanium, stainless steel, aluminum, copper, tool steel Titanium, stainless steel, aluminum, copper nickel, 4340 steel

Table 1.1: Additive manufacturing technologies and common materials (adopted from [2])

1.2 Overview of AM technologies and literature review

In this part, we detail the principles of AM technologies popularly used in industrial applications and review the literature to summarize the relevant developments and improvements have been carried out so far.

Fused deposition modeling (FDM) is an extrusion-based AM technology, it was patented by Stuart Crump and commercialized by Stratasys in 1990. FDM is the most popular and widely available AM technique for rapid and low-cost applications due to its cheap technology and cheap supply materials. In FDM technology, the movable heated nozzle is fed with a print material (filament), and the material is extruded in its melted state on the build platform. Then, each layer is formed with solidification and continuous extrusion of the print material (see Fig. 1.1).

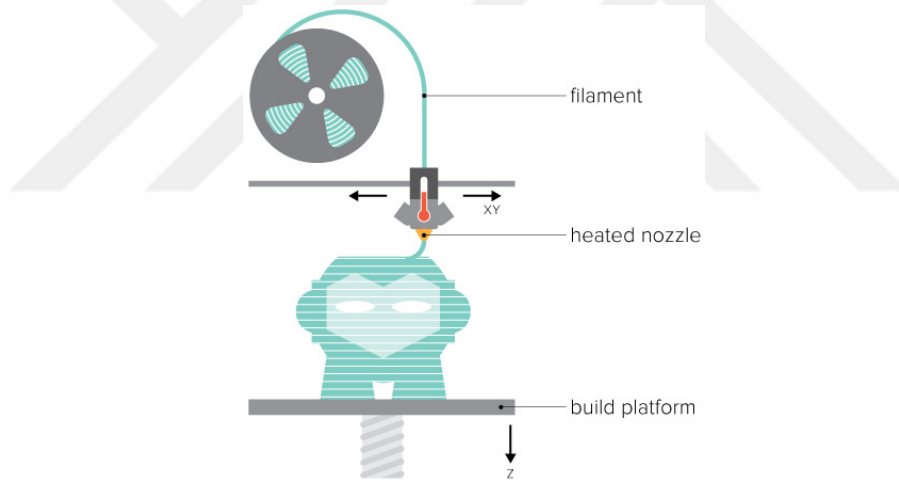


Figure 1.1: Fused deposition modeling technology [2]

FDM applications have been investigated in many different studies. Bellini and Guceri [9] presented a study to estimate the mechanical properties of products fabricated by using FDM process. In their study, the presented experimental and numerical results show that the building orientation plays an important role on the mechanical properties of the printed parts. Zhang and Chou [130] studied residual stresses and part distortion in FDM process with an FEM framework by solving a coupled thermo-mechanical model. In their other study, Zhang and Chou [129] adopted a parametric FEM study to investigate residual stresses and part distortion by analyzing three major process parameters; the road width, the layer thickness, and the scanning speed. The parametric study shows that the scan speed and the layer thickness effect residual stresses and part distortions significantly. Nikzad et al. [68] investigated the thermal and mechanical properties of Iron/ABS and Copper/ABS composites and characterized the viscoelastic properties by using the dynamic mechanical analysis (DMA) in

FDM process. Kantaros and Karalekas [46] conducted an experimental study to investigate the effects of residual stresses in FDM. Ravari et al. [77] investigated the effects of diameter variation on the elastic modulus in cellular lattice structure printed with the FDM technique. Peng et al. [72] demonstrated a study on process parameter optimization for FDM technique. In their study, they combined a fuzzy inference system with second-order response surface methodology, and they selected line width compensation, extrusion velocity, filling velocity, and layer thickness as main control parameters. Mohamed et al. [63] published a review paper on the determination of optimum process parameters for FDM technique. Hwang et al. [43] showed an experimental study to investigate the thermo-mechanical properties of metal/polymer composite filaments. In the study, two different composite filaments were prepared by mixing acrylonitrile butadiene styrene (ABS) with copper and iron particles, and the experimental results show that while thermal conductivity can be improved, the tensile strength decreases with increasing volume fraction of metal content. Gnanasekaran et al. [34] investigated the printability of electrically active structures by using composite carbon nanotube (CNT) and graphene based Polybutylene Terephthalate (PBT) filaments. Christ et al. [20] demonstrated a study on 3D printed of a sensing sensor by using conductive thermoplastic-based material. In their study, thermoplastic polyurethane (TPU) was mixed with multi-walled carbon nanotubes (MWCNT). Casavola et al. [13] conducted an experimental study to measure residual stresses by applying electronic speckle pattern interferometry (ESPI). Xia et al. [111, 112] developed a front tracking/finite volume method to simulate fluid flow, solidification, and residual stresses in FDM applications. Zhang et al. [127] investigated interfacial bonding strength between print lines extruded with ABS, carbon nanotube reinforced ABS, and short carbon fiber reinforced ABS. Comminal et al. [21] presented a numerical framework to simulate filament extrusion in FDM applications. Fitzharris et al. [27] adopted a numerical model to investigate thermal warpage in FDM processes. Osswald et al. [71] presented an analytical model to predict the polymer flow inside nozzle during the material extrusion process.

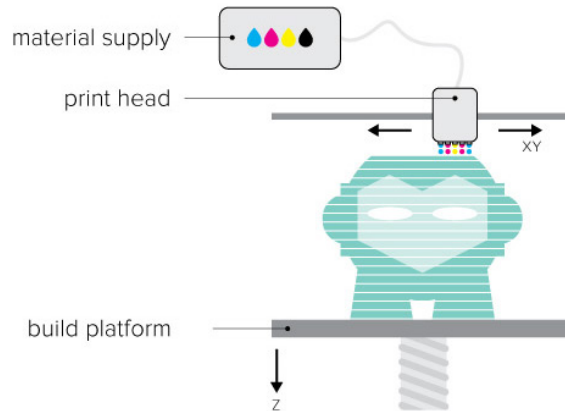


Figure 1.2: Material jetting technology [2]

Material jetting (MJ) and binder jetting (BJ) are the two droplet-based AM techniques as categorized by ASTM [89]. Material jetting, also sometimes referred to as inkjet 3-D printing, is a process in which build material are selectively deposited onto a substrate to build a 3-D object [89]. It works like a standard 2-D inkjet printer. During the manufacturing process, the build material is jetted from a nozzle as droplets by using thermal or piezoelectric method. Droplets are deposited sequentially on the substrate, and generally UV light is used to cure the material immediately after deposition. The final 3-D printed object is fabricated layer by layer with selectively deposition of the molten droplets.

In material jetting, parts are printed with high accuracy and smooth surface finish. For example, complicated groove geometry of a vinyl record has been printed with Objet Connex 500, a UV-cured resin printer [1] (see Fig. 1.3 for the STL file of the groove geometry and Fig. 1.4 for the printed vinyl record). Also, different materials can easily be combined by using multiple printer heads in this technology. Therefore, material jetting technology has a great potential for manufacturing of functional products. As the material is deposited point by point manner, material jetting has superior control over the microstructure of the final product, compared with the other AM techniques, especially when different materials are combined to functionalize the final printed parts. Hence, desired effective properties of the 3-D printed products may be achieved accurately in material jetting process. Moreover, gel-like support material may be required to use for complex geometries or overhangs; the support material is jetted as build material by using a different printer head, and removed at the end of the manufacturing process.

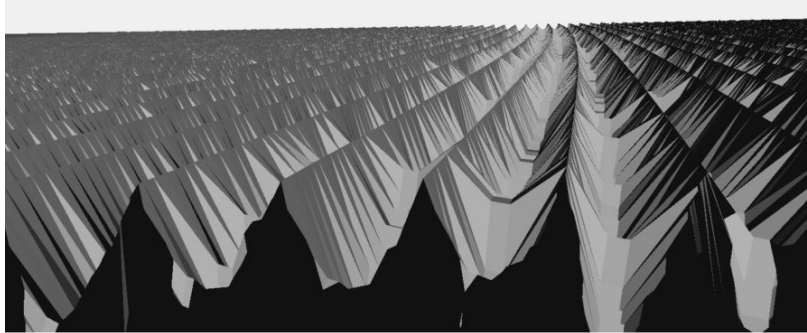


Figure 1.3: STL file of a vinyl record [1]

In droplet-based processes, the resulting morphology of the droplets is the key to improve the quality of the final product and hence the desired material properties and structural integrity. Usually, in droplet-based manufacturing processes, droplets impact on a substrate or previously deposited droplets and then spread and rebound before taking their final shapes. Therefore, understanding the interaction between different droplets and substrate which is governed by complicated fluid flow and heat transfer is significantly important to improve the overall process. This also helps one to optimize process parameters for different operating conditions and combine different materials.



Figure 1.4: 3D printed vinyl record [1]

The material jetting technique has been investigated by various authors to understand the mechanism of the process and improve the part quality. Qi et al. [75] studied the effects of process parameters on surface topography in metal micro-droplet based manufacturing. In their study, two mathematical models were proposed to predict the surface quality of printed parts. The arithmetic average height was used as a roughness parameter to characterize the surface quality, and numerical models were compared with the experimental results. Chao et al. [14] simulated the thermal process of metal droplet deposition with a 3-D finite element framework in conjunction with the element birth and death technique. They validated the numerical results by comparing with experimental results, and determined the suitable thermal conditions in order to improve re-melting and bonding between droplets. Yap et al. [117] tested three benchmark cases to investigate process capability of material jetting process. Each benchmark test was arranged for various conditions, and metrological study was conducted to determine the effect of process parameters on the dimensional accuracy and the design limitations of specific components such as thin walls. Mueller et al. [64] presented a Design of Experiment (DoE) methodology to characterize the mechanical properties of parts fabricated with 3D inkjet printing, and determined the factors which affect the overall properties. Yang et al. [115] evaluated the overall building performance of a multi-material jetting 3D printer. Luo et al. [60] presented a theoretical and experimental study on lateral instability in droplet-based manufacturing. Orme and Huang [69] presented a 1-D computational model to simulate different phase-change manipulation strategies to improve the microstructure and structural integrity of the fabricated parts. Kumar and Kumar [51] presented an experimental and theoretical study on surface roughness in poly-jet printed parts.

In binder jetting (BJ), droplets of a binding adhesive material are selectively deposited from a movable print head onto loose powder and each layer is created bonding powder particles. A new layer of powder is spread onto build bed after a layer is built, and the process is repeated until the part is printed (Fig. 1.5). Parts printed with binder jetting are brittle and have high porosity and oftentimes, printed parts requires additional post-processing

such as infiltration or sintering to improve mechanical properties [2]. Since the printing is performed at room temperature, binder jetting technology does not have a significant issue with thermal effects compared to other AM technologies. Silica sand, PMMA particle material, gypsum, stainless steel, ceramics, cobalt-chrome, tungsten-carbide are the common materials used in binder jetting technology.

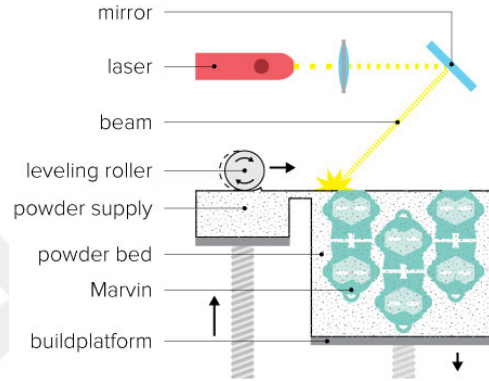


Figure 1.5: Binding jetting technology [2]

Stereolithography (SLA) is the first AM technique which was invented by Charles Hull and patented in 1986. In the patent SLA is defined as "a method and apparatus for making solid objects by successively "printing" thin layers of a curable material, e.g. a UV curable material, one on top of the other." SLA uses the photopolymerization mechanism to print parts layer by layer. In SLA, layers are formed by curing and solidifying a polymer resin with an ultraviolet (UV) laser beam (Fig. 1.6). Photopolymer thermosets in liquid form are the common materials in SLA technology. SLA provides smooth surface finish and very high dimensional accuracy. However, SLA parts are generally brittle, and their properties may be affected when they are exposed to the sun light.

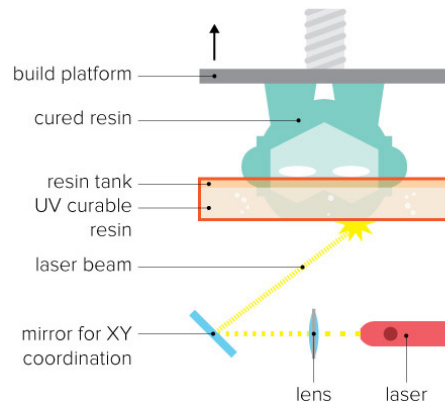


Figure 1.6: Stereolithography technology [2]

Selective laser sintering (SLS) and selective laser melting (SLM) are the two popular powder bed fusion technologies. In these techniques, powdered material is selectively sintered (or melted) by using a laser source and fused to form each layer. When a layer is printed, a new layer of powder is spread by a roller and the process is repeated until the print is done (see Figs. 1.7 and 1.8). Stainless steel, nickel-based alloys, cobalt-chrome alloys, bronze alloys, aluminum, titanium alloys are the common materials used in SLS and SLM applications.

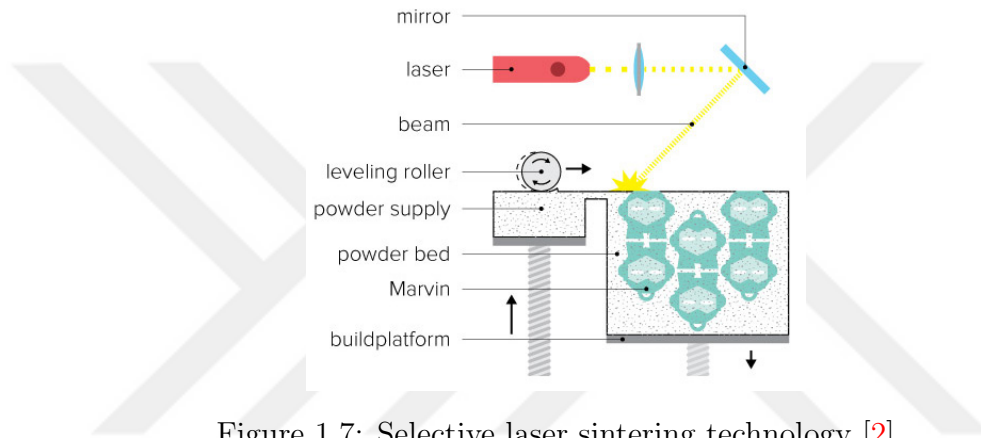


Figure 1.7: Selective laser sintering technology [2]

Powder bed fusion applications have been studied extensively in the literature. Zaeh and Branner [122] investigated residual stresses in selective laser melting applications by using finite element method to solve thermo mechanical problem. King et al. [47] conducted an experimental study to investigate the existence and conditions of keyhole-mode melting in metal AM of stainless steel. Li and Gu [54] analyzed the thermal behavior in selective laser melting of aluminum alloy powder with the finite element method. Loh et al. [58] presented a numerical study to study the behavior of aluminum alloy 6061 in SLM applications. In their study, numerical results were validated with experiments. Yuan and Gu [120] studied the behavior of molten pool during SLM of TiC/AlSi10Mg nanocomposites. Wu et al. [109] presented a numerical analysis to investigate residual stresses in SLM of AlSi10Mg. Tang et al. [98] studied porosity and solidification during SLM of stainless steel 316L. Wu et al. [110] presented a study on numerical modeling of melt-pool behavior during selective laser melting applications.

Kolossov et al. [48] presented a finite element method framework to simulate thermal evolution in selective laser sintering applications. Ganci et al. [31] studied selective laser sintering of polypropylene by using FEM. Shen et al. [83] proposed a numerical model to optimize process parameters in selective laser sintering of polymeric composite powders to improve printing quality and energy consumption. Yan et al. [114] studied the behavior of sintered carbon fiber reinforced PEEK composite during selective laser sintering.

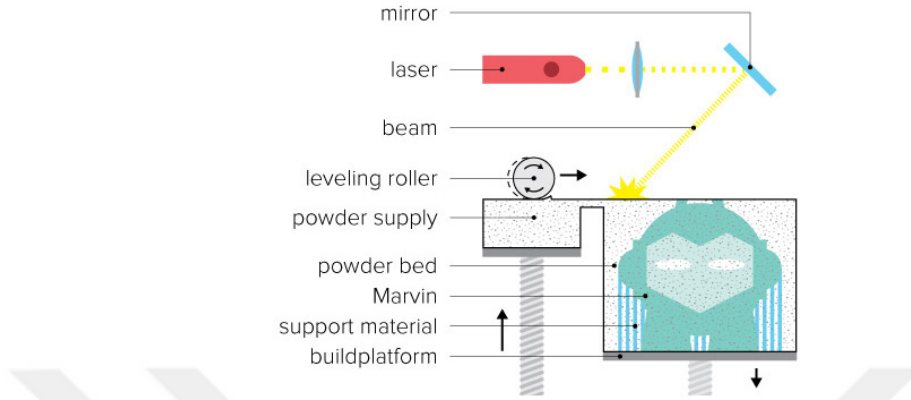


Figure 1.8: Selective laser melting technology [2]

Kolossov et al. [48] presented a finite element method framework to simulate thermal evolution in selective laser sintering applications. Ganci et al. [31] studied selective laser sintering of polypropylene by using FEM. Shen et al. [83] proposed a numerical model to optimize process parameters in selective laser sintering of polymeric composite powders to improve printing quality and energy consumption. Yan et al. [114] studied the behavior of sintered carbon fiber reinforced PEEK composite during selective laser sintering.

1.3 Scope of this work

In AM applications, the overall quality of printed parts is highly depend on the process parameters, and these parameters may vary for different materials and for different applications. Therefore, it is crucial to investigate the behavior of print materials under different process parameters and their feasibility in different applications. Usually, this requires an extensive and time-consuming experimentation procedure to determine optimum process parameters and assess the printability of a material. This procedure can be minimized with detailed numerical simulations of AM processes. In this way, numerical models can help manufacturers to have better prediction to understand the behavior of different printing materials and determine process parameters.

In this study, a computational framework is presented to simulate and understand the behavior of different print materials in AM applications. In order to narrow down the content of the work, extrusion-based AM technique is selected as the target problem. A particle-based method, namely the material point method (MPM) is adopted for simulations. The proposed numerical framework has two main parts. In the first part, the extrusion behavior of print material is simulated. Here, the fluid flow is modeled as an incompressible viscous fluid with the thermal changes due to cooling accounted for the simulations. Moreover, the main MPM code is coupled with the level set method and the ghost fluid method to track the free surface and apply the free surface boundary conditions. In the second part, a thermo-mechanical model is solved to investigate the cooling-induced residual stresses of extruded

material. The applicability of the proposed numerical framework is first validated by solving select representative problems and comparing with other numerical methods. Then, it is applied to the extrusion-based manufacturing processes. The effects of different process parameters are investigated by adopting a parametric study.



Chapter 2

Numerical Model

2.1 Introduction to the material point method

The material point method (MPM) is one of the extensions of the particle-in-cell (PIC) method which was first introduced by Harlow [39] at Los Alamos National Laboratory. The central theme behind MPM is to take advantages of both Eulerian and Lagrangian approaches in computational mechanics. In the Eulerian approach, a fixed computational grid is adopted for simulations. In this case, mesh is not attached to the material, so the material flows through the computational grid during the analysis. This type of approach can easily handle the large deformations due to using a fixed mesh. However, since the material boundary is not tracked by the computational grid, it is not suitable to simulate history-dependent materials, and oftentimes it requires an extra computational effort to track material boundary and apply boundary conditions accurately. On the other hand, in the Lagrangian approach, the computational grid is attached to the material, so the mesh moves and deforms with the material. The Lagrangian approach is useful to track history-dependent variables, and boundary conditions (e.g. free surface and traction boundary conditions) can easily be applied. However, this type of approach may require more computational effort (e.g. remeshing), especially if the material has severe distortion during the simulation. In general, the Lagrangian description is preferred in solid mechanics applications while the Eulerian description is widely used in fluid mechanics applications.

In MPM, the continuum domain is represented with a set of particles (i.e. material points). All the state variables (mass, stress, temperature, etc.) and the kinematic variables (position, velocity, deformation gradient, etc.) are stored at particles. During an MPM simulation, particles flow through a fixed background grid within each time step (see Fig. 2.1). The data stored in particles is first mapped into the background grid by using grid shape functions. The governing equations are solved on the background grid in a similar manner to the finite element method and nodal solutions are obtained. Then, the particle data is updated by remapping the nodal solutions from the background grid. Since all the interaction between particles is computed via the background grid, MPM does not require

time-consuming neighbor search compared to the other mesh-free methods such as discrete element method (DEM), smoothed particle hydrodynamics (SPH), and molecular dynamics (MD).

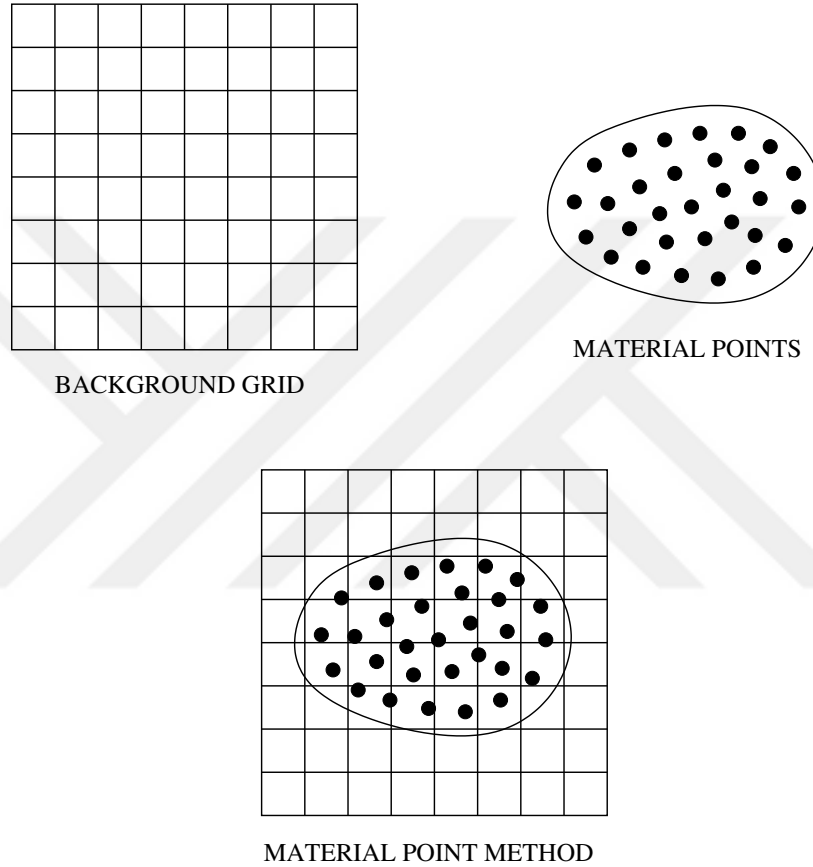


Figure 2.1: Discretization in MPM

The principles of MPM were first introduced by Sulsky et al. [93–95] to simulate and analyze history-dependent materials in solid mechanics problems. In pursuit of these seminal papers, MPM was extensively applied in a wide range of fields such as fluid-structure interaction [33, 119], granular materials [4], impact [52, 55, 126], fracture [82] free surface flow [125], multi-phase flow [123], sloshing [53, 124], plasticity [12], cutting processes [3, 65], granular flows [24], impact [25] and multiscale problems [17]. Also, due to the numerical issues relate with the original MPM formulation, various extensions of the original version have been proposed. These extensions improve the integration techniques which involve during the solution of the governing equations on the background grid. The generalized interpolation material point (GIMP) [5], the convected particle domain interpolation (CPDI) [80], and the B-spline material point method (BSMPM) [30] formulations are the most popular MPM extensions. Bardenhagen et al. [4] presented a study on simulation of granular materials by using MPM. York et al. [119] implement an MPM framework to simulate the interaction of

thin membranes with compressible fluid. Schreyer et al. [82] proposed a decohesion model with MPM to simulate crack propagation in structures. Wieckowski [108] applied MPM for the simulations of large strain engineering problems such as granular flow and plastic forming. Ionescu et al. [45] presented an MPM framework for soft tissue failure based on the two-surface failure model. Zhang et al. [125] presented an incompressible MPM formulation based on operator splitting technique. In their study, the MPM framework was coupled with the level set method to track the free surface and apply the free surface boundary conditions. Sulsky and Kaul [92] presented a time-implicit formulation for MPM and validated the formulation with various numerical examples. Ambati et al. [3] simulated cutting processes with MPM and validated the results with FEM solutions. Kularathna and Soga [50] presented an implicit MPM formulation for the simulation of incompressible materials. Nairn [65] studied the numerical simulation of orthogonal cutting processes with MPM. Xue et al. [113] conducted a micromechanical analysis by using MPM to estimate homogenized viscoelastic properties of highly filled composite materials.

The material point method is also popularly used in the field of computer graphics for physics-based animations. Stomakhin et al. [91] introduced a MPM framework to simulate melting and solidification in animations. Stomakhin et al. [90] presented a numerical model for snow simulation by using MPM. Goktekin et al. [35] presented animation of viscoelastic fluids with MPM. Ram et al. [76] studied the physics-based animations of viscoelastic fluids, foams, and sponges. Yue et al. [121] used MPM to simulate shear-dependent flows.

Moreover, the MPM have been coupled with other numerical methods. Lu et al. [59] presented a study on the coupling of molecular dynamics (MD) and MPM. Yang et al. [116] combined MPM with the discrete element method (DEM) to simulate fluid-structure interaction problems.

In the rest of the chapter, the basics and formulation of the material point method are introduced by following Chen and Brannon [16], Nguyen [67], and Zhang et al. [128]. As an introductory part, the general framework of the MPM is first presented for linear elasticity problems. Then, the numerical framework to simulate extrusion-based additive manufacturing processes is detailed in the following sections.

2.2 MPM formulation for linear elasticity problems

In a standard MPM framework, the weak forms of the governing equations are first obtained as done in a standard finite element procedure. The weak form of the linear elastodynamics problems is given as follows,

$$\int_{\Omega} \rho \delta \mathbf{u} \cdot \mathbf{a} d\Omega + \int_{\Omega} \rho \nabla \delta \mathbf{u} \cdot \boldsymbol{\sigma}^s d\Omega = \int_{\Omega} \rho \delta \mathbf{u} \cdot \mathbf{b} d\Omega + \int_{\Gamma_N} \rho \delta \mathbf{u} \cdot \bar{\mathbf{t}} d\Gamma \quad (2.1)$$

where $\boldsymbol{\sigma}^s$ is the specific Cauchy stress tensor ($\sigma_{ij}^s = \sigma_{ij}/\rho$), $\mathbf{a}$ is the acceleration vector, $\mathbf{b}$ is the body force, $\bar{\mathbf{t}}$ is the applied traction applied on the boundary Γ_N , ρ is the mass density, and $\delta \mathbf{u}$ is the virtual displacement.

In the original MPM formulation, the following approximation is introduced for mass density

$$\rho(\mathbf{x}, t) = \sum_{p=1}^{n_p} M_p \delta(\mathbf{x} - \mathbf{x}_p) \quad (2.2)$$

where δ is the dirac delta function with dimension of the inverse of volume, n_p and M_p are the total number of particles used and the particle mass, respectively. Then, by substituting Eq. (2.2) into the weak form given in Eq. (2.1), the following discrete form of the governing equation is obtained

$$\begin{aligned} \sum_{p=1}^{n_p} M_p \delta \mathbf{u}(\mathbf{x}_p) \cdot \mathbf{a}(\mathbf{x}_p) + \sum_{p=1}^{n_p} M_p \nabla \delta \mathbf{u}(\mathbf{x}_p) \cdot \boldsymbol{\sigma}^s(\mathbf{x}_p) \\ = \sum_{p=1}^{n_p} M_p \delta \mathbf{u}(\mathbf{x}_p) \cdot \mathbf{b}(\mathbf{x}_p) + \sum_{p=1}^{n_p} M_p \delta \mathbf{u}(\mathbf{x}_p) \cdot \bar{\mathbf{t}}(\mathbf{x}_p) \end{aligned} \quad (2.3)$$

The displacement, velocity and acceleration vectors of particles are approximated as follows

$$\mathbf{u}(\mathbf{x}_p) = \sum_{J=1}^{\text{nen}} N_J(\mathbf{x}_p) \mathbf{u}_J, \quad (2.4)$$

$$\mathbf{v}(\mathbf{x}_p) = \sum_{J=1}^{\text{nen}} N_J(\mathbf{x}_p) \mathbf{v}_J, \quad (2.5)$$

$$\mathbf{a}(\mathbf{x}_p) = \sum_{J=1}^{\text{nen}} N_J(\mathbf{x}_p) \mathbf{a}_J, \quad (2.6)$$

where **nen** is the total number of nodes of the element where the corresponding particle is located (4 nodes in 2D and 8 nodes in 3D problems), and $\mathbf{x}_p$ is the position vector. Here, the background grid works like a usual finite element mesh with the standard linear shape functions. Then, the virtual displacement is written as follows

$$\delta \mathbf{u}(\mathbf{x}_p) = \sum_{I=1}^{\text{nen}} N_I(\mathbf{x}_p) \delta \mathbf{u}_I, \quad (2.7)$$

and by substituting Eqs. (2.4), (2.6) and (2.7) into Eq. (2.3), the following system of equations is obtained (by imposing the condition is valid for every $\delta \mathbf{u}$)

$$m_{IJ} \mathbf{a}_J = \mathbf{f}_I^{\text{ext}} + \mathbf{f}_I^{\text{int}} \quad (2.8)$$

where m_{IJ} is the consistent mass matrix

$$m_{IJ} = \sum_{p=1}^{n_p} M_p N_I(\mathbf{x}_p) N_J(\mathbf{x}_p), \quad (2.9)$$

$\mathbf{f}_I^{\text{ext}}$ is the external force vector

$$\mathbf{f}_I^{\text{ext}} = \sum_{p=1}^{n_p} M_p N_I(\mathbf{x}_p) \mathbf{b}(\mathbf{x}_p) + \sum_{p=1}^{n_p} M_p N_I(\mathbf{x}_p) \bar{\mathbf{t}}(\mathbf{x}_p), \quad (2.10)$$

and $\mathbf{f}_I^{\text{int}}$ is the internal force vector

$$\mathbf{f}_I^{\text{int}} = - \sum_{p=1}^{n_p} V_p \nabla N_I(\mathbf{x}_p) \cdot \boldsymbol{\sigma}(\mathbf{x}_p). \quad (2.11)$$

In MPM, due to the motion of particles, the consistent mass matrix changes with time and hence this requires to compute the mass matrix and take its inverse at every time step. In order to reduce the computational time, the lumped mass approach is often preferred,

$$m_I = \sum_{J=1}^{\text{nen}} m_{IJ} = \sum_{J=1}^{\text{nen}} \sum_{p=1}^{n_p} M_p N_I(\mathbf{x}_p) N_J(\mathbf{x}_p) = \sum_{p=1}^{n_p} M_p N_I(\mathbf{x}_p), \quad (2.12)$$

and Eq. (2.8) reads,

$$m_I \mathbf{a}_I = \mathbf{f}_I^{\text{ext}} + \mathbf{f}_I^{\text{int}} = \mathbf{f}_I. \quad (2.13)$$

In order to solve Eq. (2.13), the explicit time stepping is applied in this study

$$\mathbf{a}_I^n = \frac{\mathbf{v}_I^{n+1} - \mathbf{v}_I^n}{\Delta t} \quad (2.14)$$

where the subscript n denotes the current time step, and $n + 1$ denotes the next time step. Firstly, the nodal mass values

$$m_I^n = \sum_{p=1}^{n_p} M_p N_I(\mathbf{x}_p^n) \quad (2.15)$$

and nodal linear momentum values

$$(m\mathbf{v})_I^n = \sum_{p=1}^{n_p} M_p N_i(\mathbf{x}_p^n) \mathbf{v}(\mathbf{x}_p^n) \quad (2.16)$$

are mapped from particles to the background grid.

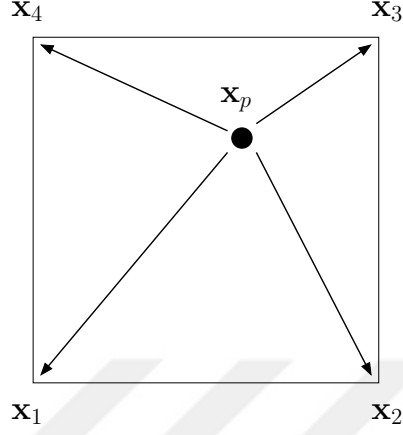


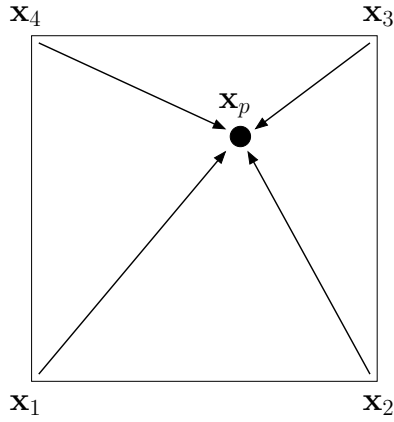
Figure 2.2: Mapping from particles to nodes

Then Eq. (2.13) is solved to update particle velocities

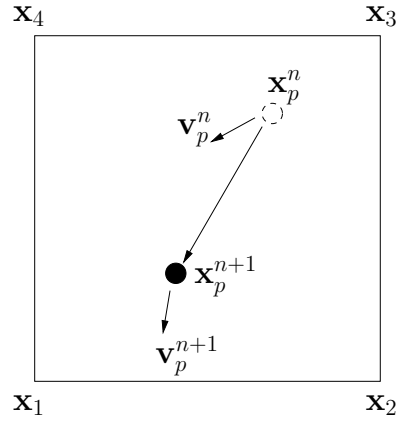
$$\mathbf{v}_p^{n+1} = \mathbf{v}_p^n + \Delta t \sum_{I=1}^{\text{nen}} \frac{N_I(\mathbf{x}_p^n) \mathbf{f}_I^n}{m_I^n}, \quad (2.17)$$

and particle positions

$$\mathbf{x}_p^{n+1} = \mathbf{x}_p^n + \Delta t \sum_{I=1}^{\text{nen}} \frac{N_I(\mathbf{x}_p^n) (m \mathbf{v})_I^{n+1}}{m_I^n}. \quad (2.18)$$



(a) Remapping from nodes to particles



(b) Position update

Figure 2.3: Mapping from nodes to particles and position update

Secondly, the deformation gradient is updated by using the relation $\dot{\mathbf{F}} = \mathbf{L}\mathbf{F}$,

$$\dot{\mathbf{F}}_p = \frac{\mathbf{F}_p^{n+1} - \mathbf{F}_p^n}{\Delta t} = \mathbf{L}_p^{n+1} \mathbf{F}_p^n \quad (2.19)$$

where $\mathbf{L}_p^{n+1}$ is the spatial velocity gradient given as

$$\mathbf{L}_p^{n+1} = \nabla \mathbf{v}_p^{n+1} = \sum_{I=1}^{\text{nen}} \nabla N_I(\mathbf{x}_p) \mathbf{v}_I^{n+1}. \quad (2.20)$$

Then, the deformation gradient at the next time step is obtained as follows

$$\mathbf{F}_p^{n+1} = (\mathbf{I} + \mathbf{L}_p^{n+1} \Delta t) \mathbf{F}_p^n \quad (2.21)$$

and the volume of each particle is updated by using the determinant of the deformation tensor

$$V_p^{n+1} = \det \mathbf{F}_p^{n+1} V_p^0 \quad (2.22)$$

where V_p^0 is the initial particle volume and V_p^{n+1} is the current particle volume. Finally, the infinitesimal strain increment

$$\dot{\boldsymbol{\epsilon}}_p = \frac{\boldsymbol{\epsilon}_p^{n+1} - \boldsymbol{\epsilon}_p^n}{\Delta t} = \frac{\Delta \boldsymbol{\epsilon}_p}{\Delta t} = \text{sym} \mathbf{L}_p^{n+1} \quad (2.23)$$

can be computed to update the stress values stored at each particle,

$$\boldsymbol{\sigma}_p^{n+1} = \boldsymbol{\sigma}_p^n + \Delta \boldsymbol{\sigma}_p \quad (2.24)$$

where

$$\Delta \boldsymbol{\sigma}_p = \mathbb{C} \Delta \boldsymbol{\epsilon}_p. \quad (2.25)$$

Here, $\mathbb{C}$ is the fourth order elasticity tensor. In the literature, this procedure is called as update stress last (USL) algorithm (see [Algorithm 1](#)). The stress can also be updated at the beginning of the time step which is referred as to update stress first (USF) algorithm. Alternatively, the modified update stress last (MUSL) scheme can be also used. In [Fig. 2.4](#), these different schemes are summarized comparing with a standard FEM scheme.

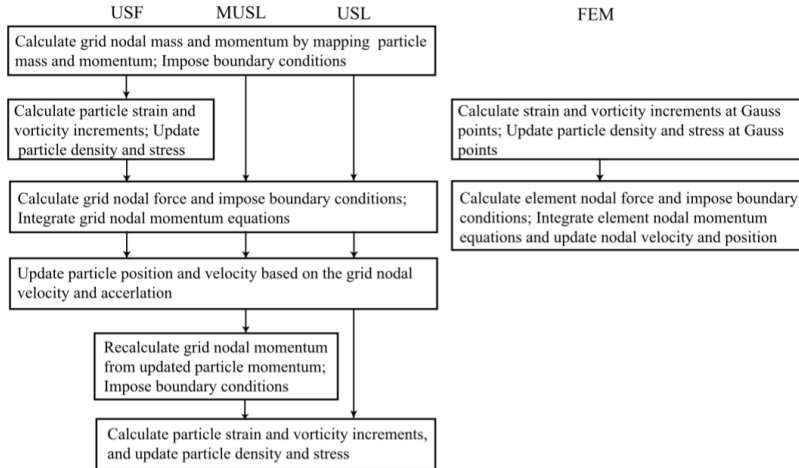


Figure 2.4: MPM schemes vs. FEM [128]

Algorithm 1 MPM procedure for linear elasticity problems

1. Initialize particles, particle data, and background grid
 2. From particles to grid
 - Nodal mass (Eq. (2.15))
 - Nodal linear momentum (Eq. (2.16))
 - Nodal external force (Eq. (2.10))
 - Nodal internal force (Eq. (2.11))
 3. Update nodal linear momenta: $(m\mathbf{v})_I^{n+1} = (m\mathbf{v})_I^n + (\mathbf{f}_I^{\text{ext}} + \mathbf{f}_I^{\text{int}})\Delta t$
 4. From grid to particles
 - Update particle velocity (Eq. (2.17))
 - Update particle position (Eq. (2.18))
 - Compute particle velocity gradient (Eq. (2.20))
 - Update particle deformation tensor (Eq. (2.21))
 - Update particle volume (Eq. (2.22))
 - Compute particle strain increment (Eq. (2.23))
 - Update particle stress (Eq. (2.24))
 5. Advance to the next time step
-

2.3 MPM formulation for incompressible fluids

In this part, the MPM framework for incompressible fluids is presented. The strong form of the balance of linear momentum (in spatial form) is given as follows

$$\text{div}\mathbf{T} + \rho\mathbf{b} = \rho\mathbf{a} \quad (2.26)$$

where $\mathbf{T}$ is the Cauchy stress tensor, $\mathbf{b}$ is the body force, and $\mathbf{a}$ is the acceleration vector, and for incompressible fluids, the constitutive relation may be generalized in the following form

$$\mathbf{T} = -p\mathbf{I} + \boldsymbol{\tau}. \quad (2.27)$$

Then, Eq. (2.26) reads

$$\rho\mathbf{a} = -\nabla p + \text{div}\boldsymbol{\tau} + \rho\mathbf{b}, \quad (2.28)$$

and the incompressibility condition yields (for isothermal case)

$$\operatorname{div} \mathbf{v} = 0 \quad (2.29)$$

where $\mathbf{v}$ is the velocity vector. By applying semi-implicit time integration scheme,

$$\rho \frac{\mathbf{v}^{n+1} - \mathbf{v}^n}{\Delta t} = -\nabla p^{n+1} + \operatorname{div} \boldsymbol{\tau}^n + \rho \mathbf{b} \quad (2.30)$$

and following Chorin-type splitting [19], Eq. (2.30) can be splitted as follows

$$\rho \frac{\mathbf{v}^* - \mathbf{v}^n}{\Delta t} = \operatorname{div} \boldsymbol{\tau}^n + \rho \mathbf{b} \quad (2.31)$$

$$\rho \frac{\mathbf{v}^{n+1} - \mathbf{v}^*}{\Delta t} = -\nabla p^{n+1} \quad (2.32)$$

where $\mathbf{v}^*$ is the intermediate velocity vector. Firstly, the weak form of Eq. (2.31) is obtained multiplying both sides by a test function $\delta \mathbf{u}$ and integrating over the domain,

$$\int_{\Omega} \rho \frac{\mathbf{v}^* - \mathbf{v}^n}{\Delta t} \cdot \delta \mathbf{u} \, d\Omega = \int_{\Omega} \operatorname{div} \boldsymbol{\tau}^n \cdot \delta \mathbf{u} \, d\Omega + \int_{\Omega} \rho \mathbf{b} \cdot \delta \mathbf{u} \, d\Omega. \quad (2.33)$$

By using the identity $\tau_{ij,j} \delta v_i = (\tau_{ij} \delta v_i)_{,j} - \tau_{ij} \delta v_{i,j}$, Eq. (2.33) takes following form

$$\int_{\Omega} \rho \frac{\mathbf{v}^* - \mathbf{v}^n}{\Delta t} \cdot \delta \mathbf{u} \, d\Omega = - \int_{\Omega} \rho \nabla(\delta \mathbf{u}) \cdot \boldsymbol{\tau}_s^n \, d\Omega + \int_{\Gamma} \rho \delta \mathbf{u} \cdot \bar{\mathbf{t}} \, d\Gamma + \int_{\Omega} \rho \delta \mathbf{u} \cdot \mathbf{b} \, d\Omega \quad (2.34)$$

where $\boldsymbol{\tau}_s$ is the specific stress tensor ($\boldsymbol{\tau}_s = \boldsymbol{\tau}/\rho$) and $\bar{\mathbf{t}}$ is the prescribed traction boundary condition ($\bar{\mathbf{t}} = \boldsymbol{\tau}_s \mathbf{n}$). The following mass density,

$$\rho(\mathbf{x}, t) = \sum_{p=1}^{n_p} m_p \delta(\mathbf{x} - \mathbf{x}_p) \quad (2.35)$$

is introduced into the weak form as in the previous section,

$$\begin{aligned} & \sum_{p=1}^{n_p} m_p \left[\frac{\mathbf{v}^*(\mathbf{x}_p) - \mathbf{v}^n(\mathbf{x}_p)}{\Delta t} \right] \cdot \delta \mathbf{u}(\mathbf{x}_p) \\ &= \sum_{p=1}^{n_p} m_p \nabla(\delta \mathbf{u})|_{\mathbf{x}_p} \cdot \boldsymbol{\tau}_s^n(\mathbf{x}_p) + \sum_{p=1}^{n_p} m_p \delta \mathbf{u}(\mathbf{x}_p) \cdot \bar{\mathbf{t}}(\mathbf{x}_p) + \sum_{p=1}^{n_p} m_p \delta \mathbf{u}(\mathbf{x}_p) \cdot \mathbf{b}(\mathbf{x}_p) \end{aligned} \quad (2.36)$$

The velocity of each particle and virtual displacement are approximated as follows

$$\mathbf{v}(\mathbf{x}_p) = \sum_{I=1}^{\text{nen}} N_I(\mathbf{x}_p) \mathbf{v}_I \quad (2.37)$$

$$\delta \mathbf{u}(\mathbf{x}_p) = \sum_{I=1}^{\text{nen}} N_I(\mathbf{x}_p) \delta \mathbf{u}_I \quad (2.38)$$

and plugged into Eq. (2.36), and the following system of equation is obtained

$$m_I \mathbf{v}_I^* = m_I \mathbf{v}_I^n + \Delta t \mathbf{f}_I^n \quad (2.39)$$

in order to solve nodal intermediate velocity $\mathbf{v}^*$. Here, m_I is the lumped mass matrix, $\mathbf{v}_I^n$ is the nodal velocity, and $\mathbf{f}_I^n$ is the total force vector ($\mathbf{f}_I^n = \mathbf{f}_I^{\text{ext},n} + \mathbf{f}_I^{\text{int},n}$). Secondly, by taking divergence of both sides of Eq. (2.32)

$$\frac{\rho}{\Delta t} (\nabla \cdot \mathbf{v}^{n+1} - \nabla \cdot \mathbf{v}^*) = -\nabla \cdot \nabla p^{n+1} \quad (2.40)$$

and by using the incompressibility condition ($\nabla \cdot \mathbf{v}^{n+1} = 0$), the pressure Poisson equation (PPE)

$$\nabla^2 p^{n+1} = \frac{\rho}{\Delta t} \nabla \cdot \mathbf{v}^* \quad (2.41)$$

is obtained to solve pressure field. In order to solve Eq. (2.41), the finite difference method is applied on the background grid. The Laplacian on the left hand side of Eq. (2.41)

$$(\nabla^2 p)_{i,j,k} = \left(\frac{\partial^2 p}{\partial x^2} \right)_{i,j,k} + \left(\frac{\partial^2 p}{\partial y^2} \right)_{i,j,k} + \left(\frac{\partial^2 p}{\partial z^2} \right)_{i,j,k} \quad (2.42)$$

is approximated by using the second-order scheme as follows

$$\left(\frac{\partial^2 p}{\partial x^2} \right)_{i,j,k} = \frac{1}{(\Delta x)^2} [p_{i+1,j,k} + p_{i-1,j,k} - 2p_{i,j,k}], \quad (2.43)$$

$$\left(\frac{\partial^2 p}{\partial y^2} \right)_{i,j,k} = \frac{1}{(\Delta y)^2} [p_{i,j+1,k} + p_{i,j-1,k} - 2p_{i,j,k}], \quad (2.44)$$

$$\left(\frac{\partial^2 p}{\partial z^2} \right)_{i,j,k} = \frac{1}{(\Delta z)^2} [p_{i,j,k+1} + p_{i,j,k-1} - 2p_{i,j,k}]. \quad (2.45)$$

As can be seen from Fig. 2.5, the finite difference scheme is applied by using cell centers

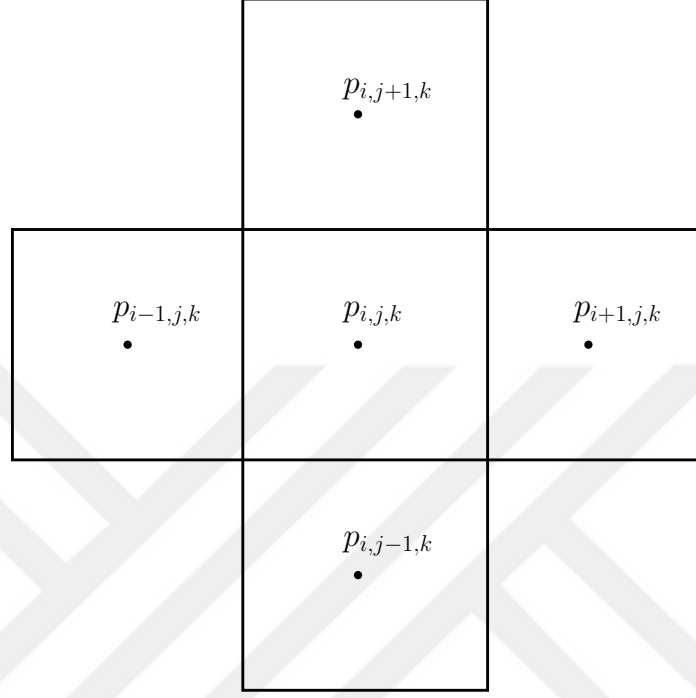


Figure 2.5: Background grid to solve pressure Poisson equation (2D view)

of the background grid. After solving for the pressure field, the nodal velocity vectors are updated by using [Eq. \(2.32\)](#)

$$\mathbf{v}^{n+1} = \mathbf{v}^* - \frac{\Delta t}{\rho} \nabla p^{n+1}. \quad (2.46)$$

Here, the nodal pressure values are calculated using pressure values computed at the cell centers (see [Fig. 2.6](#) for 2D example). Then, the following scheme is used to find the pressure gradient at the nodes by using pressure values at the cell centers,

$$\begin{aligned} \left(\frac{\partial p}{\partial x} \right)_{i+\frac{1}{2}, j+\frac{1}{2}, k+\frac{1}{2}} &= \frac{1}{4\Delta x} [p_{i+1, j+1, k+1} + p_{i+1, j, k+1} + p_{i+1, j+1, k} + p_{i+1, j, k} \\ &\quad - p_{i, j+1, k+1} - p_{i, j, k+1} - p_{i, j+1, k} - p_{i, j, k}], \end{aligned} \quad (2.47)$$

$$\begin{aligned} \left(\frac{\partial p}{\partial y} \right)_{i+\frac{1}{2}, j+\frac{1}{2}, k+\frac{1}{2}} &= \frac{1}{4\Delta y} [p_{i+1, j+1, k+1} + p_{i, j+1, k+1} + p_{i+1, j+1, k} + p_{i, j+1, k} \\ &\quad - p_{i+1, j, k+1} - p_{i, j, k+1} - p_{i+1, j, k} - p_{i, j, k}], \end{aligned} \quad (2.48)$$

$$\left(\frac{\partial p}{\partial z}\right)_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}} = \frac{1}{4\Delta z} [p_{i+1,j+1,k+1} + p_{i,j+1,k+1} + p_{i+1,j,k+1} + p_{i,j,k+1} - p_{i+1,j+1,k} - p_{i,j+1,k} - p_{i+1,j,k} - p_{i,j,k}]. \quad (2.49)$$

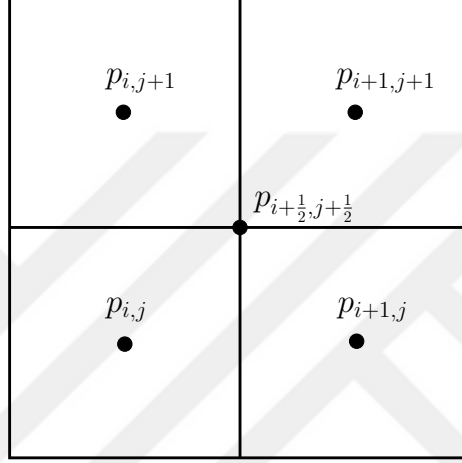


Figure 2.6: Calculation of the pressure gradient at nodes (2D view)

2.4 Surface tracking and applying free surface boundary conditions

In Eulerian description, surface tracking and applying boundary conditions may be challenging. Oftentimes, it requires applying an additional numerical technique to track the free surface and apply the free surface boundary conditions accurately. In the MPM framework developed in this study, the ghost fluid method (GFM) is applied to deal this issue. This method is used in the solution of pressure Poisson equation (Eq. (2.41)) to impose the pressure boundary conditions on the free surface. The ghost fluid method is a simple and efficient technique to deal with applying free surface boundary conditions. The central theme of GFM is based on determining computational cells (ghost cells) near the free surface to enforce the boundary conditions. The GFM was first proposed to treat multimaterial interface in gas flows by Fedkiw et al. [26]. Liu et al. [57] extended the ghost fluid method to treat more general discontinuities for Poisson's equation on irregular domains. Liu et al. [56] proposed a modified GFM to simulate shock waves on material interfaces. Menard et al. [62] studied the break-up of liquid jets by coupling the level set method, volume of fluid and the ghost fluid method. Terashima and Tryggvason [100] introduced a front tracking method for fluid interfaces by applying the GFM. Tiwari and Vanka [102] implemented the Lattice Boltzmann method with the GFM for fluid flows.

On the other hand, determining the location of the free surface is important to apply the GFM accurately. In this study, the level set method (LSM) is applied to track the free surface. The level set method is a powerful numerical tool especially when tracking the evolution of interfaces is needed. The LSM was first presented by Osher and Sethian [70], and it has been applied into different engineering problems and popularly coupled with other numerical methods.

2.4.1 Surface tracking with the level set method

In order to track the boundary of the material, the LSM is applied on the background grid. In LSM, the zero level set represents the surface of the domain (see Fig. 2.7), and the surface, surface normal vector, and curvature are accessed implicitly by operating on $\phi(\mathbf{x}, t)$.

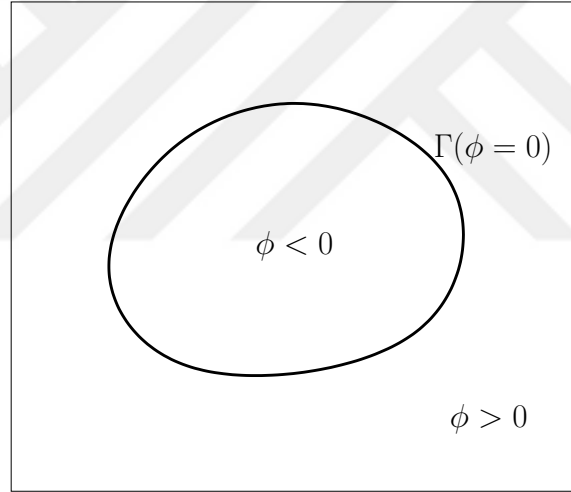


Figure 2.7: Level set function

In this study, in order to track the surface, we mainly follow the methodology presented in Zhang et al. [125]. In the beginning of the analysis, an initial signed distance function $\phi(\mathbf{x}, 0)$ is first defined by using the initial positions of the particles in the domain. In order to assign a sign distance function, cell centers of the background grid are used and $\phi(\mathbf{x}, 0)$ is evaluated with the following equation

$$\phi_c(\mathbf{x}, 0) = \min(\|\mathbf{x}_c - \mathbf{x}_p\| - r) \quad (2.50)$$

where ϕ_c is the signed distance at the corresponding cell center, $\mathbf{x}_c$ is the position of the corresponding cell center, $\mathbf{x}_p$ is the position of the particle, and r is the representative radius of the particle.

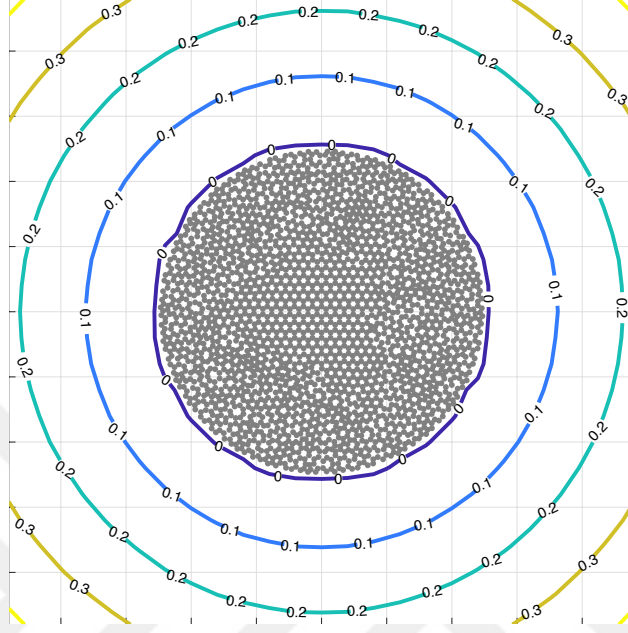


Figure 2.8: Initial level set function

In Fig. 2.8, an initial level set function is depicted as an example. In this case, a 2D droplet is considered, and as can be seen from the figure, the initial zero level set cannot capture the surface very well. Thus, the surface unit normal vector and the curvature may not be calculated accurately with this initial zero level set. In order to have a smoother zero level set, re-initialization proposed by Sussman et al. [96] can be applied

$$\frac{\partial \phi}{\partial \tau} = \text{sgn}(\phi^0)(1 - |\nabla \phi|) \quad (2.51)$$

where ϕ^0 is the initial sign distance function assigned by applying Eq. (2.50) ($\phi^0 = \phi(x, 0)$), τ is the pseudo time, and sgn is the sign function defined as

$$\text{sgn}(x) = \begin{cases} 1 & \text{if } x > 0 \\ 0 & \text{if } x = 0 \\ -1 & \text{if } x < 0 \end{cases} \quad (2.52)$$

Here, Eq. (2.51) may be solved with the first-order upwind scheme [96].

$$\phi_{i,j,k}^{n+1} = \phi_{i,j,k}^n - \Delta t(|\nabla \phi_{i,j,k}| - 1) \quad (2.53)$$

where

$$|\nabla \phi_{i,j,k}| = \begin{cases} \sqrt{\max(a_+^2, b_+^2) + \max(c_+^2, d_+^2) + \max(e_+^2, f_+^2)} & \phi_{i,j,k}^0 \geq 0 \\ \sqrt{\max(a_-^2, b_-^2) + \max(c_-^2, d_-^2) + \max(e_-^2, f_-^2)} & \phi_{i,j,k}^0 < 0 \end{cases} \quad (2.54)$$

with

$$a = D_x^- \phi_{i,j,k} = \frac{\phi_{i,j,k} - \phi_{i-1,j,k}}{\Delta x}, \quad (2.55)$$

$$b = D_x^+ \phi_{i,j,k} = \frac{\phi_{i+1,j,k} - \phi_{i,j,k}}{\Delta x}, \quad (2.56)$$

$$c = D_y^- \phi_{i,j,k} = \frac{\phi_{i,j,k} - \phi_{i,j-1,k}}{\Delta y}, \quad (2.57)$$

$$d = D_y^+ \phi_{i,j,k} = \frac{\phi_{i,j+1,k} - \phi_{i,j,k}}{\Delta y}, \quad (2.58)$$

$$e = D_z^- \phi_{i,j,k} = \frac{\phi_{i,j,k} - \phi_{i,j,k-1}}{\Delta z}, \quad (2.59)$$

$$f = D_z^+ \phi_{i,j,k} = \frac{\phi_{i,j,k+1} - \phi_{i,j,k}}{\Delta z}, \quad (2.60)$$

and subscript $+$ denotes the positive part while subscript $-$ denotes the negative part, e.g.

$$a_+ = \max(a, 0), \quad (2.61)$$

$$a_- = \min(a, 0). \quad (2.62)$$

As seen from Fig. 2.9, re-initialization gives a smoother zero level set at pseudo time $\tau = 10$. However, this scheme allows the zero level set move into the material and thus, the final result may not capture the surface accurately. Alternatively, one can apply a modified scheme (referred as first-order subcell fix scheme) proposed by Russo and Smereka [79],

$$\phi_{i,j,k}^{n+1} = \begin{cases} \phi_{i,j,k}^n - \frac{\Delta t}{\Delta x} (\text{sgn}(\phi_{i,j,k}^0) |\phi_{i,j,k}^n| - D_{i,j,k}) & \text{if } \phi_{i+1,j,k} \phi_{i,j,k} \leq 0 \text{ or } \phi_{i-1,j,k} \phi_{i,j,k} \leq 0 \text{ or} \\ & \phi_{i,j+1,k} \phi_{i,j,k} \leq 0 \text{ or } \phi_{i,j-1,k} \phi_{i,j,k} \leq 0 \text{ or} \\ & \phi_{i,j,k+1} \phi_{i,j,k} \leq 0 \text{ or } \phi_{i,j,k-1} \phi_{i,j,k} \leq 0 \text{ or} \\ \phi_{i,j,k}^n - \Delta t \text{sgn}(\phi_{i,j,k}^0) (|\nabla \phi_{i,j,k}| - 1) & \text{otherwise} \end{cases} \quad (2.63)$$

where

$$D_{i,j,k} = \frac{\phi_{i,j,k}^0}{|\nabla \phi_{i,j,k}^0|} \quad (2.64)$$

and

$$|\nabla \phi_{i,j,k}^0| = \left[\left(\frac{\partial \phi_{i,j,k}^0}{\partial x} \right)^2 + \left(\frac{\partial \phi_{i,j,k}^0}{\partial y} \right)^2 + \left(\frac{\partial \phi_{i,j,k}^0}{\partial z} \right)^2 \right]^{1/2} \quad (2.65)$$

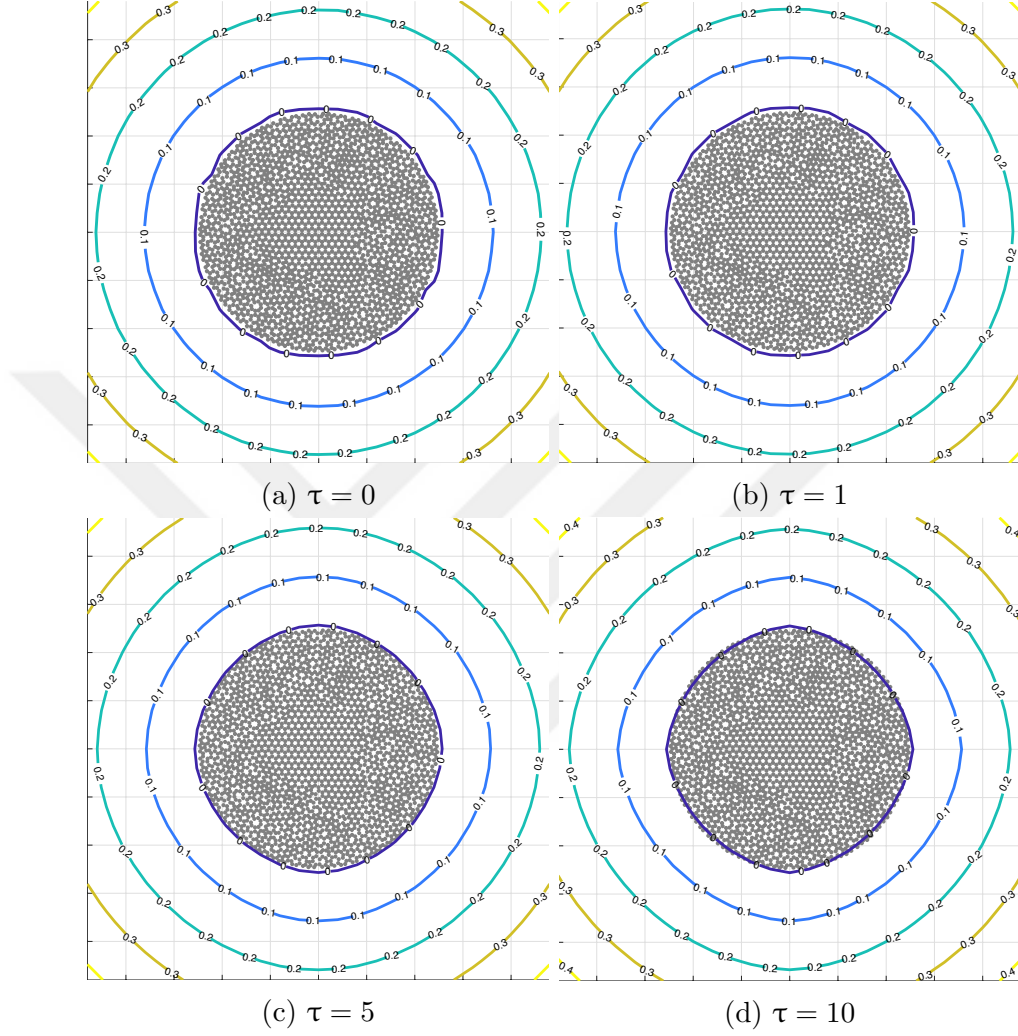


Figure 2.9: Reinitialization results with the upwind scheme proposed by Sussman et al. [96] (2D case)

Here, partial derivatives in Eq. (2.65) are determined as follows

$$\frac{\partial \phi_{i,j,k}^0}{\partial x} = \max \left(\left| \frac{\phi_{i+1,j,k}^0 - \phi_{i-1,j,k}^0}{x_{i+1,j,k} - x_{i-1,j,k}} \right|, \left| \frac{\phi_{i+1,j,k}^0 - \phi_{i,j,k}^0}{x_{i+1,j,k} - x_{i,j,k}} \right|, \left| \frac{\phi_{i,j,k}^0 - \phi_{i-1,j,k}^0}{x_{i,j,k} - x_{i-1,j,k}} \right|, \varepsilon \right), \quad (2.66)$$

$$\frac{\partial \phi_{i,j,k}^0}{\partial y} = \max \left(\left| \frac{\phi_{i,j+1,k}^0 - \phi_{i,j-1,k}^0}{y_{i,j+1,k} - y_{i,j-1,k}} \right|, \left| \frac{\phi_{i,j+1,k}^0 - \phi_{i,j,k}^0}{y_{i,j+1,k} - y_{i,j,k}} \right|, \left| \frac{\phi_{i,j,k}^0 - \phi_{i,j-1,k}^0}{y_{i,j,k} - y_{i,j-1,k}} \right|, \varepsilon \right), \quad (2.67)$$

$$\frac{\partial \phi_{i,j,k}^0}{\partial z} = \max \left(\left| \frac{\phi_{i,j,k+1}^0 - \phi_{i,j,k-1}^0}{z_{i,j,k+1} - z_{i,j,k-1}} \right|, \left| \frac{\phi_{i,j,k+1}^0 - \phi_{i,j,k}^0}{z_{i,j,k+1} - z_{i,j,k}} \right|, \left| \frac{\phi_{i,j,k}^0 - \phi_{i,j,k-1}^0}{z_{i,j,k} - z_{i,j,k-1}} \right|, \varepsilon \right). \quad (2.68)$$

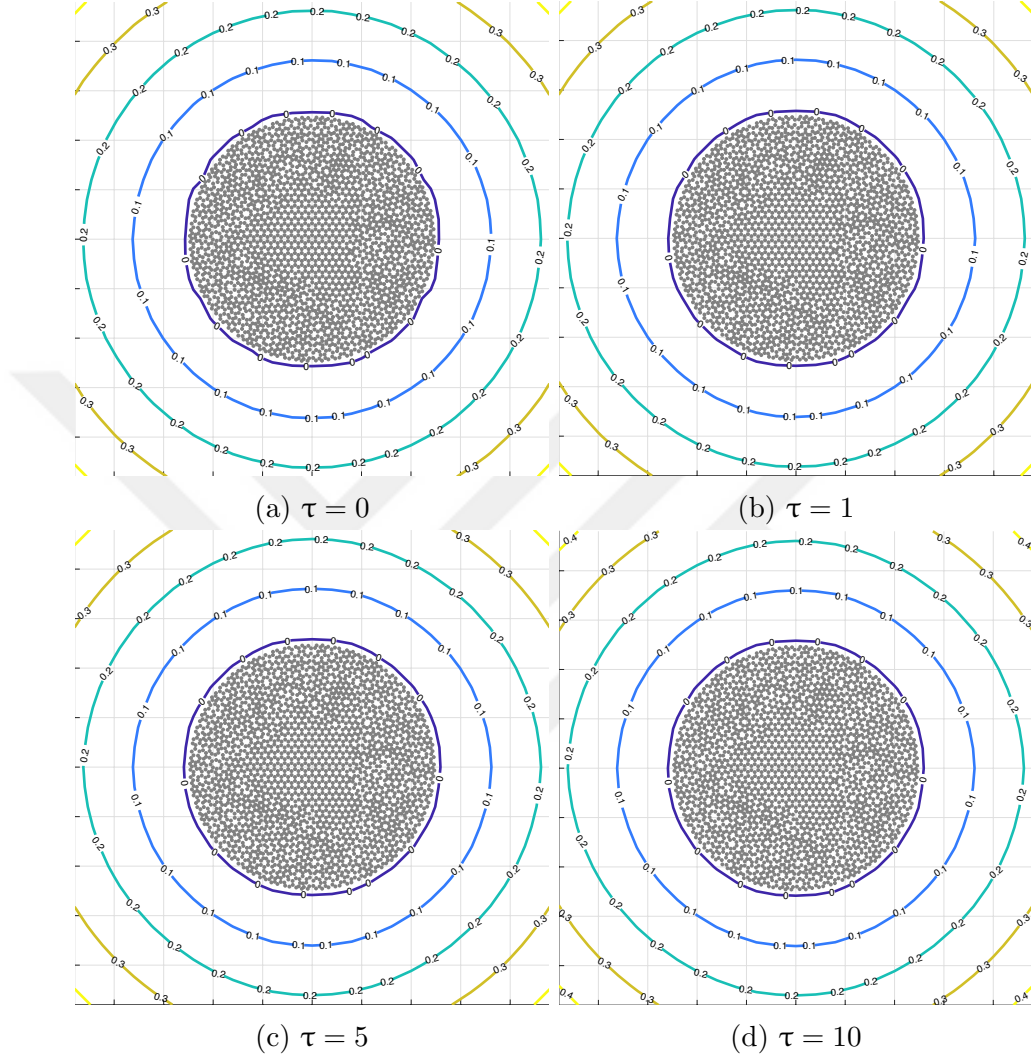


Figure 2.10: Reinitialization with the modified upwind scheme proposed by Russo and Smereka et al. [79] (2D case)

The re-initialization results obtained with the modified scheme are presented in Fig. 2.10. It is clear that, this scheme does not allow the zero level set move, and the resulting zero level set is smooth enough to calculate the surface unit normal vectors and the curvature accurately.

After re-initialization, $\phi(\mathbf{x}, t)$ is updated at each time step by solving the level set equation

$$\frac{\partial \phi}{\partial t} + \mathbf{v} \cdot \nabla \phi = 0 \quad (2.69)$$

where $\mathbf{v}$ is the velocity data mapped into the background grid from the particles. Eq. (2.69)

can be rewritten by using the formulation of the unit normal vector $\mathbf{n} = \nabla\phi/|\nabla\phi|$,

$$\frac{\partial\phi}{\partial t} + F |\nabla\phi| = 0 \quad (2.70)$$

where $F = \mathbf{v} \cdot \mathbf{n}$. The upwind finite difference approximation is applied as follows to solve Eq. (2.69)

$$\phi_{i,j,k}^{n+1} = \phi_{i,j,k}^n - \Delta t \left(\max(F, 0) \nabla_{i,j,k}^+ + \min(F, 0) \nabla_{i,j,k}^- \right) \quad (2.71)$$

where

$$\begin{aligned} \nabla_{i,j,k}^+ = & \left[\max(D_x^- \phi_{i,j,k}^n, 0)^2 + \min(D_x^+ \phi_{i,j,k}^n, 0)^2 \right. \\ & + \max(D_y^- \phi_{i,j,k}^n, 0)^2 + \min(D_y^+ \phi_{i,j,k}^n, 0)^2 \\ & \left. + \max(D_z^- \phi_{i,j,k}^n, 0)^2 + \min(D_z^+ \phi_{i,j,k}^n, 0)^2 \right]^{1/2}, \end{aligned} \quad (2.72)$$

and

$$\begin{aligned} \nabla_{i,j,k}^- = & \left[\min(D_x^- \phi_{i,j,k}^n, 0)^2 + \max(D_x^+ \phi_{i,j,k}^n, 0)^2 \right. \\ & + \min(D_y^- \phi_{i,j,k}^n, 0)^2 + \max(D_y^+ \phi_{i,j,k}^n, 0)^2 \\ & \left. + \min(D_z^- \phi_{i,j,k}^n, 0)^2 + \max(D_z^+ \phi_{i,j,k}^n, 0)^2 \right]^{1/2}. \end{aligned} \quad (2.73)$$

Moreover, the unit surface normal

$$\mathbf{n} = \frac{\nabla\phi}{|\nabla\phi|} = \frac{\phi_x \mathbf{e}_x + \phi_y \mathbf{e}_y + \phi_z \mathbf{e}_z}{\sqrt{\phi_x^2 + \phi_y^2 + \phi_z^2}}, \quad (2.74)$$

and the mean curvature

$$\kappa = \frac{\phi_x^2 \phi_{yy} - 2\phi_x \phi_y \phi_{xy} + \phi_y^2 \phi_{xx} + \phi_x^2 \phi_{zz} - 2\phi_x \phi_z \phi_{xz} + \phi_z^2 \phi_{xx} + \phi_y^2 \phi_{zz} - 2\phi_y \phi_z \phi_{yz} + \phi_z^2 \phi_{yy}}{[\phi_x^2 + \phi_y^2 + \phi_z^2]^{3/2}} \quad (2.75)$$

can easily be computed by operating on the level-set function, $\phi(\mathbf{x}, t)$.

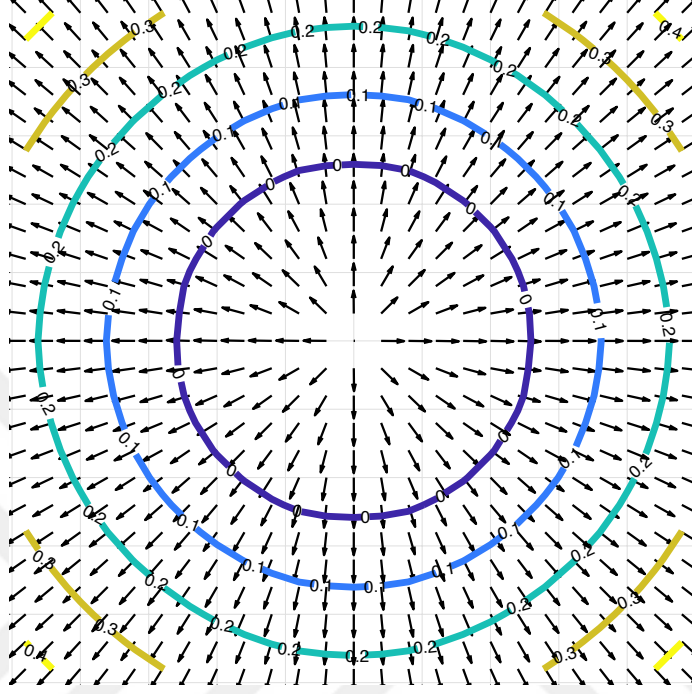


Figure 2.11: Unit normal vectors (2D case)

In Fig. 2.11, calculated unit normal vectors by using Eq. (2.74) are illustrated for a 2D problem.

2.4.2 Applying the free surface boundary conditions with the ghost fluid method

In this study, the GFM is adopted to apply the free surface boundary conditions. In this method, the pressure boundary condition on the free surface is applied by enforcing the pressure values at cell centers near the free surface. Here, we explain the method with a 2D example. Let's suppose a 2D problem with a free surface given in Fig. 2.12. In this given case, cell with pressure values $p_{i+1,j}^{Gx}$ and $p_{i,j+1}^{Gy}$ are assigned as ghost cells. In this case, the Laplacian of the pressure field at cell center i, j is written as follows

$$\nabla^2 p = \frac{1}{(\Delta x)^2} [p_{i+1,j}^{Gx} + p_{i-1,j} - 2p_{i,j}] + \frac{1}{(\Delta y)^2} [p_{i,j+1}^{Gy} + p_{i,j-1} - 2p_{i,j}] \quad (2.76)$$

where

$$p_{i+1,j}^{Gx} = \frac{1}{\theta_x} [p^{fs} + (\theta_x - 1)p_{i,j}] \quad (2.77)$$

and

$$p_{i,j+1}^{Gy} = \frac{1}{\theta_y} [p^{fs} + (\theta_y - 1)p_{i,j}]. \quad (2.78)$$

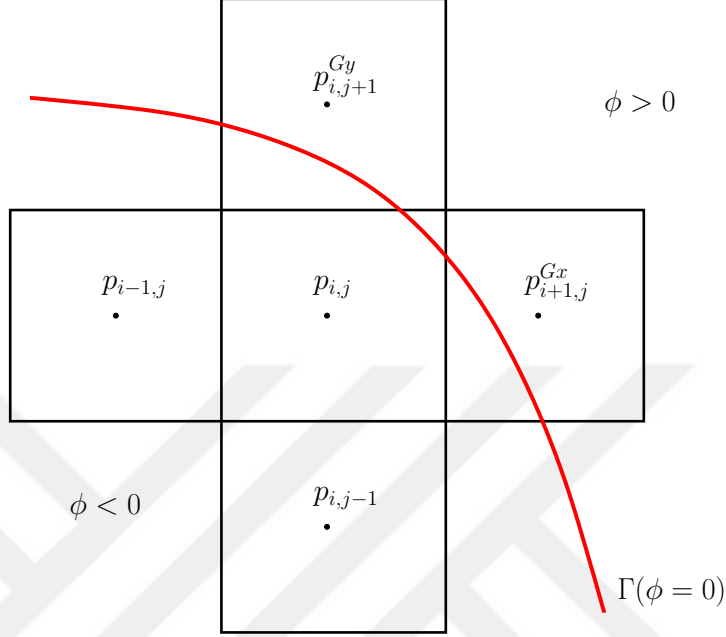


Figure 2.12: Ghost fluid cells (2D case)

Here, p^{fs} is the pressure term on the free surface, and θ_x and θ_y are given as follows

$$\theta_x = \left| \frac{x_{fs} - x_{i,j}}{\Delta x} \right|, \quad (2.79)$$

$$\theta_y = \left| \frac{y_{fs} - y_{i,j}}{\Delta y} \right| \quad (2.80)$$

where x_{fs} and y_{fs} are the x and y coordinates of the free surface (see Fig. 2.13).

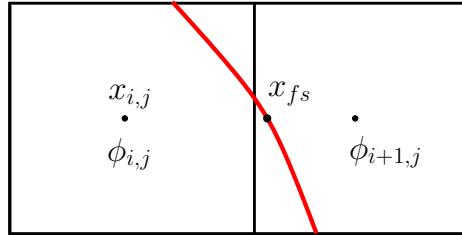


Figure 2.13: Ghost fluid cells (2D case)

In order to calculate terms given in Eqs. (2.79) and (2.80), level set function $\phi(\mathbf{x}, t)$ values

at the cell centers are used as follows

$$\theta_x = \left| \frac{\phi_{i,j}}{\phi_{i+1,j} - \phi_{i,j}} \right| \quad (2.81)$$

$$\theta_y = \left| \frac{\phi_{i,j}}{\phi_{i,j+1} - \phi_{i,j}} \right| \quad (2.82)$$

In [Fig. 2.14](#), the ghost cells determined by using the level set function are illustrated (ghost cells are marked yellow).

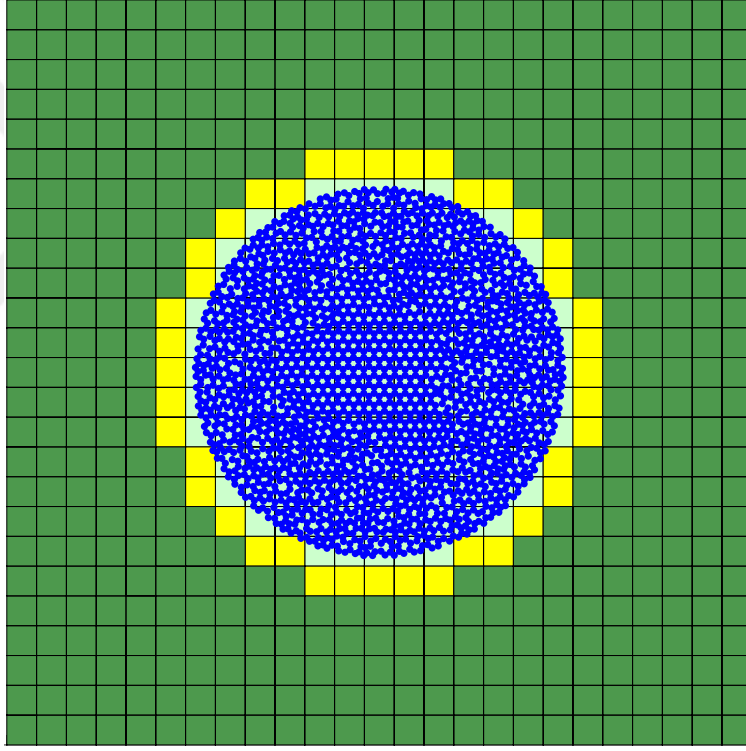


Figure 2.14: Ghost fluid cells determined by using level set function (2D case)

Finally, for this particular 2D example given in [Fig. 2.11](#), the Laplacian of pressure at node (i, j) takes the following form

$$\begin{aligned} (\nabla^2 p)_{i,j} = & \frac{1}{(\Delta x)^2} \left[\frac{1}{\theta_x} p^{fs} + p_{i-1,j} - \left(1 + \frac{1}{\theta_x} \right) p_{i,j} \right] \\ & + \frac{1}{(\Delta y)^2} \left[\frac{1}{\theta_y} p^{fs} + p_{i,j-1} - \left(1 + \frac{1}{\theta_y} \right) p_{i,j} \right]. \end{aligned} \quad (2.83)$$

In the MPM framework, pressure jumps due to the surface tension are accounted with the following term,

$$p^{fs} = p^{\text{air}} + \sigma \kappa \quad (2.84)$$

where σ is the surface tension coefficient, κ is the mean curvature, and p^{air} is the air pressure. The MPM procedure for isothermal incompressible fluids is summarized in [Algorithm 2](#).

2.5 Thermal field and phase change

In additive manufacturing processes, liquid-solid phase change effects has a crucial role for the overall process and the quality of the manufactured parts. Thus, this phenomenon is important to include in the numerical model. In order to account phase change effects, various numerical techniques have been proposed (see [44] and [49] for reviews of related methods), and they can be categorized into two groups: front tracking methods and fixed domain methods. Since the MPM framework uses a fixed background grid, one of the fixed domain methods, namely the apparent heat capacity method, is implemented to simulate phase change effects. The balance of energy (without including mechanical effects)

$$\rho c_{\text{app}} \dot{T} = -\nabla \cdot \mathbf{q} + \rho z \quad (2.85)$$

is solved in the MPM framework to account thermal changes. Here, ρ is the density, T is the temperature, c_{app} is the apparent heat capacity, k is the thermal conductivity, and z is the external heat source. The weak form of [Eq. \(2.85\)](#) is formulated by applying the explicit time scheme

$$\begin{aligned} \int_{\Omega} \rho^n c_{\text{app}}^n \left(\frac{T^{n+1} - T^n}{\Delta t} \right) \delta T d\Omega &= \int_{\Omega} \rho^n \nabla \delta T \cdot \mathbf{q}^{s,n} d\Omega + \int_{\Gamma_q} \rho^n \bar{q} \delta T d\Gamma \\ &+ \int_{\Gamma_h} h(T_{\text{ref}} - T) \delta T d\Gamma + \int_{\Omega} \rho^n z^n \delta T d\Omega \end{aligned} \quad (2.86)$$

where δT is the test function and $\mathbf{q}^s$ is the specific heat flux vector ($\mathbf{q}^s = \mathbf{q}/\rho$). By substituting the mass density ([Eq. \(2.2\)](#)) and the following approximations for T and δT

$$T(\mathbf{x}_p) = \sum_{I=1}^{\text{nen}} N_I(\mathbf{x}_p) T_I \quad (2.87)$$

$$\delta T(\mathbf{x}_p) = \sum_{I=1}^{\text{nen}} N_I(\mathbf{x}_p) \delta T_I \quad (2.88)$$

Algorithm 2 MPM procedure for isothermal incompressible fluids

1. Initialize particles, particle data, and background grid
 2. Initialize level-set function
 3. From particles to grid
 - Nodal mass (Eq. (2.15))
 - Nodal linear momentum (Eq. (2.16))
 - Nodal external force (Eq. (2.10))
 - Nodal internal force (Eq. (2.11))
 4. Update nodal intermediate linear momentum: $(m\mathbf{v})_I^* = (m\mathbf{v})_I^n + (\mathbf{f}_I^{\text{ext}} + \mathbf{f}_I^{\text{int}})\Delta t$
 5. Update nodal intermediate velocity
 6. Apply velocity boundary conditions
 7. Determine ghost cells
 8. Compute pressure
 9. Correct nodal velocity
 10. From grid to particles
 - Update particle velocity (Eq. (2.17))
 - Update particle position (Eq. (2.18))
 - Compute particle velocity gradient (Eq. (2.20))
 - Update particle deformation tensor (Eq. (2.21))
 - Update particle volume (Eq. (2.22))
 - Update particle stress (Eq. (2.24))
 11. Advance to the next time step
-

into the weak form, the MPM formulation for balance of energy is obtained as follows

$$c_I T_I^{n+1} = c_I T_I^n + \Delta t (Q_I^{\text{int},n} + Q_I^{\text{ext},n}) \quad (2.89)$$

where

$$c_I = \sum_{p=1}^{n_p} M_p c_{\text{app}}^n(\mathbf{x}_p) N_I(\mathbf{x}_p) \quad (2.90)$$

and

$$Q_I^{\text{int},n} = \sum_{p=1}^{n_p} V_p^n \nabla N_I(\mathbf{x}_p) \cdot \mathbf{q}^n(\mathbf{x}_p), \quad (2.91)$$

$$Q_I^{\text{ext},n} = \sum_{p=1}^{n_p} M_p z^n(\mathbf{x}_p) N_I(\mathbf{x}_p) - \sum_{p=1}^{n_p} V_p h^n(\mathbf{x}_p) N_I(\mathbf{x}_p). \quad (2.92)$$

The apparent heat capacity term c_{app} is given as follows

$$c_{\text{app}} = \begin{cases} c_s & T < T_s \\ c_s + \frac{L}{T_m - T_s} + (c_l - c_s) \frac{T - T_s}{T_m - T_s} & T_s \leq T \leq T_m \\ c_l & T > T_m \end{cases} \quad (2.93)$$

where c_s and c_l are the heat capacities in solid and liquid phases, respectively, and L is the latent heat. Also, T_m is the melting temperature, and T_s is the solidification temperature. All the other parameters such as thermal conductivity and viscosity are assumed as functions of temperature in the simulations.

Density change is accounted with the following equation

$$\rho(T) = (1 - \alpha(T - T_{\text{ref}})) \rho_{\text{ref}} \quad (2.94)$$

where T_{ref} and ρ_{ref} are the reference temperature and density, and α is the thermal expansion coefficient. In this case, pressure splitting is rewritten as follows

$$\rho^{n+1} \left(\frac{\mathbf{v}^* - \mathbf{v}^n}{\Delta t} \right) = \text{div } \boldsymbol{\tau}^n + \rho^{n+1} \mathbf{b} \quad (2.95)$$

$$\rho^{n+1} \left(\frac{\mathbf{v}^{n+1} - \mathbf{v}^*}{\Delta t} \right) = -\nabla p^{n+1} \quad (2.96)$$

and the balance of mass yields

$$\dot{\rho} + \rho \text{div } \mathbf{v} = 0. \quad (2.97)$$

Then, taking divergence of both sides of Eq. (2.96)

$$\frac{\rho^{n+1}}{\Delta t} (\operatorname{div} \mathbf{v}^{n+1} - \operatorname{div} \mathbf{v}^*) = -\nabla^2 p^{n+1} \quad (2.98)$$

and using Eq. (2.97)

$$\operatorname{div} \mathbf{v}^{n+1} = -\frac{\dot{\rho}^{n+1}}{\rho^{n+1}}, \quad (2.99)$$

modified version of Eq. (2.41) is obtained to account density change in the simulation

$$\dot{\rho}^{n+1} + \rho^{n+1} \operatorname{div} \mathbf{v}^* = \Delta t \nabla^2 p^{n+1}. \quad (2.100)$$

Here, the term $\dot{\rho}^{n+1}$ can be approximated as follows

$$\begin{aligned} \dot{\rho}^{n+1} &= \frac{\rho^{n+1} - \rho^n}{\Delta t} \\ &= \frac{\rho_{\text{ref}}(1 - \alpha(T^{n+1} - T_{\text{ref}})) - \rho_{\text{ref}}(1 - \alpha(T^n - T_{\text{ref}}))}{\Delta t} \\ &= \frac{\rho_{\text{ref}} \alpha (T^n - T^{n+1})}{\Delta t}. \end{aligned} \quad (2.101)$$

2.6 Simulation of cooling-induced residual stresses

In additive manufacturing applications, residual stresses due to high temperature gradient may play a crucial role for the quality of printed parts. In order to simulate residual stresses of additively manufactured parts, a thermo-mechanical model is adopted in this study. The governing equations are given as follows

$$\rho \mathbf{a} = \operatorname{div} \boldsymbol{\sigma} + \rho \mathbf{b} \quad (2.102)$$

$$\rho c_{\text{app}} \dot{T} = -\operatorname{div} \mathbf{q} + \rho z \quad (2.103)$$

where ρ is the material density, $\mathbf{v}$ is the velocity field, $\boldsymbol{\sigma}$ is the Cauchy stress tensor, $\mathbf{b}$ is the body force vector, $\mathbf{q}$ is the heat flux vector, and z is the external heat input. The infinitesimal strain tensor is given as

$$\boldsymbol{\varepsilon} = \frac{1}{2} (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) \quad (2.104)$$

and it is decomposed into elastic, plastic, and thermal parts as follows

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^{\text{el}} + \boldsymbol{\varepsilon}^{\text{pl}} + \boldsymbol{\varepsilon}^{\text{th}}. \quad (2.105)$$

Then, the Cauchy stress tensor reads

$$\boldsymbol{\sigma} = \mathbb{E}\boldsymbol{\varepsilon}^{\text{el}} = \mathbb{E}(\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^{\text{pl}} - \boldsymbol{\varepsilon}^{\text{th}}) \quad (2.106)$$

where $\mathbb{E}$ is the fourth order elasticity tensor. The thermal strain tensor is given as

$$\boldsymbol{\varepsilon}^{\text{th}} = \beta(T - T_{\text{ref}})\mathbf{I}. \quad (2.107)$$

where β is the stress-temperature modulus. The plastic strain $\boldsymbol{\varepsilon}^{\text{pl}}$ is generated by using J_2 -flow theory with linear isotropic hardening by following Simo and Hughes [86]. The thermal effects on the material parameters are introduced via a temperature-dependent damage parameter

$$\mathbb{E} = \mathcal{D}(T)\mathbb{E}_{\text{ref}} \quad (2.108)$$

where $\mathbb{E}_{\text{ref}}$ is the elasticity tensor at the reference temperature and the damage parameter $\mathcal{D}(T)$ is a function of temperature which is between 0 and 1.

2.7 Code outline

In this study, a computational framework is developed to simulate extrusion-based additive manufacturing processes. The numerical framework has two main parts. In the first part, the extrusion behavior of print material is simulated. Here, the fluid flow is modeled as an incompressible viscous fluid with the thermal changes due to cooling accounted for the simulations, and the level set method and the ghost fluid method are used to track the free surface and apply the free surface boundary conditions. Then, in the second part, a thermo-mechanical model is solved to investigate the cooling-induced residual stresses of extruded material.

In the simulations, we assume that the fluid is Newtonian, thus the constitutive relation takes the following form

$$\mathbf{T} = -p\mathbf{I} + 2\mu\mathbf{D} \quad (2.109)$$

where μ is the viscosity, and $\mathbf{D}$ is the symmetric part of the velocity gradient $\mathbf{L}$. Then, the first of the MPM framework can be summarized with the following steps:

1. Set up the background grid, the particle initial positions
2. Store particle data (mass, volume, position, velocity, deformation gradient, stress, strain, temperature, heat flux, etc.)
3. Initialize the level set function (Eq. (2.50)) and apply re-initialization (Eq. (2.63))
4. Start explicit time stepping

- a) Detect ghost cells (cells near the free surface) by using the level set function
- b) Mapping from particles to the background grid

- i. Compute nodal mass

$$m_I = \sum_{p=1}^{n_p} m_p N_I(\mathbf{x}_p)$$

- ii. Compute nodal linear momentum

$$(m\mathbf{v})_I^n = \sum_{p=1}^{n_p} m_p N_I(\mathbf{x}_p) \mathbf{v}^n(\mathbf{x}_p)$$

- iii. Compute nodal internal force vector

$$\mathbf{f}_I^{\text{int},n} = - \sum_{p=1}^{n_p} V_p \nabla N_I(\mathbf{x}_p) \cdot \boldsymbol{\tau}^n(\mathbf{x}_p)$$

- iv. Compute nodal external force vector

$$\mathbf{f}_I^{\text{ext},n} = \sum_{p=1}^{n_p} M_p N_I(\mathbf{x}_p) \mathbf{b}(\mathbf{x}_p) + \sum_{p=1}^{n_p} V_p N_I(\mathbf{x}_p) \bar{\mathbf{t}}(\mathbf{x}_p)$$

- v. Compute nodal heat capacity

$$c_I = \sum_{p=1}^{n_p} M_p c_{\text{app}}^n(\mathbf{x}_p) N_I(\mathbf{x}_p)$$

- vi. Compute nodal energy

$$(cT)_I^n = \sum_{p=1}^{n_p} M_p c_{\text{app}}^n(\mathbf{x}_p) T(\mathbf{x}_p) N_I(\mathbf{x}_p)$$

- vii. Compute nodal internal heating

$$Q_I^{\text{int},n} = \sum_{p=1}^{n_p} V_p^n \nabla N_I(\mathbf{x}_p) \cdot \mathbf{q}^n(\mathbf{x}_p)$$

- viii. Compute nodal external heating

$$Q_I^{\text{ext},n} = \sum_{p=1}^{n_p} M_p z^n(\mathbf{x}_p) N_I(\mathbf{x}_p) - \sum_{p=1}^{n_p} V_p h^n(\mathbf{x}_p) N_I(\mathbf{x}_p)$$

- c) Compute nodal intermediate linear momentum

$$(m\mathbf{v})_I^* = (m\mathbf{v})_I^n + \Delta t (\mathbf{f}_I^{\text{int},n} + \mathbf{f}_I^{\text{ext},n})$$

- d) Update nodal energy

$$(cT)_I^{n+1} = (cT)_I^n + \Delta t (Q_I^{\text{int},n} + Q_I^{\text{ext},n})$$

- e) Update nodal intermediate velocity and temperature

$$\mathbf{v}_I^* = (m\mathbf{v})_I^* / m_I$$

$$T_I^{n+1} = (cT)_I^{n+1} / c_I$$

- f) Update particle temperature and density

$$T_p^{n+1} = T_p^n + \Delta t \sum_{I=1}^{\text{nen}} N_I(\mathbf{x}_p) (Q_I^{\text{int},n} + Q_I^{\text{ext},n}) / c_I$$

$$\rho_p^{n+1} = \rho_{\text{ref}} (1 - \alpha (T_p^{n+1} - T_{\text{ref}}))$$

- g) Solve pressure Poisson equation

$$\nabla^2 p^{n+1} = \frac{\rho}{\Delta t} \nabla \cdot \mathbf{v}^*$$

- h) Update nodal velocity

$$\mathbf{v}^{n+1} = \mathbf{v}^* - \frac{\Delta t}{\rho} \nabla p^{n+1}$$

- i) Update level set function

$$\frac{\partial \phi}{\partial t} + \mathbf{v} \cdot \nabla \phi = 0$$

- j) Update particle velocity, position, deformation gradient, stress, and heat flux

- i. Update particle velocity

$$\mathbf{v}_p^{n+1} = \mathbf{v}_p^n + \Delta t \sum_{I=1}^{\text{nen}} N_I(\mathbf{x}_p) \mathbf{a}_I^n$$

- ii. Update particle position
 $\mathbf{r}_p^{n+1} = \mathbf{r}_p^n + \Delta t \sum_{I=1}^{\text{nen}} N_I(\mathbf{x}_p) \mathbf{v}_I^{n+1}$
- iii. Compute particle velocity gradient
 $\mathbf{L}_p^{n+1} = \sum_{I=1}^{\text{nen}} \nabla N_I(\mathbf{x}_p) \mathbf{v}_I^{n+1}$
- iv. Compute particle temperature gradient
 $\nabla T_p^{n+1} = \sum_{I=1}^{\text{nen}} \nabla N_I(\mathbf{x}_p) T_I^{n+1}$
- v. Update particle deformation gradient tensor
 $\mathbf{F}_p^{n+1} = (\mathbf{I} + \mathbf{L}_p^{n+1} \Delta t) \mathbf{F}_p^n$
- vi. Update particle stress tensor
 $\boldsymbol{\tau}_p^{n+1} = 2\mu \mathbf{D}_p^{n+1}$
- vii. Update particle heat flux
 $\mathbf{q}_p^{n+1} = -k \nabla T_p^{n+1}$
- k) Reset nodal values to zero
- l) Advance to the next time step

Next, in the second part, the cooling-induced residual stresses of extruded material are simulated. This part reads the final particle data from previous analysis in the beginning of the simulation. Then, the analysis is conducted with the following steps:

1. Read particle and grid data from previous analysis
2. Start explicit time stepping
 - a) Detect ghost cells (cells near the free surface) by using the level set function
 - b) Mapping from particles to the background grid as in previous analysis
 - c) Update nodal linear momentum
 $(m\mathbf{v})_I^{n+1} = (m\mathbf{v})_I^n + \Delta t (\mathbf{f}_I^{\text{int},n} + \mathbf{f}_I^{\text{ext},n})$
 - d) Update nodal energy
 $(cT)_I^{n+1} = (cT)_I^n + \Delta t (Q_I^{\text{int},n} + Q_I^{\text{ext},n})$
 - e) Update nodal velocity and temperature
 $\mathbf{v}_I^{n+1} = (m\mathbf{v})_I^{n+1} / m_I$
 $T_I^{n+1} = (cT)_I^{n+1} / c_I$
 - f) Update particle temperature and density
 $T_p^{n+1} = T_p^n + \Delta t \sum_{I=1}^{\text{nen}} N_I(\mathbf{x}_p) (Q_I^{\text{int},n} + Q_I^{\text{ext},n}) / c_I$
 $\rho_p^{n+1} = \rho_{\text{ref}} (1 - \alpha(T_p^{n+1} - T_{\text{ref}}))$
 - g) Update level set function
 $\frac{\partial \phi}{\partial t} + \mathbf{v} \cdot \nabla \phi = 0$
 - h) Update particle velocity, position, deformation gradient, stress, and heat flux

- i. Update particle velocity
 $\mathbf{v}_p^{n+1} = \mathbf{v}_p^n + \Delta t \sum_{I=1}^{\text{nen}} N_I(\mathbf{x}_p) \mathbf{a}_I^n$
- ii. Update particle position
 $\mathbf{r}_p^{n+1} = \mathbf{r}_p^n + \Delta t \sum_{I=1}^{\text{nen}} N_I(\mathbf{x}_p) \mathbf{v}_I^{n+1}$
- iii. Compute particle velocity gradient
 $\mathbf{L}_p^{n+1} = \sum_{I=1}^{\text{nen}} \nabla N_I(\mathbf{x}_p) \mathbf{v}_I^{n+1}$
- iv. Compute particle temperature gradient
 $\nabla T_p^{n+1} = \sum_{I=1}^{\text{nen}} \nabla N_I(\mathbf{x}_p) T_I^{n+1}$
- v. Update particle deformation gradient tensor
 $\mathbf{F}_p^{n+1} = (\mathbf{I} + \mathbf{L}_p^{n+1} \Delta t) \mathbf{F}_p^n$
- vi. Compute particle strain increment
 $\Delta \boldsymbol{\varepsilon} = 0.5 \Delta t \text{sym} \mathbf{L}_p^{n+1}$
- vii. Compute particle thermal and plastic strain increments
 $\Delta \boldsymbol{\varepsilon}_p^{\text{th}} = \beta (T_p^{n+1} - T_p^n) \mathbf{I}$
- viii. Update particle stress tensor
 $\boldsymbol{\sigma}_p^{n+1} = \boldsymbol{\sigma}_p^n + \mathbb{C}(\Delta \boldsymbol{\varepsilon}_p - \Delta \boldsymbol{\varepsilon}_p^{\text{th}} - \Delta \boldsymbol{\varepsilon}_p^{\text{pl}})$
- ix. Update particle heat flux
 $\mathbf{q}_p^{n+1} = -k \nabla T_p^{n+1}$
- i) Reset nodal values to zero
- j) Advance to the next time step

Chapter 3

Extensions of the material point method

Alternative versions of the original MPM formulation have been proposed to eliminate the numerical issues that reported in many studies. One of the main reasons behind the numerical instability is adopting linear shape functions. The gradient of linear shape functions creates this instability due to the jump (discontinuity) in shape functions when a particle cross between cells. In this section, we review the three popular extensions namely, the generalized interpolation material point method (GIMP), convected particle domain interpolation method (CPDI), and b-spline material point method (BSMPM).

3.1 Generalized interpolation material point method

The GIMP was first proposed by Bardenhagen and Kober [5]. In GIMP, the standard finite element shape functions are replaced with the following “effective” shape functions

$$\phi_{I_p}(\mathbf{x}_p) = \frac{1}{V_p} \int_{\Omega_p \cap \Omega} \chi_p(\mathbf{x} - \mathbf{x}_p) N_I(\mathbf{x}) d\mathbf{x} \quad (3.1)$$

$$\nabla \phi_{I_p}(\mathbf{x}_p) = \frac{1}{V_p} \int_{\Omega_p \cap \Omega} \chi_p(\mathbf{x} - \mathbf{x}_p) \nabla N_I(\mathbf{x}) d\mathbf{x} \quad (3.2)$$

where $\chi_p(\mathbf{x} - \mathbf{x}_p)$ is the characteristic function and $N_I(\mathbf{x}_p)$ is the standard finite element shape function. As seen from Eq. (3.1) and Eq. (3.2), if the dirac delta function is used as characteristic function, the original MPM formulation is recovered. The following simple characteristic function (in 1D problems)

$$\chi_p(\mathbf{x} - \mathbf{x}_p) = H(\mathbf{x} - (\mathbf{x}_p - l_p)) - H(\mathbf{x} - (\mathbf{x}_p + l_p)). \quad (3.3)$$

is commonly used in the literature. Here, H is the Heaviside function

$$H(x) = \begin{cases} 0 & x < 0, \\ 1 & x > 0 \end{cases} \quad (3.4)$$

and $2l_p$ is the current particle size. Eq. (3.3) can also be written as follows

$$\chi_p(x) = \begin{cases} 1 & x \in \Omega_p \\ 0 & x \notin \Omega_p \end{cases} \quad (3.5)$$

which Eq. (3.1) and Eq. (3.2) yield (for 1D problems)

$$\phi_{I_p}(x_p) = \frac{1}{2l_p} \int_{x_p-l_p}^{x_p+l_p} N_I(x) dx \quad (3.6)$$

$$\nabla \phi_{I_p}(x_p) = \frac{1}{2l_p} \int_{x_p-l_p}^{x_p+l_p} \nabla N_I(x) dx \quad (3.7)$$

Then, by employing standard finite element shape functions, the GIMP shape function (Eq. (3.1)) yields (for 1D problems)

$$\phi_{I_p}(x_p) = \begin{cases} 0 & |x_p - x_I| \geq h + l_p, \\ \frac{[h+l_p+(x_p-x_I)]^2}{4hl_p} & -h - l_p < x_p - x_I \leq -h + l_p, \\ 1 + \frac{x_p-x_I}{h} & -h + l_p < x_p - x_I \leq -l_p, \\ 1 - \frac{(x_p-x_I)^2+l_p^2}{2hl_p} & -l_p < x_p - x_I \leq l_p, \\ 1 - \frac{x_p-x_I}{h} & l_p < x_p - x_I \leq h - l_p, \\ \frac{[h+l_p-(x_p-x_I)]^2}{4hl_p} & h - l_p < x_p - x_I \leq h + l_p. \end{cases} \quad (3.8)$$

And its gradient (Eq. (3.2)) is given as follows

$$\nabla \phi_{I_p}(x_p) = \begin{cases} 0 & |x_p - x_I| \geq h + l_p, \\ \frac{h+l_p+(x_p-x_I)}{2hl_p} & -h - l_p < x_p - x_I \leq -h + l_p, \\ \frac{1}{h} & -h + l_p < x_p - x_I \leq -l_p, \\ -\frac{x_p-x_I}{hl_p} & -l_p < x_p - x_I \leq l_p, \\ -\frac{1}{h} & l_p < x_p - x_I \leq h - l_p, \\ -\frac{h+l_p-(x_p-x_I)}{2hl_p} & h - l_p < x_p - x_I \leq h + l_p. \end{cases} \quad (3.9)$$

The GIMP formulation with the shape functions given in Eqs. (3.8) and (3.9) is referred to as the contiguous particle GIMP (cpGIMP). In 3D problems, the cpGIMP shape functions are computed as follows

$$\phi_{I_p}(\mathbf{x}_p) = \phi_{I_p}(x_p) \phi_{I_p}(y_p) \phi_{I_p}(z_p) \quad (3.10)$$

3.2 Convected particle domain interpolation method

The CPDI was first proposed by Sadeghirad et al. [80, 81] as an alternative method to GIMP to mitigate cell-crossing issues. The main idea behind CPDI is to use explicit formulation for the GIMP formulation. In this approach, standard shape functions are replaced with the following alternative shape functions [66]

$$N_I^{\text{alt}}(\mathbf{x}) = \sum_{c=1}^{n_c} M_c(\mathbf{x}) N_I(\mathbf{x}_c) \quad (3.11)$$

where n_c is the number of corners of the convected domain, $\mathbf{x}(c)$ is the position vector of domain nodes, and $M_c(\mathbf{x})$ is the conventional shape functions defined in the convected domain. Then, now the GIMP functions and their gradients read as follows

$$\begin{aligned} \phi_I(\mathbf{x}_p) &= \frac{1}{V_p} \int_{\Omega_p} N_I^{\text{alt}}(\mathbf{x}) d\Omega \\ &= \frac{1}{V_p} \int_{\Omega_p} \left[\sum_{c=1}^{n_c} M_c(\mathbf{x}) N_I(\mathbf{x}_c) \right] d\Omega \\ &= \frac{1}{V_p} \sum_{c=1}^{n_c} \left[\int_{\Omega_p} M_c(\mathbf{x}) d\Omega \right] N_I(\mathbf{x}_c) \\ &= \sum_{c=1}^{n_c} w_c^f N_I(\mathbf{x}_c), \end{aligned} \quad (3.12)$$

$$\begin{aligned} \nabla \phi_I(\mathbf{x}_p) &= \frac{1}{V_p} \int_{\Omega_p} \nabla N_I^{\text{alt}}(\mathbf{x}) d\Omega \\ &= \frac{1}{V_p} \int_{\Omega_p} \left[\sum_{c=1}^{n_c} \nabla M_c(\mathbf{x}) N_I(\mathbf{x}_c) \right] d\Omega \\ &= \frac{1}{V_p} \sum_{c=1}^{n_c} \left[\int_{\Omega_p} \nabla M_c(\mathbf{x}) d\Omega \right] N_I(\mathbf{x}_c) \\ &= \sum_{c=1}^{n_c} w_c^g N_I(\mathbf{x}_c). \end{aligned} \quad (3.13)$$

The weight terms (w_c^f and w_c^g) can be computed for different particle domains. The detailed formulation for different types of convected domain can be find in Nguyen et al. [66].

3.2.1 1D linear convected particle domain

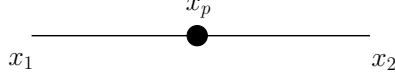


Figure 3.1: 1D linear convected domain

In 1D applications, convected domains are defined with a 2-node straight line as given in Fig. 3.1. Then, shape functions and their gradients are given as follows

$$\phi_I(\mathbf{x}_p) = \frac{1}{2} [N_I(\mathbf{x}_1) + N_I(\mathbf{x}_2)], \quad (3.14)$$

$$\nabla \phi_I(\mathbf{x}_p) = \frac{1}{l_p} [-N_I(\mathbf{x}_1) + N_I(\mathbf{x}_2)]. \quad (3.15)$$

where l_p is the length of the corresponding convected domain.

3.2.2 2D bilinear quadrilateral and constant triangular convected domains

In 2D applications, bilinear quadrilateral and constant triangular convected domains are commonly used (Fig. 3.2).

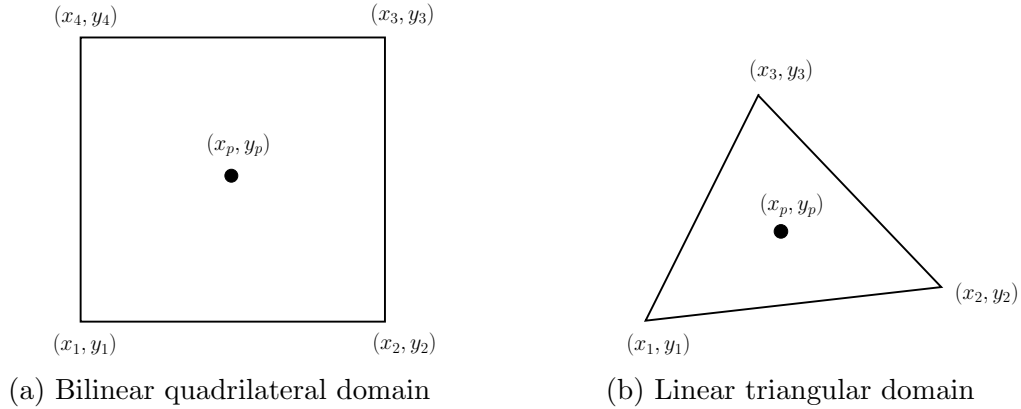


Figure 3.2: 2D convected domains

For constant triangular convected domains, shape functions and their gradients are given as follows

$$\phi_I(\mathbf{x}_p) = \frac{1}{3} [N_I(\mathbf{x}_1) + N_I(\mathbf{x}_2) + N_I(\mathbf{x}_3)] \quad (3.16)$$

$$\nabla \phi_I(\mathbf{x}_p) = \frac{1}{2V_p} \left\{ N_I(\mathbf{x}_1) \begin{bmatrix} y_{23} \\ x_{32} \end{bmatrix} + N_I(\mathbf{x}_2) \begin{bmatrix} y_{31} \\ x_{13} \end{bmatrix} + N_I(\mathbf{x}_3) \begin{bmatrix} y_{12} \\ x_{21} \end{bmatrix} \right\} \quad (3.17)$$

where V_p is the volume of the convected domain and

$$x_{ij} = x_i - x_j, \quad y_{ij} = y_i - y_j.$$

3.2.3 3D linear tetrahedron convected domains

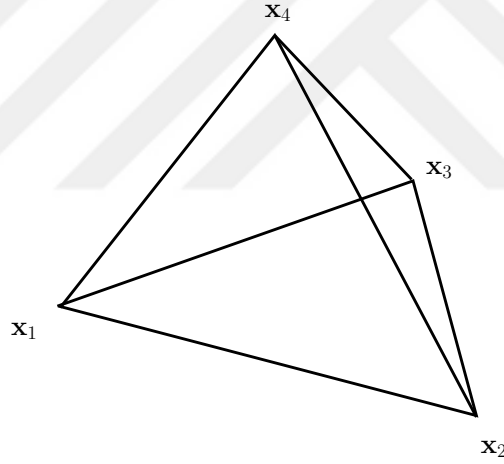


Figure 3.3: 3D linear tetrahedron convected domain

In 3D applications, linear tetrahedron convected domain may be adopted. Its shape functions and their gradients are evaluated as follows

$$\phi_I(\mathbf{x}_p) = \frac{1}{4} [N_I(\mathbf{x}_1) + N_I(\mathbf{x}_2) + N_I(\mathbf{x}_3) + N_I(\mathbf{x}_4)] \quad (3.18)$$

$$\nabla \phi_I(\mathbf{x}_p) = \frac{1}{6V_p} \left\{ N_I(\mathbf{x}_1) \begin{bmatrix} a_1 \\ b_1 \\ c_1 \end{bmatrix} + N_I(\mathbf{x}_2) \begin{bmatrix} a_2 \\ b_2 \\ c_2 \end{bmatrix} + N_I(\mathbf{x}_3) \begin{bmatrix} a_3 \\ b_3 \\ c_3 \end{bmatrix} + N_I(\mathbf{x}_4) \begin{bmatrix} a_4 \\ b_4 \\ c_4 \end{bmatrix} \right\} \quad (3.19)$$

where $a_1 = y_{42}z_{32} - y_{32}z_{42}$, $a_2 = y_{31}z_{43} - y_{34}z_{13}$, $a_3 = y_{24}z_{14} - y_{14}z_{24}$, $a_4 = y_{13}z_{12} - y_{12}z_{31}$, $b_1 = x_{32}z_{42} - x_{42}z_{32}$, $b_2 = x_{43}z_{31} - x_{13}z_{34}$, $b_3 = x_{14}z_{24} - x_{24}z_{14}$, $b_4 = x_{13}z_{12} - x_{12}z_{31}$, $c_1 = x_{42}y_{32} - x_{32}y_{42}$, $c_2 = x_{31}y_{43} - x_{34}y_{13}$, $c_3 = x_{24}y_{14} - x_{14}y_{24}$, $c_4 = x_{13}y_{21} - x_{12}y_{31}$.

3.3 B-spline material point method

B-Splines are popularly used in MPM applications as an alternative to GIMP shape functions to improve the simulations reducing cell crossing issue. In the past ten years, spline basis functions have been popularly used in different applications, and these are called isogeometric analysis since it was first proposed by [42]. Although Computer Aided Engineering (CAE) and Computer Aided Design (CAD) have had spectacular progress in the last decades, drawbacks in terms of geometry and data transfer, especially for complex structures, were major bottlenecks until recently. In order to create an analysis-suitable geometry for the use of discretization-based numerical methods, mesh generation is tedious and time-consuming, especially in regions with high curvature which require mesh refinement. The main idea underlying the isogeometric analysis (IGA) is to provide a straightforward and non-adjusting interconnection between CAD and CAE tools that enables reduction in major time-consuming engineering processes such as mesh generation and geometry construction, which span 80% of the overall analysis time [22]. The principles of IGA were first introduced by Hughes et al. [42] to perform numerical computations with desirable accuracy even with low mesh density, using the same basis functions both in geometry and analysis with low computational cost. The detailed mathematical theory of IGA was presented by Bazilevs et al. [7]. In pursuit of these seminal papers, IGA was extensively applied in a wide range of fields such as biomedical engineering [131], fracture mechanics [23], contact mechanics [99], fluid-structure interaction [6], elastostatics [87], shape optimization [118] and structural vibration [85]. Thai et al. [101] and Luu et al. [61] studied the vibration problems of laminated plates and curved beams, respectively. Wang et al. [106] proposed a novel approach by using isogeometric higher order mass matrices possessing 4th- and 6th-order accuracies in the eigenvalue problems. Zhao et al. [132] applied a multi-patch isogeometric finite element method for free vibration analysis of thick plates. As for the developments in hydrodynamics, Politis et al. [74] extended the IGA concept to boundary element method to solve 2D exterior Laplace problems. Belibassakis et al. [8] extended the previous analysis of Politis et al. [74] to solve the wavemaking resistance problem of surface-piercing 3D geometries. Takahashi and Matsumoto [97] implicated the fast multiple method (FMM) into the isogeometric boundary element method to deal with 2D large-scale Laplace problems. Recently, Gong and Dong [36] extended the standard 3D isogeometric boundary element method by employing an adaptive integration for potential problems and indicated that the effectiveness of the adaptive method appears where the lengths of adjacent panels are considerably different.

3.3.1 Non-uniform rational B-splines (NURBS)

Because of its ability to represent geometries more accurately, NURBS becomes a standard tool in CAD systems to design complex objects. Since B-Splines are the progenitors of the NURBS, definition of the B-Splines is an essential starting point on the way to comprehend the NURBS, which is the key structure to implement IGA. In this section, formulation of the NURBS is briefly explained following Piegl and Tiller [73], Rogers [78], and Hughes

et al. [42].

In order to create a NURBS patch, three parameters - knot vector(s), control points and weights - have to be defined. A knot vector is the non-decreasing coordinates of the parametric domain, and it is defined in each parametric direction of the NURBS patch. Also, it defines the partition of the parametric domain in the corresponding direction in the form of

$$\Xi = [\xi_1, \xi_2, \dots, \xi_{n+p+1}] \quad \xi_i \in \mathbb{R}, \quad (3.20)$$

where i is the knot index, $i = 1, 2, \dots, n+p+1$, p is the polynomial order, and n is the number of basis functions which comprise the B-Spline. Control points are defined as vector valued coefficients of the basis functions in order to control the shape of the patch, and weights are assigned to reflect how much the particular control point affects the curve. A p th-order 1-D NURBS patch (curve), therefore, may be expressed as follows

$$\mathbf{C}(\xi) = \sum_{i=1}^n R_i^p(\xi) \mathbf{P}_i, \quad (3.21)$$

where $R_i^p(\xi)$ is the p th-order rational basis function defined by

$$R_i^p(\xi) = \frac{N_{i,p}(\xi)w_i}{\sum_{j=1}^n N_{j,p}(\xi)w_j}, \quad (3.22)$$

$\mathbf{P}_i$ and w_i are the coordinate and the weight of the i th control point, and $N_{i,p}$ is the p th-order B-spline basis function given as follows for $p = 0$,

$$N_{i,0}(\xi) = \begin{cases} 1 & \text{if } \xi_i \leq \xi \leq \xi_{i+1}, \\ 0 & \text{otherwise,} \end{cases}$$

and for $p = 1, 2, 3, \dots$,

$$N_{i,p}(\xi) = \frac{\xi - \xi_i}{\xi_{i+p} - \xi_i} N_{i,p-1}(\xi) + \frac{\xi_{i+p+1} - \xi}{\xi_{i+p+1} - \xi_{i+1}} N_{i+1,p-1}(\xi). \quad (3.23)$$

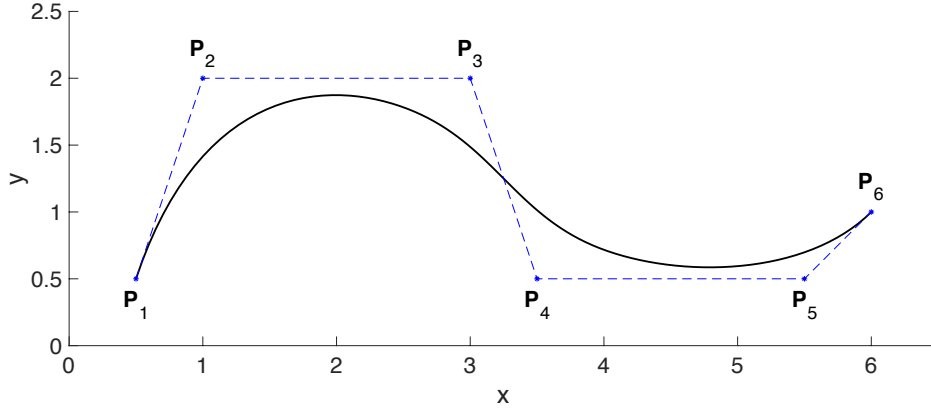


Figure 3.4: NURBS curve with knot vector $\Xi=[0, 0, 0, 0, \frac{1}{3}, \frac{2}{3}, 1, 1, 1, 1]$ and uniform weights

A 3rd-order NURBS curve and its B-spline basis functions are depicted in Figs. 3.4 and 3.5, respectively.

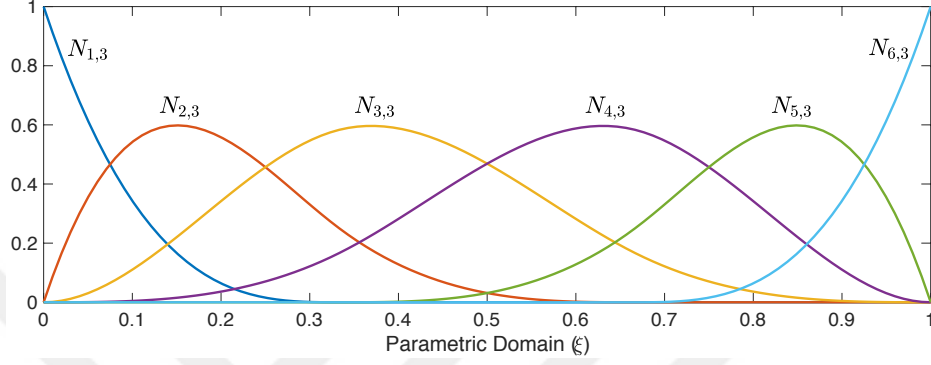


Figure 3.5: 1-D B-Spline basis functions of knot vector $\Xi=[0, 0, 0, 0, \frac{1}{3}, \frac{2}{3}, 1, 1, 1, 1]$

Likewise, NURBS surfaces and solids are defined, respectively, as follows

$$\mathbf{S}(\xi, \eta) = \sum_{i=1}^n \sum_{j=1}^m R_{i,j}^{p,q}(\xi, \eta) \mathbf{P}_{i,j}, \quad (3.24)$$

$$\mathbf{S}(\xi, \eta, \zeta) = \sum_{i=1}^n \sum_{j=1}^m \sum_{k=1}^l R_{i,j,k}^{p,q,r}(\xi, \eta, \zeta) \mathbf{P}_{i,j,k}, \quad (3.25)$$

where

$$R_{i,j}^{p,q} = \frac{N_{i,p}(\xi) M_{j,q}(\eta) w_{i,j}}{\sum_{\hat{i}=1}^n \sum_{\hat{j}=1}^m N_{\hat{i},p}(\xi) M_{\hat{j},q}(\eta) w_{\hat{i},\hat{j}}} \quad (3.26)$$

and

$$R_{i,j,k}^{p,q,r} = \frac{N_{i,p}(\xi) M_{j,q}(\eta) L_{k,r}(\zeta) w_{i,j,k}}{\sum_{\hat{i}=1}^n \sum_{\hat{j}=1}^m \sum_{\hat{k}=1}^l N_{\hat{i},p}(\xi) M_{\hat{j},q}(\eta) L_{\hat{k},r}(\zeta) w_{\hat{i},\hat{j},\hat{k}}} \quad (3.27)$$

are the 2-D and 3-D rational basis functions, respectively. $\mathbf{P}_{i,j}$ and $\mathbf{P}_{i,j,k}$ are the control points. $N_{i,p}$, $M_{j,q}$, and $L_{k,r}$ are p th, q th, and r th order B-spline basis functions, respectively, defined with knot vectors $\Xi = [\xi_1, \xi_2, \dots, \xi_{n+p+1}]$, $\mathcal{H} = [\eta_1, \eta_2, \dots, \eta_{m+q+1}]$ and $\mathcal{Z} = [\zeta_1, \zeta_2, \dots, \zeta_{l+r+1}]$. Also, n , m , and l denote the number of basis functions in each parametric directions ξ , η , and ζ .

Chapter 4

Numerical validation

In this chapter, the proposed MPM framework is applied to different problems to validate the applicability of the numerical model. Three select representative examples were studied, and the results were validated with other numerical methods. In the first example, droplet impingement was considered to simulate incompressible flow problem without including thermal effects and surface tension. A forced heat convection problem (cooling of a hot droplet) was studied in the second numerical example. In this problem solution of the balance of energy and evaluation of the boundary integrals due to the heat flux boundary condition were validated. In the last example, evolution of a non-equilibrium droplet was simulated to check the validity of the mean curvature computation with the level set method and the application of the free surface boundary conditions with the ghost fluid method. All the numerical results presented with the proposed MPM framework were validated with a commercial FEM package COMSOL[®] or results obtained with other numerical methods in the literature.

4.1 Isothermal droplet impingement

Droplet deposition processes are used in many industrial applications such as additive manufacturing, spray coating, etc. This problem involves a complex fluid flow and it has been studied and simulated with many different numerical methods. In the problem, a droplet is released with an initial velocity v_0 (see Fig. 4.1), then the droplet impacts and spreads out on the substrate, and it takes its final morphology.

In the numerical examples, a droplet with the radius $R = 0.25$ mm and the density $\rho = 1000 \text{ kg/m}^3$ was studied, and three different viscosity values were tested. The droplet is released with the initial velocity $v_0 = 1$ m/s from the height $h = 0.25$ mm. In each numerical simulation, the droplet was represented with 1536 particles, and a background grid with 40×16 elements was used. In Figs. 4.2 to 4.4, the numerical results are presented with three different viscosity values $\mu = 0.02, 0.04$, and $0.1 \text{ Pa} \cdot \text{s}$, respectively. The surface tension is not considered in the simulations ($\sigma = 0 \text{ N/m}$). The droplet behavior was simulated for

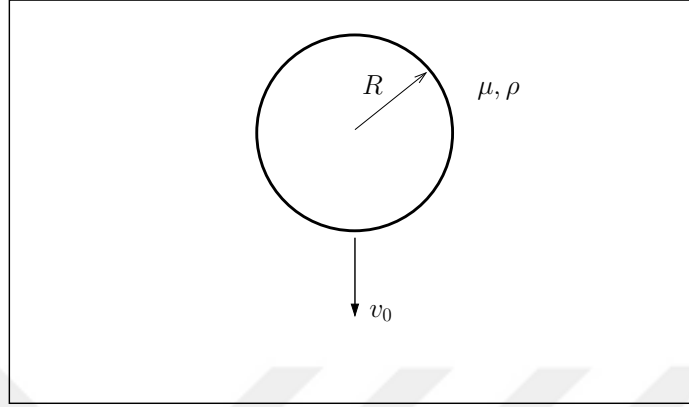


Figure 4.1: Isothermal droplet impingement problem

0.005 seconds with the time-step $\Delta t = 0.0000001$ s.

In each numerical test, snapshots are provided at times $t = 0.0005, 0.001$, and 0.005 seconds during the simulations to capture the impact and spreading behavior of the droplet. As can be seen from Figs. 4.2 to 4.4, spreading area decreases with increasing viscosity values. Importantly, due to the initial antisymmetric distribution of the particles to represent the droplet, the final droplet morphology is not perfectly symmetric. Usually, droplets have also rebound behavior due to surface tension forces which is another important phenomenon to be studied in impingement problems. In the examples, this behavior is not observed due to having zero surface tension coefficient, $\sigma = 0$ N/m.

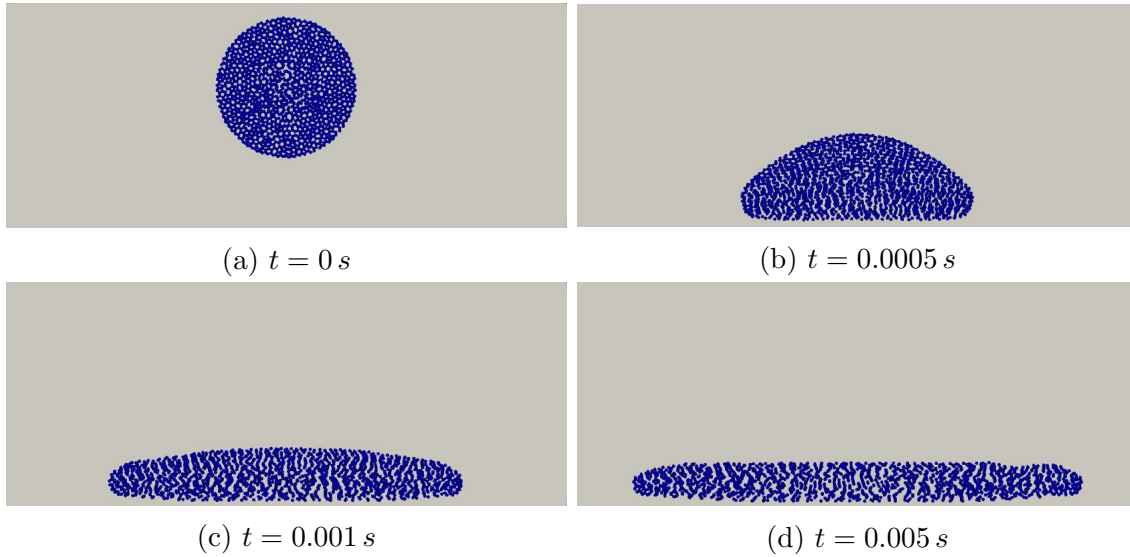


Figure 4.2: Isothermal droplet impingement with viscosity $\mu = 0.02$ Pa $\cdot$ s

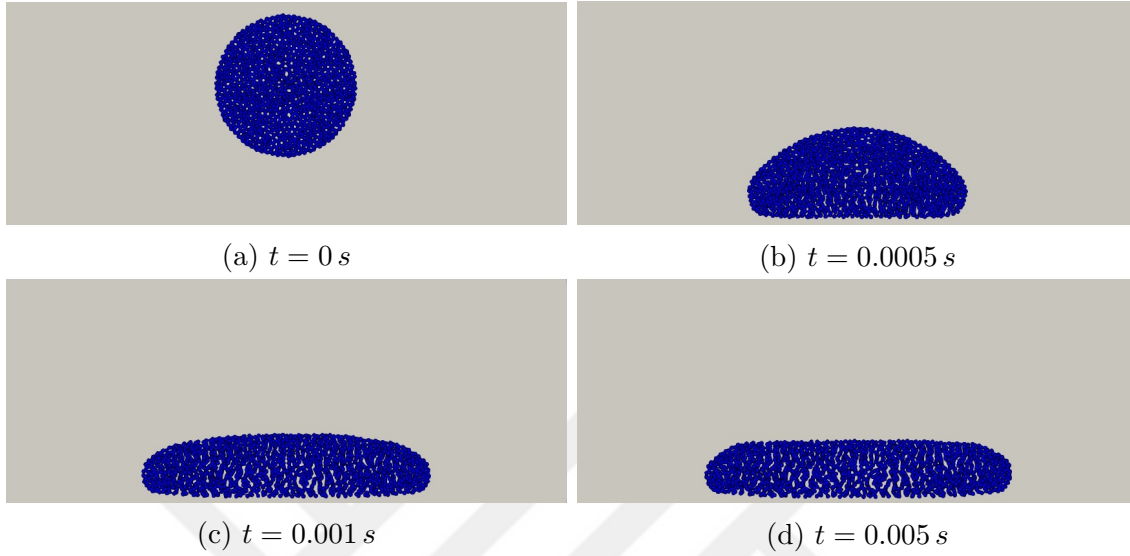


Figure 4.3: Isothermal droplet impingement with viscosity $\mu = 0.04 \text{ Pa} \cdot \text{s}$

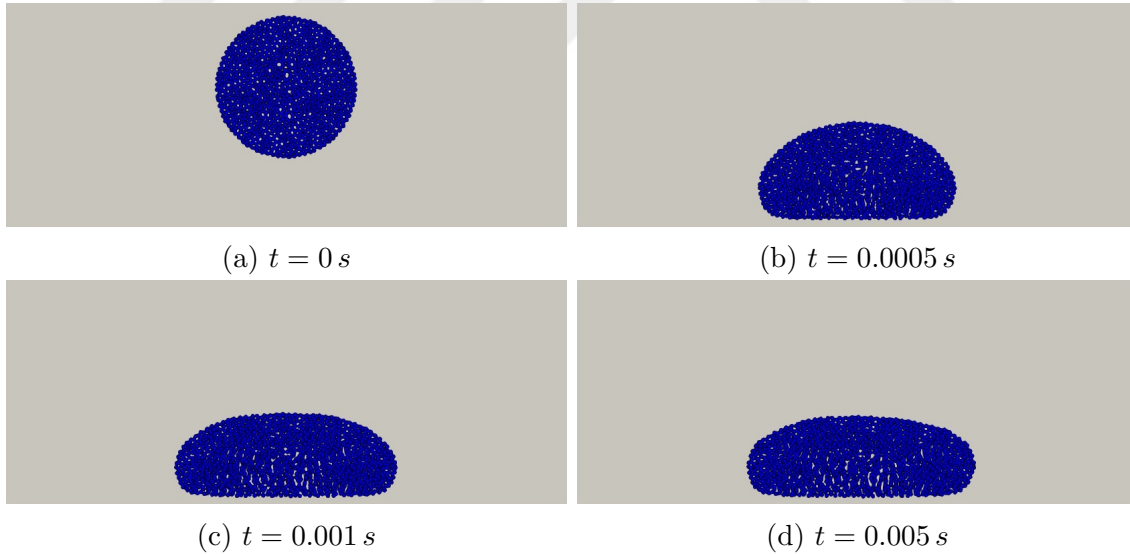


Figure 4.4: Isothermal droplet impingement with viscosity $\mu = 0.1 \text{ Pa} \cdot \text{s}$

In order to validate the isothermal droplet impingement simulations presented with the proposed MPM framework, the same problem was solved with COMSOL[®]'s 2-phase fluid flow modeling module. This solver couples the finite element method with the level set method to track and represent the interface boundary between fluids. In COMSOL[®] applications, the numerical analysis was conducted by modeling the surrounding area of the droplet as air. The snapshots are provided at times $t = 0.0005, 0.001, 0.005$ seconds and compared with the results obtained by using the MPM framework.

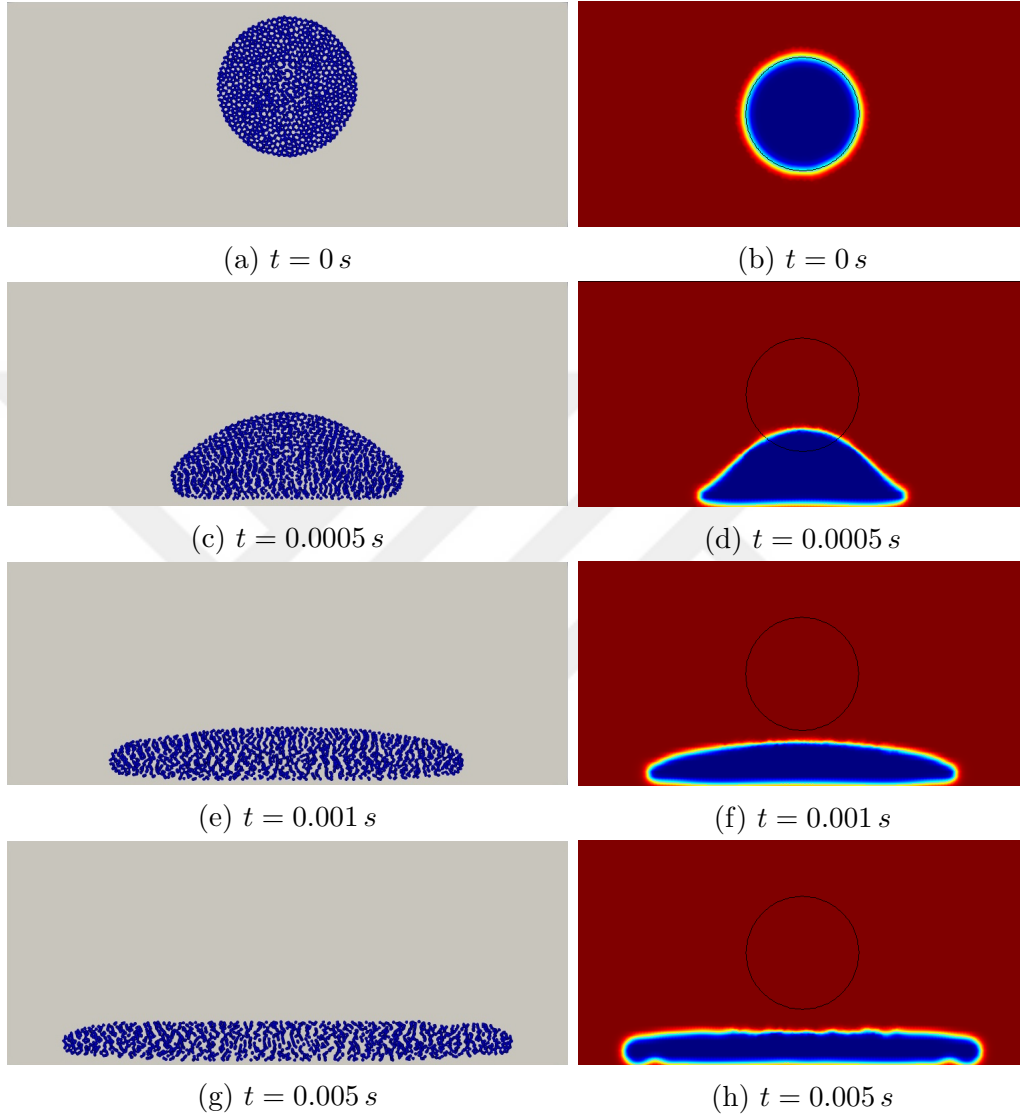


Figure 4.5: MPM vs 2-phase flow solver with viscosity $\mu = 0.02 \text{ Pa} \cdot \text{s}$

As seen from Figs. 4.5 to 4.7, the numerical results obtained by using the proposed MPM framework compare very well the COMSOL[®] simulations. The main difference between these two simulations is the surrounding fluid. In the MPM simulations, it is assumed that the droplet is in vacuum so the problem is solved in the nodes that particles occupy. However, in COMSOL[®] simulations, the surrounding area is modeled as air and the problem is solved by including properties of air. The spreading behavior (snapshots at $t = 0.0005$) looks slightly different when the two numerical results are compared, especially for the viscosity $\mu = 0.02 \text{ Pa} \cdot \text{s}$.

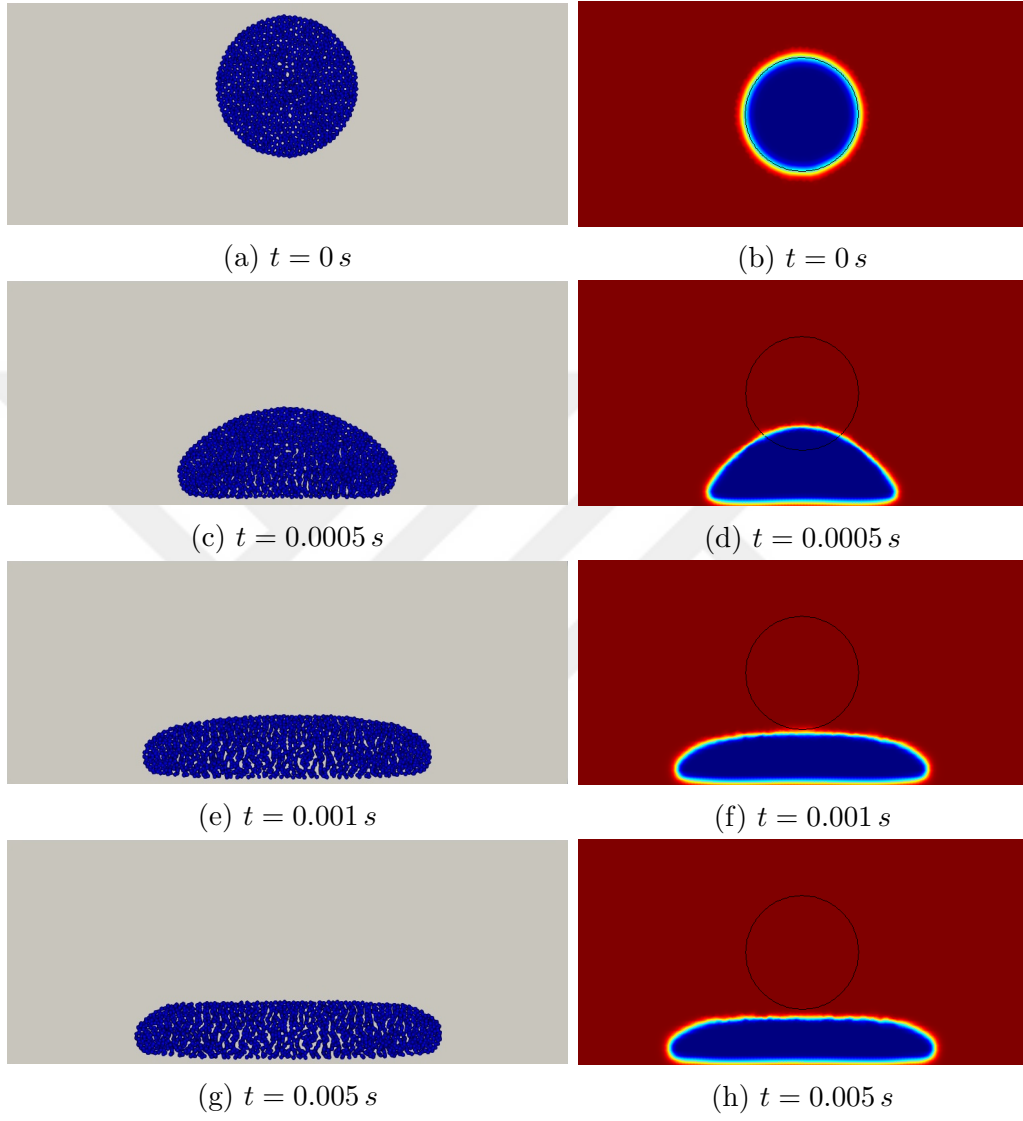


Figure 4.6: MPM vs 2-phase flow solver with viscosity $\mu = 0.04 \text{ Pa} \cdot \text{s}$

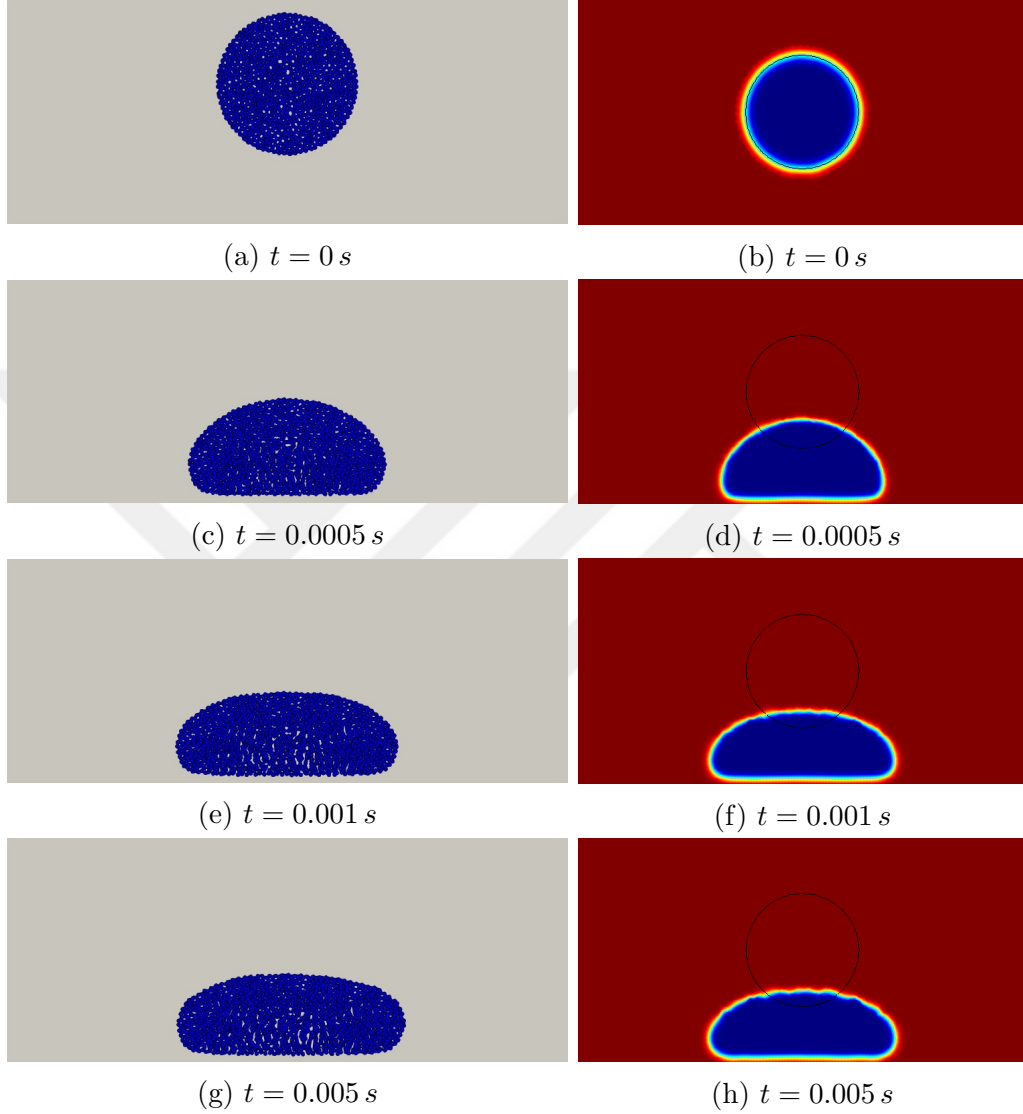


Figure 4.7: MPM vs 2-phase flow solver with viscosity $\mu = 0.1 \text{ Pa} \cdot \text{s}$

As a further study, mesh dependency of the numerical model is studied by solving the same droplet impingement problem with different background meshes. The central reason behind the importance of the size of the background grid is the coupling of the main MPM code with the level set method to track the free surface. The background grid is not only used to map data between particles and nodes but also to track the free surface with the level set method and impose the free surface boundary conditions with the ghost fluid method. In order to see the effects of mesh size, four different background meshes were considered in this part of the study. The number of particles to represent the droplet was 1536 as in the previous simulations.

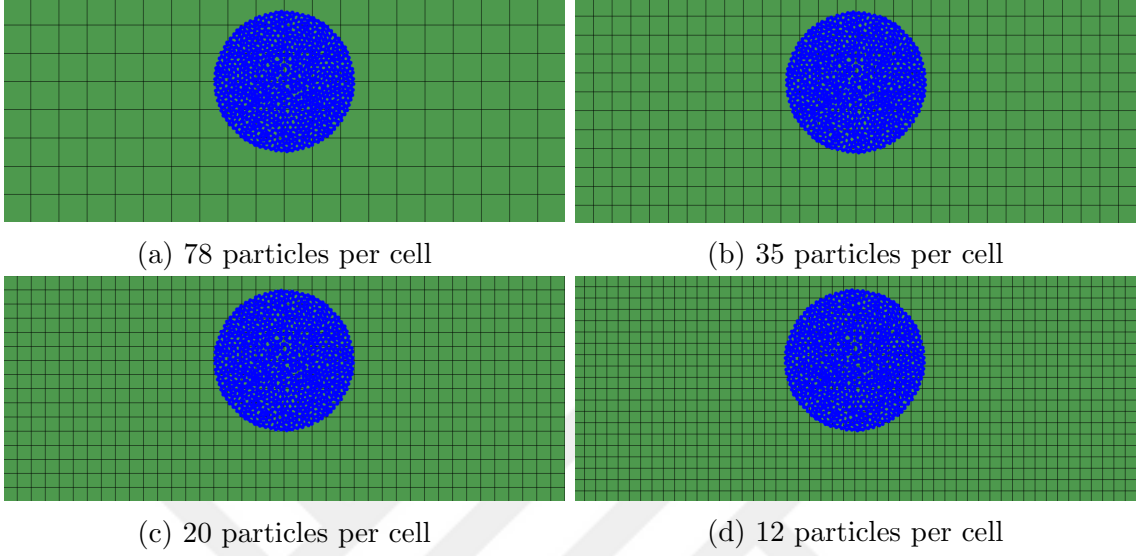


Figure 4.8: Mesh dependency study

In order to study the mesh dependency in the proposed MPM framework, four different background grids with 20×8 , 30×12 , 40×16 , and 50×24 elements were adopted, respectively (see Fig. 4.8). The approximate number of particles per each cell are also given due to having different mesh size in each case (see Figs. 4.8a to 4.8d).

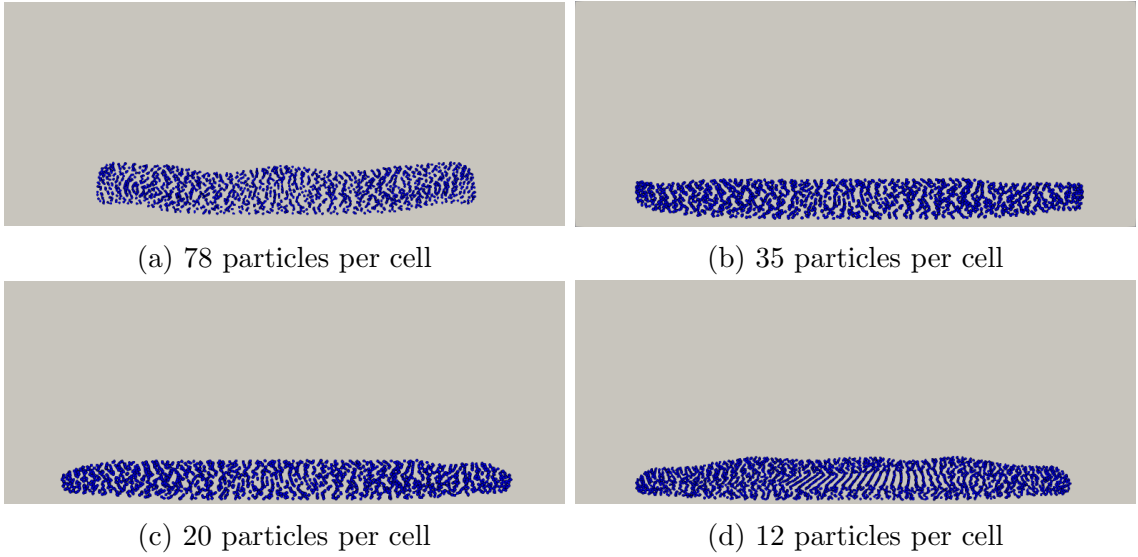


Figure 4.9: Mesh dependency results with viscosity $\mu = 0.02 \text{ Pa} \cdot \text{s}$

From the mesh dependency analysis (see Figs. 4.8a to 4.8d), it can be concluded that the background mesh plays a crucial role due to the coupling of the main MPM code with other

mesh-based numerical methods to solve the pressure field and track the free surface. Since better free surface representation is obtained with finer background meshes, the numerical framework provides more accurate results.

4.2 Forced heat convection

In extrusion based applications, cooling of extruded material are mainly controlled through natural or forced heat convection. In this part, cooling of a hot droplet was studied with the proposed MPM framework, and the results were validated with the FEM. In the numerical simulation, a droplet with the radius $R = 0.25$ mm, the density $\rho = 1000$ kg/m³, the heat capacity $c = 1000$ J/K, and the thermal conductivity $k = 0.2$ W/(m · K) was studied. In particle-based simulations or Eulerian approaches, due to the lack of material boundary representation, evaluation of the boundary integral term due to heat flux boundary condition is usually cumbersome. Therefore, the problem considered here is important to validate the determination of the boundary nodes and the computation of the boundary integral term given in [Eq. \(2.92\)](#). The simulation was simulated for 0.01 seconds with the heat convection term $h = 10000$.

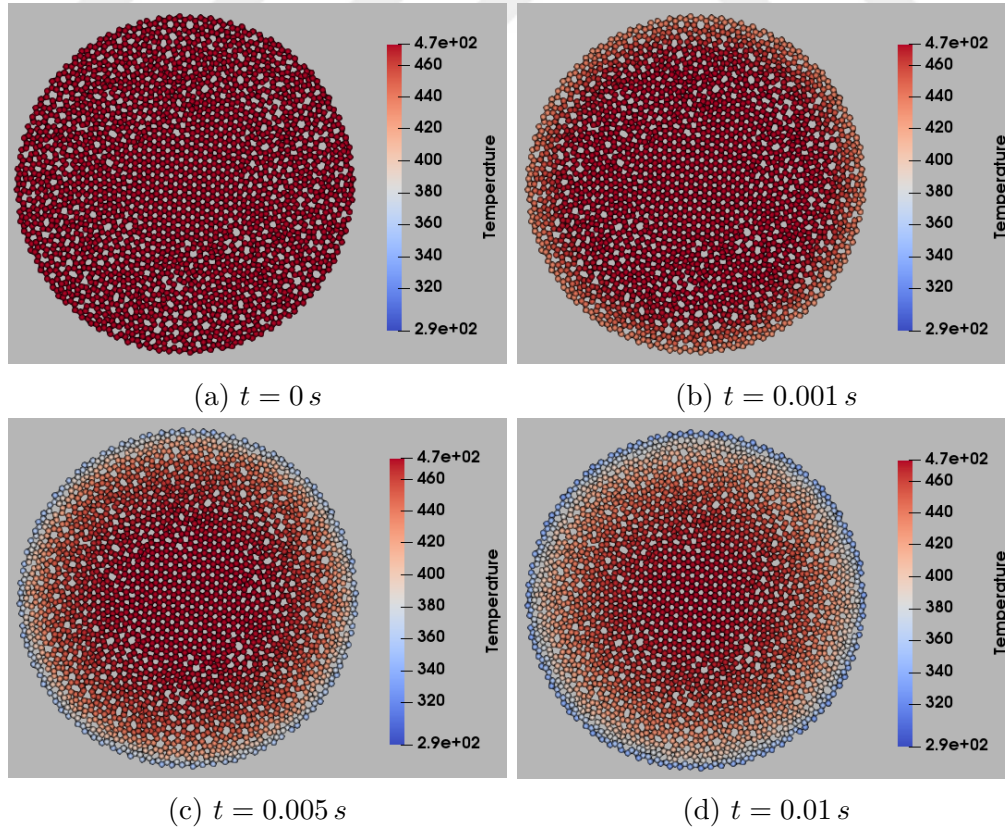


Figure 4.10: Heat convection

The same heat transfer problem was modeled with COMSOL[®], and the results were compared with the MPM results in Fig. 4.11 at times $t = 0.001, 0.005$, and 0.01 seconds. The boundary temperature reaches to 331 K in the FEM simulation while the average boundary temperature was obtained about 333 K in the MPM simulation.

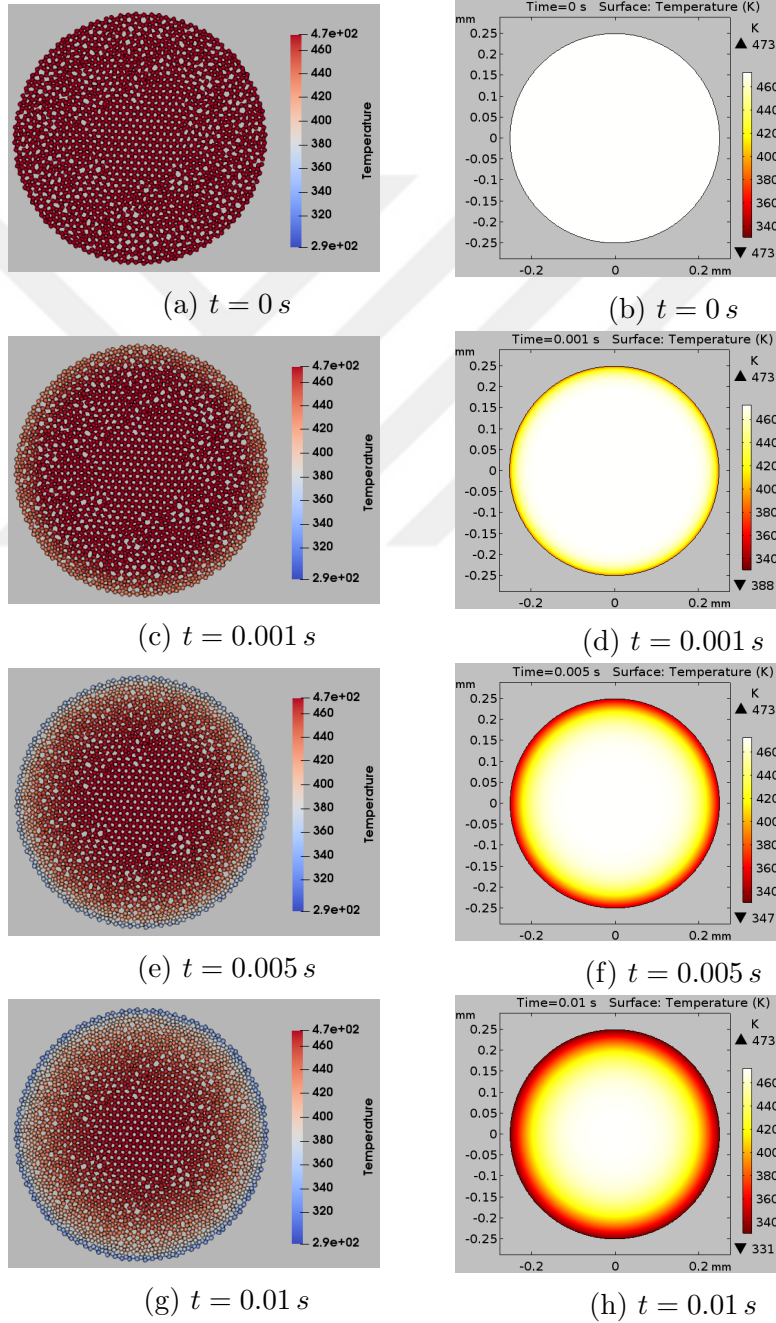


Figure 4.11: MPM vs FEM results for forced convection problem

4.3 Evolution of non-equilibrium droplet

In the last numerical validation problem, evolution of a non-equilibrium droplet was studied. In this problem, the surface tracking with the level set method and applying the free surface boundary conditions with the ghost fluid method were validated. A $0.1 \text{ cm} \times 0.1 \text{ cm}$ square droplet with the viscosity $\mu = 0.05 \text{ Pa} \cdot \text{s}$, the density $\rho = 1000 \text{ kg/m}^3$, and the surface tension coefficient $\sigma = 0.0024 \text{ N/m}$ was considered in the problem. The droplet was represented with 5000 particles, and a $0.02 \text{ cm} \times 0.02 \text{ cm}$ background mesh with 50×50 elements was adopted for the simulation.

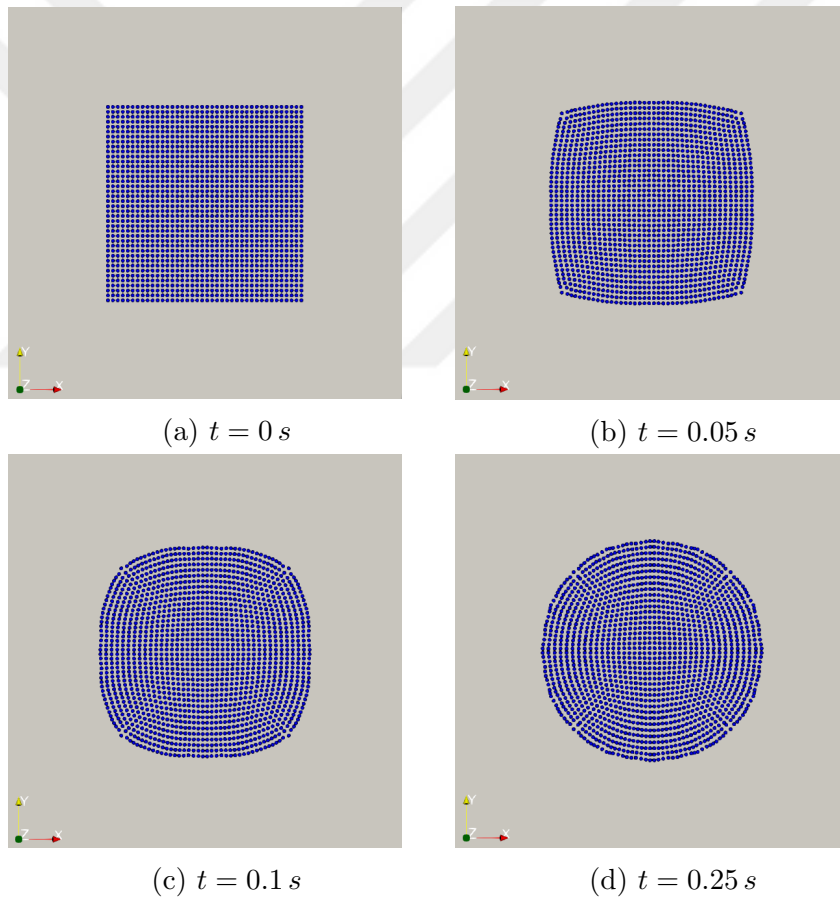


Figure 4.12: Evolution of non-equilibrium droplet with the MPM framework

The evolution of the square droplet under surface tension is showed in [Fig. 4.12](#) providing four different snapshots at times $t = 0, 0.05, 0.1$, and 0.25 seconds. The droplet reaches its equilibrium shape at the end of the simulation. These results were compared with the results provided by Chen [15]. In the study, the same problem was solved with a GIMP framework, and continuum surface force (CSF) model was adopted to simulate surface tension. In CSF, the surface tension is modeled as an extra body force term in the balance of linear

momentum. In Chen [15], a color function is adopted to track the free surface and evaluate the free surface parameters (i.e. surface normal and mean curvature).

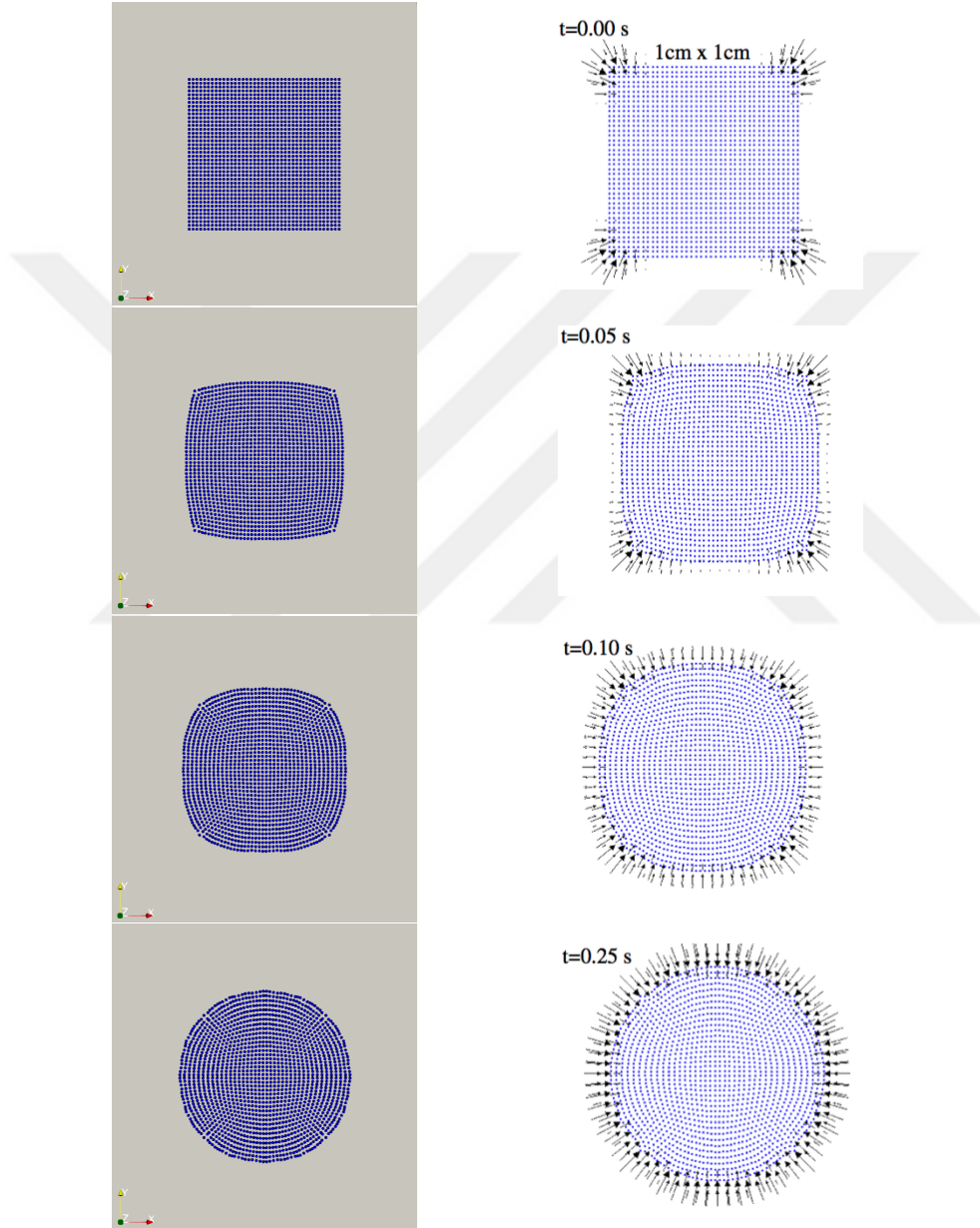


Figure 4.13: Comparison with GIMP-CSF modeling

As seen from the comparison given in Fig. 4.13, the free surface tracking with the level set method and the surface tension modeling with the ghost fluid method work very well in the proposed MPM framework compared to the simulations provided by Chen [15].

Chapter 5

Numerical Experiment

In this chapter, an extrusion-based AM technique, namely the fused deposition modeling (FDM) is studied by using the computational framework presented in Chapter 2. In the numerical simulations, a parametric study was adopted to investigate the effects of the process parameters on the extrusion behavior of the print material and the cooling-induced residual stresses. In the literature, the FDM process was simulated by following different numerical approaches. In the studies presented by Zhang and Chou [129, 130], an FEM framework which based on birth and death element technique was adopted. In this technique, the motion of the nozzle (tool planning) is given as input data, and a fixed mesh is adopted. In the beginning of the simulation, all the elements are assigned as “deactivated”. During the simulations, elements below the position of the nozzle are “activated”, and then the governing equations are solved in the activated elements. The actual extrusion behavior is not simulated in this technique, when an element is activated, it is assumed that the volume of the element is occupied by the extruded material. In the study presented by Xia et al. [111, 112], a front tracking finite volume method framework was adopted to simulate both the extrusion of the print material and residual stresses. In their study, the extrusion behavior and the cooling-induced residual stresses are studied with 2D and 3D examples. Fitzharris et al. [27] followed a process simulation model which couples ANSYS® Polyflow and ANSYS® Mechanical to simulate the FDM process. In this numerical model, the extrusion behavior is first simulated by using ANSYS® Polyflow and then the temperature profiles and geometries are exported into ANSYS® Mechanical to simulate residual stresses by solving a thermo-mechanical model. According to the author’s best knowledge, this is the first study to investigate the FDM process by employing an MPM-based numerical model. The overall numerical framework follows the methodology presented by Fitzharris et al. [27].

5.1 Problem definition and simulation parameters

In the FDM process, the layer-by-layer manufacturing process is carried out with continuous extrusion of melted print material from a movable nozzle (see Fig. 5.1). In this

study, the extrusion velocity (v_E), the nozzle velocity (v_N), the nozzle temperature (T_N), the substrate temperature (T_S), the nozzle gap (h_N), and the cooling rate (h_{air}) are selected as main process parameters.

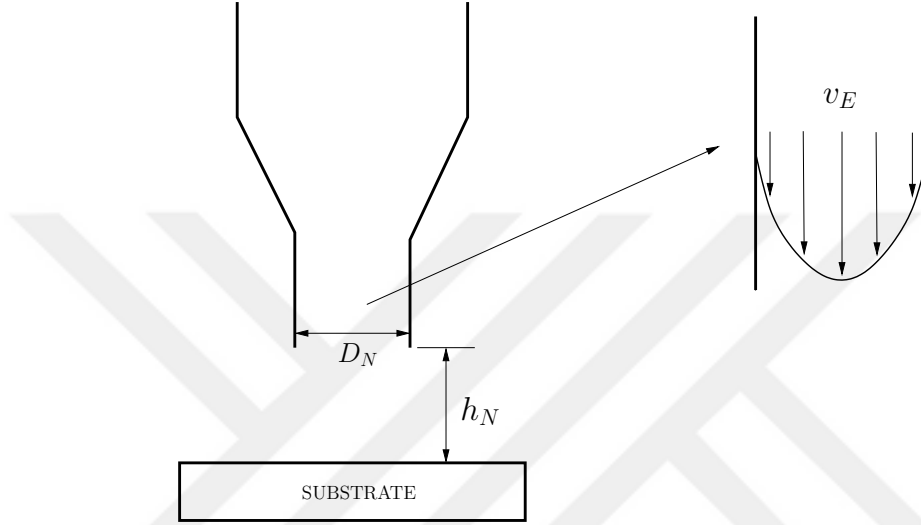


Figure 5.1: Nozzle geometry and extrusion velocity profile

In the numerical simulations, it is assumed that the fluid flow inside the nozzle tip is fully developed. Therefore, the following velocity profile

$$v_E = 2v_{AVE} \left[1 - \left(\frac{r}{D_N/2} \right)^2 \right] \quad (5.1)$$

is subjected to the particles inside the nozzle. In each simulation, 5 mm of print material is extruded on the substrate with a constant nozzle velocity. The parameters used in the simulations are listed as follows:

- Air temperature, $T_{air} = 293$ K
- Reference temperature, $T_{ref} = 293$ K
- Melting temperature, $T_{liq} = 493$ K
- Glass transition temperature, $T_g = 353$ K
- Substrate temperature, $T_S = 323$ K
- Reference density, $\rho_{ref} = 1000$ kg/m³
- Heat capacity in solid state, $c_s = 1200$ J/K

- Heat capacity in liquid state $c_l = 1800 \text{ J/K}$
- Latent Heat $L = 1000 \text{ J}$
- Thermal conductivity, $k = 0.2 \text{ W/(m} \cdot \text{K)}$
- Thermal expansion coefficient, $\alpha = 40 \times 10^{-6} \text{ m/(m} \cdot \text{K)}$
- Viscosity in solid phase, $\mu_s = 0.5 \text{ Pa} \cdot \text{s}$
- Viscosity in liquid phase, $\mu_l = 0.02 \text{ Pa} \cdot \text{s}$
- Reference Young's Modulus, $E_{ref} = 3.5 \text{ GPa}$
- Reference yield strength, $\sigma_{Y_{ref}} = 50 \text{ MPa}$

5.2 Parameter study

A parametric study was adopted to analyze the effects of three main parameters; the nozzle velocity (v_N), the nozzle gap (h_N), and the cooling rate (h_{air}). The extrusion of the print material and the cooling-induced residual stresses are presented for different cases. The residual stress analysis results are given by calculating the Von Mises stress of the material.

5.2.1 Nozzle velocity variation study

In the first study, the effects of the nozzle velocity (v_N) were investigated. In the simulations, the extrusion velocity (v_E), nozzle temperature (T_N), substrate temperature (T_S), nozzle gap (h_N), and the cooling rate (h_{air}) were kept constant (see [Table 5.1](#)).

Parameter	Value
v_{AVE}	10 mm/s
T_N	493 K
T_S	323 K
h_N	0.4 mm
h_{air}	100 W/(m ² · K)

Table 5.1: Process parameters for variation in v_N

In [Fig. 5.2](#), the snapshots are provided for the the extrusion process for $v_N = 12 \text{ mm/s}$ at times $t = 0.125, 0.25$, and 1 seconds. As can be seen from the temperature profiles presented in [Fig. 5.2](#), the bottom part of the extruded material has a higher cooling rate due to the contact with the substrate, and the upper part of the material cools down slowly due to heat convection through air.

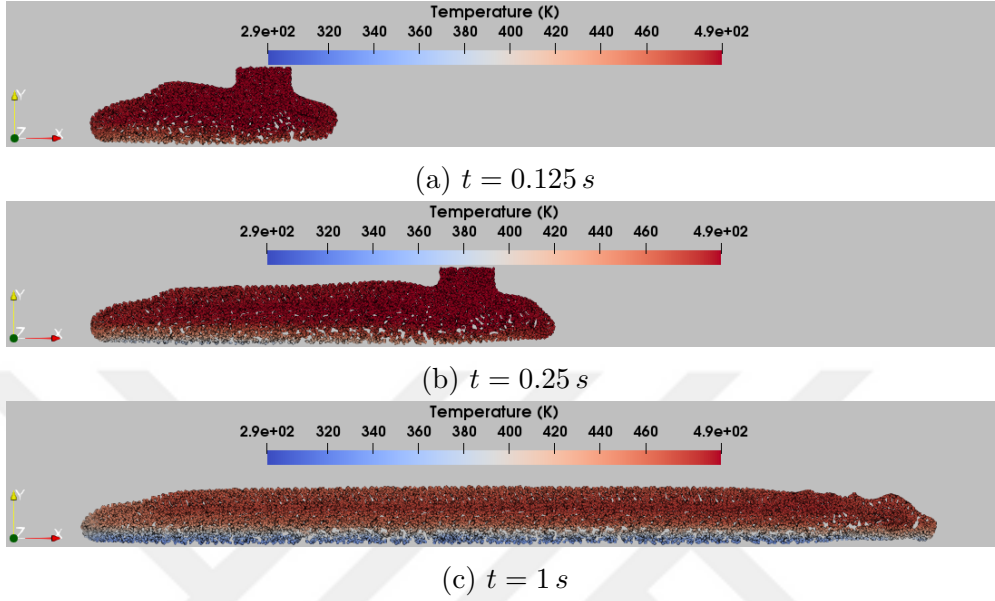


Figure 5.2: Extrusion process for $v_N = 12$ mm/s

In Fig. 5.3, the snapshots are given for the simulation of the cooling-induced residual stresses at times $t = 3, 4$, and 5 seconds. It is observed that the residual stresses are higher at the tips and the bottom part of the extruded material due to high cooling rates. This is actually the main reason to have thermal warping issue in material extrusion AM applications. Therefore, it is important to study, and it can be improved by controlling the substrate temperature.

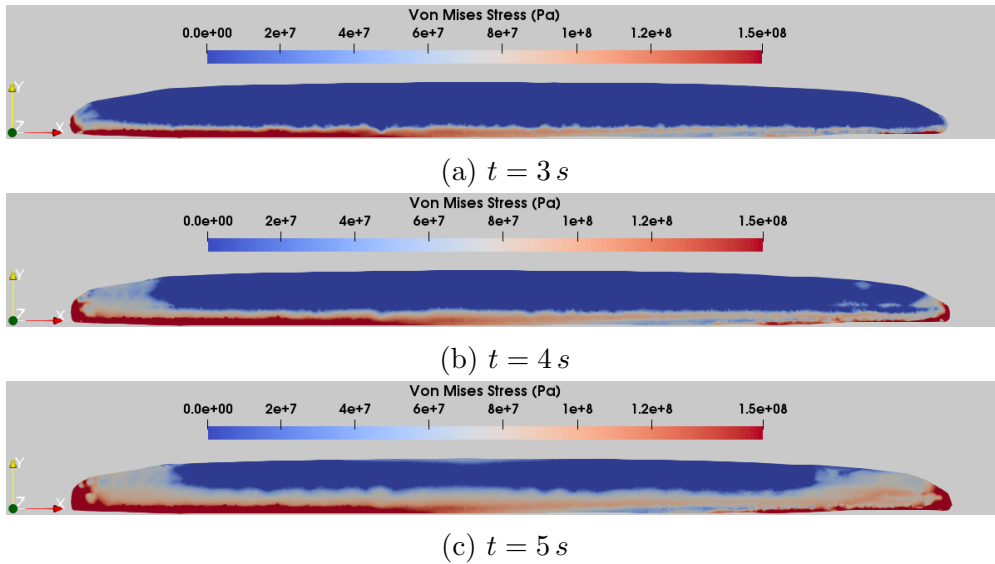


Figure 5.3: Residual stress distribution for $v_N = 12$ mm/s

In Fig. 5.4, the profiles of the extruded material and temperature distributions are provided for the nozzle velocities, $v_N = 0.14, 0.16, 0.18, 0.20, 0.22$, and 0.24 mm/s, respectively. The temperature profiles are given at $t = 1$ second (see also Appendix A for simulation results in detail). As it is expected, less material is extruded with increasing nozzle velocity, and therefore, the thickness of the extruded material decreases. It is also clear that, the roughness of the surface increases with higher nozzle velocities. This is actually an undesired extrusion case that may cause defects and poor printing quality. Moreover, better extrusion behavior is observed for lower nozzle velocities, especially for $v_N = 0.14$ and 0.16 mm/s.

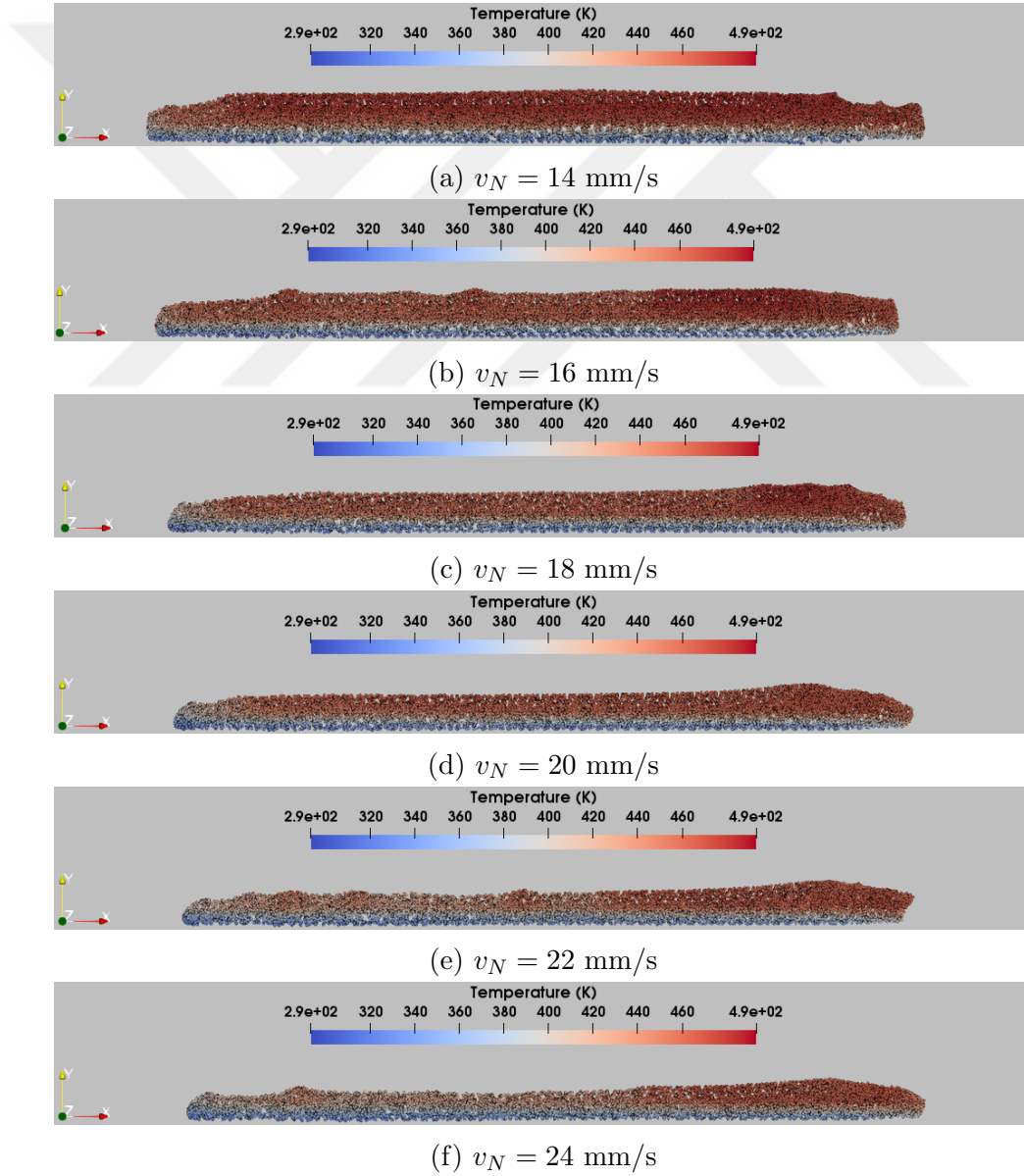


Figure 5.4: Extruded material for different nozzle velocity (v_N) values

The results of the residual stress analyses are given in Fig. 5.5 for the nozzle velocities, $v_N = 0.14, 0.16, 0.18, 0.20, 0.22$, and 0.24 mm/s, respectively. The results show that high stress concentration is obtained at the tips and the bottom part of the extruded material in all cases. Furthermore, it is clear that residual stress concentration increases in the center of the extruded material with increasing nozzle velocity. Thus, higher residual stresses are obtained when the nozzle velocity increases.

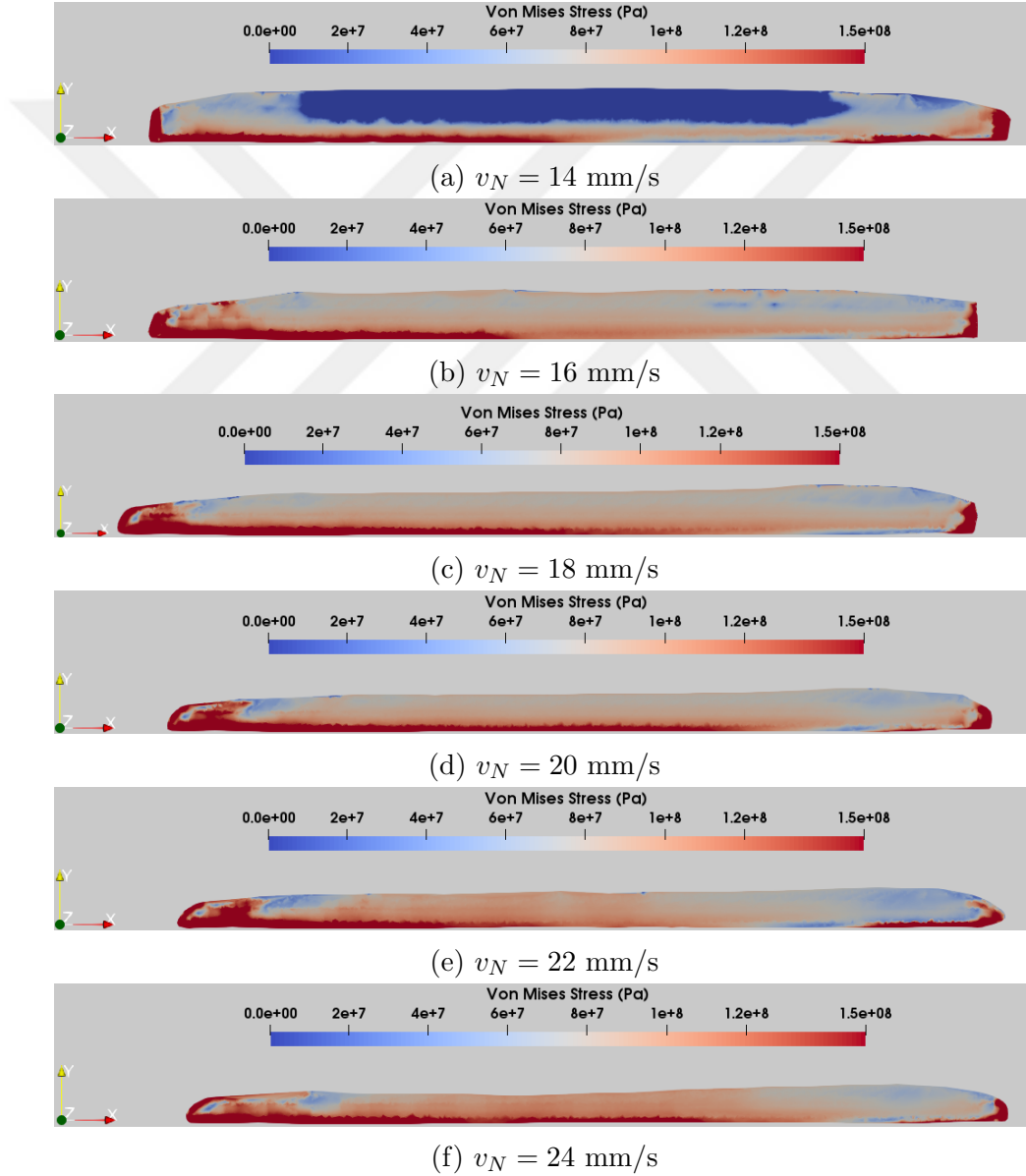


Figure 5.5: Residual stresses for different nozzle velocity (v_N) values

5.2.2 Nozzle gap variation study

In the second study, the effects of the nozzle gap (h_N) were investigated. The extrusion velocity (v_E), the nozzle velocity (v_N), the nozzle temperature (T_N), the substrate temperature (T_S), and the cooling rate (h_{air}) were kept constant (see Table 5.2) in the simulations. The problem was analyzed with different values of the ratio h_N/D_N .

Parameter	Value
v_{AVE}	10 mm/s
v_N	18 mm/s
T_N	493 K
T_S	323 K
h_{air}	100 W/(m ² · K)

Table 5.2: Process parameters for variation in h_N

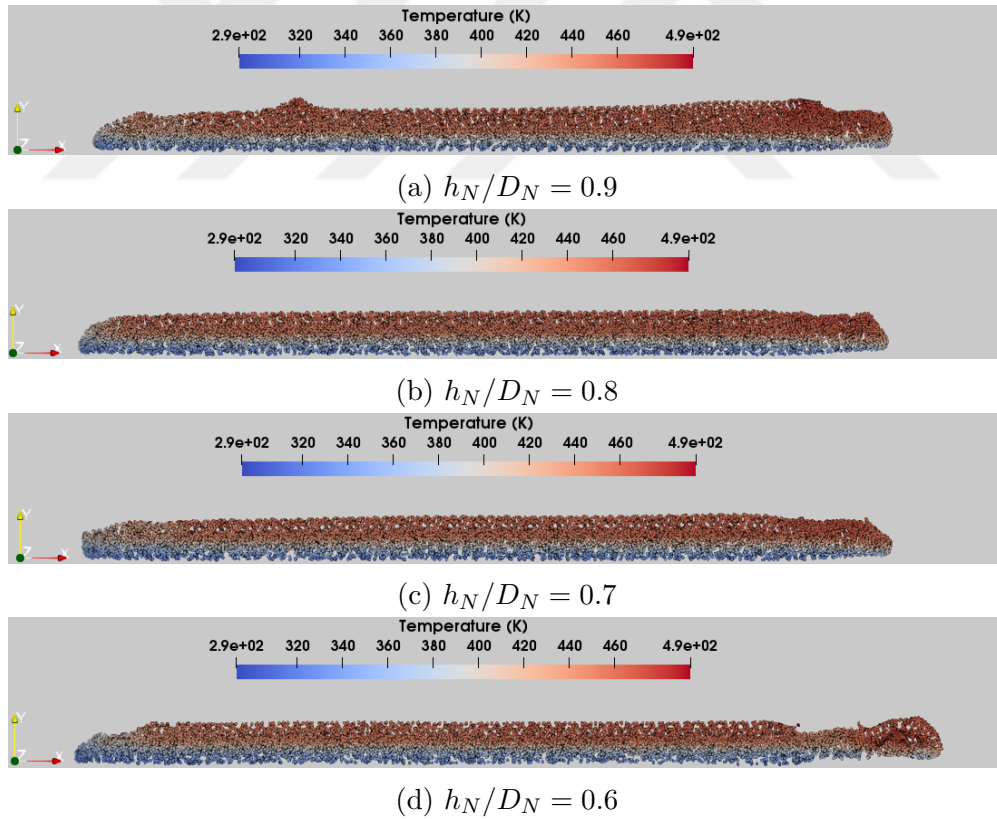


Figure 5.6: Extruded material for different h_N/D_N values

In this part, by taking the previous parameter study as a basis, the nozzle velocity was fixed to 18 mm/s in the simulations. In Fig. 5.6, the numerical results are provided for the ratios $h_N/D_N = 0.9, 0.8, 0.7$, and 0.6 , respectively. The temperature profiles are given

at $t = 1$ second (see also Appendix A for simulation results in detail). It is clear that better extrusion behavior is observed, especially for the ratios $h_N/D_N = 0.28$ and 0.32 . For $h_N/D_N = 0.36$, surface roughness is slightly alleviated compared to the result given in Fig. 5.4 but the nozzle gap is still wide to get better extrusion behavior with this nozzle velocity. On the other hand, an undesired print condition is obtained for $h_N/D_N = 0.24$ due to accumulation of excessive amount of print material in front of the nozzle tip. This issue can be resolved by increasing the nozzle velocity or the nozzle gap accordingly.

The residual stress analysis results are given in Fig. 5.7. Here, it can be observed that the residual stress distribution is not significantly affected by the change of the nozzle gap, similar residual stress distributions are obtained in all cases.

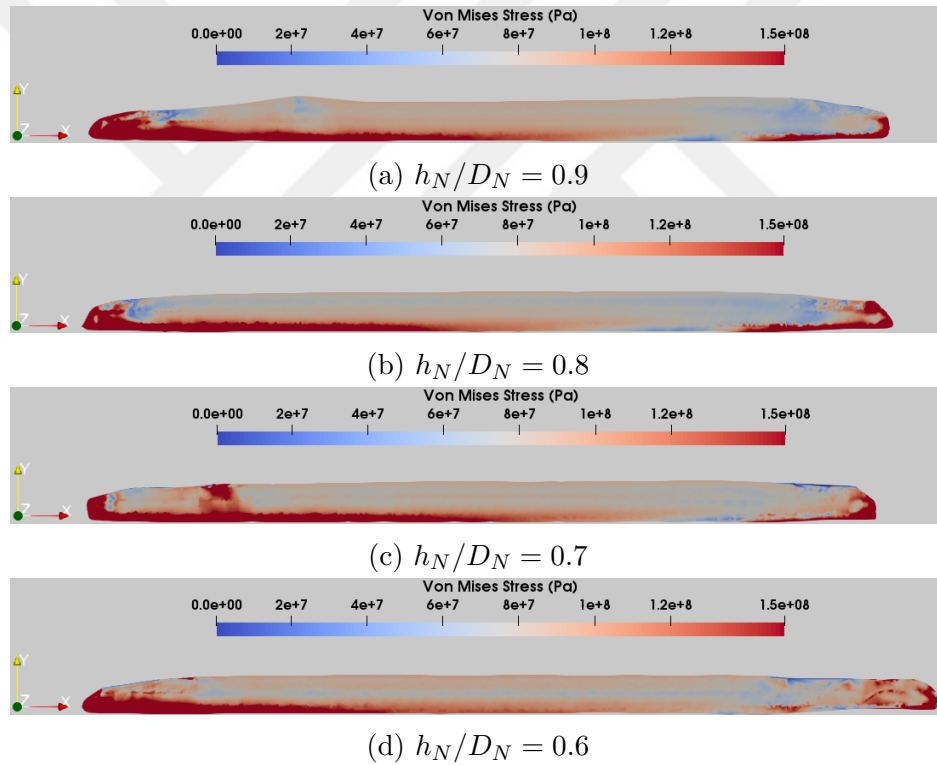


Figure 5.7: Residual stresses for different h_N/D_N values

By inspecting the results of this parameter study, it can be concluded that the surface roughness is mitigated by controlling the gap between the nozzle and the surface, and better surface finish is obtained. In addition, the thickness of the extruded material, in other words the thickness of the layer can be controlled with the combination of the nozzle gap and the nozzle velocity.

5.2.3 Cooling rate variation study

In the last parametric study, the effects of cooling rate were analyzed. The extrusion velocity (v_E), the nozzle velocity (v_N), the nozzle temperature (T_N), the substrate temperature (T_S), and the nozzle gap (h_N) were kept constant (see Table 5.3) in the simulations. In many FDM applications, the cooling rate is a process parameter to be determined. Usually, an external fan attached to the nozzle controls the cooling rate. For this reason, it is important to analyze the effects of different cooling rates.

Parameter	Value
v_{AVE}	10 mm/s
v_N	18 mm/s
T_N	493 K
? T_S	323 K
h_N	0.28 mm

Table 5.3: Process parameters for variation in h_{air}

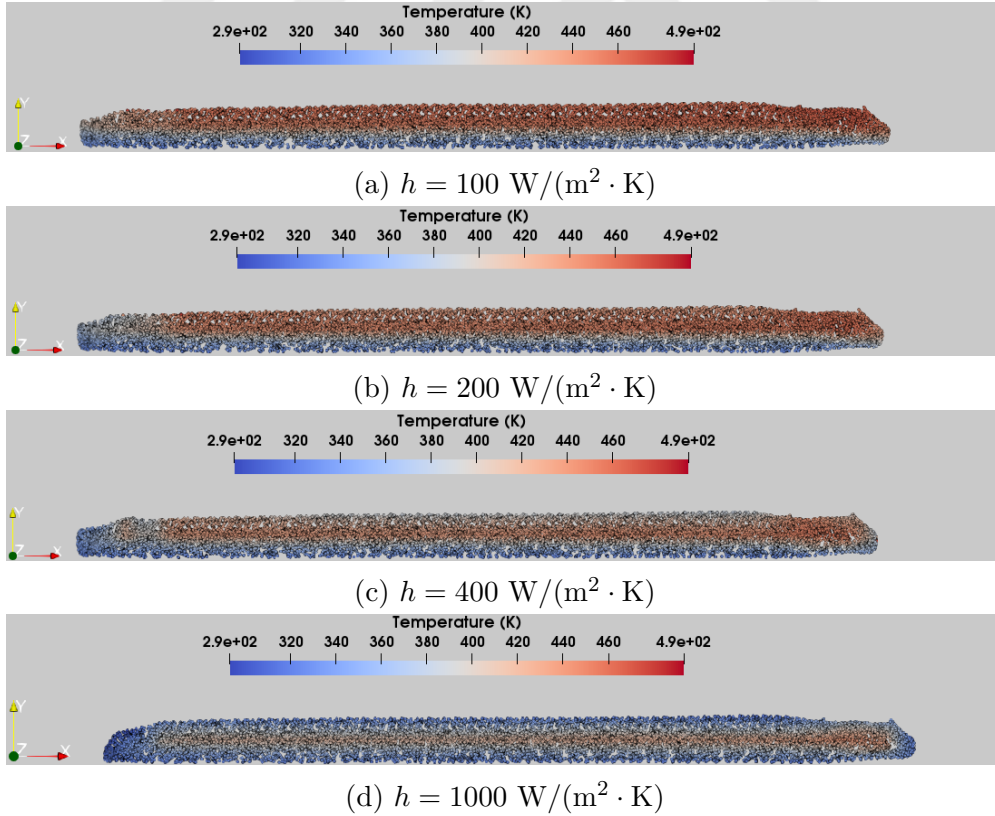


Figure 5.8: Extrusion process for different cooling rates

In this case, the nozzle velocity is fixed to 18 mm/s as in previous parameter study. In Fig. 5.8, the numerical results are provided for heat convection coefficients $h_{air} = 100, 200,$

400, and 1000 W/(m² · K). The temperature profiles are given at $t = 1$ second (see also Appendix A for simulation results in detail).

As can be seen from the temperature profiles given in Fig. 5.8, rapid solidification is observed at the top surface of the extruded material when the cooling rate is increased. The surface roughness of the extruded material is not significantly affected by changing the cooling rate with the parameters given Table 5.3. On the other hand, in the residual stress analyses, it is observed that slightly higher residual stresses are obtained for increasing cooling rates.

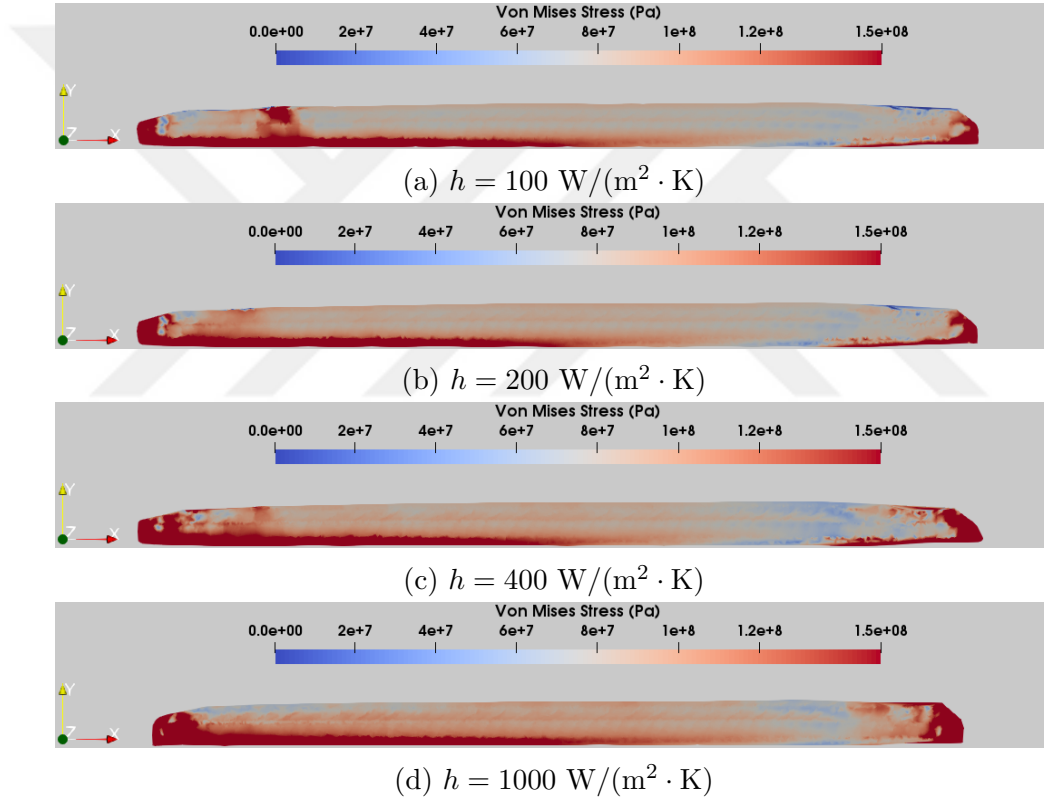


Figure 5.9: Residual stress distributions for different cooling rates for $v_N = 18 \text{ mm/s}$

In a further study, to see the effects of different cooling rates better, the nozzle gap and the nozzle velocity were changed to 0.4 mm and 14 mm/s, respectively. The temperature profiles are given in Fig. 5.10 at $t = 1$ second (see also Appendix A for simulation results in detail) for the heat convection coefficients $h_{air} = 100, 200, 400$, and 1000 W/m² · K, respectively. In this case, a significant effect of applying different cooling rates is observed in Fig. 5.11. The numerical results show that higher cooling rates increase the surface roughness and the residual stress of the printed material.

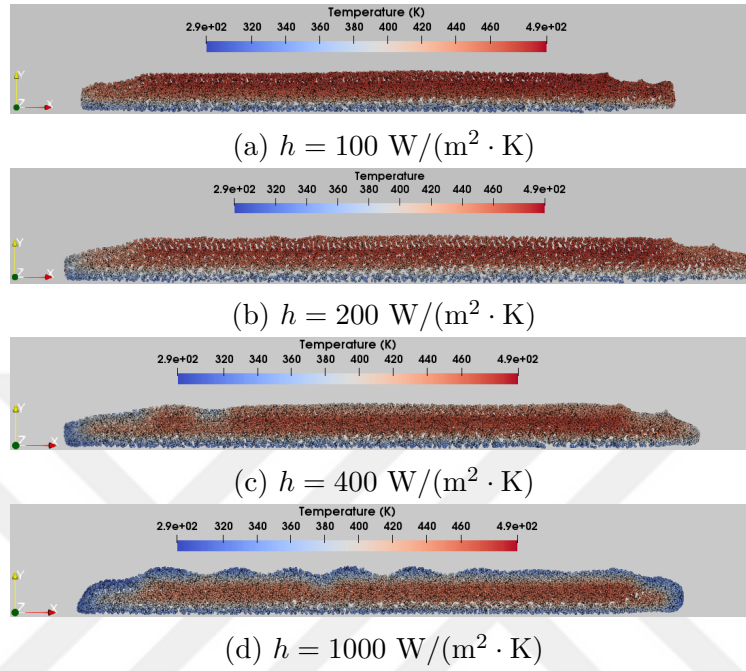


Figure 5.10: Extrusion process for different cooling rates for $v_N = 14 \text{ mm/s}$ and $h_N = 0.4 \text{ mm}$

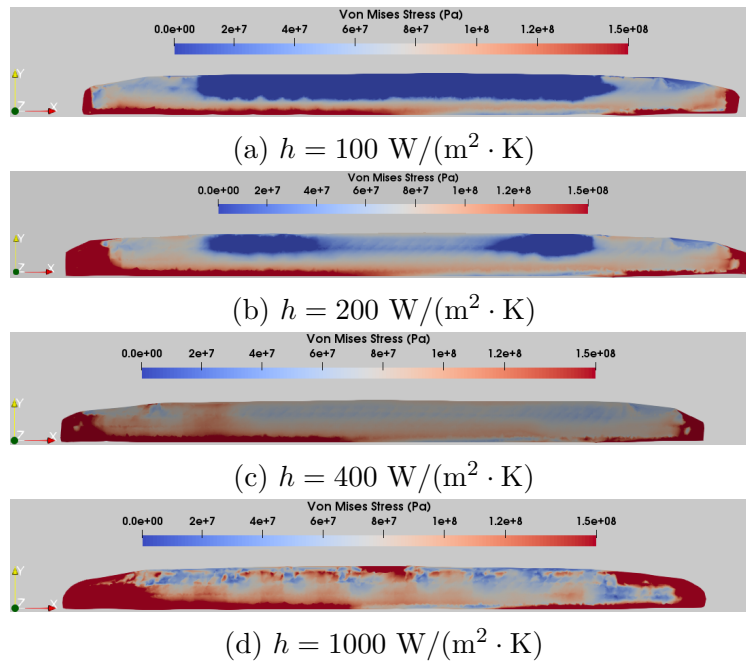


Figure 5.11: Residual stress distributions for different cooling rates for $v_N = 14 \text{ mm/s}$ and $h_N = 0.4 \text{ mm}$

Chapter 6

Conclusions and future work

6.1 Conclusions

In this dissertation, an MPM framework was developed to simulate extrusion-based AM processes to optimize process variables and simulate cooling-induced residual stresses. The overall computational framework has two main parts. In the first part, the extrusion of print material is simulated by modeling the polymer flow as an incompressible viscous fluid. The main MPM code is coupled with FDM to solve the pressure field and update the velocity field (Eq. (2.32)). Additionally, in this part, the numerical model is capable of tracking the free surface to apply the free surface pressure boundary conditions. In the second part, the cooling-induced residual stresses of the extruded material are simulated by solving a thermo-mechanical model. The residual stress computation starts with the morphology of the extruded material and the temperature field obtained in the first part of the numerical analysis.

The numerical framework was first validated by studying three select problems: isothermal droplet impingement, forced heat convection, and evolution of a non-equilibrium droplet. In these numerical examples, different parts of the numerical model was studied. In the isothermal droplet impingement problem, the solution of the pressure-splitting technique and the coupling with the FDM were validated. In this problem thermal effects were neglected, and the surface tension was not applied. The numerical simulations were validated by comparing with the results obtained with COMSOL[®]'s 2-phase flow modeling module. In the second problem, cooling of a hot droplet was considered to solve the balance of energy with the MPM. In particle-based methods, imposition of boundary conditions is usually cumbersome. Therefore, in this problem, determination of the boundary particles by using the level set method and the evaluation of the boundary integral (heat flux boundary condition) were also tested. In the last problem, evolution of a non-equilibrium droplet was studied. In this case, the applicability of the ghost fluid method and the mean curvature calculation by using the level set method were tested. On the other hand, the effects of mesh size were studied. The results show that mesh size have an important role in the simulations due to

the boundary representation with the level set method.

Next, in Chapter 5, the proposed numerical framework was applied to an extrusion-based additive manufacturing technique, namely the fused deposition modeling (FDM). The nozzle velocity, the extrusion velocity, the nozzle gap, the substrate temperature, the nozzle temperature, and the cooling rate were selected as main process parameters, and a parameter study was adopted to investigate the effects of different process parameters. In the first parameter study, the effects of the nozzle velocity were investigated. As can be seen from the results given in Figs. 5.4 and 5.5, the thickness of the extruded material decreases with increasing nozzle velocity values. On the other hand, the surface roughness and the residual stresses increase with higher nozzle velocities. In the second study, the effects of the nozzle gap were investigated and it was showed that better extrusion profiles can be obtained by adjusting the nozzle gap accordingly (see Fig. 5.6). In the last study, the effects of cooling rate were investigated, and it was concluded that in some cases, high cooling rates may cause undesired print quality increasing the surface roughness.

6.2 Future work

Firstly, the numerical framework needs to be extended to 3D to understand the problem, so the effects of different parameters can be fully understood in the simulations. Secondly, since the flow of print materials are usually non-Newtonian, more realistic fluid models such as Oldroyd-B, Giesekus, and Pom-Pom models must be adopted in the numerical model. In this way, the important effects like shear thinning can be investigated, and better prediction in the extrusion process is obtained.

On the other hand, to improve the numerical method and eliminate the cell crossing issue, two of the advance versions of the original MPM, namely convected domain particle integration method (CPDI) and b-spline material point method (BSMPM) are currently being developed by the author.

Another interesting study would be deposition of polymer-metal mixtures. This type of functional filaments are currently used in many different applications. In the numerical model, metal particles can be modeled as rigid bodies. In the MPM, rigidity of the metal particles can be controlled via the deformation tensor. Therefore, rigid body motion can be imposed for the rigid particles.

Bibliography

- [1] 3d printed record. http://www.amandaghassaei.com/projects/3D_printed_record/.
- [2] 3DHUBS. <https://www.3dhubs.com/>.
- [3] Ravindra Ambati, Xiaofei Pan, Huang Yuan, and Xiong Zhang. Application of material point methods for cutting process simulations. *Computational Materials Science*, 57:102–110, 2012.
- [4] SG Bardenhagen, JU Brackbill, and Deborah Sulsky. The material-point method for granular materials. *Computer methods in applied mechanics and engineering*, 187(3-4):529–541, 2000.
- [5] SG Bardenhagen and EM Kober. The generalized interpolation material point method. *Computer Modeling in Engineering and Sciences*, 5(6):477–496, 2004.
- [6] Y Bazilevs, VM Calo, Y Zhang, and Thomas JR Hughes. Isogeometric fluid–structure interaction analysis with applications to arterial blood flow. *Computational Mechanics*, 38(4-5):310–322, 2006.
- [7] Yuri Bazilevs, L Beirao da Veiga, J Austin Cottrell, Thomas JR Hughes, and Giancarlo Sangalli. Isogeometric analysis: approximation, stability and error estimates for h-refined meshes. *Mathematical Models and Methods in Applied Sciences*, 16(07):1031–1090, 2006.
- [8] KA Belibassakis, Th P Gerostathis, KV Kostas, CG Politis, PD Kaklis, AI Ginnis, and C Feurer. A bem-isogeometric method for the ship wave-resistance problem. *Ocean Engineering*, 60:53–67, 2013.
- [9] Anna Bellini and Selçuk Güçeri. Mechanical characterization of parts fabricated using fused deposition modeling. *Rapid Prototyping Journal*, 9(4):252–264, 2003.
- [10] H Bikas, Panagiotis Stavropoulos, and George Chryssolouris. Additive manufacturing methods and modelling approaches: a critical review. *The International Journal of Advanced Manufacturing Technology*, 83(1-4):389–405, 2016.

- [11] David Bourell, Jean Pierre Kruth, Ming Leu, Gideon Levy, David Rosen, Allison M Beese, and Adam Clare. Materials for additive manufacturing. *CIRP Annals*, 66(2):659–681, 2017.
- [12] J Burghardt, R Brannon, and J Guilkey. A nonlocal plasticity formulation for the material point method. *Computer Methods in Applied Mechanics and Engineering*, 225:55–64, 2012.
- [13] Caterina Casavola, Alberto Cazzato, Vincenzo Moramarco, and Giovanni Pappaletta. Residual stress measurement in fused deposition modelling parts. *Polymer Testing*, 58:249–255, 2017.
- [14] Yan-pu Chao, Le-hua Qi, Han-song Zuo, Jun Luo, Xiang-hui Hou, and He-jun Li. Remelting and bonding of deposited aluminum alloy droplets under different droplet and substrate temperatures in metal droplet deposition manufacture. *International Journal of Machine Tools and Manufacture*, 69:38–47, 2013.
- [15] Liangbiao Chen. *Using the generalized interpolation material point method for fluid-solid interactions induced by surface tension*. PhD thesis, University of Alaska Fairbanks, 2013.
- [16] Zhen Chen and Rebecca Brannon. An evaluation of the material point method. *SAND Report, SAND2002-0482, (February 2002)*, 2002.
- [17] Zhen Chen, Shan Jiang, Yong Gan, Hantao Liu, and Thomas D Sewell. A particle-based multiscale simulation procedure within the material point method framework. *Computational Particle Mechanics*, 1(2):147–158, 2014.
- [18] Helena N Chia and Benjamin M Wu. Recent advances in 3d printing of biomaterials. *Journal of biological engineering*, 9(1):4, 2015.
- [19] Alexandre Joel Chorin. Numerical solution of the navier-stokes equations. *Mathematics of computation*, 22(104):745–762, 1968.
- [20] Josef F Christ, Nahal Aliheidari, Amir Ameli, and Petra Pötschke. 3d printed highly elastic strain sensors of multiwalled carbon nanotube/thermoplastic polyurethane nanocomposites. *Materials & Design*, 131:394–401, 2017.
- [21] Raphaël Commin, Marcin P Serdeczny, David B Pedersen, and Jon Spangenberg. Numerical modeling of the strand deposition flow in extrusion-based additive manufacturing. *Additive Manufacturing*, 20:68–76, 2018.
- [22] J Austin Cottrell, Thomas JR Hughes, and Yuri Bazilevs. *Isogeometric analysis: toward integration of CAD and FEA*. John Wiley & Sons, 2009.

- [23] E De Luycker, DJ Benson, T Belytschko, Y Bazilevs, and MC Hsu. X-fem in isogeometric analysis for linear fracture mechanics. *International Journal for Numerical Methods in Engineering*, 87(6):541–565, 2011.
- [24] Sachith Dunatunga and Ken Kamrin. Continuum modelling and simulation of granular flows through their many phases. *Journal of Fluid Mechanics*, 779:483–513, 2015.
- [25] Sachith Dunatunga and Ken Kamrin. Continuum modeling of projectile impact and penetration in dry granular media. *Journal of the Mechanics and Physics of Solids*, 100:45–60, 2017.
- [26] Ronald P Fedkiw, Tariq Aslam, Barry Merriman, and Stanley Osher. A non-oscillatory eulerian approach to interfaces in multimaterial flows (the ghost fluid method). *Journal of computational physics*, 152(2):457–492, 1999.
- [27] Emily R Fitzharris, Narumi Watanabe, David W Rosen, and Meisha L Shofner. Effects of material properties on warpage in fused deposition modeling parts. *The International Journal of Advanced Manufacturing Technology*, 95(5-8):2059–2070, 2018.
- [28] Panagis Foteinopoulos, Alexios Papacharalampopoulos, and Panagiotis Stavropoulos. On thermal modeling of additive manufacturing processes. *CIRP Journal of Manufacturing Science and Technology*, 20:66–83, 2018.
- [29] William E Frazier. Metal additive manufacturing: a review. *Journal of Materials Engineering and Performance*, 23(6):1917–1928, 2014.
- [30] Yong Gan, Zheng Sun, Zhen Chen, Xiong Zhang, and Yu Liu. Enhancement of the material point method using b-spline basis functions. *International Journal for Numerical Methods in Engineering*, 113(3):411–431, 2018.
- [31] Mario Ganci, Wei Zhu, Gianluca Buffa, Livan Fratini, Song Bo, and Chunze Yan. A macroscale fem-based approach for selective laser sintering of thermoplastics. *The International Journal of Advanced Manufacturing Technology*, 91(9-12):3169–3180, 2017.
- [32] Wei Gao, Yunbo Zhang, Devarajan Ramanujan, Karthik Ramani, Yong Chen, Christopher B Williams, Charlie CL Wang, Yung C Shin, Song Zhang, and Pablo D Zavattieri. The status, challenges, and future of additive manufacturing in engineering. *Computer-Aided Design*, 69:65–89, 2015.
- [33] Anvar Gilmanov and Sumanta Acharya. A hybrid immersed boundary and material point method for simulating 3d fluid–structure interaction problems. *International journal for numerical methods in fluids*, 56(12):2151–2177, 2008.
- [34] Karthikeyan Gnanasekaran, T Heijmans, S van Bennekom, H Woldhuis, S Wijnia, Heiner Friedrich, et al. 3d printing of cnt-and graphene-based conductive polymer nanocomposites by fused deposition modeling. *Applied Materials Today*, 9:21–28, 2017.

- [35] Tolga G Goktekin, Adam W Bargteil, and James F O'Brien. A method for animating viscoelastic fluids. In *ACM Transactions on Graphics (TOG)*, volume 23, pages 463–468. ACM, 2004.
- [36] YP Gong and CY Dong. An isogeometric boundary element method using adaptive integral method for 3d potential problems. *Journal of Computational and Applied Mathematics*, 319:141–158, 2017.
- [37] DD Gu, Wilhelm Meiners, Konrad Wissenbach, and Reinhart Poprawe. Laser additive manufacturing of metallic components: materials, processes and mechanisms. *International materials reviews*, 57(3):133–164, 2012.
- [38] Nannan Guo and Ming C Leu. Additive manufacturing: technology, applications and research needs. *Frontiers of Mechanical Engineering*, 8(3):215–243, 2013.
- [39] Francis H Harlow. The particle-in-cell computing method for fluid dynamics. *Methods Comput. Phys.*, 3:319–343, 1964.
- [40] Samuel H Huang, Peng Liu, Abhiram Mokasdar, and Liang Hou. Additive manufacturing and its societal impact: a literature review. *The International Journal of Advanced Manufacturing Technology*, 67(5-8):1191–1203, 2013.
- [41] Yong Huang, Ming C Leu, Jyoti Mazumder, and Alkan Donmez. Additive manufacturing: current state, future potential, gaps and needs, and recommendations. *Journal of Manufacturing Science and Engineering*, 137(1):014001, 2015.
- [42] Thomas JR Hughes, John A Cottrell, and Yuri Bazilevs. Isogeometric analysis: Cad, finite elements, nurbs, exact geometry and mesh refinement. *Computer methods in applied mechanics and engineering*, 194(39):4135–4195, 2005.
- [43] Seyeon Hwang, Edgar I Reyes, Kyoung-sik Moon, Raymond C Rumpf, and Nam Soo Kim. Thermo-mechanical characterization of metal/polymer composite filaments and printing parameter study for fused deposition modeling in the 3d printing process. *Journal of Electronic Materials*, 44(3):771–777, 2015.
- [44] Sergio R Idelsohn, Mario A Storti, and Luis A Crivelli. Numerical methods in phase-change problems. *Archives of Computational Methods in Engineering*, 1(1):49–74, 1994.
- [45] Irina Ionescu, James E Guilkey, Martin Berzins, Robert M Kirby, and Jeffrey A Weiss. Simulation of soft tissue failure using the material point method. *Journal of Biomechanical Engineering*, 128(6):917–924, 2006.
- [46] Antreas Kantaros and Dimitris Karalekas. Fiber bragg grating based investigation of residual strains in abs parts fabricated by fused deposition modeling process. *Materials & Design*, 50:44–50, 2013.

- [47] Wayne E King, Holly D Barth, Victor M Castillo, Gilbert F Gallegos, John W Gibbs, Douglas E Hahn, Chandrika Kamath, and Alexander M Rubenchik. Observation of keyhole-mode laser melting in laser powder-bed fusion additive manufacturing. *Journal of Materials Processing Technology*, 214(12):2915–2925, 2014.
- [48] Serguei Kolossov, Eric Boillat, Rémy Glardon, P Fischer, and M Locher. 3d fe simulation for temperature evolution in the selective laser sintering process. *International Journal of Machine Tools and Manufacture*, 44(2-3):117–123, 2004.
- [49] Andreas König-Haagen, Erwin Franquet, Eric Pernot, and Dieter Brüggemann. A comprehensive benchmark of fixed-grid methods for the modeling of melting. *International Journal of Thermal Sciences*, 118:69–103, 2017.
- [50] Shyamini Kularathna and Kenichi Soga. Implicit formulation of material point method for analysis of incompressible materials. *Computer Methods in Applied Mechanics and Engineering*, 313:673–686, 2017.
- [51] Krishnan Kumar and Gurunathan Saravana Kumar. An experimental and theoretical investigation of surface roughness of poly-jet printed parts: This paper explains how local surface orientation affects surface roughness in a poly-jet process. *Virtual and Physical Prototyping*, 10(1):23–34, 2015.
- [52] Fan Li, Jingzhe Pan, and Csaba Sinka. Modelling brittle impact failure of disc particles using material point method. *International Journal of Impact Engineering*, 38(7):653–660, 2011.
- [53] JG Li, Y Hamamoto, Y Liu, and X Zhang. Sloshing impact simulation with material point method and its experimental validations. *Computers & Fluids*, 103:86–99, 2014.
- [54] Yali Li and Dongdong Gu. Parametric analysis of thermal behavior during selective laser melting additive manufacturing of aluminum alloy powder. *Materials & Design*, 63:856–867, 2014.
- [55] YP Lian, X Zhang, X Zhou, S Ma, and YL Zhao. Numerical simulation of explosively driven metal by material point method. *International Journal of Impact Engineering*, 38(4):238–246, 2011.
- [56] TG Liu, BC Khoo, and KS Yeo. Ghost fluid method for strong shock impacting on material interface. *Journal of Computational Physics*, 190(2):651–681, 2003.
- [57] Xu-Dong Liu, Ronald P Fedkiw, and Myungjoo Kang. A boundary condition capturing method for poisson’s equation on irregular domains. *Journal of computational Physics*, 160(1):151–178, 2000.

- [58] Loong-Ee Loh, Chee-Kai Chua, Wai-Yee Yeong, Jie Song, Mahta Mapar, Swee-Leong Sing, Zhong-Hong Liu, and Dan-Qing Zhang. Numerical investigation and an effective modelling on the selective laser melting (slm) process with aluminium alloy 6061. *International Journal of Heat and Mass Transfer*, 80:288–300, 2015.
- [59] H Lu, NP Daphalapurkar, B Wang, S Roy, and R Komanduri. Multiscale simulation from atomistic to continuum–coupling molecular dynamics (md) with the material point method (mpm). *Philosophical Magazine*, 86(20):2971–2994, 2006.
- [60] Jun Luo, Le-Hua Qi, Xiao-Shan Jiang, Ji-Ming Zhou, and Hua Huang. Research on lateral instability of the uniform-charged droplet stream during droplet-based freeform fabrication. *International Journal of Machine Tools and Manufacture*, 48(3):289–294, 2008.
- [61] Anh-Tuan Luu, Nam-Il Kim, and Jaehong Lee. Nurbs-based isogeometric vibration analysis of generally laminated deep curved beams with variable curvature. *Composite Structures*, 119:150–165, 2015.
- [62] Thibault Ménard, Sebastien Tanguy, and Alain Berlemont. Coupling level set/vof/ghost fluid methods: Validation and application to 3d simulation of the primary break-up of a liquid jet. *International Journal of Multiphase Flow*, 33(5):510–524, 2007.
- [63] Omar A Mohamed, Syed H Masood, and Jahar L Bhowmik. Optimization of fused deposition modeling process parameters: a review of current research and future prospects. *Advances in Manufacturing*, 3(1):42–53, 2015.
- [64] Jochen Mueller, Kristina Shea, and Chiara Daraio. Mechanical properties of parts fabricated with inkjet 3d printing through efficient experimental design. *Materials & Design*, 86:902–912, 2015.
- [65] John A Nairn. Numerical simulation of orthogonal cutting using the material point method. *Engineering Fracture Mechanics*, 149:262–275, 2015.
- [66] Vinh Phu Nguyen, Chi Thanh Nguyen, Timon Rabczuk, and Sundararajan Natarajan. On a family of convected particle domain interpolations in the material point method. *Finite Elements in Analysis and Design*, 126:50–64, 2017.
- [67] Vinh Phu Nguyen and Cardiff University. Material point method: basics and applications, 2014.
- [68] M Nikzad, SH Masood, and I Sbarski. Thermo-mechanical properties of a highly filled polymeric composites for fused deposition modeling. *Materials & Design*, 32(6):3448–3456, 2011.

- [69] M Orme and C Huang. Phase change manipulation for droplet-based solid freeform fabrication. *TRANSACTIONS-AMERICAN SOCIETY OF MECHANICAL ENGINEERS JOURNAL OF HEAT TRANSFER*, 119:818–823, 1997.
- [70] Stanley Osher and James A Sethian. Fronts propagating with curvature-dependent speed: algorithms based on hamilton-jacobi formulations. *Journal of computational physics*, 79(1):12–49, 1988.
- [71] Tim A Osswald, John Puentes, and Julian Kattinger. Fused filament fabrication melting model. *Additive Manufacturing*, 22:51–59, 2018.
- [72] Anhua Peng, Xingming Xiao, and Rui Yue. Process parameter optimization for fused deposition modeling using response surface methodology combined with fuzzy inference system. *The International Journal of Advanced Manufacturing Technology*, 73(1-4):87–100, 2014.
- [73] Les Piegl and Wayne Tiller. *The NURBS book*. Springer, 1995.
- [74] Costas Politis, Alexandros I Ginnis, Panagiotis D Kaklis, Kostas Belibassakis, and Christian Feurer. An isogeometric bem for exterior potential-flow problems in the plane. In *2009 SIAM/ACM Joint Conference on Geometric and Physical Modeling*, pages 349–354. ACM, 2009.
- [75] Le-hua Qi, Song-yi Zhong, Jun Luo, Dai-cong Zhang, and Han-song Zuo. Quantitative characterization and influence of parameters on surface topography in metal micro-droplet deposition manufacture. *International Journal of Machine Tools and Manufacture*, 88:206–213, 2015.
- [76] Daniel Ram, Theodore Gast, Chenfanfu Jiang, Craig Schroeder, Alexey Stomakhin, Joseph Teran, and Pirouz Kavehpour. A material point method for viscoelastic fluids, foams and sponges. In *Proceedings of the 14th ACM SIGGRAPH/Eurographics Symposium on Computer Animation*, pages 157–163. ACM, 2015.
- [77] MR Karamooz Ravari, M Kadkhodaei, M Badrossamay, and R Rezaei. Numerical investigation on mechanical properties of cellular lattice structures fabricated by fused deposition modeling. *International Journal of Mechanical Sciences*, 88:154–161, 2014.
- [78] David F Rogers. *An introduction to NURBS: with historical perspective*. Elsevier, 2000.
- [79] Giovanni Russo and Peter Smereka. A remark on computing distance functions. *Journal of Computational Physics*, 163(1):51–67, 2000.
- [80] A Sadeghirad, Rebecca M Brannon, and J Burghardt. A convected particle domain interpolation technique to extend applicability of the material point method for problems involving massive deformations. *International Journal for Numerical Methods in Engineering*, 86(12):1435–1456, 2011.

- [81] A Sadeghirad, Rebecca M Brannon, and JE Guilkey. Second-order convected particle domain interpolation (cpdi2) with enrichment for weak discontinuities at material interfaces. *International Journal for numerical methods in Engineering*, 95(11):928–952, 2013.
- [82] HL Schreyer, DL Sulsky, and S-J Zhou. Modeling delamination as a strong discontinuity with the material point method. *Computer Methods in Applied Mechanics and Engineering*, 191(23-24):2483–2507, 2002.
- [83] Fei Shen, Shangqin Yuan, Chee Kai Chua, and Kun Zhou. Development of process efficiency maps for selective laser sintering of polymeric composite powders: Modeling and experimental testing. *Journal of Materials Processing Technology*, 254:52–59, 2018.
- [84] Seyed Farid Seyed Shirazi, Samira Gharehkhani, Mehdi Mehrali, Hooman Yarmand, Hendrik Simon Cornelis Metselaar, Nahrizul Adib Kadri, and Noor Azuan Abu Osman. A review on powder-based additive manufacturing for tissue engineering: selective laser sintering and inkjet 3d printing. *Science and Technology of Advanced Materials*, 16(3):033502, 2015.
- [85] S Shojaee, E Izadpanah, N Valizadeh, and J Kiendl. Free vibration analysis of thin plates by using a nurbs-based isogeometric approach. *Finite Elements in Analysis and Design*, 61:23–34, 2012.
- [86] Juan C Simo and Thomas JR Hughes. *Computational inelasticity*, volume 7. Springer Science & Business Media, 2006.
- [87] Robert N Simpson, Stéphane PA Bordas, Jon Trevelyan, and Timon Rabczuk. A two-dimensional isogeometric boundary element method for elastostatic analysis. *Computer Methods in Applied Mechanics and Engineering*, 209:87–100, 2012.
- [88] Sunpreet Singh, Seeram Ramakrishna, and Rupinder Singh. Material issues in additive manufacturing: A review. *Journal of Manufacturing Processes*, 25:185–200, 2017.
- [89] ASTM Standard. F2792. 2012. standard terminology for additive manufacturing technologies. *ASTM F2792-10e1*, 2012.
- [90] Alexey Stomakhin, Craig Schroeder, Lawrence Chai, Joseph Teran, and Andrew Selle. A material point method for snow simulation. *ACM Transactions on Graphics (TOG)*, 32(4):102, 2013.
- [91] Alexey Stomakhin, Craig Schroeder, Chenfanfu Jiang, Lawrence Chai, Joseph Teran, and Andrew Selle. Augmented mpm for phase-change and varied materials. *ACM Transactions on Graphics (TOG)*, 33(4):138, 2014.
- [92] D Sulsky and A Kaul. Implicit dynamics in the material-point method. *Computer Methods in Applied Mechanics and Engineering*, 193(12-14):1137–1170, 2004.

- [93] Deborah Sulsky, Zhen Chen, and Howard L Schreyer. A particle method for history-dependent materials. *Computer methods in applied mechanics and engineering*, 118(1-2):179–196, 1994.
- [94] Deborah Sulsky and Howard L Schreyer. Axisymmetric form of the material point method with applications to upsetting and taylor impact problems. *Computer Methods in Applied Mechanics and Engineering*, 139(1-4):409–429, 1996.
- [95] Deborah Sulsky, Shi-Jian Zhou, and Howard L Schreyer. Application of a particle-in-cell method to solid mechanics. *Computer physics communications*, 87(1-2):236–252, 1995.
- [96] Mark Sussman, Peter Smereka, and Stanley Osher. A level set approach for computing solutions to incompressible two-phase flow. *Journal of Computational physics*, 114(1):146–159, 1994.
- [97] Toru Takahashi and Toshiro Matsumoto. An application of fast multipole method to isogeometric boundary element method for laplace equation in two dimensions. *Engineering Analysis with Boundary Elements*, 36(12):1766–1775, 2012.
- [98] C Tang, JL Tan, and CH Wong. A numerical investigation on the physical mechanisms of single track defects in selective laser melting. *International Journal of Heat and Mass Transfer*, 126:957–968, 2018.
- [99] I Temizer, P Wriggers, and TJR Hughes. Contact treatment in isogeometric analysis with nurbs. *Computer Methods in Applied Mechanics and Engineering*, 200(9):1100–1112, 2011.
- [100] Hiroshi Terashima and Grétar Tryggvason. A front-tracking/ghost-fluid method for fluid interfaces in compressible flows. *Journal of Computational Physics*, 228(11):4012–4037, 2009.
- [101] Chien H Thai, H Nguyen-Xuan, N Nguyen-Thanh, T-H Le, T Nguyen-Thoi, and Timon Rabczuk. Static, free vibration, and buckling analysis of laminated composite reissner–mindlin plates using nurbs-based isogeometric approach. *International Journal for Numerical Methods in Engineering*, 91(6):571–603, 2012.
- [102] A Tiwari and SP Vanka. A ghost fluid lattice boltzmann method for complex geometries. *International Journal for Numerical Methods in Fluids*, 69(2):481–498, 2012.
- [103] Nahum Travitzky, Alexander Bonet, Benjamin Dermeik, Tobias Fey, Ina Filbert-Demut, Lorenz Schlier, Tobias Schlordt, and Peter Greil. Additive manufacturing of ceramic-based materials. *Advanced Engineering Materials*, 16(6):729–754, 2014.

- [104] Mohammad Vaezi, Srisit Chianrabutra, Brian Mellor, and Shoufeng Yang. Multiple material additive manufacturing—part 1: a review: this review paper covers a decade of research on multiple material additive manufacturing technologies which can produce complex geometry parts with different materials. *Virtual and Physical Prototyping*, 8(1):19–50, 2013.
- [105] Mohammad Vaezi, Hermann Seitz, and Shoufeng Yang. A review on 3d micro-additive manufacturing technologies. *The International Journal of Advanced Manufacturing Technology*, 67(5-8):1721–1754, 2013.
- [106] Dongdong Wang, Wei Liu, and Hanjie Zhang. Superconvergent isogeometric free vibration analysis of euler–bernoulli beams and kirchhoff plates with new higher order mass matrices. *Computer Methods in Applied Mechanics and Engineering*, 286:230–267, 2015.
- [107] Xin Wang, Man Jiang, Zuowan Zhou, Jihua Gou, and David Hui. 3d printing of polymer matrix composites: A review and prospective. *Composites Part B: Engineering*, 110:442–458, 2017.
- [108] Zdzislaw Wikeckowski. The material point method in large strain engineering problems. *Computer methods in applied mechanics and engineering*, 193(39-41):4417–4438, 2004.
- [109] Jiaojiao Wu, Linzhi Wang, and Xuguang An. Numerical analysis of residual stress evolution of als10mg manufactured by selective laser melting. *Optik-International Journal for Light and Electron Optics*, 137:65–78, 2017.
- [110] Yu-Che Wu, Cheng-Hung San, Chih-Hsiang Chang, Huey-Juan Lin, Raed Marwan, Shuhei Baba, and Weng-Sing Hwang. Numerical modeling of melt-pool behavior in selective laser melting with random powder distribution and experimental validation. *Journal of Materials Processing Technology*, 254:72–78, 2018.
- [111] Huanxiong Xia, Jiakai Lu, Sadegh Dabiri, and Gretar Tryggvason. Fully resolved numerical simulations of fused deposition modeling. part i-fluid flow. *arXiv preprint arXiv:1711.05940*, 2017.
- [112] Huanxiong Xia, Jiakai Lu, and Gretar Tryggvason. Fully resolved numerical simulations of fused deposition modeling. part ii-solidification, residual stresses, and modeling of the nozzle. *arXiv preprint arXiv:1711.07094*, 2017.
- [113] Liping Xue, Oleg Borodin, Grant D Smith, and John Nairn. Micromechanics simulations of the viscoelastic properties of highly filled composites by the material point method (mpm). *Modelling and Simulation in Materials Science and Engineering*, 14(4):703, 2006.

- [114] Mengxue Yan, Xiaoyong Tian, Gang Peng, Dichen Li, and Xiaoyu Zhang. High temperature rheological behavior and sintering kinetics of cf/peek composites during selective laser sintering. *Composites Science and Technology*, 165:140–147, 2018.
- [115] Hongyi Yang, Jingying Charlotte Lim, Yuchan Liu, Xiaoying Qi, Yee Ling Yap, Vishwesh Dikshit, Wai Yee Yeong, and Jun Wei. Performance evaluation of projet multi-material jetting 3d printer. *Virtual and Physical Prototyping*, 12(1):95–103, 2017.
- [116] Youqing Yang, Pengtao Sun, and Zhen Chen. Combined mpm-dem for simulating the interaction between solid elements and fluid particles. *Communications in Computational Physics*, 21(5):1258–1281, 2017.
- [117] Yee Ling Yap, Chengcheng Wang, Swee Leong Sing, Vishwesh Dikshit, Wai Yee Yeong, and Jun Wei. Material jetting additive manufacturing: An experimental study using designed metrological benchmarks. *Precision Engineering*, 2017.
- [118] Minh Yoon and Seonho Cho. Isogeometric shape design sensitivity analysis of elasticity problems using boundary integral equations. *Engineering Analysis with Boundary Elements*, 66:119–128, 2016.
- [119] Allen R York, Deborah Sulsky, and Howard L Schreyer. Fluid–membrane interaction based on the material point method. *International Journal for Numerical Methods in Engineering*, 48(6):901–924, 2000.
- [120] Pengpeng Yuan and Dongdong Gu. Molten pool behaviour and its physical mechanism during selective laser melting of tic/alsi10mg nanocomposites: simulation and experiments. *Journal of Physics D: Applied Physics*, 48(3):035303, 2015.
- [121] Yonghao Yue, Breannan Smith, Christopher Batty, Changxi Zheng, and Eitan Grinspun. Continuum foam: A material point method for shear-dependent flows. *ACM Transactions on Graphics (TOG)*, 34(5):160, 2015.
- [122] Michael F Zaeh and Gregor Branner. Investigations on residual stresses and deformations in selective laser melting. *Production Engineering*, 4(1):35–45, 2010.
- [123] Duan Z Zhang, Qisu Zou, W Brian VanderHeyden, and Xia Ma. Material point method applied to multiphase flows. *Journal of Computational Physics*, 227(6):3159–3173, 2008.
- [124] Fan Zhang, Xiong Zhang, and Yan Liu. An augmented incompressible material point method for modeling liquid sloshing problems. *International Journal of Mechanics and Materials in Design*, 14(1):141–155, 2018.
- [125] Fan Zhang, Xiong Zhang, Kam Yim Sze, Yanping Lian, and Yan Liu. Incompressible material point method for free surface flow. *Journal of Computational Physics*, 330:92–110, 2017.

- [126] HW Zhang, KP Wang, and Z Chen. Material point method for dynamic analysis of saturated porous media under external contact/impact of solid bodies. *Computer methods in applied mechanics and engineering*, 198(17-20):1456–1472, 2009.
- [127] Wei Zhang, Chase Cotton, Jessica Sun, Dirk Heider, Bohong Gu, Baozhong Sun, and Tsu-Wei Chou. Interfacial bonding strength of short carbon fiber/acrylonitrile-butadiene-styrene composites fabricated by fused deposition modeling. *Composites Part B: Engineering*, 137:51–59, 2018.
- [128] Xiong Zhang, Zhen Chen, and Yan Liu. *The material point method: a continuum-based particle method for extreme loading cases*. Academic Press, 2016.
- [129] Y Zhang and K Chou. A parametric study of part distortions in fused deposition modelling using three-dimensional finite element analysis. *Proceedings of the Institution of Mechanical Engineers, Part B: Journal of Engineering Manufacture*, 222(8):959–968, 2008.
- [130] Y Zhang and YK Chou. Three-dimensional finite element analysis simulations of the fused deposition modelling process. *Proceedings of the Institution of Mechanical Engineers, Part B: Journal of Engineering Manufacture*, 220(10):1663–1671, 2006.
- [131] Yongjie Zhang, Yuri Bazilevs, Samrat Goswami, Chandrajit L Bajaj, and Thomas JR Hughes. Patient-specific vascular nurbs modeling for isogeometric analysis of blood flow. *Computer methods in applied mechanics and engineering*, 196(29):2943–2959, 2007.
- [132] Gang Zhao, Xiaoxiao Du, Wei Wang, Bo Liu, and Hongbing Fang. Application of isogeometric method to free vibration of reissner–mindlin plates with non-conforming multi-patch. *Computer-Aided Design*, 82:127–139, 2017.

Appendix A

Parameter Study Results

A.1 Nozzle velocity variation study

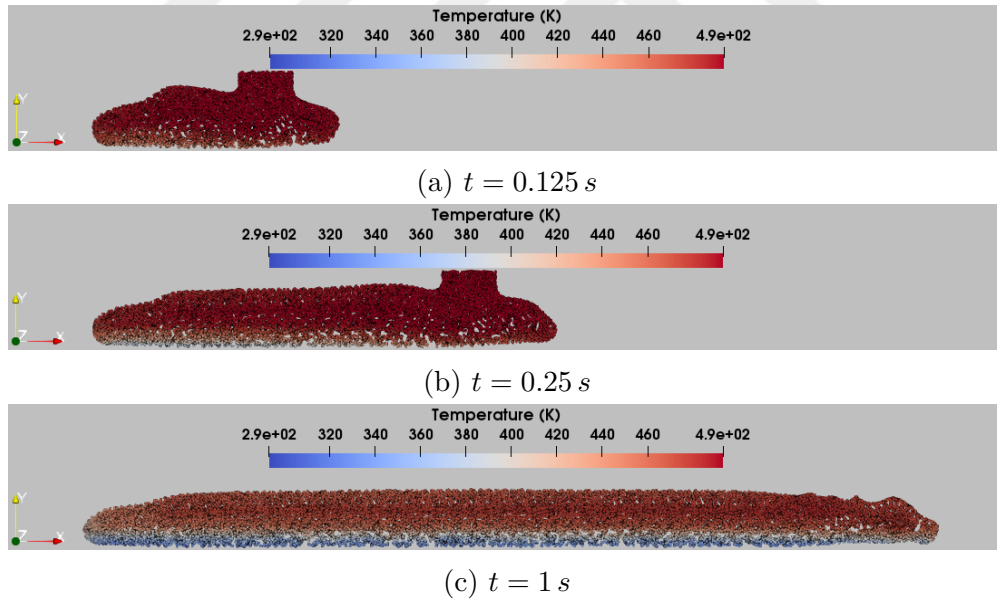
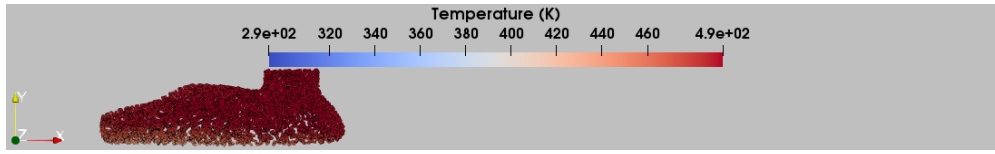
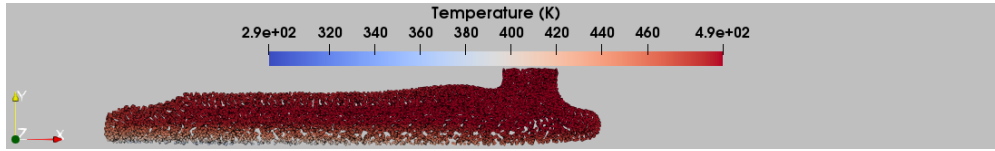
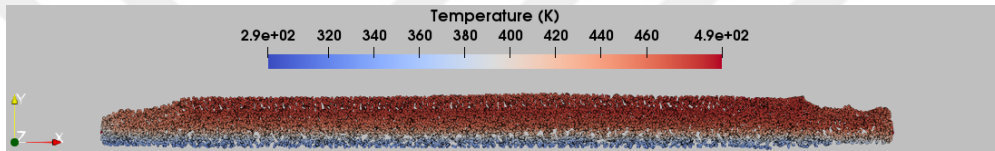
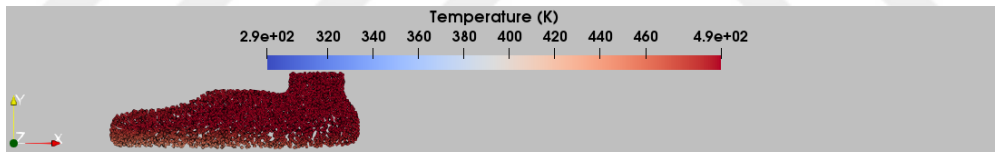
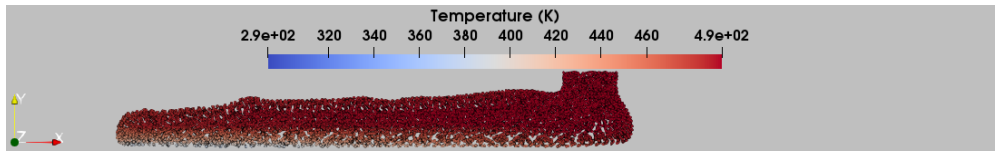
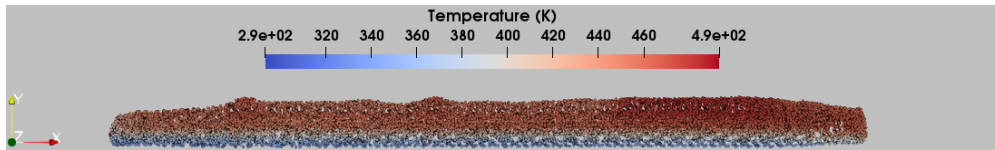
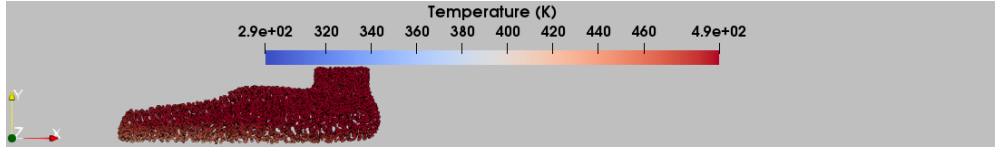
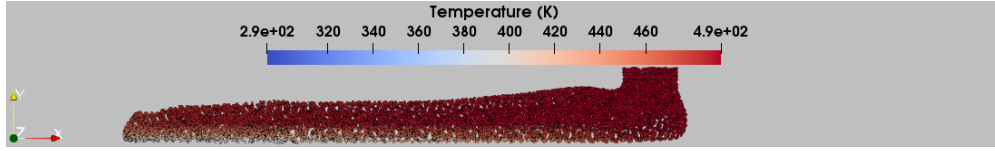
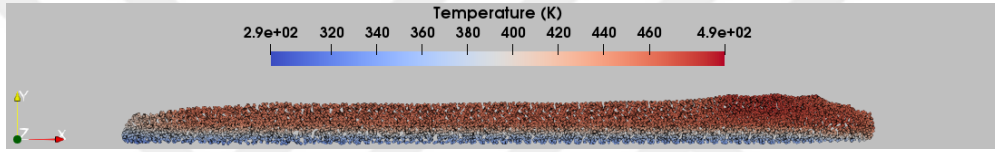
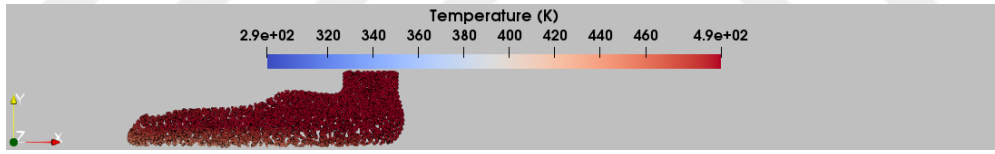
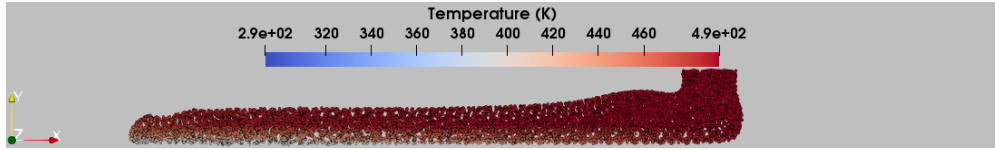
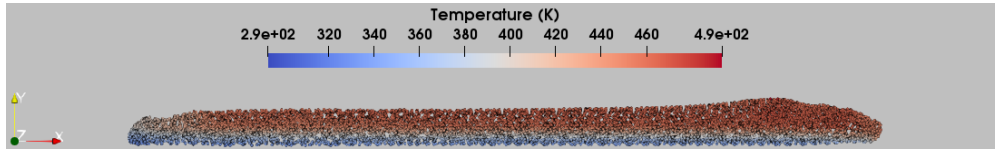
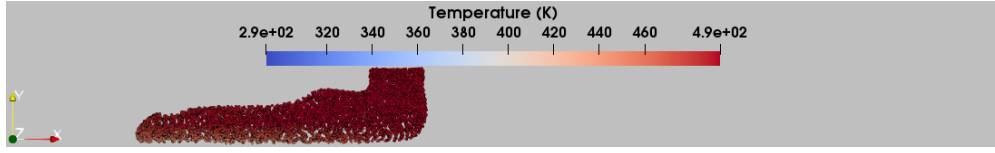
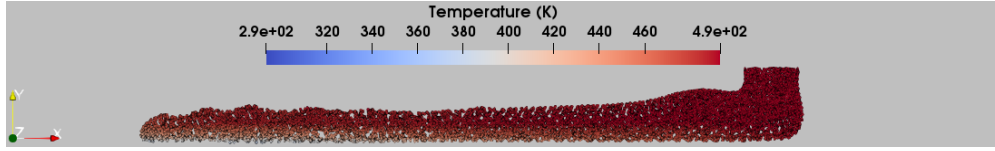
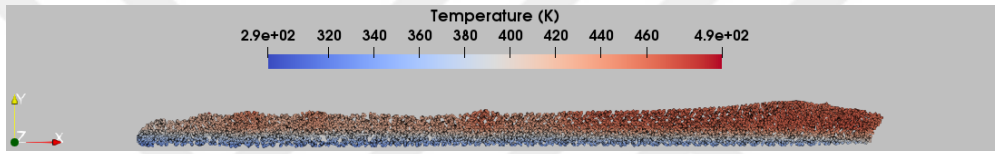
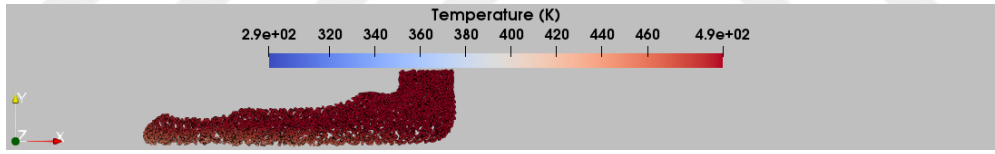
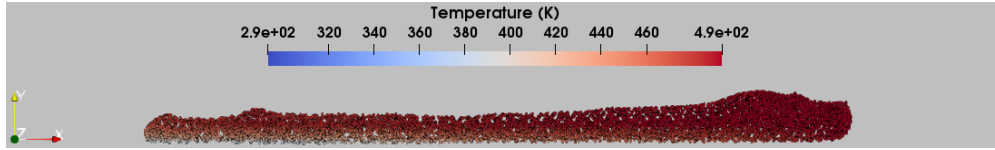
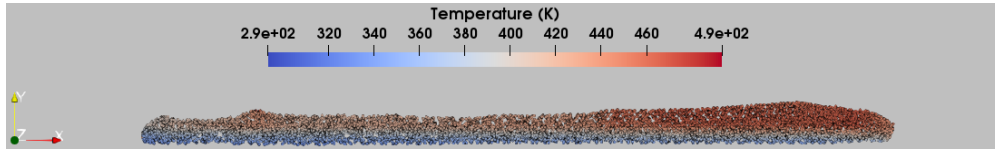


Figure A.1: Extrusion process for $v_N = 12 \text{ mm/s}$

(a) $t = 0.125 \text{ s}$ (b) $t = 0.25 \text{ s}$ (c) $t = 1 \text{ s}$ Figure A.2: Extrusion process for $v_N = 14 \text{ mm/s}$ (a) $t = 0.125 \text{ s}$ (b) $t = 0.25 \text{ s}$ (c) $t = 1 \text{ s}$ Figure A.3: Extrusion process for $v_N = 16 \text{ mm/s}$

(a) $t = 0.125 \text{ s}$ (b) $t = 0.25 \text{ s}$ (c) $t = 1 \text{ s}$ Figure A.4: Extrusion process for $v_N = 18 \text{ mm/s}$ (a) $t = 0.125 \text{ s}$ (b) $t = 0.25 \text{ s}$ (c) $t = 1 \text{ s}$ Figure A.5: Extrusion process for $v_N = 20 \text{ mm/s}$

(a) $t = 0.125 \text{ s}$ (b) $t = 0.25 \text{ s}$ (c) $t = 1 \text{ s}$ Figure A.6: Extrusion process for $v_N = 22 \text{ mm/s}$ (a) $t = 0.125 \text{ s}$ (b) $t = 0.25 \text{ s}$ (c) $t = 1 \text{ s}$ Figure A.7: Extrusion process for $v_N = 24 \text{ mm/s}$

A.2 Nozzle gap variation study

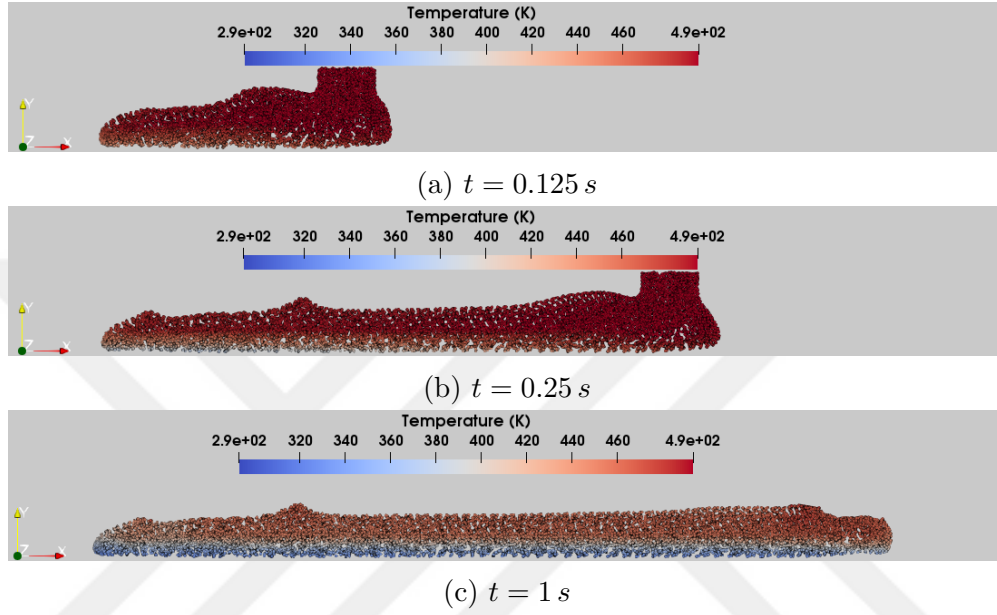


Figure A.8: Extrusion process for $h_N/D_N = 0.9$

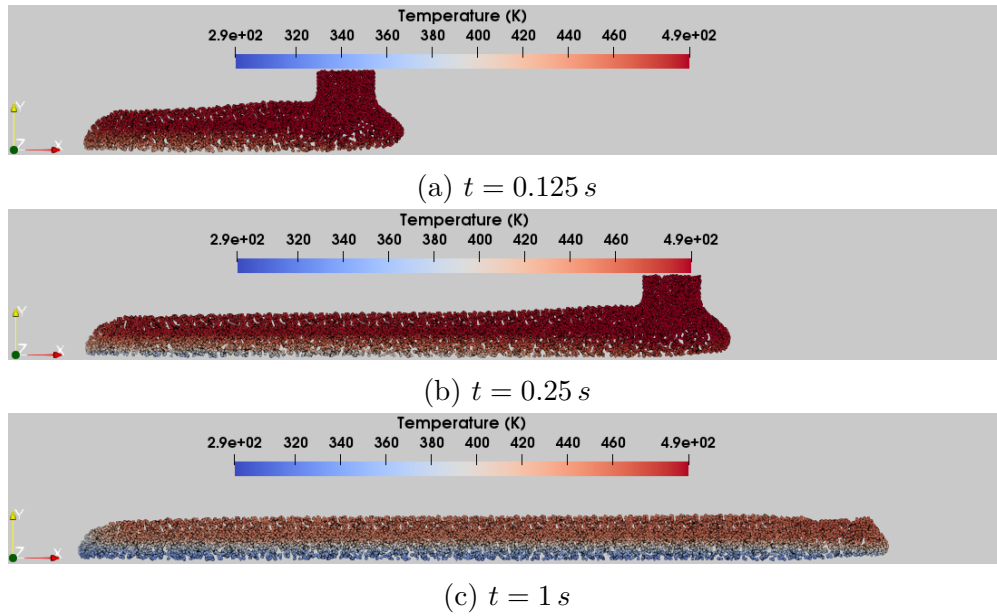
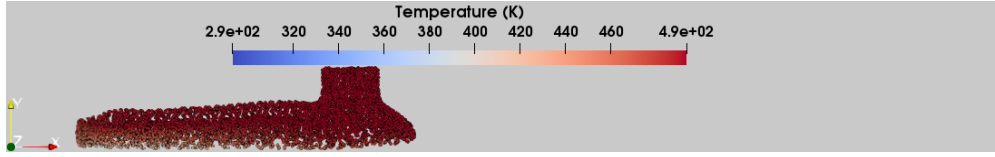
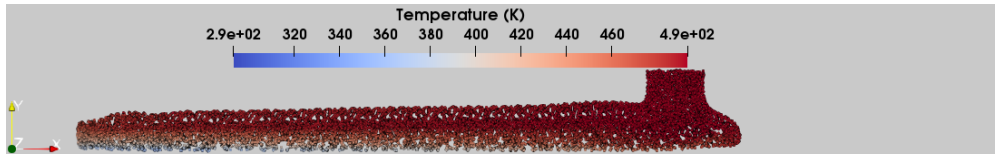
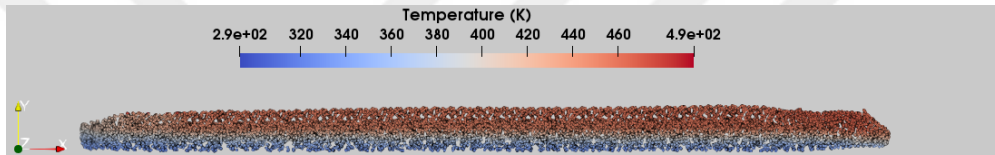
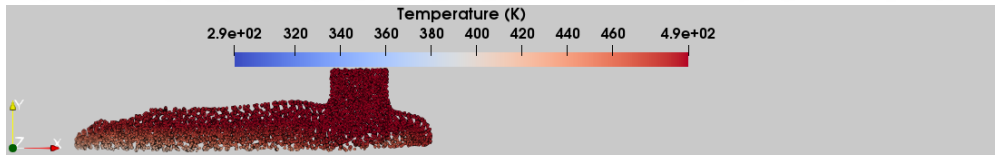
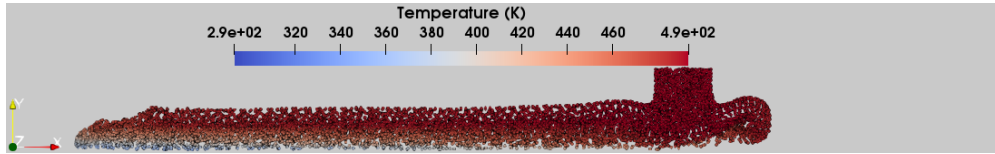
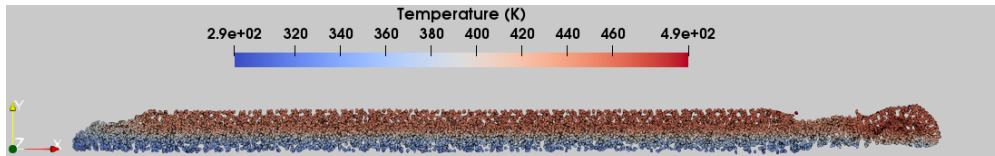


Figure A.9: Extrusion process for $h_N/D_N = 0.8$

(a) $t = 0.125 \text{ s}$ (b) $t = 0.25 \text{ s}$ (c) $t = 1 \text{ s}$ Figure A.10: Extrusion process for $h_N/D_N = 0.7$ (a) $t = 0.125 \text{ s}$ (b) $t = 0.25 \text{ s}$ (c) $t = 1 \text{ s}$ Figure A.11: Extrusion process for $h_N/D_N = 0.6$

A.3 Cooling rate variation study

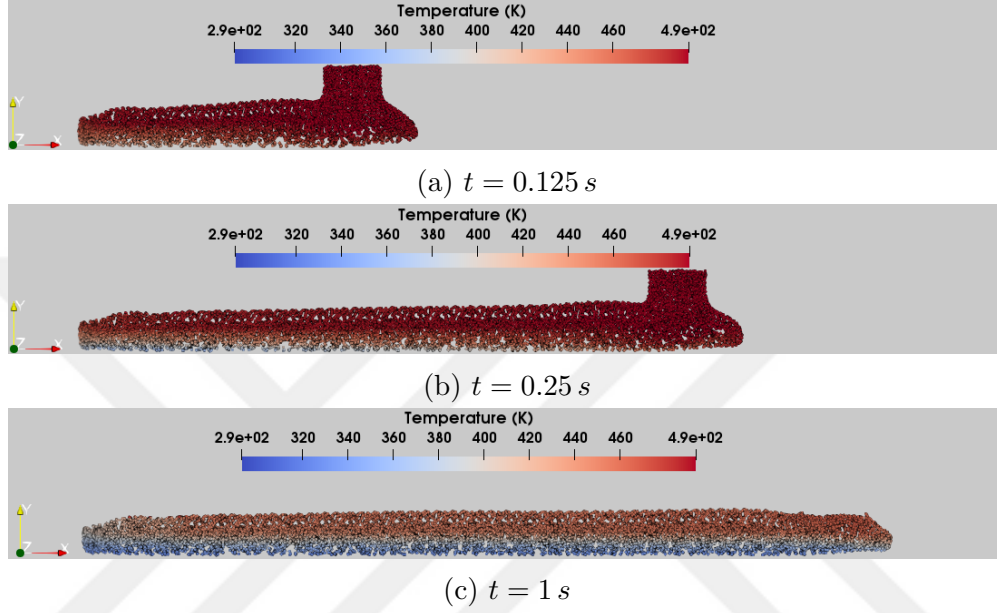


Figure A.12: Extrusion process for $h_{air} = 100 \text{ W}/(\text{m}^2 \cdot \text{K})$

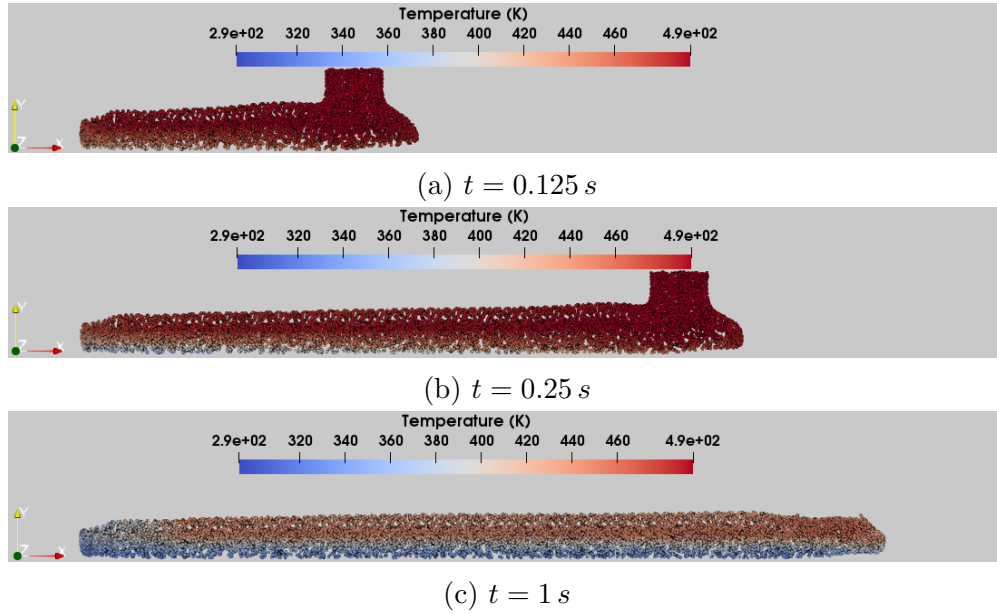
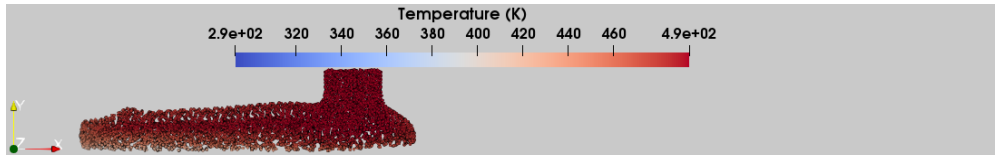
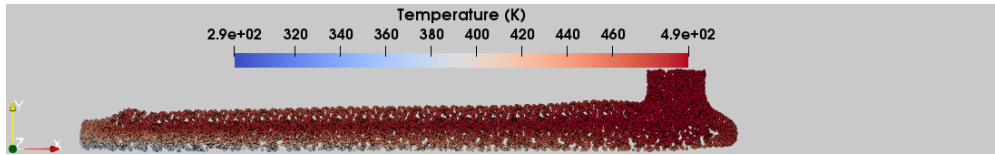
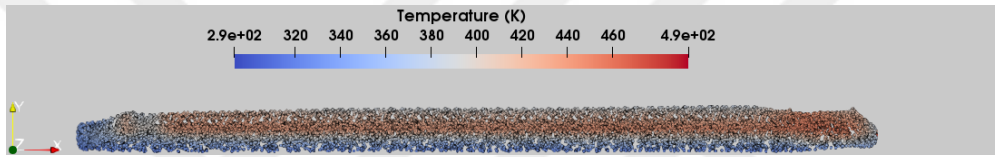
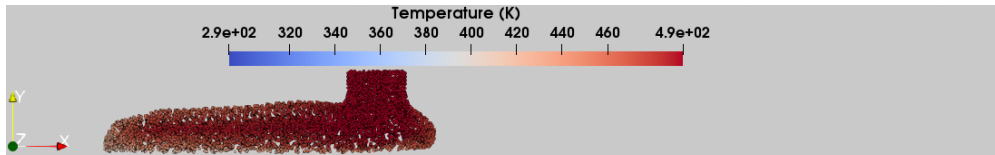
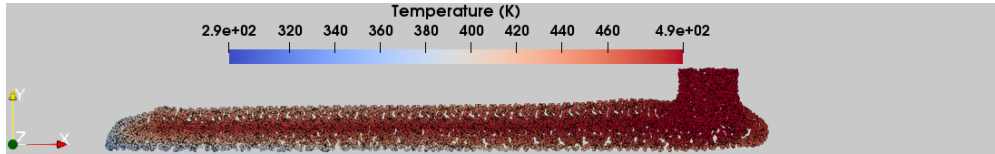
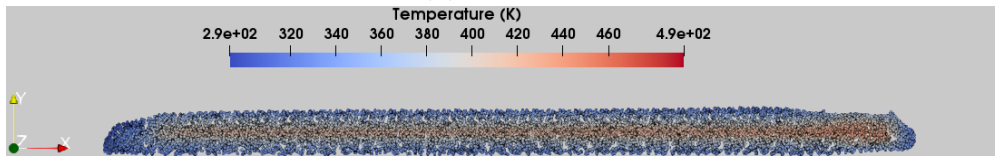
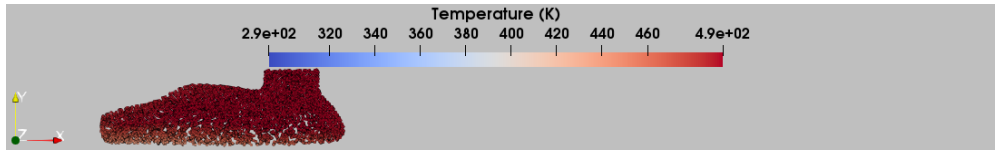
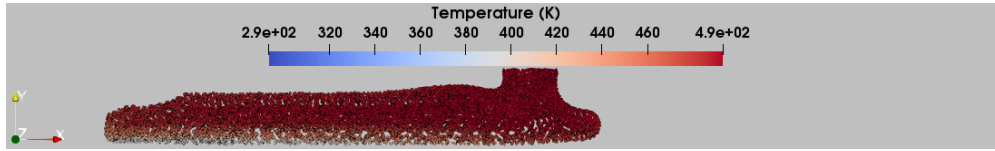
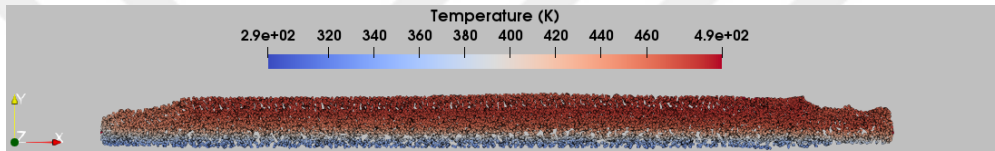
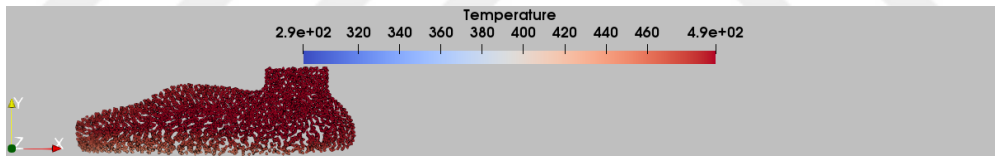
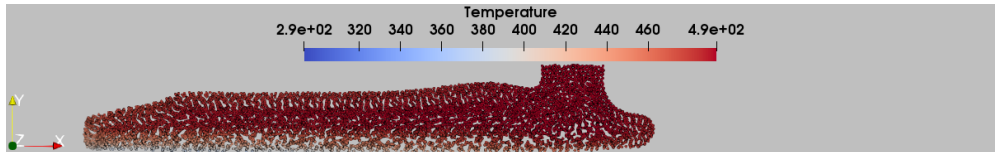
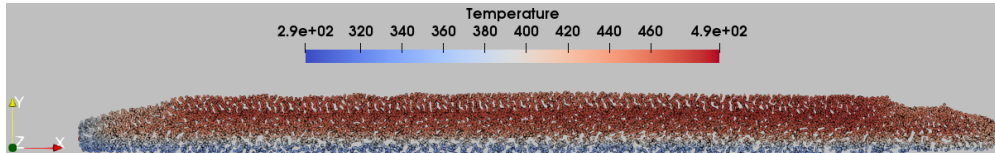
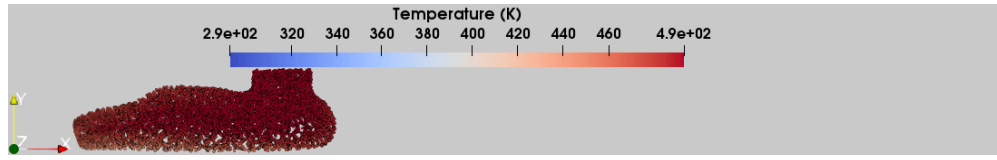
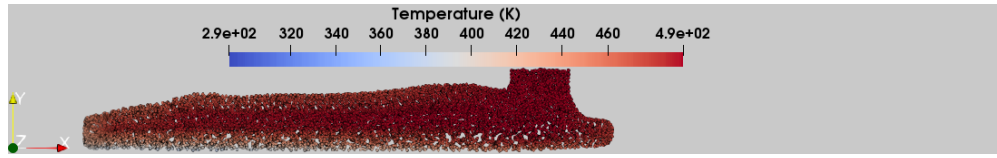
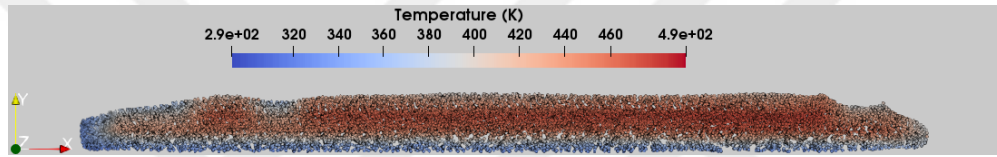
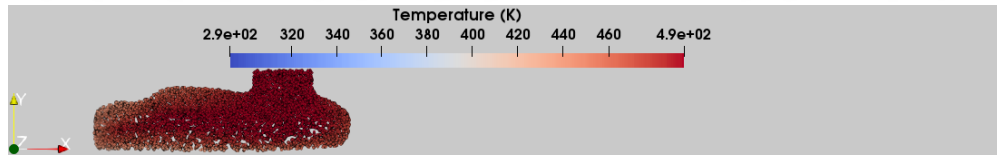
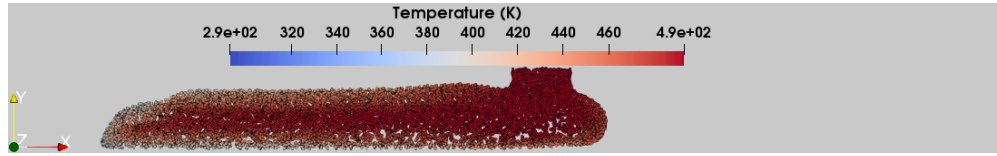
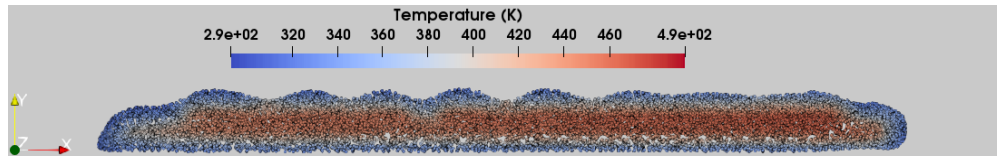


Figure A.13: Extrusion process for $h_{air} = 200 \text{ W}/(\text{m}^2 \cdot \text{K})$

(a) $t = 0.125 \text{ s}$ (b) $t = 0.25 \text{ s}$ (c) $t = 1 \text{ s}$ Figure A.14: Extrusion process for $h_{air} = 400 \text{ W}/(\text{m}^2 \cdot \text{K})$ (a) $t = 0.125 \text{ s}$ (b) $t = 0.25 \text{ s}$ (c) $t = 1 \text{ s}$ Figure A.15: Extrusion process for $h_{air} = 1000 \text{ W}/(\text{m}^2 \cdot \text{K})$

(a) $t = 0.125 \text{ s}$ (b) $t = 0.25 \text{ s}$ (c) $t = 1 \text{ s}$ Figure A.16: Extrusion process for $h_{air} = 100 \text{ W}/(\text{m}^2 \cdot \text{K})$ (a) $t = 0.125 \text{ s}$ (b) $t = 0.25 \text{ s}$ (c) $t = 1 \text{ s}$ Figure A.17: Extrusion process for $h_{air} = 200 \text{ W}/(\text{m}^2 \cdot \text{K})$

(a) $t = 0.125 \text{ s}$ (b) $t = 0.25 \text{ s}$ (c) $t = 1 \text{ s}$ Figure A.18: Extrusion process for $h_{air} = 400 \text{ W}/(\text{m}^2 \cdot \text{K})$ (a) $t = 0.125 \text{ s}$ (b) $t = 0.25 \text{ s}$ (c) $t = 1 \text{ s}$ Figure A.19: Extrusion process for $h_{air} = 1000 \text{ W}/(\text{m}^2 \cdot \text{K})$