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Unified simulation of melt flow and solidification processes using a Smoothed Particle Hydrodynamics based method with a thermoplastic-viscous-elastic material model

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Abstract

The numerical simulation of manufacturing processes involving molten materials requires an accurate description of melt flow, phase transitions, and the resulting geometry during solidification and cooling. The Smoothed Particle Hydrodynamics (SPH) method has proven to be a promising approach for such problems, particularly when strong deformations and topological changes of the melt occur. As a mesh-free Lagrangian method, SPH allows a natural representation of free surfaces and evolving geometries.

However, the accurate modeling of density changes during solidification remains a major challenge, since these changes strongly influence the final geometry and the thermomechanical stresses developing during cooling.

To address this problem, we propose an extension of the SPH approach by integrating a thermoplastic-viscous-elastic material model. This unified formulation enables the consistent description of both liquid metal behavior and temperature-dependent thermomechanical properties, allowing the simulation of melt flow and solidification processes within a single framework.

Keywords

process simulation, smoothed particle hydrodynamics, welding, solidification, volume contraction

1 Introduction

Welding and casting processes are heavily influenced by the thermal effects at play. For reliably assuring the quality of the process products, it is essential to understand and being able to control the complex thermomechanical phenomena. During the process, the material undergoes several phase changes, from solidified to half-solidified to liquid and back. Thus, the whole process

encompasses a multi-physics problem in which every part influences the others. One approach for the process simulation is to use dedicated methods for every state of matter and transfer the information from one method to the next. While this approach ensures, that every phase is simulated with a well-suited method, the mapping between these methods may introduce errors into the simulation chain. Additionally, capturing the interaction between different phases may require the use of surrogate models. Thus, it is advantageous to capture the whole simulation process with a single model. This approach eliminates the need for mapping and surrogate models as long as the unified simulation method is able to capture all simulation effects.

For welding and casting applications, the accurate depiction of several different phenomena is required. These include the phase change during melting and solidification, the free-surface flow of the molten material and the mechanical stresses arising during solidification and cooling. Additionally, all processes are governed by the heat transfer and its accompanying effects on the materials. The goal of this publication is to outline a unified simulation framework for the whole process of welding and casting.

The simulation framework is based on the Smoothed Particle Hydrodynamics (SPH) method. Traditionally, grid-based or mesh-based approaches have been employed [1-3]. For the whole process simulation chain, the requirements for handling strongly deforming melt pools, droplet impact and fragmentation as well as strongly deforming volumes, these methods require additional effort for the accurate depiction. SPH as a meshless, Lagrangian method natively handles strongly changing topologies and thus is well-suited.

This work proposes a unified, SPH-based framework for welding and casting processes. This includes the simulation of the melt-pool dynamics consisting of the interplay between pressure, viscosity, surface tension and temperature flow. First results capturing gas metal arc welding and thermal spraying processes will be shown and discussed. This method will be extended by the volume contraction happening in fluid and solid phases alike through the temperature dependent material density. Finally, further developments will be shown towards a unified SPH model for fluid and solid states.

2 Aim of the Investigation

The goal of this work is to present a unified, SPH-based framework for welding and casting processes. In the following the advantages of this Lagrangian, mesh-less method will be outlined and discussed. Further, the newly created method will be thoroughly analyzed in theoretical and practical use cases. The authors envision a full process simulation method using SPH as the main discretization method, that is able to capture melting, melt pool dynamics, solidification, internal stresses and deformation during cooling.

3 Materials and Experimental Details

3.1 Smoothed Particle Hydrodynamics

Smoothed Particle Hydrodynamics (SPH) [4, 5] is a meshless, Lagrangian simulation method. In detail, the SPH discretization works by sampling the simulation domain with mass points called particles. These points aggregate the surrounding mass, represent the local volume, and carry additional quantities like the density or temperature. As a Lagrangian method, the particles are advected with the fluid flow.

These properties allow SPH as a method to be well suited for the natural treatment of free surface flows. As a meshless method, large deformations and topological changes as in the droplet formation of the melting welding wire are natively supported. Furthermore, SPH allows for a unified and flexible treatment of the underlying multi-physics problem.

The core idea of SPH is that, in theory, given infinitely many sampling points, the particle discretization represents the continuum. With a finite number of particles, any field quantity A at position $\mathbf{x}$ can be calculated using the SPH interpolation using the surrounding particles j:

$$A(\mathbf{x}) \approx \sum_j \frac{m_j}{\rho_j} A(\mathbf{x}_j) W(\mathbf{x} - \mathbf{x}_j, \hbar),$$

where m is the particle's mass, ρ_j the density and $W(\mathbf{x} - \mathbf{x}_j, \hbar)$ the kernel function. The latter is a compactly supported, Gaussian-like scalar function which weighs the contribution of a particle dependent on their distance. The second argument $\hbar$, the smoothing length, influences the steepness of the Gaussian-like shape of the kernel function. A common assumption is to couple the smoothing length to the compact support radius $\tilde{h}$ and the particle radius R. In the following, properties are computed on the particles themselves. There, the abbreviations $A_i = A(\mathbf{x}_i)$, $W_{ij} = W(\mathbf{x} - \mathbf{x}_j, h)$ will be used for example for the computation on particle i. Further, all neighboring particles which have a non-zero contribution will be denoted as the neighborhood $\mathcal{N}_i$. For further details, the reader is referred to the works of Koschier et al. [6, 7] and Price [8].

SPH is commonly used to solve the momentum equation, that is:

$$\rho \frac{D\mathbf{v}}{Dt} = \nabla \cdot \sigma + \mathbf{f}_{\text{ext}},$$

where $\mathbf{v}$ denotes the velocity, $\mathbf{f}_{\text{ext}}$ external forces and σ the stress tensor. For the simulation of incompressible fluids, the suitable stress tensor leads to the well-known Navier Stokes equations:

$$\frac{D\rho}{Dt} + \rho \nabla \cdot \mathbf{v} = 0$$
$$\rho \frac{D\mathbf{v}}{Dt} = -\nabla p + \mu \nabla^2 \mathbf{v} + \mathbf{f}_{\text{st}} + \mathbf{f}_{\text{ext}},$$

where p denotes the pressure, μ the dynamic viscosity and $\mathbf{f}_{\mathrm{st}}$ the surface tension force. A common strategy for solving the momentum equation with SPH is operator splitting [7]. With it, non-pressure forces are solved with their own system before the pressure is being solved to comply with the incompressibility condition of the continuity equation. This allows each contributing force to have its own dedicated solver, improving the flexibility of the framework.

3.2 Simulation Framework

For the full process simulation, the framework must support the simulation of solids, liquids and temperature propagation. Concerning the depiction of the melt pool dynamics, the authors rely on the works of Bender et al. [9, 10] for solving pressure forces, Weiler et al. [11] for viscosity and Jeske et al. [12] for surface tension. These methods have been altered to fit the needs of the process simulation, most notably by the inclusion of temperature dependent parameters. That is, both the viscosity and surface tension method have been modified to accommodate spatially and time varying parameters, $\mu\big(T(x,t)\big)$ and $\sigma\big(T(x,t)\big)$ respectively. These are read from temperature dependent tables during the simulation.

The temperature is being calculated by solving Fourier's equation:

$$\frac{D\left(\rho c_p T\right)}{Dt} = \nabla \cdot (\lambda \nabla T) + \dot{q}''',$$

where T denotes the temperature, c_p the specific heat capacity, λ the thermal conductivity and $\dot{q}'''$ the contribution from volumetric heat sources. This equation is solved based on the work of Jeske et al. [13] by discretizing the left hand side of the equation in time and the right hand side with SPH while changing the parameter of interest from temperature to the specific enthalpy. Following the authors derivation, the next specific enthalpy is being calculated by:

$$h(t + \Delta t) = h(t) + \frac{\Delta t}{\rho}(\nabla \cdot (\lambda \nabla T) + \dot{q}''')$$

Following their work, both explicitly and implicitly solving Fourier's equation have been investigated. However, during most applications time step constraints for the fluid solver dominated the convergence requirements of all systems, that is, the thermal solver oftentimes already converged with the maximum time step sizes from the fluid solver.

For interaction with solids, a surrogate model of freezing particles in space and time has been used.

During development of the method, the option has been added to change the rest density of the material in dependence of the temperature, that is $\rho = const. \rightarrow \rho(T)$. This change breaks with several assumptions of classical SPH-based algorithms. Most importantly, SPH strives for having enough neighbors around the current position to ensure a good interpolation accuracy. Thus, with constant mass per particle, the volume which a particle represents changes with changing rest density. This must be accounted for in the compact support radius, which leads to a relation between density and smoothing length [8]. For this volume contraction, a new method is proposed which

relates a unit volume which the particle initially represents against the compact support radius. That is,

$$\tilde{h} \stackrel{!}{=} 4R, \quad V_0 \stackrel{!}{=} 8R^3 \rightarrow \tilde{h}(T) = 2\sqrt[3]{\frac{m}{\rho(T)}}$$

Here, the initial volume V_0 is assumed to be a cube with edge length $2R$, that is two times the particle radius. Additionally, a common heuristic in SPH is to set the compact support radius to be four times the particle radius. From that, the according smoothing length $\hbar$ can be determined.

4 Results

The aforementioned simulation framework has been implemented into the open source software SPlisHSPlasH [14]. The extension of the framework includes the thermal solver, an implicit and stable surface tension model, the coupling of viscosity and surface tension with temperature, a new and stable volume contraction method as well as a method for simulating elasticity catered to the needs of the welding process. In the following, key results during the development of the simulation method will be presented.

4.1 Surface Tension

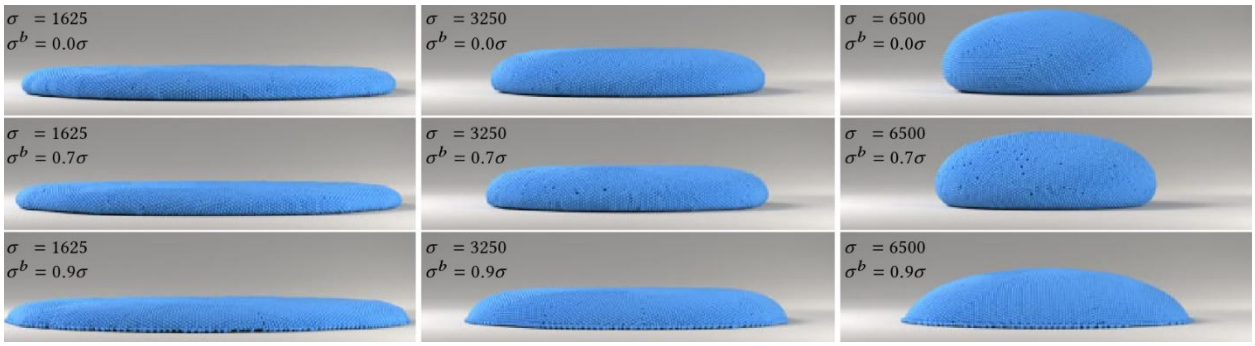

Figure 1: Simulation of a droplet on a flat plane with varying surface tension parameters. From left to right, the cohesion is increasing and from top to bottom, the adhesion is increasing. The simulation results depict the influence of these parameters on the droplet shape as well as the versatility of the method. Reproduced with permission [12].

A crucial aspect for the accurate depiction of the melt pool dynamics is the interplay between pressure, viscosity and surface tension. The latter is important for different effects like the droplet formation of the molten welding wire to the general melt pool dynamics. An important requirement here is that the simulation method remains stable and versatile under various geometric conditions and large surface tension forces. To that goal, Jeske et al. [12] developed a novel surface tension method. They derive the surface tension force from the imbalance of interior and exterior particles. This force is solved using a linearized implicit system which improves the stability of the method with large surface tension forces. This allows for capturing a wide range of surface tension effects for example depicted in Figure 1. As shown by the authors, their method outperforms other state-of-the-art methods [15-18] in for example the formation of droplets, an important requirement for

the process simulations. Thus, for different applications from welding to thermal spraying, their method has been proven to be indispensable [19-21].

4.2 TIG Spot Welding

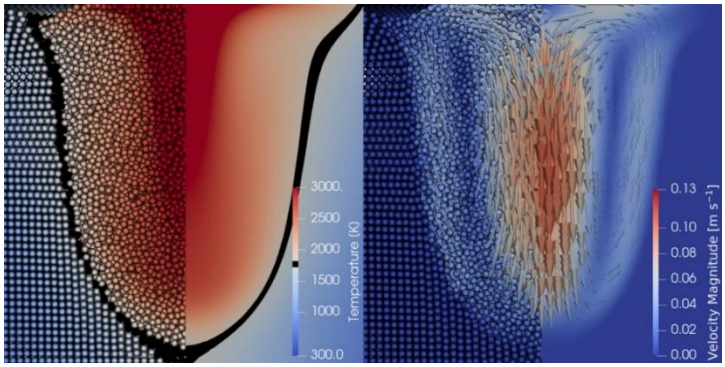

Figure 2: Comparison of SPH (left, particle view) and FEM (right, rendered view) simulation of the temperature distribution and velocity profile of the melt pool of a TIG welding scenario. SPH produces comparable results to the well-established FEM solution. Reproduced with permission [13].

To investigate the applicability of SPH for welding process simulations, Jeske et al. [13] conducted a quantitative analysis using the example of tungsten inert gas (TIG) spot welding. The authors compared their novel SPH-based method against Wolfram Mathematica® and COMSOL FEM® simulations. While this example is more suited to be simulated with an Eulerian simulation method due the continuous melt pool geometry, the authors conclude that their method is comparable to the other well-established methods in terms of simulation accuracy for the temperature flow and melt pool dynamics. The results can be seen in Figure 2. Additionally, they argue that while their method offers comparable results, the SPH-based method will be advantageous for the further depiction of real-world processes with topology changes and strong discontinuities in for example droplets or metal splatter. To conclude, the authors have proven with their study that the Smoothed Particle Hydrodynamics method is able to produce quantitatively similar results to well-established methods in the field.

4.3 Thermal Spraying

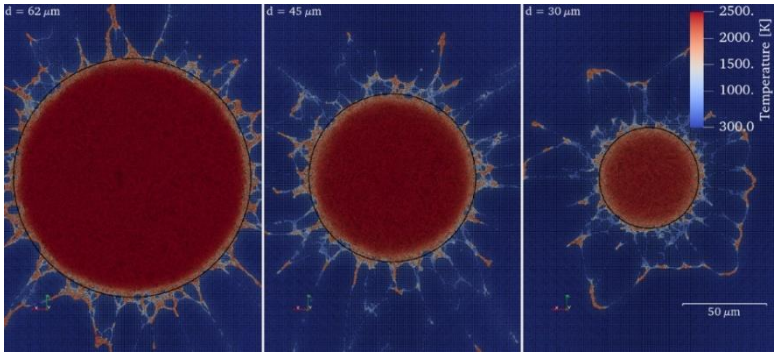

Figure 3: Splats of differently sized initial droplets simulated with SPH for thermal spraying. Reproduced with permission [20].

Another field of application to which the Smoothed Particle Hydrodynamics method was applied to is thermal spraying. In the work of Jeske et al. [20], the authors showcase the capabilities of SPH

and compare their method against the ANSYS Fluent® solver using the finite volume method (FVM) with the volume of fluent (VOF) method. There, the authors demonstrate the advantages of using SPH as a discretization method. The thermal spraying process involves large deformations of the droplet during impact with the substrate leading to geometry and topology changes during splat formation, see Figure 3. Additionally, the thermal spraying is a multi-physics process, requiring the correct interaction of temperature, pressure, surface tension and viscosity. The authors demonstrate the applicability of an SPH-based method by quantitatively comparing against the VOF method. They conclude a good agreement between the methods and provide explanations for the differences arising from both simulation methods. Furthermore, the authors point out the increased computational efficiency of their method. They report for a comparable simulation parameter that their method is able to use a 22 times higher discretization density while only needing a quarter of the simulation time while comparing against ANSYS Fluent®.

The method of Jeske et al. [20] has been further extended by Bobzin et al. [19]. They demonstrate the droplet impact on a realistic, irregularly shaped surface for which the splat fills in the crevices of the work piece. Additionally, they investigate the influence of the temperature of the substrate in regards to the splat diameter. Finally, and most remarkably, the method is able to simulate void regions that occur in the buildup of multiple splats in the spraying process. Thus, the authors have demonstrated that the method lays an important foundation for further research in that area.

4.4 Volume Contraction

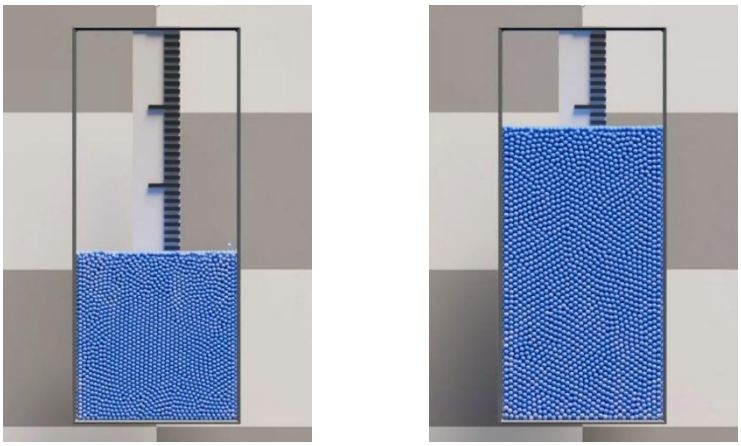

Figure 4: Simulation snapshots of a fluid column expanding and afterwards shrinking again through halving and doubling the rest density of the fluid.

For evaluating the stability and capabilities of the volume contraction method, the following synthetic test case has been devised. Here, the density of a fluid column is being altered over time to check for the stability of the simulation with changing rest densities and support radii, see Figure 4. As the simulation method, a modified version of divergence-free SPH [9, 10] has been chosen to support the material changes. The newly created volume contraction method has been compared against the version of Li et al. [22] and Winchenbach et al. [23] for incorporating different particle sizes and support radii.

In this example, the density of the fluid has been halved over time and afterwards doubled again. Both methods of Li et al. [22] and Winchenbach et al. [23] failed this scenario while with the geometrically-based method the scene could be successfully simulated. While the volume contraction processes happening in real material are usually much smaller, the results of the synthetic scenario demonstrated the following fundamental issues with the previous methods.

While the methods of Li et al. [22] and Winchenbach et al. [23] depend on the particle distribution, the here presented method is purely dependent on geometrical properties. The advantage is, that particle distributions with too few particles like single droplets or at the free surface must not be accounted for separately. Both previous methods need to define a maximum neighborhood search radius for not unnecessarily increasing the radius for isolated droplets. Without, the ill-distributed particles will increase their neighborhood radius to an unphysical degree which lead to an inability to resolve the demonstrated scene.

4.5 Blind Weld

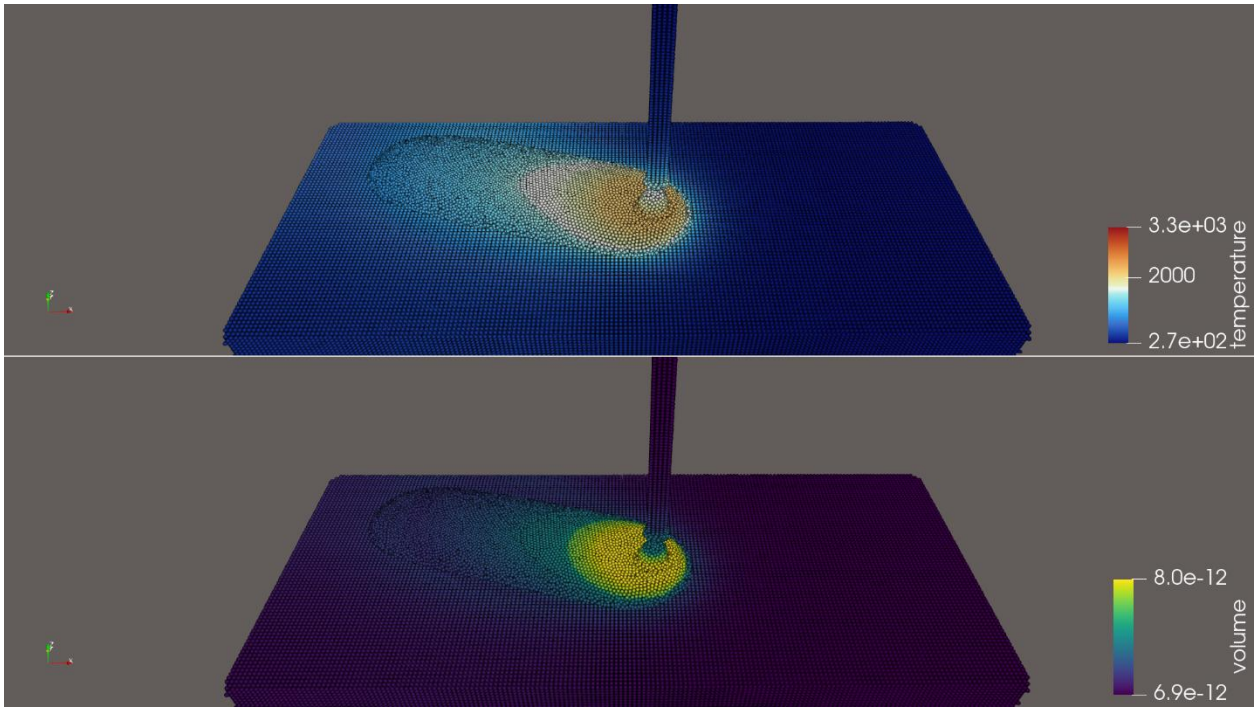

Figure 5: Temperature and volume distribution during a blind weld simulation as a demonstrator of a full process simulation. The simulation entails a full multi-physics process of the melt pool dynamics.

To demonstrate the applicability of the volume contraction method, a simulation of a blind weld using the cold metal transfer (CMT) variant of gas metal arc welding (GMAW) has been devised. This example showcases a complex scenario with several physical systems interacting with each other. The included effects and surrogate models apart from the temperature dependent volume have been described by Mokrov et al. [21]. The latter has been newly added. While the effects currently are only affecting the liquid melt pool, the results (Figure 5) show the applicability of the volume contraction method to the process simulation.

4.6 Discussion and Towards a Unified SPH Model for Fluid and Solid States

The results demonstrate the capability of SPH for melt-based processes. Especially for processes with large deformations and topological changes as in thermal spraying or CMT based welding, SPH has been shown indispensable for its native handling due to its Lagrangian, meshless nature. The first results show a promising direction for a unified SPH model for a full process simulation.

A remaining task for this framework is the handling of fluid-solid transitions and the mechanical behavior. First experiments have been conducted with a linear elasto-plastic model. Here, the elasto-dynamic behavior is handled – as in the works of Zerbe [24] and Yang et al. [25] – by updating the stress tensor over time. The plastic behavior is modeled using the von Mises yield criterion. This model has the advantage that it must not refer back to a reference configuration. Since new material will solidify over time, updating the internal stress seem to be a more natural depiction, since otherwise a constantly evolving reference configuration must be established.

5 Summary

Conclusively, the presented framework has shown the potential of SPH-based process simulations, both in qualitative and quantitative scenarios. SPH offers a unique suite of properties like its ability to depict large deformations, topological changes and the ability to capture a wide range of physical effects in a stable manner. Thus, SPH as a method thrives in processes which specify exactly these requirements as for example the CMT process, thermal spraying, but also other ones like WAAM (Wire and Arc Additive Manufacturing) [26] or LDNA (Laser-assisted double-wire welding with non-transferred arc) [27]. With further development of the solidification behavior, one can foresee a wide range of applications for SPH-based process simulations.

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Conflict of Interest

The author declares no conflict of interest.

Data Availability Statement

The data that support the findings of this study are available at http://hdl.handle.net/21.11102/94ac8b57-c163-4854-842a-698831b4f027 upon request.

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