Development and validation of a meshless 3D material point method for simulating the micro-milling process

S. Leroch\textsuperscript{a,*}, S. J. Eder\textsuperscript{a,b}, G. Ganzenn"uller\textsuperscript{c,d}, L. J. S. Murillo\textsuperscript{c,d}, M. Rodríguez Ripoll\textsuperscript{a}

\textsuperscript{a}AC2T research GmbH, Viktor-Kaplan-Straße 2/C, 2700 Wiener Neustadt, Austria
\textsuperscript{b}Institute for Engineering Design and Logistics Engineering, Vienna University of Technology, Getreidemarkt 9, 1060 Vienna, Austria
\textsuperscript{c}INATECH, Universität Freiburg, Emmy-Noether-Str. 2, 79110 Freiburg i. Br., Germany
\textsuperscript{d}Fraunhofer Ernst-Mach-Institut, Eckerstr. 4, 79104 Freiburg i. Br., Germany

Abstract

A meshless Generalized Interpolation Material Point Method for simulating the micro-milling process was developed. This method has several advantages over well-established approaches (such as finite elements) when it comes to large plastic strains and deformations, since it inherently does not suffer from tensile instability problems. The feasibility of the developed material point model for simulating micro-milling is verified against finite element simulations and experimental data. The model is able to successfully predict experimentally measured cutting forces and determine chip temperatures in agreement with conventional finite element simulations. After having verified the approach, the model was applied to perform extensive numerical 3D simulations of the micro-milling process. The goal is to evaluate the response of the micro-milling cutting forces as function of the hardening behavior of the micro-milled material. The meshless 3D simulations reveal a dependency of tool force slopes (with respect to the uncut chip thickness) on the hardening parameters. Based on these findings, a new approach is outlined to determine hardening parameters directly from two micro-milling experiments with distinct, sufficiently large uncut chip thicknesses.

Keywords: micro-milling, cutting forces, chip formation, meshless simulation method, Johnson-Cook model

*Corresponding author

Email address: sabine.leroch@ac2t.at (S. Leroch)

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1. Introduction

The current trend in miniaturizing components requires the development and improvement of suitable machining technologies that are able to perform accurately at the micrometer scale. In this context, micro-milling has emerged as one of the most cost-efficient techniques for manufacturing components with complex micro-features. The success of micro-milling is based on its high performance and versatility, since it can be applied to machining for a great variety of materials. Micro-milling is becoming increasingly relevant due to the high demand in aerospace, automotive, medical, optical, and microelectronics industries for miniaturized systems with superior surfaces and high aspect ratios.

A profound understanding of the micro-milling process is essential for ensuring the reliability of the process. The prediction of the cutting forces during micro-milling is of special interest, since they constitute useful parameters for estimating the design requirements for the tool and equipment. Several empirical and analytical cutting force models were reviewed by Germain et al. (2013). The authors reported that in general, empirical models provide a link between the micro-milling parameters and the cutting forces, so that the hardening behavior of the material is implicitly considered via model parameters that need to be fitted. Conversely, analytical models take into account a larger number of process parameters and include material behavior, but are often handicapped by the simplifications required to obtain a analytical expressions.

A significant amount of fundamental knowledge on milling in general and micro-milling in particular has been obtained using computer simulations. They provide a fast and cost-efficient tool for performing parameter studies in order to optimize process conditions. In the early 2000s, Özel and Altan (2000) utilize the finite element method for simulating high-speed flat end milling. The results of this work showed a qualitative agreement between the simulations and experimental data in terms of predicted forces and location of highest tool temperatures and stresses. The feasibility of applying a 2D finite element model for simulating the micro-milling process of aluminum and steel was shown for the first time by Dhanorker and Özel (2008). Their results revealed a reasonable accuracy in the prediction of temperature distributions and cutting forces. Micro-milling simulations of titanium alloys were performed by Thespontithi and Özel (2013) with emphasis on the impact of cBN coating on tool wear. Their results showed a detailed study of the
cutting temperature and forces combined with tool wear. However, despite the detailed analyses of the micro-
milling process, the use of a 2D simulation model led to simplifications, since the complexity of a oblique
3D cutting process can not be captured. The extension into a full 3D model was subsequently performed
by the authors Thepsonthi and Özel (2015). The 3D model allowed the prediction of 3D chip formation
with its related cutting forces, temperatures and wear distributions. These results could be exploited to
investigate the impact of milling strategy and tool wear. In summary, the available literature shows that the
major advantage of finite element simulations is that they allow the determination of variables that are not
readily accessible to experiments, such as chip temperatures, strains, and strain rates. Contrary to empirical
and analytical cutting force models, computer simulations are capable of coping with most of the process
complexity while simultaneously using advanced material models.

The most widespread simulation tool for investigating micro-milling processes is the Finite Element
Method (FEM). In combination with visco-plastic constitutive material models, such as the one by Johnson
and Cook (1985), this approach has been extensively used with the increasing availability of commercial
FEM codes and computational power. However, as an alternative to both FEM and conventional meshless
particle methods, a different approach is taken here, combining grid and particle behavior, the so-called
Material Point Method (MPM). The reason is that these established discretization methods come with
specific disadvantages. Classic FEM is inappropriate for the large deformations experienced here. While
re-meshing is possible, this often leads to excessively small time step sizes and thus large computational
overhead, as shown by Torigaki and Kikuchi (1992). CFD-like Eulerian simulations are difficult to perform for
solid body behavior and suffer from high numerical diffusion as material is advected on the grid. Lagrangian
meshless methods such as smooth particle hydrodynamics (SPH) appear as a worthwhile alternative for
treating large deformations as shown by Hoover (2006). SPH was originally developed by Gingold and
Monaghan (1977) to simulate the formation of stars in the context of astrophysics. However, these methods
are not free from problems either. Traditional SPH with Eulerian kernels suffers from tensile instabilities,
where tensile stress states lead to unphysical disintegration of solids, as shown by Swegle et al. (1994) and
Mamalis et al. (2011) in the context of micro-scratching. The prevention of tensile instabilities requires large
amounts of artificial viscosity and strong \textit{ad-hoc} correction mechanisms, which severely influence the accuracy of the results. The Total-Lagrangian SPH of Ganzenmüller (2015) is a much more accurate reformulation of SPH which utilizes a constant reference configuration to perform the weak-form integration of stresses and strains. While this markedly improves accuracy and eliminates the dreaded tensile instability, the concept of a constant reference configuration is not compatible with truly large deformations, in particular plastic flow, where parts of the material are disconnected and reconnected to different parts upon solidification. Updates of the reference configuration may be performed as shown in Leroch et al. (2016), who used this approach for performing scratch simulations on copper. Recently, Varga et al. (2017b) applied the same methodology for simulating scratch tests on austenitic steel, reaching a good agreement in terms of scratch morphology. The method was also applied by Varga et al. (2017a) for performing extensive simulation of scratch tests with the aim of linking the material parameters with the scratch morphology and scratch hardness. However, the main disadvantage of this approach is that it incurs in computational overhead and does not appeal as an elegant solution.

In this work, a particular MPM called the Generalized Interpolation Material Point Method (GIMP) is applied for the following reasons: it does not suffer from the tensile instability problem, can handle very large deformations, and has been shown to exhibit first-order convergence upon resolution refinement, as shown by Wallstedt and Guilkey (2008). With all these features, as will be shown in the following, GIMP presents itself as a promising method for studying machining problems featuring violent deformations. Introduced in the 1990s by Sulsky et al. (1994), MPM was subsequently further developed and refined by a number of authors, in particular Bardenhagen and Kober (2004), who introduced a Petrov-Galerkin discretization scheme, and Wallstedt and Guilkey (2007), who improved the projection operation for linear functions. Common to all flavors of MPM is the use of Lagrangian particles as in SPH, which contain all the information about the system, e.g., stress, strain, momentum, and histories of these quantities. Additionally, and in contrast to classical particle methods such as SPH, an auxiliary background grid is used to compute strain rates and stresses. Information between particles and grid is exchanged via the use of smooth interpolates, which can be related to the SPH kernel or FEM shape functions. MPM is classified as a true particle method, because
the entire grid only serves as a computational scratchpad and is discarded at the end of each time step. The state of the system is then advanced by moving the particles only.

The accuracy of computer simulations depends on the robustness of the hardening models used for predicting the cutting forces and chip temperatures, among others. These models usually rely on parameters that need to be determined via fitting to reference experiments. In the particular case of micro-milling, the use of visco-plastic constitutive models with strain rate and temperature dependence means that the identification of the material parameters requires complex and demanding dynamic stress-strain experiments, such as the Hopkinson bar. As illustrative example of this effort, Hokka et al. (2012) used high temperature and high strain rate compression tests performed on the titanium alloy Ti-15-3 for determining the material parameters of a modified Johnson-Cook model. The results obtained were used to simulate orthogonal cutting, reaching a very good agreement between the predicted and the measured cutting stresses. Consequently, the direct identification of the material parameters from data acquired during the milling process itself would be of paramount technological and scientific relevance. Several attempts to this end have been made in the past by some authors. Shrot and Bäker (2012) applied FEM simulations for inverse identification of the material parameters during milling. The results reveal the ambiguity encountered in the inverse identification of the Johnson-Cook material parameters for steel. In their case, sets of different parameters where found that led to indistinguishable cutting forces and chips. In a follow-up work, Bäker (2015) proposed a method that successfully removed this duality, but still relied on quantities that are not directly measurable in experiments. Therefore, a more profound understanding of the role of the material parameters in the milling process is required for achieving this ambitious goal. The prediction of cutting forces during micro-milling has also been a subject of recent interest by Afazov et al. (2010). Using a semi-empirical equation, the authors correlated the cutting force with the uncut chip thickness and the cutting velocity. The results were verified experimentally using AISI 4340 steel. Later, Afazov et al. (2012) also successfully validated the model using AISI H13 steel with a hardness ranging from 35 and 60 HRC. The influence of tool wear was subsequently taken into account in Afazov et al. (2013). Denkena et al. (2015) developed an inverse determination methodology based on Oxley’s machining theory to predict cutting forces for complex
three-dimensional tools. When combined with tensile test data, material parameters could be determined using this method. The methodology led to the formulation of a mathematical model for determining the uncut chip thickness.

The aim of the present work is to implement a material point method on the molecular dynamics program LAMMPS developed by Plimpton (1995) and apply the implementation to 3D micro-milling. To our best knowledge, no MPM implementation has been used so far to simulate micro-milling. The model is benchmarked against standard and well-established finite element simulations, and the predicted cutting forces are additionally compared to experimentally measured values. The main advantage of the proposed model is that it is naturally able to handle very large deformations and material detachment, in contrast to current state-of-the-art finite element simulation approaches. The gain in performance and computational efficiency is exploited for performing extensive meshless 3D simulations. The simulations are used to identify the influence of the hardening behavior on the micro-milling cutting forces and temperatures as a function of the uncut chip thickness. Based on the observed dependence of the micro-milling forces on the uncut chip thickness, a method for determining hardening parameters from micro-milling experiments using two sufficiently large chip thicknesses is suggested.

2. Numerical method

2.1. Basic equations

The MPM algorithm described in this section was implemented into LAMMPS, an open-source particle code presented in Plimpton (1995), by one of the authors. The MPM model itself was originally proposed by Sulsky et al. (1994), and subsequently further developed by Bardenhagen and Kober (2004) and Wallstedt and Guilkey (2007), among others. First, a combined problem of mechanical deformation and heat conduction is considered. The conservation equations representing these physical mechanisms are given as a set of partial differential equations:
\[
\frac{\partial \mathbf{v}}{\partial t} = \frac{1}{\rho} \nabla \cdot \mathbf{\sigma} + \mathbf{b} \tag{1}
\]
\[
\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \mathbf{v}) \tag{2}
\]
\[
\frac{\partial q}{\partial t} = \kappa \nabla^2 q - \nabla \cdot (q \mathbf{v}) + W_p(t) \tag{3}
\]

Equations (1) and (2) describe the mechanical flow, where \( \mathbf{v} \) is the velocity, \( \rho \) the mass density, and \( \mathbf{b} \) a vector of body forces or imposed boundary forces. The Cauchy stress tensor \( \mathbf{\sigma} \) contains both pressure and viscous stresses. The temperature field evolves in time according to the advection-diffusion equation, Eq. (3), where \( q \) is the heat and \( \kappa \) is the thermal conductivity coefficient, and also according to heating due to plastic deformation, \( W_p(t) \). Note that temperature \( T = q m C_p \) is proportional to heat, with mass \( m \) and specific heat capacity \( C_p \). In this model, the constitutive equation that yields the stress \( \mathbf{\sigma} \) depends explicitly on temperature.

The mechanical flow, i.e., Eqns. (1) and (2), is discretized using a variant of the Material Point Method (MPM). Here, the central idea is to associate the quantities mass \( m \), heat \( q \), velocity \( \mathbf{v} \), stress \( \mathbf{\sigma} \), and strain \( \varepsilon \) with particles. These particles can be thought of as small volume elements of the material. The particles move through space according to their velocity, which implies a Lagrangian, co-moving frame of reference. This fact significantly simplifies the treatment of the advection terms appearing in Eq. (2), as self-advection is automatically exactly accounted for in the Lagrangian frame. Heat conduction, i.e., Eq. (3), is discretized using central finite differences on an auxiliary grid that is temporarily evaluated as part of the MPM algorithm.

2.2. Numerical description of mechanical flow

While the use of particles in the MPM scheme simplifies the advection terms, the absence of a topological mesh complicates the computation of the derivatives appearing in Eqns. (1) and (2). This is solved by using an auxiliary background grid. Information from particles is transferred to the grid by means of grid basis functions \( W \). Gradients are calculated on the grid using derivatives of the basis functions, similar to the weak form solution as employed in the standard Finite Element Method. Subsequently, the gradients are
transferred back to the particles. Dyadic products of one-dimensional cubic B-splines, $S$, as basis functions are used, similar to Steffen et al. (2008),

$$W_{np} = S\left(\frac{x_n - x_p}{h}\right) \times S\left(\frac{y_n - y_p}{h}\right) \times S\left(\frac{z_n - z_p}{h}\right).$$

(4)

Grid nodal positions are denoted by $x_n$, while particle positions are denoted as $x_p$. The components $(x_n, y_n, z_n)$ and $(x_p, y_p, z_p)$ correspond to the entries of the vectors $x_n$ and $x_p$. The discretization is performed on a regular cubic grid with node spacing $h$. $W$ is of compact support, meaning that a particle can only interact with nearby nodes up to a distance of $2h$ respectively. The B-spline itself is defined in units of $h$ as follows:

$$S(r) = \begin{cases} 
\frac{1}{2} |r|^3 - |r|^2 + \frac{2}{3} & \text{if } 0 \leq |r| < 1 \\
\frac{1}{6} - \frac{1}{6} |r|^3 + |r|^2 - 2 |r| + \frac{4}{3} & \text{if } 1 \leq |r| < 2 \\
0 & \text{otherwise}
\end{cases}$$

(5)

The full cycle of steps required in the MPM Method to solve a single time-step is visualized in Fig. 1. At the beginning of a single time-step at time $t$, the following information is located at a particle with index $p$: velocity $v_t^p$, Cauchy stress $\sigma_t^p$, deformation gradient $F_t^p$, heat (thermal energy) $q_t^p$, and external force $b_t^p$. These quantities are evolved according to the following steps.

2.2.1. Particles to grid

This is the initial stage of the MPM algorithm. Mass $m$, velocities $v$, heat, and external forces (e.g., forces due to the indenter) are interpolated to the grid nodes:
Figure 1: Flow diagram of the Material Point Method (MPM).

\[ m_n^t = \sum_p W_{pn} m_p \]  
\[ q_n^t = \frac{1}{m_n} \sum_p W_{pn} m_p q_p^t \]  
\[ v_n^t = \frac{1}{m_n} \sum_p W_{pn} m_p v_p^t \]  
\[ b_n^t = \frac{1}{m_n} \sum_p W_{pn} m_p b_p^t \]

Note that weighting by grid node mass ensures conservation of heat, order parameter, and momentum.

Forces on grid nodes are computed similarly, except that the kernel gradient is used to obtain the divergence of the stress field:

\[ f_n^t = \sum_p V_p^t \sigma_p^t \nabla W_{pn} . \]

Here, \( V_p^t \) is the particle volume. The rate-of-heat \( q_n^t \) could in principle be calculated using a similar expression involving the Laplacian of the kernel function. However, this was found to be numerically unstable, so the rate-of-heat was computed directly on the grid using central finite differences instead.
2.2.2. Update of grid state

At this stage, heat, rate-of-heat, velocity, and forces are known on the grid. An explicit forward-Euler update of the grid state is performed:

\[ q_{n}^{t+\Delta t} = q_{n}^{t} + \Delta t \dot{q}_{n}^{t} \]  
\[ v_{n}^{t+\Delta t} = v_{n}^{t} + \frac{\Delta t}{m_{n}} f_{n}^{t} \]  

2.2.3. Reverse transfer of updated grid state and particle update

The updated grid velocities, grid accelerations, and heat rates are interpolated back to the particles.

\[ q_{p}^{t+\Delta t} = \sum_{n} W_{pn} q_{n}^{t+\Delta t} \]  
\[ \tilde{v}_{p}^{t+\Delta t} = \sum_{n} W_{pn} v_{n}^{t+\Delta t} \]  
\[ \tilde{a}_{p}^{t} = \sum_{n} W_{pn} (v_{n}^{t+\Delta t} - v_{n}^{t}) / \Delta t \]  

Note that the interpolated new particle velocities and accelerations are temporary values for now and thus decorated with the tilde (~) symbol. Following this, particle position and heat are updated according to a simple forward-Euler step:

\[ x_{p}^{t+\Delta t} = x_{p}^{t} + \Delta t \tilde{v}_{p}^{t+\Delta t} \]

The update of particle velocities can be performed in two different ways:

\[ v_{p}^{t+\Delta t} = \tilde{v}_{p}^{t+\Delta t} \]  
\[ v_{p}^{t+\Delta t} = v_{p}^{t} + \Delta t \tilde{a}_{p}^{t} \]  

The first option is known as the pure Particle-In-Cell (PIC) update, which stems from the fact that the predecessor of MPM, the PIC Method, used this velocity update. This update leads to a very stable simulation at the price of strong dissipation. The second option is known as a pure Fluid Implicit Particle (FLIP) update, which was introduced by Brackbill et al. (1988). Pure FLIP is nearly free from dissipation, but introduces numerical noise into the simulation. A linear combination of both methods is used here with 99% FLIP, i.e., \( \beta = 0.99 \) in the equation below:

\[ v_{p}^{t+\Delta t} = (1 - \beta) \tilde{v}_{p}^{t+\Delta t} + \beta (v_{p}^{t} + \Delta t \tilde{a}_{p}^{t}) \]
2.2.4. Computation of velocity gradient

This specific MPM scheme implements the Modified-Update-Stress-Last (MUSL) approach for the computation of the velocity gradients, and subsequently the update of the particle stress state. Compared to the original Update-Stress-First algorithm by Wallstedt and Guilkey (2008), a large gain in numerical stability and accuracy is obtained at the cost of slightly increased computational effort, for more details see Nairn (2003). In a first step, the new particle velocities are again interpolated to the grid nodes:

\[
m_{n}^{t+\Delta t} = \sum_{p} W_{pn}^{t+\Delta t} m_{p}^{t+\Delta t}
\]

\[
v_{n}^{t+\Delta t} = \frac{1}{m_{n}} \sum_{p} W_{pn}^{t+\Delta t} m_{p}^{t+\Delta t} v_{p}^{t+\Delta t}
\]

Following this, the velocity gradient at the particles is obtained as

\[
L_{p}^{t+\Delta t} = \sum_{n} v_{n}^{t+\Delta t} \otimes \nabla W_{pn}^{t+\Delta t}.
\]

2.2.5. Update particle stress and strain state

The update of strains and stresses starts with the update of the deformation gradient:

\[
F_{p}^{t+\Delta t} = \exp (\Delta t L_{p}^{t+\Delta t}) F_{p}^{t}
\]

From the updated deformation gradient, the updated volume is calculated:

\[
V_{p}^{t+\Delta t} = J V_{p}^{0}
\]

Here, \(J\) is the determinant of \(F_{p}^{t+\Delta t}\), and \(V_{p}^{0}\) is the initial particle volume.

An updated stress formulation is employed, in which the stress is accumulated based on strain increments, allowing a simple implementation of history-dependent constitutive models involving plastic deformation, as shown in Taylor and Flanagan (1987). The strain increment is given by

\[
\epsilon_{p}^{inc} = \Delta t \frac{1}{2} (L^{T} + L).
\]

Note that the time superscript in the above line is omitted to reduce clutter. It is implicitly assumed that time \(t+\Delta t\) is referred to. Using the strain increment, a new value of the stress is computed via a constitutive
law $f$:

$$\sigma_p^{t+\Delta t} \leftarrow f(\sigma_p^t, \epsilon_p^{inc})$$

(25)

3. Material model

In what follows, particle properties are discussed, but for simplicity the index $p$ is omitted. The material model is decomposed into isotropic and deviatoric parts, corresponding to volumetric and shear deformations. The relationship between density $\rho$ and pressure $p$ is given by the equation of state, while the relation between a tensorial shear deformation $\epsilon_d$ and the stress deviation tensor $\sigma_d$ is given by the constitutive law. The decomposition is additive, i.e.,

$$\sigma = -pI + \sigma_d ,$$

(26)

where $I$ is the diagonal unit tensor.

The equation of state is assumed to be a linear relation between deformation gradient $J$ and pressure

$$p = K(1 - J) ,$$

(27)

with $K = 172.5$ GPa the bulk modulus of AISI 4340 steel. To determine the deviatoric part of the stress tensor in Eq. (26), the purely empirical Johnson-Cook model by Johnson and Cook (1985) is used, which is numerically robust and therefore widely used for thermal elastic-plastic modeling, where the calculation of $\sigma_d$ is illustrated in Leroc et al. (2016). The relation for the flow stress $\sigma_f$ is given as

$$\sigma_f(\epsilon, \dot{\epsilon}, T) = [\sigma_Y + B(\epsilon)^n][1 + C \ln(\dot{\epsilon}^*)][1 - (T^*)^m] ,$$

(28)

where $\epsilon$ is the equivalent plastic strain, which is calculated in dependence of the strain tensor, $\dot{\epsilon}$ its time derivative, the plastic strain-rate, and $\sigma_Y$ the material yield stress at zero strain. $B$ and $n$ are strain hardening parameters, $C$ a strain rate parameter, and $m$ a temperature coefficient given in Table 1. The normalized strain rate and temperature in Eq. (28) are defined as

$$\dot{\epsilon}^* = \frac{\dot{\epsilon}}{\dot{\epsilon}_0},$$

$$T^* = \frac{T - T_0}{T_m - T_0} ,$$

(29)
where $\dot{\epsilon}_0$ is the plastic strain rate and $T_0$ the reference temperature used to determine $\sigma_Y$, $B$ and $n$, and $T_m$ the reference melting temperature.

Table 1: Johnson-Cook parameters for AISI 4340 steel Afazov et al. (2010).

<table>
<thead>
<tr>
<th>$\sigma_Y$ [MPa]</th>
<th>$B$ [MPa]</th>
<th>$C$</th>
<th>$n$</th>
<th>$m$</th>
<th>$\dot{\epsilon}_0$ [1/s]</th>
<th>$T_0$ [K]</th>
<th>$T_m$ [K]</th>
</tr>
</thead>
<tbody>
<tr>
<td>792</td>
<td>510</td>
<td>0.014</td>
<td>0.26</td>
<td>1.03</td>
<td>1.0</td>
<td>294</td>
<td>1793</td>
</tr>
</tbody>
</table>

4. Computational Setup and Simulation Procedure

![Figure 2: Sketch of the cutting process. UCT is the uncut chip thickness, $\alpha$ the rake angle, $\gamma$ the clearance angle, $v_c$ the cutting velocity, $F_c$ and $F_t$ the cutting and tangential forces, respectively, $r$ the tool edge radius, and $RP$ the reference point.](image)

In Fig. 2, a sketch of the orthogonal micro-milling process is shown, where the cutting tool of width 10 $\mu$m is moved with velocity $v_c$ into the workpiece cutting out a chip of the uncut chip thickness $UCT$. The edge of the cutting tool has a curvature radius $r = 3.5$ $\mu$m, a rake angle $\alpha = 8^\circ$ and a clearance angle $\gamma = 40^\circ$, similar to Afazov et al. (2010). The cutting and the tangential forces $F_c$ and $F_t$ acting on the tool’s center of mass are recorded. To calculate the forces for various uncut chip thicknesses $UCT$, the resolution of the substrate was varied, i.e., 0.1 $\mu$m for thicknesses up to 0.8 $\mu$m, 0.5 $\mu$m for thicknesses up to 5.5 $\mu$m, and 1 $\mu$m for larger $UCT$. The lowest particle layer of the substrate is kept fixed to avoid that the material...
block starts moving while micro-milling. The thickness of the substrate is chosen to be around triple that of the selected \( UCT \), its width in x-direction is 30 \( \mu \text{m} \). The material parameters for AISI 4340 are shown in Table 2.

Table 2: Material parameters for AISI 4340 steel taken from Afazov et al. (2010): \( \rho_0 \) is the reference bulk density, \( E \) Young’s modulus, \( \nu \) the Poisson ratio, \( Q \) the artificial viscosity coefficient, \( \gamma \) the hourglass coefficient, and \( C_p \) the specific heat capacity at room temperature.

<table>
<thead>
<tr>
<th>( \rho_0 ) [kg/m(^3)]</th>
<th>( E ) [GPa]</th>
<th>( \nu )</th>
<th>( Q )</th>
<th>( \gamma )</th>
<th>( C_p ) [J/kg K]</th>
</tr>
</thead>
<tbody>
<tr>
<td>7830</td>
<td>207</td>
<td>0.3</td>
<td>0.1</td>
<td>10</td>
<td>473</td>
</tr>
</tbody>
</table>

4.1. \textit{Heat transfer in the substrate and interaction with the cutting tool}

The cutting tool is assumed to be perfectly rigid and isothermal with a temperature set to 294 K. Heat transfer between the particles of the substrate was enabled by applying a heat conductivity coefficient \( \kappa = 44.5 \text{ W/(mK)} \) for unalloyed steel taken from Ng et al. (1999). The work of plastic deformation \( W_p \) caused by the cutting tool is converted into heat with a Taylor-Quinney-coefficient of 1 as can be seen in Eqn. (3).

While the particles in the substrate interact via Eqs. (1) to (3), applying the constitutive Eqs. (27)–(29) for pressure and von Mises flow stress, the interaction between the completely rigid tool and the substrate is assumed purely repulsive. To calculate the interaction a mesh of the same resolution as in the substrate is placed on the tool surface. The interaction force between a particle in the substrate and the closest point of a triangle in the tool surface at a distance \( r \) is then assumed to be

\[
f = E \varepsilon = E (r - r_c) r_c, \quad r < r_c
\]

with the characteristic stiffness \( E = sK(1 - \varepsilon)^2 \) of the interaction in dependence of the bulk modulus \( K \), a scaling factor \( s \), which is usually set to unity, and \( r_c \) the contact radius, assuming that the particle is an elastic cube with edge length \( r_c \). In addition, Coulomb friction is applied using a coefficient of friction \( \mu = 0.4 \), as in Afazov et al. (2010).

5. Results and Discussion

5.1. Validation of MPM

To validate the MPM algorithm, it is first attempted to reproduce results from recent FEM simulations carried out by Afazov et al. (2010), where micro-milling cutting forces for various cutting velocities and
tool tip curvatures were calculated. The same Johnson-Cook constitutive model and material parameters as in the cited reference given in Tables 1 and 2 are used, which represent AISI 4340 steel with a hardness of 30 HRC. To reduce computational costs, the validation study was restricted to a cutting velocity of 4.732 m/s applied in Afazov et al. (2010). Test runs with other velocities have shown that the agreement with FEM results does not depend on the chosen velocity. The results obtained using MPM show similar cutting forces as function of different uncut chip thicknesses as in the FEM simulations, as seen in Fig. 3 (a). The simulated forces initially exhibit non-linear behavior for small uncut chip thickness, followed by a linear region, as approximated by a two-phase exponential equation in Afazov et al. (2010). The non-linearity at small uncut chip thickness arises from the micro-milling forces being significantly affected by the tool radius, which creates a negative rake between the tool and the workpiece, as pointed out by Afazov et al. (2010).

The maximum chip temperatures obtained using MPM agree reasonably well with the FEM results, as can be seen in Fig. 3 (b). However, as numerical instabilities may sometimes cause unrealistic peak temperatures for individual particles, it was considered more meaningful to calculate the median temperature within the chip as a measure for a “typical” temperature. To do this, the elements constituting the chip at a given time must first be identified using the following criteria. An element contributes to the chip, if

- the absolute element velocity is greater than 8 m/s and less than 15 m/s,
- the element is not part of the milling tool,
• and the element’s z-coordinate is greater than 4 \( \mu m \) to eliminate artifacts from the lower boundary, finally adding all elements that are not part of the milling tool with a z-coordinate higher than 7 \( \mu m \) above the original work piece surface (to exclude any possible bulges along the milling track), regardless of particle velocity. Once the elements are known, the median chip temperature can be analyzed as a function of the tool tip position \( y \). The temperature first rises strongly during cutting and then saturates to a constant value for large \( y \). At a cutting velocity of 10 m/s, the saturation value rises from 450 K to 850 K with yield stresses ranging from 210 MPa to 2100 MPa, while varying the UCT has much smaller influence on the median chip temperature.

![Figure 4](image1.png)

Figure 4: Comparison between cutting forces in \( y \) direction (a) and \( z \) direction (b) with FEM and experiment (Fig. 23 in Afazov et al. (2010)) for cutting velocities of 4.723 m/s at a UCT of 12.5 \( \mu m \) and rotation angles \( \theta \) of 75, 103, 434, 461, 795 and 819\(^\circ\) as deduced from Afazov et al. (2010).

The micro-milling forces in \( y \) and \( z \) direction obtained with the MPM simulations in this work are benchmarked against experimentally measured cutting forces and FEM predictions as shown in Fig. 4. The experimental data was obtained with the setup as described in Fig. 12 in Afazov et al. (2010). The sinusoidal force originates from the rotation of the cutting tool with a rotation angle \( \theta \). The comparison of the experimental cutting forces with the simplified simulation models, where the cutting tool is replaced with a single tooth as shown in Fig. 2 at fixed \( \theta \), is performed by extracting all possible angles \( \theta \) at the selected UCT of 12.5 \( \mu m \) from Fig. 4 in Afazov et al. (2010). Afterwards, the milling forces in \( y \) and \( z \)
direction are evaluated using

$$
\begin{bmatrix}
F_Y \\
F_Z
\end{bmatrix} = \Delta x
\begin{bmatrix}
\sin \theta & \cos \theta \\
- \cos \theta & \sin \theta
\end{bmatrix}
\begin{bmatrix}
F_t \\
F_c
\end{bmatrix},
$$

(31)

with $\Delta x$ being the depth of the cut in the experiment of 0.1 mm and the forces from the MPM simulation of $F_t = 15.3$ N/mm, $F_c = 33.9$ N/mm. As can be seen in Fig. 4, the agreement of the present 3D MPM model with experimental data is good.

5.2. Influence of the yield stress and the hardening parameters on the cutting force

![Figure 5: Cutting and tangential forces at 5.5 µm uncut chip thickness and cutting velocity of 10 m/s for yield stresses $\sigma_Y$ of 210, 500, 1050 and 2100 MPa as a function of the tool tip position $y$.](image)

Once the MPM model was validated against well-established FEM simulations, it was applied to investigate the impact of strength and hardening behavior on the cutting force during micro-milling of steel. To this end, the yield stress $\sigma_Y$ as well as the hardening parameter $B$ and hardening exponent $n$ were varied with the aim of covering the plastic deformation behavior of most steels. Firstly, the $\sigma_Y$ parameter of the Johnson-Cook model was set to the values 210, 500, 1050, and 2100 MPa, while the other material parameters remained as in Table 1. The geometrical parameters were kept as described in Section 4, and the cutting velocity was increased to 10 m/s for better computational efficiency. For each yield stress, the cutting forces are modeled as functions of the uncut chip thickness $UCT$.

The time-evolution of the cutting ($F_c$) and the tangential force ($F_t$) during micro-milling for an $UCT$ of 5.5 µm is shown in Fig. 5 and illustrates the increase of both forces for steels with higher yield stress. As one can see in the graph after around 40 µm of cutting all the forces have reached a steady state value.
Figure 6: Von Mises stresses (left) and temperatures (right) during chip formation for an uncut chip thickness of 5.5 µm and a cutting velocity of 10 m/s for yield stresses $\sigma_Y$ of 210 MPa (top), and 2100 MPa (bottom).

Some exemplary snapshots of the MPM simulations for the same UCT and two different yield stresses are shown in Fig. 6, once colored according to von Mises stresses and once to illustrate the temperature distribution. As expected, the maximum von Mises stresses imparted during micro-milling are located at the tool tip–chip interface and increase for higher yield stresses. After relaxation, the stresses in the chip and behind the tool are nearly the same. The temperature is highest in the chip and directly at the tool tip, and cools down rapidly to moderate temperatures behind the tool. As also observed for the stresses, the temperature increases with higher yield stress. The chip shape depends on the yield stress. For softer materials it is shorter and thicker, while for harder materials it becomes longer and finer. The chip shape also slightly varies in dependence of the hardening parameters $B$ and $n$.

Steady-state values of the cutting and tangential forces were calculated as the median value of the time-
Figure 7: Steady-state cutting (left) and tangential forces (right) as a function of the uncut chip thickness $UCT$ for various yield stresses $\sigma_Y$ with $B = 500$ MPa and $n = 0.26$ (top), for varying values of $B$ with $\sigma_Y = 500$ MPa and $n = 0.26$ (middle), and for varying values of $n$ with $\sigma_Y = 500$ MPa and $B = 500$ MPa (bottom).

series, thus automatically discarding outliers as well as the entire running-in phase at the onset of milling.

Error bars were obtained by calculating the standard deviation of the respective force in the steady-state
region over a minimum of 2 μm of milling distance for $UCT < 1 \mu m$ and 15 μm for all other values of $UCT$. These steady-state values are plotted as functions of the $UCT$ (ranging from 0.15 to 10 μm) for four yield stresses in Fig. 7 (a–b). As mentioned, the results show that the $UCT$ can be related to the cutting and tangential forces using a two-phase exponential function, as done in Afazov et al. (2010). This function serves to capture the initial rapid increase of the micro-milling forces for small $UCT$, which is followed by a linear region. The linear region, which starts for $UCT$ greater than 1 μm, is characterized by a slope that increases for higher yield stresses.

Analogous simulations were performed varying the hardening parameter $B$ and the hardening exponent $n$. The variation of the cutting and tangential forces during micro-milling as a function of the $UCT$ is shown in Fig. 7 (c–d) for hardening parameters $B$ of 100, 500, and 1000 MPa, while keeping $n$ fixed at $n = 0.26$. The results show that the cutting force is higher and increases more rapidly for larger $B$ values. This behavior is similar to that observed for the yield stress. Regarding the tangential force, the $F_t$ values are also higher for larger hardening parameters, but their increase as a function of $UCT$ seems to be negligible, in contrast to the dependence observed for the yield stress variation.

The impact of the hardening exponent $n$ on the cutting and tangential forces, shown in Fig. 7 (e–f), features a significant difference to the results discussed above, since differences in the dependence of $F_c$ on $UCT$ for various values of $n$ are very small, particularly for small $UCT$. For larger $UCT$ the values start to diverge somewhat, since $F_c$ rises faster for higher values of $n$. Still, in this case higher $F_c$ values are obtained.
for higher $n$. By contrast, the simulations show a radically different behavior for $F_t$. In this case, a higher $F_t$ is achieved for lower hardening exponents. Furthermore, while the slope of $F_t$ as a function of $UCT$ does not vary much, higher slopes can be obtained for lower values of $n$. The reason for this behavior lies in the significantly different plastic strains imparted in cutting and tangential direction. While in cutting direction, plastic strains during micro-milling are higher than 1, in tangential direction these are smaller. The plastic strain value of 1 is the crossing point of the stress values. For smaller values, lower $n$ leads to higher stresses, while beyond 1 the behavior is reversed.

The slopes of the micro-milling forces were obtained by applying a chi-square fit to the data points with $UCT > 2 \, \mu m$, also taking into account the respective error bars. Thus, points with small error bars have greater weight in the fitting procedure than those with larger error bars, as explained in detail in Vernes et al. (2012). These slopes over the $UCT$ as a function of the yield stress are shown in Fig. 8 (a) including additional data points for $\sigma_Y = 100 \, MPa$ to better represent the region of steep increase of the slope at small values of the yield stress. As already seen in Fig. 7 (a–b), the slope of the force curves is higher for the cutting forces than for the tangential ones. The slope of the cutting force indicates saturation behavior. As can be expected for yield stresses tending to zero, the cutting force will remain almost constant independent of the $UCT$, leading to slopes close to zero. For very high yield stresses, the slope is expected to decrease its rate, although much higher yield stresses for steel would be non-physical. These results indicate that for steels with similar hardening behavior, i.e., those exhibiting uniaxial stress–strain behavior that can be modeled using a similar set of Johnson-Cook material parameters and only differing in the yield stress, the latter can be determined by measuring the cutting forces during micro-milling of two sufficiently large $UCT$s and determining the slope of this curve.

Figure 8 (b–c) summarizes the results of the variation of $B$ and $n$ as the slope in the linear range of the cutting and tangential forces over the $UCT$ as a function of $B$ and $n$. As observed in the individual plots, the increase in slope as function of the hardening parameter $B$ is evident for the cutting force $F_c$. The curve seems to follow an exponential saturation, in a similar way as observed for the yield stress variation. By contrast, the variation of the slope for the tangential force is negligible, even though an exponential
saturation seems to fit the data. The slope behavior as a function of the hardening exponent is substantially different. The slope of the cutting force over $UCT$ remains fairly steady within the evaluated parameter range, which is believed to comprise the plastic deformation behavior of most steel grades. Also in this case, the slope of the tangential force shows only a small dependence on $n$. What is surprising is the decrease for higher $n$ values due to the different hardening behavior of metals with increasing $n$ values at plastic strains below and above one, as mentioned earlier.

5.3. Discussion

Computational tools such as FEM or the MPM presented here are very powerful, but rely on material models that contain parameters for performing accurate calculations. The determination of the material parameters under the severe conditions occurring during micro-milling in terms of plastic strain, strain rates, and temperatures is not trivial, even under well-controlled lab conditions. To this end, extensive numerical simulations were performed in order to investigate the relation between material parameters and cutting forces during micro-milling of steel. For this contribution, a material point method was implemented. The method is 3D and, besides calculating stresses and temperatures using a visco-plastic strain-rate-dependent Johnson-Cook model, can intrinsically account for material separation and damage, making it specially suitable for modeling machining processes such as micro-milling. In general, MPM is more efficient when compared to conventional FEM simulations, since the time-step size is not directly controlled by the deformation state. In contrast, in FEM the critical time step becomes very small for heavily distorted elements, as it is very common when simulating machining processes. The only way to avoid distorted elements is by using remeshing strategies, which are rather time-consuming processes. Thus, MPM is intrinsically much more suitable for solving problems dealing with large deformations than FEM. However, an actual real-world comparison between these two methods in terms of computational cost will be heavily influenced by the implementation efficiency of the program so that such a comparison, besides comparing methods, will also include many other variables affecting computational performance. Therefore, a direct comparison is beyond the scope of the present work and would add little value to the present work.

It was verified that the simulations provide reliable results by comparing the calculations with data
available in the literature obtained using the well-established finite element method. The comparison showed
an excellent agreement between the cutting forces calculated by MPM and FEM for several uncut chip
thicknesses. The maximum chip temperature was slightly underestimated, but it is pointed out once more
that such maxima are prone to high variance due to numerical instabilities. After verifying the MPM
model, the model was systematically used for predicting cutting forces and chip temperatures as function of
yield stress and hardening parameters during micro-milling. The parameter range for the yield stress and
hardening parameters $B$ and $n$ was selected with the aim of covering the plastic behavior of most steels. The
goal of this selection was to investigate their impact on the cutting and tangential forces in an attempt to
discover methods for estimating plasticity parameters by merely measuring the forces during micro-milling.
To this end, first cutting and tangential forces were correlated with the $UCT$ for several values of the yield
stress $\sigma_Y$, the hardening coefficient $B$, and the hardening exponent $n$. The resulting behavior reproduces
the double-exponential function proposed by Afazov et al. (2010), characterized by a rapid increase of the
micro-milling forces for small values of $UCT$, followed by a steady, linear increase as function of the $UCT$.

The slope of the linear range varies depending on the plastic behavior of the material being simulated.
Based on this, the slope could be directly correlated with each individual hardening parameter. This means
that for a steel where two of the plastic parameters are constant and only one of them varies, for example
steels with identical or similar hardening behavior but different yield stresses, the value of the yield stress
could be simply determined by measuring the cutting force during two micro-milling measurements at
different $UCT$, determining the slope of the curve and obtaining the sought yield stress of the steel by
interpolation from Fig. 8. A similar approach may be valid for the hardening parameters $B$ and $n$.

A large effort has been previously made by several authors to develop methods for identifying these
material parameters during micro-milling. The applied methods are numerically complex and, until now, no
method has been established to this end. The present work indicates that such a method may exist, but that
contrary to the mainstream opinion, such a determination may require not one but two micro-milling steps
under different uncut chip thickness conditions. The approach is still simple enough, but requires further
work to be able to determine the impact of one parameter when simultaneously modifying a second one.
6. Conclusion

In the present work, a novel meshless 3D material point method for simulating the micro-milling process was developed and implemented. The model is intrinsically able to account for very large deformations and material detachment without the need for re-meshing and thus increasing computational power. Despite its low computational cost, the model can successfully reproduce the cutting forces and chip temperatures predicted by finite element simulations. Moreover, the experimentally measured cutting forces that occur during micro-milling are in good agreement with the simulated results.

The computational efficiency of the MPM model is exploited for investigating the relation between hardening behavior and micro-milling cutting forces using extensive meshless 3D simulations. The results showed that the cutting force as a function of the uncut chip thickness is characterized by a rapid initial exponential rise followed by a linear regime. This approach relies on considering the slope of the linear regime as a function of either the yield stress or the hardening parameters. By knowing this functional relationship, the unknown yield stress of a steel with a given hardening behavior can be determined by measuring the cutting force for two distinct uncut chip thicknesses, provided they are large enough to be located in the linear regime.

The method is straightforward and has the main advantage that material parameters are determined under the same conditions of strain, strain rate, and temperature as in the micro-milling process, thus ensuring the reliability of subsequent simulations. The method can be extended in order to address the impact of modifying one material parameter on the remaining ones.

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