THESIS FOR THE DEGREE OF DOCTOR OF PHILOSOPHY IN SOLID AND STRUCTURAL MECHANICS

Modeling of cast iron materials related to machining simulations

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Abstract

A microstructure level simulation model of cast iron machining based on micrograph image analysis has been developed. The simulation tool has been developed for the orthogonal machining process involving 2D representations of a range of cast iron microstructures. The benefits achieved from this approach are: a better understanding of the machinability of the work-piece material related to its composition and microstructures, and qualitative predictions of e.g. the cutting force connected to a variation of the microstructural properties. Compacted graphite iron was taken as a prototype material due to unsolved issues regarding the machining of this type of cast iron in industry. As to the modeling, focus is placed on the pearlitic phase since it is the dominating constituent with respect to strength, and the continuous deformation behavior is described using the Johnson-Cook (JC) visco-plasticity model. Various formats of this model, using both hyperelastic-inelastic and hypoelastic-inelastic formulations, have been used to investigate possible differences in response and computational efficiency. In order to further describe the material degradation during machining, a continuum damage evolution is proposed as an enhancement of the JC model. Finite element results obtained from many simulations have been compared to machining tests with promising results. However, a severe mesh dependence has been observed in the simulations caused by the local damage modeling. A special investigation of this mesh dependence has been undertaken based on the resulting behavior of the Johnson Cook (JC) plasticity model combined with two different types of damage formulations. The results show a similar extent of the mesh dependence for both damage models, and that the viscous regularization effects, due to rate dependence of the model, are absent. As a remedy to the observed mesh dependence, the final contribution is concerned with ductile dynamic fracture modeling using FE-element embedded discontinuities. To characterize the homogenized continuous/discontinuous macro-behavior, a discontinuous enhancement is proposed at a sub-scale based on homogenization theory. In the corresponding FE-application, localized cohesive zone damage is kinematically realized as an element embedded discontinuity, which is introduced elementwise, thereby facilitating the model implementation in standard FE packages. In the considered numerical examples the proposed continuous/discontinuous ductile fracture modeling exhibits no significant element size dependence.

Keywords: Microstructure, Machining simulation, Johnson Cook plasticity, Fracture modeling, Calibration, Hypoelasticity, Hyperelasticity, Dissipation, Mesh dependency, Embedded discontinuity

till Oskar och Stella

Preface

The work presented in this thesis was carried out during 2007–2013 at the Department of Applied Mechanics at Chalmers University of Technology. The research was initially financially supported by Volvo Powertrain Corporation and The Knowledge Foundation (KK-stiftelsen). The second part of the work has been performed within the Swedish national research program FFI (Strategic Vehicle Research and Innovation).
I would like to express my deepest gratitude to my supervisors Professor Ragnar Larsson and Assistant Professor Martin Fagerström for their patience, guidance, endless enthusiasm and always door open for project discussions and questions. I wish to acknowledge all my co–workers at the Department of Applied Mechanics and involved colleagues at Department of Materials and Manufacturing Technology.
Most of all, I would like to thank my wife for supporting me and giving me the strength during all these years.

Göteborg in April 2013

Goran Ljustina

Thesis

This thesis consists of an extended summary and the following appended papers:

Paper A
A FE based machining simulation methodology accounting for cast iron microstructure
G. Ljustina, R. Larsson and M. Fagerström
Submitted for international publication

Paper B
Hypo- and hyper-inelasticity applied to modeling of compacted graphite iron machining simulations
G. Ljustina, M. Fagerström and R. Larsson
European Journal of Mechanics A/Solids 37, 57-68, 2013

Paper C
On the pathological mesh dependency in FE computations based rate sensitive continuum damage models
G. Ljustina, M. Fagerström and R. Larsson
To be submitted for international publication

Paper D
Ductile dynamic fracture modeling using embedded discontinuities in CGI machining simulations
R. Larsson, G. Ljustina and M. Fagerström
To be submitted for international publication

CONTRIBUTIONS TO CO-AUTHORED PAPERS

Paper A

- Predominantly responsible for planning the paper
- Predominantly responsible in theoretical development of the paper
- Prepared and carried out numerical simulations
- Wrote major parts of the paper

Paper B

- Took part in the planning of the paper
- Took part in theoretical development of the paper
- Took part in numerical implementations
- Prepared and carried out numerical simulations
- Took part in writing the paper

Paper C

- Predominantly responsible for planning the paper
- Predominantly responsible in theoretical development of the paper
- Prepared and carried out numerical simulations
- Wrote major parts of the paper

Paper D

- Took part in the planning of the paper
- Took part in theoretical development of the paper
- Took part in numerical implementations
- Prepared and carried out numerical simulations
- Took part in writing the paper

Contents

Part I
Introduction

1 Motivation and background

In the heavy truck industry today the improved fuel economy and the low emission demands are constantly increasing. These demands can be met by a combination of increased combustion pressure and reduced engine weight. Traditionally, gray cast iron is used as a cylinder block material, but it is unable to withstand the peak combustion pressures that in the modern applications are exceeding 200 bars. Thus, gray cast iron with its inferior material properties, in some cases, is replaced with a stronger material with sufficient thermal conduction and damping capacity. The material that is best suited to meet these requirements for engine manufacturing is a Compacted Graphite Iron (CGI). However, the big drawback connected to recent introduction of CGI in production of heavy diesel engines is the fact that it is more difficult to machine than gray iron. This difference primarily depends on shape, size and quantity of the graphite grains in the microstructure [11]. Machining in general is a complicated process where the work piece material is subjected to the large plastic deformations and damage at high deformation rates and temperatures. In the case of heterogeneous materials like cast iron the interaction between different phases in the microstructure leads to the additional complexity of the deformation process. Machining results, characterized by chip shape, amount of the plastic deformation, damage, temperatures, stresses, friction, etc., are dependent on work piece material properties and machining conditions at hand. Work piece material properties are, in turn, governed by chemical composition and microstructure. In machining, the proper management of the involved process parameters is of major importance. For example, knowledge of cutting forces, chip morphology, temperatures, surface roughness, residual stresses and surface integrity, etc., is an important prerequisite for reducing machining costs and improving product quality. The manufacturing industry currently addresses these issues by increasing the implementation of simulation tools for the specific operations included in their processing chain. In order to obtain reliable simulation results the modeling of every aspect mentioned above demands attention and careful consideration. The cost of machining cast iron can be as much as ten times the cost of the casting for heavily machined parts [47] which illustrates the importance of manufacturing process optimization via simulation.

2 Purpose, goal and limitations

As a consequence of the emerging challenges with respect to machining of cast iron (and CGI specifically), this project was started in 2007 with the purpose to develop a simulation tool and carry out representative numerical simulations of the orthogonal machining process. The influence of micro-structural material properties should be accounted for in order to gain a better understanding of materials composition and microstructure on machinability. Using the FE-representations of the resolved microstructure in the simulations is demanding from the computational point of view. Thus, one of the main goals have been to develop the appropriate computational framework to devise a machining simulation methodology applicable from the industrial point of view. This implies the application and/or development of robust and computationally efficient routines with appropriate constitutive model formulations, either available or easy to implement in commercial softwares. Another very important goal demanding special attention in machining simulations of the heterogeneous material is the realistic representation of damage and crack propagation. The aim is also to establish the simulation model with the microstructure representations based on real microstructures of the relevant cast iron material.

It became clear very early in the project that due to the complexity of the challenge at hand certain limitations had to be made. For example, the simulation model created in the early stages of the project pertains to the orthogonal machining simulation. The orthogonal machining situation where the cutting edge is perpendicular to cutting direction generally can be represented by a two-dimensional simulation model. In case of the heterogeneous material where the microstructure is resolved employment of the two-dimensional model results in simplified representation of the material distribution in the third dimension. This means that in the two-dimensional representation of the microstructure there is no variation of the material in the out of plane direction which leads to unrealistic amplification of the phase material properties behind the corresponding areas.

Further, when it comes to material properties of the different constituents involved in the microstructure a special attention is placed on the (strongest) pearlite phase. The process of determining the material properties of the pearlite was based on information found in the literature [32, 16, 2]. No own experiments has been conducted due to limited resources. The graphite phase properties has not been thoroughly investigated. Instead the characteristic shape of the graphite grains is considered to be more important. The ferrite phase was not included in FE representations of the microstructure due to small amounts of this phase in the cast iron materials used in relevant industrial applications. The tool is represented by a rigid body and the Columb model is used to model friction between the tool and the work piece material.

The simulations realized during the first part of the project has indicated a mesh dependency in the model. The solution of this important issue is then adopted as one additional challenge of the project and it has been dealt with to this end.

3 Machining simulation of cast iron microstructure

3.1 Material properties and microstructure

For the truck engine industry, strength, thermal and damping characteristics of CGI, are mid-way between ductile and gray iron as illustrated in Table 3.1. CGI has higher

Table 3.1: Material properties of gray iron, CGI and ductile cast iron.

Property	*Gray*	*CGI*	*Ductile*
Tensile strength (MPa)	250	450	750
Elastic modulus (GPa)	105	145	160
Elongation %	0	1.5	5
Thermal conductivity (W/mK)	48	37	28
Relative damping capacity	1	0.35	0.22
Hardness (BHN 10/3000)	179-202	217-241	217-255

strength, stiffness and better fatigue properties than gray iron and it has at the same time more favorable thermal conductivity and damping capacity compared to ductile iron.

In CGI and gray iron the microstructure primarily consists of a mixture of pearlite, ferrite and graphite phases, as shown in Figure 3.1. The graphite phase in the CGI appears, in a two dimensional cut, as "worm-shaped" or as consisting of randomly oriented vermicular particles. The "worms" are in reality connected to their nearest neighbors and form a complex three-dimensional coral-like morphology. For comparison, in gray iron, the graphite is formed as flakes that have a smooth surface and sharp edges that act as sites for stress concentration and crack initiation and makes the material weak and brittle. The shape of the graphite grains and the pearlite content plays an important role in determining mechanical properties of cast iron like strength and hardness. Other material properties, such as Poisson's ratio or thermal expansion, are effectively constant over a wide range of microstructure and chemistry [10].

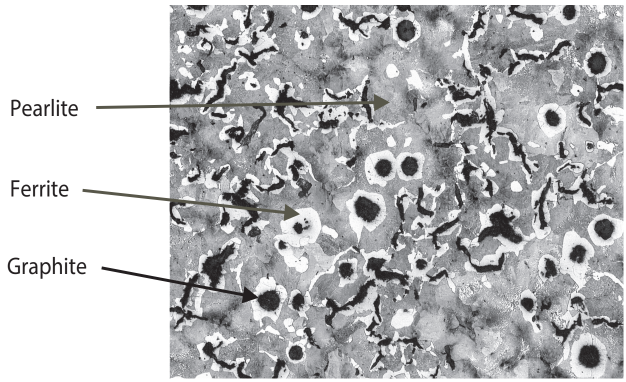

Figure 3.1: *Example of CGI microstructure*

3.1.1 The graphite phase

The characteristic coral-like morphology of graphite in CGI, together with the rounded edges and irregular bumpy surfaces, lead to strong adhesion between the graphite and the "steel" matrix, consisting of pearlite and ferrite phases. As a consequence, the crack initiation and growth is reduced providing improved mechanical properties compared to gray cast iron [10]. The appearance of flake graphite (typical for gray iron) in the microstructure leads to decreased mechanical properties of CGI by 20-25 %. The graphite in CGI material also appears to some extent as nodular (spheroidal) particles, cf. Figure 3.1, which is a typical shape for graphite grains in ductile iron. Nodularity is one of the most important micro structural parameters that affects mechanical properties of the CGI material. This is defined in a 2D projection of the microstructure as the area fraction of graphite that is considered to be close to round in shape eq. (3.1) [41].

$$Percentage\, of\, nodularity = \frac{\Sigma Area_{nodules} + 0.5 \cdot \sum Area_{intermediates}}{\sum Area_{total\, area\, of\, the\, graphite\, particles}} \tag{3.1}$$

Generally speaking, the mechanical properties of the cast iron increase as the nodularity measure is increasing. However, when it exceeds 20% the thermal conductivity reduces which leads to poorer castability and machinability. Currently, an acceptable compacted graphite iron (CGI) should contain at least 80% of compacted graphite and less than 20% spheroid graphite with no flake graphite presence [11]. The nodularity level in CGI is controlled primarily by the cooling rate which unavoidably varies in casting sections. This means that nodularity and also strength are higher in thin sections and lower in thick sections, which is an advantage in engine design. The effect of varying the nodularity parameter during the machining simulations of CGI microstructure is one of the main issues investigated in paper A.

3.1.2 The pearlite phase

Pearlite consists of ferrite (almost pure iron) and cementite (hard and brittle iron carbide) lamellas. The mixture of these two phases makes the pearlite phase strong and durable. The pearlite content is considered to be one of the most important microstructural parameters regarding influence on the ultimate tensile strength of cast iron materials [4]. Increasing the pearlite content increases the tensile strength and hardness of the material. Looking further down in the microstructure of the pearlite, the distance between cementite lamellas is also an important micro-structural parameter affecting the mechanical properties of the pearlite phase. A decrease of the distance between lamellas caused by a higher cooling rate generally leads to higher strength and hardness of the pearlite phase. However, according to [4] the interlamellar distance in pearlite does not have as large effect on the material physical properties or machinability as the pearlite content.

3.1.3 The ferrite phase

Ferrite is a ductile material with a relatively low yield strength. Usually, ferrite forms concentric shells around graphite grains (see Figure 3.1) due to depletion of the carbon as

Table 3.2: Material parameters of involved constituents of the microstructure.

Parameter	*Graphite*	*Pearlite*
Elastic modulus E (GPa)	25	190
Poisson's ratio, ν	0.2	0.3
Density ρ (kg/m^3)	2560	7850
Specific heat C_v (J/kg K)	837	452
Isotropic heat conduction k (W/mK)	130	52
Factor η in energy equation	0.9	0.9
Hardness (HV)	60	300
Yield strength σ (MPa)	125	514
Strain hardening exponent n	0.1555	0.136

it diffuses into the graphite nodules. The CGI used in the heavy truck engines and in the related machining experiments [5] contain only a small amounts of ferrite (less than 5 %).

3.2 Machining simulation of cast iron

During machining, the materials are subjected to high strains, strain rates, temperatures and pressures. In order to be able to properly describe the material behavior in the machining simulations, besides essential material properties like Young's modulus, Poisson's ratio, density etc., "dynamic" properties valid at the high strain rates have to be determined. The dynamic behavior is described by stress–strain curves obtained in laboratory tests at different strain rates and temperatures which can be used for calibration of material parameters. Another challenge is the proper modeling of the rather complicated tool–chip interface friction. Cutting forces, stress distributions and tool wear are greatly influenced by friction. As mentioned earlier, an important goal of this work and one of the biggest challenges is to, under present circumstances, realistically describe damage and damage evolution in a computationally efficient way.

Models for prediction of process parameters during metal cutting have been developed for over the past 60 years. Early analytical models by Merchant [29] and Oxley [35, 36] covered basic mechanics of metal cutting, using simplifying assumptions and mathematical relationships. More reliable and accurate models came with the computer-based simulations together with the finite element method in the early 1970s [46]. During the following few decades a number of new approaches and modeling methods have been developed as described in e.g. References [13, 26, 27]. Today the metal cutting processes can be described in a much more realistic manner and research involves simulations of non-conventional processes such as micro-scale cutting [7] etc.

One of the earliest studies on modeling the machining of cast iron with its heterogeneous microstructure containing pearlite, ferrite and graphite was presented by Chuzhoy et al. [7, 8]. Therein, the orthogonal cutting simulation carried out on a ductile iron microstructure was capable of predicting cutting forces, temperatures, stress–strain distributions together with evolving damage. The utilized technique was able to capture the effect of the material microstructure on machinability with the potential for alternative applications.

An example of a more recent investigations related to microstructure modeling is the work by Simoneau et al. [40] on chip formation in orthogonal turning of AISI 1045 steel. The approaches in the works by Chuzhoy and co-workers and by Simoneau and co-workers have large similarities to the approach adopted in the present work.

Despite all the additional challenges connected to machining simulations based on the resolved microstructure models compared to simulations on the homogeneous material representations, this approach has a great potential. The possibility to simulate the phenomena occurring during machining that are connected to the characteristic microstructure is one advantage. Another advantage is that, once the material properties of the relevant constituents have been determined, a variation of the heterogeneous material can be modeled and simulated without redoing the experiments to determine macroscopic material properties.

The alternative to resolving the entire microstructure is to make use of the "Computational Multiscale Modeling" strategy described in [24], which involves derivation of the local macroscopic constitutive behavior from the underlying microstructure by use of representative volume elements (RVE). In this way the stress-strain relationship on macro-level is obtained. Unfortunately, the graphite flakes are relatively large in relation to normal cutting depths during orthogonal machining operations. This implies that the scale separation assumption of the multiscale modeling approach is difficult to make, whereby this approach cannot be properly motivated in the present case. Furthermore, the use of the multiscale procedure would make it hard to study the characteristic crack propagation through graphite grains.

A central point in the modeling concerns the temperature modeling in conjunction with the proper modeling of energy dissipation. The principle of non-negative dissipation is central in solid mechanics, in particular, in conjunction with thermodynamical analyses of heat generation and temperature assessment as is in the e.g. machining simulations. The consistent heat generation is an advantage of the hyper formulations of the material behavior. As opposed to the hypoelastic–inelastic formulations, the basic idea in the hyperelastic-inelastic framework is to assume the presence of a stored energy function. However, the price to be paid using the consistent formulation is that these models are generally not as computationally efficient as those of the hypoelastic–inelastic framework. In hypo formulations, on the other hand, a description of the dissipated energy converted to heat is managed through in advance estimated inelastic heat fraction parameter determining the amount of the plastic work rate that is transformed into heat. A way to conform a more computationally efficient hypo formulated model with the thermodynamically consistent hyper-elasticinelastic framework, as proposed in paper B, is to use the same expression for the dissipation for the hypo framework as in the hyperelastic-inelastic case.

Metal cutting simulations have been modeled using different formulations. Model formulation refers to the way in which the FE mesh is associated with the work piece material. The Eulerian, Lagrangian, and the arbitrary Lagrangian-Eulerian (ALE) are the three main formulations. In the Eulerian simulations [45, 43, 22], the mesh is stationary, with the material flowing through the meshed control volume. The main disadvantage of the truly Eulerian formulation in machining simulation is the fact that the initial shape of the chip and the contact conditions must be known or assumed in advance which excludes the natural formation of the chip as the result of deformation. In this work the Lagrangian formulation is used, which means that the mesh is attached to the work piece material and the elements deform together with the material during cutting. The Lagrangian approach, used in t.ex. [38, 39, 23, 44], often leads to severe distortion of elements and introduction of both geometrical and material non-linearities which increases the computational load. The FE mesh in an ALE simulations, cf. e.g. References [21, 34], is neither fixed spatially nor attached to the material, instead, it is allowed to move more freely relative to the material [48].

The explicit time integration is used for the machining simulations due to its capability of simulating fast events with a reasonable execution time [1]. In the explicit procedure the response is integrated by using many small time increments. The largest time step is dependent of the highest natural frequency of structure and need to be small enough for the computations to be stable. The solution is built up by using the information from earlier time steps. No iteration procedure is required as in implicit integration scheme.

4 Failure modeling

This chapter is an attempt to explain some of the concepts frequently used in appended papers and to put the presented work into its context with respect to heterogeneous materials failure modeling, mesh dependency and its regularization.

4.1 Fracture modeling in metal cutting simulations

Despite the fact that the pearlite is ductile, CGI exhibits brittle behavior at the macroscopic level during machining. This is due to the heterogeneous nature of the material, where the characteristic shape of the brittle graphite induces the observed brittle response of the CGI at the macroscopic level. During machining of macroscopically brittle materials like gray iron and CGI discontinuous chips are produced. Simulation of the creation of discontinuous chips eliminates the possibility of using a predefined cutting plane, often used in continuous chip creation simulations based on a Eulerian formulation of the cutting problem. Pertinent to the Lagrangian approach, re-meshing techniques are often used, where the chips are not separated via the proper fracture modeling cf. Reference [25]. Instead, the focus is placed on the modeling of large continuous deformations (possibly combined with damage evolution), where large plastic deformations are combined with a continuous re-meshing scheme, resolving the cutting process. Consequently, a method appropriate in case of dynamic crack propagation typical for brittle materials should be used in order to enable the simulation of discontinuous chips formation.

As to the fracture modeling, we note that cohesive zone formulations are often combined with the eXtended Finite Element Method (XFEM), cf. Reference [30], the inter-element crack method, the element embedded crack band approach, or the element deletion method. In particular, the XFEM is a methodology for modeling cracks of arbitrary geometry, where the displacement field incorporates the discontinuity as additional terms in the displacement approximation, and modeling of the crack by separation along the element edges is the main principle of the inter-element crack method. An extension of the element embedded crack band approach is proposed in paper D of this thesis, where a discontinuous displacement field is allowed for the element subscale domain, like in the XFEM approach.

The element deletion method, used in machining simulations in papers A–C of this thesis, is one of the simplest methods for fracture simulation, where the crack is modeled by a set of deleted elements. In case of JC dynamic failure model [20], when the failure criterion is met at an integration point, all the stress components will be set to zero and that material point fails. In case of the continuum damage model [9] the evolving damage is causing progressive softening of the material that leads to failure. Element deletion (removal) of the element takes place as soon as its first integration point fails. Element deletion method, often used in industry, is chosen due to its simplicity and availability in commercial softwares.

4.2 Mesh dependence

The damage models used in this thesis are local, which means that they do not depend upon any action/variables at the neighboring material points. Under certain circumstances, this type of failure modeling is well known in the literature to produce severely mesh dependent results, corresponding to a lack of convergence of the fracture energy dissipation, as discussed in e.g. Reference [33]. In the case of the Johnson Cook dynamic failure criterion, including the sudden deletion of an element when the critical effective plastic strain is reached, the released energy due to deleting an element depends on the element size, which like in the continuum damage models causes mesh dependence. In the continuum damage modeling, when a material point starts to soften, its deformation may become localized to this material point and damage grows only in that point, resulting in additional softening. Eventually, this leads to the situation that the damage induced deformation becomes localized in a band of elements, whose width and direction depend on the used mesh. As the mesh is further refined the width of the localization zone becomes smaller and smaller, corresponding to zero fracture energy and infinitely brittle behavior of the structural response.

4.3 Visco-plastic regularization

There exists several different ways of dealing with the pathological mesh dependency. The usual ways to avoid or, at least, to reduce the mesh dependency, are e.g. nonlocal strategies, used in e.g. [3, 6], where the constitutive behavior is dependent of its neighborhood through introduction of the nonlocal variable (e.g. the equivalent plastic strain or damage). Another strategy is introduction of discontinuity by establishment of cohesive zone models, like the solution including the element embedded discontinuities presented in paper D.

A well known solution to the pathological mesh dependency problem is a visco-plastic regularization used by e.g. [12, 42]. This means that by introducing the the rate dependency in the plasticity model the increasing deformation rate in the softer element (with damage) makes element stiffer again which, in turn, prohibits the deformation to accumulate in one element. Since the Johnson-Cook plasticity model [19] includes rate dependence the natural solution to pathological mesh dependency caused by using the local damage models could be expected. The effectiveness of the regularization by rate dependency is controlled by an interaction of the viscosity, deformation rate and element size. Unfortunately, as shown in the simulations conducted in paper C, these demands were not fulfilled and mesh dependent results were obtained. In paper D, this issue is advanced further, by the introduction of element embedded discontinuities controlled by a cohesive zone law whenever the criterion for discontinuous bifurcation is arrived at.

5 Summary of the appended papers

5.1 A FE based machining simulation methodology accounting for cast iron microstructure

A modeling analysis methodology for the simulation of the orthogonal machining of CGI-material has been proposed in paper A. The heterogeneous microstructure of CGI is accounted for by a micro-level approach based on micrograph analysis of the actual CGI material. The material microstructure is thereby resolved on a grain level. A finite element model is established based on the micrographs (cf. Figure 5.1 for an example of the discretization of the CGI microstructure).

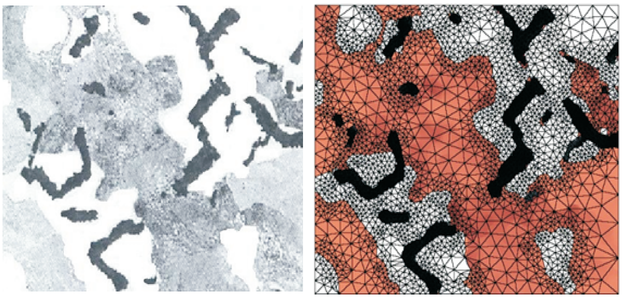

Figure 5.1: *a) Micro-graph representing CGI, b) corresponding FE-discretized graph based on the software OOF2*

The continuous deformation behavior of pearlite and graphite phases is described in paper A using the Johnson-Cook (JC) viscoplasticity and damage model [19], including temperature dependency. Most of the material parameters used in the simulation have been found in literature. The remaining parameters have been fitted in with respect to the observed behavior of the chip formation.

A quite extensive parametric study has been carried out involving micrographs with nodularity ranging from 0% to 50%. Comparison of trends between simulation and machining experiments based on the similar CGI material in a related project [5], which were not adapted for validation of two-dimensional orthogonal cutting simulations, was done. The predictive capability of the model regarding the nodularity induced increase of the cutting forces is remarkable. It was not possible to completely predict the experimentally observed increase of cutting force magnitude when lower cutting speed was used. Thereby, it appears that the true effect of elevated temperatures on the continuum response as well as on the critical fracture strain has not been fully captured by the present model. The presented model can be used to study the influence of primary phases in the heterogeneous microstructure of different types of cast iron on machinability.

5.2 Hypo- and hyper-inelasticity applied to modeling of compacted graphite iron machining simulations

In paper B, the difference regarding resulting behavior and computational efficiency between hypoelastic–inelastic formulations of the JC model based on Zaremba-Jaumann, Green-Naghdi and Oldroyd stress rates have been studied. The aim of the study was to elucidate possible differences in response in connection with uniaxial- and shear tests of the JC-model. The variants of hypo–elasticinelastic formulation of the JC model involving Zaremba-Jaumann and Green-Naghdi stress rates were also compared in machining simulations by looking at mean values of cutting force and maximum temperature. As an additional alternative, a thermodynamically consistent hyperelastic-inelastic formulation of the JC model has also been investigated as well as an additional version of the hypo-formulation based on Oldroyd stress rate that is consistent with the hyperelastic-inelastic modeling framework.

The simulations were carried out in ABAQUS/Explicit (version 6.9-2), cf. [1] according to the proposed modeling procedure from paper A. The hypo-formulation of the JC-model based on the Zaremba-Jaumann stress rate already exists as a built- in constitutive model in Abaqus. To facilitate the comparison, the remaining models were implemented in Fortran as separate user subroutines (VUMAT) to define the mechanical constitutive behavior of the material. During the calculations the main program calls the programmed user subroutine as described in Figure 5.2.

Simulations show that a hyper-elasticinelastic models are generally not as computationally efficient as those based on the hypo-elasticinelastic framework. A surprisingly small discrepancy in results based on different model variants from uniaxial and shear test simulations as well as machining simulations were observed. One exception is the comparison of maximum temperature values obtained from hypo- and hyper-elastoplastic models in the machining simulations which show a clear trend of lower temperatures for the hyperelastic–inelastic model. This trend is explained by the fact that the inelastic heat fraction η, defined by the default value of 0.9 in the calculations based on hypoelastic–inelastic formulation, is too big. This leads to the conclusion that the thermodynamically more consistent version of the Oldroyd stress rate based hypoelastic–inelastic model should be used in future machining simulations with the JC constitutive model.

Also, a set of JC material constants for the pearlite phase has been calibrated based on stress-strain data for rail steels found in literature [32, 16, 2]. The results from orthogonal machining simulations were also compared to the results from machining experiments

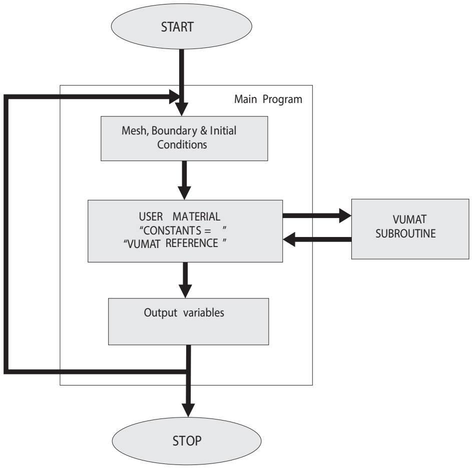

Figure 5.2: *Main program interaction with user subroutine VUMAT*

carried out in a related project [14]. A general trend of lower level of simulated cutting force and maximum temperature, as compared to the experimental findings, has been observed.

5.3 On the pathological mesh dependency in FE computations based rate sensitive continuum damage models

During the shear tests of the pearlite material conducted in paper B a different structural behavior was suspected when different element sizes were used for, in every other respect, the same conditions. This typical pathological mesh dependency behavior was manifested through a clear variation of the force-displacement curves, plastic strain distribution and crack patterns developing only through one row of elements regardless to element size. In paper C the pathological mesh dependency indicated in earlier simulations (paper B) has been investigated. In the investigation, two types of damage models were combined with JC plasticity and compared with respect to mesh dependency. The first damage model is Johnson Cook dynamic failure model [20] used also in papers A and B where the "damage" development does not affect the material response until the critical value of the effective plastic strain is reached. The second is a continuum damage model developed by Cocks and Ashby [9] and earlier successfully used in machining simulations of the cast iron material. The notion "continuum" stands here for the fact that damage development in this model is continuously affecting the material response. The investigation is conducted based on a series of 2D shear and tensile tests of a plane strain plate with pearlite material properties represented by FE models with different element sizes. The results show that, for both damage models, a similar extent of mesh dependency is obtained for both damage models. A possible regularization of the observed mesh dependency due to employment of the rate dependent damage models appeared to be low in case of element sizes, deformation rates and material parameters used in investigation. The paper is to be presented as invited lecture at "MekIT'13 - National conference on Computational Mechanics" on May 13-14, 2013 in Trondheim, Norway

5.4 Ductile dynamic fracture modeling using embedded discontinuities in CGI machining simulations

In paper D, we propose a ductile dynamic fracture modeling approach using FE-embedded discontinuities as a way of handling the pathological mesh dependency. This means that the localized cohesive zone damage is kinematically realized as an element embedded discontinuity, which is introduced element-wise, thereby facilitating the model developments in standard FE-packages.

Despite the overall impression from paper C that the Johnson-Cook dynamic failure model is behaving more consistently, the continuum damage model represents a more realistic behavior with continuous effect on material response leading to softening. Consequently, it is proposed to use a continuum damage approach on the basis of the Johnson-Cook (JC) plasticity model for the ductile continuous behavior up to the critical stress—strain states where the softening behavior caused by local continuum damage model starts (as described in Mesh dependency section) and produces a mesh size dependent results. Whenever a critical state has been diagnosed, a cohesive zone (CZ) is established inside the element. The energy dissipation is then confined to the development of a propagating CZ. The main new parameters introduced are essentially the fracture energies in mode I and mode II. Thereby, both the continuum damage development occurring before the critical state is reached and post critical CZ damage are considered in the formulation and defined separately.

To investigate the potential to eliminate pathological mesh dependence by the proposed element embedded discontinuity approach the numerical simulations of three different loading cases on a 2D pearlite plane strain plate (with different geometry and fewer elements than the plate models used in paper B and C) were conducted. For comparison with the standard continuum damage modeling, the calculations are carried out based on the same continuum model with or without the embedded cohesive zone enhancement of the elements.

Results from simulations, show that when the adopted element embedded discontinuity approach (where the cohesive zone enhancement of the model is added) the pathological mesh dependence is removed.

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- the "83rd Annual Meeting of the International Association of Applied Mathematics and Mechanics" on March 26-30, 2012 in Darmstadt, Germany
- the "European Congress on Computational methods in Applied Sciences and Engineering" on September 10-14, 2012 in Vienna, Austria

- the "25th Nordic Seminar on Computational Mechanics" on October 25-26, 2012 in Lund, Sweden

6 Concluding remarks and Future work

The two-dimensional machining simulation model created, involving the material behavior based on the Johnson-Cook model and the finite element discretization of the micro-structure as described in the first paper, serves primarily as a platform for further development. The process of the chip formation is dependent on the delicate interplay between ductile fracture, decohesion and plastic deformation. In order to obtain realistic simulation results, each aspect should be thoroughly investigated and modeled. The resolved micro-structure approach has the ability to illustrate the influence of the primary phases in the heterogeneous micro-structure on the deformation and failure during machining. For example, it is able to capture the characteristic behavior where the effective plastic strain and damage development are following the preferred path by developing between graphite grains. The proposed algorithm is general enough to be used for many different microstructures which is practical due to a variety of different cast iron materials used in industry.

In this work, besides the establishment of the simulation model, different alternatives of the elastic-inelastic constitutive frameworks were compared from the consistency and computational efficiency point of view. Also, a crucial issue of pathological mesh dependence has been investigated and a solution to it was proposed.

Despite the mentioned achievements of this thesis there is still a number of modeling issues and phenomena occurring during the machining of the cast iron that demands appropriate attention and remains to be addressed and developed in the simulation model.

- The friction at the tool-chip interface during cutting is a complex process and needs further development towards description of the stick-slip friction conditions, typically occurring during machining.

- One of the crucial tasks in the future is to further develop the adopted methodology for the representation of ductile fracture as induced by material softening and damage. This procedure needs to be further explored and developed with respect to the modeling of the proper fracture mode.

- Modeling of the cutting tool and its material properties in order to e.g. properly model heat transfer between work piece and tool.

- In order to fully understand the micro-structure influence on the chip formation, further improvements of the micro-structure representations are needed. Unlike more homogeneous materials, a special feature of the cast iron machining is the formation of segmented chips, where the fracture zone is partially characterized by decohesion/separation of graphite flakes or nodules from the matrix structure. This graphite/matrix separation, besides fracture of the graphite and pearlite, plays a significant part in the fracture process of the heterogeneous structure of the cast iron [31]. Modeling a separation of the graphite flakes from the matrix structure during machining is thereby an important aspect of future development.

- Considerable efforts were made to the determination of the Johnson-Cook plasticity parameters for the pearlite phase including the calibration based on experimental results found in the literature and also the experiments combined with inverse modeling. Due to the smaller amount of ferrite existing in the relevant cast iron microstructures this phase is neglected in the current work. Despite the small amounts it is possible that ferrite, with its ductility plays an important role and should be included in the models. A proper study of the graphite and ferrite material properties together with inclusion of ferrite in models is a future challenge.
- A further interesting research task is to develop a multi-scale procedure to capture the effect of the material micro-structure with respect to cutting forces, temperature and compressive stress in machined surface etc. In order to save computational effort while at the same time maintaining proper model representation, the material micro-structure can be resolved in the machining zone while at the same time a homogenized material response is considered away from the machining zone.
- The pathological mesh dependence present in the simulations is thoroughly investigated. One way of dealing with this mesh dependence problem is by introducing the embedded discontinuities on the element level. The proposed solution is implemented in Matlab and the remaining challenge is to make the routine more computationally efficient in order to implement it as an element routine in commercial software. Further developments are necessary to make the modeling approach more reliable and efficient.

Consequently, due to remaining modeling challenges, the model at its existing form is mainly a tool to study the trends rather than predict exact values of cutting forces, temperatures, etc. At the present moment only the qualitative comparisons with experiments are possible. The orthogonal machining experiments on CGI material with different nodularities, fitted for comparisons with two-dimensional simulations, are planned in order to validate the model. Planned machining experiments/simulations includes lower feed rates compared to simulations conducted in paper A. Lower cutting depth means that the longer finite element representations of the resolved microstructure can be used without increasing the total number of the elements compared to earlier simulations. This opens for simulation of formation of several chips (more than two) in each simulation and, thereby, a better statistical ground for determination of mean values of cutting force, temperature, etc.

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