# Zoning Method for Efficient Material Properties Calculation

J. Kronsteiner and E. Kabliman
*Leichtmetallkompetenzzentrum Ranshofen GmbH, AIT Austrian Institute of Technology GmbH, Lamprechtshausenerstr. 61, 5282 Braunau am Inn - Ranshofen, AUSTRIA.*

## Abstract

When material models are enhanced by calculating additional effects such as microstructure evolution for every Gauss point and time step, considerable numerical effort must be expected. Interfacing third-party software from within user defined material subroutines can even be more time consuming. In many applications, however, considerable parts of the material domain give similar results. Strain, strain rate and temperature are the most important properties for the material behavior. During the thermo-mechanical processing such as rolling and especially extrusion, material deformation is concentrated in small areas. This means that strain, strain rate and thus temperature remain almost constant for large parts of the material during most of the simulation runtime. The idea behind the zoning method proposed in present work and implemented into LS-DYNA® user defined subroutine is to calculate material properties only once for an individual zone. By adaptively subdividing the material domain due to e.g. strain, strain rate and/or temperature results, runtime used for calculation and interfacing of third party software can be effectively saved. A comparison between history variables from the last call of the zoning method with current values can be even used to reduce the number of calculations over time. Elements are dynamically clustered using adaptive zoning and element iteration is thus reduced to elements with evolving values. For elements without major changes of relevant quantities or sufficiently small deviations to already computed data, existing values are used. The effectiveness of the proposed zoning method is demonstrated for a case of 2D compression test of a cylindrical sample. A cylindrical specimen made of a standard AA2024 alloy is compressed at elevated temperature to a certain degree. For calculation of a flow stress an in-house dislocation density based model is implemented into a user-defined elasto-viscoplastic material model. Based on the elemental dislocation density, the material domain is separated in individual zones and calculated results are mapped to all elements covered by the respective zone. In the end, the third-party software (herein MatCalc©) is called to calculate the local fraction of precipitates in a given zone. The results have shown that it is possible to consider micro-chemistry at reasonable costs.

## Introduction

The so-called “Zoning” method is a spatial clustering technique which helps to reduce the numerical effort in FEM simulations by taking advantage of quasi-homogeneous zones inside a deformed part. In many forming operations, deformation is concentrated in a very small area compared to the overall part size. In rolling, the deformation is performed inside the rolling gap. In metal extrusion, the major part of the deformation happens inside the die. In both cases, the deformation zone at a certain point in time is only very limited compared to the overall part size. For certain properties which are only affected by the material deformation, it is reasonable to calculate only the affected areas. One way to reduce the numerical effort is to recalculate numerically expensive properties only if the change of major input parameters is greater than a specified limit and only for elements which are affected by those changes. To still obtain a good resolution, a spatial subdivision can be a solution.
The method proposed in present work is based on the idea of Clustered Generalized FEM (GFEM) published in [1]. In there, a much more general approach is described to reduce the number of elements by clustering elements with similar properties. Clustered GFEM is a very basic technique which can be applied to all properties of the whole FEM model. This is achieved by defining a new shape function for the clustered Partition Of Unity, basically reducing the degrees of freedom. A much simpler approach was used by [2] for the use of complex simulation models in optimization loops. The authors have spatially subdivided the simulation model according to pre-simulated results and thus reduced the computational effort for multiple calculations during optimization. In [3], the authors have applied a spatial clustering technique for the equivalent plastic strain in a torsion test of a quadratic beam. Even in this very complex deformation example where the whole part is affected by the deformation, the number of calculations could be spatially reduced from 12168 elements

to 9 clusters in static clustering. In dynamic clustering, there is also the possibility to evolve the clusters over time which means that if the input parameters have the same value at the start of the simulation, only one cluster is created. When parameters evolve over time, existing clusters are split in order to satisfy the criteria for each individual cluster. Therefore, the computational gain is especially high at the start of the simulation and as more clusters are added during deformation, the acceleration is reduced. The number of clusters compared to number of elements for the dynamic clustering was between 2119 and 6013 clusters compared to 12168 elements. The gain in time was between 16 and 4, depending on the number of clusters. Especially for the dynamic clustering, the threshold for splitting has a huge influence on the number of clusters and thus the gain in time. The authors of [3] have compared the results for effective plastic strain with results from a reference Hierarchical Multi-Scale model and found that the relative error due to the clustering was between 0.7 and 0.1 % depending on the number of clusters and in the case of dynamic adaptive clustering also on the threshold for splitting of clusters.
In present work we would like to focus on simultaneous evolution of local microstructure and microchemistry and thus the coupling of finite elements with the thermo-kinetic modeling is required. In order to perform the calculation of precipitation distribution we have chosen the MatCalc© of MatCalc Engineering GmbH. The goal of the present work to reduce the computational effort and the effort for interfacing between LS-DYNA user-defined subroutine and third-party software. It is expected that numerical gain of the proposed zoning method may be even greater in comparison to above mentioned techniques since the considered example involves calling a third-party code. This means that the reduction of elements to the number of clusters also reduces the effort of interfacing between different software packages.

## Zoning method

The idea behind the zoning method is subdivide the mesh into certain zones with similar values based on the results of certain major properties. Those zones can be defined flexibly during runtime by defining certain maximum zone sizes and if results exceed those limits, a new zone is created automatically. Over time, the evolution of zones helps to reduce the numerical effort as well, since at the start of deformation most properties are evenly distributed and therefore only very few zones suffice to represent the full resolution model. Over time, when influencing properties evolve, the number of zones is automatically increased.
At the moment, the method is implemented such that zones are created based on dislocation density values calculated by the in-house microstructure model ([4], [5]) implemented in LSDYNA® UMAT47v. During each timestep and for each individual element, mean dislocation density is calculated based on the material deformation. When the maximum values for the mean dislocation density exceed the specified limit of the zone with the highest number, a new zone is automatically created which inherits the history of its ancestor. Zoning is implemented as a separate subroutine in LS-DYNA which is only called if the change of maximum dislocation density compared to the last call exceeds a predefined limit. Since a vectorized user-defined material model is used, UMAT is called for a certain block of elements. It is thus necessary to first collect the results of all elements into a global array. If the change of dislocation density between two calls is sufficiently high, Zoning is called after the element loop and has access to the results in the global array. Based on the elemental dislocation density values, elements are clustered in individual zones. As already mentioned in the introduction, if the deformation occurs very localized, only very few zones can suffice to obtain a representative description of the current dislocation density distribution. For every zone, mean values of the major parameters used for simulations of the precipitation kinetics are calculated. In the current implementation, temperature, strain, strain rate, dislocation density and grain size are considered and a thermo-kinetic modelling of phase distribution by using MatCalc is called for those values. In order to minimize the time lag between loading the necessary script in MatCalc, the calculation and finally receiving the results, a fully initialized session is already started when initializing LS-DYNA and additional sessions are started when new zones are created inside the zoning subroutine. MatCalc is based on a 1-dimensional approach and thus benefits from the interface by providing results for a higher-dimensional model. The resulting new values for the material parameter $\chi$ are then imported

in LS-DYNA UMAT for every zone. Finally, those values are redistributed to all elements inside the individual zone and saved as a history variable in LS-DYNA. Basically, the above described method can be applied to any property calculated inside a user-defined material model. The basic steps are illustrated in *Fig. 1*.

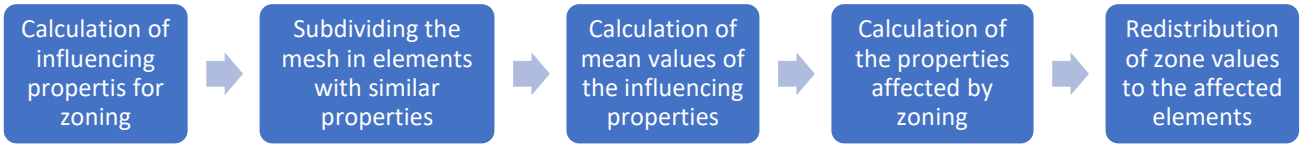


Fig. 1: Schematic illustration of the proposed zoning method.

## Show case – hot compression test

The proposed zoning method was applied to a simulation of the hot compression test performed inside the deformation dilatometer (DIL 805 A/C of Texas Instruments). A specimen made of a standard AA2024 alloy of 5 mm diameter and 10 mm length was compressed at a fixed mean strain rate and temperature and force results were recorded. This test is usually applied for the determination of flow stress over true strain for a certain alloy at a predefined temperature and strain rate. A 2D axi-symmetric model was used in a thermo-mechanical calculation. An explicit mechanical solver combined with an implicit thermal solver using SMP in LS-DYNA R910 was applied. Adaptive remeshing was not used in this example, however the proposed method is also compatible with remeshing techniques in LS-DYNA. The main material and process parameters are summarized in *Tab. 1:*

*Tab. 1:* Major initial material and process parameters for the hot compression simulation.

| **t** | **T** | $\dot{\varphi}$ | $\varphi$ | $\rho_0$ |
|---|---|---|---|---|
| 10 s | 490 °C | 1.0 | 1.0 | 1.0E11 $m^{-2}$ |

where **T** is the deformation temperature, **t** is the duration of the isothermal heat treatment before the deformation, $\dot{\varphi}$ is the mean strain rate, $\varphi$ is the mean true strain, $\rho_0$ is the initial dislocation density. . In order to account for possible dissolution of the precipitation phases (herein Cu- and Mg-containing phases) at the deformation temperature, we introduce a parameter, $\chi$, which is reverse proportional to the fraction of solute atoms, $f_i$:

$$\chi = \left( \sum_i f_i^n \right)^{-\frac{1}{n}} \tag{1}$$

In Equation (1), *n* is the number of relevant alloy elements. During the phase dissolution, the fraction of solute atoms in the Al-matrix will increase and the solute atoms will act as obstacles for the motion of dislocations and impede their annihilation. Therefore a deformed material will be less recovered. All the values given in *Tab. 1* were calculated by the MatCalc toolbox and used as initial values for all elements at the start of the simulation. Material parameters for the mean dislocation density based flow model were determined by a parameter fitting based on the flow curves determined from the hot compression test inside the deformation dilatometer (DIL 805 A/C of Texas Instruments).

**Results from numerical simulations**

The following results show how zones are formed based on values of mean dislocation density. The consideration of the precipitation kinetics by calling a third-party software (MatCalc©) for every timestep and element would require enormous computational effort. Especially since in this early stage of the feasibility study, very crude interface methods were used. The proposed zoning method offered an ideal platform for minimizing the interfacing effort while still giving reasonable results. First, the results for the effective plastic strain and temperature are given in Fig. *2*. As can be seen from Fig. *2*(a) the distribution of plastic strain results has a characteristic X-shape, while temperature increase due to compression is concentrated in the center of the specimen (see *Fig. 2*(b)). It is clearly visible that for a mean plastic strain value of 1.0, the local strain might achieve the values from zero up to 2.0.

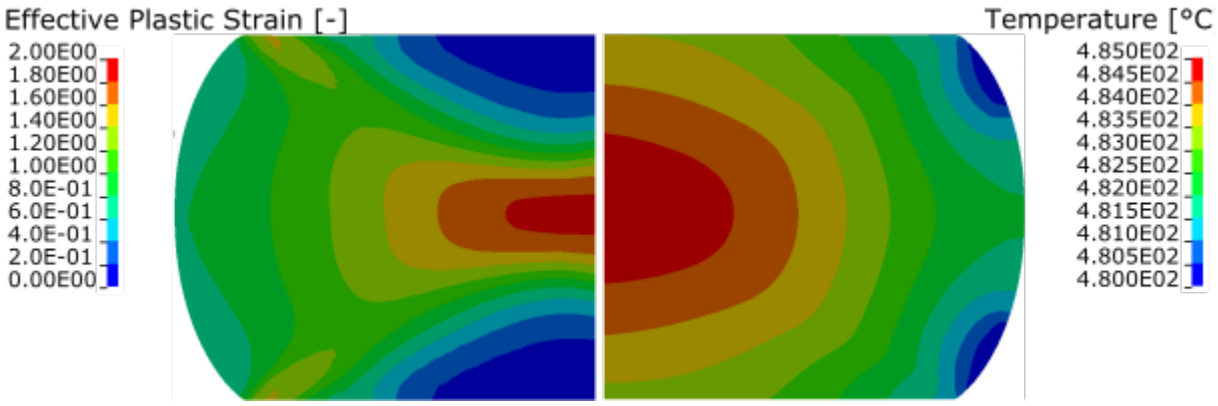


Fig. 2: Results from the hot compression test simulation for plastic strain (a) and temperature (b) .

Dislocation density and effective stress are influenced by plastic strain, strain rate and temperature. Thus a similar distribution was expected. Fig. *3* shows the similarity for dislocation density (a) and effective stress (b).

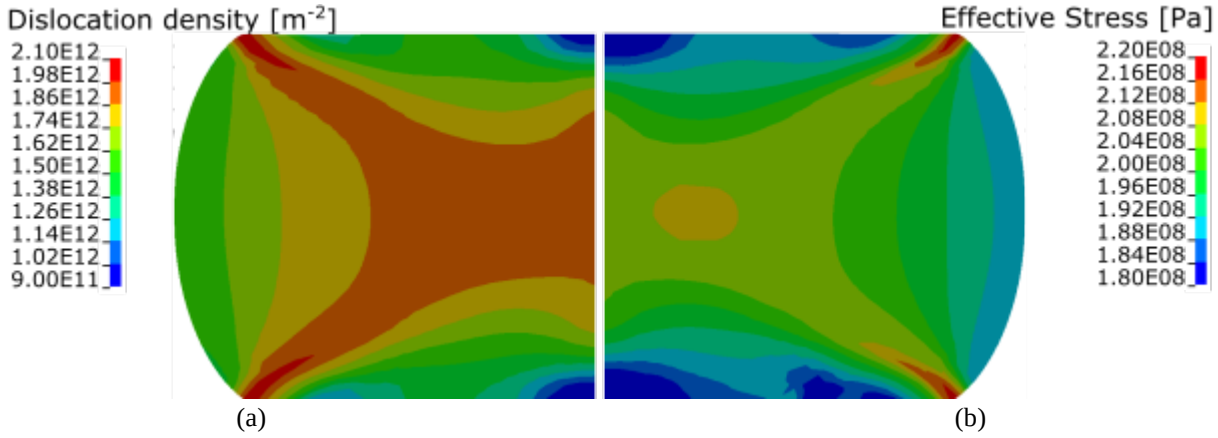


Fig. 3: Results from the hot compression test simulation for dislocation density (a) and effective stress (b).

In Fig. *2* and Fig. *3* it is clearly visible that only very few areas with considerably different values of major parameters occur. This circumstance justifies the reasonability of zone definition, which is illustrated in Fig. *2* (b). When performing the thermo-kinetic modelling by MatCalc for given zones a slight change of a material parameter, $\chi$, is observed. It is reverse proportional to the fraction of solute atoms and thus its change might

indicate the change in the fraction of phases. Since a slight increase is observed one might expect the dissolution of some phases (herein Cu- and Mg-containing phases).

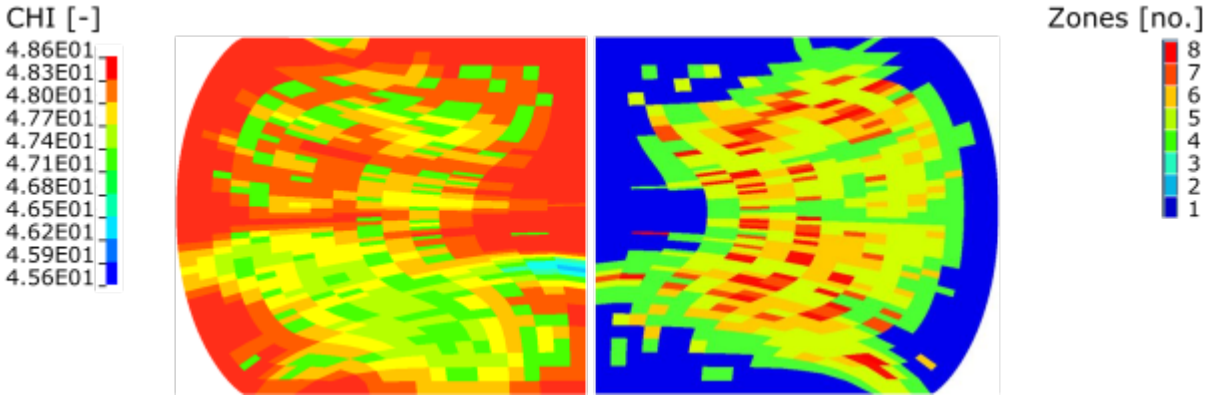


Fig. 4: Distribution of material parameter χ (a) based on the defined zones (b).

The increase in numerical effort between considering the simultaneous thermo-kinetic modeling using zoning and neglecting it, is limited. Although the presented implementation is only a very simple version of the planned method, the increase in calculation time is already reasonable. By using individual MatCalc sessions for the individual zones the calculation was parallelized and accelerated. When communication with a third-party software and the crude sorting algorithm are considered, an increase from 18 min to 6 hours in calculation time with maximum 14 zones is still acceptable. Without zoning, even for such simple model, the calculation of precipitation kinetics for all elements would increase the calculation time by a factor of several times of the number of elements.

## Conclusion and outlook

In addition to mean dislocation density based models of the flow stress, static recrystallization and grain growth, the calculation of change in local microchemistry (precipitation distribution) might bring more insight on the microstructure development during the thermo-mechanical processing, such as warm forming and heat treatment operations. However, this is related with a huge increase of computational effort. The proposed method shows a considerable potential for reducing the additional numerical cost of element based properties. By adaptively spatially clustering elements, properties are only calculated for each individual zone instead of each element. This is especially beneficial when large areas of similar influencing parameters or very localized deformation are observed.

Still a major restriction of the current implementation is that zoning is only based on dislocation density. Only temperature, strain rate, strain, dislocation density and grain size of the currently considered zone are thus considered. Additional material properties such as size and number of dispersoids should be added in future.

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