On the **Contribution** of Grain Boundary Sliding--type creep to *Firn Densification*--an Assessment using an Optimisation Approach

Timm Schultz¹, Ralf Müller¹, Dietmar Gross², and Angelika Humbert³,⁴

¹Institute of Applied Mechanics, Technische Universität Kaiserslautern, Kaiserslautern, Germany
²Division of Solid Mechanics, Technische Universität Darmstadt, Darmstadt, Germany
³Alfred-Wegener-Institut Helmholtz-Zentrum für Polar- und Meeresforschung, Bremerhaven, Germany
⁴Faculty of Geosciences, University of Bremen, Bremen, Germany

**Correspondence:** Timm Schultz (tschultz@rhrk.uni-kl.de)

**Abstract.** *Physics based simulation* approaches to firn densification often rely on the assumption that grain boundary sliding is the leading process driving the first stage of densification. Alley (1987) first developed a *material model of firn* that describes this process. However, often *so-called semi-empirical* models are favored against the *physical* description of grain boundary sliding due to simplicity and *owing to their simplicity and the* uncertainties regarding model parameters. In this study, we are assessing the applicability of the grain boundary sliding model of Alley (1987) to firn using a numeric firn densification model and an optimisation approach, for which we formulated variants of the constitutive relation by Alley (1987). The efficient model implementation based on an updated Lagrangian numerical scheme enables us to perform a large number of simulations testing different model parameters, to find simulation results suiting and identify the simulation results that best reproduced 159 firn density profiles from Greenland and Antarctica. For most of the investigated locations, a good agreement of the simulated and measured firn density profiles was found. This were in good agreement. This result implies that the constitutive relation by Alley (1987) characterizes the first stage of firn densification well, if suitable model parameters are used. An analysis of the parameters that lead to best matches reveals a dependency on the mean surface mass balance. This may indicate an insufficient description of the load situation, as finding may indicate that the load is insufficiently described, as the lateral components of the stress tensor are usually neglected in one-dimensional models of the firn column.

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1 Introduction
Two basic categories of firn densification models can be identified. The first one, incorporating the majority of Firn densification models, fall into two basic categories. Models in the first category, which includes most existing models, is following the so-called semi-empirical concept follow the so-called semi-empirical approach of Herron and Langway (1980), which itself is based on Sorge’s Law (Bader, 1954) and the Robin Hypothesis hypothesis (Robin, 1958). Examples are the models by of Arthern et al. (2010), Ligtenberg et al. (2011), and Simonsen et al. (2013). Typically The empirical parameters of these models are adjusted to typically adjusted on the basis of certain datasets of depth density profiles. The In the second category of firn densification model, an attempt is made to quantify the physical processes related to the densification of firn firn densification. These processes incorporate different include various types of creep and diffusion. Micro mechanical-Micromechanical models are used for small-scale investigations (Johnson and Hopkins, 2005; Theile et al., 2011; Fourtenau et al., 2020) while continuum mechanics based models, whereas models based on continuum mechanics can be used for large-scale simulations. Examples of the latter are models by the models of Arthern and Wingham (1998), Arnaud et al. (2000), and Goujon et al. (2003).

Alley (1987) first applied the theory of grain boundary sliding adopted from Raj and Ashby (1971) to firn densification at densities below the critical density of $\rho_c = 550 \text{ kg m}^{-3}$. Since then the The description of this process by Alley (1987) was subsequently used in other firn densification models (Arthern and Wingham, 1998; Arnaud et al., 2000; Goujon et al., 2003; Bréant et al., 2017). Nevertheless However, the assumption that grain boundary sliding is the dominant process in firn densification at densities below $\rho_c = 550 \text{ kg m}^{-3}$ has been questioned numerous times (Ignat and Frost, 1987; Roscoat et al., 2010). For example, by conducting Theile et al. (2011) conducted experiments on a small number of snow samples suggested that the and suggested that densification is more likely driven by processes within the grain rather than by the intergranular process of grain boundary sliding.

When first published the description of grain boundary sliding for firn, he tested the material model by fitting the model results to four firn profiles available at this time, evaluating the resulting model parameters. As indicated by the title of his paper and pointed out in its discussion, grain boundary sliding might not be the only process driving the densification of firn at low density and model parameters might differ, but by using the given constitutive law it is possible to reproduce measured depth density profiles to a satisfying degree.–

In this study we aim to evaluate whether the description of grain boundary sliding and its description given by Alley (1987) is suitable for the simulation of firn densification at low density, (ii) how a modification of the constitutive relation introduced by Bréant et al. (2017) affects simulation results, (iii) whether hidden or additional dependencies of the constitutive relation on climatic or other conditions can be identified in the constitutive relation, and (iv) how a modification of the constitutive relation by of Alley (1987) leading to improvement of the description, could look like. We want to point out might be improved. Note that our study aims at assessing to assess the constitutive relation for grain boundary sliding proposed by Alley (1987). An evaluation clarifying if that clarifies whether grain boundary sliding is the dominating dominant process driving firn densification below the critical density of $\rho_c = 550 \text{ kg m}^{-3}$ has to be carried out must be conducted using other methods. Attempts Experimental attempts to do so have been made for example by by, for example, Kinosita (1967), Ignat and Frost (1987), and Theile et al. (2011) by conducting experiments. In contrast to these experimental investigations we follow a
combination of data and physical model based approach, a data-driven model approach is used in our study. Since the original study by Alley (1987) was published, the amount of available data became much larger. Alongside to has increased greatly. The data include a large number of firn profiles this includes forcing data which, together with additional modelling techniques, allows and forcing data, and they allow us to simulate firn profiles at a very high quality using additional modeling techniques.

2 Methods

In order to test the description of grain boundary sliding given by Alley (1987) we use a numeric model, simulating, we used a numerical model to simulate the evolution of a one-dimensional one-dimensional firn column with respect to time. The model incorporates uses variants of the constitutive relation of Alley (1987), all of which combine several model parameters in a single factor. We then force the model with data provided by the regional climate model RACMO2.3 (Van Wessem et al., 2014; Noël et al., 2015), representing the climate of the last recent decades at 159 different locations where firn density measurements were retrieved. These firn measurements are available through the Surface Mass Balance and Snow Depth on Sea Ice Working Group (SUMup) snow density subdataset (Koenig and Montgomery, 2019). By varying the factor incorporated used in the variants of the constitutive equation, we produce a large number of simulation results, which are compared to the corresponding density measurements. The quality of the factors used in the simulations is evaluated in terms of the deviation of the computed density profiles from the measured profiles. Evaluating factor values leading to best results, reveals-The factor values that yielded the best results reveal possible improvements in the description of grain boundary sliding for firn densification at low density. In the following sections, the constitutive equation for grain boundary sliding given by Alley (1987), the optimization scheme, and the used density and forcing data are described. A detailed description of the model can be found is presented in the appendix (Section A).

2.1 Grain Boundary Sliding Constitutive relation for grain boundary sliding

The different components and characteristics of the constitutive law by Alley (1987) describing the process of grain boundary sliding,

\[ \dot{\varepsilon}_{zz} = -\frac{2}{15} \delta_b \frac{8 D_{BD} \Omega}{k_b T h^2} \frac{1}{r \mu^2} \left( \frac{\rho_{ice}}{\rho} \right)^3 \left( 1 - \frac{5}{3} \frac{\rho}{\rho_{ice}} \right) \sigma_{zz} , \quad D_{BD} = A_{BD} \exp \left( -\frac{Q_{BD}}{RT} \right) \]  

(1)

will be explained briefly. The factor of 2/15 results from the geometric deviation pointed out by Alley (1987). Another geometric parameter, \( \delta_b \), describes the width of the grain boundary.

The following part of the equation describes the reciprocal bond or boundary viscosity (Raj and Ashby, 1971). The optimization approach of Alley (1987) aimed to find optimal values for was intended to identify the optimal values of the boundary viscosity. Alley (1987) compared the results from this optimization of this optimization to the description of the boundary viscosity given by Raj and Ashby (1971), which incorporates the factor \( D_{BD} \), the volume of the H₂O molecule \( \Omega \), the Boltzmann constant \( k_b \), the temperature \( T \), and the amplitude of grain boundary obstructions, \( h \). The latter is a measure of the roughness of the grain boundary. \( D_{BD} \) is an Arrhenius equation-factor describing the rate of boundary diffusion. Values
for the activation energy representative of the typical activation energy for this process, $Q_{BD}$, and the corresponding prefactor, $A_{BD}$, can be found in literature \( \text{the literature} \) (e.g., Maeno and Ebinuma, 1983), and are further discussed in Sect. 2.2. $R$ is the universal gas constant.

The strain rate resulting from grain boundary sliding also depends on the grain radius $r$. The ratio of the grain radius to the neck radius $\mu$ was introduced by Arthern and Wingham (1998) and is assumed to be constant. There are different methods Various methods can be used to determine the size of grains in crystalline materials (e.g., Gow, 1969). The model by of Alley (1987) was developed under the assumption of assuming perfectly spherical grains. Although this assumption is not true for firm, this assumption of firn, it provides a reasonable basis for modeling. Therefore, throughout this paper, the grain radius $r$ describes represents the radius of theoretical spherical grains throughout this study.

The next factor of Equation in Eq. (1) describes the dependency on the inverse relative density to the power of threedensity relative to the ice density cubed. The factor of $5/3$ corresponds to the inverse relative $1 - (5 \rho / 3 \rho_{\text{ice}})$ causes the strain rate due to grain boundary sliding to decrease with increasing density until it vanishes at the critical density of $\rho_c = 550 \text{ kg m}^{-3}$. When the critical density and with it the theoretical densest packing of spheres is reached, the maximum coordination number of a single grain is established. At this point grains can not close random packing is established (Anderson and Benson, 1963), and grains can no longer slide against each other and thus, the process of grain boundary sliding ends. Other deformation processes, \( \text{especially in particular} \) dislocation creep (Maeno and Ebinuma, 1983), lead to result in further densification with increasing stress. This behaviour is achieved in the constitutive relation by the factor incorporating the relative density $\rho / \rho_{\text{ice}}$. The vertical strain rate $\dot{\varepsilon}_{zz}$ decreases with increasing density $\rho$, until it becomes zero at the critical density $\rho_c$.

It has to be mentioned though, that Alley (1987) suggested also other processes leading to densification act at densities that additional processes contribute to densification below the critical density. A decline of the strain rate due to It is feasible that the effect of grain boundary sliding while the influence on the strain rate decreases, whereas that of other processes increases, seems feasible. The studies by of Arthern and Wingham (1998) and Bréant et al. (2017) use this description, in which only grain boundary sliding drives densification in the first stage of firn densification exclusively. In the study by of Bréant et al. (2017), the constitutive relation by of Alley (1987) is changed in a way that leads to a modified such that the transition into the second stage of densification. We will is modified. We evaluate this modification throughout this study in this work.

Finally, the stress in vertical direction the vertical direction, $\sigma_{zz}$, resulting from the overburden firn is driving drives grain boundary sliding. Whereas Alley (1987) used the product of the accumulation rate, acceleration due to gravity, and time since the deposition of a specific firn sample to describe the overburden stress, we use a more general form at this point (see Section here [see Sect. A2, Equation Eq. (A5)]). The other physical properties influencing affecting the process are density $\rho$, temperature $T$, and grain radius $r$. 

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\[ \text{Equation Eq. (1)} \]
2.2 Optimisation

To test the concept of the material model developed by Alley (1987) we formulate variants of Equation, we formulated variants of Eq. (1) and compared the model results to density measurements of various firn cores. These variants of the constitutive equation (Equations [Eqs. (2) to (5)]) preserve its general form but group several material parameters into a single parameter. In this way, as a result, the simulation result does not depend on those parameters, but on the single factor. The factor leading to that yields the optimal simulation result recreating that best reproduces the measured firn profile. The factor leading to that yields the optimal simulation result depends on the measured firn density profile and the corresponding climate conditions. It is therefore site-specific. This allows for the assessment if the site-specific. This feature makes it possible to assess whether the description of grain boundary sliding given by Alley (1987) can be used to recreate reproduce measured firn profiles under the assumption of, assuming an optimal set of parameters. It further allows to analyse the site-specific factors leading to us to analyze the site-specific factors yielding the best simulation results for possible hidden dependencies.

Arnaud et al. (2000), Goujon et al. (2003) as well as and Bréant et al. (2017) also summed incorporated the material parameters of the model by of Alley (1987) up into a single parameter. In the study by Bréant et al. (2017) additionally also modified the factor of 5/3 to change the density at which the deformation due to grain boundary sliding becomes zero. In the following the four variants, indicated by the subscripts (·)v1 to (·)v4, are shown presented:

\[
\dot{\varepsilon}_{zzv1} = -C_{v1}D_{BD}\frac{1}{T}\frac{\rho_{ice}}{\rho}^3\left(1 - \frac{5}{3}\frac{\rho}{\rho_{ice}}\right)\sigma_{zz}, \quad D_{BD} = A_{BD}\exp\left(-\frac{Q_{BD}}{RT}\right), \tag{2}
\]

\[
\dot{\varepsilon}_{zzv2} = -C_{v2}D_{BD}\frac{1}{T}\frac{\rho_{ice}}{\rho}^3\left(1 + \frac{0.5}{6} - \frac{5}{3}\frac{\rho}{\rho_{ice}}\right)\sigma_{zz}, \quad D_{BD} = A_{BD}\exp\left(-\frac{Q_{BD}}{RT}\right). \tag{3}
\]

Variant 1 (Equation [Eq. (2)]) and Variant 2 (Equation [Eq. (3)]) of the constitutive equation combine all material constants using the factors C_{v1} and C_{v2}, respectively. The Arrhenius equation factor for boundary diffusion, D_{BD} (see Equation, [see Eq. (1)]) is preserved) is retained in these variants. Following Maeno and Ebinuma (1983), we use a value of \(Q_{BD} = 44.1 \text{kJ mol}^{-1}\) for the boundary diffusion activation energy. It is This variable was defined by Maeno and Ebinuma (1983) by two thirds as two-thirds of the activation energy for lattice diffusion measured by Itagaki (1964). The corresponding prefactor is \(A_{BD} = 3.0 \times 10^{-2} \text{m}^2 \text{s}^{-1}\).

Alley (1987) assumed a similar value for the boundary diffusion activation energy.

Except for in addition to the temperature \(T\), the vertical strain rate \(\dot{\varepsilon}_{zz}\) only depends only on the firm density \(\rho\), the grain radius \(r\) and the stress in the vertical direction \(\sigma_{zz}\). Variant 2 differs from Variant 1 by the use of the in that it uses the modification introduced by Bréant et al. (2017). This modification leads to a theoretical ending of causes a theoretical end to the process of grain boundary sliding at the density of \(\rho_{c} = 596 \text{kg m}^{-3}\). It was introduced to grant better transition into obtain a better transition to the second stage of firn densification. The strain rate due to grain boundary sliding is therefore higher at the critical density when using the modification this modification of Bréant et al. (2017) is used.
To test the influence on the density factor, it is disregarded in Variants 3 and 4, as shown in Eqs. (4) and (5):

\[ \dot{\varepsilon}_{zzv_3} = -C_v \frac{1}{T} \frac{1}{r} \left( \frac{\rho_{ice}}{\rho} \right)^3 \left( 1 - \frac{5}{3} \frac{\rho}{\rho_{ice}} \right) \sigma_{zz}, \]

(4)

\[ \dot{\varepsilon}_{zzv_4} = -C_v \frac{1}{T} \frac{1}{r} \left( \frac{\rho_{ice}}{\rho} \right)^3 \left( 1 + \frac{0.5}{6} - \frac{5}{3} \frac{\rho}{\rho_{ice}} \right) \sigma_{zz}. \]

(5)

Again in Variant 4, the modification by Bréant et al. (2017) is used while Variant 3 incorporates the original formulation by Alley (1987).

The aim of the optimization is to find optimal values of the factors \( C_v \) for every variant of the constitutive relation (Eqs. (2) to (5)) resulting in a simulated density profile that best reproduces the measured profiles in the best possible way. As an example, we explain the optimization process for one selected firn core in more detail. The upper part of ice core ngt03C93.2 (Wilhelms, 2000) is shown in Fig. 1(a).

Every simulation starts with a spin-up period in which constant values are used for the forcing. When the model is forced with prescribed values of temperature, accumulation rate, firn density, and grain radius at the surface. We check for steady-state conditions by comparing the change in density between time steps. If the maximum density change is smaller than \( |\Delta \rho_{\text{max}}| < 0.1 \text{ kg m}^{-3} \), we assume that the steady state is reached. In this case, a transient run using evolving varying forcing data follows. We use a constant value of 48 time steps per year for spin-up and transient simulation runs (see Sect. A7). The forcing at the location of ngt03C93.2 is shown in Fig. 1(e). The resulting firn profile is then compared to the measured profile. We use the root mean square deviation (RMSD) between measured and modeled density for comparison, which allows a simple and easy to compute comparability between the simulation result and the density measurement. To calculate the deviation, the simulated density values are interpolated linearly to the measurement locations along the profile. To guarantee a high quality of the results, we restrict the calculation of the deviation to the domain defined by the location of the uppermost available measurement point and the oldest horizon within the firn profile affected by the forcing. In case of forcing, for ngt03C93.2, this horizon is the surface of 1958 at a depth of approximately 11 m below the surface, indicated by dashed horizontal lines in Fig. 1(a).

Only results located above the surface are used to calculate the deviation. The reason is that the forcing data from RACMO2.3 (Van Wessem et al., 2014; Noël et al., 2015) begin in 1958 are incorporated in the calculation of the deviation. Examining for Greenland. Consequently, the results are not affected by the spin-up period. For firn profiles retrieved in Antarctica, climate forcing from RACMO2.3 begins in 1979. Thus, only those results located above the simulated horizon of 1979 are considered for comparison with the Antarctic firn profiles. The examination of other firn cores revealed that the surface of the oldest available forcing may be located at greater depth, when the density of \( \rho_c = 550 \text{ kg m}^{-3} \) is already has been reached. In those cases, the computation of the root mean square deviation is restricted. RMSD was limited to the domain showing density values smaller than 540 \text{ kg m}^{-3}. We decided to use a smaller density threshold.
than the density threshold below the critical density due to the asymptotic characteristic because of the asymptotic nature of the resulting density profiles obtained using Variants 1 and 3 of the constitutive equation (Equations [Eqs. (2) and (4)]). The value of 540 kg m\(^{-3}\) rendered to ensure comparability between results of the different was chosen to ensure that the results obtained using the variants of the constitutive relation while unique values for the factors are comparable, whereas unique values of the factor \(C_v\) were found quickly throughout the optimisation quickly determined throughout the optimization.

As the implementation of our model is efficient and the approach is as well simple and reliable, we decided to determine the best factor \(C_v\) for the four variants of the constitutive equation —by simply testing 250 values within certain ranges. These ranges are shown in Equations Eqs. (6) and (7). They differ because of the inclusion or disregard of the Arrhenius law, which include and exclude the Arrhenius factor, respectively. Optimal factors can be found within these range boundaries for every analysed range for every analyzed firn profile. To ensure this this is the case, all simulations were performed multiple times testing using different ranges of the factors.

\[
1.0 \times 10^{-9} \text{Ks}^2 \text{kg}^{-1} \leq C_{v_1,v_2} \leq 2.5 \times 10^{-4} \text{Ks}^2 \text{kg}^{-1} 
\]  \hspace{1cm} (6)

\[
2.5 \times 10^{-21} \text{Ksm}^2 \text{kg}^{-1} \leq C_{v_3,v_4} \leq 5.0 \times 10^{-15} \text{Ksm}^2 \text{kg}^{-1} 
\]  \hspace{1cm} (7)

Figure 1 (b) shows the root mean square deviation (RMSD) b shows the RMSD plotted over the 250 tested values for the four different factors. The different variants are color coded variants are color-coded, and the best result is results are marked. The smallest value values of the deviation is shown within are shown in the figure. The corresponding density profiles are shown in Fig. 1 (a).

As can be seen in Fig. 1 (a) the The firn profile of ngt03C93.2 starts at a depth of about approximately 1.3 m. This yields the problem of finding Therefore an appropriate surface density, needed as boundary condition in the simulation boundary condition must be found. As firn density profiles differ greatly especially near the surface, the derivation of an appropriate surface density is difficult. Following our approach we Although Alley (1987) simulated the density starting at a depth of 2 m below the surface, we included this domain in our simulation so that we could apply transient surface forcing to our model. To find suitable values of the surface density, we included this parameter in our optimization. For each of the four variants and 250 factors \(C_v\), we tested 21 different values for values of the surface density between \(\rho_0 = 250 \text{kg m}^{-3}\) and \(\rho_0 = 450 \text{kg m}^{-3}\), using steps of \(\Delta \rho_0 = 10 \text{kg m}^{-3}\). Afterwards the best result is chosen. This method proofed to work well throughout the study. Firm profiles which start The best result was chosen. We used the method of testing 21 surface density values for all the analyzed firn profiles. We included profiles including measurements of the density at small depths, providing near-surface density data are well represented. Applying the method to all firn profiles no matter at which depth they begin, accounts for comparability of the results. Overall In this way, we established that the results are comparable. Profiles including near-surface density values are, however, well-represented. A total of 4 \(\times\) 250 \(\times\) 21 = 21 000 simulations were performed in case of for ice core ngt03C93.2 to find the optimal results shown in Fig. 1. The same procedure was applied to all 159 firn profiles analyzed in the study.
Figure 1. Panel (a) of the figure shows the depth density profile of ice core ngt03C93.2 (Wilhelms, 2000) retrieved in Greenland in: and the best corresponding model results obtained using four different variants of the constitutive law for grain boundary sliding by Alley (1987) in different colors. The dark gray line shows the mean density of the ice core calculated using a window of 0.5 m starting at the surface. Dashed horizontal lines represent horizons of firn deposited in the indicated years, where 1958 is the first year that forcing from RACMO2.3 (Van Wessem et al., 2014; Noël et al., 2015) is available. Simulation results are drawn using colors as shown: Colored dashed horizontal lines show horizons obtained in the legend. Horizons plotted in gray to the right of the vertical dashed line represent the same surfaces as those determined by Miller and Schwager (2004) during analysis of the core. Panel (b) shows the root mean square deviation RMSD between measured and modeled density plotted over the range of tested factor values. Note the different axes for different tested factors. The (c) Representative forcing representative for the location of ice core ngt03C93.2 and which was used in the simulation is shown in panel (e). Horizontal dashed lines show the mean values of the surface mass balance and surface temperature over the course of the simulation time.
3 Data

3.1 Firn Profiles

In order to test the description of grain boundary sliding given by Alley (1987), we used 159 firn profiles of which 80, 80 of which were retrieved in Greenland. The remaining 79 measurements were taken in Antarctica. The profiles are included in the “Surface Mass Balance and Snow Depth on Sea Ice Working Group (SUMup) SUMup snow density subdataset” (Koenig and Montgomery, 2019). Individual references for all 159 firn profiles are listed in the supplementary material. The dataset does not feature the four profiles used in the study by of Alley (1987), as the original data of for these firn cores are unpublished. To obtain firn profiles relevant for this study from the dataset, we filter it based on the following conditions:

1. Profiles have to consist of at least ten data points.
2. The overall length of the profiles has to exceed three meters each profile must exceed 3 m.
3. Profiles have to start at a depth of less than three meters below the surface.
4. The starting density of the profiles must not exceed \( \rho_c = 550 \text{ kg m}^{-3} \).
5. The annual mean surface mass balance at the profile location has to be positive.
6. Forcing data are available. Furthermore, a number of density profiles were used only datasets for which at least five years of forcing data are available. Furthermore, a number of density profiles were manually excluded from the filtered dataset by hand. These profiles include those with very low spatial resolution, atypical profiles showing decreasing density with depth, and measurements with a surface density very close to the critical density of \( \rho_c = 550 \text{ kg m}^{-3} \).
Figure 2. Locations of the firn profiles used for model comparison. Eighty profiles were measured in Greenland, and 79 depth density datasets were retrieved in Antarctica. The blue marker shows the location of ice core ngt03C93.2 (Wilhelms, 2000, N 73.940°, E −37.630°). The green marker shows the location of site 3 of the iSTAR traverse, from which the firn core shown in Figure 3 was retrieved (Morris et al., 2017, N −74.565°, E −86.913°). Map data: Amante and Eakins (2009); Arndt et al. (2013), SCAR Antarctic Digital Database.

we only use a certain domain for the comparison between the simulated and measured data. If this domain turns out to be less than 2.5 m long in case of any of the tested variants of the constitutive equation, the firn profile in question is neglected in the further analysis.

Figure 2 illustrates the locations from which the 159 density profiles were retrieved. The 80 measurements from Greenland are relatively uniformly distributed over the ice sheet. Coastal locations are not well covered owing to the requirement of a strictly positive surface mass balance. In the Antarctica, sites in East Antarctica are underrepresented. However, a wide variety of environments is covered, including the Filchner–Ronne Ice Shelf, the West Antarctic coast, and Dronning Maud Land.

3.2 Boundary Conditions and Forcing

To force the firm densification model, surface values for density, temperature, accumulation rate, and grain radius at the locations of the 159 firm profiles are needed. Although Alley (1987) used constant forcing, we followed the example of Arthern and Wingham (1998) and Goujon et al. (2003) performing transient simulations.
As measured firm density profiles represent past climate conditions, the choice of forcing data is crucial for the presented method in the proposed method is crucial. Uncertainties in the forcing will reflect in affect the simulation results and therefore in the comparison with the measured firm profiles. Neither the model formulation nor the optimisation optimization scheme can compensate for these effects. We use data provided by the regional climate model RACMO2.3 (Van Wessem et al., 2014; Noël et al., 2015). Details on RACMO2.3, including the limitations of the model and the resulting data products, were presented by Van Wessem et al. (2014); Noël et al. (2015); van Wessem et al. (2018). RACMO2.3 provides forcing data for the Greenland ice sheet covering the period from 1958 to 2016. In case of Antarctica, the time period is shorter, starting in running from 1979 and ending in to 2016. Data for the mean annual skin temperature and surface mass balance of the Greenland ice sheet are available at mean spatial resolutions of 11.3km and 1.0km respectively, respectively, for this study. Mean spatial resolutions for Antarctica are 8.0km and 28.5km for The mean spatial resolutions of the mean annual skin temperature and surface mass balance for Antarctica are 8.0km and 28.5km, respectively. Spatial interpolation of the fields obtained from RACMO2.3 output leads to forcing data for the locations of the investigated firm profiles. It has to be mentioned that such an interpolation may introduce systematic errors.

The time period for the transient simulation runs, as described in Section Sect. 2.2, is specified by the earliest data available from RACMO2.3 and the drilling date of the firm core under consideration. In case of For ice core ngt03C93.2 (Wilhelms, 2000), which was retrieved in central Greenland in 1993, the simulation time covers the period from 1958 to 1993 (see Fig. 1 (c)). Constant values of the surface temperature and surface mass balance for the preceding spin-up are spin-up period were calculated as mean values over this time range.

Using We present a second example we want to illustrate how the to illustrate the effect of the temporal resolution of the forcing affects the optimisation on the optimization results and why we decided to use used yearly averaged data provided by RACMO2.3. Figure 2 shows the depth density profile of the firm core retrieved retrieved at site 3 of the iSTAR Traverse in 2013 (Morris et al., 2017). The location of the site, at Pine Island Glacier in West Antarctica, is shown in Fig. 2. Instead of using forcing data from RACMO2.3, for this particular simulation we used ERA5-Land monthly averaged data from 1981 to present (Muñoz Sabater, 2019; Hersbach et al., 2020), as it is they are freely available at monthly resolution. From this data we computed these data, we computed the annual average data for a second simulation run. The forcing data at both resolutions is are shown in Fig. 3 (c). Panel (a) of the figure shows the best 3c. Figure 3a shows the simulated firm profiles identified using the optimisation approach in comparison with the best best reproduce the measured density profile. On the left hand side results, which were identified using the optimization approach. The results obtained using the annually averaged forcing data are shown, while the right hand side illustrates the results on the left, whereas those obtained using monthly averaged data from ERA5. In case of the are shown on the right. The data with higher resolution data reveal much more detail is covered within the simulated firm density profiles. However, the aim of this study is not primarily to reproduce the analysed analyzed measured firm profiles with the highest possible detail, but to evaluate the constitutive relation by of Alley (1987) using an optimisation approach finding site specific optimization approach that identifies site-specific optimal constitutive factors $C_v$ (see Section Sect. 2.2). Panel (b) of Fig. 3b shows the root mean square deviation Figure 3b shows the RMSD of the simulated profiles from the measured profile over the range of tested optimisation optimization factors. Dashed lines belong to
**Figure 3.** Panel (a) of the figure shows the depth-density profile (gray) of the firn core retrieved at site 3 of the iSTAR traverse (Morris et al., 2017) in gray colour. Colour-coded colored lines show the optimised optimal simulation results for all four tested variants of the constitutive relation are pictured. The simulated density profiles on the left result from were obtained using yearly averaged surface forcing while the profiles, whereas those on the right, plotted using dashed lines, result from were obtained using monthly averaged forcing. In panel (b) the root mean square deviation (RMSD) between the best simulation result and the measured firm profile is shown over the range of tested optimisation optimization factors $C_v$. Colours again Colors indicate results for the different variants of the constitutive relation. Dashed lines are used for results computed with monthly averaged forcing, whereas solid lines indicate the use of yearly averaged surface forcing. The forcing (c) Forcing data from ERA5-Land monthly averaged data from 1981 to the present (Muñoz Sabater, 2019; Hersbach et al., 2020) is shown in panel (c), from the earliest available forcing in 1981 to the date the firm core was drilled in 2013. Strong Bold lines show the yearly averaged data computed from the monthly averaged data.
the represent simulations performed using the high resolution forcing data, while solid lines are dedicated to whereas solid lines represent the annual averaged data. The difference between the optimisation results is small. We therefore decided to use the annual averaged data provided by RACMO2.3 available for this study, as the data cover a longer time period, especially for Greenland, a greater time period. This allows us to analyse. As a result, we can analyze more firn profiles at greater detail. In case of For ice core ngt03C93.2 (Wilhelms, 2000), the horizon of the year 1981, the earliest forcing available in ERA5, lies at a depth of about 5 m below the surface as can be seen in Fig. 1 (a). The horizon of the earliest forcing available by RACMO2.3, the year 1958, is located at a depth of about 11 m below the surface. A much greater part of the simulated firn profile is therefore influenced by surface forcing. Furthermore, the use of yearly averaged data produces less overhead.

As pointed out in Section 2.2 we noted in Sect. 2.2 we used 21 surface density values in the range of 250 kg m$^{-3}$ $\leq \rho_0 \leq$ 450 kg m$^{-3}$ for every tested firn profile. The value leading to that yielded the best result was then used for further analysis. Due to the Owing to a lack of relevant data, simplicity and better comparison options and for simplicity and ease of comparison, the grain radius at the surface was assumed to be the same at all locations and to be constant over time. We chose to use a grain radius of $r_0 = 0.5$ mm based on the measurements and empirical relation of Linow et al. (2017) and the assumption of Arthern and Wingham (1998). As climatic conditions, and therefore the surface grain size, differ at every investigated location this vary among the investigated locations, this choice is a simplification. Due to the optimisation approach the influence of this parameter is of less significance. Owing to the use of the optimisation approach, this parameter has a less significant effect, as it can be understood as a constant part of the grain radius, which is the same for every analyzed firm profile.

Figure 4 illustrates the range and distribution of surface boundary conditions at the investigated sites. In comparison, The locations in Greenland show a higher mean surface temperature and surface mass balance than locations in Antarctica. The surface density is higher at Antarctic location than the Antarctic locations than at those in Greenland. In general, Overall, a wide variety of typical climatic conditions for both ice sheets is covered.

3.3 Distribution and Influence-effects of Input Data

Ice core ngt03C93.2 shown in (Fig. 1 (a)) is an example of a high resolution density measurement showing extensive small-scale layering. Only a few of the 159 firn profiles are of such high quality and cover such kind include this type of layering. Although our model approach works on a proposed model works at high temporal and spatial resolution, it does not cover layering, as shown in Fig. 1 (a). Simulation of small scale layering could easily be added to the model following the a. The density profile retrieved at site 3 of the iSTAR traverse (Morris et al., 2017) (Fig. 3) illustrates that the model, if it is forced with data of higher temporal resolution, still does not cover the measured density variability. Small-scale layering of firn appears to be driven by a number of different processes (Hörhold et al., 2011). An extension of the model to cover such processes may be introduced in the future. We would prefer the approach of Freitag et al. (2013), introducing a dependency of the activation energy $Q_{NT}$ for the process of boundary diffusion (Equation (1)) on a proxy for impurities. Such data who introduced the concept of impurity-controlled densification. Forcing data for this model are
Figure 4. Distribution and comparison of the boundary conditions at the 159 firm profile sites. All values are averaged over the specific simulation time for each location, beginning in the year 1958 and 1979 for Greenland and Antarctica, respectively, and ending at the date of measurement (see Section 3.2). The top row of plots in (gray colour) shows the boundary conditions at all locations, whereas the middle and bottom rows, in red and blue, exclusively represent only the locations in Greenland and Antarctica, respectively. Data for the surface temperature in the middle, (center) and surface mass balance in the (right column) are provided by RACMO2.3 (Van Wessem et al., 2014; Noël et al., 2015).

The activation energy can therefore be understood as a temporally averaged value, leading to a mean density. The use of the root mean square deviation for comparison of simulation results and measured density profiles assures the optimisation result is independent of layering. To illustrate this the running mean density of ice core ngt03C03.2 is shown. However, the model in its current form does reproduce the mean density well, as demonstrated in Fig. 1-(a). Note that computing the running mean neglects information. Thus we compute the root mean square deviation on the basis of the original data.

In this study we focus on the very first, we focused on the initial, stage of firm densification and the uppermost meters densification and the uppermost part of the firm column. We limited the model domain to a maximum depth of −25 m below the surface. Furthermore we did not develop the density further after the critical density of $\rho_c = 550 \text{ kg m}^{-3}$ is reached. This choice raises the question if the use of a Neumann boundary condition set to zero at the profile base to solve for the temperature as described in Section A4 is justified for this particular model setup (Sect. A4).

The critical density of $\rho_c = 550 \text{ kg m}^{-3}$ is usually reached within the upper ten meters of the firm column. The temperature within this domain is influenced by the surface conditions, which are covered by the forcing data.
greater depths, the temperature corresponds to the mean annual surface temperature and changes very little. The amount of high resolution temperature measurements in firn is sparse (e.g., Cuffey and Paterson, 2010, pp. 399 ff.). There have been few high-resolution temperature measurements of firn. Orsi et al. (2017) published a temperature profile of a 147 m length from borehole NEEM2009S1, which shows a temperature difference of little more than 1 K over the entire profile. The study by Vandecrux et al. (2021) suggests the same. Such obtained the same result. This small temperature change, below the depth of at depths greater than approximately 10 m below the surface has little effect on our model approach. To test the sensitivity of the optimisation approach the temperature we performed reruns of the simulations with the site specific temperature dependence of the optimization approach. We performed the simulations again using the site-specific surface temperature forcing increased and decreased by plus or minus 1 K. The effect of the optimal factors $C_v$ differs depending on the variant of the constitutive relation, but in general is it is generally small. For example, the greatest difference between the optimal factors resulting from obtained using the correct and the adjusted forcing in case of adjusted forcing for ice core ngt03C93.2 (Wilhelms, 2000) can be found when were found using Variant 1. It shows This variant yields a value of $\Delta C_{v1,\text{max}} = 0.02 \times 10^{-4} \text{K s}^2 \text{kg}^{-1}$, which corresponds to two times twice the sampling space of the factors $C_v$ used in the optimisation. In case of optimization, Variant 4 the results are even the same yields the same results. Because of this small influence in general, the greater influence effect overall, the stronger effect of the surface temperature in the investigated domain and the restriction, and the limitation of the comparison to the domain actually influenced by the surface forcing affected by surface forcing, a Neumann boundary condition at the profile base is is justified despite the low depth, is justified.

4 Results

Figure 5 illustrates shows the distribution of the root mean square deviation (RMSD) -- RMSD calculated from the simulated firn profiles matching that best reproduce the measured profiles best. The four different plots of the figure distinguish between the four different plots in the figure represent the four variants of the constitutive equation for grain boundary sliding (Equations [Eqs. (2) to (5)]), as described in Section Sect. 2.2. Additionally the median value, the median values of the data is are shown. The differences in the distribution distributions of the deviation are small with regard to the different tested variants: for the four variants show little difference. The median values differ in a small range. Variant Variants 2 shows the smallest value and Variant and 3 the greatest show the smallest and largest values, respectively. The use of the modification introduced by Bréant et al. (2017) within in the constitutive equation results in 6.2–6.8% better agreement between improves the agreement between the simulated and measured firn profiles by 6.2–6.8%. To put the values in perspective, the deviation of the four best fitting modelled best-fitting modeled firn profiles from ice core ngt03C93.2 (Wilhelms, 2000) displayed in Fig. 1 is about approximately 28 kg m$^{-3}$. That means, more than half of the resulting simulations show even better agreement with the corresponding firn density profiles than this one. An overview of the deviation between among all 159 measured firm profiles and the corresponding best simulation results can be found in the supplementary material.

The range of factors resulting in the best fitting contributing to the best-fitting firn profile is smaller for Variants 2 and 4 of the constitutive equation, which use the modification by of Bréant et al. (2017), compared to Variants 1 and 3, as shown in
Figure 5. Distribution of the smallest root mean square deviation (RMSD) for every analysed firn profile found using the optimization scheme outlined in Section 2.2. The four plots show the results for the four tested variants of the constitutive equation. Vertical lines indicate the median value of the 159 values.

The box plots in Fig. 6. In contrast to factors $C_{v1}$ and $C_{v2}$, factors $C_{v3}$ and $C_{v4}$ incorporate the Arrhenius law factor from the original description of grain boundary sliding given by Alley (1987). Therefore, a direct comparison between the two groups of factors is not possible. The quartile coefficient of dispersion, shown for the four variants, which is shown on the right side of Fig. 6, is a relative measure for the scatter of the values. The coefficient reveals that the resulting factors of Variants 1 and 2 are defined in a range narrower versus narrower range than those of Variants 3 and 4. All four resulting sets of factors show a slightly non-uniform distribution, tending towards slightly nonuniform distributions that tend toward smaller values.

To find a possible dependency of the resulting factors, leading to the best match between simulated and measured density profiles, Fig. 7 shows the

To check for possible mean surface temperature dependence of the 159 factors found by the optimization, plotted against optimization, these values are plotted against each other in Fig. 7. The values of the mean surface temperature were calculated from the forcing data specific for each firn profile site. The left plot illustrates the results for Variants 1 and 2 in red and blue colour, while the right part of the figure shows the results, whereas the right plot shows the factors for Variants 3 and 4 using green and purple markers, respectively. The legend features shows the Pearson correlation coefficient $r_{Pearson}$, a measure for the linear correlation of the two variables, and the distance correlation $dCor$ (Székely et al., 2007). The distance correlation was designed by Székely et al. (2007) to overcome problems with the Pearson correlation coefficient. It describes the correlation of two vectors while not being restricted to linear dependency and is not limited to linear dependence. It is defined in the range between zero and one, where zero indicates the independence of the variables.
Figure 6. Box plots showing the distribution of the best factors, $C_{v_1}$ to $C_{v_4}$, for the four variants of the constitutive equation describing grain boundary sliding (see Equations [Eqs. (2) to (5)]) derived using the optimization scheme described in Sect. 2.2. On the right side the quartile coefficient of dispersion $v_r$ of each variant is shown for the variants right in the corresponding color. The quartile coefficient of dispersion is calculated using the first ($Q_1$) and third ($Q_3$) quartile values of the data sets, which are shown in black and represent a robust relative measure of dispersion.

The correlation of the resulting factors with the mean surface temperature is higher compared to the correlation with other properties. This statement is especially true for factors $C_{v_3}$ and $C_{v_4}$ of Variants 3 and 4, respectively. However, the Pearson correlation coefficient only indicates the linear correlation. The scatter of factors $C_{v_3}$ and $C_{v_4}$ with respect to the mean surface temperature might resemble a higher-order function, as indicated by the higher values of the distance correlation.

The figures show the resulting factors in the same manner as Fig. 7 but, which shows the factors with respect to the mean surface mass balance. Just as, are higher than those in Fig. 7.

Like the mean surface temperature, the mean surface mass balance was calculated from the forcing data used during the simulations. The correlation coefficients for the results obtained using Variants 3 and 4 exceed the ones for the results obtained using the variants of the constitutive equation incorporating the Arrhenius law explicitly. The factor explicitly.

Variant 3 shows the best indication of a relationship between surface mass balance and the factor yielding the factor resulting in the-density profile best matching that best reproduces the corresponding field measurement and the surface mass balance can be seen for Variant 3.

A striking feature within Fig. 8 can be found, a striking feature appears around a mean surface mass balance of $0.4 \text{ m weq. a}^{-1}$. Values of the factors resulting in the best match between simulation results and measured density yielding the simulated density profiles that best reproduce the measured profiles show a wide range for all four variants of the constitutive relation. The corresponding profiles are part of a study by which took place in western Greenland by Harper et al. (2012).
Figure 7. Best factors for every investigated firn profile determined using the optimization scheme and plotted against the mean surface temperature during the forcing period (see Section 4). On the left side of the figure the Left: results for Variants 1 and 2 of the constitutive equation are shown in blue and red colour respectively, while the right plot illustrates the right: results for Variants 3 and 4 in green and purple colours respectively. The Pearson correlation coefficient \( r_{\text{Pearson}} \), representing the linear correlation between factors \( C_{v1} \) to \( C_{v4} \) and the mean surface temperature, as well as the distance correlation \( dCor \), are given within the legend.

Figure 8. Resulting factors of the optimization over the Factors obtained by optimization versus mean surface mass balance, calculated for everyone of the 159 firn profiles from its the forcing. The left hand side plot shows best fitting Left: best-fitting values for Variants 1 and 2 (factors \( C_{v1} \) and \( C_{v2} \) respectively). The plot on the right shows the corresponding Right: best-fitting values for Variants 3 and 4 or (factors \( C_{v3} \) and \( C_{v4} \) respectively). The linear Linear correlation between the factors and mean surface mass balance is illustrated indicated by the Pearson correlation coefficient \( r_{\text{Pearson}} \) and the general correlation is indicated by the distance correlation \( dCor \).
The study region is relatively small, which explains the similar climatic conditions. Although the mean annual surface mass balance is positive, melting occurs throughout the year influencing and affects the firn density.

5 Discussion

Using the four variants of the constitutive relation by Alley (1987), we were able to generate density profiles matching those generated from the presented optimization scheme (Sect. 3.2). The limited knowledge on the initial grain radius, and the poor constraint on the density at the surface. As measured firn densities represent past climate conditions, deviant forcing would always result in unrealistic forcing always results in a mismatch between the simulated and measured firn properties, independent of the optimization approach and physical model. However, when the proposed optimization scheme was used, the differences between the simulated and measured density profiles indicating show distinct minima, indicating that the forcing represents the climatic history of the firn profiles, in principle.

The optimization scheme results in site-specific values for the factors $C_{v1}$ to $C_{v4}$. As the optimization is specific for the analyzed site and variant of the constitutive relation, the four simulated density profiles for each site are very similar, as illustrated in Fig. 5. This feature allows us to compare the factors resulting from obtained using the four variants. The differences between the factors do not primarily arise from differences in the simulated density profiles, but reflect the differences in the variants, leading to consequently, the results are almost the same result.

However, due to the principle of the optimization scheme, possible errors in the forcing data or other parameters like the activation energy used for the computation of the grain radius (see Equation A11) are also included in the optimal factors $C_{v1}$ to $C_{v4}$. For example, the surface temperature forcing at a site is constantly off by five degree Kelvin over the simulation time, this consistently deviates by 5 K during the simulation, this error can be compensated by a corresponding adjustment of the specific optimization factor $C_v$ (see Section 3.3). However, the great amount of analyzed firm profiles compensates for such random error. Systematic error included errors. Systematic errors in the forcing data cannot be identified. Therefore, improvements improving the temporal resolution of the forcing with respect to resolution in time and covering of longer periods, could lead to and covering longer periods could result in better and more detailed simulation results in future as is shown in Fig. 7.

It should be mentioned again this study analyzed only dry firn densification. The current model cannot handle melting. We accommodate this feature by setting the annual mean surface mass balance at the investigated sites to be strictly positive (Sect. 3.1). However, this limitation means that we cannot ensure that no melting occurs over the course of a year. The results shown in Fig. 8 illustrate how this limitation affects the optimization results. The limitation is problematic, especially in recent years, when melting occurred over almost the entire Greenland Ice Sheet (e.g., Nghiem et al., 2012). The simulation of
meltwater percolation through the firm and its interaction with firm densification is important, especially in the upper part of the firm body (e.g., Vandecrux et al., 2020). The proposed method could be improved by the application of this model approach in future investigations. However, we identified some correlations between the optimization results and the surface mass balance.

Note, again, that we have not investigated whether grain boundary sliding is indeed the dominating process during the first stage of firm densification. We assess whether a process with a functional dependence on density, firm overburden stress, temperature, and grain radius represents the observed density profiles well. Any other deformation process with the same functional dependence would be equally well suited. Nevertheless, by maintaining the general structure of the constitutive relation by Alley (1987), we conclude that this description of grain boundary sliding is a good basis for a physically based model describing firm densification up to the critical density of \( \rho_c = 550 \text{ kg m}^{-3} \).

Comparing the results for Variants 1 and 2, as well as those for Variants 3 and 4, we find that the model results in better reproduction of the measured density profiles. With regard to This result must be reviewed carefully in terms of the study design and the background of a physics-based model describing firm densification, this result has to be reviewed carefully. As Alley (1987) pointed out, grain boundary sliding might be the dominant process driving firm densification at low densities, but it is presumably not the only one. The constitutive law by Alley (1987) is designed in a way such that the densification due to grain boundary sliding becomes zero at the density of \( \rho_c = 550 \text{ kg m}^{-3} \), motivated by the densest packing of spheres obtained at that density and increasing accommodation incompatibilities. The modification by Bréant et al. (2017) changes this behaviour in the way that the process such that grain boundary sliding vanishes at a density of about \( \rho_c^* = 596 \text{ kg m}^{-3} \), which could have advantages for the transition into the next stage of firm densification. We suggest a simultaneous decrease in grain boundary sliding and increase of one or more other processes would provide a good characterisation. Namely, dislocation creep drives the densification at higher density (Maeno and Ebinuma, 1983) due to increasing stresses. An onset of dislocation creep at densities lower than \( \rho_c = 550 \text{ kg m}^{-3} \) affecting not necessarily would not necessarily affect the entire bulk firm matrix, but increasing volume fractions of the porous matrix should be investigated further in future.

Variants 1 and 2 of the constitutive relation by Alley (1987) incorporate the Arrhenius factor for boundary diffusion, \( D_{BD} \), from the description of the bond viscosity given by Raj and Ashby (1971). For the formulation of Variants 3 and 4, we neglected the Arrhenius equation. As can be seen factor. As shown in Fig. 5, the difference in the resulting root mean square deviation is small, whether the Arrhenius equation-RMSD is small regardless of whether \( D_{BD} \) is considered or not. This is consistent as we determined. This result is reasonable, as we determined individual factors \( C_v \) for every site.

The similarity of the results allows us to compare the factors \( C_{v_1} \) and \( C_{v_2} \), which were determined including the Arrhenius equation using the Arrhenius factor \( D_{BD} \), to factors \( C_{v_3} \) and \( C_{v_4} \), resulting from which were obtained using the variants of the constitutive relation without the Arrhenius equation. As the Arrhenius equation factor, \( D_{BD} \) is a function of temperature, it is reasonable to take a look at the dependency examine the dependence of the factors on the mean surface temperature as which is shown in Fig. 7.
The determined factors \( C_{v_3} \) and \( C_{v_4} \), resulting from variants without the Arrhenius equation for boundary diffusion which were determined using the variants without \( D_{BD} \), show a stronger dependency dependence on the mean surface temperature than the factors \( C_{v_1} \) and \( C_{v_2} \). At the same time, In addition, the factors \( C_{v_1} \) and \( C_{v_2} \) show less dispersion than factors \( C_{v_3} \) and \( C_{v_4} \), as is shown in Fig. 6. The inclusion of the Arrhenius equation \( D_{BD} \) in the constitutive relation leads to better improves the determination of these factors. It is therefore a meaningful description within the constitutive relation. Although the inclusion of the Arrhenius equation results in better determination of factors, factor improves the determination of \( C_{v_1} \) and \( C_{v_2} \), we still see a dependency some dependence on the mean surface temperature to some degree. A better determination of the parameters of the Arrhenius equation may result in resolving this dependency factor may resolve this dependence. If this is not the case another dependency, another dependence on the temperature may be introduced to improve the constitutive relation for grain boundary sliding.

We interpret the dependency on the dependence on surface mass balance such, as indicating that the load situation is currently not represented well. The stress is represented by a second 
order tensor. A firn column represented in a one-dimensional modelling by a one-dimensional modeling approach would be surrounded by neighbouring neighboring firn columns, a lateral confinement restricting deformation in resulting in lateral confinement that limits deformation in the horizontal direction. The horizontal components of the stress tensor are not zero. As firn is a compressible material, the determination of these horizontal stress components is not trivial. The frequently used term "overburden pressure" is misleading, as the mechanical pressure is defined as the spherical part of the Cauchy stress tensor (e.g., Haupt, 2002, p. 301) and is not in general, in general, identical to the normal stress in the vertical direction. With increasing depth, the magnitude of the horizontal stress components and their influence would rise. Modelling approaches including considerations of effects would increase. Modeling approaches that consider the full stress tensor can be found in were reported by Greve and Blatter (2009), Salamantin et al. (2009), and Meyer and Hewitt (2017). It might be worthwhile to use worth using the constitutive relation for grain boundary sliding by of Alley (1987) in such a modelling modeling context. This must approach will not necessarily result in a full three dimensional model three-dimensional model, as the problem can be formulated axially symmetrical. This would require an assuming axial symmetry, which would require adjustment of the constitutive relation. A more extensive interpretation of the factors obtained in the best matches that yielded the best agreement is therefore challenging. The determination of a single factor \( C_v \) for one or all of the variants is not useful. It would not result in better simulation results compared to other published firn densification models. The site-specific site-specific values of the factors determined using the presented optimisation approach optimization approach simply show the differences in the variants of the constitutive relation.

6 Conclusions

Using variants of the constitutive relation for grain boundary sliding by of Alley (1987) and a efficient optimisation an efficient optimization scheme, we were able to reproduce reproduced 159 firn density profiles reasonably well. Thus we conclude we conclude that the description of grain boundary sliding as introduced by Alley (1987) is appropriate for the simulation of firn densification at low density.
The modification of the constitutive relation by Bréant et al. (2017) leads to slightly better simulation results when only the first stage of firn densification is considered. Further considerations, including the transition from the first to the second stage, have to answer the question, must be considered to answer questions regarding which extent different processes drive firn densification.

In our optimisation approach, we use a single factor representing various model parameters and search for the factor value leading to the best match between resulting in the best agreement between the simulated and measured firn profiles. In this way, the site-specific simulation results are independent of the possibly deficient, now collectively considered, model parameters. It is not possible to derive a distinct value for the factor representing the climatic conditions at all locations of the investigated firn profiles. The use of a global factor would lead to worse simulation results compared to existing firn density models. Rather we find a linear dependency of the factors on the site-specific surface mass balance specific to the location. By contrast, we did not find a clear linear dependence on temperature (Fig. 7), but the results show that a site-specific parameter is required.

As the amount of surface accumulation affects the load situation conditions, we assume it is not represented well in the model. Unlike other firn densification models, the physical approach of grain boundary sliding depends not does not depend directly on the surface mass balance, but depends on the actual stress. Further interpretation of the results obtained factors is difficult using the presented simulation setup. The description of grain boundary sliding given by Alley (1987) could benefit from a higher dimensional approach including be improved by using a higher-dimensional approach including the horizontal components of the stress tensor. Modelling approaches of this kind include those of Greve and Blatter (2009), Salamantin et al. (2009), and Meyer and Hewitt (2017).

We want to emphasise, that any kind optimisation approaches are only possible due to would like to emphasize that optimization of any type is possible only because of the enormous efforts of the SUMup team (Koenig and Montgomery, 2019), that which has made a vast amount of firn core data available. This is These data are strategically crucial for firn densification modelling advances, which adds to advances in firn densification modeling, reinforcing the recommendations of FirnMICE (Lundin et al., 2017) for enhanced efforts for toward physically based models.

Code availability. The code used to simulate firn profiles will become available via github.com and gitlab.com when this manuscript is published.

535 Appendix A: Model description

A1 Numerical Treatment of Densification

All model equations are solved on an adapting grid, updated in a grid that is updated at every time step. The approach follows the concept of being based on an updated Lagrangian description with, where the update velocity
of the grid being in the material flow velocity. This results in material fixed material-fixed coordinates. The Lagrangian like description allows for a Lagrangian-like description affords very high spatial and temporal resolution in the simulations. It can be shown that by integrating the local Eulerian form of the mass balance in one dimension over a material control volume with moving boundaries \( z_1(t) \) and \( z_2(t) \) leads to, we obtain (Ferziger and Perić, 2002, p. 374)

\[
\frac{dz_2(t)}{dt} \int_{z_1(t)}^{z_2(t)} \rho \, dz + \int_{z_1(t)}^{z_2(t)} \left( \frac{\partial}{\partial z} \left( \rho (v - v_b) \right) \right) \, dz = 0 .
\] (A1)

Here \( \rho \) describes represents the density, \( z \) is the vertical coordinate, \( t \) the time is the time, and \( v \) is the material flow velocity, whereas \( v_b \) represents the grid velocity or the velocity of the integration boundary. When the grid velocity equals the material flow velocity \( (v_b = v) \), the second part of Equation term of Eq. (A1), describing which describes the advection, vanishes. The resulting equation is equal to the Lagrangian form of the mass balance (Ferziger and Perić, 2002, p. 374). On a one-dimensional grid, built up by one-dimensional grid consisting of a number of grid points, as illustrated in Fig. A1, we define denote the grid point velocity to be as \( v_b \) and to equal, which is equal to the flow velocity \( v_b \equiv v \). The location locations of all grid points is updated in every are updated at each time step by integrating the grid point velocity \( v_b \) using a forward Euler scheme. In this way advection is entirely represented. Thus, advection is represented entirely by the adapting grid.

The grid point velocity \( v_b \) is calculated using the constitutive equation of for grain boundary sliding, as described in Section 2.1 Sect. 2.1, and the definition of the strain rate in one dimension. The description of grain boundary sliding provides the strain rate in the vertical direction along the grid, \( \dot{\varepsilon}_{zz} \), as a function of the vertical stress \( \sigma_{zz} \), density \( \rho \), temperature \( T \), and grain radius \( r \)

\[
\dot{\varepsilon}_{zz} = f (\sigma_{zz}, \rho, T, r) = \frac{\partial v}{\partial z} = \frac{\partial v_b}{\partial z} .
\] (A2)

The strain rate of a material line element can be defined as the spatial derivative of the velocity, as shown in Equation Eq. (A2) (Haupt, 2002, pp. 32–38). On a one-dimensional grid, defined by one-dimensional grid, which is defined as a number of grid points, the space between neighboring neighboring grid points can be considered as a material line element (see Fig. A1). Therefore, the grid point velocity \( v_b \) can easily be is easily computed by integrating the strain rate \( \dot{\varepsilon}_{zz} \) in the vertical direction along the length of the grid cell:

\[
v_b = \int_{z_1}^{z_2} \dot{\varepsilon}_{zz} \, dz .
\] (A3)

For the implementation of Equation To implement Eq. (A3), an integration constant determined by a suitable boundary condition is needed. It is reasonable to apply a Dirichlet boundary condition forcing that forces the grid point velocity \( v_b \) to be zero at either the top or the base of the computational domain representing to represent a fixed reference point at the top or the base of the modelled modeled firm profile, respectively. All other points defining the adapting grid are moving with respect to this anchor point. In case of the present study we decided to place this study, we placed the anchor point at the base of the simulated firm profiles \( (z_0 \text{ in Fig. A1}) \). Depth coordinates of The depth coordinates of the profiles shown in the following figures below were adjusted for better readability.
Figure A1. Principle of the grid evolution. On the left side, a grid at time \( t \) is shown. The right hand side of the figure. The grid points move with at the grid point velocity \( v_b \), which equals the material flow velocity \( v \). At time \( t + \Delta t \), an additional grid point \( z_{n+1}(t + \Delta t) \) representing accumulation is added. Distances between neighboring grid points can be understood as material line elements \( |dZ| \) and \( |dz| \) in the reference and in the current configuration, respectively.

For the representation of accumulation at the top of a simulated firn profile, an inflow boundary condition must be implemented. To achieve this, in every time step an additional grid point is added at the top of the grid. Its coordinate within the grid \( z_{n+1}(t + \Delta t) \) is calculated as

\[
z_{n+1}(t + \Delta t) = z_n(t + \Delta t) + \Delta t \frac{a_0(t)}{\rho_0} \rho_{\text{water}},
\]

with where \( a_0 \) is the accumulation rate given in as the \( \text{m s}^{-1} \) water equivalent, \( \Delta t \) is the length of the time step, \( \rho_{\text{water}} \) is the density of water, and \( \rho_0 \) is the density of the deposited snow. The position of a new grid point \( z_{n+1}(t + \Delta t) \) in Fig. A1 is the position of the firn surface at the last time step \( z_n \) plus the thickness of the firn layer deposited during the last time step. This thickness is defined by the time step \( \Delta t \) and the time-dependent accumulation rate \( a_0(t) \). As we use an accumulation rate given in the unit of meter water equivalent per second, it has to be converted to the unit of meter firn equivalent taking the site-specific surface firn density \( \rho_0 \) and water density \( \rho_{\text{water}} \) into account.

This process results in a growing number of grid points. Therefore, grid points are removed from the extending model domain at its base when a maximum number is reached.

A2 Stress

For the evaluation of the stress in vertical direction, we use the local form of the static linear momentum balance in its Eulerian description. We neglect the part of acceleration, as acceleration component.
as the changes in velocity are assumed to be small, leading to: thus, we have
\[ \frac{\partial \sigma_{zz}}{\partial z} + \rho g = 0. \]  
(A5)

Computation of the stress \( \sigma_{zz} \) can easily be achieved by integrating the product of density \( \rho \) and acceleration due to gravity \( g \) along the simulated profile. We assume that the surface of the profile is traction-free.

**A3 Density**

As pointed out in Section A1 and illustrated by Equation (A1), the change of the density integrated over a control volume with respect to time must be zero. Or in other words, the mass incorporated in a control volume cannot change. As the position of the grid points, and therefore the material control volume, does change, the density is changing accordingly. The evaluation of the density integral over a control volume at two time steps leads to:

\[ \rho(t) (z_2(t) - z_1(t)) = \rho(t + \Delta t) (z_2(t + \Delta t) - z_1(t + \Delta t)) . \]  
(A6)

As the space between two neighboring grid points can be understood as a material line element, Equation (Haupt, 2002, pp. 32–38), Eq. (A6) can be rewritten in the form of Equation (A7): Where, where \( |dZ| = |z_2(t) - z_1(t)| \) and \( |dz| = |z_2(t + \Delta t) - z_1(t + \Delta t)| \) are the lengths of a material line element in the reference configuration and its image in the current configuration, respectively:

\[ \rho(t)|dZ| = \rho(t + \Delta t)|dz|. \]  
(A7)

Sorting Equation (A7) leads to, we obtain the formulation of the density change with respect to time depending on the definition of the strain \( \varepsilon_{zz} \) in one dimension (Haupt, 2002, p. 34):

\[ \rho(t + \Delta t) - \rho(t) = -\rho(t + \Delta t) \left( \frac{|dz| - |dZ|}{|dZ|} \right) = -\rho \varepsilon_{zz} . \]  
(A8)

The evolution of the density can therefore be computed by integrating the strain rate \( \dot{\varepsilon}_{zz} \) (Section 2.1) in over time.

**A4 Temperature**

As pointed out in Section A1, all advection in the model domain is represented by the moving grid. Therefore, the description of the temperature evolution reduces to simple heat diffusion:

\[ \rho c_p \left( \frac{\partial T}{\partial t} \right) + \frac{\partial}{\partial z} \left( k(\rho) \frac{\partial T}{\partial z} \right) = 0 . \]  
(A9)
Following Paterson (1994), we assume a constant heat capacity of \( c_p = 2009 \text{J kg}^{-1} \text{K}^{-1} \), and following the example of Zwinger et al. (2007), we assume the density-dependent thermal conductivity described by Sturm et al. (1997) as

\[
k(\rho) = (0.138 \text{W m}^{-1} \text{K}^{-1}) - (1.010 \times 10^{-3} \text{W m}^3 \text{kg}^{-1} \text{K}^{-1}) \rho + (3.233 \times 10^{-6} \text{W m}^5 \text{kg}^{-2} \text{K}^{-1}) \rho^2.
\] (A10)

The temperature profile is initialized using a constant mean value computed from the site-specific surface forcing. To solve for the temperature, a Neumann boundary condition is used at the lower boundary at the profile base. The first derivative, vertical gradient of the temperature is forced to be zero.

### A5 Grain Radius

Alley (1987) used measured grain size data to fit his simulation results to four firn profiles. As information about the grain size is sparse, we use a modelling approach for the description of the grain radius. The evolution of the grain radius \( r \) is simulated using the well-known description of Stephenson (1967) and Gow (1969) as given in the example of Arthern et al. (2010). Stephenson (1967) and Gow (1969) describe the grain size in terms of the mean cross-sectional area. By contrast, Arthern et al. (2010) however assume the mean cross-sectional area to be \( A = (2/3)\pi r^2 \) and formulate the grain growth rate as

\[
\frac{\partial r^2}{\partial t} = k_0 \exp \left( -\frac{E_g}{RT} \right).
\] (A11)

This formulation allows for simple calculation of the grain radius \( r \). Values for activation energy \( E_g = 42.4 \text{kJ mol}^{-1} \) and pre-factor \( k_0 = 1.3 \times 10^{-7} \text{m}^2 \text{s}^{-1} \) of the Arrhenius law are based on data published by Paterson (1994) and were also adapted from Arthern et al. (2010). In contrast to Arthern et al. (2010), we do not use the mean annual temperature but the actual temperature \( T(z,t) \) along the simulated profile.

In order to solve Equation (A11), suitable boundary conditions must be provided. We choose to prescribe a constant surface grain radius. See Section 3.2 for further information on the boundary conditions.

### A6 Age

For reasons of comparison and general interest, the firn age \( \chi \) is simulated. Again due to the fact that was also simulated, because advection is represented by an adapting grid, the description is very simple.

\[
\frac{\partial \chi}{\partial t} = 1.
\] (A12)

Newly deposited snow has an age of zero, prescribed in the form of a Dirichlet boundary condition. The age discretized at the grid points then increases according to the time step.
Time is discretised using constant time steps. For this study, a value of 48 time steps per year was found to be a good compromise between simulation costs and economical simulation and desirable resolution and was used throughout in all simulations. The grid resolution depends on the time step, as a new grid point is generated in every time step representing accumulation at each time step to represent accumulation, as described in Section A1 and shown in Equation Eq. (A4). Time-dependent properties such as the density, temperature, grain radius, and age were developed using an explicit Euler scheme.

Author contributions. T.S. developed the numerical approach and code and conducted and analyzed all simulations. All authors jointly developed the concept of the modeling approach, discussed the results, and wrote the manuscript.

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