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Stabilization of Coupled Convection-Diffusion-Reaction Equations for Continuum Dislocation Transport

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Abstract

The plasticity of crystalline materials can be described at the meso-scale by dislocations transport models, typically formulated in terms of dislocation densities. This leads to sets of coupled non-linear partial differential equations involving diffusive and convective transport mechanisms. Since exact solutions for these systems are not available, numerical approximations are needed to efficiently solve them. The properties of these systems of equations cause most traditional numerical methods to fail, even for the case of a single equation. For systems of equations the problem is even more challenging due to the lack of fundamental principles guiding numerical discretization strategies. Special strategies must be developed and carefully applied to obtain physically meaningful and numerically stable approximations. The objective of this paper is to construct a coefficient perturbation-based stabilization technique for general systems of equations and to apply it to the modelling of one-dimensional dislocation transport. A detailed numerical study is carried out in order to demonstrate its ability to render well-behaved and physically admissible numerical approximations.

keywords.- Convection-diffusion-reaction equations, Coupled systems, Finite element method, Crystal plasticity, Continuum dislocation transport.

1 Introduction

In applied materials science the accurate description of the plastic behaviour of materials is of paramount importance. Inelastic effects of plastic nature in crystalline solids can be accounted for at various scales, among which at the level of a single crystal [1]. This plastic behaviour can be modelled efficiently by considering dislocation densities instead of tracking the behaviour of individual dislocations [2–4]. This results in a continuum description at the meso-scale governed by a set of coupled, transient, and non-linear partial differential equations. These equations contain both first and second order spatial derivatives [3, 5]. The presence of the first order derivative poses serious difficulties to numerical approximation methods, especially when the second order diffusion-like term is dominated by the first order convection-like term.

The approximation of such convection-dominated problems using classical numerical schemes, e.g. by centered finite differences or Bubnov-Galerkin finite elements, may lead to the appearance of spurious and non-physical oscillations that yield useless numerical approximations. Such oscillations appear because of the lack of stability of the numerical scheme for the discretization used. To remedy this problem one has to rely on stabilization techniques to obtain physically meaningful approximations [6–10].

Focusing on the numerical approximation of the system of equations expressed in terms of positive and negative dislocation densities, a stabilization technique based on coefficient perturbation was first developed in [13]. In that communication it is shown, and confirmed numerically, that the stabilized finite element approximation obtained by coefficient perturbation converges toward the classical Bubnov-Galerkin scheme if the diffusion-like terms dominate over the convection-like terms on a sufficiently fine mesh. The development there is based on enforcing the discrete maximum principle, which is the translation of the continuous maximum principle related to the physics of the problem [14, 15].

However, the stabilization technique proposed in [13] cannot be straightforwardly applied to dislocation transport equations involving total and geometrically necessary dislocation densities as the field variables, rather than positive and negative dislocation densities. Such formulations however are more common in the field [2, 3, 5]. The inability of the method to deal with this form is due to the fact that when

signed dislocations are considered, it is possible to arrange the non-linear terms in such a way that the negative dislocation density acts as a transport coefficient in the positive dislocation density equation and vice-versa. Therefore, the system consisting of two partial differential equations can be handled numerically as two independent problems from a numerical stability viewpoint, although its numerical time integration is performed in a staggered manner. This uncoupling is not possible when total and geometrically necessary dislocation densities are the governing field variables, since terms containing only the geometrically necessary dislocation density appear in the total dislocation density equation and vice-versa. This problem thus cannot be decomposed into two problems, which would have allowed for the use of stable approximations of single convection-diffusion partial differential equations. Instead, a single problem consisting of two strongly coupled equations should be solved simultaneously in a monolithic way.

This change of perspective has profound conceptual and technical consequences. It suggests to treat the fully general case with m coupled convection-diffusion-reaction equations, whereas the particular case $m = 1$ received most attention during the past decades among numerical methods practitioners. Systems of coupled equations are met in several branches of science and engineering [16–27]. Since for the multiple equations case analytical solutions are even harder to obtain than for the single equation case, numerical approximations constitute the only available option to solve such systems. Nevertheless, only limited attention has been given to the stabilization of systems of equations. The lack of reliable and robust numerical approximation techniques results from the lack of a maximum principle when passing from a single equation to systems of coupled equations in the most general form [28].

The numerical difficulties present in the single equation case when convection, reaction, or a combination of them dominates over diffusion are inherited by the multiple equations case. Remedies to such instability problems for systems of equations were developed by extending and adapting techniques originally developed for the single equation case. Upwinding of convective terms on layer adapted meshes was proposed by finite difference practitioners [29, 30]. Finite volumes made use of discontinuous and high order approximations and adaptive meshes [31, 32]. Galerkin least-squares, algebraic sub-grid scales, and the extension of the streamline upwind Petrov-Galerkin technique to symmetric systems of convection-diffusion equations, have been the most successful techniques proposed by the finite element community [17, 21, 26, 33]. Notwithstanding all this progress, the straightforward application of some of these techniques to dislocation transport problems is made difficult due to their particular characteristics, mainly (i) the asymmetry of the matrix containing the the convection coefficients and (ii) the non-standard boundary conditions with which they are supplemented.

Taking the single equation case as the departure point, a stabilization technique based on coefficient perturbations was proposed and proven to be effective for systems of linear one-dimensional convection-diffusion-reaction equations in steady state arising from different branches of science and engineering [34]. The main objective of this communication is to extend and to apply this stabilization technique for dislocation transport problems expressed in terms of the total and geometrically necessary dislocation densities, including its non-linearity in the transient regime. The stabilization technique is expected to be versatile despite the above two additional complexities associated with dislocation transport. It allows dealing with continuum dislocation transport problems using affordable and relatively inexpensive mesh refinement levels.

The paper is organized as follows. In Section 2, the problem statement of an infinite crystal with parallel glide planes and subjected to a shear stress is described. The corresponding partial differential equations are obtained based on some simplifying assumptions. Boundary and initial conditions are next discussed both from physical and mathematical perspectives. Section 3 is devoted first to the numerical treatment of a general system of convection-diffusion-reaction equations with constant coefficients in a one-dimensional setting using finite elements. Subsequently, a stabilization technique for a single steady state and linear convection-diffusion-reaction equation, originally proposed in [13], is reviewed. The extension of the stabilization technique extension to *systems* of coupled convection-diffusion-reaction equations, as proposed in [34], is discussed at the end of this section. Section 4 assesses the effectiveness of the stabilization technique for the system of dislocation transport equations through two numerical examples comparing stabilized results with those obtained with the classical Bubnov-Galerkin scheme. This is followed by two additional numerical examples, allowing to thoroughly assess the efficiency and consistency of the stabilization technique. Subsequently, several numerical simulations obtained for different dislocation transport modelling assumptions, mainly related to the length scale parameters, are presented. To close this section, the performance of the stabilization technique is evaluated when the

diffusion and convection terms are defined in a different manner. Such a change in the definition of the transport operators is made possible by the non-linearity of the dislocation transport equations. Section 5 presents the conclusions of this work and outlooks some future work.

2 Continuum model for dislocation transport

The main focus of this paper is to construct the stabilization of the dislocation transport equations and therefore to obtain physically meaningful approximations on which to build further developments. It is desired to be able to obtain such reliable approximations regardless of the field variables used.

The total dislocation density on a particular plane is defined as the total length of dislocation line per unit crystal volume [4, 35]. A single glide system with infinite parallel edge dislocations is considered. First, positive and negative dislocation densities, denoted respectively by ρ^+ and ρ^- , are used. This choice is made since ρ^+ and ρ^- have a clear, intuitive physical interpretation. For simplicity, annihilation of dislocations of different signs is not considered. This implies that positive and negative dislocations are assumed to move on different glide planes. The crystal is considered infinite in the direction perpendicular to these glide planes. A pure shear stress τ is applied parallel to the glide planes. Figure 1 depicts these assumptions together with impenetrable boundaries, which will be described later. It is presumed that the main cause of the instability problems, i.e. first order convection-like terms dominant over second order diffusion-like terms, are still present despite the simplifying assumptions adopted.

Figure 1: Positive and negative dislocations on distinct glide planes, bounded by impenetrable barriers.

The shear stress will give rise to the convection-like terms that together with the impenetrable boundaries cause the positive dislocations to pile-up at one extremity of the spatial domain while the negative dislocations pile up at the opposite boundary. These dislocation concentrations, once translated to the continuum scale through dislocation densities, are reflected in boundary layers, as will be further illustrated in the numerical assessment section.

2.1 Governing equations

Dislocation transport in the previously sketched configuration can be described by two conservation equations, one for each dislocation density, as

$$\frac{\partial \rho^+}{\partial t} + \frac{\partial}{\partial x} (\Phi^+) = s^+, \quad (1)$$

$$\frac{\partial \rho^-}{\partial t} + \frac{\partial}{\partial x} (\Phi^-) = s^-, \quad (2)$$

where ρ^+ and ρ^- are the positive and negative dislocation densities to be transported and conserved in the spatial domain Ω with boundary Γ , s^+ and s^- are their corresponding source terms. $\Phi^+ = \rho^+ v^+$ and $\Phi^- = \rho^- v^-$ are in turn their corresponding fluxes, with v^+ and v^- being the velocities of positive and negative dislocations. These velocities are obtained by averaging the Peach-Koehler forces experienced by each dislocation along a single glide plane divided by the drag coefficient B . This force is the result

of the external stress τ and of the stresses induced by the other dislocations. Accordingly, the velocities can be expressed as [2, 3, 5]

$$v^\pm = \pm \frac{b\tau}{B} - \mathcal{L}^2 \frac{\bar{G}b^2}{6B} \left[(b'_1 + b'_2) \frac{\partial \rho^\pm}{\partial x} + (b'_1 - b'_2) \frac{\partial \rho^\mp}{\partial x} \right]. \quad (3)$$

The first term is standard in the literature while the second takes into account the internal stresses generated by dislocation density gradients. In this expression b is the Burgers' vector length, $\bar{G} = G/(2(1 - \nu))$ is a material constant and τ is the externally applied shear stress. The length scale is denoted generically by $\mathcal{L}$ with the aim of keeping the model as general as possible. Taking $\mathcal{L} = h$, with h being the glide plane spacing, a constant length scale model is recovered. By setting $\mathcal{L} = 1/\sqrt{\rho^+ + \rho^-}$, a variable length scale model is obtained. Two constants, $b'_1 = (2 + a)b_1$ and $b'_2 = (2 - a)b_2$, have been introduced in order to reproduce typical dislocation transport models presented in the literature. If the forces exerted by the positive dislocations on the negative dislocations, and vice-versa, are taken into account, then $a = 1$. By setting $a = 0$ this mutual action between positive and negative dislocations is neglected. Furthermore, by setting $b_1 = 1$ and $b_2 = 1$ *Dogge* type models, as they will be referred to hereafter, are obtained [2]. If, instead, $b_1 = 0$ and $b_2 = 12/(2 - a)$ are set, then *Groma* type models are obtained [3]. The superscripts $\pm$ and $\mp$ are used to encompass two expressions in a single one. To further facilitate the forthcoming algebraic manipulations two stress and material dependent constants are introduced:

$$C_0 = \frac{b\tau}{B}, \quad \text{and} \quad C_1 = \frac{\bar{G}b^2}{12B}. \quad (4)$$

Two additional constants are introduced to easily switch parameters between the *Dogge* and *Groma* models, constant and variable length scales, and mutually acting forces between positive and negative dislocations

$$C_2 = (b'_1 + b'_2)C_1\mathcal{L}, \quad \text{and} \quad C_3 = (b'_1 - b'_2)C_1\mathcal{L}, \quad (5)$$

allowing to express the positive and negative fluxes generically as

$$\Phi^\pm = \rho^\pm \left(\pm C_0 - C_2 \frac{\partial \rho^\pm}{\partial x} - C_3 \frac{\partial \rho^\mp}{\partial x} \right). \quad (6)$$

It is common practice in the literature to use the *total dislocation density* ρ and the *geometrically necessary dislocation density* κ rather than the positive and negative dislocations densities, since these total dislocations and geometrically necessary dislocations densities are directly related to macroscopic properties such as incompatibility and hardening. They are related to the positive and negative dislocation densities by

$$\rho = \rho^+ + \rho^-, \quad \text{and} \quad \kappa = \rho^+ - \rho^-. \quad (7)$$

Using these relations it is possible to rewrite the transport equations, first for ρ by adding Equations (1) and (2) and then for κ by subtracting Equation (2) from Equation (1), yielding

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} (\Phi_\rho) = s_\rho, \quad (8)$$

$$\frac{\partial \kappa}{\partial t} + \frac{\partial}{\partial x} (\Phi_\kappa) = s_\kappa, \quad (9)$$

where the fluxes are obtained similarly as $\Phi_\rho = \Phi^+ + \Phi^-$ and $\Phi_\kappa = \Phi^+ - \Phi^-$, which can again be expressed in terms of ρ and κ . By introducing the following two constants

$$C_4 = b'_1 C_1 \mathcal{L}, \quad \text{and} \quad C_5 = b'_2 C_1 \mathcal{L}, \quad (10)$$

the corresponding fluxes are expressed in a compact form as

$$\Phi_\rho = C_0 \kappa - C_4 \rho \frac{\partial \rho}{\partial x} - C_5 \kappa \frac{\partial \kappa}{\partial x}, \quad (11)$$

$$\Phi_\kappa = C_0 \rho - C_5 \rho \frac{\partial \kappa}{\partial x} - C_4 \kappa \frac{\partial \rho}{\partial x}. \quad (12)$$

Finally, the pair of coupled non-linear partial differential equations modeling dislocations transport is obtained by substituting the fluxes (11-12) into the conservation Equations (8-9). Analytical solutions for these equations are not available mainly because of their non-linear character. Thus, a numerical approximation method should be used to deal with them. This will be done in the next section using the finite element method.

2.2 Boundary and initial conditions

The first type of boundary condition to be considered corresponds to the situation depicted in Figure 1, i.e. an impenetrable boundary which acts as a barrier preventing the dislocations from flowing out of the domain. In terms of total and geometrically necessary dislocation densities, and in accordance with the positive and negative dislocations conditions sketched in Figure 1, the fluxes vanish at impenetrable boundaries, $\Phi_\rho(\Gamma_R) = \Phi_\kappa(\Gamma_R) = 0$. The sub-index R makes reference to the fact that this matches a coupled mixed boundary condition of Robin type. This can be understood from the flux expressions (11-12) since both dislocation densities and their normal derivatives are involved.

The second boundary condition considered consists of a free surface trough which dislocations can freely escape. This matches the condition $\rho(\Gamma_D) = \kappa(\Gamma_D) = 0$ which can be obtained from the boundary condition $\rho^\pm(\Gamma_D) = 0$, with the sub-index D making reference to a boundary condition of Dirichlet type.

Due to the transient character of the conservation Equations (8-9), the total and geometrically necessary dislocation density distributions in the whole spatial domain at the initial time must be supplied as well. These initial conditions will be identified with the 0 sub-index, i.e. $\rho_0(\Omega) = \rho(\Omega, t = 0)$ and $\kappa_0(\Omega) = \kappa(\Omega, t = 0)$.

3 Stabilization of the finite element approximation by coefficient perturbation

This section first outlines the classical finite element discretization following a Bubnov-Galerkin scheme, of a general system of coupled linear convection-diffusion-reaction equations with constant coefficients. Afterwards the stabilization technique based on coefficient perturbations proposed in [13], is reviewed in Section 3.2, making a special effort to convey its conceptual working mechanism. This methodology is then extended from the single equation case to the case containing several coupled convection-diffusion-reaction equations in Section 3.3.

3.1 Classical finite element discretization

Consider the system of equations that describe the conservative transport of the generic field variables u_q for $q = 1, 2, \dots, m$, with reaction terms

$$\rho_{pq} \frac{\partial u_q}{\partial t} + \frac{\partial}{\partial x} (F_p) + \gamma_{pq} u_q = f_p, \quad (13)$$

with the corresponding fluxes denoted as

$$F_p = -\alpha_{pq} \frac{\partial u_q}{\partial x} + \beta_{pq} u_q. \quad (14)$$

Repeated indices are contracted according to the traditional summation convention. The mass coefficients $\rho_{pq} \in \mathbb{R}^+$ are assumed to vanish when $p \neq q$. In these equations $\alpha_{pq} \in \mathbb{R}^+$ are the diffusion coefficients, $\beta_{pq} \in \mathbb{R}$ are the convection coefficients, and $\gamma_{pq} \in \mathbb{R}$ are the reaction coefficients, for $p, q = 1, 2, \dots, m$. All these physical coefficients will be referred to as *direct* when $p = q$ and as *coupled* when $p \neq q$. Finally, $f_p \in \mathbb{R}$, for $p = 1, 2, \dots, m$, are the source terms. In the whole of this section all these physical coefficients and source terms will be considered as constants.

The direct substitution of the flux given by Equation (14) in the general conservation Equation (13) leads to

$$\rho_{pq} \frac{\partial u_q}{\partial t} + \frac{\partial}{\partial x} \left(-\alpha_{pq} \frac{\partial u_q}{\partial x} + \beta_{pq} u_q \right) + \gamma_{pq} u_q = f_p. \quad (15)$$

$$\mathbf{M}\dot{\mathbf{u}} - \mathbf{A}\mathbf{u}'' + \mathbf{B}\mathbf{u}' + \mathbf{G}\mathbf{u} = \mathbf{f}, \quad (16)$$

where time and space derivatives are denoted by the superimposed dot and the prime symbol respectively. The matrices $\mathbf{M}$, $\mathbf{A}$, $\mathbf{B}$, and $\mathbf{G}$ are the *matrices of mass, diffusion, convection, and reaction coefficients* and $\mathbf{u} = [u_1, u_2, \dots, u_m]^T$ is the *vector of unknowns* that gathers all the field variables. The vector $\mathbf{f} = [f_1, f_2, \dots, f_m]^T$ does the same for the m source terms. These matrices and vectors corresponds to the strong form of the problem and should not be confused with the global matrices and vectors assembled by the finite element discretization.

Even if the weighted residuals statement would allow the use of a different weighting function for each of the m equations, only a single weighting function w will be used in what follows, with the sole purpose to keep the exposition as simple as possible. Thus the general conservation Equation (13) is multiplied by w and integrated over the whole spatial domain. Its weighted residual form is obtained after integration by parts

$$\int_{\Omega} w \rho_{pq} \frac{\partial u_q}{\partial t} d\Omega - \int_{\Omega} \frac{\partial w}{\partial x} F_p d\Omega + [w F_p]_{\Gamma} + \int_{\Omega} w \gamma_{pq} u_q d\Omega = \int_{\Omega} w f_p d\Omega. \quad (17)$$

Here, the integration by parts is performed on the whole flux term, as seldom done in the finite element context for fluid dynamics, in order to easily handle *natural* boundary conditions of the Robin type.

Linear combinations of the nodal values of the weighting function w and the field variables u_p are used with their corresponding interpolation functions W_k and P_k , associated with the n nodes in the finite element mesh

$$w = \sum_{k=1}^n W_k w_k \quad \text{and} \quad u_p = \sum_{k=1}^n P_k (u_p)_k. \quad (18)$$

Since the result must hold for all w_k , it can be eliminated and the finite element resulting discretization reads

$$\mathbf{M}_{pq} \dot{\mathbf{u}}_q + (\mathbf{D}_{pq} + \mathbf{C}_{pq} + \mathbf{R}_{pq}) \mathbf{u}_q = \mathbf{f}_p, \quad (19)$$

where the sub-indices p and q help emphasizing that these *global matrices*, $\mathbf{M}_{pq}$ for mass, $\mathbf{D}_{pq}$ for diffusion, $\mathbf{C}_{pq}$ for convection and $\mathbf{R}_{pq}$ for reaction differ from those presented in Equation (16). The nodal values are sorted in m vectors $\mathbf{u}_q = [u_q^{(1)}, u_q^{(2)}, \dots, u_q^{(n-1)}, u_q^{(n)}]^T$, for $q = 1, 2, \dots, m$. Here n is the total number of nodes in the finite element discretization. Moreover, these m vectors can be collected into a single degree-of-freedom vector as

$$\mathbf{u} = [u_1^{(1)}, u_1^{(2)}, \dots, u_1^{(n)}, u_2^{(1)}, u_2^{(2)}, \dots, u_2^{(n)}, \dots, u_m^{(1)}, u_m^{(2)}, \dots, u_m^{(n)}]^T, \quad (20)$$

which will be hereafter simply called the numerical approximation. The same conventions will be applied to the m vectors $\mathbf{f}_p$ that contain the source terms f_p and the associated boundary conditions for each of the $p = 1, 2, \dots, m$ equations.

Bubnov-Galerkin approaches, with $P_k = W_k$, render physically meaningful solutions if the convection coefficients β_{pq} and reaction coefficients γ_{pq} , are negligible compared with the diffusion coefficients α_{pq} , on a sufficiently refined mesh, i.e. having at hand a diffusion dominated case. However, these conditions might not be satisfied for problems of practical interest in which spurious oscillations appear, preventing any use of the numerical approximation. Solving this problem has been the motivation for the development of several stabilization techniques. The vast majority of these proposals have in mind the single equation case, i.e. with $m = 1$ [11, 12]. Extension of these stabilization techniques to systems of convection-diffusion equations have been proposed as well [26]. However the continuum dislocation transport equations do not satisfy some of the key requirements of these techniques, e.g. the symmetry of the matrix of convection coefficients $\mathbf{B}$ [33].

3.2 Stabilization for the case of a single equation

The aforementioned spurious oscillations that appear when discretizing a convection dominated equation with the classical Bubnov-Galerkin method are caused by the inability of this method to unconditionally satisfy the discrete maximum principle. Its fulfillment ensures uniform convergence of the finite element approximation, i.e. the reduction of the truncation error as the mesh is refined [14, 36]. Such a maximum principle can be only rigorously established for the case of a single differential equation. When handling systems of differential equations, barrier functions or compatibility conditions should be established and used instead [30, 37–39]. Irrespective of the problem considered, a stabilization technique is required in order to obtain physically meaningful approximations. In this work, no special attention will be paid to the afore mentioned barrier functions or compatibility conditions as their derivation is beyond the scope of the present work. Therefore, the only guiding criterion for the stabilization technique development will be the removal of spurious oscillations. Interior domain values of the approximated solutions will therefore be allowed to be larger or smaller than the corresponding boundary values, by considering coupling terms between unknowns as sources or sinks.

The particular nature of the system of equations modeling continuum dislocation transport has recently motivated the development of a stabilization technique based on coefficient perturbations [13]. It consists in adding a perturbation to the problem's physical coefficients in a similar fashion as done in artificial diffusion methods. This stabilization technique ensures that the computed perturbations are optimally determined, avoiding the use of excessive artificial diffusion. This stabilization technique will be reviewed by using the simplified Dirichlet problem reading

$$\frac{d}{dx} \left(-\alpha \frac{du}{dx} + \beta u \right) + \gamma u = f \quad \text{in} \quad \Omega = (0, 1), \quad (21)$$

$$u(x=0) = u^L \quad \text{and} \quad u(x=1) = u^R. \quad (22)$$

Note that the use of sub-indices has been dispensed with here without the risk of confusion. As previously done, a Bubnov-Galerkin approach is used to discretize Equation (21). Once this discretization is carried out on a uniform mesh with element size ℓ and linear shape functions, a linear system of equations is obtained. Its i -th algebraic equation can be written as

$$-\left(\frac{\alpha}{\ell^2} + \frac{\beta}{2\ell} - \frac{\gamma}{6}\right) u^{(i-1)} + 2\left(\frac{\alpha}{\ell^2} + \frac{\gamma}{3}\right) u^{(i)} - \left(\frac{\alpha}{\ell^2} - \frac{\beta}{2\ell} - \frac{\gamma}{6}\right) u^{(i+1)} = f^{(i)}. \quad (23)$$

The discrete maximum principle should be satisfied by the stencil (23) in order to render the numerical scheme stable. To fulfill it, the following inequality should hold

$$\frac{\alpha}{\ell^2} - \frac{|\beta|}{2\ell} - \frac{\gamma}{6} \geq 0. \quad (24)$$

Based on this inequality, it is worth considering the convection-diffusion sub-case ($\gamma = 0$) due to its extensive study in the fluid dynamics community. In such a case, Inequality (24) reduces to

$$Pe \stackrel{\text{def}}{=} \frac{\beta\ell}{2\alpha} \leq 1, \quad (25)$$

where Pe is the mesh Péclet number that will be further used in the remainder of the paper.

Inequality (24) can be satisfied by reducing the mesh size ℓ , i.e. through mesh refinement. However, for a given combination of the physical coefficients, α , β , and γ , such a refinement could become computationally unaffordable. An alternative strategy keeping ℓ unaltered would consist in modifying one or several of the physical coefficients, α , β , and γ , in order to ensure the fulfilment of Inequality (24). This is the fundamental working mechanism of the presented stabilization technique. Given a set of physical coefficients, α , β , and γ , and a mesh size ℓ , it determines some modifications of the physical coefficients, hereafter called *perturbations* and distinguished by the use of an asterisk as super-index, α^* , β^* , and γ^* , such that the Inequality (24) is fulfilled.

Once these perturbations are taken into account they define, together with the physical coefficients, a set of *perturbed* coefficients, $\tilde{c} = c + c^*$ for $c = \alpha, \beta, \gamma$, which in turn define a *perturbed* problem for which it is known on beforehand that its finite element approximation is stable on the given mesh size ℓ .

Using the perturbed coefficients instead of the original ones and after some rearrangement, the i -th stencil of the algebraic system can be written as

$$-\frac{\tilde{\alpha}}{\ell} \left(u^{(i-1)} - 2u^{(i)} + u^{(i+1)} \right) - \frac{\tilde{\beta}}{2} \left(u^{(i-1)} - u^{(i+1)} \right) + \frac{\tilde{\gamma}\ell}{6} \left(u^{(i-1)} + 4u^{(i)} + u^{(i+1)} \right) = \ell f^{(i)}. \quad (26)$$

The fulfillment of the discrete maximum principle, i.e. Inequality (24), is sought via the determination of the coefficient perturbations α^* , β^* , and γ^* . These perturbations should be selected as small as possible in order to keep the perturbed problem as close as possible to the original problem defined with the unperturbed physical coefficients.

The computation of the perturbations uses the exact solution of the homogeneous convection-diffusion-reaction equation, given by the form

$$u(x) = c_1 e^{\lambda_1 x} + c_2 e^{\lambda_2 x}, \quad (27)$$

in which the boundary conditions (22) determine the integration constants c_1 and c_2 . Still for the single equation case, the exponential coefficients $\lambda_{1,2}$ are the roots of the characteristic polynomial associated to Equation (21) with $f = 0$:

$$\lambda_{1,2} = \frac{\beta}{2\alpha} \pm \sqrt{\left(\frac{\beta}{2\alpha}\right)^2 + \frac{\gamma}{\alpha}}. \quad (28)$$

The coordinates of the stencil points, i.e. x_{i-1} , x_i and x_{i+1} , are substituted in the exact solution (27)

$$u^{(i)} = c_1 e^{\lambda_1 x_i} + c_2 e^{\lambda_2 x_i}, \quad \text{and} \quad u^{(i\pm 1)} = c_1 e^{\lambda_1 x_i} e^{\pm \lambda_1 \ell} + c_2 e^{\lambda_2 x_i} e^{\pm \lambda_2 \ell}, \quad (29)$$

and these evaluations are in turn substituted in the i -th perturbed stencil (26) to obtain

$$\begin{aligned} & \frac{\tilde{\alpha}}{\ell} \{c_1 e^{\lambda_1 x_i} [1 - \cosh(\lambda_1 \ell)] + c_2 e^{\lambda_2 x_i} [1 - \cosh(\lambda_2 \ell)]\} + \\ & \frac{\tilde{\beta}}{2} \{c_1 e^{\lambda_1 x_i} \sinh(\lambda_1 \ell) + c_2 e^{\lambda_2 x_i} \sinh(\lambda_2 \ell)\} + \\ & \frac{\tilde{\gamma} \ell}{6} \{c_1 e^{\lambda_1 x_i} [2 + \cosh(\lambda_1 \ell)] + c_2 e^{\lambda_2 x_i} [2 + \cosh(\lambda_2 \ell)]\} = 0. \end{aligned} \quad (30)$$

It is important to remark that this expression is valid for the i -th node in the mesh and does not represent in any way the differential operator on the whole spatial domain. This fact allows modifying the local boundary conditions with great flexibility. By doing so in order to get $c_2 = 0$, one algebraic equation with coefficients depending only on λ_1 is obtained from the general expression (30). Next, changing the boundary conditions to get $c_1 = 0$ furnishes an equation with coefficients only depending on λ_2 . These two equations constitute a linear system with the three unknown perturbed coefficients, reading

$$\frac{\tilde{\alpha}}{\ell} [1 - \cosh(\lambda_1 \ell)] + \frac{\tilde{\beta}}{2} \sinh(\lambda_1 \ell) + \frac{\tilde{\gamma} \ell}{6} [2 + \cosh(\lambda_1 \ell)] = 0, \quad (31)$$

$$\frac{\tilde{\alpha}}{\ell} [1 - \cosh(\lambda_2 \ell)] + \frac{\tilde{\beta}}{2} \sinh(\lambda_2 \ell) + \frac{\tilde{\gamma} \ell}{6} [2 + \cosh(\lambda_2 \ell)] = 0. \quad (32)$$

The most straightforward way to solve this undetermined linear system is to keep one of the coefficients unperturbed, i.e. its corresponding perturbation is arbitrarily set to zero. This will allow to determining the two remaining perturbations through the solution of the, now determined, 2×2 linear system at hand. It can be demonstrated that the presented perturbation-based stabilization technique renders unconditionally stable numerical approximations. Moreover, for the convection-diffusion case the classical SUPG artificial diffusion formula is obtained [13]. Nevertheless, it is presumed that determining all three perturbations at once could be envisioned using an optimization strategy. Even though this option is presumed to be optimal, the proper formulation of the required objective function is far from trivial in view of an intended local stabilization technique. Moreover, the real gain with respect to the adopted simple approach remains unclear. The implementation and assessment of such a potential optimization strategy are beyond the scope of the present work.

3.3 Extension to systems of coupled equations

The objective of this section is to summarize the heuristic extension of the previously developed stabilization technique from the single equation case to the system of coupled equations case. The unperturbed simplified boundary value problem in the m equations case reads as

$$\frac{d}{dx} \left(-\alpha_{pq} \frac{du_q}{dx} + \beta_{pq} u_q \right) + \gamma_{pq} u_q = f_p \quad \text{in} \quad \Omega = (0, 1), \quad (33)$$

$$u_p(x=0) = u_p^L \quad \text{and} \quad u_p(x=1) = u_p^R, \quad (34)$$

which generates, after discretization on a uniform mesh, m numerical stencils having the general form

$$-\frac{\alpha_{pq}}{\ell} \left(u_q^{(i-1)} - 2u_q^{(i)} + u_q^{(i+1)} \right) - \frac{\beta_{pq}}{2} \left(u_q^{(i-1)} - u_q^{(i+1)} \right) + \frac{\gamma_{pq} \ell}{6} \left(u_q^{(i-1)} + 4u_q^{(i)} + u_q^{(i+1)} \right) = \ell f_p^{(i)}, \quad (35)$$

which, after assembly of the global system of linear equations, represents the $[i + (p-1)m]$ -th equation.

On the other hand, the analytical solution of the corresponding homogeneous system of differential equations, i.e. (33) with $f_p = 0$, can be expressed in all generality as

$$\mathbf{u} = c_1 e^{\lambda_1 x} \mathbf{v}^{(1)} + c_2 e^{\lambda_2 x} \mathbf{v}^{(2)} + \dots + c_{2m} e^{\lambda_{2m} x} \mathbf{v}^{(2m)}, \quad (36)$$

where the c_k constants solely depend on the boundary conditions given by (34), and λ_k and $\mathbf{v}^{(k)}$ are the $2m$ eigenvalues and eigenvectors of a $2m \times 2m$ matrix constructed with the transport matrices defined in (16) as follows

$$\mathbf{K} = \begin{bmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{A} \end{bmatrix}^{-1} \begin{bmatrix} \mathbf{0} & \mathbf{I} \\ \mathbf{G} & \mathbf{B} \end{bmatrix}, \quad (37)$$

where $\mathbf{I}$ and $\mathbf{0}$ are the $m \times m$ identity and null matrices. Thus, it is possible to evaluate the q -th solution of the system of equations (33) with $f_p = 0$ at the nodes defining the finite element stencils (35), i.e. at x_{i-1} , x_i and x_{i+1} :

$$u_q(x_i) = u_q^{(i)} = \sum_{k=1}^{2m} c_k v_q^{(k)} e^{\lambda_k x_i}, \quad \text{and} \quad u_q(x_{i\pm 1}) = u_q^{(i\pm 1)} = \sum_{k=1}^{2m} c_k v_q^{(k)} e^{\lambda_k x_i} e^{\pm \lambda_k \ell}. \quad (38)$$

These evaluations are then substituted into the perturbed finite element stencils. These perturbed stencils are obtained in the same manner as the unperturbed ones, and given by (35), but using the perturbed coefficients $\tilde{\alpha}_{pq}$, $\tilde{\beta}_{pq}$, and $\tilde{\gamma}_{pq}$ instead of the physical coefficients α_{pq} , β_{pq} , and γ_{pq} . After substitution and some elementary algebra one obtains for the p -th perturbed stencil

$$\begin{aligned} & \frac{\tilde{\alpha}_{pq}}{\ell} \sum_{k=1}^{2m} c_k v_q^{(k)} e^{\lambda_k x_i} [1 - \cosh(\lambda_k \ell)] + \\ & \frac{\tilde{\beta}_{pq}}{2} \sum_{k=1}^{2m} c_k v_q^{(k)} e^{\lambda_k x_i} \sinh(\lambda_k \ell) + \\ & \frac{\tilde{\gamma}_{pq} \ell}{6} \sum_{k=1}^{2m} c_k v_q^{(k)} e^{\lambda_k x_i} [2 + \cosh(\lambda_k \ell)] = 0. \end{aligned} \quad (39)$$

Each of these m equations (for $p = 1, 2, \dots, m$) correspond to a differential equation in the system (33). It is possible to generate $2m$ algebraic equations from each of the m equations (39) through the index $k = 1, 2, \dots, 2m$ since the c_k constants solely depend on the boundary conditions in (34). To illustrate this equation generating process, one chooses first the boundary conditions in such a way that $c_1 \neq 0$ and $c_2 = c_3 = \dots = c_{2m} = 0$, generating m algebraic equations for $k = 1$. A change to the boundary conditions to get $c_1 = 0$, $c_2 \neq 0$, and $c_3 = c_4 = \dots = c_{2m} = 0$, generates m more algebraic equations for $k = 2$. Each of the subsequent $k = 3, 4, \dots, 2m$ will generate m algebraic equations. At the end of this process one ends up with a system of $2m^2$ algebraic equations with $3m^2$ unknowns, i.e. the m^2 perturbed diffusion coefficients $\tilde{\alpha}_{pq}$, the m^2 perturbed convection coefficients $\tilde{\beta}_{pq}$, and the m^2 perturbed reaction coefficients $\tilde{\gamma}_{pq}$, ($p, q = 1, 2, \dots, m$). This system of algebraic equations can be compactly expressed as

$$\frac{\tilde{\alpha}_{pq}}{\ell} v_q^{(k)} [1 - \cosh(\lambda_k \ell)] + \frac{\tilde{\beta}_{pq}}{2} v_q^{(k)} \sinh(\lambda_k \ell) + \frac{\tilde{\gamma}_{pq} \ell}{6} v_q^{(k)} [2 + \cosh(\lambda_k \ell)] = 0, \quad (40)$$

where the eigenvalues λ_k and their corresponding eigenvectors $\mathbf{v}^{(k)}$ can be computed numerically. However, it is only possible to determine at most $2m^2$ perturbed coefficients since this is the number of algebraic equations at hand. Thus at least m^2 perturbations must be set to zero to make the system (40) solvable.

Note that the case $m = 1$ corresponds to that illustrated in Section 3.2. Moreover, when all the transport matrices $\mathbf{A}$, $\mathbf{B}$, and $\mathbf{G}$ are diagonal, i.e. the equations in the system are uncoupled, it is possible to shown that the system of m differential equations can be treated instead as m separate problems consisting of a single differential equation.

4 Computational assessment of the stabilization technique

This section is devoted to the application of the perturbation-based stabilization technique once extended to dislocation transport. The main intention is to assess its efficiency to deal with the dislocation transport equations written in terms of total and geometrically necessary dislocations presented in Section 2. When using these field variables, the original stabilization technique presented in [13] was shown ineffective due to the presence of crossed convection terms. Particular attention is therefore paid here to the illustration of the efficiency and consistency of the stabilization scheme reviewed in Section 3.3.

	Crossed interaction	
b'_1	With	Without
Dogge	3	1
Groma	0	0

Table 1: Values of b'_1 .

	Crossed interaction	
b'_2	With	Without
Dogge	1	1
Groma	4	12

Table 2: Values of b'_2 .

4.1 Numerical implementation of the dislocation transport problem

The system of interest in the present work, i.e. in terms of total and geometrically necessary dislocations, is obtained by substituting the dislocation fluxes (11-12) into their corresponding conservation Equations (8-9) to obtain the non-linear partial differential equations

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} \left[-C_4 \rho \frac{\partial \rho}{\partial x} + \left(C_0 - C_5 \frac{\partial \kappa}{\partial x} \right) \kappa \right] = s_\rho, \quad (41)$$

$$\frac{\partial \kappa}{\partial t} + \frac{\partial}{\partial x} \left[-C_5 \rho \frac{\partial \kappa}{\partial x} + C_0 \rho - C_4 \frac{\partial \rho}{\partial x} \kappa \right] = s_\kappa, \quad (42)$$

where the terms composing the fluxes have been re-written in a slightly different format than in Equations (11-12). This format is chosen in order to clearly identify convection-like or diffusion-like coefficients, either direct or crossed, and to be able to cast this system of coupled partial differential equations in the generic matrix form given by Equation (16). In this generic form, the unknown vector is taken as $\mathbf{u} = [\rho, \kappa]^T$; it follows naturally that the source vector is $\mathbf{f} = [s_\rho, s_\kappa]^T$. Thus, the diffusion matrix $\mathbf{A}$ and the convection matrix $\mathbf{B}$ can be expressed as:

$$\mathbf{A} = \rho \begin{bmatrix} C_4 & 0 \\ 0 & C_5 \end{bmatrix}, \quad \text{and} \quad \mathbf{B} = \begin{bmatrix} 0 & C_0 - C_5 \frac{\partial \kappa}{\partial x} \\ C_0 & -C_4 \frac{\partial \rho}{\partial x} \end{bmatrix}. \quad (43)$$

Note that this form can be established irrespective of: (i) the dislocation transport model type used (e.g. [2] for Dogge model or [3] for Groma model), (ii) the length scale adopted (constant or variable), (iii) the presence or absence of interactions between dislocations of different sign. It is emphasized that the generality of the notation used in Equations (41-42) and in the definitions in (43) through the constants C_0 , C_4 , and C_5 allows addressing various commonly used transport models. Their precise definition and role in switching among the different transport models, length scales and interactions can be found in Section 3.1. Also note that the convection matrix $\mathbf{B}$ depends on the gradient of the dislocation densities. This matrix, together with the diffusion matrix $\mathbf{A}$, is required in advance by the stabilization technique to compute the corresponding perturbations according to Equation (40). In order to deal with such dependency, the stabilization technique should be applied in each of the non-linear iterative steps, making it highly adaptive.

It is useful to analyze in some depth the properties of these diffusion and convection matrices. First note that the effectiveness of the stabilization technique will be determined by the positive definiteness of the diffusion matrix which can be seen as the vector equivalent of having a positive diffusion coefficient in the scalar case, i.e. diffusion always takes place in the negative gradient's direction. This property can be easily verified through the diffusion matrix determinant given by $|\mathbf{A}| = C_4 C_5 \rho^2$. Its sign is hence determined by the constants C_4 and C_5 given by Equation (10). After continued substitution, the diffusion matrix determinant can finally be written as

$$|\mathbf{A}| = b'_1 b'_2 (\rho C_1 \mathcal{L})^2. \quad (44)$$

It is clear that the positiveness of the diffusion matrix is not affected by the length scale $\mathcal{L}$, nor by the material properties since $C_1 \neq 0$. This property is only affected by the model used and by the interactions between dislocations of different signs considered. This can be observed by identifying the b'_1 and b'_2 values for the two considered models, shown in tabular form in Table 1 for b'_1 and Table 2 for b'_2 .

Note that the Groma model poses a serious difficulty to the stabilization technique presented here since the conservation equation for the total dislocation density ρ becomes a purely hyperbolic partial differential equation. Such equations have been successfully handled by the finite difference and finite volume communities by means of several techniques that have shown to be effective throughout the years, the up-wind differences being the oldest and simplest one. In general terms all these techniques,

and up-winding in particular, rely on the addition of artificial diffusion. Therefore all of them can be interpreted as perturbation techniques that introduce ellipticity into the originally hyperbolic partial differential equation. This is the main reason to consider the introduction of a threshold diffusion when dealing with the Groma type models. This threshold will be taken as $\alpha_{min} = 10^{-12}$ in all subsequent computations.

Despite its first order accuracy $\mathcal{O}(\Delta t)$, the fully implicit backward Euler method is used to deal with the time discretization of the system at hand. This choice is based on its unconditional stability regardless of the time step size Δt and the spectral properties of the matrices obtained after the time-space discretization [42–46].

To deal with the non-linear nature of the dislocations transport equations, the Picard iterative method of successive approximations is employed for all simulations. The iterative process at each time step is stopped as soon as the tolerance $\epsilon_n = 10^{-6}$ is reached, i.e. when $d^{(j)} < \epsilon_n$, with $d^{(j)}$ being the difference between two successive non-linear approximations, measured as

$$d^{(j)} = \sqrt{\|\boldsymbol{\rho}_t^{(j)} - \boldsymbol{\rho}_t^{(j-1)}\|_2^2 + \|\boldsymbol{\kappa}_t^{(j)} - \boldsymbol{\kappa}_t^{(j-1)}\|_2^2}, \quad (45)$$

where the vectors $\boldsymbol{\rho} = [\rho_1, \rho_2, \dots, \rho_{n-1}, \rho_n]^T$ and $\boldsymbol{\kappa} = [\kappa_1, \kappa_2, \dots, \kappa_{n-1}, \kappa_n]^T$ are the nodal values of the dislocation densities in the finite element discretization. The sub-index t makes reference to the current time instance, and not to the nodal labels used for the individual components of the vectors. At each time increment the final approximation in the previous time step is used as the initial guess for the non-linear iteration, i.e. $\boldsymbol{\rho}_{t+\Delta t}^{(0)} = \boldsymbol{\rho}_t^{(j)}$ and $\boldsymbol{\kappa}_{t+\Delta t}^{(0)} = \boldsymbol{\kappa}_t^{(j)}$.

The unpreconditioned *BiCGStab* method has been used to solve the linear systems resulting at each non-linear iteration [47, 48]. The maximum number of allowed iterations is $2n$, but the iterative process is stopped as soon as $\|\mathbf{r}^{(k)}\|/\|\mathbf{b}\| < \epsilon_s = 10^{-6}$ is reached, with $\mathbf{r}^{(k)}$ the k -th residual vector and $\mathbf{b}$ the right hand side vector.

The physical parameters are identical to those used in [13] in which they were selected in an attempt to represent values most commonly used in previous studies [2, 49]. The length of the domain is $L = 1 \mu m$, with material properties as follows: $h = 0.1 \mu m$, $b = 0.3 nm$, $B = 10^{-4} Pa s$, $\nu = 1/3$, $G = 25 GPa$. The initial condition for all problems is given by $\rho_0 = 400 \mu m^{-2}$ and $\kappa_0 = 0 \mu m^{-2}$. All simulations were run with a time step $\Delta t = 10^{-1} \mu s$.

For all subsequent numerical examples, except those presented in Section 4.5, in which a comparison between models is carried out, the Dogge model is used with a constant length scale and considering interactions between dislocations of different sign, i.e. $\mathcal{L} = h$, $a = 1$ and $b_1 = b_2 = 1$.

The presented assessment will be conducted by methodologically modifying the applied stress τ and the mesh size ℓ , which directly affect the fulfilment of the discrete maximum principle and therefore the stability properties of the numerical approximation method. In all cases the diffusion coefficients will be kept unaltered and only the convection coefficients will be perturbed. It will be specified in each instance if either the direct or crossed convection coefficient is perturbed.

The precise definition of a mesh Péclet number in the most traditional way is, for the coupled equations at hand, an intricate matter. Indeed, it is only possible for the second equation to compute it according to Equation (25). After simplifying, it can be expressed as

$$Pe_\kappa = \frac{\ell}{2} \frac{b'_1}{b'_2} \left(\frac{1}{\rho} \frac{\partial \rho}{\partial x} \right). \quad (46)$$

Note that for the Groma model, this number vanishes, since $b'_1 = 0$. Moreover, due to the non-linear nature of the dislocation transport problem, this Péclet number depends on the total dislocation density and its gradient, that evolve over time. However, if a uniform distribution of the total dislocation density is reached, or if a uniform initial condition is used, the Péclet number vanishes here as well. The situation is even more complicated for the first equation, since in this case the direct convection coefficient $\beta_{\rho\rho}$ is always zero, and thus $Pe_\rho = 0$, irrespective of the model, irrespective of the length scale used and independently of the interactions considered between different types of dislocations.

Because of the aforementioned argument and the form of the convection matrix $\mathbf{B}$ in (43), the physical coefficients to be perturbed have been first chosen to be $\beta_{\rho\kappa}$, the crossed convection coefficient for the ρ Equation (41), and $\beta_{\kappa\kappa}$, the direct convection coefficient for the κ Equation (42). All other physical coefficients remain unperturbed, except in the last section of this assessment. This subsequent change of coefficient to be perturbed in Section 4.7 will allow evaluating the influence of this different choice.

As dislocation transport starts, this situation becomes yet more intricate because dislocations are expected to pile up at the impenetrable boundaries, forming *boundary layers*. Since the applied stress τ will be taken constant through the whole spatial domain, a *V*-shape profile for the total dislocation density is expected. As the transport continues, dislocations are expected to pile up in a smaller region, reducing the boundary layer width. At this moment three different regions can be roughly identified. The first one is close to the boundaries where the total dislocation density and its gradient attain their largest values. These two tendencies reduce and increase, respectively, the local Péclet number. The second region is the central one in which the total dislocation density and its gradient attain both their lowest values causing an increase and reduction, respectively, of the local Péclet number. The third and more critical region is the transitional region in which a low total dislocation density and a high value of its gradient both involve an increase of the Péclet number. Thus, as the simulations advance in time, and the uniform distribution of the total dislocations density changes to the mentioned *V*-shape profile, it is expected that the adaptive nature of the stabilization technique will play a more prominent role.

4.2 Influence of the applied stress

Illustrating the removal of spurious oscillations and negative values of the total dislocation density achieved by the presented stabilization technique, compared with the classical Bubnov-Galerkin scheme, is the main aim of the present example. Three different cases are presented, all using the same uniform coarse mesh of 16 linear elements. Only the applied stress is different in each of the cases, taking the values $\tau = 0.01, 0.1$, and 1.0 GPa. All the presented results are obtained at time $t = 10^6 \mu s$.

Figure 2 shows the results in terms of total dislocation and geometrically necessary dislocation densities in blue and red respectively. The results obtained with the classical (non-stabilized) Bubnov-Galerkin method are depicted in the left column, while the right column shows the results obtained with the stabilization technique. These numerical schemes are referred to as *classical* and *stabilized* respectively.

Note that in the first case depicted in the top row of Figure 2, for a small applied stress ($\tau = 0.01$ GPa), no noticeable difference can be observed between the classical and stabilized approximations for both dislocation densities. The applied stress is not large enough to generate sharp boundary layers and therefore the middle of the spatial domain remains sufficiently occupied by dislocations, avoiding a large reduction of the diffusion coefficients given by $\alpha_{\rho\rho} = C_4 \rho$ and $\alpha_{\kappa\kappa} = C_5 \rho$.

The results for the second case, with $\tau = 0.1$ GPa, are shown in the middle row of Figure 2. For the classical scheme, saw-tooth-like oscillations start appearing in the central region of the spatial domain where the total dislocation density is close to zero, which causes a decrease of the diffusion coefficients. This effect pollutes the numerical approximation, with the nodal values of the total dislocation density at some nodes being negative, which is physically meaningless. The numerical approximation obtained with the stabilization scheme, as shown on the right, is smooth, non-negative for the total dislocation density, and free of any oscillation. It is important to note that the maximum and minimum values attained by both total dislocation and geometrically necessary dislocations differ between the classical and stabilized approximations. Larger values are obtained by the classical scheme, but this classical numerical approximation is meaningless since it reveals spurious oscillations and negative values for a strictly non-negative quantity.

The results for the third case, with $\tau = 1.0$ GPa, are shown in the last row of Figure 2. Note that this stress level may well be attained in practical applications. On the left, corresponding to the classical scheme, the oscillations are much larger than in the previous case, making the numerical approximation completely useless for any application. This effect is partially due to the fact that the convective character of the problem has increased by one order of magnitude through the increase of the applied stress. The second important cause is the decrease of the effective local diffusion coefficients due to the starvation of dislocations in the central part of the spatial domain. The corresponding stabilized result is shown on the right in the last row. It does not exhibit any oscillations and the total dislocation density is non-negative

in the entire spatial domain. As expected, the width of the boundary layer is decreased and dislocation densities reach higher values compared to the cases with a lower applied stress.

These results confirm that the stabilization technique is effective when required. If spurious oscillations are not present in the classical formulation because the problem is not dominated by convection, the effect of the stabilization is negligible, as confirmed by the plots depicted in the first row of Figure 2. On the other hand, the beneficial effect of the stabilization technique becomes apparent as soon the convective character of the system of partial differential equations starts polluting the numerical approximation obtained by the classical scheme, distorting it with oscillations and non-physical negative density values.

4.3 Influence of the discretization

The aim of this example is to examine the performance of the stabilization technique when the mesh is refined and to assess the non-linearity influence as time advances. Thus, while the applied stress is kept constant and equal to $\tau = 10^{-0.5}$ GPa, the element size ℓ will be progressively and systematically reduced.

The diagrams in Figure 3 show the total dislocation density profiles obtained at equally spaced time instances between $t_o = 0 \mu s$ and $t_f = 10^6 \mu s$, the brightest one corresponding to the initial time and the darkest one to the last time instance. As in the previous example, classical approximations are depicted on the left and stabilized ones on the right. The results obtained using increasingly refined meshes of 16, 32, 64, and 128 elements with linear shape functions are depicted.

Note that for the coarsest mesh, depicted in the first row of Figure 3, the approximations obtained with the classical scheme start to show an oscillatory behaviour from early time instances onwards, precisely in the above mentioned transitional region. Such spurious oscillations start to scatter and become more pronounced as time advances due to the reduction of the diffusion coefficients as the total dislocation density ρ approaches zero. In contrast, the approximations obtained with the stabilized scheme are, for all time instances, strictly non-negative and free of spurious oscillations even in the central region, where the total dislocation density almost vanishes. This is also true for the transitional regions, where the high value reached by the geometrically necessary dislocation density gradient increases the crossed convection coefficient $\beta_{\rho\kappa}$, making the numerical approximation more prone to oscillatory behaviour. From the discrepancy of the vertical axis of the top two diagrams it can be noticed that the maximum values of the numerical approximations attained for the classical and stabilized schemes differ considerably. The surplus obtained by the classical scheme is presumably due to the lack of stability of that scheme, the solution of which is not reliable due to the presence of oscillations and negative values.

Moving to the second row of Figure 3, the number of elements is doubled while all other parameters remain identical. Again, from the left diagram corresponding to the classical scheme, it is noticeable that oscillations appear in the transitional region, and propagate to the central region due to the decrease of the total dislocation density in this region. For this case the oscillations do not grow as severely as in the previous case because the mesh has been refined. For the stabilized scheme, at all time instances, the approximations are strictly positive and free of spurious oscillations. Note that the maximum values attained are higher than in the stabilized results using a coarser mesh. This discrepancy will be further analysed in what follows.

By doubling again the number of elements used in the mesh, the numerical approximations shown on the third row of Figure 3 are obtained. The classical scheme approximation is now also free of oscillations at all time instances, except at the final time instance at which tiny but still noticeable oscillations can be observed in the transitional region. This is consistent with the explanation of the results obtained with the two previous meshes. Again, the stabilized scheme results are strictly non-negative and free of any oscillation throughout the spatial domain for all time instances. Furthermore, it is emphasized that the difference between the maximum values attained by the classical or stabilized schemes is now progressively reduced as time advances, to become insignificant at the last time instance.

Finally, the fourth and last row of Figure 3 shows the results obtained using the finest mesh for the present example, consisting of 128 elements. The first important feature to observe is that for this refinement level, the classical scheme now recovers a stable approximation, which does not exhibit spurious oscillations. For this level of refinement, the classical scheme approximation can be regarded as reliable

(a) Classical, $\tau = 10^{-2}$ GPa.

(b) Stabilized, $\tau = 10^{-2}$ GPa.

(c) Classical, $\tau = 10^{-1}$ GPa.

(d) Stabilized, $\tau = 10^{-1}$ GPa.

(e) Classical, $\tau = 10^0$ GPa.

(f) Stabilized, $\tau = 10^0$ GPa.

Figure 2: Comparison of the total dislocation density ρ in blue and the geometrically necessary dislocation density in red, both in μm^{-2} , obtained with the classical (left) and stabilized (right) scheme using a discretization with 16 elements, increasing the stress τ from top to bottom. The diffusion and convection matrices are given by Equations (43).

for comparative purposes with respect to the approximation obtained with the stabilized scheme. Both approximations are very similar for all time instances, not only in terms of the maximum values attained in the boundary layers, but also in the profile shape in the whole spatial domain.

To close this analysis, two important observations remain to be discussed, namely the maximum value discrepancies when using a series of refined meshes with stabilization, and the steady state solution delay observed when analysing the finest mesh results. Both effects can be associated with the artificial diffusion introduced by the stabilization scheme in order to render stable numerical approximations. When using the stabilization scheme, not the original problem is solved but rather another problem with slightly modified coefficients. This in turn is the conceptual basis of the stabilization technique since it is based on perturbing the original problem, and instead solving a problem with coefficients selected to resemble as close as possible the original one, but with which the approximation remains free of spurious oscillations when discretized using a given mesh. The classical and stabilized results obtained with an even more refined mesh containing 256 elements (not shown here) are almost identical at all time instances, a fact that confirms the artificial diffusion addition argument. This confirms the fact that the present stabilization technique intervenes only when it is strictly needed, whereas it is inactive if the mesh is fine enough to get numerically stable approximations.

4.4 Non-linear and time evolution adaptivity

In this section a detailed analysis of the stabilization technique behaviour is carried out in order to provide evidence of its flexibility and adaptive nature. This analysis is performed by modifying the applied stress and mesh refinement. Henceforth, only results obtained with the stabilization scheme will be considered.

4.4.1 Stress variation

In the first situation, the mesh is fixed and consists of 256 elements. The stress level is modified in order to observe its influence on the evolution of the direct diffusion and convection coefficients for the geometrically necessary dislocation densities κ given by Equation (42). These coefficients are in turn used by the stabilization technique to determine the direct convection perturbation $\beta_{\kappa\kappa}^*$. In order to simplify the analysis, the crossed convection perturbation is set to zero, i.e. $\beta_{\kappa\rho}^* = 0$, even though its corresponding coefficient does not vanish, being indeed a time invariant constant through the whole spatial domain, i.e. $\beta_{\kappa\rho} = C_0$. Thus the effects of both direct and crossed convection coefficients will be active on the direct convection perturbation only.

Figure 4 shows on the first row the direct diffusion coefficient $\alpha_{\kappa\kappa} = \rho C_5$, while on the second row the direct convection coefficient $\beta_{\kappa\kappa} = -C_4 \partial\rho/\partial x$ is depicted. Similar diagrams for the crossed convection coefficient are not shown since, even if it influences the perturbation evolution to analyse, it remains constant throughout the computation. The third row of Figure 4 shows the direct convection perturbation $\beta_{\kappa\kappa}^*$, which is the main quantity of interest in the present analysis. The stress level is increased from one column to the next by one order of magnitude. It is unnecessary to show similar plots for the crossed advection coefficient since, even if it influences the perturbation evolution to analyse, it remains constant.

The first important observation is that the direct diffusion coefficient decreases in the central region and increases close to the impenetrable boundaries, exhibiting a boundary layer behaviour. This is of course due to the fact that the direct diffusion coefficient is simply a constant multiplied by the total dislocation density. As expected, the boundary layer width decreases and the maximum values attained are larger as the stress is increased, see first row of Figure 4. An almost perfect linear relationship exists between the magnitude of the maximum values attained by $\alpha_{\kappa\kappa}$ and the applied stress.

A second important observation can be made in the second row of Figure 4, where the time evolution of the direct convection coefficient is shown for three different stress levels. Since the plotted quantity is a constant times the total dislocation density gradient, these diagrams keep a close relationship with those presented in the first row. The boundary layer pattern is not as apparent as in the previous row but, mainly from the third column, it is clear that the same behaviour is also exhibited by the direct convection coefficient $\beta_{\kappa\kappa}$. Note again that the order of magnitude of the maximum values attained for $\beta_{\kappa\kappa}$ is approximately linearly related to the order of magnitude of the applied stress as observed in the vertical axis scale.

Figure 3: Comparison of the time evolution of the total dislocation density ρ in μm^{-2} , obtained with the classical (left) and stabilized (right) scheme for an applied stress $\tau = 10^{-0.5}$ GPa, successively doubling the number of elements from top to bottom. The cyan line corresponds to the initial condition and the blue one to the last computed time instance ($t = 10^6 \mu\text{s}$); intermediate approximations are at equidistant time intervals. The diffusion and convection matrices are given by Equations (43).

Figure 4: Comparison of the time evolution of the direct diffusion coefficient $\alpha_{\kappa\kappa}$, in $\mu\text{m}^2/\text{s}$, and the direct convection coefficient $\beta_{\kappa\kappa}$ and its perturbation $\beta_{\kappa\kappa}^*$, both in $\mu\text{m}/\text{s}$, obtained using a discretization consisting of $n_e = 2^8$ elements, increasing the stress from left to right. The yellow line corresponds to the initial condition and the red one to the last time instance computed ($t = 10^6 \mu\text{s}$); intermediate approximations are at equidistant time intervals. The diffusion and convection matrices are given by Equations (43).

Once the behaviour of $\alpha_{\kappa\kappa}$ and $\beta_{\kappa\kappa}$ have been analysed, the perturbation $\beta_{\kappa\kappa}^*$ can be scrutinized based on the third row of Figure 4. As expected, a localized behaviour can also be recognized, but in this case not in the form of boundary layers, but *internal layers*. These internal layers in which $\beta_{\kappa\kappa}^*$ strongly evolves appear precisely in the transitional region where a low total dislocation density is combined with a large value of its spatial gradient. The development of such regions for $\beta_{\kappa\kappa}^*$ starts to be evident even in the left-most diagram corresponding to the lowest applied stress, where one would expect high values in the central region based on the direct diffusion decrease there. For the central diagram, with an increased applied stress, the width of the internal layer reduces from outside the spatial domain towards its centre, since the total dislocation density gradient becomes, though high in magnitude, constant close the boundaries where the total dislocation density itself attains its maximum values. This combined effect becomes more prominent by increasing the applied stress: the right-most column reveals an internal layer of $\beta_{\kappa\kappa}^*$ that is much thinner than the previous ones.

4.4.2 Mesh variation

The manner in which the stabilization technique affects the stability issues when the mesh is refined for a fixed applied stress is investigated next. This is carried out by scrutinizing the crossed convection perturbation for the total dislocation density equation $\beta_{\rho\kappa}^*$, in relation with the two physical coefficients controlling it, i.e. the direct diffusion coefficient $\alpha_{\rho\rho} = \rho C_4$ and the crossed convection coefficient $\beta_{\rho\kappa} = C_0 - C_5 \partial\kappa/\partial x$. The direct convection perturbation will be set to zero, i.e. $\beta_{\rho\rho}^* = 0$, and therefore the effect of the direct diffusion and crossed convection coefficients will be active only on the crossed convection perturbation, in a similar way as done in the previous example.

Figure 5 shows on the first row the direct diffusion coefficient throughout the spatial domain for equally spaced time instances and three different meshes with 16, 64, and 256 elements. The second row shows the crossed convection coefficient. These two physical coefficients are the ones affecting the computation of the crossed convection perturbation, which is the main quantity of interest in this analysis. This perturbation is shown in the third row of Figure 5.

The analysis is much simpler than in the previous example since now both the direct diffusion and crossed convection coefficient show exactly the same boundary layer pattern. Here, their effects are mutually reinforced, and not counteracting as in the previous example. For instance, the central region where the direct diffusion coefficient tends to vanish is the same region where the crossed convection remains high as the simulation evolves in time. On the other hand, the pile up of dislocations close to the boundaries increases the direct diffusion coefficient, an effect reinforced by the local reduction of the crossed convection coefficient due to the positive geometrically necessary dislocation gradient $\partial\kappa/\partial x$ caused by the pile up of dislocations.

A final observation relates to the magnitude of the maximum values of the required crossed convection perturbation given in the third row of Figure 5. The maximum values of this perturbation decrease as the mesh is refined. Its convergence towards zero can be shown to be super-linear using more refined meshes for a fixed stress, and considering the same mesh refinement procedure for different applied stresses.

The presented examples demonstrate that the stabilization technique successfully renders stable numerical approximations irrespective of the local values of the diffusion and convection coefficients being direct or crossed. This proves its flexibility and adaptivity. More specifically, the second example reveals that the stabilization technique is consistent, i.e. the perturbations' magnitudes vanish as the mesh is refined.

4.5 Models and length scale comparison

This section has the aim to show that the presented stabilization technique renders numerical approximations free of spurious oscillations irrespective of the model used: (i) Dogge or Groma, (ii) with either a constant or variable length scale. As in the previous section, only stabilized results are shown here.

Figure 6 depicts the numerical approximation of the geometrically necessary dislocation density obtained using a mesh with 256 elements with a moderate applied stress $\tau = 10^{-0.5}$ GPa for the four possible combinations obtained by changing the model type (Dogge or Groma) and the length scale (constant or variable). In all four results shown, interactions between dislocations of different signs have been taken into account.

The first row of Figure 6 shows the results obtained when using the Dogge model while the second row corresponds to the Groma model. The left column depicts the results obtained using a constant length scale while the right column contains the results obtained with a variable length scale.

Although all the profiles are qualitatively similar, some differences provide valuable information for a comparative analysis. An important observation is the fact that individual numerical approximations for the Groma model at different time instances can be well distinguished. This is not the case for the results obtained with the Dogge model. Only a few individual numerical approximations at different time instances can be recognized with a constant length scale, while such a distinction is even more difficult when using a variable length scale. This suggests that the Dogge model tends to *accelerate* the dislocation transport process with respect to the Groma model, i.e. both models have different kinetics. At first glance it could be argued that the slower kinetics in the Groma model may be caused by the adopted diffusion threshold for the total dislocation density equation. However, this difference in dislocation transport velocities was also observed when using positive and negative dislocation densities as the primary unknowns.

4.6 Rearrangement of convection and diffusion matrices

The purpose of this section is to assess the performance of the presented stabilization technique when the diffusion and convection matrices are defined in a different way from the one used in Sections 4.2-4.5. In order to carry out this assessment it should be noted that, due to the non-linearity of Equations

Figure 5: Comparison of the time evolution of the direct diffusion coefficient $\alpha_{\rho\rho}$, in $\mu\text{m}^2/\text{s}$, the crossed convection coefficient $\beta_{\rho\kappa}$ and its perturbation $\beta_{\rho\kappa}^*$, both in $\mu\text{m}/\text{s}$, obtained when applying a stress of $\tau = 10^{-0.5}$ GPa quadrupling the number of elements composing the finite element mesh from left to right (16, 64 and 256 elements). The cyan line corresponds to the initial condition and the blue one to the last time instance computed ($t = 10^6 \mu\text{s}$); intermediate approximations are at equidistant time intervals. The diffusion and convection matrices are given by Equations (43).

(41-42), the definition of the diffusion and convection matrices is not unique. It is also possible to define these matrices differently from the choice made in (43) as follows

$$\mathbf{A} = \begin{bmatrix} \rho C_4 & \kappa C_5 \\ \kappa C_4 & \rho C_5 \end{bmatrix}, \quad \text{and} \quad \mathbf{B} = \begin{bmatrix} 0 & C_0 \\ C_0 & 0 \end{bmatrix}. \quad (47)$$

A summary of the numerical assessment is now presented for this alternative definition.

Figure 7 should be compared with the bottom row of Figure 2. The classical scheme results have been re-computed as well in order to assess the effect of the rearrangement of the transport coefficients even when no stabilization technique is used. As expected, such an effect is negligible. The classical scheme results are shown in the left column and the stabilized scheme results in the right column. For the results shown, corresponding to $\tau = 1.0$ GPa, the classical scheme results show the same oscillatory behaviour as their counterparts depicted in Figure 2. The stabilized scheme results presented in Figure 7, like those depicted in Figure 2, are numerically well-behaved and free of any spurious oscillation. However, it is possible to recognize that the current definition of the diffusion and convection matrices leads to slightly smoother solutions. It is suspected that this effect is caused by the fact that formerly convective terms are now taken as diffusive terms.

Figure 8 corresponds to the right column of Figure 3. The classical results are here omitted since they are practically identical to those presented in the left column of Figure 3. It is confirmed that irrespective of the two tested arrangements of the convection and diffusion matrices, the results obtained

Figure 6: Dogge (top) and Groma (bottom) models with constant (left) and variable (right) length scales: time evolution of the geometrically necessary dislocation density κ in μm^{-2} for an applied stress $\tau = 10^{-0.5}$ GPa on a mesh composed of $n_e = 2^8$ elements. The yellow line corresponds to the initial condition while the red one to the last time instance computed ($t = 10^6 \mu\text{s}$), intermediate approximations are at equidistant time intervals.

with the classical (plots not shown) and stabilized schemes are qualitatively the same. It also confirms that stabilization is necessary to obtain numerically well-behaved approximations and, more importantly, that the proposed stabilization technique is able to render strictly positive numerical approximations free of spurious oscillations. The stabilized scheme results also confirm that the alternative arrangement of the convection and diffusion matrices slightly increases the smoothness of the numerical approximations obtained.

The results presented in this section allow one to conclude that irrespective of the two tested arrangements of the convection and diffusion matrices, the numerical approximation of the problem at hand requires the use of a stabilization technique able to deal with its convection dominated character. Furthermore, the ability of the presented stabilization technique to render numerical approximations free of spurious oscillations is not affected by this rearrangement of the convection and diffusion matrices.

4.7 Influence of the choice of the perturbation

In this section, another selection of the physical coefficients to be perturbed is made in order to evaluate the influence of this choice. To this end the simulations presented in Section 4.6 are reconsidered perturbing the diffusion coefficients, instead of the convection coefficients as previously done. For the sake of brevity in the exposition, only the most illustrative results are shown and discussed.

Figure 9 depicts the total dislocation density profiles obtained at equally spaced time instances but perturbing the diffusion coefficients rather than the convection coefficients as done in Section 4.6. Thus, these plots can be compared to those presented in Figure 8.

Figure 7: Comparison of the total dislocation density ρ in blue and the geometrically necessary dislocation density in red, both in μm^{-2} , obtained with the classical (left) and stabilized (right) scheme using a discretization with 16 elements. The diffusion and convection matrices are given by Equations (47).

As expected, these results are free of spurious oscillations and render strictly positive numerical approximations. Thus, the presented stabilization technique fulfills its main goal irrespective of the coefficients, in this case, either convection or diffusion, that one chooses to perturb.

However, as can be observed in Figure 9, the individual profiles at each time instance differ from each other, especially for early time instances (in cyan) and for the coarsest meshes (top). Two main discrepancies can be observed. First, it is easier to separately recognize the profiles at different time instances in the results depicted in Figure 9 than in those depicted in Figure 8, i.e. perturbing diffusion seems to slow down the pile-up process. Second, the values attained on the boundaries for the last time instance (in blue) are higher when perturbing the diffusion coefficients than the corresponding values obtained when perturbing the convection coefficients for the two coarsest meshes. The latter discrepancy becomes less marked as the mesh is refined.

In order to further investigate this matter, the ratios $\beta_{\rho\kappa}^*/\beta_{\rho\kappa}$ and $\alpha_{\rho\rho}^*/\alpha_{\rho\rho}$, respectively obtained when perturbing the convection and diffusion coefficients, have been computed and their maximum values on the whole spatial domain and through the entire time marching computation are depicted as functions of the number of nodes n for increasingly refined meshes in Figure 10. This allows assessing the local behavior of the stabilization technique under mesh refinement. These plots allow confirming that, independently of the coefficient chosen to be perturbed, the relative influence of the stabilization technique decreases as the mesh is refined. Moreover, once a certain mesh refinement level is reached, from approximately $n = 10^2$ nodes onwards, this influence decreases quadratically.

5 Conclusions and outlook

This paper first presented a summary of the different physical assumptions found in the literature modelling dislocation transport in crystalline materials at the meso-scale. In order to easily deal with these different models, a generic formulation has been proposed and used in this work. Subsequently, the development of a stabilization technique for general systems of coupled convection-diffusion-reaction equations has been reviewed. This has been done explaining first the single equation case and henceforth extending the stabilization technique to the multiple equations case.

The ability of the stabilization technique to deal with the different models presented in the literature, rendering smooth and well-behaved numerical approximations free of spurious oscillations, has been demonstrated through a thorough numerical assessment. It has been demonstrated as well that the effectiveness of the stabilization technique is unaffected when using a different arrangement of the transport coefficients, supporting its generality and versatility.

As future work, it is planned to extend this stabilization technique to multidimensional configurations and to apply it to more general and complex dislocation transport problems modelling screw and mixed

Figure 8: Time evolution of the total dislocation density ρ in μm^{-2} , obtained by the stabilized scheme perturbing the convection coefficients successively doubling the number of elements. The cyan line corresponds to the initial condition and the blue one to the last computed time instance ($t = 10^6 \mu s$); intermediate approximations are at equidistant time intervals. The diffusion and convection matrices are given by Equations (43). These plots are equivalent to those presented in the right column of Figure 3.

dislocations, as well as other phenomena such as annihilation and dislocations production. From a numerical perspective, an in depth mathematical analysis of this stabilization technique may be valuable to provide additional insights and routes for further improvements. The detailed study of the effect of the choice of the physical coefficient to be perturbed could provide valuable insights into the feasibility of determining the perturbations in a more rational manner through an optimization strategy. Whether or not this could improve the solution thus remains to be investigated. Of special value could be the investigation of the effect the stabilization technique has on the spectral properties of the linear systems resulting from the discretization. This would provide valuable information for the acceleration of the iterative method used to solve such large and sparse linear systems.

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Figure 9: Time evolution of the total dislocation density ρ in μm^{-2} , obtained by the stabilized scheme perturbing the diffusion coefficients successively doubling the number of elements. The cyan line corresponds to the initial condition and the blue one to the last computed time instance ($t = 10^6 \mu s$); intermediate approximations are at equidistant time intervals. The diffusion and convection matrices are given by Equations (43). These plots are equivalent to those presented in the right column of Figure 3 and to those presented in Figure 8.

Figure 10: Effect of mesh refinement on the maximum values on the whole spatial domain and through the entire time marching computation of the ratio $\beta_{\rho\kappa}^*/\beta_{\rho\kappa}$ obtained when perturbing convection (left), and the ratio $\alpha_{\rho\rho}^*/\alpha_{\rho\rho}$ obtained when perturbing diffusion (right). The diffusion and convection matrices are given by Equations (43).

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