A Finite Element Method for computing Shear Band formation

Th. Baxevanis, Th. Katsaounis, and A. Tzavaras

Abstract. The objective of this work is to provide an in depth numerical study of the interplay between thermal softening and strain-hardening in shearing deformations of strain-rate dependent materials. We consider the unidirectional simple shearing of an infinite slab. This model, despite its simplicity, incorporates the essential features of shear band modeling. We employ an adaptive finite element method of any order for the spatial discretization. Adaptivity in the spatial variable, is a necessity to correctly capture these singular phenomena. Further the implicit Euler method with variable time-step is used for the time discretization. The resulting numerical scheme is of implicit-explicit type, of any order in space and simple to implement.

1. Introduction

Dissipative mechanisms, such as viscosity or thermal diffusion, tend to stabilize the thermomechanical processes opposing the destabilizing influence of the nonlinearity of the material response. The competition is especially delicate when the strength of the dissipative mechanisms weakens in the course of the motion. At high strain rates, thermal softening can eventually outweigh the tendency of the material to harden, thus creating a destabilizing mechanism which competes with internal dissipation. Experimental and numerical investigations indicate that when the degree of thermal softening is large this competition results to instability and formation of shear bands. Shear bands are narrow regions of concentrated shearing deformation. Once the band is fully formed, the two sides of the region are displaced relatively to each other, however the material still retains full physical continuity from one side to the other. We refer to [19] for an excellent survey of the mechanical issues.

The intent of this work is to provide an in-depth numerical study of the interplay of thermal softening and strain-hardening in shearing deformations of strain-rate dependent materials, using modern ideas of adaptive finite element methods so as to fully resolve the bands. We consider a simple model, the unidirectional simple shear of an infinite slab, which, despite its simplicity, incorporates the essential material behavior necessary for shear band modeling. The model simulates the main significant aspects of experiments in shear band formation, like the pressure-shear test, [8], or the thin-walled tube torsion test [13]. It ignores, however, certain potentially important factors that may play a role in the subsequent development of shear bands, [18]. The model is then solved numerically using a finite element method, appropriate for the multiscale nature of the problem.

The width of the shearing band may be of the order of only a few micrometers or even less. A resolution of the order of $10\mu m$ or less would be required for many materials in order to follow the deformation across the band in detail. When a fixed mesh is used and the tip of a peak of a state variable becomes narrower than the mesh spacing then it will be the length scale of the grid that regularizes the calculation rather than the physical and constitutive features of the material. Thus, an adaptive refinement strategy for the spatial as well as for the temporal discretization parameters is necessary to capture correctly the shear band formation. Wright and Walter, [20], were perhaps the first to follow, with numerical simulations the evolution of an adiabatic shear band from the initial, nearly homogeneous stage to the final, fully localized stage. For numerical computations in various one-dimensional models we also refer to [3],[10], [12], [11] and the two- and three-dimensional computational studies in [1], [2].

It is our objective to introduce various developments from adaptive finite elements into the study of formation and evolution of shear bands, and use this model problem as a paradigm to further develop and extend the related theory of adaptive finite element method to quasilinear convection diffusion systems. The proposed finite element schemes show excellent numerical resolution of the shear band and provide a numerical justification that shear band formation is occurring concurrently with the collapse of momentum diffusion mechanism. This is in accordance with the preliminary analysis in [17] and justifies the role of diffusion collapse in shear band formation. Further the numerical schemes provide a justification that growing amplitude oscillations predicted by linearized instability analysis are concentrated and consumed, through a nonlinear mechanism, into one fully developed shear band.

The paper is organized as follows: in Section 2 we introduce the mathematical model. The finite element approximations are described in Section 3 while in Section 4 some numerical results are presented.

2. The mathematical model

We consider the adiabatic plastic shearing of an infinite plate of thickness d. In a Cartesian coordinate system the plate occupies the region $\Omega = [0, d]$ between the planes $x = 0$ and $x = d$. Let $v(x, t)$ be the velocity field in the shearing direction, $\gamma(x, t)$ be the shear strain, $\theta(x, t)$ be the temperature and $\sigma(x, t)$ be the shear stress. Under the assumption that elastic effects are negligible the Lagrangian description of the balance laws of momentum, energy and the kinematic compatibility condition yield:

$$\rho\, v_t = \sigma_x, \qquad x \in \Omega,\ t > 0, \tag{1}$$

$$c\,\rho\,\theta_t = \beta\,\sigma\,\gamma_t + k\,\theta_{xx}, \qquad x \in \Omega,\ t > 0, \tag{2}$$

$$\gamma_t = v_x, \qquad x \in \Omega,\ t > 0, \tag{3}$$

where ρ, c, β, k are constants denoting the referential density, the specific heat, the portion of plastic work converted into heat ("cold work") and thermal diffusivity, respectively. In the case where $k = 0$ the process is adiabatic. A simpler model consisting of two equations can also be considered

$$\rho\, v_t = \sigma_x, \qquad x \in \Omega,\ t > 0, \tag{4}$$

$$c\,\rho\,\theta_t = \beta\,\sigma\, v_x + k\,\theta_{xx}, \qquad x \in \Omega,\ t > 0. \tag{5}$$

The above systems of equations are supplemented with the constitutive law

$$\sigma = G\ \theta^{-\alpha}\ \gamma^m\ \gamma_t^\ell = G\ \theta^{-\alpha}\ \gamma^m\ v_x^\ell, \quad \text{or} \quad \sigma = G\ \theta^{-\alpha}\ v_x^\ell \tag{6}$$

where α, m, ℓ denote the thermal softening, strain hardening and strain rate sensitivity parameters respectively and G is a material constant. This power law model has been used extensively to model steels that exhibit shear bands. Equation (6) is entirely empirical, but it allows considerable flexibility in fitting experimental data over an extended range. According to experimental data for most steels we have $\alpha = O(10^{-1}),\ m = O(10^{-2})$ and $\ell = O(10^{-2})$. Further, the plate is subjected to a prescribed constant velocity V at the one boundary while the other boundary is at rest, so the boundary conditions are

$$v(0, t) = 0, \quad v(d, t) = V, \quad t \geq 0. \tag{7}$$

We also impose initial conditions

$$v(x, 0) = v_0(x) > 0,\ \theta(x, 0) = \theta_0(x) > 0,\ \gamma(x, 0) = \gamma_0(x) > 0, \quad x \in \Omega, \tag{8}$$

which are to be compatible with the boundary data so that $v_x(x, 0) > 0$.

For these initial data it can be proved, by maximum principle, that $\theta_t > 0$ and $\gamma_t > 0$ hence $\theta(x, t) > 0$ and $\gamma(x, t) > 0$ so (2) is well defined and (1) is parabolic in v. The problem of adiabatic shearing ($k = 0$) has been extensively studied analytically for a variety of constitutive assumptions by a great number of authors [9], [15, 16, 17], [14]. In [7] the authors use the finite element method to prove existence and uniqueness for a system similar to (4),(5). Tzavaras, [17], introduced a mathematical characterization of shear banding based on the existence theory and large time behavior of solutions of the system of nonlinear partial differential equations describing the shearing. For the constitutive model at hand it has been proved using linearized analysis, that the homogeneous solution is stable under the quasistatic assumption, provided that $q = m + \ell - \alpha > 0$. This stability criterion was first published in [14] (see [5] for the more general case of nonhomogeneous materials). On the other hand, according to the aforementioned mathematical characterization introduced by Tzavaras, the only result for the dynamical problem known so far is that a classical solution exists over all times when $q = m+\ell-\alpha > 0$ if the initial conditions are smooth enough but otherwise arbitrary, [17]. Thus it is an open question whether the solution blows up in finite time or even at infinity.

A simple solution to (1)-(3) is given by choosing $k = 0,\ v(0,t) = 0,\ v(1,t) = 1,\ \forall t$ then

$$v(x,t) = x, \qquad \gamma(x,t) = \gamma_0(x) + t, \tag{9}$$

$$\theta(x,t) = \left\{ \theta_0(x)^{\alpha+1} + \frac{\alpha+1}{m+1}\left[(\gamma_0(x)+t)^{m+1} - \gamma_0(x)^{m+1}\right] \right\}^{\frac{1}{\alpha+1}}. \tag{10}$$

3. Finite element approximation

We consider the finite element discretization of (1)-(3). Let $\mathcal{T}_h$ be a partition of Ω consisting of intervals $I = [x_{i-1}, x_i]$ of length $h_i = x_i - x_{i-1}$, $i = 1, \dots, M_h$ where $M_h = card(\mathcal{T}_h)$ with $h = \sup_i h_i$. Further let $0 = t_0 < t_1 < \cdots < t_n < \dots$ be a partition of $[0, \infty)$ with $\delta_n = t_n - t_{n-1},\ n = 1, 2, \dots$. We consider the classical one dimensional C^0 finite element space $\mathcal{S}_{h,p} \subset H^1(\Omega)$, defined on partitions $\mathcal{T}_h$ of Ω

$$\mathcal{S}_h = \mathcal{S}_{h,p} = \left\{ \phi \in C^0(\Omega) : \phi|_I \in \mathbb{P}_p(I), I \in \mathcal{T}_h \right\}, \quad \dim\mathcal{S}_h = p\, M_h + 1, \tag{11}$$

where $\mathbb{P}_p(I)$ denotes the space of polynomials on I of degree at most p.

For simplicity we consider the finite element discretization of (4)-(5): we seek functions $v_h, \theta_h \in \mathcal{S}_h$ such that

$$(v_{h,t}, \phi) = \frac{G}{\rho}\,\theta_h^{-a} v_h^{\ell} \phi(x)\big|_{x=0}^{x=d} - (\frac{G}{\rho}\,\theta_h^{-a} v_{h,x}^{\ell}, \phi'), \quad \forall \phi \in \mathcal{S}_h, \tag{12a}$$

$$(\theta_{h,t}, \psi) = (\frac{\beta G}{c\rho}\, v_{h,x}^{\ell+1}\theta_h^{-a}, \psi) + k\theta_{h,x}\psi\big|_{x=0}^{x=d} - k(\theta_{h,x}, \psi'), \quad \forall \psi \in \mathcal{S}_h, \tag{12b}$$

The (12a)-(12b) is a coupled fully nonlinear system of ordinary differential equations which we discretize by an Implicit-Explicit Euler (IEE) scheme. Indeed in the nonlinear equations of the system the unknown variable is treated implicitly while the other variables are treated explicitly. The proposed scheme decouples completely the system and each equation is solved separately, possibly in parallel. Let $J = \dim\mathcal{S}_h$, $\mathcal{V} = (V_1, \dots, V_J)$, $\mathcal{U} = (\theta_1, \dots, \theta_J)$, we write

$$v_h(x,t) = \sum_{i=1}^{J} V_i(t)\phi_i(x), \quad \theta_h(x,t) = \sum_{i=1}^{J} \theta_i(t)\psi_i(x),$$

Then the IEE scheme applied to (12a)-(12b) is : Given the solution $\mathcal{V}^n$, $\mathcal{U}^n$ at time level t^n the solution $\mathcal{V}^{n+1}$, $\mathcal{U}^{n+1}$ is given by

$$\mathcal{M}\mathcal{V}^{n+1} = \mathcal{M}\mathcal{V}^n + \delta_{n+1}\mathcal{F}(\mathcal{V}^{n+1}, \mathcal{U}^n), \qquad \mathcal{V}^0 = \mathcal{V}(t=0) = \mathcal{P}v_0(x), \tag{13a}$$

$$\mathcal{M}\mathcal{U}^{n+1} = \mathcal{M}\mathcal{U}^n + \delta_{n+1}\mathcal{H}(\mathcal{V}^n, \mathcal{U}^{n+1}), \qquad \mathcal{U}^0 = \mathcal{U}(t=0) = \mathcal{P}\theta_0(x), \tag{13b}$$

where $\mathcal{F}(\mathcal{V},\mathcal{U}) = \frac{G}{\rho}\,\theta_h^{-a} v_{h,x}^{\ell}\phi_j\big|_{x=0}^{x=d} - (\frac{G}{\rho}\,\theta_h^{-a} v_{h,x}^{\ell}, \phi_j')$, $\mathcal{H}(\mathcal{V},\mathcal{U}) = (\frac{\beta G}{c\rho}\, v_{h,x}^{\ell+1}\theta_h^{-a}, \psi_j) + k\theta_{h,x}\psi_j\big|_{x=0}^{x=d} - k(\theta_{h,x}, \psi_j')$, $\quad j = 1, \dots, J$, $\mathcal{M} = (\phi_i, \phi_j)$, $i, j = 1, \dots, J$ is the mass matrix and $\mathcal{P}$ is either the interpolation or the L^2 projection operator : $\mathcal{P} : C^0([0,d]) \to \mathcal{S}_h$. The nonlinear equations (13a), (13b) are solved using Newton's method.

We describe briefly the adaptive mechanisms, spatial and temporal, used to follow the development of the singularity of v_x and consequently for γ and θ. The adaptive mesh refinement strategy presented here is motivated by the work in [6]. The location of the singularity point $x^\star \in [0,d]$ is completely determined by non-uniformities in the initial conditions $v_0,\ \theta_0$. As time increases v_x grows near $x^\star$ and the adaptive mechanism refines the spatial mesh in a neighborhood of $x^\star$ and cuts the time step according to a certain criterion.

We assume that the partition $\mathcal{T}_h$ satisfies: $\exists c_0 \in \mathbb{R},\ h \le c_0 h_I,\ \forall I \in \mathcal{T}_h$. At time level n an interval I of the partition $\mathcal{T}_h$ is refined, the spatial size h_I is halved, if the following criterion is satisfied

$$h_I \|v^n_{h,x}\|_{L^\infty(I)} > \epsilon_h \|v^n_{h,x}\|_{L^1(I)}, \tag{14}$$

where ϵ_h is a constant that is determined empirically, [4]. The criterion (14) is motivated by a local $L^\infty - L^1$ inverse inequality that elements of $\mathcal{S}_h$ satisfy on I. On the other hand, the time step control is motivated by preserving the energy $E(t)$:

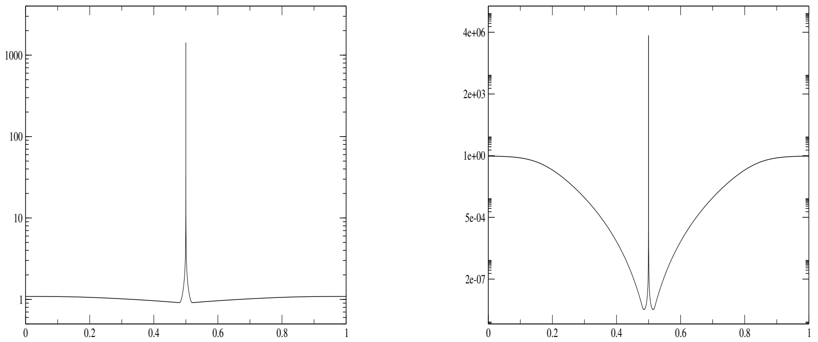
$$E(t) := \int_0^d \left[\frac{\beta\rho}{2} v^2(x,t) + c\rho\theta(x,t)\right] dx. \tag{15}$$

Using (1), (2) and the boundary conditions we get $\frac{\partial E}{\partial t} = \beta V \sigma|_{x=d}$. Thus to preserve the energy in time up to first order we define the time step size δ_{n+1} as

$$\delta_{n+1} = \epsilon_\delta \frac{|E_h^{n+1} - E_h^n|}{\beta V \sigma_h^{n+1}|_{x=d}}, \qquad \epsilon_\delta \sim 1. \tag{16}$$

4. Numerical Experiments

We present numerical results in the case of the formation of a shear band without thermal diffusion : $k = 0,\ -\alpha + \ell < 0$. For simplicity we consider the system of two equations (4)- (5) and we take $\alpha = 0.5$ and $\ell = 0.1$. The initial conditions $v_0,\ \theta_0$, are small perturbations of the uniform shearing solutions, (9), (10) around the point $x = \frac{1}{2}$. We compute the solution of (4), (5) at time $t = 0.32$, which are shown in Figures 1(b) and 1(a). The singular behavior of the solution is correctly captured using the adaptive techniques (14) and (16) with $\epsilon_h = 1.0025$. The temperature at the shear band point $x = \frac{1}{2}$ has risen about 1100 times the initial temperature, while v_x has reached a value of $\sim 2.7 \times 10^6$. In Figure 2(a) the resulting stress is shown, while Figure 2(b) shows the stress at the shear band point $x = \frac{1}{2}$. The oscillations in Figure 2(b) are believed to be the high frequency modes the solution which due to the local behavior of the instability are concentrated at the shear band point, [4]. We notice that the stress exhibits a large dip at the point where the shear band is forming. With progression of time the two parts of the material



(a) θ (b) v_x

FIGURE 1. Solution at $t = 0.32$

deform increasingly independent, and unloading occurs at the regions outside the band (see Fig. 4(b)). In other words, we have *collapse of momentum diffusion across the shear band*. In Figure 3(a) we show the evolution in time of the v_x at the shear band point $x = \frac{1}{2}$. We notice the exponential shape of the curve in a logarithmic scale which might be an indication that v_x blows up at the shear band. Further in Figure 3(b) the solution v at time $t = 0$ and $t = 0.32$ are shown. We notice that v_x is developing a δ-function type behavior. The case $k \neq 0$ is under consideration, [4].

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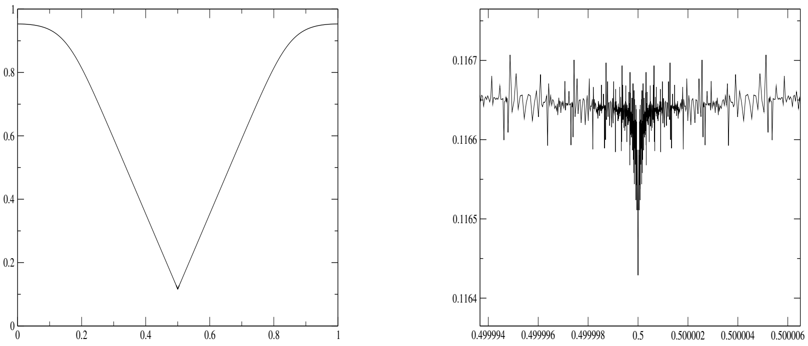
References

[1] Batra R.C. and Gummalla R.R., *Effect of material and geometric parameters on deformations near the notch-tip of a dynamically loaded prenotched plate*, International Journal of Fracture, 101, pp. 99-140, 2000.

[2] Batra R.C. and Ravinsankar M.V.S.,*Three-dimensional simulation of the Kalthoff experiment*, International Journal of Fracture, 105, pp. 161-186, 2000

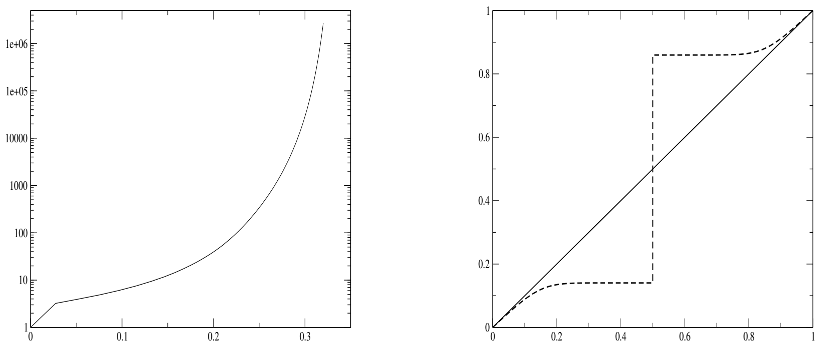
[3] Batra, R.C. and Ko, K.I., *An adaptive refinement technique for the analysis of shear bands in plain strain compression of a thermoplastic solid*, Appl. Mech. Rev. 45, 123, 1992.

[4] Baxevanis Th., Katsaounis Th., Tzavaras A., *An adaptive FEM for computing Shear Bands*, Preprint.



(a) Stress (b) Stress(zoom)

FIGURE 2. Stress at $t = 0.32$



(a) v_x at $x = \frac{1}{2}$ (b) v at $t = 0$(solid), $t = 0.32$(dotted)

FIGURE 3. Evolution of $v_x,\ v$

[5] Baxevanis,Th. and Charalambakis, N., *The role of material non-homogeneities on the formation and evolution of strain non-uniformities in thermoviscoplastic shearing*, To appear in Quart. Appl. Math.
[6] Bona J.L, Dougalis V.A, Karakashian O.A, McKinney W.R, *Conservative high order numerical schemes, for the generalized Korteweg-de-Vries equation*, Philos. Trans. Roy. Soc. London, Ser. A, 351, pp. 107-164, 1994.
[7] Charalambakis, N., Murat, F, *Approximation by finite elements, existence and uniqueness for a model of stratified thermoviscoplastic materials* , To appear in Ricerche di Matematica.
[8] Clifton R.J., *High strain rate behavior of metals*, Appl. Mech. Revs. 43(5), S9,1990
[9] Dafermos, C.M. and Hsiao,L., *Adiabatic shearing of incompressible fluids with temperature dependent viscosity*, Quart. Appl. Math 41, 45-58, 1983.
[10] Drew, D.A. and Flaherty, J.E., *Adaptive finite element methods and the numerical solution of shear band problems*, in Phase Transformations and Material Instabilities in Solids (Madison, WI.1983), Publ. Math. Res. Center Univ.-Wisconsin (Academic Press, Orlando, FL, 1984), Vol. 52, p.37,1984.
[11] Estep, D.J., Lunel, S.M.V. and Williams, R.D., *Analysis of shear layers in a fluid with temperature-dependent Viscosity*, Comp. Phys. 173, 17-60, 2001.
[12] French, D.A., *Computation of large shear deformations of a thermoplastic material*, Numer. Meth. Part. Differential Equatios 12, 393, 1996
[13] Hartley K.A., Duffy J., Hawley R.J., *Measurement of the temperature profile during shear band formation in steels deforming at high strain-rates*, J. Mech. Phys. Solids 35, 283-301, 1987.
[14] Molinari A. and Clifton R.J., *Localisation de la deformation viscoplastique en cisaillement simple, Resultats exacts en theorie non-lineaire*, Comptes Rendus Academie des Sciences, II, 296, 1-4, 1983.
[15] Tzavaras, A.E., *Plastic shearing of materials exhibiting strain hardening or strain softening*, Arch. Rat. Mech. Anal. 94, 39-58, 1986.
[16] Tzavaras, A.E., *Strain softening in viscoelasticity of the rate type*, J. Integr. Eq. Appl. 3, 195-238, 1991.
[17] Tzavaras, A.E., *Nonlinear analysis techniques for shear band formation at high strain rates*, Appl. Mech. Reviews 45, 82-94, 1992.
[18] Walter J.W., *Numerical experiments on adiabatic shear band formation in one dimension*. International Journal of Plasticity, 8, 657-693, 1992.
[19] Wright T.W., *The Physics and Mathematics of Shear Bands*, Cambridge University Press, 2002.
[20] Wright, T.W. and Walter, J.W., *On stress collapse in adiabatic shear bands*, J. Mech. Phys. Solids 35, 701-720, 1987.

Ecole Centrale de Nantes, FRANCE
E-mail address: theocharis@tem.uoc.gr

Dept. of Applied Mathematics, Univ. of Crete, Heraklion 71409, GREECE, and Institute of Applied and Computational Mathematics, FORTH, Heraklion 71110, GREECE
E-mail address: thodoros@tem.uoc.gr

Dept. of Mathematics, Univ. of Wisconsin Madison, WI, USA
E-mail address: tzavaras@math.wisc.edu