User-Defined Nonlocal Models in LS-DYNA

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Abstract: In this paper, we present an implementation technique that aims to easily incorporate the benefits of a nonlocal formulation to existing local constitutive models. In order to avoid pathological mesh dependency, an approximation of the nonlocal strategy is adopted. The technique is designed in such manner that the nonlocal extension of previously existing local models is carried out straightforwardly, requiring only minor modifications in the local routines. The implementation in LS-DYNA is depicted in detail for which a FORTRAN code excerpt is provided. In order to validate the proposed nonlocal scheme, we have considered two different constitutive models: one of them intended for the description of ductile materials, the other one suitable for the simulation of fiber-reinforced composites. The numerical analysis of different specimens shows that the proposed nonlocal strategy is able to eliminate spurious mesh dependency under different stress states and using different material models.

Keywords: Nonlocal Models, Damage, Metal Plasticity, Fiber-Reinforced Materials

1 Introduction

In several practical engineering applications, the simulation of failure often requires the introduction of suitable damage laws in order to capture the softening behavior generally observed in experiments. These laws, which can be defined either through explicit or implicit functions of some measure of strain or stress, have the ability of reproducing the global strength decay appreciated on a typical force-displacement diagram. However, whenever some sort of material softening takes place, the results are always pathologically dependent of the spatial discretization. Accuracy is therefore dramatically reduced since finer meshes lead to nonphysical results where dissipative variables (such as damage and plastic strain) localize into a single layer of elements.

The aforementioned shortcoming can be conveniently overcome by the introduction of a nonlocal enhancement. In the nonlocal strategy, the constitutive behavior ceases to be independent of its neighborhood and a given local quantity (e.g. the equivalent plastic strain) is replaced by an integral average within a certain prescribed radius of influence. This radius can be interpreted as a new material property, generally called as *internal length*, that dictates the size of the damaging zone. In this context, Andrade et al. [2] recently presented an efficient algorithm for the numerical implementation of a Lemaitre-based ductile damage nonlocal model. However, the algorithm demands simultaneous access to all integration points of the mesh, a condition not easily met in most commercial FE-packages used by the industry.

In the present contribution, we adopt an approximation of the nonlocal theory that is suitable to be used with existing local models, requiring only little modification. The technique is designed to be easily incorporated as a general user-defined feature in LS-DYNA. The shortcoming of accessing the neighbor integration points at once is overcome by adopting an implementation strategy that saves and uses information of the previous time step [3]. In a general sense, the disadvantage of such approximated nonlocal formulation is the requirement of small time steps for enough accuracy. However, this does not represents a problem in the present case since the explicit integration scheme of LS-DYNA naturally demands very small time steps in order to guarantee stable solutions. As a consequence, the results obtained with the present technique are sufficiently accurate to attenuate the mesh dependency issue.

A methodology similar to the one presented in this paper has been already adopted by Cesar de Sa et al. [3] in the context of a Lemaitre-based ductile damage model, where the implementation in LS-DYNA has been presented in detail. In the present contribution, however, we are extending the methodology to two other material models, where our intention is to demonstrate the generality of the technique.

The first constitutive theory is a J_2 -based elastoplastic damage model for the description of ductile materials. The second one is a recently proposed transversely-isotropic constitutive model suitable for the description of fiber-reinforced materials [9]. Numerical simulation shows that the nonlocal technique is also able to avoid the spurious mesh dependency for these two different material models, proving that the proposed strategy is suitable for a wider spectrum of applications.

2 Local Modeling of Damage

2.1 Ductile damage model

In this paper, we will adopt a constitutive framework similar to the one proposed by Engelen et al. [4]. The model of Engelen and co-authors was formulated in such manner that nonlocality was introduced through an implicit gradient approach. Their results have shown that the gradient methodology is able to successfully eliminate pathological mesh dependency. Our intention by adopting a similar constitutive model is to show that our nonlocal technique, yet to be presented in this paper, has the same regularizing characteristics as Engelen and co-authors' formulation.

We firstly introduce the constitutive equations within the local theory. The yield function of the present ductile damage model is given by

$$\Phi = q - (1 - D(\kappa))\sigma_y(\kappa) \tag{1}$$

where $q = \sqrt{J_2(s)}$ is the equivalent von Mises stress, $s = \sigma - pI$ is the stress deviator, σ is the stress tensor, $p = \frac{1}{3} \text{tr} \sigma$ is the pressure, σ_y is the yield stress and κ is the accumulated plastic strain. The scalar $D(\kappa)$ is the local damage, which here is considered to be

$$D(\kappa) = \frac{\kappa}{\kappa_c} \tag{2}$$

where κ_c is the critical value of accumulated plastic strain at which full material failure occurs.

Associative plasticity is assumed, therefore, plastic flow reads

$$\dot{\varepsilon}^p = \frac{\partial \Phi}{\partial \sigma} = \dot{\gamma} \sqrt{\frac{3}{2}} \frac{s}{\|s\|}.$$
(3)

Within the present constitutive framework, plasticity and damage are assumed to take place respecting the conditions $\Phi \leq 0$, $\dot{\gamma} \geq 0$ and $\Phi \dot{\gamma} = 0$.

The present ductile damage model has been implemented in LS-DYNA via user-defined subroutines (umat41) where the classical elastic-predictor/return-mapping scheme has been adopted in the numerical implementation. In the algorithm, the following trial state

$$\boldsymbol{\sigma}_{n+1}^{trial} = \boldsymbol{\sigma}_n + \boldsymbol{D}^e : \Delta \boldsymbol{\varepsilon} \tag{4}$$

is initially assumed and plastic admissibility is checked using the yield function in Eq. (1). If $\Phi > 0$, then the following residual equation is solved for $\Delta \gamma$ through the Newton-Raphson method:

$$\mathbf{r} := q_{n+1}^{trial} - 3G\Delta\gamma - [1 - D_{n+1}(\kappa_{n+1})]\,\sigma_y(\kappa_{n+1})$$
(5)

where $\kappa_{n+1} = \kappa_n + \Delta \gamma$. When a certain prescribed tolerance is reached, the stress tensor is updated as

$$\boldsymbol{\sigma}_{n+1} = \left(1 - \frac{3G\Delta\gamma}{q_{n+1}^{trial}}\right) \boldsymbol{s}_{n+1}^{trial} + p_{n+1}^{trial} \boldsymbol{I}.$$
 (6)

2.2 Transversely-isotropic elastoplastic material model for short fiber reinforced polymers

In contrast to metals, thermoplastic materials in general exhibit a strong pressure-dependent material behavior, which results in different yielding in uniaxial tension and compression, under shear and under biaxial loadings. Furthermore, the assumption of volume constancy during plastification does not hold for thermoplastic polymers. Especially in the tensile range (uniaxial and biaxial tensile stress states) this effect cannot be neglected. Due to reorientation of molecule chains and due to fiber reinforcements, most thermoplastics also exhibit anisotropic material behavior. This direction-dependent behavior does not only affect the plastic yielding, but also the strain rate sensitivity. A material and failure model, aiming to predict these effects, is therefore summarized in the following. A more detailed description is given in references [9] and [10].

Yield surface formulation

The yield surface as a function of the transversely-isotropic invariants is formulated as

$$f = \alpha_1 I_1 + \alpha_2 I_2 + \alpha_3 I_3 + \alpha_{32} I_3^2 + \alpha_4 I_4 + \alpha_{42} I_4^2 - 1$$
(7)

with the yield surface parameters α_1 , α_2 , α_3 , α_{32} , α_4 and α_{42} . The definition of the invariants is given in [9]. Each of these parameters represents a loading state. The parameter α_1 stands for transverse shear, α_2 for in-plane shear, α_3 and α_{32} represent uniaxial compression and tensile loading transverse to the preferred direction and the parameters α_4 and α_{42} control yielding in fiber direction in compression and tension. The yield surface parameters are directly related to the current yield stress, given by the respective hardening curve for each stress state. Thus, different yielding and hardening in uniaxial compression and tension transverse to the fiber direction and in fiber direction as well as different yielding under in-plane and transverse shear can be regarded. The hardening curves for each stress state, giving yield stresses vs. corresponding plastic strain, can be directly fed via tabulated data in the LS-DYNA input deck.

In order to enable a realistic representation of plastic Poisson's coefficients, a non-associated flow rule is applied. The plastic flow potential, which gives the direction of the projection onto the yield surface, is formulated as

$$g = \beta_1 I_1 + \beta_2 I_2 + \beta_3 I_3 + \beta_{32} I_3^2 + \beta_4 I_4^2 - 1 \quad . \tag{8}$$

The numerical treatment follows an elastic-predictor/plastic-corrector scheme assuming an additive decomposition of the strain increment. The stresses at the end of each time step t_{n+1} are

$$\sigma_{\mathbf{n+1}} = \sigma_{\mathbf{n+1}}^{\text{trial}} - \Delta \lambda_{\mathbf{n+1}} \mathbb{C}_{\mathbf{e}} : \boldsymbol{m}_{\mathbf{n+1}} \quad , \tag{9}$$

whereas $\sigma_{n+1}^{\text{trial}}$ are the elastic trial stresses, \mathbb{C}_e is the transversely-isotropic elasticity tensor, $\Delta \lambda_{n+1}$ is the sought plastic multiplier and m_{n+1} is the direction of the plastic flow, given by the plastic potential

$$\boldsymbol{m}_{n+1} = \partial g(\sigma_{n+1}) / \partial \sigma_{n+1} \quad . \tag{10}$$

Inserting the stresses σ_{n+1} into the yield surface formulation and enforcing the yield surface to be zero at the end of the time step (consistency condition $f_{n+1} = 0$) formally leads to a nonlinear equation in $\Delta \lambda_{n+1}$ which is solved by the Newton-Raphson method. With the plastic multiplier at hand, the plastic strains are updated at the end of each time step

$$\boldsymbol{\varepsilon}_{n+1} = \boldsymbol{\varepsilon}_n + \Delta \lambda_{n+1} \| \boldsymbol{m}_{n+1} \| \quad . \tag{11}$$

Failure criterion and damage formulation

The failure surface follows the same equation as the yield surface formulation, see Eq. (7). Therefore, the experimentally identified ultimate strengthes in each loading state are required for calculating the six failure surface parameters in Eq. (7). In particular, these are the fiber parallel strengthes in tension and compression, R_{\parallel}^t and R_{\parallel}^c , the uniaxial tensile and compressive strength perpendicular to the fiber direction, R_{\perp}^t and R_{\perp}^c , and the material strength of transverse shear $R_{\perp\perp}$ and in-plane shear $R_{\parallel\perp}$. If the failure criterion is active, a degradation of the stresses is performed using a damage approach, where damage is added into the model in an explicit fashion through the linear expression

$$D_{n+1} = \alpha(\varepsilon_{n+1}^p - \varepsilon_{fail}) \tag{12}$$

where α is damage-related parameter and ε_{n+1}^p is the norm of the plastic strain tensor. In the equation above, ε_{fail} denotes a strain value, associated with failure, obtained by applying the failure criterion. The stress tensor is then substituted by

$$\boldsymbol{\sigma}_{n+1}^{dam} = (1 - D_{n+1})\boldsymbol{\sigma}_{n+1}.$$
(13)

3 Nonlocal Formulation

Spurious localization is inherent to the structural problem whenever some sort of strain-driven softening, formulated within the standard local framework, is present. This shortcoming happens because the partial differential equations that govern the structural problem become ill-posed when the hardening modulus is negative, for which uniqueness of solution with respect to the spatial discretization is lost. This is the case of the damage models presented in the last section. Consequently, the numerical results tend to unrealistically concentrate in a single layer of elements as the mesh is refined.

A constitutive model formulated within the nonlocal framework, on the other hand, has the major advantage of being effectively free of spurious mesh dependency and the size of the localizing zone (dictated by the internal length) can be easily controlled. However, the nonlocal method is very often avoided due to its nonstandard implementation requirements.

In this paper, our intention is to present a numerical implementation that aims to considerably simplify the process of turning a local model into nonlocal in LS-DYNA. The technique has been designed in such manner that the nonlocal enhancement has to be implemented in LS-DYNA (via user-defined subroutines) just once. After this initial implementation, any userdefined local material model implemented in LS-DYNA can be transformed into nonlocal in a few minutes. The cornerstone of the technique is based on the approximation of the nonlocal formulation proposed by Tvergaard and Needleman [8]. To start with, let us consider that a generic variable z is the desired local quantity to be turned nonlocal. Using the approximated nonlocal strategy, the updated value of the local variable, z_{n+1} , is re-phrased as

$$z_{n+1}^* = K^{nl} z_{n+1} \tag{14}$$

where K^{nl} is a nonlocal penalty factor defined as

$$K^{nl} = \frac{\bar{z}_n}{z_n} \tag{15}$$

In the equation above, z_n and \bar{z}_n are respectively the local and nonlocal values at the last converged incremental step. Therefore, the stress integration is performed locally where the chosen variable z is penalized with the coefficient K^{nl} . Note that, in order to obtain stable results with the present strategy, it is imperative to keep the size of the time step small enough. As a matter of fact, an explicit finite element framework naturally demands very small time steps dictated by a given stability criterion. Therefore, the technique is perfectly suitable if the explicit scheme is adopted.

The nonlocal average at a given spatial point \boldsymbol{x} is defined as

$$\bar{z}_n(\boldsymbol{x}) = \int_V \beta(\boldsymbol{x}, \boldsymbol{\xi}) z_n(\boldsymbol{\xi}) \, dV(\boldsymbol{\xi}) \tag{16}$$

where $\beta(\boldsymbol{x},\boldsymbol{\xi})$ is the non-local operator expressed by

$$\beta(\boldsymbol{x},\boldsymbol{\xi}) = \frac{\alpha(\boldsymbol{x},\boldsymbol{\xi})}{\int_{V} \alpha(\boldsymbol{x},\boldsymbol{\zeta}) \, dV(\boldsymbol{\zeta})}$$
(17)

and $\alpha(\mathbf{x}, \boldsymbol{\xi})$ is the weighting function, here considered to be the bell-shaped function, i.e.,

$$\alpha(\boldsymbol{x},\boldsymbol{\xi}) = \left\langle 1 - \frac{\|\boldsymbol{x} - \boldsymbol{\xi}\|^2}{\ell_r^2} \right\rangle^2$$
(18)

In the equation above, ℓ_r is the characteristic or internal length, which is a material parameter that has to be experimentally determined.

Nonlocal ductile damage model

In the case of ductile damage model of Section 2.1, the updated damage assumes the form

$$D_{n+1}(\kappa_{n+1}^*) = \frac{\kappa_{n+1}^*}{\kappa_c}$$
(19)

for which

$$\kappa_{n+1}^* = K^{nl} \kappa_{n+1} \tag{20}$$

where K^{nl} is the nonlocal penalty factor given by

$$K^{nl} = \frac{\bar{\kappa}_n}{\kappa_n} \tag{21}$$

Nonlocal transversely-isotropic model

In similar manner to the ductile damage model, the transversely-isotropic model of Section 2.2 has incorporated damage in an explicit fashion. To avoid spurious results, we will substitute Eq. (12) by

$$D_{n+1} = \alpha(\varepsilon_{n+1}^{p*} - \varepsilon_{fail}^{p}) \tag{22}$$

where

$$\varepsilon_{n+1}^{p\ *} = K^{nl} \varepsilon_{n+1}^p \tag{23}$$

and

$$K^{nl} = \frac{\overline{\varepsilon}_n^p}{\varepsilon_n^p}.$$
(24)

4 Numerical Implementation in LS-DYNA

It is worth mentioning that LS-DYNA has the option of using nonlocal formulations through the keyword MAT_NONLOCAL since Version 960 [5]. Unfortunately, this option is restricted to some elastoplastic models only and is not accessible for user-defined constitutive models.

Concerning the implementation of the proposed nonlocal technique, the first step is the spatial discretization of the integral of Eq. (16). Adopting the well-known Gaussian quadrature, we have

$$\bar{z}_i = \sum_{j=1}^{npg_i} w_j J_j \beta_{ij} z_j \tag{25}$$

where $\beta_{ij} \equiv \beta(\boldsymbol{x}, \boldsymbol{\xi})$ is the averaging factor that relates the Gauss points *i* and *j* respectively located at global coordinates \boldsymbol{x} and $\boldsymbol{\xi}$. The quantities \bar{z}_i and z_j are the constitutive variables associated to the Gauss points *i* and *j*, respectively. The quantity w_j is the Gaussian weight and J_j is the Jacobian, both evaluated at the Gauss point *j*. Finally, npg_i is the number of Gauss points that lie inside the nonlocal volume of interaction measured from point *i*. In the numerical implementation, *z* is substituted by the associated constitutive variable according to the model that is enhanced with nonlocality.

In order to facilitate comprehension, a schematic flowchart for the implementation of the nonlocal technique in LS-DYNA is depicted in Figure 1. In Appendix A, we have listed a FORTRAN code excerpt with the main steps of the implementation in file dyn21.f. Two main steps are need for the implementation of the nonlocal strategy. The first one concerns the computation of the factors w_j , J_j and β_{ij} of Eq. (25). These factors are merely geometrical¹, i.e., they depend on the finite element mesh itself and not on the material model. Therefore, once this step has been implemented, it can be re-used whenever the nonlocal formulation is activated.

The second step concerns the computation of the nonlocal penalty factor, K^{nl} . Since it uses the local values of the previous time step, the local variable has to be stored in array var_loc after calling the user material routine umat41. Note that in the code excerpt of Appendix A the arrays var_loc and var_nonloc contain the local and nonlocal values of every element of

 $^{^{1}}$ In order to compute the nonlocal factors, one needs to have the element connectivities and the nodal coordinates.

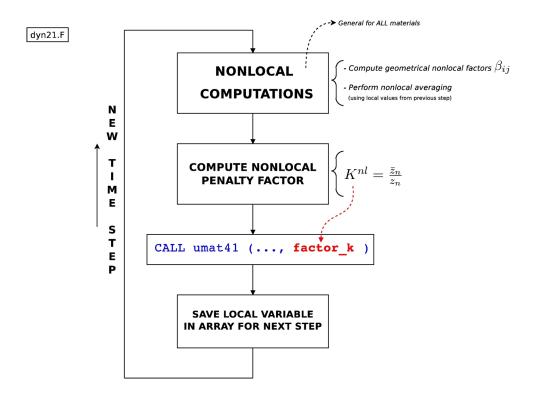


Figure 1: Schematic flowchart of the implementation of the nonlocal strategy.

the mesh. The statement SAVE var_loc guarantees that the information stored in var_loc will be available in the next time step. It is important to remark that the calculations performed for the computation of the nonlocal values (through the discretized integral of Eq. 25) and of the nonlocal penalty factor are the same for any material model. The only difference is which variable is used in these calculations. For instance, in the case of the ductile damage model of Section 2.1, one needs to store the updated accumulated plastic strain, κ_{n+1} , in var_loc. In the case of the transversely-isotropic model of Section 2.2, the updated values of the plastic strain norm are saved in var_loc every time step.

It is also worthwhile emphasizing that the present nonlocal technique can be employed either in scalar or in vectorized LS-DYNA implementations. Thus, the advantages of parallel processing are not lost within the present nonlocal framework.

5 Examples

5.1 Ductile damage

We first assess the nonlocal strategy with the damage model of Section 2.1. Therefore, we simulate two specimens commonly used in the experimental determination of the properties of metals (see Figure 2). The first specimen can be simulated using an axisymmetric formulation meanwhile the second one can be analyzed considering a plane strain state. It is worth mentioning that both specimens deliver similar triaxiality ratios at the critical region $(0.7 \leq p/q \leq 0.8)$;

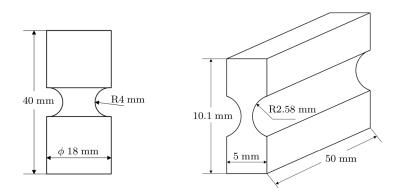


Figure 2: Geometry of the specimens for the ductile damage analysis.

however, the value of the Lode angle is different (i.e., around 1.0 in the axisymmetric specimen and about 0.0 in the plane strain one). As discussed in other references (e.g. in [6]), not only the triaxiality but also the Lode angle plays an important role in the characterization of the stress state and also in the failure onset. The specimens have been considered to be made of steel (E = 200 GPa, $\nu = 0.3$) with a yield stress function given by $\sigma_y(\kappa) = 700 + 300\kappa^{0.3}$ MPa.

The damage contours resulting from the simulation of the axisymmetric and plane strain specimens are respectively given in Figures 3 and 4. The force-displacement diagram is also plotted for both specimens (see Figure 5). Close inspection on these figures reveals that spurious mesh dependency is much stronger in the plane strain specimen than in the axisymmetric one. This fact has also been reported by Andrade et al. [1] who compared local and nonlocal models based on the constitutive theories of Lemaitre and Gurson. Note that those materials models are quite different from the one employed in the present analysis. Even so, the general conclusion that a stress state with Lode angle around 0.0 renders more pronounced pathological mesh dependency persists. Finally, it is also evident from the results that the proposed nonlocal technique has effectively eliminated the spurious mesh dependency associated with strain-softening.

5.2 Fiber-reinforced materials

In order to further assess the proposed nonlocal technique, we simulate three specimens commonly used in the experimental determination of the properties of fiber-reinforced materials (see Figure 6). The transversely-isotropic material model of Section 2.2 is then adopted for the numerical analysis. The selected specimens comprise three different stress states, namely tension, compression and shear. Each specimen has been discretized with three different mesh refinements in order to verify if the nonlocal formulation is able to prevent spurious results.

In Figure 7, the results for the tension specimen are illustrated. Clearly, if the local theory is assumed, the numerical solutions become highly mesh dependent when the softening regime takes place. The nonlocal solution, on the other hand, is able to provide mesh-insensitive results since damage spreads over the elements at the central region. The results for the shear specimen are provided in Figure 8. We observe a very accentuated mesh sensitivity of the local solution, where damage tends to concentrate into a single layer of elements. When the nonlocal strategy is

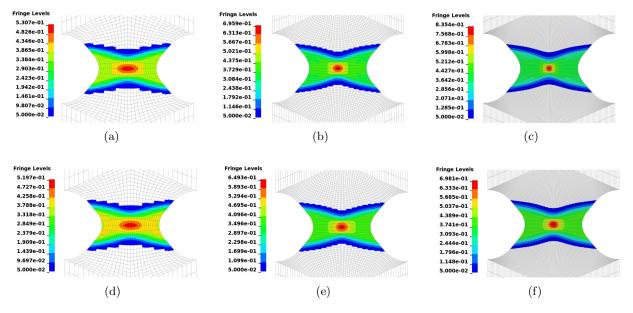


Figure 3: Damage contours for the axisymmetric specimen: (a–c) local; (d–f) nonlocal.

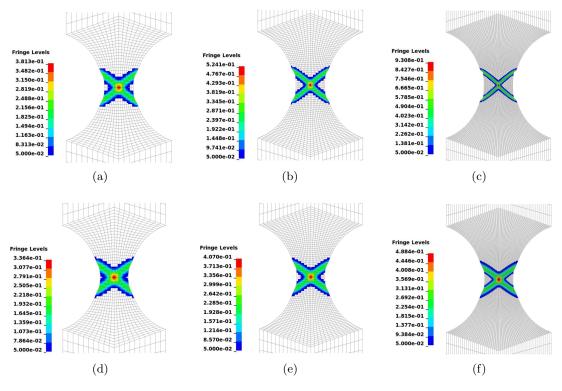


Figure 4: Damage contours for the plane strain specimen: (a-c) local; (d-f) nonlocal.

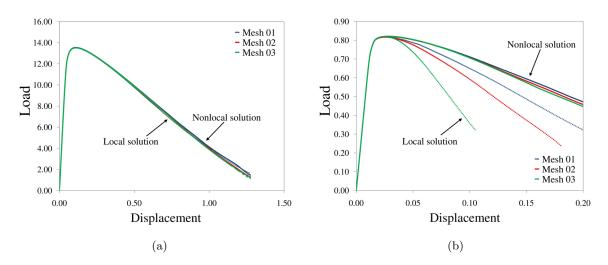


Figure 5: Force-displacement diagrams: (a) axisymmetric specimen; (b) plane strain specimen.

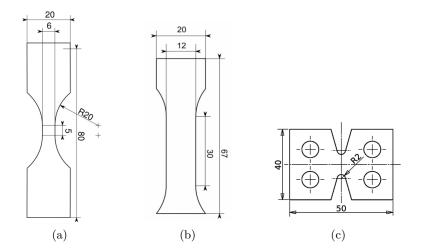


Figure 6: Specimens for (a) tension, (b) compression and (c) shear test.

activated, the spurious mesh dependency is prevented, rendering more physically sound results. Finally, Figure 9 depicts the results obtained in the compression test. Again, pathological mesh dependency is evident within the standard local theory, which has been significantly alleviated with the use of the nonlocal formulation.

6 Conclusions

In this paper, a strategy for the implementation of nonlocal models in LS-DYNA has been presented. The technique has been designed to be generally applicable to several user-defined material models, requiring only little modification in the original local routines. Two different

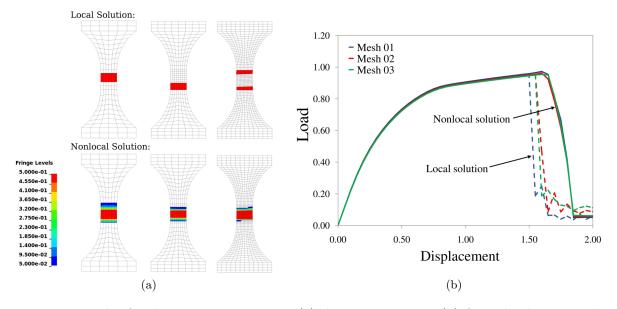


Figure 7: Results for the tension specimen: (a) damage contours; (b) force-displacement diagram.

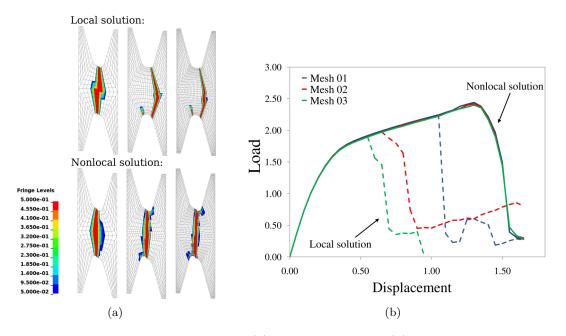


Figure 8: Results for the shear specimen: (a) damage contours; (b) force-displacement diagram.

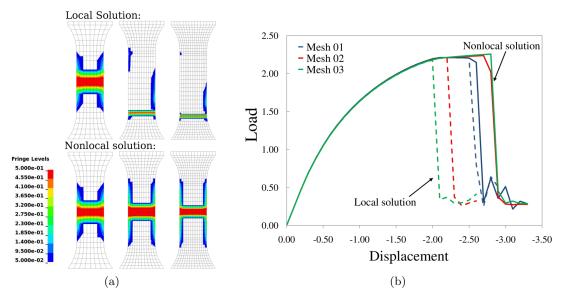


Figure 9: Results for the compression specimen: (a) damage contours; (b) force-displacement diagram.

constitutive models, one of them suitable for the description of ductile metals and the other one intended for the simulation of fiber-reinforced materials, have been coupled with the present nonlocal technique. The numerical analysis has demonstrated that the nonlocal strategy has been able to prevent unlimited localization and physically sound results have been obtained. It is important to mention that, once the general routines of the nonlocal scheme have been implemented, the nonlocal extension of the aforementioned material models was straightforward. Thus, the obtained mesh-insensitive results and the generality of implementation make the present nonlocal technique a strong candidate against other competitive regularization methods.

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Appendix A

An excerpt of the FORTRAN code for the implementation of the nonlocal strategy in LS-DYNA as a user-defined option is provided. Only the main steps have been listed and the code is intended to serve as a general guide. The implementation has to be incorporated in dyn21.f.

```
SUBROUTINE urmathn (...)
. . . .
COMMON/bk06/idmmy, iaddp, ifil, maxsiz, ncycle, time(2, 30)
. . . .
! Declare dimensions for nonlocal formulation
DIMENSION betaij(...), var_loc(mxelem), var_nonloc(mxelem)
DIMENSION connect(mxelem,8), coord(mxnode,3)
! Save data for the next step
SAVE betaij, var_loc, connect, coord
. . . .
! Get connectivities and nodal coordinates (only at cycle #1)
IF(ncycle.EQ.1)THEN
  CALL get_connectivities (..., connect ,....)
  CALL get_coordinates (..., coord , r_mem(dm_x) ,...)
ENDIF
! Compute nonlocal factors beta_ij (only at cycle #2)
IF(ncycle.EQ.2)THEN
  CALL compute_nonlocal_factors (..., betaij, connect, coord,...)
ENDIF
! Compute nonlocal variable (e.g. at every cicle)
IF(ncycle.GE.2)THEN
  CALL compute_nonlocal_variable (..., betaij , var_loc , var_nonloc ,...)
ENDIF
. . . .
DO 90 i=lft,llt
  ! Get external element ID (solids)
  ielem=lqfinv(nnm1+i,2)
  ! Compute penalty factor K
 factor_k=var_nonloc(ielem)/var_loc(ielem)
  . . . .
  ! Local user material routine
41 CALL umat41 (..., factor_k)
  . . . .
  ! Store local variable to be used in the next step
 var_loc(ielem) = hsv(...)
. . . .
90 CONTINUE
. . . .
END SUBROUTINE urmathn
```

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