A numerical framework for continuum damage - discontinuum transition

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Dedicated to Professor Piotr Perzyna
on the occasion of his 70th birthday

A framework is derived for the proper and consistent description of a discontinuity (a crack) as the result of a damaging process in a continuous medium. The damaging process in the continuous medium is described using a gradient-enhanced damage theory, so that well-posedness of the boundary-value problem is maintained until the damage process is completed and a discontinuity arises. At that moment the partition-of-unity property of finite element shape functions is exploited to partition the displacement field into two continuous fields, separated via a Heaviside function. It is demonstrated that the additional boundary conditions that arise in a gradient-enhanced damage theory, can be accounted for in a natural and transparent manner.

1. Introduction

The failure behaviour of many engineering materials can be classified as quasi-brittle. Prominent examples are concrete and ceramics, but also most fibre-reinforced materials behave as such. The salient characteristic common in failure of these materials is that, ahead of a macroscopically observable crack, there is a rather large fracture process zone, in which micro-cracks initiate, grow and coalesce. This observation prevents the use of linear elastic fracture mechanics. Indeed, from a physical point of view, a model in which the micro-cracking ahead of the crack tip would be modelled as a degrading continuum, e.g., using continuum damage mechanics, while the macroscopic crack would be captured as a true discontinuity, would be most appealing. It is precisely such an approach that we will describe in this contribution.
For the micro-cracking ahead of the crack tip, we shall use a smeared, or continuum approach. In particular, we shall employ a standard isotropic damage model, e.g., [4]. However, since standard damage models lack an internal length scale, the governing equations in the fracture process zone can lose ellipticity during quasi-static loadings. To remedy this, the model must be enhanced by a form of non-locality [3] or by adding viscosity [5]. Herein, we employ the second gradient of the equivalent strain measure of the damage model for this purpose [7], [8]. For numerical solutions of non-local and gradient-enhanced models, a very fine discretisation is required, since the spacing of nodes or grid points must be smaller than the characteristic or internal length scale of the continuum in order to resolve the strains in the fracture processes zone properly.

In isotropic damage models, the material locally loses all coherence when the damage parameter $\omega$ becomes equal to one. Then, the governing partial differential equations that arise from the equilibrium, the kinematic and the constitutive equations, lose meaning for a continuum and a discrete crack arises. In fact, a 'vanishing' length scale then arises, since a discrete crack has a zero width. To capture such a 'zero' length scale using numerical techniques designed for continuum problems is impossible. However, traditional finite element techniques can be adapted to cope with this when use is made of the partition-of-unity property of the shape functions of finite elements [1]. Then, the displacement field can be written as the sum of two continuous displacement fields, which are separated via a Heaviside function and a crack, i.e. a discontinuity in an otherwise smooth displacement field, can be described in an exact manner. Following the work of Belytschko and Black [2] for linear elastic fracture mechanics and Wells et al. [9], [10] for cohesive-zone models and application to viscoplasticity, this concept is now applied to form a true discontinuity at the end of a process in which a gradient-enhanced damage model has been used to describe the initiation, growth and coalescence of micro-cracks.

The paper will first give a succinct summary of the implicit gradient damage model. Then, the development leading to the introduction of a discontinuity in a gradient-enhanced continuum will be outlined. Special attention will be given to the treatment of the additional boundary condition, which arises due to the introduction of the gradient term, at the internal boundary, i.e. at the crack.

2. Gradient-enhanced damage model

We start the discussion by recalling the governing equations of the so-called implicit gradient-enhanced damage model, originated by Peerlings at al. [7], [8]. In it, the equilibrium equation (in the absence of body forces):
and the kinematic relation (for small strains)
(2.2) \[ \varepsilon = \nabla^s u \]
with \( u \) being the displacement field and the superscript \( s \) denoting the symmetric part of the gradient operator, are augmented by an injective relation between the stress tensor \( \sigma \) and the strain tensor \( \varepsilon \):
(2.3) \[ \sigma = (1 - \omega) D^e : \varepsilon \]
In equation (2.3) \( D^e \) is the elasticity tensor with the virgin elastic constants \( E \) (Young's modulus) and \( \nu \) (Poisson's ratio). \( \omega \) is a monotonically increasing damage parameter, with an initial value 0, for the intact material, and an ultimate value 1, at complete loss of material coherence. It is a function of a history parameter \( \kappa \):
(2.4) \[ \omega = \omega(\kappa) \]
with \( \kappa \) linked to a non-local strain measure \( \bar{\varepsilon} \) via a loading function
(2.5) \[ f = \bar{\varepsilon} - \kappa \]
such that loading occurs if \( f = 0, \dot{f} = 0 \) and \( \omega < 1 \). Formally, the loading-unloading process can be captured by the Kuhn-Tucker conditions:
(2.6) \[ f \kappa = 0, \quad f \leq 0, \quad \kappa \geq 0. \]
The non-local strain measure is coupled to a local strain measure \( \varepsilon \) via a Helmholtz equation:
(2.7) \[ \frac{\partial \varepsilon}{\partial \varepsilon} - c \nabla^2 \varepsilon = \bar{\varepsilon} \]
with \( c \) denoting a material parameter with the dimension of length squared, and \( \bar{\varepsilon} \) a function of the strain tensor:
(2.8) \[ \bar{\varepsilon} = \bar{\varepsilon}(\varepsilon). \]
The equilibrium equation (2.1), the kinematic equation (2.2) and the constitutive model (2.3)-(2.8) are complemented by the boundary conditions
(2.9) \[ \sigma \cdot n_{\partial \Omega} = t_p \quad \text{and} \quad u = u_p \]
on complementary parts of the boundary \( \partial \Omega_t \) and \( \partial \Omega_u \), with \( \partial \Omega = \partial \Omega_t \cup \partial \Omega_u \) and \( \partial \Omega_t \cap \partial \Omega_u = \emptyset \), while for the non-local strain \( \bar{\varepsilon} \) the natural boundary condition
(2.10) \[ \frac{\partial \bar{\varepsilon}}{\partial n} \equiv n_{\partial \Omega} \cdot \nabla \bar{\varepsilon} = 0 \]
with the unit normal vector \( n_{\partial \Omega} \) at the boundary \( \partial \Omega \), is commonly assumed [6].
3. Transition to a discontinuity

When $\omega = 1$, the material has lost all coherence. At this moment, the governing equations for the continuous medium lose validity and a discrete crack arises. Then, the displacement field can be written as

$$\mathbf{u}(x, t) = \mathbf{u}^a(x, t) + H_{\partial\Omega^d}(x) \mathbf{u}^b(x, t)$$

with $\mathbf{u}^a$ and $\mathbf{u}^b$ denoting the continuous displacement fields, and $H_{\partial\Omega^d}$ a Heaviside function centered at the discontinuity $\partial\Omega^d$ which separates the $\Omega^+$ domain from the $\Omega^-$ domain ($\Omega = \Omega^+ \cap \Omega^-$). At this discontinuity a normal $\mathbf{n}_{\partial\Omega^d}$ is defined such that it points to the $\Omega^+$ domain. From Eq. (3.1) the strain field can be derived as:

$$\epsilon(x, t) = \nabla^s \mathbf{u}^a(x, t) + H_{\partial\Omega^d}(x) \nabla^s \mathbf{u}^b(x, t) + \delta_{\partial\Omega^d} \left( \mathbf{u}^b \otimes \mathbf{n}_{\partial\Omega^d} \right)^s$$

with $\delta_{\partial\Omega^d}$ the Dirac function at $\partial\Omega^d$. Again, the superscript $s$ denotes the symmetric part.

Consistent with the decomposition (3.1) we now partition the field that describes the non-local strain measure as:

$$\bar{\epsilon}(x, t) = \bar{\epsilon}^a(x, t) + H_{\partial\Omega^d}(x) \bar{\epsilon}^b(x, t)$$

where, as emphasised by Peerlings et al. [6], the boundary condition is also applied at the internal boundary $\partial\Omega^d$.

We now cast the governing equations (2.1) and (2.7) in a weak format by multiplying them by test functions $\eta$ and $\xi$, respectively, and integrating over the body. When adopting a Bubnov-Galerkin approach, we have, cf. Eqs. (3.1) and (3.3):

$$\eta = \eta^a + H_{\partial\Omega^d} \eta^b,$$

$$\xi = \xi^a + H_{\partial\Omega^d} \xi^b,$$

where the dependence on $x$ and $t$ has been left out for clarity of notation. Thus, the weak forms become:

$$\int_\Omega \left( \eta^a + H_{\partial\Omega^d} \eta^b \right)^T \left( L^T \sigma \right) \, d\Omega = 0,$$

$$\int_\Omega \left( \xi^a + H_{\partial\Omega^d} \xi^b \right) (\bar{\epsilon} - c \nabla^2 \bar{\epsilon} - \bar{\epsilon}) \, d\Omega = 0,$
where a change has been made to matrix-vector notation, with \( L \) denoting a differential operator matrix, for 2D:

\[
L = \begin{bmatrix}
\frac{\partial}{\partial x} & 0 \\
0 & \frac{\partial}{\partial y} \\
\frac{\partial}{\partial y} & \frac{\partial}{\partial x}
\end{bmatrix}.
\]

(3.8)

Use of the divergence theorem and the boundary conditions (2.9) and (2.10) gives in lieu of equations (3.6) and (3.7):

\[
\int_{\Omega} \left[ L \eta^a + H_{\partial \Omega^d} \, L \eta^b \right]^T \sigma \, d\Omega + \int_{\Omega} \delta_{\partial \Omega^d} \left( L^* \eta^b \right)^T \sigma \, d\Omega = \int_{\partial \Omega} \left( \eta^a + H_{\partial \Omega^d} \eta^b \right)^T t_p \, d(\partial \Omega),
\]

(3.9)

\[
\int_{\Omega} \left( \xi^a + H_{\partial \Omega^d} \xi^b \right) \tilde{\varepsilon} \, d\Omega + \int_{\Omega} \left( \nabla \xi^a + H_{\partial \Omega^d} \nabla \xi^b \right)^T \nabla \tilde{\varepsilon} \, d\Omega
\]

\[
+ \int_{\Omega} c \delta_{\partial \Omega^d} \xi^b \eta_{\partial \Omega^d}^T \nabla \tilde{\varepsilon} \, d\Omega = \int_{\Omega} \left( \xi^a + H_{\partial \Omega^d} \xi^b \right) \tilde{\varepsilon} \, d\Omega,
\]

(3.10)

with \( L^* \) defined as

\[
L^* = \begin{bmatrix}
n_x & 0 \\
0 & n_y \\
n_y & n_x
\end{bmatrix}.
\]

(3.11)

Using the general distribution property

\[
\int_{\Omega} \delta_{\partial \Omega^d} \ldots \, d\Omega = \int_{\partial \Omega^d} \ldots \, d(\partial \Omega),
\]

(3.12)

and

\[
\int_{\Omega} H_{\partial \Omega^d} \ldots \, d\Omega = \int_{\Omega^+} \ldots \, d\Omega
\]

(3.13)

we rewrite equations (3.9) and (3.10) as:
\begin{align}
(3.14) \quad & \int_{\Omega} (\eta^a)^T L^T \sigma \, d\Omega + \int_{\Omega^+} (\eta^b)^T L^T \sigma \, d\Omega \\
& + \int_{\partial\Omega^d} (\eta^b)^T (L^*)^T \sigma \, d(\partial\Omega) = \int_{\partial\Omega} \left( \eta^a + H_{\partial\Omega^d} \eta^b \right)^T t_p \, d(\partial\Omega),
\end{align}

\begin{align}
(3.15) \quad & \int_{\Omega} \xi^a \bar{\epsilon} \, d\Omega + \int_{\Omega^+} \xi^b \bar{\epsilon} \, d\Omega + \int_{\Omega} c \left( \nabla \xi^a \right)^T \nabla \bar{\epsilon} \, d\Omega \\
& + \int_{\Omega^+} c \left( \nabla \xi^b \right)^T \nabla \bar{\epsilon} \, d\Omega + \int_{\partial\Omega^d} c \xi^b \mathbf{n}_{\partial\Omega^d}^T \nabla \bar{\epsilon} \, d(\partial\Omega) \\
& = \int_{\Omega} \xi^a \bar{\epsilon} \, d\Omega + \int_{\Omega^+} \xi^b \bar{\epsilon} \, d\Omega.
\end{align}

After complete decohesion of the bulk material, the internal crack or discontinuity that then arises is stress-free. Accordingly, for the interface traction \( t_{\partial\Omega^d} \), it holds that

\begin{equation}
(3.16) \quad t_{\partial\Omega^d} \equiv (L^*)^T \sigma = 0.
\end{equation}

Thus, the third integral in Eq. (3.15) cancels. Similarly, the fifth integral of Eq. (3.16) cancels because of the boundary condition (2.10), which, as has been emphasised by Peerlings et al. [6], must also hold at the internal boundary \( \partial\Omega^d \). Thus, we obtain instead of Eqs. (3.15) and (3.16):

\begin{align}
(3.17) \quad & \int_{\Omega} (\eta^a)^T L^T \sigma \, d\Omega + \int_{\Omega^+} (\eta^b)^T L^T \sigma \, d\Omega \\
& = \int_{\partial\Omega} \left( \eta^a \right)^T t_p \, d(\partial\Omega) + \int_{\partial\Omega} H_{\partial\Omega^d} \left( \eta^b \right)^T t_p \, d(\partial\Omega),
\end{align}

\begin{align}
(3.18) \quad & \int_{\Omega} \xi^a \bar{\epsilon} \, d\Omega + \int_{\Omega^+} \xi^b \bar{\epsilon} \, d\Omega + \int_{\Omega} c \left( \nabla \xi^a \right)^T \nabla \bar{\epsilon} \, d\Omega \\
& + \int_{\Omega^+} c \left( \nabla \xi^b \right)^T \nabla \bar{\epsilon} \, d\Omega = \int_{\Omega} \xi^a \bar{\epsilon} \, d\Omega + \int_{\Omega^+} \xi^b \bar{\epsilon} \, d\Omega.
\end{align}

4. Spatial discretisation

For the spatial discretisation we use a standard Bubnov-Galerkin approach, so that the test and trial functions are in the same space:

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(4.1) \[ \mathbf{u} = \mathbf{N} (\mathbf{a} + H_{\partial \Omega^d} \mathbf{b}), \]

(4.2) \[ \eta = \mathbf{N} (\mathbf{w} + H_{\partial \Omega^d} \mathbf{z}), \]

(4.3) \[ \bar{\varepsilon} = \tilde{\mathbf{N}} (\bar{\mathbf{e}} + H_{\partial \Omega^d} \mathbf{g}), \]

(4.4) \[ \bar{\xi} = \tilde{\mathbf{N}} (\bar{\mathbf{f}} + H_{\partial \Omega^d} \mathbf{h}) \]

where the partition-of-unity property of the shape functions contained in \( \mathbf{N} \) and \( \tilde{\mathbf{N}} \) has been exploited. The arrays \( \mathbf{a} \) and \( \mathbf{e} \) contain the "regular" nodal degrees-of-freedom of the displacements and the non-local strain measure, while \( \mathbf{b} \) and \( \mathbf{g} \) contain the part that is due to the enhancement. Inserting Eqs. (4.1)-(4.4) into Eqs. (3.18)-(3.19) and setting:

(4.5) \[ \mathbf{B} = \mathbf{L} \mathbf{N} \quad \text{and} \quad \tilde{\mathbf{B}} = \nabla \tilde{\mathbf{N}} \]

gives, after requiring that the result holds for all admissible \( \mathbf{w}, \mathbf{z}, \mathbf{f} \) and \( \mathbf{h} \):

(4.6) \[ \int_{\Omega} \mathbf{B}^T \sigma \ d\Omega = \int_{\partial \Omega} \mathbf{N}^T \mathbf{t}_p \ d(\partial \Omega), \]

(4.7) \[ \int_{\Omega^+} \mathbf{B}^T \sigma \ d\Omega = \int_{\partial \Omega} H_{\partial \Omega^d} \mathbf{N}^T \mathbf{t}_p \ d(\partial \Omega), \]

(4.8) \[ \int_{\Omega} (\tilde{\mathbf{N}}^T \tilde{\mathbf{N}} + c \tilde{\mathbf{B}}^T \tilde{\mathbf{B}}) \ d\Omega \mathbf{e} \]

\[ + \int_{\Omega^+} (\tilde{\mathbf{N}}^T \tilde{\mathbf{N}} + c \tilde{\mathbf{B}}^T \tilde{\mathbf{B}}) \ d\Omega \mathbf{g} = \int_{\Omega} \tilde{\mathbf{N}}^T \bar{\varepsilon} \ d\Omega, \]

(4.9) \[ \int_{\Omega^+} (\tilde{\mathbf{N}}^T \tilde{\mathbf{N}} + c \tilde{\mathbf{B}}^T \tilde{\mathbf{B}}) \ d\Omega \mathbf{e} \]

\[ + \int_{\Omega^+} (\tilde{\mathbf{N}}^T \tilde{\mathbf{N}} + c \tilde{\mathbf{B}}^T \tilde{\mathbf{B}}) \ d\Omega \mathbf{g} = \int_{\Omega^+} \tilde{\mathbf{N}}^T \bar{\xi} \ d\Omega. \]

To facilitate the linearisation process, needed for an incremental-iterative procedure in a Newton-Raphson sense, we define:

(4.10) \[ f_{a}^{\text{int}} = \int_{\Omega} \mathbf{B}^T \sigma \ d\Omega, \]
\begin{align*}
(4.11) \quad f_\text{int}^b &= \int_{\Omega^+} B^T \sigma \, d\Omega, \\
(4.12) \quad f_\text{ext}^a &= \int_{\partial \Omega} N^T t_p \, d(\partial \Omega), \\
(4.13) \quad f_\text{ext}^b &= \int_{\partial \Omega} H_{\partial \Omega^d} N^T t_p \, d(\partial \Omega), \\
(4.14) \quad f_e &= \int_{\Omega} N^T \bar{\varepsilon} \, d\Omega, \\
(4.15) \quad f_g &= \int_{\Omega^+} N^T \bar{\varepsilon} \, d\Omega,
\end{align*}

and

\begin{align*}
(4.16) \quad K_{ee} &= \int_{\Omega} (\bar{N}^T \bar{N} + c \bar{B}^T \bar{B}) \, d\Omega \\
(4.17) \quad K_{eg} &= \int_{\Omega^+} (\bar{N}^T \bar{N} + c \bar{B}^T \bar{B}) \, d\Omega
\end{align*}

Then, Eqs. (4.6)-(4.9) can be cast in the following format:

\begin{align*}
(4.18) \quad f_\text{int}^a &= f_\text{ext}^a, \\
(4.19) \quad f_\text{int}^b &= f_\text{ext}^b, \\
(4.20) \quad K_{ee} e + K_{eg} g &= f_e, \\
(4.21) \quad K_{eg} e + K_{eg} g &= f_g.
\end{align*}
5. Consistent linearisation

To solve the coupled discrete Eqs. (4.18)-(4.21), a Newton-Raphson procedure is normally employed, which requires a linearisation of the set. Equation (4.18) can be linearised as follows, cf. Eq. (2.3),

\[(5.1) \quad \sigma_j = \sigma_{j-1} + d\sigma \]
\[= \sigma_{j-1} + (1 - \omega_{j-1}) \mathbf{D}^e \mathbf{d} \mathbf{e} - d\omega \mathbf{D}^e \mathbf{e}_{j-1} \]
\[= \sigma_{j-1} + (1 - \omega_{j-1}) \mathbf{D}^e \mathbf{B} (\mathbf{d}a + H_{\partial \Omega^d} \mathbf{d}b) - d\omega \mathbf{D}^e \mathbf{e}_{j-1}.\]

Since

\[(5.2) \quad d\omega = \frac{d\omega}{d\kappa} \frac{d\kappa}{d\epsilon} \bar{\mathbf{N}} (\mathbf{d}e + H_{\partial \Omega^d} \mathbf{d}g),\]

we have for \(\sigma_j\)

\[(5.3) \quad \sigma_j = \sigma_{j-1} + (1 - \omega_{j-1}) \mathbf{D}^e \mathbf{B} (\mathbf{d}a + H_{\partial \Omega^d} \mathbf{d}b) - \mathbf{D}^e \mathbf{e}_{j-1} \frac{d\omega}{d\kappa} \frac{d\kappa}{d\epsilon} \bar{\mathbf{N}} (\mathbf{d}e + H_{\partial \Omega^d} \mathbf{d}g) \]

and the linearised form of (4.18) becomes:

\[(5.4) \quad \mathbf{K}_{aa} \mathbf{d}a + \mathbf{K}_{ab} \mathbf{d}b + \mathbf{K}_{ae} \mathbf{d}e + \mathbf{K}_{ag} \mathbf{d}g = \mathbf{f}_{a}^{\text{ext}} - \mathbf{f}_{a,j-1}^{\text{int}} \]

where

\[(5.5) \quad \mathbf{K}_{aa} = \int_\Omega \mathbf{B}^T (1 - \omega_{j-1}) \mathbf{D}^e \mathbf{B} d\Omega, \]
\[(5.6) \quad \mathbf{K}_{ab} = \int_{\Omega^+} \mathbf{B}^T (1 - \omega_{j-1}) \mathbf{D}^e \mathbf{B} d\Omega, \]
\[(5.7) \quad \mathbf{K}_{ae} = - \int_\Omega \mathbf{B}^T \mathbf{D}^e \mathbf{e}_{j-1} \frac{d\omega}{d\kappa} \frac{d\kappa}{d\epsilon} \bar{\mathbf{N}} d\Omega, \]
\[(5.8) \quad \mathbf{K}_{ag} = - \int_{\Omega^+} \mathbf{B}^T \mathbf{D}^e \mathbf{e}_{j-1} \frac{d\omega}{d\kappa} \frac{d\kappa}{d\epsilon} \bar{\mathbf{N}} d\Omega. \]

In a similar fashion, we obtain for Eq. (4.19)

\[(5.9) \quad \mathbf{K}_{ab} \mathbf{d}a + \mathbf{K}_{ab} \mathbf{d}b + \mathbf{K}_{ag} \mathbf{d}e + \mathbf{K}_{ag} \mathbf{d}g = \mathbf{f}_{b}^{\text{ext}} - \mathbf{f}_{b,j-1}^{\text{int}}. \]
Finally, \( f_e \) can be linearised using

\[
(5.10) \quad d\bar{c} = \left( \frac{d\bar{c}}{d\epsilon} \right)^T B (da + H_{\Omega} db)
\]

so that Eqs. (4.20) and (4.21) turn into:

\[
(5.11) \quad K_{ea} da + K_{ga} db + K_{ee} de + K_{eg} dg \\
= f_{e,j-1} - K_{ee} e_{j-1} - K_{eg} g_{j-1}
\]

and

\[
(5.12) \quad K_{ga} da + K_{ga} db + K_{eg} de + K_{eg} dg \\
= f_{g,j-1} - K_{eg} e_{j-1} - K_{eg} g_{j-1},
\]

\[
(5.13) \quad K_{ea} = - \int_{\Omega} \tilde{N}^T \left( \frac{d\bar{c}}{d\epsilon} \right)^T B d\Omega,
\]

\[
(5.14) \quad K_{ga} = - \int_{\Omega^+} \tilde{N}^T \left( \frac{d\bar{c}}{d\epsilon} \right)^T B d\Omega.
\]

Summarising Eqs. (5.4), (5.9), (5.11) and (5.12) in a matrix-vector format, we obtain:

\[
(5.15) \quad \begin{bmatrix} K_{aa} & K_{ab} & K_{ae} & K_{ag} \\ K_{ab} & K_{ab} & K_{ag} & K_{ag} \\ K_{ea} & K_{ga} & K_{ee} & K_{eg} \\ K_{ga} & K_{ga} & K_{eg} & K_{eg} \end{bmatrix} \begin{bmatrix} da \\ db \\ de \\ dg \end{bmatrix} = \begin{bmatrix} f_{a,ext} - f_{a,j-1}^{int} \\ f_{b,ext} - f_{b,j-1}^{int} \\ f_{e,j-1} - K_{ee} e_{j-1} - K_{eg} g_{j-1} \\ f_{g,j-1} - K_{eg} e_{j-1} - K_{eg} g_{j-1} \end{bmatrix}
\]

6. Concluding remarks

A theoretical framework has been given for the description of a truly discontinuous crack arising as the result of a damaging process involving initiation, growth and coalescence of micro-cracks. For the latter process, a gradient-enhanced damage model has been utilised. An example representing the proposed method will be presented in a forthcoming publication.
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References


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