

Configurational Forces in a Phase Field Model for Fatigue

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In the last decades, the phase field method has drawn much attention for its application in fracture mechanics because it offers a simple unified framework for crack propagation. The core idea of phase field models for fracture is to introduce a continuous scalar field representing the discontinuous crack. Recently, a phase field model for fatigue has been proposed along this path. The fatigue failure differs from the other fracture scenarios since cracks only occur after a considerable number of load cycles. As fracturing happens, changes of the material microstructure are involved, which causes the evolution of the structural configuration. Thus, a new mathematical description not based on traditional spatial coordinates but the material manifold is desired, which will serve as an elegant analysis tool to understand the energetic forces for crack propagation. Configurational forces are a suitable choice for this purpose, as they describe the energetic driving forces associated with phenomena changing the material itself. In this work, we present a phase field model for fatigue. Furthermore, the phase field fatigue model is analyzed within the concept of configurational forces, which provides a straightforward way to understand the phase field simulations of fatigue fracture.

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1 A Phase Field Model for Fatigue

The phase field fracture model introduces an additional field variable to represent cracks. The crack field s is 1 if the material remains undamaged and if is 0 where cracks occur [1]. Furthermore, it is postulated that the displacement field \mathbf{u} and crack field s locally minimize the total energy of a loaded body Ω . This yields the equilibrium of the stress field and the evolution of the crack field for fatigue fracturing. The total energy \mathcal{E} is given as [2] [3]

$$\mathcal{E} = \int_{\Omega} \psi(\varepsilon, s, \nabla s, D) dV = \int_{\Omega} \left[(g(s) + \eta) \psi^e(\varepsilon) + \psi^s(s, \nabla s) + h(s) \psi^{\text{ad}}(D) \right] dV, \quad (1)$$

where ψ denotes the total energy density. The stain energy density

$$\psi^e(\varepsilon) = \frac{1}{2} \varepsilon : (\mathbb{C} \varepsilon) \quad (2)$$

is the energy stored inside of a body and $g(s)$ is the degradation function, which models the loss of stiffness of the broken material. The crack surface density

$$\psi^s(s, \nabla s) = G_c \left(\frac{(1-s)^2}{4\epsilon} + \epsilon |\nabla s|^2 \right) \quad (3)$$

is the energy required to separate the material in order to generate the crack, which is assumed to be proportional to the crack surface. The parameter G_c denotes the fracture toughness, which is the ability of a material to resist fracturing. The numerical parameter ϵ models the width of the smooth transition zone. The fatigue energy density

$$\psi^{\text{ad}}(D) = q \langle D - D_c \rangle^b \quad \text{with} \quad D = D_0 + dD \quad (4)$$

is introduced to account for the accumulated fatigue driving forces, which is associated with a fatigue damage parameter D . This parameter D models the damage related to fatigue, inspired by Miner rule [4], which will be accumulated during the entire simulation; D_0 is the previous damage; $dD = \frac{dN}{n_D} \left(\frac{\hat{\sigma}}{A_D} \right)^k$ is the damage increment, which is associated with the cycle increment dN , where the parameters n_D , A_D and k are read from the Wöhler curve of experiments. In the phase field model, the first principal stress from the undegraded stress field $\hat{\sigma} = [\mathbb{C}\varepsilon]_1$ is used as the fatigue driving force. D_c is a damage threshold, which models the crack nucleation process. The additional fatigue energy will not give attributions when the damage D is below this threshold. After the crack nucleation stage, the parameters q and b are numerical parameters controlling how fast the additional fatigue energy growth.

2 Phase Field Fatigue Simulation of 1D Bar

A 1D fracture problem is given as follows: a homogeneous bar of length $2L$ under a given displacement load u_0 at both sides and the middle of the bar is broken $s = 0$ (see Fig. 1). Let the degradation function for both elastic strain energy density ψ^e

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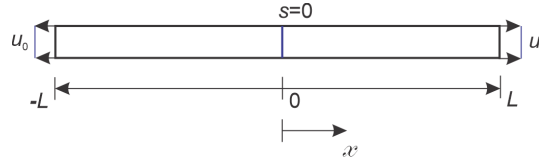


Fig. 1: A homogeneous bar is under displacement load.

and fatigue energy density ψ^{ad} be $g(s) = h(s) = s^2$, the equilibrium equation of the stress field reads

$$\frac{d\sigma}{dx} = 0 \quad \text{with} \quad \sigma = (s^2 + \eta)2\mu\epsilon + s^2 \frac{\partial \psi^{\text{ad}}}{\partial \epsilon} \quad \text{and} \quad \epsilon = \frac{du}{dx} \quad (5)$$

and the evolution of crack field s in a cyclic domain reads

$$\frac{ds}{dN} = -M \left\{ s2\mu\epsilon^2 - \mathcal{G}_c \left(2\epsilon \frac{d^2s}{dx^2} - \frac{s-1}{2\epsilon} \right) + 2s\psi^{\text{ad}} \right\}. \quad (6)$$

We consider first the bar in a quasi-static state without any load, the elastic energy contribution is therefore neglected. Eq. (6) can be then simplified as a second order linear differential equation

$$\frac{d^2s}{dx^2} - \left(\frac{1}{4\epsilon^2} + \frac{\psi^{\text{ad}}}{\mathcal{G}_c\epsilon} \right) s + \frac{1}{4\epsilon^2} = 0. \quad (7)$$

For the given boundary conditions $s'(\pm L) = 0$ and a crack $s(0) = 0$ at the bar middle, ignoring the higher order infinitesimal and assuming the crack is ideal e.g. $\epsilon \rightarrow 0$ yields the crack field profile

$$s(x) = 1 - \exp\left(\frac{-|x|}{2\epsilon}\right). \quad (8)$$

Look again to Eq. (5), it implies that the stress $\sigma = \bar{\sigma}$ is constant over the whole bar

$$\sigma(x) = \bar{\sigma}. \quad (9)$$

Let Eq. (8) be an approximated solution and taking boundary condition for u into consideration yields the displacement profile [5]

$$u(x) = \frac{u_0}{F(L) - F(0)} \int_0^x \frac{1}{\left[1 - \exp\left(-\frac{x}{2\epsilon}\right) \right]^2 + \eta} dx \quad \text{with} \quad F = \int \frac{1}{s^2 + \eta} dx. \quad (10)$$

The significant feature of the fatigue phase field model is to introduce a fatigue driving force $\hat{\sigma}$. The driving force here is not the stress associated with the degradation function, which has turned out to be constant over the whole bar as shown in Eq. 9. The driving force $\hat{\sigma}$ is given as

$$\hat{\sigma} = 2\mu\epsilon = \frac{\bar{\sigma}}{(s^2 + \eta)}. \quad (11)$$

Letting the model parameter $\epsilon = 0.1$ and $\eta = 0.00001$, Fig. 2 shows the pattern of the field values along the right side of the bar with a given displacement load $u_0 = 0.1$. As intended, different from the stress field, which appears constant over the bar, the driving force has a peak value at the crack front ($x = 0$) and almost vanished at the other locations of the bar.

3 Phase Field Fatigue Model with Configurational Forces

Consider a body defined in a stress-free reference configuration C_R . It deforms under mechanical loading and occupies into a new configuration C_r shown in Fig. 3. This transformation can be usually defined by a deformation gradient \mathbf{F} . Let the body be unloaded, the occupying back into the stress-free configuration C'_R can be defined by a reversed deformation gradient \mathbf{f} . If the material of the body is perfectly elastic, the reverse deformation can be formulated as $\mathbf{f} = \mathbf{F}^{-1}$ and the original reference configuration C_R and the stress-free configuration C'_R are identical. However, if irreversible microstructural changes like fatigue cracking are involved during the deformation, the gradients \mathbf{f} and \mathbf{F}^{-1} are close but not the equal. Therefore, a new perspective based on the material manifold but not the spatial coordinates is required, which must provide a unified and elegant framework for the analysis of various kinds of material imperfections like fatigue fracturing.

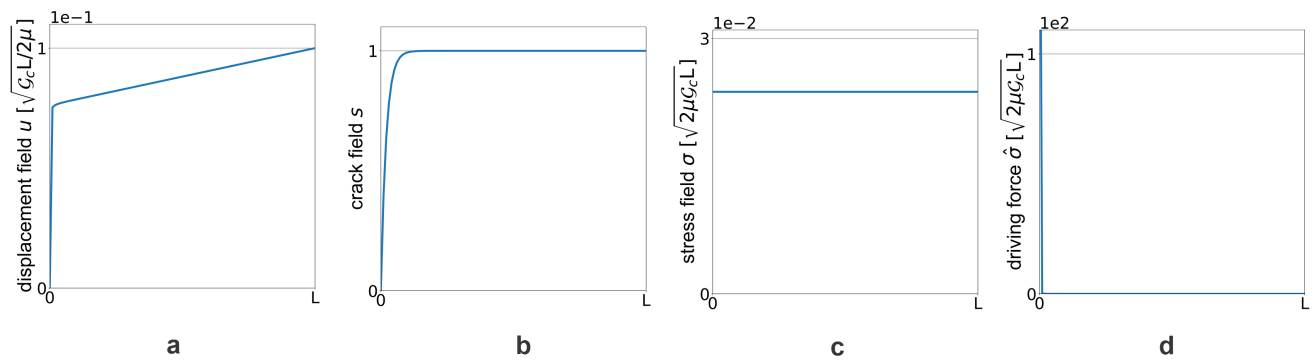


Fig. 2: The field quantities (a: displacement field; b: crack field; c: stress field; d: driving force) of the right side of the bar.

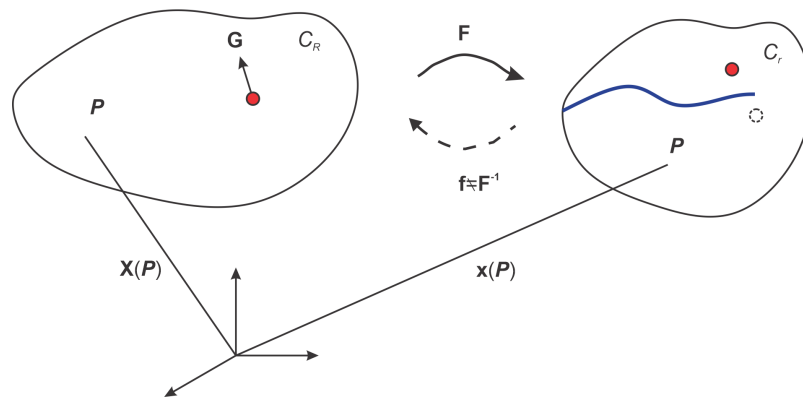


Fig. 3: If crack occurs, the deformation \mathbf{f} and the inverse of the original deformation \mathbf{F}^{-1} are not equal. Configurational force describes the dislocation of material associated with material itself (red point).

Starting point again is the total energy density of the body ψ . Computing the gradient of the extended energy density for fatigue with respect to the displacement field \mathbf{u} , the crack field s , the fatigue damage D , and the location of the crack tip \mathbf{x}^{tip} yields

$$\begin{aligned} \nabla \psi(\varepsilon, s, \nabla s, D, \mathbf{x}^{\text{tip}}) &= \frac{\partial \psi}{\partial \varepsilon} : \nabla \varepsilon + \frac{\partial \psi}{\partial s} \nabla s + \frac{\partial \psi}{\partial \nabla s} \nabla \nabla s + \frac{\partial \psi}{\partial D} \nabla D + \frac{\partial \psi}{\partial \mathbf{x}^{\text{tip}}} \nabla \mathbf{x}^{\text{tip}} \\ &= -\nabla \mathbf{u}^T \nabla \cdot \sigma + \nabla \mathbf{u}^T + \frac{\partial \psi}{\partial s} \nabla s - \nabla \cdot \left(\frac{\partial \psi}{\partial \nabla s} \right) \nabla s + \nabla \cdot \left(\nabla s \frac{\partial \psi}{\partial \nabla s} \right) + \frac{\partial \psi}{\partial \psi^{\text{ad}}} \frac{\partial \psi^{\text{ad}}}{\partial D} \nabla D + \frac{\partial \psi}{\partial \mathbf{x}^{\text{tip}}} \nabla \mathbf{x}^{\text{tip}}. \end{aligned} \tag{12}$$

Noting the equations of the equilibrium of the stress field, the evolution of the crack field and applying partial integration on that, Eq.(12) can be further simplified as

$$\nabla \cdot \left(\underbrace{\psi \mathbf{I} - \nabla \mathbf{u}^T \sigma - \frac{\partial \psi}{\partial \nabla s} \nabla s}_{\Sigma} \right) + \underbrace{\frac{1}{M} \frac{ds}{dN} \nabla s - \frac{\partial \psi}{\partial \psi^{\text{ad}}} \frac{\partial \psi^{\text{ad}}}{\partial D} \nabla D - \frac{\partial \psi}{\partial \mathbf{x}^{\text{tip}}} \nabla \mathbf{x}^{\text{tip}}}_{\mathbf{g}} = \mathbf{0}. \tag{13}$$

This equation gives a configurational force balance

$$\text{div} \Sigma + \mathbf{g} = \mathbf{0}, \tag{14}$$

where Σ is the generalized Eshelby stress tensor and \mathbf{g} is the generalized configurational force. The generalized Eshelby stress tensor captures the local changes as the fatigue fracturing, and the generalized configurational force is the energetic force for the crack evolution.

Noting Eq. (12), the generalized Eshelby stress tensor can be split as

$$\Sigma = \underbrace{(g(s) + \eta) \psi^e \mathbf{I} - \nabla \mathbf{u}^T \sigma}_{\Sigma^e} + \underbrace{\psi^s \mathbf{I} - \frac{\partial [(g(s) + \eta) \psi^e + \psi^s]}{\partial \nabla s} \nabla s}_{\Sigma^s} + \underbrace{h(s) \psi^{\text{ad}} \mathbf{I} - \frac{\partial h(s) \psi^{\text{ad}}}{\partial \nabla s} \nabla s}_{\Sigma^{\text{ad}}} \tag{15}$$

and similarly for the general configurational forces

$$\mathbf{g} = \underbrace{\frac{1}{M} \frac{ds}{dN} \nabla s}_{\mathbf{g}^{\text{dis}}} - \underbrace{\frac{\partial \psi}{\partial \psi^{\text{ad}}} \frac{\partial \psi^{\text{ad}}}{\partial D} \nabla D}_{\mathbf{g}^D} - \underbrace{\frac{\partial \psi}{\partial \mathbf{x}^{\text{tip}}} \nabla \mathbf{x}^{\text{tip}}}_{\mathbf{g}^{\text{tip}}}. \quad (16)$$

Σ^e is the classical Eshelby stress tensor in the case of an undamaged material $s = 1$. The second term Σ^s can be seen as a fracture surface contribution of the generalized Eshelby stress tensor [1]. The last part Σ^{ad} is related to the fatigue part of the generalized Eshelby stress tensor, which is introduced here to provide the necessary fatigue driving forces against fatigue crack self-healing. The dissipative configurational force \mathbf{g}^{dis} represents the energetic forces associated with the energy dissipation during the crack propagation. The contribution \mathbf{g}^D can be interpreted as the energetic fatigue driving force due to the accumulated fatigue damage. The total configurational force acting on the crack tip \mathbf{g}^{tip} stands for a measure of the change of total energy density around the crack tip and as a total energetic driving force for crack propagation.

4 Evaluation of the Phase Field Model on Configurational Forces

Let Ω_0 be a sufficient large domain around the crack tip and \mathbf{n} is the normal vector of the boundary domain $\partial\Omega_0$ as shown in Fig. 4,

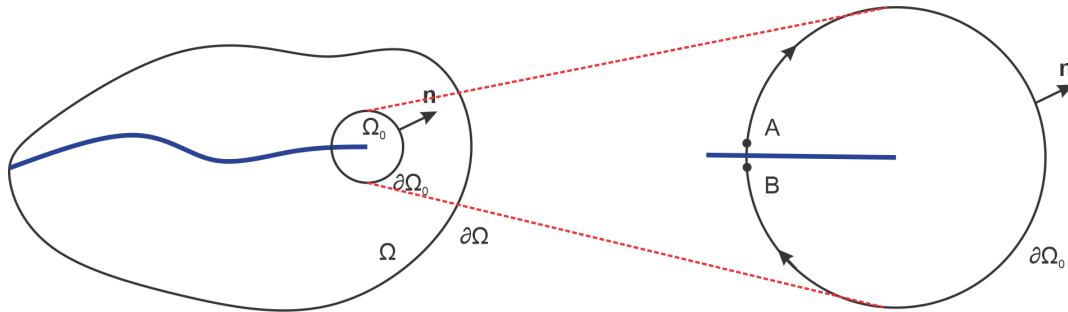


Fig. 4: Assuming $\Omega_0 \subset \Omega$ is a sufficiently large domain around the crack tip and $\partial\Omega_0$ is its boundary.

For a pure mode I loading case, the integral over the control volume for the first term in Eq. (15) can be seen as a elastic part of the general configurational force, which corresponds the negative J -integral, also known as the energy release rate [6].

$$\mathbf{G}^e = - \int_{\partial\Omega_0} \Sigma^e \mathbf{n} dA = - \int_{\partial\Omega_0} \left[\frac{1}{2} (s^2 + \eta) \boldsymbol{\varepsilon} : (\mathbb{C}\boldsymbol{\varepsilon}) \mathbf{I} - \nabla \mathbf{u}^T \boldsymbol{\sigma} \right] \mathbf{n} dA \stackrel{\epsilon \rightarrow 0}{=} - \mathcal{J} \mathbf{e}_x. \quad (17)$$

The J -integral is a measure of the intensity of deformation at a crack tip. As shown in [1], the second part of Eq. (15) is the respective fracture surface part of the total configurational force, equaling the crack resistance \mathcal{G}_c [7]

$$\mathbf{G}^s = - \int_{\partial\Omega_0} \Sigma^s \mathbf{n} dA = - \int_{\partial\Omega_0} \left[\mathcal{G}_c \left(\frac{(1-s)^2}{4\epsilon} + \epsilon |\nabla s|^2 \right) \mathbf{I} - 2\mathcal{G}_c \nabla s \otimes \nabla s \right] \mathbf{n} dA \stackrel{\epsilon \rightarrow 0}{=} \mathcal{G}_c \mathbf{e}_x. \quad (18)$$

The crack resistance stands for an energetic force which acts in the opposite direction of the crack propagation, giving the resistance against crack extension at the crack tip.

For further investigation of the third component in Eq. (15), the entire volume integration over domain Ω_0 is split into two parts (see right side of Fig. 4)

$$\mathbf{G}^{\text{ad}} = - \int_{\partial\Omega_0} \Sigma^{\text{ad}} \mathbf{n} dA = - \int_{\partial\Omega_0|_{A \rightarrow B}} \Sigma^{\text{ad}} \mathbf{n} dA - \int_{\partial\Omega_0|_{B \rightarrow A}} \Sigma^{\text{ad}} \mathbf{n} dA. \quad (19)$$

For the section $A \rightarrow B$, the driving force $\hat{\sigma}$ vanishes outside the crack tip due to the pure mode I load situation as discussed before in Fig. 2; thus, $\int_{\partial\Omega_0|_{A \rightarrow B}} \Sigma^{\text{ad}} \mathbf{n} dA = 0$. The section of $B \rightarrow A$ can be computed with ignoring the damage threshold D_c as

$$\int_{\partial\Omega_0|_{B \rightarrow A}} \Sigma^{\text{ad}} \mathbf{n} dA = \int_{\partial\Omega_0|_{B \rightarrow A}} s^2 \psi^{\text{ad}} \mathbf{I} dx = \int_{\partial\Omega_0|_{B \rightarrow A}} s^2 q \left[\frac{N}{n_D} \left(\frac{\bar{\sigma}}{A_D (s^2 + \eta)} \right)^k \right]^b \mathbf{I} dx. \quad (20)$$

Therefore, the fatigue configurational force is given as

$$\mathbf{G}^{\text{ad}} = \int_{\partial\Omega_0|_{B \rightarrow A}} s^2 q \left[\frac{N}{n_D} \left(\frac{\bar{\sigma}}{A_D (s^2 + \eta)} \right)^k \right]^b \mathbf{I} dx. \quad (21)$$

The fatigue configurational force \mathbf{G}^{ad} is an additional energetic driving force related to fatigue, which acts against the cracks self-recovery.

For the generalized configurational forces, processing to define an integral over the domain Ω_0 of the dissipative part \mathbf{g}^{dis} yields

$$\mathbf{G}^{\text{dis}} = \int_{\Omega_0} \mathbf{g}^{\text{dis}} dV, \tag{22}$$

and of the damage part \mathbf{g}^D yields

$$\mathbf{G}^D = \int_{\Omega_0} \mathbf{g}^D dV \quad \text{with} \quad \mathbf{g}^D = -\frac{\partial \psi}{\partial \psi^{\text{ad}}} \frac{\partial \psi^{\text{ad}}}{\partial D} \nabla D = -h(s)qb < D - D_c >^{b-1} \nabla D \tag{23}$$

Allocating the Eq. (15) and (16) with the above definitions, an energetic balance equation around the crack tip is derived as

$$\mathbf{G}^{\text{tip}} = \mathbf{G}^e + \mathbf{G}^s + \mathbf{G}^{\text{ad}} - \mathbf{G}^{\text{dis}} - \mathbf{G}^D \tag{24}$$

where $\mathbf{G}^{\text{tip}} = \int_{\Omega_0} \mathbf{g}^{\text{tip}} dV$ is the total configuration force acting on the crack tip as the total energetic fatigue driving force.

The x_1 component of different terms \mathbf{G} as shown in Fig. 5. The integration domain needs to be large enough to cover the whole transition zone but not intersect the boundary, where with an integration radius of 6.25ϵ (crack width) the result shows a smooth and constant configurational force profile of the fracture surface part $\mathbf{G}^s \approx 1$. It is noted that the onset of cracking happens when the total configurational forces on the crack tip vanishes ($\mathbf{G}_x^{\text{tip}} = 0$), where the damage part \mathbf{G}^D and fracture surface part \mathbf{G}^s cancel themselves out. The fatigue crack can be observed to propagate faster at the later stage of the simulation, as the total configurational forces \mathbf{G}^{tip} is more often to be zero.

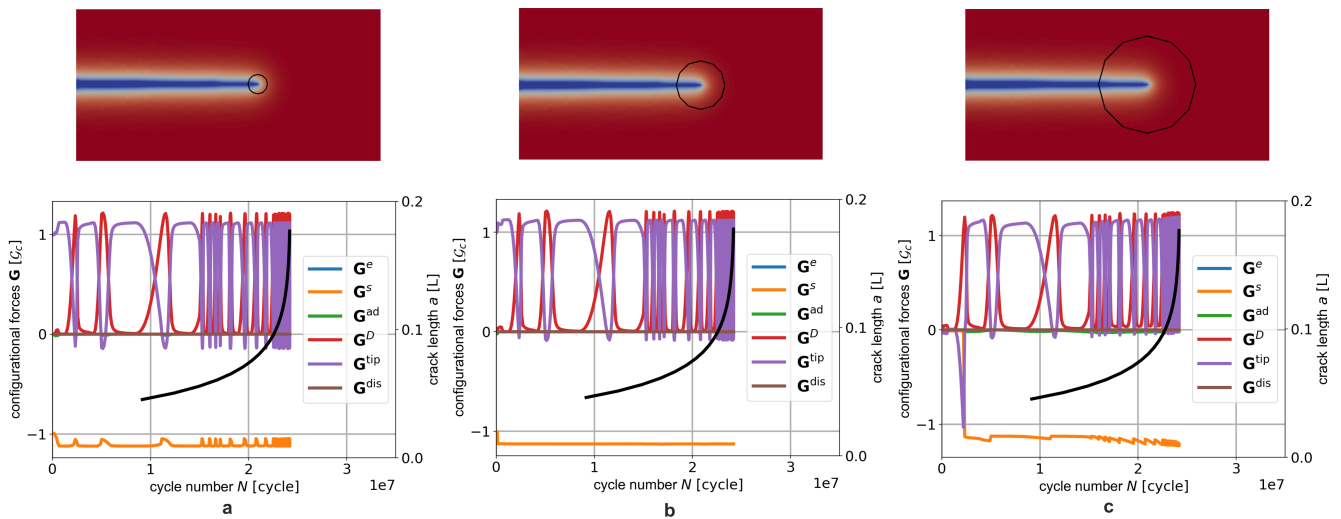


Fig. 5: Configurational force with different integration radius in respect to the length scalar (crack width) ϵ (a: 2.5ϵ ; b: 6.25ϵ ; c: 12.5ϵ). The black line denotes the crack length.

For a detailed illustration, the depicted Fig. 6 are taken from a small number of cyclic domain intervals where the crack only slightly propagates in the right horizontal direction. It can be noticed that the configurational force for the crack tip \mathbf{g}^{tip} are dominated by its horizontal component, which provides the driving force for crack propagation. This part of configurational force reduces from cycle N_1 to N_3 at the previous crack tip, and grows again at the new crack tip from cycle N_3 to N_5 . The vertical direction components provide the energetic force for the crack to widen. However, they vanish during the integral over the domain near the crack tip. The elastic part of the configurational force \mathbf{g}^e is not pronounced, it is because the mechanical loads involved in fatigue scenarios are relatively smaller in contrast to the other fracture cases. The fracture surface part \mathbf{g}^s points in the opposite direction to the crack propagation since it provides the energetic forces to resist the crack growth. Moreover, it reduces during the fracturing (N_1 to N_3) as the fracture resistance decreases due to the broken material. The additional fatigue configurational forces provide additional energetic forces from the fatigue, whose vertical components can be interpreted as the energetic force against the crack self-closure. The damage part \mathbf{g}^D is the energetic force due to the accumulated fatigue damage, which works at the crack propagation direction as an energetic fatigue driving force. At cycle N_3 , the fatigue damage energetic force reaches its maximum value and the total configurational force at the crack tip is zero, enabling the outset of cracking.

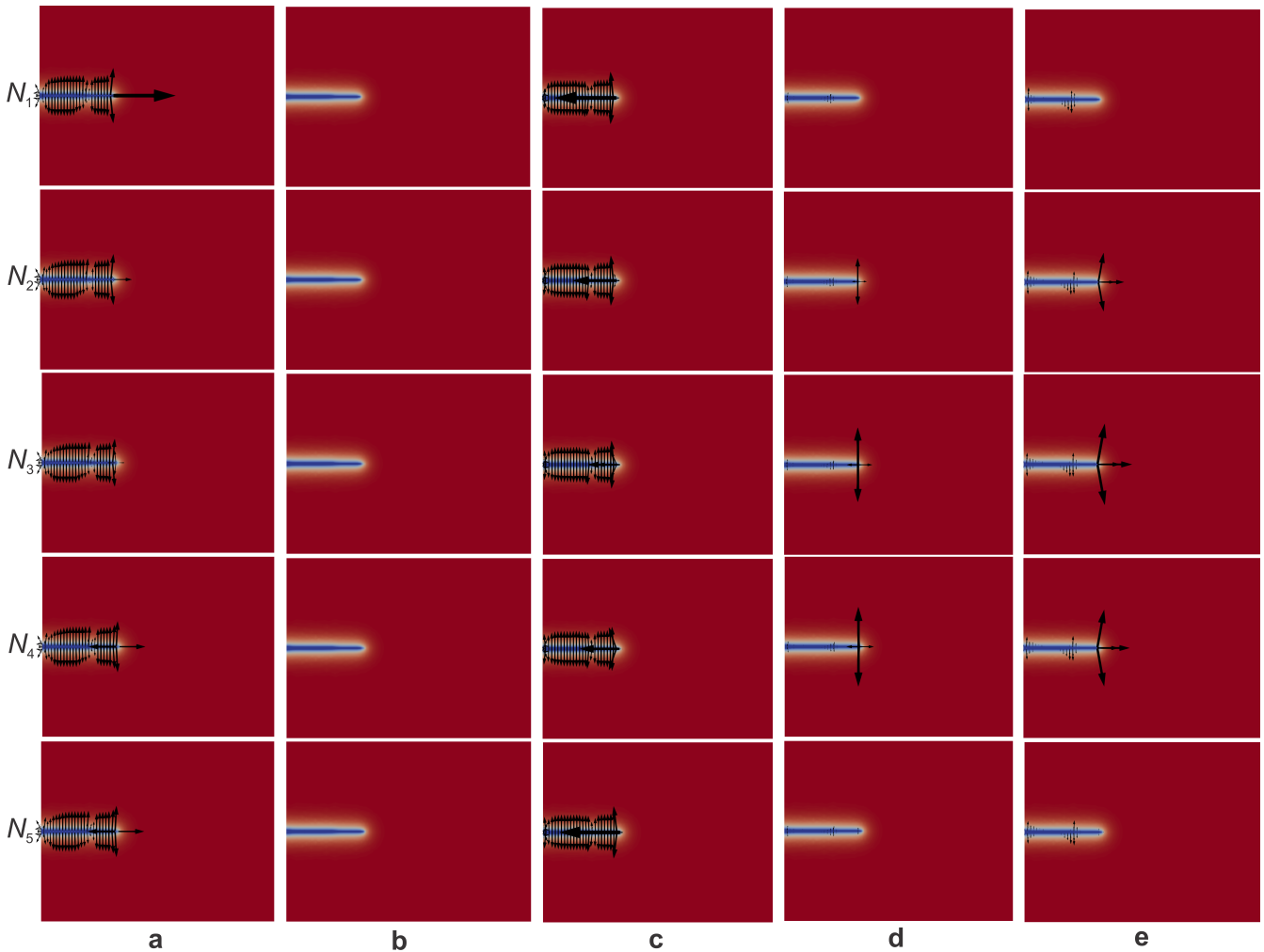


Fig. 6: The configurational forces for crack propagation in a short cycle domains interval at every nodes (**a**: configurational forces at the crack tip \mathbf{g}^{tip} ; **b**: elastic part of the configurational force \mathbf{g}^e ; **c**: fracture surface part of the configurational forces \mathbf{g}^s ; **d**: fatigue part of the configurational forces \mathbf{g}^{ad} ; **e**: damage part of the configurational forces \mathbf{g}^D).

5 Conclusion

In this work, we combine the phase field fatigue model with the concept of configurational forces. By using this tool, our results illustratively explain how the energy components of the total energy density influence the crack evolution.

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