Dependence of Equilibrium Griffith Surface Energy on Crack Speed in Phase-Field Models for Fracture Coupled to Elastodynamics

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Abstract

Phase-field models for crack propagation enable the simulation of complex crack patterns without complex and expensive tracking and remeshing as cracks grow. In the setting without inertia, the crack evolution is obtained from a variational energetic starting point, and leads to an equation for the order parameter coupled to elastostatics. Careful mathematical analysis has shown that this is consistent with the Griffith model for fracture. Recent efforts to include inertia in this formulation have replaced elastostatics by elastodynamics. In this brief note, we examine the elastodynamic augmentation, and find that it effectively causes the Griffith surface energy to depend on the velocity of the crack. That is, considering two identical specimens that are each fractured by a single crack that grows at different velocities in the two specimens, it is expected that the final equilibrium configurations are nominally identical; however, the phase-field fracture models augmented with elastodynamics achieve final configurations – in particular, the Griffiths surface energy contributions – that depend on the crack velocity. The physical reason is that the finite relaxation time for the stresses in the elastodynamic setting enables the cracked region to widen, beyond the value observed in the quasistatic setting. Once the crack widens, the "no-healing" condition prevents it from relaxing even after the specimen reaches equilibrium. In phase-field models, crack width in the reference configuration is unrelated to the physical opening of the crack but is instead a measure of Griffiths surface energy. This observation suggests that elastodynamic phase-field fracture models should not be used in settings where the crack velocity is large.

1 Introduction

Griffith's criterion [Gri21] for crack propagation balances the decrease in elastic energy against the increase in crack surface energy: a pre-existing crack will advance if the total potential energy of the body

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is reduced by doing so, discussed further in [Lip14, Lip16, Fre98] and many other sources. Francfort and Marigo cast this criterion in a rigorous variational setting [FM98]. Building on this, [BFM00, BFM08] developed a regularized phase-field model where cracks are smeared out and are hence amenable to simple numerical methods that do not require the complex and expensive tracking of discontinuities. This approach has been applied and extended to model a wide variety of problems, e.g. [AA12, ZKL16]. Instead of treating the crack as a surface discontinuity, the crack is modeled as a second phase with vanishing elastic energy density, and the interface between the intact material and the second phase is regularized with standard gradient terms. All of the work above was in the context of elastostatics, i.e. without inertia.

Recent efforts to include the effects of inertia have essentially retained the same energetics for the phase field parameter but replaced the elastostatic equation by elastodynamics. An example of such an approach using elastodynamics – in the context of phase field models for twinning rather than fracture – can be found in [AD15a, AD15b]; other approaches start from the Lagrangian that includes the kinetic energy. While this appears to be appropriate in the context of twinning, we describe in this paper why it does not seem to be so for fracture. Briefly, cracks in this class of phase-field models have a finite thickness in the *reference* configuration, and this thickness provides a measure of the Griffith surface energy[1]. Therefore, for the Griffith surface energy to be truly a material parameter related to the energy, every crack must have the same reference width once the body is at equilibrium, regardless of the kinetics of the crack growth. However, in the elastodynamic setting, the stress field takes a finite time to relax to the equilibrium values, and there is a driving force and consequent widening of the crack while this relaxation occurs. In contrast, in the elastostatic setting, which we can loosely consider as the limit of relaxation occurring infinitely quickly, the driving force drops to 0 and crack widening does not go beyond a constant value that is set by the model parameters. Hence, in effect, replacing elastostatics by elastodynamics leads to an unphysical Griffith surface energy that is no longer a material parameter but rather that depends on the crack growth kinetics.

2 Standard Variational Phase-Field Formulation without Inertia

The phase-field formulation, e.g. following [LPM+15], starts with the energy E (up to boundary loads) of the body Ω:

$$E[\boldsymbol{u},\phi] = \int\limits_{\Omega} (\phi^2+\eta_\epsilon) W(\nabla \boldsymbol{u}) \mathrm{d}\Omega + \mathcal{G}_c \int\limits_{\Omega} \left[\frac{(1-\phi)^2}{4\epsilon} + \epsilon |\nabla\phi|^2 \right] \mathrm{d}\Omega \tag{2.1}$$

E is a functional of the displacement $\boldsymbol{u}$ and phase ϕ fields, with $\phi = 1$ corresponding to the intact material and $\phi = 0$ corresponding to the cracked material, and W is the elastic energy density, $\mathcal{G}_c$ is the Griffith surface energy density, and ϵ is a small regularizing parameter that smears out the interfaces due to the term containing $|\nabla\phi|^2$.

The first integral is the standard elastic energy of the intact material, and which goes almost to 0 in the crack; setting it precisely to 0 would cause numerical issues, and hence a small regularization η_ϵ is used. The second integral corresponds to the Griffith surface energy. Unlike standard phase-field models that typically have an explicit multi-well energy density for ϕ, there is only a term that drives ϕ to 1. In the

[1] Note that the crack width in the reference configuration is unrelated to the opening of the crack in the lab / current configuration; rather it is related to the transformation of material particles to the zero-elastic-stiffness second phase.

cracked region where $\phi = 0$, there is an energy cost, and this – together with the term containing $|\nabla\phi|^2$ – provides the energetic cost for the crack corresponding to the Griffith surface energy. However, the first integral provides an energetic cost for $\phi = 1$ when $W(\nabla \boldsymbol{u})$ is large, e.g. when large stresses develop, and therefore it effectively and elegantly induces a 2-well structure.

We note some relevant features of this model for fracture:

- While not immediately apparent, [BFM00,BFM08] show rigorously through variational arguments that the volume integral above recovers the Griffith surface energy contribution when $\epsilon \to 0$.
- The faces of the crack – represented in this setting by regions where $|\nabla\phi| \neq 0$ – are not sharp but have a well-defined thickness related to ϵ.
- As the crack grows, the elastic energy is reduced, and thus lowers the driving force for the crack. Therefore, once the crack faces separate by a distance of order ϵ, the crack does not open further.
- To prevent crack healing, typically a pointwise constraint $\dot{\phi} \leq 0$ is postulated, though a related but simpler condition is used in practice [BFM08].

Elastic equilibrium is obtained from the variation of $E[\boldsymbol{u}, \phi]$ with respect to $\boldsymbol{u}$:

$$\mathbf{0} = \operatorname{div}(\boldsymbol{\sigma}), \qquad \boldsymbol{\sigma} := (\phi^2 + \eta_\epsilon)\frac{\partial W}{\partial(\nabla \boldsymbol{u})} \tag{2.2}$$

where $\boldsymbol{\sigma}$ is the stress.

The driving force f on ϕ is obtained from the variation of $E[\boldsymbol{u}, \phi]$ with respect to ϕ:

$$f = \frac{\delta E}{\delta \phi} = 2\phi W(\boldsymbol{\varepsilon}) + \mathcal{G}_c\left(-\frac{1}{2}\frac{(1-\phi)}{\epsilon} - 2\epsilon\nabla^2\phi\right) \tag{2.3}$$

Setting $f = 0$ provides $\phi = \arg\min_\phi E[\boldsymbol{u}, \phi]$. Crack evolution could alternatively occur through a gradient flow: $\dot{\phi} = -\kappa f$ where κ is the mobility or kinetic coefficient; crack growth occurs only for $f > 0$ due to the irreversibility constraint. The discussion in this paper holds for both evolution statements, though for clarity we focus on the case with $f = 0$ which is more widely applied.

3 Role of Inertia in Setting the Griffith Surface Energy

The dynamic phase-field model with inertia simply replaces elastostatics, $\mathbf{0} = \operatorname{div}(\boldsymbol{\sigma})$, with elastodynamics, $\rho\ddot{\mathbf{u}} = \operatorname{div}(\boldsymbol{\sigma})$. The energy E and equation for ϕ remain the same.

As a specific example, we consider an extremely simple setting of a mode-I crack growing upward due to an applied horizontal load far from the crack (Fig. 1). For the strain energy, we assume a simple linear elastic isotropic solid. The values of the various constants in the energy do not correspond to any specific real material but are only to compare the role of crack velocity when elastodynamics and inertia are considered. The domain is a finite 2D body and displacements are in-plane. The computational domain is has dissipation applied far from the crack to eliminate the effect of wave reflection. We begin the calculations with an existing notch / crack (cracks are not sharp in the phase-field approach). The numerical methods are as described in [AD15b] except that we minimize E with respect to ϕ at every time step rather than use the evolution described there. The details of the numerical method and other parameters are described in Appendix A.

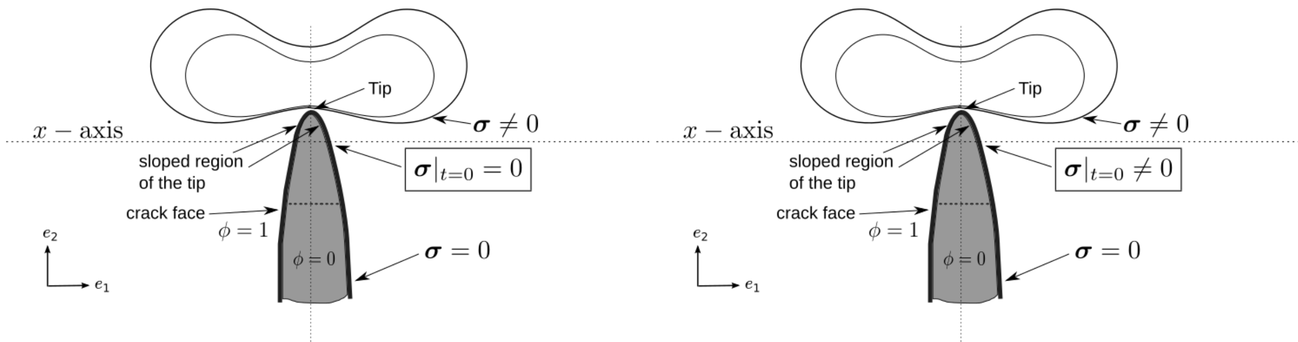

Figure 1: Schematic of stress fields around an advancing crack. Left: Quasistatic stress fields in the near-tip region relax immediately after the crack passes ($t = 0$). Right: Inertial stress fields in the near-tip region take a finite time to relax after the crack passes. Note that $\boldsymbol{\sigma}$ is used as shorthand to represent the traction in the appropriate direction.

In this setting, we compare elastodynamic crack growth at two different crack velocities. Both calculations have identical expressions for the energetics, and the only difference is in the magnitude of applied load that is used to drive the crack at different velocities. As is immediately apparent from Fig. 2, the crack width in the reference configuration is significantly wider when the crack grows faster.

Consider first the setting without inertia. The applied load causes a stress concentration near the tip. The intact regions have a stored elastic energy density, while points within the cracked region have an energy roughly equal to $\mathcal{G}_c$. However, the intact region all along the crack face does not bear a tensile stress because it borders the cracked region (Fig. 1); in a more complex loading scheme, only the relevant traction need vanish. Without inertia, E is minimized with respect to both $\boldsymbol{u}$ and ϕ, and the energy cost of the cracked region keeps it from growing wider since doing so does not further reduce the elastic energy in the unloaded regions. In other words, the driving force $f \leq 0$. This vanishing of the stress on the crack-face is essential to have $f \leq 0$ and prevents the crack from widening into a void.

In the elastodynamic setting, the evolution of $\boldsymbol{u}$ is governed by time-dependent linear momentum balance $\rho\ddot{\mathbf{u}} = \operatorname{div}(\boldsymbol{\sigma})$ and not by energy minimization. Therefore, the stress fields around the advancing crack tip take a finite time to relax to zero. Until the stress fields relax, the system can minimize its energy with respect to ϕ by lateral widening of the crack. This is particularly active in the region directly away from the crack tip but still in the vicinity of the tip. Directly at the tip, there is the crack advance as physically expected, and far from the crack tip the stress fields have reached equilibrium. In other words, the driving force f in this region remains positive until the stress drops below the threshold level such that the strain energy density is lesser than $\mathcal{G}_c$. Until this happens, the crack gets wider.

The final width of the crack is governed by the competition between the elastic wave speed and the crack speed. Considering elastostatics as a limit case where the elastic wave speed is much faster than the crack speed, the stress relaxes immediately; hence, the crack width is independent of the crack speed. In elastodynamics, the large the ratio of crack speed to elastic wave speed, the wider the resulting crack, and the no-healing condition prevents it from shrinking to the correct width corresponding to the Griffith energy. From the discussion of the model formulation, the width of the crack is directly related to the Griffith energy, and therefore the Griffith energy for two samples at equilibrium will depend on the kinetic path to reach equilibrium, i.e. the crack speed.

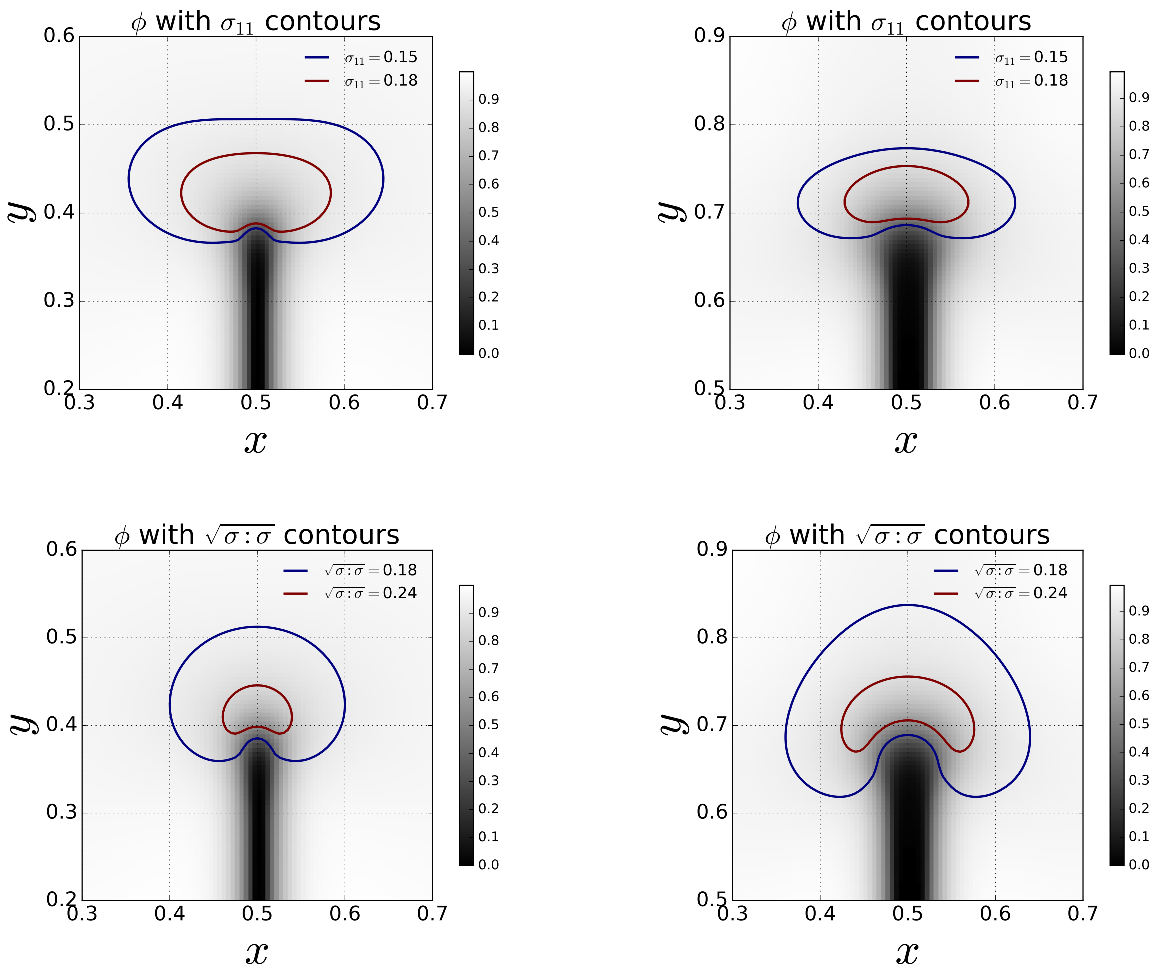

Figure 2: Top row: Crack growth at $M = 0.11$ (left) and at $M = 0.25$ (right) showing the ϕ-field and superposed σ_{11} contours. Bottom row: Crack growth at $M = 0.11$ (left) and at $M = 0.25$ (right) showing the ϕ-field and superposed $\sqrt{\boldsymbol{\sigma} : \boldsymbol{\sigma}}$ contours. The increase in reference crack width and hence Griffith energy with velocity is immediately apparent, as also that the stress fields are different. The no-healing condition prevents this issue from resolving itself once equilibrium is reached, as would occur in standard phase-field elastodynamic models. All stresses are in non-dimensional units with a factor of 10^4.

4 Discussion

Our key observation is that phase-field models of fracture coupled to elastodynamics predict different Griffith fracture energies depending on the velocity of the crack. For instance, consider two specimens that are subject to fracture due to cracks at different velocities but eventually reach an identical unloaded equilibrium state; hence the energy is simply the Griffith surface energy contribution. However, the phase field models for fracture would predict that the Griffith surface energy for these two specimens is different, because the equilibrium phase field solution in the two cases is not identical but depends on the crack velocity. This issue causes considerable error: the error scales as crack area (in 2D), and Fig. 2 shows a change of roughly a factor of 2 when the crack velocity goes from $M = 0.11$ to $M = 0.25$. Further, the issue becomes worse as the velocity increases. This suggests that phase-field models for dynamic fracture that simply couple the variational approach to elastodynamics are unsuitable for fast-growing cracks.

In the language of continuum mechanics, the phase field approach models the crack as an entity that occupies finite volume in the *reference* configuration. This is distinct from the opening width of the crack in the current configuration. The width in the reference configuration is a measure of the region in which material particles satisfy the condition $\phi(\boldsymbol{x}) = 0$ and is unrelated to the displacement field $\boldsymbol{u}$. The width in the current configuration is obtained from the displacement field $\boldsymbol{u}(\boldsymbol{x})$. An idealized crack in classical fracture mechanics has vanishing width in the reference configuration.

Phase-field approaches have been applied to model various phenomena that involve the transformation of material particles from one state to another, e.g. solid-liquid transformations, structural transformations, and so on [SRG17, YD10, ZCD08, CK11, BH16]. In these cases, there are typically two – or more – bulk phases that occupy a finite volume, and the phase-field model regularizes the interface between the phases. Fracture phase-field models however have an important difference. In the context of fracture, the "bulk" phases are the intact and cracked regions, the interface between these is regularized, and material particles transform from intact ($\phi = 1$) to cracked ($\phi = 0$). However, the cracked region is not a bulk phase in reality: in an idealized sharp crack, the crack is represented by a surface in the reference configuration. Hence, the phase-field model for fracture regularizes the crack surface in the reference by a *finite bulk* crack volume, and further regularizes the interface between the cracked region and the uncracked region. This causes phase-field fracture models to be highly sensitive to the elastic evolution as observed here. This is in contrast to standard phase-field models for the phenomena mentioned above, which appear to be robust when coupled to elastodynamics [AD15a, AD15b, PL13].

The finite reference volume of the crack leads to additional difficulties in the dynamic setting. For instance, if the mass density is taken to be independent of time, then the total mass of the body is conserved, but the cracked region consists of material particles with inertia and kinetic energy but zero stiffness, and hence no way to interact with the rest of the body. Alternately, this issue can be resolved if the mass density is taken to scale with ϕ, but then mass disappears as the crack grows. Neither situation is physically appealing; further, these mechanisms occur precisely at the crack tip where they will have the greatest influence on crack growth.

Notwithstanding the objections above to the use of a bulk phase to capture an interfacial region in the phase-field approach, it has been shown to provide the correct results for Griffith surface energy in the static setting [BFM08]. An important additional complication is the no-healing condition. While completely reasonable in that it does not allow cracks to heal, for instance as can occur if the loading conditions are reversed, it also means that dynamically created cracks cannot shrink to the width that provides the correct Griffith surface energy. This is in contrast to standard phase-field models that do not use a no-healing condition and hence are not trapped in states that are not energetically correct.

It has been recognized that the phase-field formulation discussed above can lead to spurious crack growth under compression. While recent papers have attempted to improve this, e.g. by using the spectral decomposition of the strain tensor [MHW10], the issue noted here will appear in those models as well if used in combination with elastodynamics, for the same reasons. That is, the issue that we have highlighted in this paper is not sensitive to the details of the model [2]. Related to this, we note that there can be additional lateral widening of the crack far from the tip if elastic waves (e.g., due to reflection from boundaries) impinge on the crack faces.

The rate-dependence of dynamic fracture is an important physical effect that has been observed in experiments [RR00] and should be captured in modeling. The different levels of dissipation at different loading rates and crack advance velocities will give rise to different temperature and mechanical fields, but once the transient heat transfer and elastodynamics effects die out and the specimens reach equilibrium, we expect that the specimens should be nominally identical. The class of models discussed here show rate-dependence both of the crack kinetics but also of the end state. We believe that perhaps some other evolution statement for ϕ will provide the correct behavior in the dynamical setting, but it is unclear to us how to find this. While the cause is relatively straightforward – a conspiracy between the no-healing condition and the finite relaxation time for stresses in elastodynamics – a good way to avoid this is not obvious: simply removing the no-healing condition would introduce even more unphysical artifacts even in the static setting. We further note that our observations are fairly robust to the specific evolution law: for instance, gradient evolution models with a finite mobility will display the same feature qualitatively, with the widening decreasing with decrease in mobility. Loosely, minimization at each time step as we used can be considered as using infinite mobility, and the other limiting case of extremely small mobility corresponds to the quasistatic limit where the Griffith energy is correctly captured.

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A Numerical Method and Values of Parameters

In the expression for the energy:

$$E[\boldsymbol{u}, \phi] = \int_{\Omega} (\phi^2 + \eta_\epsilon) W(\nabla \boldsymbol{u}) \mathrm{d}\Omega + \mathcal{G}_c \int_{\Omega} \left[\frac{(1-\phi)^2}{4\epsilon} + \epsilon |\nabla \phi|^2 \right] \mathrm{d}\Omega \tag{A.1}$$

we use $\eta_\epsilon = 10^{-8}$, $\mathcal{G}_c = 0.8$, $\epsilon = 10^{-4}$, and linear isotropic elasticity is assumed with Lame constants $\lambda = 10^4$, $\mu = 8 \times 10^3$ in non-dimensionalized units. The mass density is 10^4.

[2] A phase-field formulation for fracture proposed by [KKL01] is popular in some fields for fracture calculations. It is not clear if that model has the deficiency noted here, but it has numerous other problems, e.g. noted in [BLR11], and hence we have not examined it further.

The computational domain is a square of size 1. We define the origin at the bottom left corner. As described in the main text, the initial condition includes a notch – at $x_1 = 0.5$ running from $x_2 = 0$ to $x_2 = 0.15$ – to initiate the growth of the crack. A notch is defined here as a region over which $\phi \approx 0$.

Tractions $\boldsymbol{t}$ are imposed on the left and right boundaries at $t = 0$ to cause tensile elastic waves to initiate and travel towards the center of the domain. The boundary conditions are as follows:

$$x_1 = L \text{ (Right face)} : t_1 = P, t_2 = 0 \tag{A.2}$$
$$x_1 = 0 \text{ (Left face)} : t_1 = -P, t_2 = 0 \tag{A.3}$$
$$x_2 = L \text{ (Top face)} : t_1 = 0, u_2 = 0 \tag{A.4}$$
$$x_2 = 0 \text{ (Bottom face)} : t_1 = 0, t_2 = 0 \tag{A.5}$$
(A.6)

When these waves hit the notch, they cause crack growth to commence. We have used $P = 750$ and $P = 1000$ to get the different crack speeds described in the main document. The displacement at $(x_1, x_2) = (L/2, L)$ is set to zero to prevent rigid-body translations in the 1 direction.

For the time evolution of the momentum equation, we use finite differences in time with an explicit central difference scheme; this is a standard approach for elastodynamics. In the particular context of phase-field fracture approaches, a related Newmark method is used by [BRLM16]. The time step used is $\Delta t = 5 \times 10^{-5}$ for the material parameters above.

The spatial discretization uses standard finite elements with uniform rectangular elements and piecewise-linear shape functions for $\boldsymbol{u}$ and ϕ. There are 200 elements in both directions.

At each time step, we minimize with respect to ϕ. The minimization is performed using a gradient descent algorithm. To satisfy the irreversibility constraint (“no healing”), following [BLR11], we perform the minimization while restricting $\phi = 0$ on the set where $\phi < \phi_0$ with $\phi_0 = 0.01$.

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