PHASE FIELD MODEL FOR MODE III CRACK GROWTH IN TWO DIMENSIONAL ELASTICITY

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A phase field model for anti-plane shear crack growth in two dimensional isotropic elastic material is proposed. We introduce a phase field to represent the shape of the crack with a regularization parameter $\epsilon > 0$ and we approximate the Francfort–Marigo type energy using the idea of Ambrosio and Tortorelli. The phase field model is derived as a gradient flow of this regularized energy. We show several numerical examples of the crack growth computed with an adaptive mesh finite element method.

Keywords: crack growth, phase field model, numerical simulation

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1. CRACK GROWTH MODEL

We propose the following mathematical model for the mode III (anti-plane shear mode) crack growth in an elastic plate. Let Ω be a bounded two dimensional domain with a piecewise smooth boundary Γ , and let Γ_D be a nonempty open portion of Γ which consists of a finite number of connected components. We define $\Gamma_N := \Gamma \setminus \Gamma_D$. For t > 0, we consider the equations:

$$\begin{aligned} \alpha_{1} \frac{\partial u}{\partial t} &= \operatorname{div} \left((1-z)^{2} \nabla u \right) & x \in \Omega, \\ \alpha_{2} \frac{\partial z}{\partial t} &= \left(\varepsilon \Delta z - \frac{\gamma^{2}}{\varepsilon} z + |\nabla u|^{2} (1-z) \right)_{+} & x \in \Omega, \\ u(x,t) &= g(x,t) & x \in \Gamma_{D} \\ \frac{\partial u}{\partial n} &= 0 & x \in \Gamma_{N}, \\ \frac{\partial z}{\partial n} &= 0 & x \in \Gamma, \\ \zeta + \operatorname{I.C.} (2) & x \in \Omega, \end{aligned}$$
(1)

where u(x,t) represents the small anti-plane displacement at the position $x \in \overline{\Omega}$ and time $t \ge 0$, and g(x,t) is a given anti-plane displacement on the boundary Γ_D . The variable z(x,t) satisfies $0 \le z(x,t) \le 1$ in Ω and represents the crack shape, as $z \approx 0$ in the region without crack and $z \approx 1$ near the crack. The minimum length scale of z is given as $O(\varepsilon)$ with a small regularization parameter $\varepsilon > 0$. The function z(x,t) is called the phase field for the crack shape. For stable numerical simulations, we also introduce small time relaxation parameters $\alpha_1 \ge 0$ and $\alpha_2 > 0$. The initial conditions for (1) are given as follows:

$$\begin{cases} u(x,0) = u_0(x) & x \in \Omega \quad (\text{omitted if } \alpha_1 = 0), \\ z(x,0) = z_0(x) \in [0,1] & x \in \Omega, \end{cases}$$
(2)

The first equation of (1) expresses the force balance in the uncracked region $(z \approx 0)$, and the second equation expresses the crack evolution due to the modulus of the stress $|\nabla u|$. The material constant $\gamma > 0$ is called the fracture toughness, which prescribes the critical value of the energy release rate in the Griffith's criterion. It is harder for the crack to grow, if the value of γ is larger.

A crack once generated can be no longer repaired. We put ()₊ to the right hand side of the second equation, where $(a)_{+} = \max(a, 0)$. It guarantees the non-repair condition for the crack: $\frac{\partial z}{\partial t} \ge 0$.

The derivation of this mathematical model is shown in Section 2, and some computational results will be given in Section 3.

2. DERIVATION OF THE MODEL

We consider a crack propagation in a plate by the deformation perpendicular to the plate. Let Ω be a bounded two dimensional domain as described in Section 1 We denote by $x = (x_1, x_2) \in \mathbb{R}^2$ a Cartesian coordinate parallel to the plate, and by x_3 the coordinate perpendicular to the plate. The plate is supposed to be an isotropic elastic material with a constant thickness and is treated as a two dimensional domain Ω .

We consider a crack in Ω , which is denoted by a closed subset $\Sigma \subset \Omega$. We assume that the deformation of the plate is limited to the x_3 -direction, and the anti-plane displacement is denoted by $u(x) \in \mathbb{R}$ for $x \in \Omega \setminus \Sigma$. In the case that the speed of the crack evolution is very slow, we can apply the quasi-static assumption that the following equations are valid for every fixed t:

$$\begin{aligned}
\zeta & -\mu\Delta u &= f \quad \text{in} \quad \Omega \setminus \Sigma, \\
u &= g \quad \text{on} \quad \Gamma_D, \\
\mu \frac{\partial u}{\partial n} &= h \quad \text{on} \quad \Gamma_N, \\
\frac{\partial u^{\pm}}{\partial n} &= 0 \quad \text{on} \quad \Sigma^{\pm},
\end{aligned}$$
(3)

where f(x) is a given external load perpendicular to the plate on Ω , g(x) is a given anti-plane displacement on Γ_D , and h(x) is a given boundary load in the x_3 -direction on Γ_N . The outward normal derivative on the boundary of $\Omega \setminus \Sigma$ is denoted by $\frac{\partial}{\partial p}$. In particular, $\frac{\partial u^+}{\partial n}$ and $\frac{\partial u^-}{\partial n}$ stand for the outward normal derivatives of u on the sides Σ^+ and Σ^- , respectively, where the both sides of the crack Σ are denoted by Σ^+ and Σ^- . The parameter $\mu > 0$ is the rigidity, which is one of the Lamé constants.

The solution u to (3) is obtained as a unique minimizer of the following elastic potential energy including the external loads:

$$E_1(v, \Sigma) = \frac{\mu}{2} \int_{\Omega \setminus \Sigma} |\nabla v|^2 \, \mathrm{d}x - \int_{\Omega} f v \, \mathrm{d}x - \int_{\Gamma_N} h v \, \mathrm{d}s \qquad (v \in V(g, \Omega \setminus \Sigma)) \,,$$

where $V(g, \Omega \setminus \Sigma) := \{ v \in H^1(\Omega \setminus \Sigma); v = g \text{ on } \Gamma_D \}$. We have assumed that $g = \tilde{g}|_{\Gamma_D}$ with $\tilde{g} \in H^1(\Omega)$ and that $h \in L^2(\Gamma_N)$.

According to the classical theory of brittle fracture by A. A. Griffith [8], the elastic energy which is released along the crack evolution is the source of energy supply for creating new crack. Francfort–Marigo [7] proposed the following energy based on the Griffith's theory:

$$\begin{cases} E(\Sigma) = E_1(u, \Sigma) + E_2(\Sigma), \\ E_1(u, \Sigma) = \min_{v \in V(g, \Omega \setminus \Sigma)} E_1(v, \Sigma) & (u \in V(g, \Omega \setminus \Sigma)), \\ E_2(\Sigma) := \int_{\Sigma} \gamma(x) \, \mathrm{d}s. \end{cases}$$
(4)

The total energy of our system E, which we call free energy in the analogy of the time dependent Ginzburg–Landau (TDGL) theory or the phase field model approach ([11] etc.), is given by sum of the elastic potential energy E_1 over $\Omega \setminus \Sigma$ and a surface energy E_2 on the crack. At a time t, the bulk energy $E_1(u, \Sigma)$ which is generated by the strain of the elastic plate is given as the minimum potential energy of E_1 .

Let us suppose that a crack Σ grows and becomes $\tilde{\Sigma}(\supset \Sigma)$. Since $V(g, \Omega \setminus \Sigma) \subset V(g, \Omega \setminus \tilde{\Sigma})$,

$$E_1(u, \Sigma) = \min_{v \in V(g, \Omega \setminus \Sigma)} E_1(v, \tilde{\Sigma}) \ge \min_{v \in V(g, \Omega \setminus \tilde{\Sigma})} E_1(v, \tilde{\Sigma}) = E_1(\tilde{u}, \tilde{\Sigma}),$$

holds. The released potential energy $E_1(u, \Sigma) - E_1(\tilde{u}, \tilde{\Sigma}) \ge 0$ along the crack growth from Σ to $\tilde{\Sigma}$ is used to reduce the surface energy E_2 depending on the fracture toughness $\gamma(x) > 0$.

In [7], they proposed a mathematical model for crack growth with this energy and studied it in detail. In practical numerical computation, however, we have the following numerical difficulties: 1) numerical treatment of stress concentration at the crack tip (i.e. $|\nabla u| = \infty$), 2) no explicit formula for crack path determination, 3) numerical treatment of crack initiation or subcrack, 4) numerical task to remesh $\Omega \setminus \Sigma(t)$ for the finite element method or other numerical methods.

In order to represent the crack shape, we consider a phase field z(x), which satisfies $z \approx 1$ around the crack and $z \approx 0$ for the other region. Introducing a sufficiently small spatial regularization parameter $\epsilon > 0$, we suppose that the crack has $O(\epsilon)$ thickness. Let $\mathcal{E}_1(u, z)$ and $\mathcal{E}_2(z)$ be approximations of the bulk energy $E_1(u, \Sigma)$ and the surface energy $E_2(\Sigma)$, respectively. Using the idea of Ambrosio– Tortorellio [1], we consider the following regularized energy which depends on the anti-plane displacement $u \in V(g, \Omega)$ and the phase field for the crack shape $z \in$ $H^1(\Omega)$ with $0 \leq z(x) \leq 1$:

$$\begin{cases} \mathcal{E}(u,z) := \mathcal{E}_1(u,z) + \mathcal{E}_2(z), \\ \mathcal{E}_1(u,z) := \frac{\mu}{2} \int_{\Omega} (1-z)^2 |\nabla u|^2 \, \mathrm{d}x - \int_{\Omega} f u \, \mathrm{d}x - \int_{\Gamma_N} (1-z)^2 h u \, \mathrm{d}s, \\ \mathcal{E}_2(z) := \frac{1}{2} \int_{\Omega} \gamma(x) \left(\epsilon |\nabla z|^2 + \frac{1}{\epsilon} z^2\right) \mathrm{d}x. \end{cases}$$
(5)

In [1], it is mathematically proved that this energy approximates (4) if $\epsilon \to 0$ in the sense of Γ -convergence.

We suppose that the given external force f, h and the given boundary displacement g changes slowly in time and that u and z approach to the (quasi-)equilibrium state in relatively smaller time scales. In the TDGL theory or the phase field approach, the dynamics near equilibrium of a system is described by the gradient flow of the free energy (see [11] etc.). In general, for a free energy F(u), its gradient flow is given by $\alpha \frac{\partial u}{\partial t} = -\frac{\delta F}{\delta u}$, where $\alpha > 0$ is a suitable time constant and $\frac{\delta F}{\delta u}$ is the first variation of F with respect to u.

Suppose that $\Gamma_N = \Gamma_N^0 \cup \Gamma_N^1, \Gamma_N^0 \cap \Gamma_N^1 = \emptyset$ and that h = 0 on Γ_N^0 . We assume that h may not vanish on Γ_N^1 and the crack does not touch the boundary Γ_N^1 . We assume the following conditions:

$$\begin{cases} u = g & \frac{\partial z}{\partial n} = 0 \quad \text{on} \quad \Gamma_{\rm D}, \\ \mu \frac{\partial u}{\partial n} = h = 0 \quad \frac{\partial z}{\partial n} = 0 \quad \text{on} \quad \Gamma_{\rm N}^{0}, \\ \mu \frac{\partial u}{\partial n} = h & z = 0 \quad \text{on} \quad \Gamma_{\rm N}^{1}. \end{cases}$$
(6)

Under these assumptions, the gradient flow of the energy (5) with respect to u becomes

$$\alpha_1 \frac{\partial u}{\partial t} = \mu \operatorname{div} \left((1-z)^2 \nabla u \right) + f.$$
(7)

We remark that $\alpha_1 = 0$ corresponds to the original quasi-static assumption in (3) and the case with $0 < \alpha_1 \ll 1$ is considered as its natural approximation. Actually, in case of $\alpha_1 = 0$, the elliptic equation degenerates if z = 1 and a small time constant $\alpha_1 > 0$ is effective to stabilize its numerical computation.

Similarly, under these conditions we have the gradient flow for z(x,t) with a suitable time constant $\alpha_2 > 0$:

$$\alpha_2 \frac{\partial z}{\partial t} = \epsilon \operatorname{div}\left(\gamma(x)\nabla z\right) - \frac{\gamma(x)}{\epsilon} z + \mu |\nabla u|^2 (1-z).$$
(8)

Summarizing (7) and (8), we obtain the following phase field model for crack growth:

$$\begin{cases} \alpha_1 \frac{\partial u}{\partial t} = \mu \operatorname{div} \left((1-z)^2 \nabla u \right) + f(x,t) & x \in \Omega, \\ \alpha_2 \frac{\partial z}{\partial t} = \left(\epsilon \operatorname{div} \left(\gamma(x) \nabla z \right) - \frac{\gamma(x)}{\epsilon} z + \mu |\nabla u|^2 (1-z) \right)_+ & x \in \Omega, \\ + \text{ B.C. (6)}, \\ + \text{ I.C. (2)}. \end{cases}$$
(9)

In the second equation, to guarantee the non-repair condition for the crack $(\frac{\partial z}{\partial t} \ge 0)$, we have modified (8) as $\alpha_2 \frac{\partial z}{\partial t} = (\cdots)_+$, where $(a)_+ = \max(a, 0)$. A class of such evolution equations with constraint is studied mathematically in [13] etc. Similar approaches to compute the Francfort–Marigo model with regularized energy are found in [2, 3, 4, 5] etc. We remark that the energy of this system satisfies the gradient flow structure as $\frac{d}{dt} \mathcal{E}(u, z) = -\int_{\Omega} (\alpha_1 |u_t|^2 + \alpha_2 |z_t|^2) dx$ when h, f and g are constant in time.

In (9), setting $\Gamma_N^0 = \Gamma_N$, f = 0, $\gamma(x) \equiv \gamma > 0$, $\mu = 1$ and replacing $\epsilon \gamma$ by ε , we obtain (1). This model no longer has any numerical difficulties for computer simulation. Several numerical results is shown in the next section.

3. NUMERICAL SIMULATION

For our numerical simulation, we used an adaptive mesh finite element solver for reaction diffusion systems [9, 10] with an adaptive mesh FEM toolbox ALBERTA [12].

Let $u^k(x)$ and $z^k(x)$ be approximations of u and z at $t = k\tau$ $(k = 0, 1, 2, \cdots)$, respectively, with time increment $\tau > 0$. To obtain u^k and z^k from u^{k-1} and z^{k-1} , we adopt the following implicit scheme for the first two equations of (9):

$$\begin{cases} \alpha_{1} \frac{u^{k} - u^{k-1}}{\tau} = \mu \operatorname{div} \left((1 - z^{k-1})^{2} \nabla u^{k} \right), \\ \alpha_{2} \frac{\tilde{z}^{k} - z^{k-1}}{\tau} = \epsilon \operatorname{div} \left(\gamma(x) \nabla \tilde{z}^{k} \right) - \frac{\gamma(x)}{\epsilon} \tilde{z}^{k} + \mu |\nabla u^{k-1}|^{2} (1 - \tilde{z}^{k}), \\ z^{k} = \max(\tilde{z}^{k}, z^{k-1}). \end{cases}$$
(10)

The condition $\tilde{z}^k \in [0, 1]$ is derived by the maximum principle of elliptic equations for \tilde{z}^k , and it leads $z^k \in [0, 1]$. In this paper, we adapt this simple scheme (10) with sufficiently small τ . But it will be interesting to apply the projected SOR method ([6] etc.) to the second equation of (9) for more accurate computation.

We solve (10) by using the adaptive mesh FEM with P1 elements and adaptive time step control (see [9, 10]). In the following simulations, we put $\epsilon = 10^{-3}$, $\alpha_1 = 0$, $\alpha_2 = 10^{-3}$ in (9), and set the computational domain as $\Omega = (-1, 1) \times (-1, 1)$ with

 $\Gamma_D = \{(x_1, x_2) | x_1 \in (-1, 1), x_2 = \pm 1, \}$. The boundary condition for u is given by $g(x, t) = 10x_2t$ for $x \in \Gamma_D$ and $t \ge 0$.

We consider four cases with different γ and $z_0(x)$. We set the fracture toughness γ is constant in the first three cases, and consider variable $\gamma = \gamma(x)$ in the last case.

	$\max(\text{mesh number})$	$\min(\text{mesh size})$	$\min(au)$	$\max(\tau)$
i)	8192	0.005524	0.001477	0.089005
ii)	40824	0.001953	0.001407	0.066417
iii) (a)	18496	0.002762	0.001477	0.063254
iii) (b)	17788	0.002762	0.001477	0.069738
iv) (a)	128856	0.001953	0.001407	0.088783
iv) (b)	114264	0.000691	0.001407	0.098128

Table. Computational data on adaptive mesh.

Table shows the computational data on adaptive mesh for these numerical simulations.

i) One crack ($\gamma = 0.5$)

We set one straight crack in the plate at t = 0. For the initial condition for z, we define $z_0(x) := \zeta_0(x_1 + 0.5, x_2)$ where $\zeta_0(x) := e^{-(x_2/\delta)^2}(1 + e^{x_1/\delta})^{-1}$ with $\delta = 0.1$. (In the other simulations ii) – iv), their initial conditions are also defined similarly with suitable shift and superposition of the above $\zeta_0(x)$.) We can see that the crack grows straight and reaches the right-hand side boundary (Figure 1).

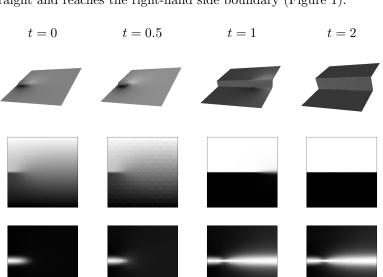


Fig. 1. Birdviews of u(top), u (middle) and z (bottom).

ii) Two cracks in the same direction $(\gamma = 0.5)$

At t = 0 we set two cracks on the left-hand side boundary with the same length. If the length is long enough, they reach to the right-hand side boundary. They, however, merge into one crack when the length of the two cracks is not enough long (Figure 2).

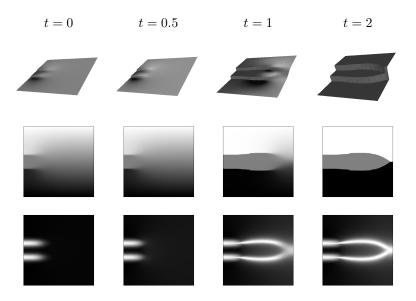


Fig. 2. Birdviews of u(top), u (middle) and z (bottom) in the temporal evolution of the cracks when initial length of cracks is 0.5.

iii) Two cracks in the alternated directions ($\gamma = 0.5$).

When we set two cracks that one starts from the left-hand side boundary and another starts from the right-hand side boundary, then crack growth patterns are classified in three cases. Only when the initial cracks are sufficiently long, they reach the opposite boundaries (Figure 3(a)). If we set sufficiently short cracks in alternative directions, as we can easily imagine, they reach and connect to each other. But, in some middle length case, a subcrack (side-branched crack) appears (Figure 3(b)).

iv) One crack with variable fracture toughness $(\gamma = \gamma(x))$.

We show the results of two cases that the fracture toughness varies in the plane. The crack is going to the straight way, however, on the way to another side the front of crack find the weak (small toughness) point and turn into there. We set γ as (a) a checkerboard pattern ($\gamma(x) = 0.5(1 + 0.2 \cos 10x \cdot \cos 10y)$) and (b) a stripe pattern ($\gamma(x) = 0.5(1 + 0.2(\cos 10x + \cos 10y))$). Figure 4 shows that the crack propagates to the right-hand side boundary through the weaker points of γ .

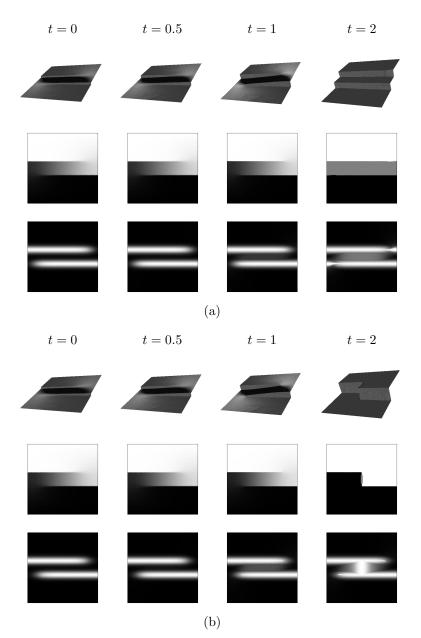


Fig. 3. Birdviews of u(top), u (middle) and z (bottom) in the temporal evolution of the cracks with initial cracks of length (a) 1.8 and (b) 1.7.

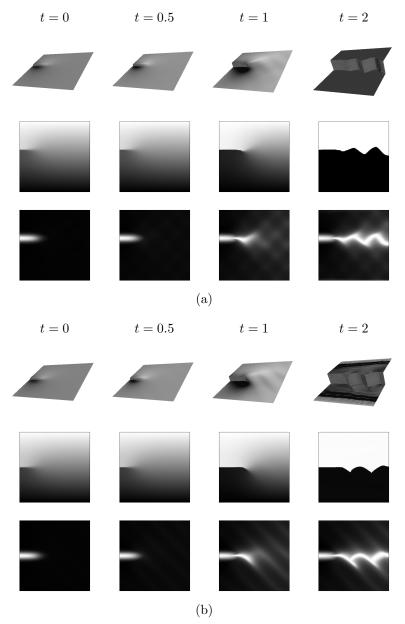


Fig. 4. Birdviews of u(top), u (middle) and z (bottom) in the temporal evolution of the cracks when (a) $\gamma(x) = 0.5(1 + 0.2 \cos 10x \cdot \cos 10y)$ and (b) $\gamma(x) = 0.5(1 + 0.2(\cos 10x + \cos 10y))$.

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REFERENCES

- L. Ambrosio and V. M. Tortorelli: On the approximation of free discontinuity problems. Boll. Un. Mat. Ital. 7 (1992), 6-B, 105–123.
- [2] B. Bourdin: The variational formulation of brittle fracture: numerical implementation and extensions. Preprint 2006, to appear in IUTAM Symposium on Discretization Methods for Evolving Discontinuities (T. Belytschko, A. Combescure, and R. de Borst eds.), Springer.
- B. Bourdin: Numerical implementation of the variational formulation of brittle fracture. Interfaces Free Bound. 9 (2007), 411–430.
- [4] B. Bourdin, G.A. Francfort, and J.-J. Marigo: Numerical experiments in revisited brittle fracture. J. Mech. Phys. Solids 48 (2000), 4, 797–826.
- [5] M. Buliga: Energy minimizing brittle crack propagation. J. Elasticity 52 (1998/99), 3, 201–238.
- [6] C. M. Elliott and J. R. Ockendon: Weak and Variational Methods for Moving Boundary Problems. Pitman Publishing Inc. 1982.
- [7] G. A. Francfort and J.-J. Marigo: Revisiting brittle fracture as an energy minimization problem. J. Mech. Phys. Solids 46 (1998), 1319–1342.
- [8] A. A. Griffith: The phenomenon of rupture and flow in solids. Phil. Trans. Royal Soc. London A 221 (1920), 163–198.
- [9] M. Kimura, H. Komura, M. Mimura, H. Miyoshi, T. Takaishi, and D. Ueyama: Adaptive mesh finite element method for pattern dynamics in reaction-diffusion systems. In: Proc. Czech–Japanese Seminar in Applied Mathematics 2005 (M. Beneš, M. Kimura, and T. Nakaki, eds.), COE Lecture Note Vol. 3, Faculty of Mathematics, Kyushu University 2006, pp. 56–68.
- [10] M. Kimura, H. Komura, M. Mimura, H. Miyoshi, T. Takaishi, and D. Ueyama: Quantitative study of adaptive mesh FEM with localization index of pattern. In: Proc. of the Czech–Japanese Seminar in Applied Mathematics 2006 (M. Beneš, M. Kimura, and T. Nakaki, eds.), COE Lecture Note Vol. 6, Faculty of Mathematics, Kyushu University 2007, pp. 114–136.
- [11] R. Kobayashi: Modeling and numerical simulations of dendritic crystal growth. Physica D 63 (1993), 410–423.
- [12] A. Schmidt and K. G. Siebert: Design of Adaptive Finite Element Software. The Finite Element Toolbox ALBERTA (Lecture Notes in Comput. Sci. Engrg. 42.) Springer– Verlag, Berlin 2005.
- [13] A. Visintin: Models of Phase Transitions. Birkhäuser-Verlag, Basel 1996.

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