Development and application of a grain-based hybrid finite-discrete element method for investigating fracture processes of heterogeneous rocks under static and dynamic loads

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ABSTRACT: A both two- and three-dimensional grain-based hybrid finite-discrete element method (HFDEM-GB2D/3D) is developed and parallelized on the basis of the general-purpose graphic-processing-units. It is then calibrated by modelling the failure process of heterogeneous rocks in uniaxial compression tests. After that, it is applied to investigate the dynamic fracture process of heterogeneous rocks in triaxial Hopkinson bar tests. It is concluded that HFDEM-GB2D/3D can consider the actual microstructures of heterogeneous rocks to investigate the intra-, trans- and inter-granular crack propagations besides modelling the failure process of heterogeneous rocks.

Keywords: Grain-based modelling, FDEM, intergranular failure, trans-granular failure, rock fracture, heterogeneity.

1 INTRODUCTION

Heterogeneity is a material fabric characteristic that should be better understood in terms of its role in influencing the fracture progression process. In recent years, the grain-scale heterogeneities of rocks have been characterized using various methods, including statistical methods such as Weibull's distribution and grain-based methods. It is generally agreed (Yahaghi et al., 2023) that grain-based methods can better characterize some microstructure properties of rocks and address their effects on the macroscopic behaviors, bulk properties and failure processes of rocks, although grain-based methods are much more time-consuming than statistical methods. However, rock microstructures are complex and include more properties than those considered in the currently available grain-based methods, such as the grain morphology, grain size and spatial distribution, crystallographic anisotropy and orientation, elastic properties and interface properties. Thus, it is of fundamental importance to incorporate more if not all important microstructure properties of rocks when investigating the macroscopic responses (e.g., a complete stress–strain curve), localized microscopic cracking nucleation, coalescence and propagation, the entire failure processes of these rocks and their sensitivities to the presence of bedding planes, flaws, pores, and cavities inherent in the rocks. This paper aims to propose both a two- and three-dimensional grain-based hybrid finite-discrete element method (HFDEM-GB2D/3D) parallelized based on general-purpose graphic-processing-unit for investigating the inter-, intra- and trans-granular failures of heterogeneous rocks under static and dynamic loads.

2 GRAIN-BASED HYBRID FINITE-DISCRETE ELEMENT METHOD

The both two- and three-dimensional grain-based hybrid finite-discrete element method is developed by incorporating granular-scale heterogeneities including polycrystal grains to be generated using open-source software Neper (Quey et al., 2011) into an in-house hybrid finite-discrete element method (Liu et al., 2015) parallelized based on general-purpose graphic-processing-units (GPGPU) (Fukuda et al., 2020).

HFDEM was initially developed by the authors (Liu et al., 2015) using Visual C++ and OpenGL on the basis of the open-source Y libraries (Munjiza, 2004), which had been calibrated by simulating a series of fundamental rock mechanics tests, joint shearing tests and near-surface rock blasting tests and become a valuable numerical tool to investigate rock fracture. To overcome the limitation of sequential programming and achieve a reasonable simulation time for 3D modelling, HFDEM has been parallelized by the authors (Fukuda et al., 2020) using a compute unified architecture device (CUDA) C/C++ to run on GPGPU for both 2D and 3D simulations. Subsequently, the GPGPU-parallelized HFDEM can run in a completely parallel manner on GPGPU devices, and no sequential processing is necessary except for the input and output procedures. The simulation results can be visualized using both open-source visualization software such as Paraview and the built-in postprocessor of HFDEM. To facilitate large-scale modelling, the visualization module of HFDEM is separated from the computing module, so HFDEM can run on ordinary workstations based on the windows operation system or high-performance servers/supercomputers based on Linux operation systems. After that, various novel, useful and efficient features including semi-adaptive contact activation approach, local damping and contact damping and elasto-plastic material model have recently been implemented into GPGPU-parallelized HFDEM. This has been applied to model triaxial compressions, deep tunnelling under high in-situ stress, rock cutting, dynamic fracture under impact loads, rock bursts, destress blasting and freeze-thaw tests.

In HFDEM-GB, polygon- or polyhedral-based grains of the target rock are first generated using the open-source Neper software (Quey et al., 2011), as a powerful tool for polycrystal generation and meshing and can generate multiscale tessellations. It can generate tessellations with the Voronoi and grain-growth methods, although most of the previous studies used the Voronoi tessellation method. The grain-growth tessellation method can generate grains with wider grain size distributions and higher grain sphericities, but it takes a longer time to generate grains than the Voronoi tessellation method, which greatly affects the simulation time step size, as later discussed by Yahaghi et al. (2023). To reduce the simulation time, the regularization method is available in Neper to remove the small edges and faces. The generated mesh information is imported as an input to the FDEM simulation of the rock failure process.

3 GRAIN-BASED MODELLING OF FRACTURE PROCESS OF HETEROGENEOUS ROCKS UNDER STATIC AND DYNAMIC LOADS

Three examples are presented in this section to demonstrate the grain-based modelling of the fracture process of heterogenous rocks under static and dynamic loads, which include uniaxial compression tests modelled in both 2D and 3D using HFDEM-GB and triaxial Hopkinson bar tests under combined static and dynamic loads using HFDEM-GB3D.

3.1 Grain-based 2D and 3D modelling of rock failures in uniaxial compression tests

The Neper software is first used to create a rectangular domain with a width of 54 mm and a height of 135 mm, which is then divided into tessellated regions using Voronoi method. After that, the tessellated regions are meshed using Delaunay triangulation and subsequently regularized on the basis of the predefined number of tessellation seeds (2000 seeds are used here) to remove all small edges improving the mesh. To mimic the microstructure of rocks, these tessellated regions are assumed to represent grains consisting of various minerals and defects. Finally, the generated tessellations are imported into HFDEM for modelling their fracture under uniaxial compression tests.

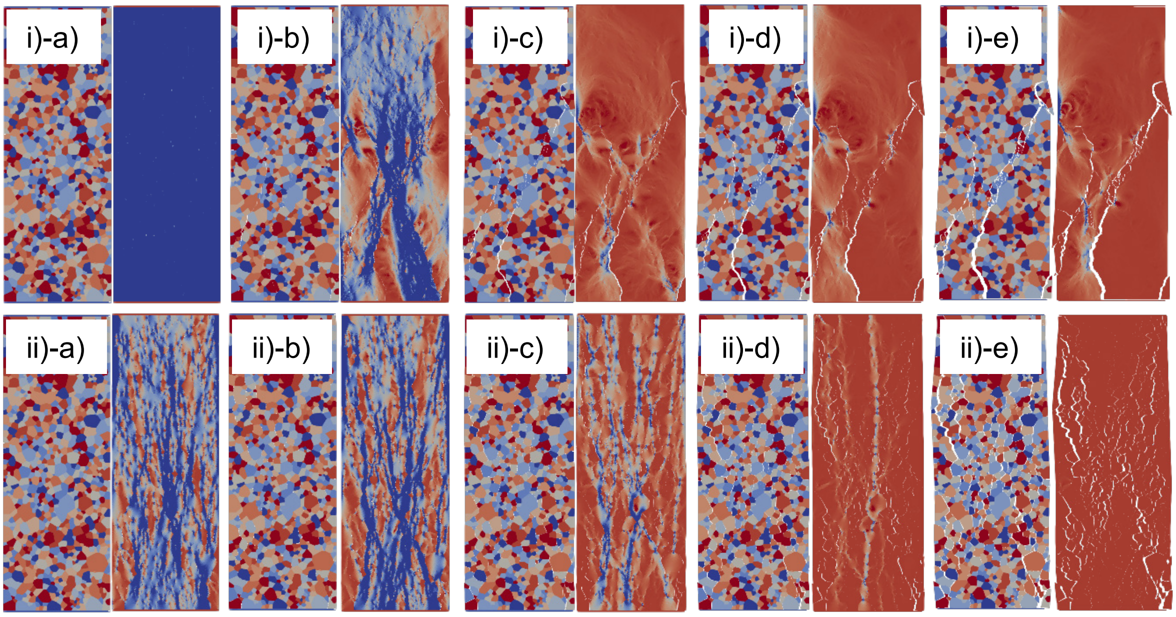

Figure 1. Grain-based 2D modelling of uniaxial compression tests: i) Rock sample with cohesive grains and ii) Assembled aggregate sample with non-cohesive grains.

Figure 1 illustrates the modelled failure progressive processes of rock samples with cohesive grains (i) and assembled aggregate samples with non-cohesive grains (ii) in the uniaxial compression tests in terms of the distributions of the grains (left in each pair) and minor principal stresses (i.e., the most compressive stress) (right in each pair). Figure 2 depicts the corresponding stress-strain curves. The stress state (a) in Figure 1 i) corresponds to the stage before the onset of nonlinearity in the stress-strain curve of the rock sample with cohesive grains in Figure 2. At this stage, the generation of microcracks is minor and the stress distribution is uniform in the sample. After this stage till the peak stress, the onset of microcrack growth occurs when the resultant concentrated stresses in the middle and bottom of the rock sample are greater than the local crack initiation stress, as shown in Figure 1 i)-b). Since the peak stress in Figure 2, the growth and coalescence of unstable microscopic cracks commence to form macroscopic cracks (c), which is accompanied by a rapid decrease in rock bearing capacity, as shown in Figure 2. Finally, the formed macroscopic cracks further propagate (d) resulting in the completed failure (e) of the rock specimen and the loss of its stress-bearing capacity. The physical-mechanical behavior of the assembled aggregate samples with non-cohesive grains is similar to that of the rock samples with cohesive grains explained above. However, since the grains of the assembled aggregate samples are not bonded together by cohesive elements, the level of resultant stresses is rather low and stress chains align with the loading direction since the forces between the grains are transferred completely depending on their interactions.

Grain-based 3D modelling of the failure process of the rocks with cohesive grains in the uniaxial compression test is shown in Figure 3 in terms of the 3D distribution of the minor principal stresses (left in each triplet) and the 2D distribution of the grains (central in each triplet) and minor principal stresses (right in each triplet) in a central cross-section in the vertical (YZ) plane, which are more or less the same as those obtained from the grain-based 2D modelling. However, the grain-based 3D model is generated using grain-growth tessellation method while the grain-based 2D model is built using the Voronoi tessellation method. As commented by Yahaghi et al. (2023), the grain-growth tessellation method generates rounder grains than the Voronoi tessellation method. The rounder boundaries of the grains help increase the peak strength while the sharper boundaries of the grains result in more zigzag crack propagation during the post-failure stage, especially when the crack

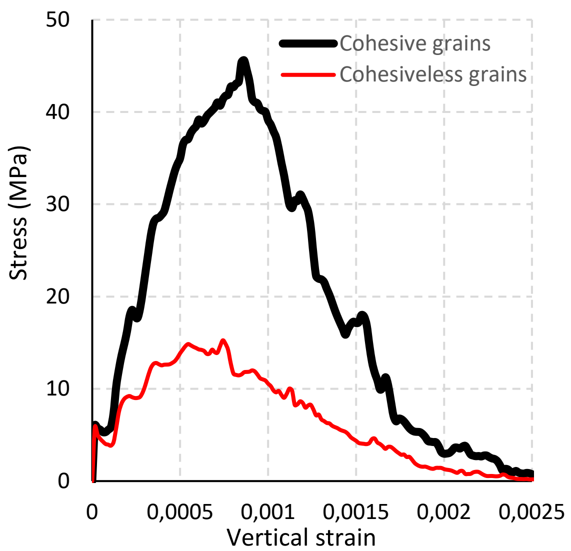

Figure 2. Stress-strain curves obtained from the uniaxial compression tests of rock samples with cohesive grains and assembled aggregate samples.

propagates along the grain boundaries. Moreover, the peak strength from the grain-based modelling initially increases with the increasing number of grains but remains almost the same with more than a threshold number of grains, for example 800 grains for modelling Tasmanian sandstones. Besides, the grain-based 3D modelling can clarify the effect of unbreakable grains, which are assumed in most discrete element modelling. The comparisons of two grain-based 3D simulations with breakable and unbreakable grains show that significant number of transgranular cracks are observed in the modelling with breakable grains while, in the modelling with unbreakable grains, pervasively distributed cracks appear in the specimen due to the instability of forming transgranular cracks. Correspondingly, the zigzag grain boundaries and unbreakable grains both increase interlocking forces among grains resulting in higher failure strength and ambiguous macro friction coefficient.

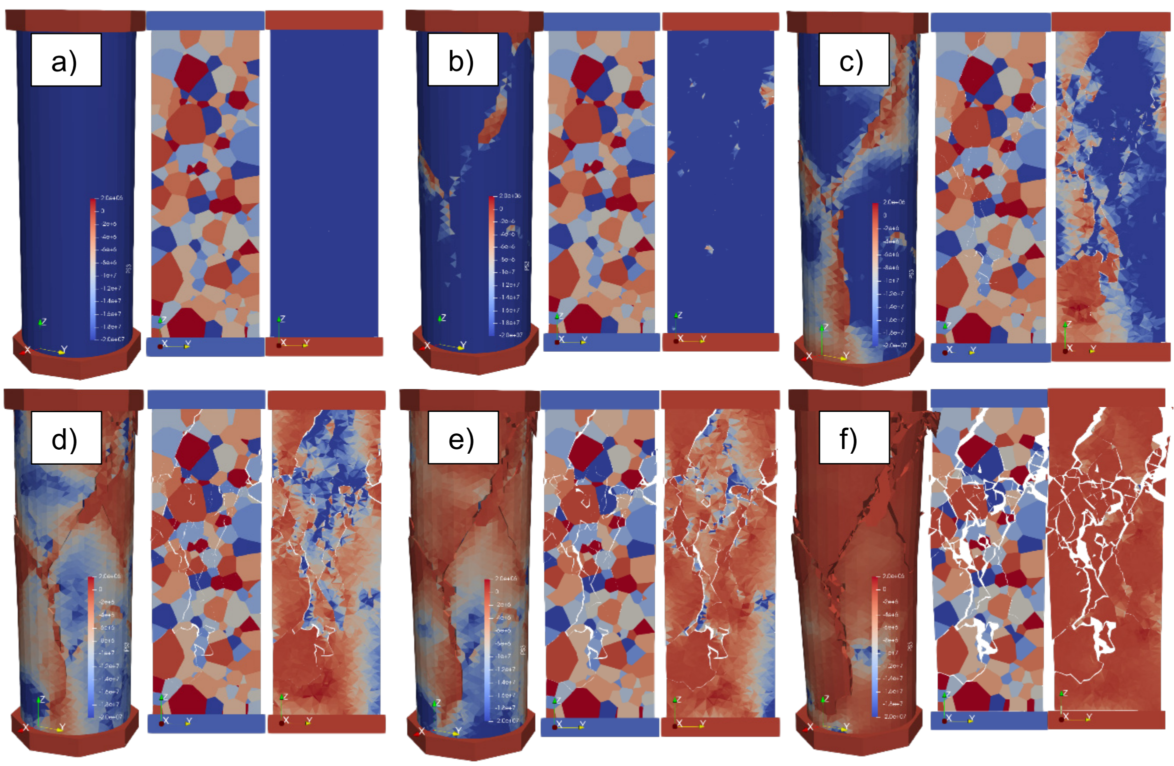

Figure 3. Grain-based 3D modelling of uniaxial compression tests.

3.2 *Grain-based 3D modelling rock dynamic fractures in triaxial Hopkinson bar tests*

A full-scale 3D numerical model of the triaxial Hopkinson bar testing apparatus reported by Liu et al. (2020) is built using HFDEM with the rock sample represented using the grain-based model, as shown in Figure 4. Only a dynamic biaxial compression test is modelled in this study, during which, the quasi-static simulation is first conducted in the first step to achieve the target pre-stress state of

10 MPa along X axis and 30 MPa along Y axis by adding corresponding biaxial confining pressures on the Hopkinson bars and then a dynamic load is applied at the outer end of the incident bar and transmitted to the rock sample while the confining pressures are kept constant. Figure 5 plots the dynamic stress-time profiles monitored in the incident, transmission and output bars during the dynamic biaxial compression tests with and without weak intergranular cohesive elements.

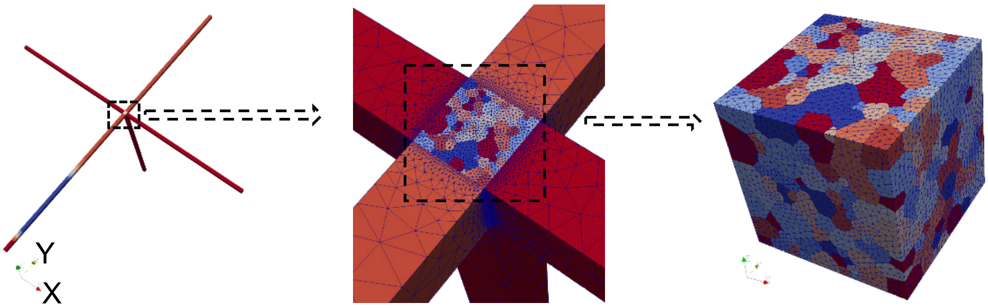

Figure 4. Grain-based 3D modelling of triaxial Hopkinson bar tests.

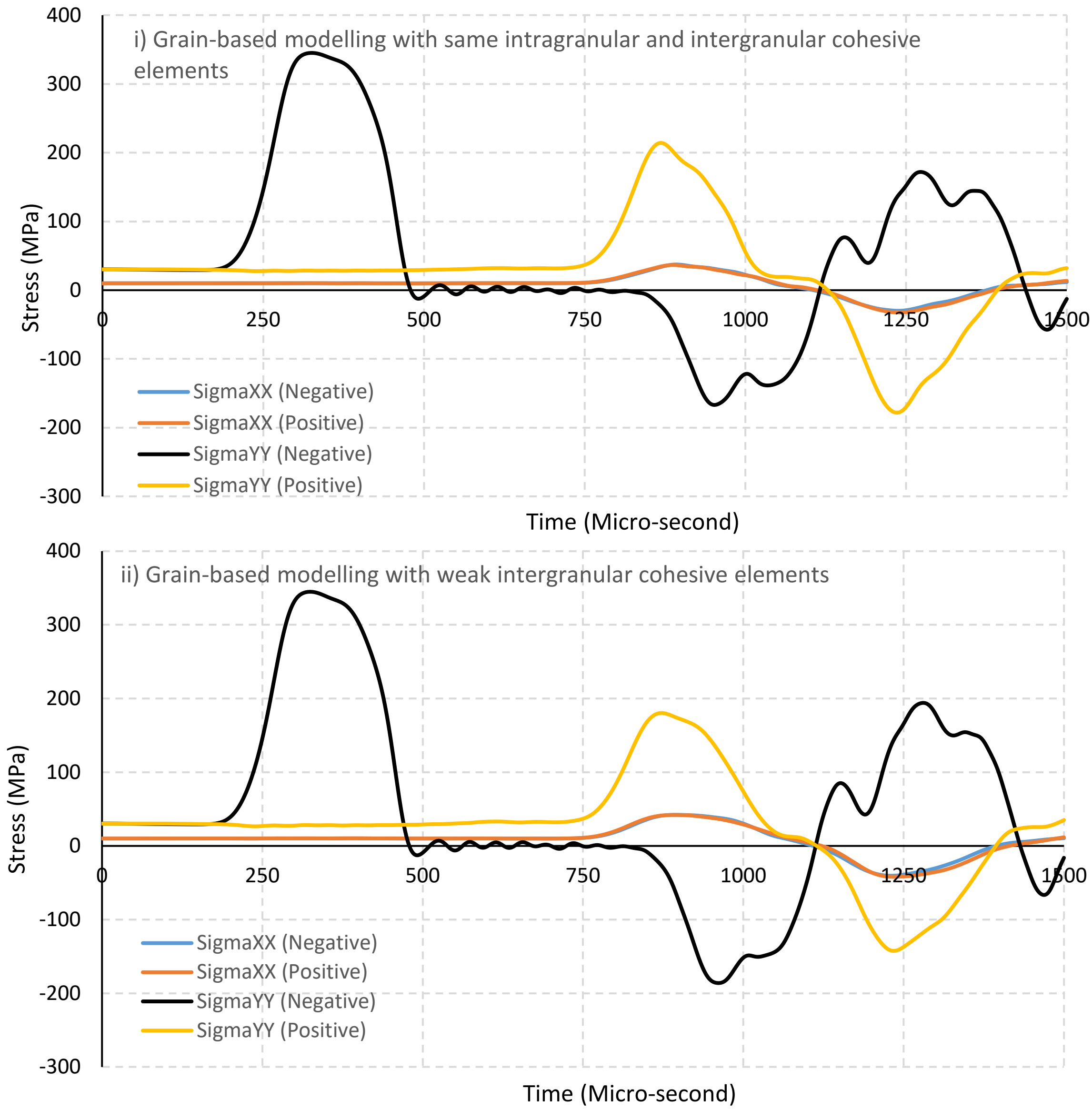

Figure 5. Comparison of dynamic stress - time profiles from the grain-based 3D modelling of triaxial Hopkinson bar tests of rocks without (i) and with (ii) weak intergranular cohesive elements.

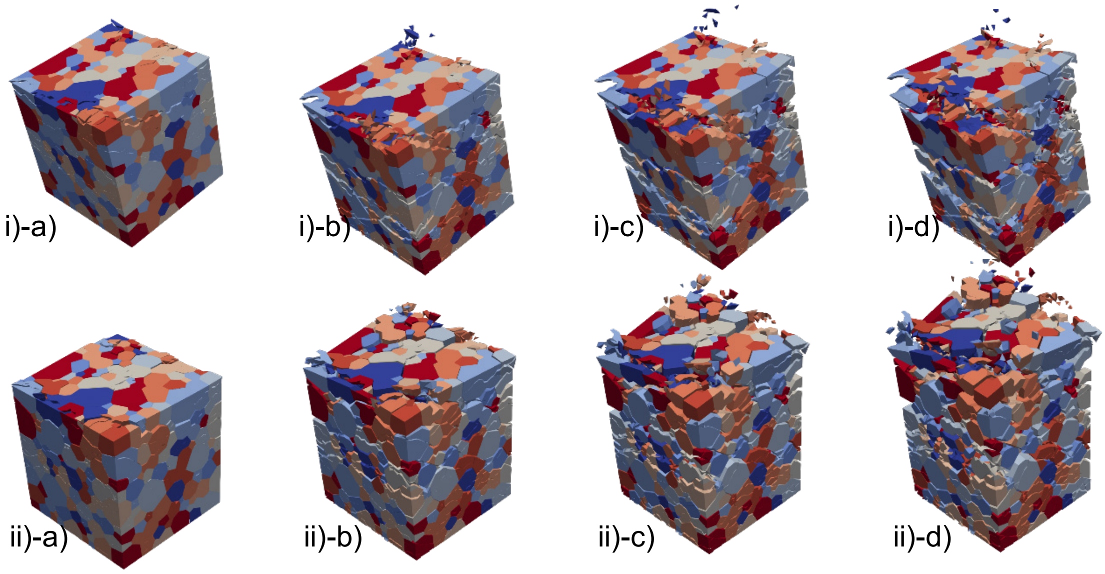

Figure 6. Comparison of the dynamic failure process of the rocks without (i) and with (ii) weak intergranular cohesive elements in the biaxial Hopkinson bar tests.

Figure 6 compares the modelled dynamic failure process of the rocks with and without weak intergranular cohesive elements in the biaxial Hopkinson bar tests. In both cases, fractures are initiated at the top parts of the contact surfaces between rock and incident/transmission bars and then intersect to form rock fragments, which are ejected into the only unconfined directions. However, due to the weak intergranular cohesive elements, many grains remain intact while rock fragments are formed in the case of the rock sample with weak intergranular cohesive elements. Finally, the middle and bottom parts of the rock specimens are broken into fragments as well.

4 CONCLUSIONS

A grain-based hybrid finite-discrete element method (HFDEM-GB) is proposed to investigate the failure process of heterogeneous rocks taking into account of the actual microstructure of heterogeneous rocks. It is first calibrated by modelling the failure process of granular rocks in the uniaxial compression tests and then applied to investigate the dynamic fracture of granular rocks in the triaxial Hopkinson bar tests. It is concluded HFDEM-GB can distinguish the intra-, trans- and inter- granular crack propagations besides modelling the failure process of heterogeneous rocks.

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