Computational Modelling of Concrete and
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Reappraisal of phase-field, peridynamics and other fracture models in light of classical fracture tests and new gap test

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ABSTRACT: The newly developed gap test and ten types of classical fracture tests of concrete are used to evaluate the performances of three popular numerical models. The crack band model with microplane damage constitutive model M7 is found to match all the experimental results well. However, the phase-field models show large deviations from the test results, and peridynamic models are even worse. Examination of four recent variants of these models does not change the overall critical appraisal.

1 INTRODUCTION

Recently, a new type of experimental setup, called the gap test [1, 2], has been developed at Northwestern University to reveal in a clear and unambiguous way the effect of crack-parallel stress on the fracture properties of material. Testing specimens of different sizes and applying the size effect method showed that the fracture energy, G_f, and the effective size, c_f, of fracture process zone (FPZ) of concrete depends strongly on level of crack-parallel stresses $\sigma_{xx}(=T)$.

This prediction is confirmed by finite element analysis with the M7 crack band model, which further indicated a strong effect of σ_{zz} and σ_{xz}. The gap test, applied to shale, composites and plastic-hardening metals, to reveal that the crack-parallel stress effects are rather different for different materials. These results shed new light on the validity of numerical models for fracture, such as phase-field (PF) and peridynamics (PD), newly popular in computational mechanics. The gap tests [2] also revealed that the fracture energy of quasibrittle materials, plastic hardening metals and composites depends strongly on the history of crack-parallel stresses (see Figure 1).

2 APPROACH AND MAIN RESULTS

This study uses the new gap test and ten types of classical fracture tests of concrete, most of them previously ignored, to conduct a critical comparison of the phase field (PF) model and peridynamics (PD) with the finite element crack band model (CB) in which the material model is the microplane model M7.

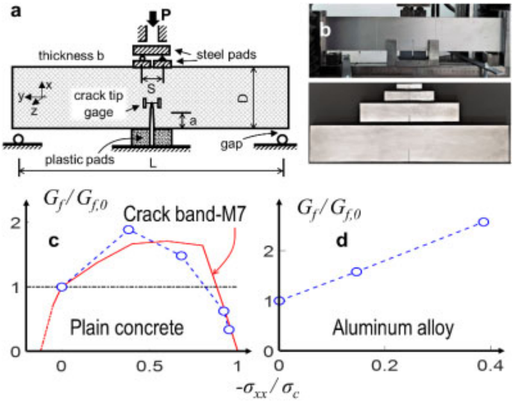

Figure 1. a,b) Setup of the gap test for 2D-geometrically scaled concrete specimens of various sizes. c) Measured and predicted variation of fracture energy G_f with increasing crack-parallel compression; d) the same for polycrystalline metal with millimeter-width yielding zone and micrometer-width fracture process zone.

Optimal fitting of the data by state-of-art phase-field and peridynamics computer programs calibrated by basic material properties reveals severe discrepancies.

Although the phase-field models have certain advantages (being superior for static and dynamic propagation of curved and branching line cracks in perfectly brittle materials obeying LEFM), and could be generalized to different constant (non-varying) levels of crack-parallel stress, they are found incapable of matching the results of the gap test and the classical fracture tests of concrete and rock, provided that the same set of model parameters is used for all the tests conducted on the same material.

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In these comparisons, the PD, considered as a kind of strongly nonlocal model, is found to disagree with the test data and be even inferior to PF. This reinforces the previous, strictly theoretical, critique of the basic concept of peridynamics [3], both bond- and state-based.

One of the faults of peridynamics is the use of interparticle potential, which is realistic only on the atomic scale. Still another is does not take into account shear-resisted particle rotations (which are what lends LDPM, the lattice particle discrete model, its superior performance). Still another is the unphysical boundary conditions and crack face conditions, along with the problem of unphysical interaction across the fracture process zone (FPZ) softened to various degrees.

The continuum-based finite element crack band model with realistic tensorial damage constitutive law M7 [4, 5] is able to fit the data from all the classical tests and the gap tests closely. The crack band model combined with Grassl's tensorial model and CDPM2 performs in most types of tests almost equally well.

The previously discussed severe limitations of the discrete crack and cohesive crack models are also pointed out. Also, the ubiquity of varying crack-parallel stresses in practical problems and their effects in concrete, shale, fiber composites, plastic-hardening metals and materials on submicrometer scale is emphasized.

3 MODELS AND EXPERIMENTAL DATA USED IN COMPARISONS

Eleven types of experiments on quasibrittle materials (concrete and rock) have been simulated to test the performance of computational models and discussed in the lecture. A few of them are selected here for comments.

- Size effect tests of types 1 and 2 [6]: geometrically scaled specimens with and without notches, subjected to three-point-bend load configuration.
- Compression-torsion fracture tests (mode III) [7]: notched cylindrical specimens subjected to a fixed axial confinement and angle-controlled torque.
- Uniaxial compression fracture tests [2] of cylindrical specimens subjected to uniaxial compressive load with zero or various constant lateral confining pressures rigid confinement.
- Diagonal shear fracture of reinforced concrete (RC) beams [8], reinforced by graded steel bars and subjected to four-point-bend load configuration.
- Gap tests [2] of fracture of notched beams subjected to the loading configuration in Figure 1 and described in Section 1.

Seven computational models are examined in the lecture. They include:

- CB-M7: the crack band model [9] based on the microplane damage constitutive model M7 for concrete [4], as slightly updated in [10] (downloadable codes can be found at http://www.civil.northwestern.edu/people/bazant/m7-coding/m7_cyc_schell_v1.f). The material parameters are optimized for material tests of typical laboratory specimens whose size is close to the size FPZ, or the representative volume of material. This size approximately represents the material characteristic length l_0, which is, of course, kept the same for all specimen sizes.
- CB-Gr: is a tensorial damage constitutive model implemented within the same crack-band finite element framework as CB-M7, except that M7 has been replaced with the concrete constitutive model CDPM2 developed by Grassl et al. [5]. This model is an update of [11] and represents arguably the best plastic-damage constitutive model of concrete formulated in the classical way—in terms of tensors, two loading surfaces in the stress space, and tesorial invariants.
- PF: is the basic phase-field model developed by Francfort and Marigo [12]. Conveniently, this model has been implemented as a user subroutine in Abaqus by Pañeda *et al.* [13].
- PF-Wu: is a phase-field model that is modified to fit better one particular test and is based on the cohesive zone theory of Jiang-Ying Wu [14]. Download both PF models from: https://www.empaneda.com/codes/.
- PD: is an ordinary state-based peridynamic model using a critical stretch with sudden force drop to initiate fracture, developed by Silling [15]. This model has been implemented in the Peridigm [16] code downloadable from the Sandia National Laboratory website.
- PD-Gr: is a state-based non-ordinary (or correspondence-based) peridynamic model, in which Grassl's CDPM2 has been implemented as the constitutive law.
- PDba-Gr: is the same as PD-Gr, except that the deformation gradient needed for the constitutive relation is corrected by Bazilevs et al. according their new bond-associated formulation of peridynamics [17]. Both PD-Gr and PDba-Gr models were implemented as user material subroutines to be used with Peridigm code.

4 CRITICAL COMPARISONS

The size effect on structural strength [18] is salient characteristic of quasibrittle fracture and thus the most important experiment to verify a fracture model. It follows a simple size effect law formulated in 1984 and amply verified for many different quasibrittle materials. This law, whose most important feature is the deviation from the $-1/2$ power law of linear elastic fracture mechanics (LEFM), underlies a simple unambiguous procedure (1990) for measuring the fracture energy and the material characteristic length of quasibrittle materials (even in presence of crack-parallel stresses).

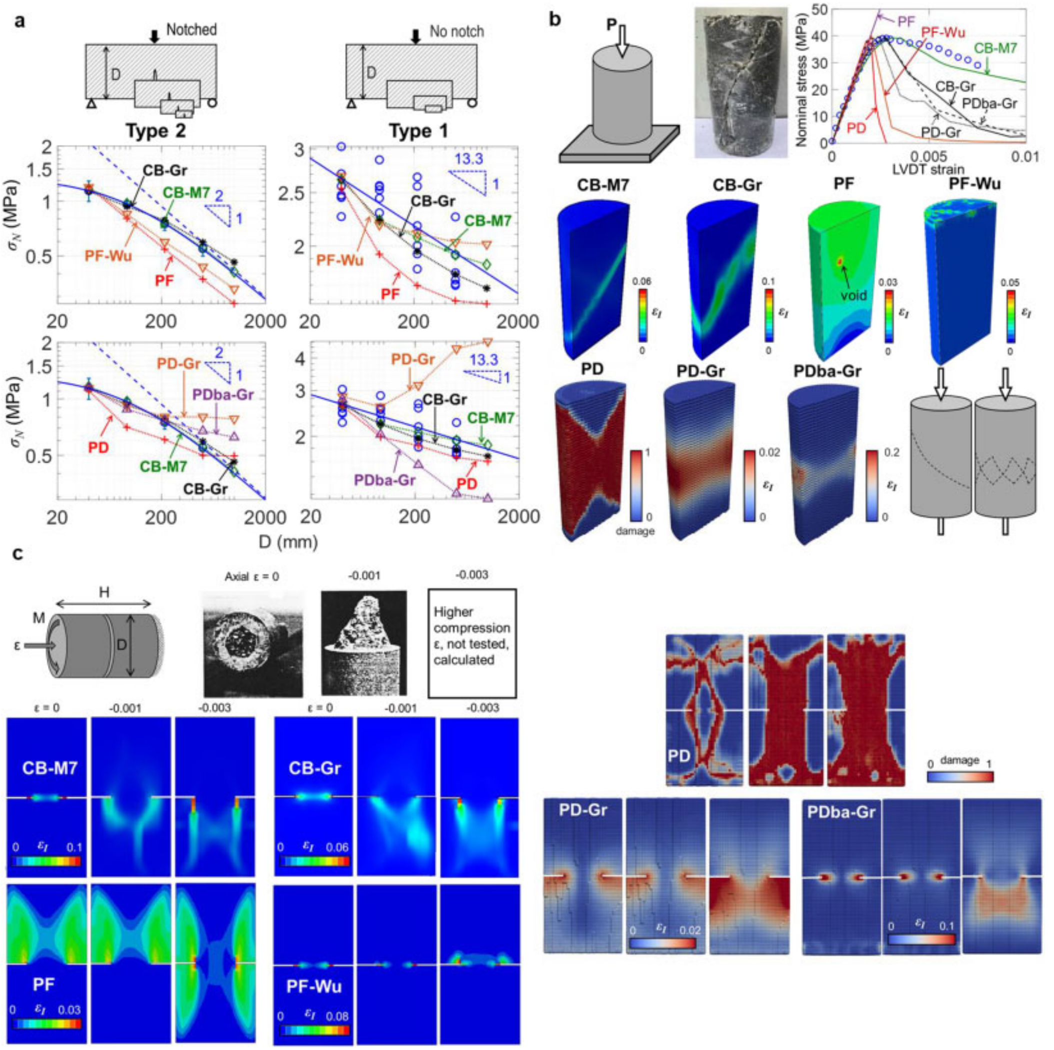

Figure 2. Simulations of a) quasibrittle size effect, b) uniaxial compression fracture, c) mode III shear fracture without and with transverse compression, and d) vertex effect tests (all in concrete).

Figure 2a shows that both PF models result in a power-law behavior in log-log scale. While the slope of the PF model is $-1/2$, which complies with the LEFM, the slope of PF-Wu is different from $-1/2$ which is thermodynamically impossible since it implies a zero-energy flux into the fracture tip. All PD models deviate significantly from the experimental data, and the PD-Gr model even results in an unphysical increase of structural strength. Both CB models yield good results.

Unlike tension, the existence of a discontinuous band of localized strain in concrete could only appear when a material model has the capability of forming frictional or cohesive shear surfaces. Such a capability is absent from both PF models. The same conclusion can be drawn for the basic PD model. Even though the tensorial formulation of Grassl's model allows the emergence of a localized band, only CB implementation of this model shows the presence of such a band. PDba-Gr shows its appearance only vaguely while it is missing completely from the PD-Gr (see Figure 2b).

The transition from a flat to conical and then to distorted cylindrical surfaces of the localized crack when the axially confining strain increases is well captured by both CB models, yet the CB-Gr model produces some secondary diffused cracks. Such a transition is evident in the experimental observation. Neither of the PF models could produce such a transition. Among the PD models, the basic PD model exhibits a rather brittle failure with fragmented pieces which are abruptly released at the peak load but are absent in experiment. The PD-Gr, on the other hand, shows delocalized damage band while the PDba-Gr results in unchanged flat crack surfaces (see Figure 2c).

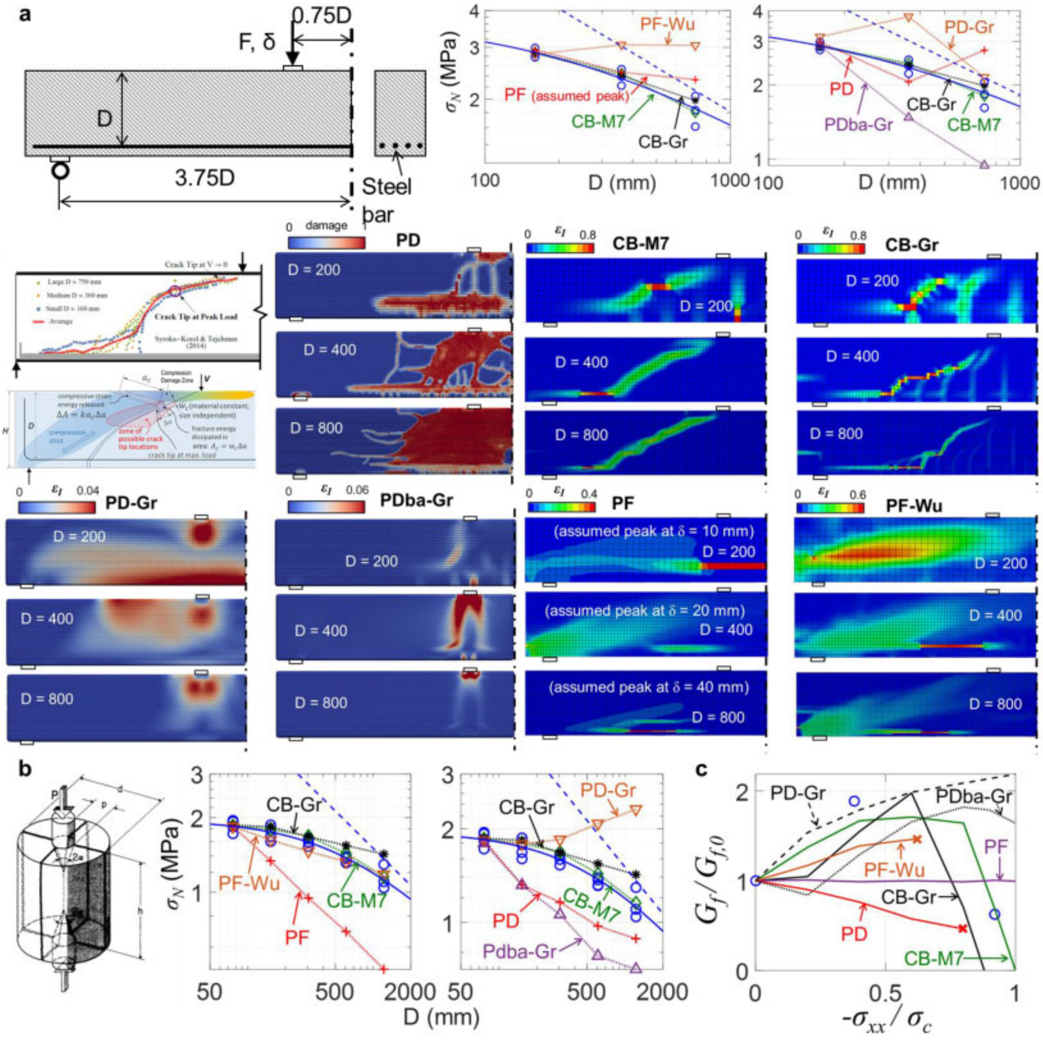

Figure 3. Simulations of a) diagonal shear failure of RC beams without stirrups, b) double punch tests of concrete cylinders, and c) gap test.

The ability to capture diagonal shear of RC beams and the gap test depends on the ability of the model to capture the interaction between components of the stress tensor. Only CB-M7 could reasonably do the job. Though the trend in CB-Gr was reasonable, its prediction of the change in fracture energy could be improved. Other models can capture neither the crack development process nor the peak load corresponding to each structural size (see Figure 3).

5 CLOSING COMMENT

These comparisons document more broadly an unhealthy dichotomy that has recently prevailed between computational mechanics and the concrete testers-designers. The former has relied on minimal selective and insufficient experimental verifications while latter paid insufficient attention to theoretical developments and their critical scrutiny.

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