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Computational fracture modelling of polymer-bonded explosives and solid propellants: A critical review of local and nonlocal continuum formulations and discrete particle approaches

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Abstract: Fracture behaviour is a critical determinant of the safety, reliability and service life of polymer-bonded explosives (PBXs) and solid propellants. Both are highly filled polymer composites whose damage evolution is governed by heterogeneous particle-binder architectures, rate- and temperature-dependent binders, interfacial debonding, matrix failure and particle or crystal fracture. A broad range of computational methods has been developed to describe crack initiation, propagation, coalescence and fragmentation, but suitability varies with the dominant mechanism, length scale and intended prediction. This paper reviews five approaches: the extended finite element method (XFEM), cohesive zone modelling (CZM), phase-field fracture modelling (PFM), peridynamics (PD) and the discrete element method (DEM). For each, the theoretical foundation, crack representation, numerical implementation, parameter requirements and applications to PBXs and solid propellants are examined, with emphasis on particle-binder debonding, constituent fracture, interacting crack networks, fragmentation and post-failure contact. The comparison indicates that XFEM enables the non-mesh-conforming representation of one or a few discrete sharp cracks; CZM represents progressive separation along predefined or explicitly resolved interfaces; PFM captures distributed nucleation and complex crack topology; PD accommodates dynamic fracture and fragmentation through a nonlocal continuum formulation; and DEM resolves contact-network evolution and particle rearrangement. These capabilities are conditional on compatible constitutive laws, identifiable and appropriately calibrated parameters, verified numerical implementation and solution, and validation against independent local as well as global experimental observables. Prospective hybrid formulations and machine-learning-assisted strategies are also discussed, together with the requirements for conservative coupling, uncertainty quantification and thermo-mechanical-chemical validation. The review provides a comparative basis for selecting and developing fracture models for the safety and structural-integrity assessment of PBXs and solid propellants.

Keywords: Polymer-bonded explosives; Solid propellants; Computational fracture

mechanics; Extended finite element method; Cohesive zone model; Phase-field method; Peridynamics; Discrete element method

1. Introduction

Polymer-bonded explosives (PBXs) and solid propellants are two important classes of polymer-bonded energetic composites used in defence systems, aerospace propulsion and related engineering applications [1-5]. PBXs serve primarily as high explosives and generally contain a high volume fraction of energetic crystals dispersed in a polymeric binder, whereas solid propellants are designed for controlled combustion and commonly contain oxidiser crystals, polymeric binder and, in many formulations, metallic fuel. Despite their different functions, both materials rely on a highly filled particulate architecture in which particle-binder load transfer and interface integrity govern the macroscopic response. During manufacture, storage, transportation and service, thermal cycling, ageing, confinement and mechanical loading can initiate distributed damage and subsequent crack growth [6-9]. Fracture not only degrades structural integrity but may also localise mechanical dissipation and promote hot-spot formation under severe loading [10-12]. Accurate prediction of crack initiation and propagation is therefore essential to the safety assessment and lifetime evaluation of both PBXs and solid propellants.

Experimental investigations have provided valuable information on the tensile, compressive and fracture responses of PBXs and solid propellants under different loading conditions [13-15]. Full-field optical measurements and microstructure-based characterisation further enable the evolution of strain localisation, debonding and crack paths to be examined [16-21]. Nevertheless, experiments remain constrained by safety requirements, limited access to internal damage, and the difficulty of independently controlling loading rate, temperature, confinement and ageing. Computational modelling provides a complementary means of separating competing mechanisms, linking mesoscale damage to macroscopic response and exploring conditions that are difficult to isolate experimentally [7,22,23].

Fracture modelling of these composites is challenging because their responses are governed by heterogeneous microstructures and several interacting failure mechanisms. In PBXs, crystal anisotropy, defects, porosity and particle-binder adhesion promote competition among interfacial debonding, binder failure and transgranular crystal fracture [6,24-26]. In solid propellants, damage is more strongly influenced by binder viscoelasticity, oxidiser-binder dewetting, void growth and the constraints imposed by grain geometry and casing [2,5]. Both material classes exhibit pronounced rate and temperature dependence [27,28], while dynamic or thermal loading may couple fracture with heat generation and subsequent energetic response [11,29]. Their failure processes also span multiple length scales, from particle-scale

debonding and microcracking to macroscopic crack propagation, requiring models that relate local mechanisms to structural observables [22].

A range of computational approaches has been employed to describe these processes. Within local continuum mechanics, the reviewed fracture formulations include the extended finite element method (XFEM), cohesive zone modelling (CZM) and phase-field fracture modelling (PFM). XFEM enriches the finite-element approximation to represent sharp cracks independently of the underlying mesh and avoids remeshing during propagation [30-33]. CZM describes progressive separation through a traction-separation law and is well suited to interface-dominated damage when the relevant fracture path or interface network can be represented [34-38]. PFM replaces a sharp discontinuity with a regularised crack field and can naturally reproduce crack nucleation, branching and coalescence [39-43].

Peridynamics (PD) and the discrete element method (DEM) provide complementary descriptions when discontinuities, fragmentation or particle interactions dominate, but they operate at different representational levels. PD, as a nonlocal continuum theory, formulates the governing equations through finite-range integral interactions, allowing discontinuities to emerge without a separate crack-tracking procedure [44-48]. The DEM represents the material as interacting discrete particles or bonded units and directly resolves contact forces, bond breakage, rearrangement and post-failure interaction [49-52]. These features make PD and DEM attractive for distributed cracking and fragmentation, although their spatial resolution, constitutive calibration and computational cost require careful control.

The applicability of these methods depends on the dominant fracture mechanism, the observable of interest and the scale at which the material is represented. Existing reviews have generally concentrated on an individual numerical framework or on material systems other than PBXs and solid propellants [45,50,53-55]. Moreover, several advanced formulations have been established mainly in conventional structural composites and cannot be transferred to energetic composites without material-specific parameterisation and validation [41,56-58]. Hybrid formulations and data-enabled strategies provide promising routes for bridging scales and may reduce repeated high-fidelity evaluations in appropriate applications, but their application to PBXs and solid propellants remains at an early stage [59-62]. A comparative assessment is therefore needed to relate each numerical method to material architecture, fracture mechanism, parameter requirements and experimentally measurable outputs.

This paper provides a comparative review of computational fracture modelling for PBXs and solid propellants. Its objectives are to summarise the theoretical foundations and fracture representations of XFEM, CZM, PFM, PD and DEM; examine their applications to particle-binder debonding, matrix failure, crystal fracture, crack coalescence and fragmentation; and evaluate their capabilities and limitations in terms of constitutive description, parameter identification, numerical

objectivity, validation and computational cost. Potential multimethod coupling and data-enabled approaches are also discussed in relation to the unresolved modelling requirements of these materials.

The remainder of this paper is organised as follows. Section 2 examines the material characteristics and dominant fracture mechanisms of PBXs and solid propellants, establishes their common fracture-mechanics basis, and formulates the corresponding modelling requirements. Sections 3-7 review XFEM, CZM, PFM, PD and DEM, respectively. Section 8 discusses prospective multimethod coupling and data-enabled strategies. Section 9 provides a comparative capability assessment and a mechanism-based procedure for method selection.

2. Material characteristics, fracture mechanisms and modelling implications

2.1 Material architectures and dominant failure processes

Polymer-bonded explosives (PBXs) and solid propellants are both highly filled polymer composites, yet their fracture problems are not identical. PBXs consist of a dense assembly of energetic crystals connected by relatively thin binder ligaments, so mesoscale defects and crystal-binder interfaces strongly influence mechanical integrity and impact sensitivity. Solid propellants contain oxidiser and, depending on formulation, fuel particles within a polymeric load-transfer network that must also maintain the integrity of a macroscopic propellant grain. Their fracture response is therefore governed not only by particle-scale damage but also by the rate- and temperature-dependent deformation of the binder and by the structural consequence of creating new burning surface [1,8,63].

In PBXs, quasi-static failure commonly emerges from competition among crystal-binder debonding, tearing or cavitation of constrained binder ligaments, crack initiation at pores or pre-existing defects, and—in sufficiently strong interfaces or severe loading—fracture of energetic crystals. Microcracks may subsequently interact and coalesce into a specimen-scale crack. The balance among interfacial separation, binder damage, crystal fracture and frictional contact is controlled by crystal morphology and defects, binder properties, interface strength, porosity, confinement, loading rate and temperature [20,26,64,65]. The direct evidence is nevertheless concentrated on HMX-based or generically designated PBXs; fracture parameters and mechanisms should not be extrapolated to CL-20-based formulations without dedicated experiments.

For solid propellants, the binder response controls stress redistribution before and during fracture. Loading rate, temperature, confinement and prior ageing can shift the balance among particle dewetting, matrix cavitation or tearing, crack-tip blunting and unstable macrocrack growth. At the structural scale, these processes interact with grain geometry, internal pressure, thermal gradients and propellant – insulation constraints. Depending on loading and service history, the resulting response may be

dominated by distributed dewetting, a macroscopic crack or long-term constitutive degradation [8,21,63,66].

A second distinction concerns the consequences of damage. At the crystal scale, anisotropic elasticity, crystallographic defects and thermally induced transformation strains can alter crack nucleation and growth [67]. Under impact, pore collapse, plastic or viscoelastic dissipation, and friction during crack closure or particle sliding may generate local heat. Whether this local heating develops into ignition depends on its magnitude and duration relative to thermal diffusion and reaction timescales. In solid propellants, fracture may also expose new burning surface and thereby couple mechanical damage to regression and combustion response [10-12,68,69].

2.2 Common fracture-mechanics basis

Although XFEM, CZM, PFM, PD and DEM represent fracture differently, each must satisfy the relevant balances of mass, momentum and energy; the fracture law specifies how available energy is dissipated as a crack, a process zone or failed interactions evolve. For a quasistatic conservative body with total potential energy Π and crack-surface area A , the energy-release rate is

$$G = -\partial\Pi/\partial A = G_c \quad (1)$$

where G_c is the fracture resistance. The second relation is Griffith's propagation condition, not a universal constitutive law. In PBXs and solid propellants, viscoelasticity, plasticity, friction, inertia, heat transport and reaction can introduce additional storage or dissipation; a purely elastic interpretation of G and G_c is therefore defensible only within the regime in which those contributions are negligible or represented explicitly [70].

For a sharp crack in homogeneous isotropic linear elasticity, the leading stress term in the Williams expansion varies as $r^{-1/2}$, and its amplitude is described by the mode-I, mode-II and mode-III stress-intensity factors K_I , K_{II} and K_{III} . For mixed-mode I/II loading, the Irwin relation for an isotropic solid is [71,72]

$$G = (K_I^2 + K_{II}^2)/E \quad (2)$$

$$E' = \begin{cases} E, & \text{plane stress} \\ E/(1 - \nu^2), & \text{plane strain} \end{cases} \quad (3)$$

The J -integral provides a contour measure of the crack-driving force and equals G under quasistatic conservative conditions; the associated configurational force expresses the material driving force acting on a defect. These equivalences are

conditional. Large process zones, material heterogeneity, viscoelastic or inelastic dissipation, inertia and thermo-chemical coupling may require generalised domain or interaction integrals and an energy balance containing the additional terms [71-74]. Process-zone and regularised formulations preserve energy accounting while replacing the idealised singular tip. For a specified loading mode, a cohesive law assigns a finite traction-bearing zone whose traction–separation work defines G_c ; the cohesive strength and separation work, together with the bulk stiffness, set the process-zone scale. PFM approximates the Griffith surface functional by a diffuse crack density over the regularisation length ℓ . PD distributes force and failure energy across interactions within the horizon δ , so the relation between an interaction-level failure law and macroscopic G_c depends on the kernel, horizon and spatial dimension. DEM assigns deformation and dissipation to particle contacts or bonds; continuum K , J and G are then derived macroscopic measures rather than intrinsic contact variables [75-79].

For PBXs and solid propellants, this common basis supplies a comparison framework rather than a single fracture criterion. Each formulation can be assessed through the representation of the crack or process zone, the driving measure, the resistance and dissipation law, the characteristic physical or regularisation length, and the scale of the validation observable [80].

2.3 Mechanism-based modelling requirements

Material architecture and loading regime define a causal chain from the dominant failure mechanisms to the target observables and only then to a suitable fracture representation. Table 1 consolidates this mechanism-centred mapping for PBXs and solid propellants. The entries indicate mechanism-dependent tendencies rather than a universal ranking; every selection remains conditional on appropriate constitutive relations, independently identifiable parameters, numerical verification and validation against observables relevant to the intended use.

Table 1. Integrated mechanism-observable-method mapping for PBXs and solid propellants.

Material problem and loading context	Dominant mechanism and target observable	Mechanism-compatible representation	Critical qualification
PBX mesoscale fracture	Interface debonding, binder-ligament failure and microcrack coalescence; local damage and specimen response.	CZM or DEM for distributed interface/contact damage; XFEM for a dominant crack after localisation [1,13,20,64].	Separate interface and bulk failure parameters; validate local damage as well as global response.

Material problem and loading context	Dominant mechanism and target observable	Mechanism-compatible representation	Critical qualification
PBX crack from a cavity or notch	Sharp crack initiation and propagation; crack path, failure load and growth history.	XFEM for one or a few dominant cracks; PFM or PD when distributed initiation and interacting topology must be represented [26,81].	Use independently measured fracture properties and demonstrate mesh/internal-length sensitivity.
PBX impact, hot-spot formation and ignition	Mechanical damage or fracture; dissipative heating, temperature, reaction progress and ignition delay.	Coupled PD for distributed damage and thermo-chemical fields; DEM or an explicit mesoscale formulation when contact or friction is central [65,68].	Mechanical agreement does not validate temperature or ignition; energy partition and local thermal validation are required.
Solid-propellant dewetting and rate-dependent failure	Viscoelastic interface separation, matrix deformation and distributed mesodamage.	Rate-/temperature-dependent CZM for represented interfaces; PFM for distributed matrix/fracture fields; DEM when explicit force networks are required [8,21,63].	Calibrate across rate, temperature and loading mode; avoid fitting all parameters to one global curve.
Solid-propellant dominant or mixed-mode crack	Crack-tip blunting and mode-I/mixed-mode growth at specimen or grain scale.	XFEM or CZM for one or a few cracks; PD or PFM for non-prescribed interacting topology [16,66].	Validate crack path and load response under withheld rates or mode mixities.
Crystal fracture or fracture-deflagration coupling	Anisotropic cleavage or co-evolution of damage, heat release and burning surface.	PFM or PD with anisotropic constitutive relations for crystal fracture; coupled multiphysics formulations for deflagration [67,69].	Direct PBX crystal-fracture evidence and local thermochemical validation remain limited.

Method choice should therefore follow whether the target observable requires representation of a resolved interface, a sparse dominant crack, an evolving crack network, or post-failure contact and particle rearrangement, with method-specific parameter and resolution requirements assessed separately.

Fracture representation must be distinguished from constitutive and multiphysics modelling. XFEM, CZM, PFM, PD and DEM describe discontinuity, degradation or separation, whereas viscoelasticity, viscoplasticity, tension–compression asymmetry and crystal anisotropy are specified through the associated bulk, interface or contact constitutive relations. A distributed damage variable represents constitutive degradation and should not be equated with a resolved crack unless localisation or separation and the associated dissipation are defined objectively. Thermal transport and reaction kinetics enter through additional field equations and coupling terms; resolving mechanical damage or fracture alone therefore does not establish ignition prediction.

Calibration, verification and validation denote distinct operations. Calibration is the estimation or adjustment of uncertain model parameters using a specified experimental dataset. Verification determines whether the mathematical model has been implemented and solved correctly: code verification tests the implementation against analytical, manufactured or benchmark solutions, whereas solution verification evaluates discretisation, iterative and time-integration errors through convergence and balance checks. Validation determines the degree to which the verified model represents the physical response for its intended use by comparison with experiments not used for calibration, with numerical and experimental uncertainties reported where possible. Accordingly, agreement with a stress-strain or force-displacement curve used to identify parameters is calibration evidence, not validation; predictive qualification requires independent validation of relevant global and local observables without retuning.

The same material may require different representations at different scales: a mesoscale CZM or DEM model may resolve distributed debonding, while an XFEM, PFM or PD model represents the resulting structural crack. Conversely, a method that reproduces a crack path is not necessarily credible for lifetime or ignition prediction unless its constitutive, thermal and kinetic parameters are independently constrained. The following method-specific sections therefore evaluate XFEM, CZM, PFM, PD and DEM in terms of the mechanisms actually demonstrated for PBXs and solid propellants, the parameters required, the validation observable and the computational scale—not solely their mathematical ability to create discontinuities.

3. Extended finite element method: enriched representation of sparse dominant cracks

The XFEM is most compelling when fracture localises into one or a few sharp cracks whose trajectories are not known a priori. This regime is relevant to cavity- or flaw-controlled fracture in PBXs and to pre-cracked solid-propellant specimens and grains. It is, however, distinct from the distributed particle-binder debonding and matrix microcracking that often precede macroscopic localisation in these materials. Therefore, XFEM should be assessed as a crack-representation strategy embedded within an appropriate constitutive and fracture framework.

3.1 Crack representation and material-specific parameterisation

In conventional finite elements, a discrete crack normally has to follow element boundaries or be accommodated by remeshing. XFEM instead augments the finite-element approximation with discontinuous and near-tip functions through the partition-of-unity framework, allowing a crack to cut through elements independently of the background mesh [82-84]. A representative displacement approximation is

$$\mathbf{u}^h(\mathbf{x}) = \underbrace{\sum_{i \in N} N_i(\mathbf{x}) \mathbf{u}_i}_{\text{Standard FEM}} + \underbrace{\sum_{j \in N_{\text{cut}}} N_j(\mathbf{x}) H(\mathbf{x}) \mathbf{a}_j}_{\text{Heaviside enrichment}} + \underbrace{\sum_{k \in N_{\text{tip}}} N_k(\mathbf{x}) \left(\sum_{\alpha=1}^4 F_{\alpha}(\mathbf{x}) \mathbf{b}_k^{\alpha} \right)}_{\text{Tip enrichment}} \quad (4)$$

where N_i denotes the conventional shape function, $\mathbf{u}_i$ is the standard nodal displacement, $H(\mathbf{x})$ is the Heaviside function describing the displacement jump across the crack, the functions $F_{\alpha}(\mathbf{x})$ are the near-tip enrichment functions, $\mathbf{a}_j$ and $\mathbf{b}_k^{\alpha}$ are the corresponding enriched degrees of freedom. Level-set descriptions are commonly used to update the crack surface and front [31,85-87], while stress-intensity factors or energy-release measures can be evaluated using domain or interaction integrals [88,89]. These features remove the need for mesh conformity to a moving crack, but they do not determine when a crack initiates, how it turns, or how resistance evolves with opening rate and temperature.

In Eq. (4), the conventional displacement approximation acts on all nodes, whereas the enrichment terms are restricted to nodes whose supports intersect the crack interior or its tip. The Heaviside term represents the displacement jump; the classical near-tip functions reproduce the square-root radial displacement field of linear-elastic fracture mechanics. The enriched and conventional nodal unknowns are solved together through the finite-element weak form, with integration that accounts for the crack inside cut elements [82-87].

For PBXs and solid propellants, a predictive XFEM model consequently requires four internally consistent components: (i) a bulk constitutive law appropriate to the loading regime; (ii) an initiation criterion; (iii) a propagation resistance and mixed-mode evolution law; and (iv) a direction rule together with an explicit treatment of initial defects. Linear-elastic formulations require independently measured fracture toughness or critical energy release rate and are defensible only when the process zone is small relative to the structural dimensions. Cohesive enrichment relaxes the crack-tip singularity and can represent finite process-zone dissipation, but introduces cohesive strength, fracture energy and mode-mixity parameters [13]. In both cases, a rate-independent brittle law cannot be assumed to remain valid for an HTPB binder undergoing large-strain viscoelastic deformation or for a PBX whose binder response and interface strength vary with temperature and strain rate. The accumulated, time-dependent damage reported for solid propellants

[90] is therefore a constitutive requirement to be represented and calibrated; it is not supplied by the enrichment itself [91,92].

Parameter identification should separate bulk deformation from fracture. Unnotched tests over the relevant rate-temperature window are needed to identify the constitutive response, whereas notched specimens, crack-opening measurements and size-dependent fracture tests are needed to identify initiation strength and fracture resistance. The same crack-path data should not be used both to select the growth criterion during calibration and to claim validation. After code verification of the XFEM implementation, solution verification should establish convergence with respect to the background mesh, enrichment radius, subcell integration, crack increment and time step. The calibrated model should then be validated, without retuning, against independent observables from another geometry or a withheld loading condition: the load-displacement curve, initiation site, crack trajectory, crack length versus displacement or time and, where available, near-tip displacement fields measured by digital image correlation (DIC). Where a geometrical enrichment radius r_e and a discrete crack-growth increment Δa are used, their resolution should be reported as r_e/h and $\Delta a/h$, respectively, where h is the local background-element size. Quadrature order or subcell subdivision in cut elements must be varied separately because it is not represented by either ratio.

3.2 Applications of XFEM to PBXs and solid propellants

Applications of XFEM to PBXs and solid propellants have so far concentrated on defect-controlled fracture, in which a cavity, notch or pre-existing crack provides a clearly identifiable initiation site. Chen et al. [26] used XFEM to investigate crack initiation and propagation in compression-loaded PBX specimens containing cavities. The model combined pressure-sensitive bulk plasticity with a maximum-principal-stress criterion for crack initiation and a cohesive traction–separation law for subsequent growth [26]. This separated the nonlinear response of the surrounding PBX from progressive traction loss across the developing crack. Their simulations placed crack initiation at stress-concentration regions on the cavity boundary and allowed the resulting cracks to traverse the background mesh without prescribing an element-aligned path. Huang et al. [13,93] subsequently combined compression experiments with an XFEM-based cohesive formulation for PBX-9502 plates containing elliptical cavities. As shown in Fig. 1, they compared the observed and simulated crack patterns and further examined crack-length evolution with normalised displacement, rather than relying only on peak load. The latter study therefore provides local, spatial validation of a defect-driven macroscopic crack. Collectively, these investigations demonstrate the utility of XFEM for cavity-controlled fracture, but the inference remains bounded: the defect geometry is prescribed, only a small number of cracks dominate, and the PBX is represented at an effective-continuum scale. Agreement at this level does not establish that the model resolves crystal fracture, particle-binder debonding or the distributed microcrack population preceding localisation.

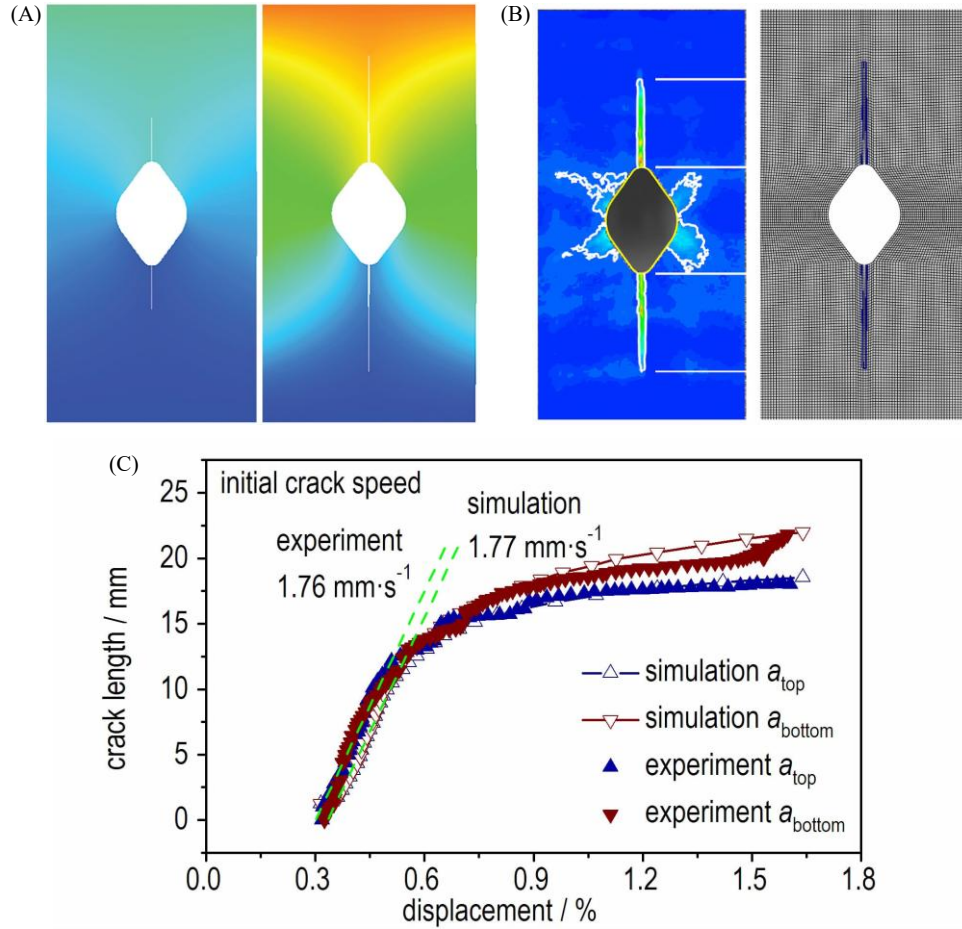


Fig. 1. XFEM simulations of cavity-controlled crack initiation and growth in PBX specimens under compression. (A) Simulated crack paths for a cavity-containing PBX specimen [26]. (B) Experimental crack pattern (left) and XFEM result (right) for a PBX-9502 plate with an elliptical cavity [13]. (C) Experimental and simulated crack length as a function of normalised displacement [13].

For solid propellants, Lü [94] applied XFEM within a fracture-mechanics framework to HTPB propellant grains subjected to thermal and internal-pressure loading, using crack-driving parameters to assess the response of pre-existing defects under service-like boundary conditions. Gao et al. [16] combined tensile tests, microscopic observation and DIC with XFEM simulations of pre-cracked HTPB propellant. Their comparison of measured and simulated crack evolution provides the strongest local validation in this group. Zhang et al. [95] also examined fracture evolution from pre-existing cracks, whereas Hou et al. [3] analysed damaged modified double-base propellant under impact overload and reported the sensitivity of stress redistribution and crack growth to the initial defect and loading condition. Except where independent local measurements are available, these calculations establish numerical feasibility and load-case sensitivity rather than independently validated predictions of crack evolution.

Taken together, the two material classes support a specific conclusion rather than a general claim of predictive capability. XFEM is demonstrated for two-dimensional, specimen-scale problems in which a cavity or pre-crack selects one or a few dominant cracks, and the strongest experimental comparisons concern crack path or crack-length evolution [13,16]. These comparisons constitute validation only when those observables are withheld from calibration. Evidence for predictive transfer is more limited across defect geometries, loading rates and temperatures, and for three-dimensional structural grains. Moreover, applying temperature and pressure as boundary conditions is not equivalent to validating coupled thermomechanical fracture: such a claim would require measured temperature fields and temperature-dependent constitutive and fracture parameters. No ignition prediction is established unless the mechanically generated dissipation is further linked to, and validated against, thermal localisation or reaction observables.

3.3 Capabilities and limitations of XFEM for PBXs and solid propellants

The available PBX and solid-propellant studies therefore support its use in cavity-, notch- and pre-crack-dominated problems, for which the defect is geometrically resolved and crack-path or crack-length observables are available [3,13,16,26]. In this regime, XFEM can reduce remeshing costs and accommodate curved crack trajectories at specimen or grain scale. This geometric flexibility should not, however, be interpreted as a general ability to predict fracture mechanisms. The enrichment represents the discontinuity, whereas crack nucleation, propagation direction, fracture resistance, closure and rate-temperature dependence are determined by additional constitutive and fracture laws. The demonstrated scope is therefore geometry-flexible propagation of sparse cracks; distributed particle-binder damage and spontaneously evolving multi-crack networks remain outside the capabilities established for PBXs and solid propellants [96,97].

Four limitations are particularly consequential. First, standard XFEM becomes cumbersome when failure is distributed over thousands of particle-binder interfaces or when many cracks nucleate, branch and coalesce; enrichment proliferation and interacting level sets can erode its computational advantage [98,99]. Second, compressive fracture around cavities involves crack closure, contact and friction. Traction-free crack faces can produce an incorrect driving force after closure unless contact is explicitly enforced [100,101]. Third, nonlinear viscoelasticity, large deformation and rate-temperature dependence must be supplied by the bulk and fracture laws and calibrated over the intended service envelope. Combining a sophisticated enrichment with rate-independent parameters does not resolve this incompatibility [59,102,103]. Fourth, three-dimensional crack-front tracking, branching and contact substantially increase integration and solver costs [101,104], while validation data for internal crack surfaces remain scarce. DIC is valuable for

accessible surfaces, but volumetric imaging or interrupted-section measurements are needed when the target is an internal three-dimensional network [105,106].

Predictive application to structural solid-propellant grains remains conditional on an appropriate viscoelastic constitutive description, crack-face contact and mixed-mode resistance, together with demonstrated convergence in three-dimensional analyses. It is not yet established as a stand-alone predictive framework for distributed particle-binder dewetting, spontaneous multi-crack nucleation, fragmentation, or fracture-to-ignition coupling. Those regimes require explicit interface descriptions, a nonlocal continuum formulation such as PD, a discrete particle formulation such as DEM, or a carefully validated hybrid model. Within this bounded domain, XFEM offers an attractive balance between geometric flexibility and computational efficiency; outside it, the apparent freedom of the crack path can obscure stronger assumptions in the initiation law, propagation resistance and material calibration.

4. Cohesive zone modelling: interface-controlled damage and fracture

CZM is most compelling when fracture is governed by separation along a known or explicitly resolved interface. This condition commonly arises in PBXs, where crystal-binder debonding can precede macroscopic localisation, and in solid propellants, where particle-binder dewetting or propellant-insulation separation may control failure. CZM replaces a traction-free crack tip with a finite process zone governed by a traction-separation law (TSL), thereby linking the onset of separation to the energy dissipated during complete decohesion [38,107]. Its predictive value, however, depends less on the label “cohesive” than on whether the relevant interface is represented, its parameters are independently identifiable, and the numerical process zone is adequately resolved.

4.1 Traction-separation representation and material-specific parameterisation

For a damage-based cohesive law, the nominal traction vector $\mathbf{t}_n$ can be expressed schematically as

$$\mathbf{t}_n = (1-D)\mathbf{K}\delta_n \quad (5)$$

where δ_n is the displacement jump, $\mathbf{K}$ is the initial normal–tangential stiffness and D is a damage variable. Damage initiation is usually defined by a traction- or separation-based criterion, whereas subsequent softening is constrained by the mode-dependent fracture energy [75,108-110]:

$$G_c = \int_0^{\delta_f} t(\delta) d\delta \quad (6)$$

The traction t and separation δ constitute a work-conjugate pair for the mode considered, while δ_f defines the separation at complete decohesion. Under mixed-mode conditions, the normal and tangential work contributions are combined according to the adopted fracture-energy interaction criterion. As shown in Fig. 2, bilinear and trapezoidal laws are common idealisations, but choosing a curve shape does not by itself confer physical fidelity. The initial stiffness must be high enough to suppress artificial interface compliance; the peak normal and shear tractions determine initiation; and the areas under the normal and tangential curves determine the mode-I and mode-II dissipation. A mixed-mode interaction law is additionally required when opening and sliding coexist. These quantities are correlated in a global load–displacement response, so substantially different parameter sets may reproduce the same peak load while predicting different initiation sites, process-zone lengths and crack-growth histories [111-113]. For a common rate-independent bilinear damage law, D evolves from 0 to 1 with the maximum attained effective separation. Unloading and reloading follow the current degraded stiffness until that previous maximum is exceeded. The compressive normal response is treated separately to prevent interpenetration after opening damage. Cohesive elements or surface interactions evaluate these relations from the displacement jump between opposing faces, so the active state variables describe separation and its history [38,107].

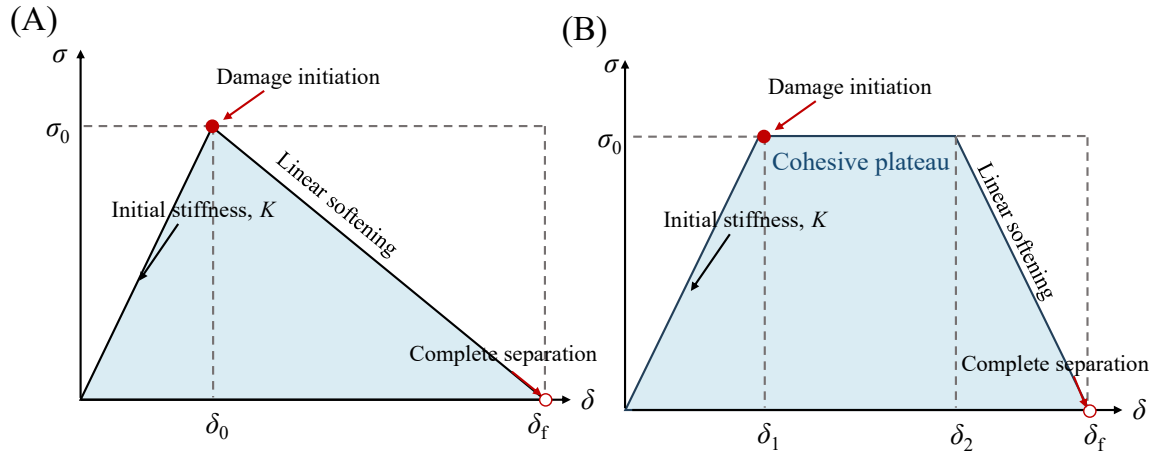


Fig. 2. Representative traction-separation laws used in cohesive zone modelling [103-105]: (A) bilinear and (B) trapezoidal laws.

In fracture-mechanics terms, CZM replaces the singular crack tip by a finite process zone: the traction-separation work defines the mode-dependent fracture resistance, while cohesive strength and bulk stiffness govern the process-zone length. Atomistically informed process-zone formulations provide a related multiscale construction by deriving bulk and interphase response from a common interatomic energy [114,115].

Material-specific constitutive consistency is essential. For PBXs, a mesoscale model must distinguish the elastic or inelastic response of energetic crystals, the

constrained response of thin binder ligaments, and crystal-binder interface separation. Assigning one cohesive law to every internal boundary can represent distributed debonding, but it also assumes that those boundaries are the admissible fracture network; transgranular crystal fracture and bulk binder tearing require separate failure descriptions. For solid propellants, the surrounding binder is commonly viscoelastic and may undergo large deformation, while the apparent interface strength and fracture energy vary with rate, temperature, ageing and mode mixity. A rate-independent TSL coupled to a rate-dependent bulk law can therefore shift dissipation artificially between binder deformation and interface damage. Time- or rate-dependent cohesive formulations provide a route to greater consistency [112,116,117], but their use in PBXs and solid propellants requires calibration over the intended rate-temperature envelope rather than transfer from a single reference condition.

4.2 Applications of CZM to PBXs and solid propellants

Applications to PBXs and solid propellants are most usefully organised by the physical interface represented and by whether the reported comparisons support calibration or independent validation. At the PBX specimen scale, Xiao et al. [64,118] embedded cohesive fracture within multiscale descriptions of dynamic compression and dynamic notched semi-circular bending. As illustrated in Fig. 3, their simulations reproduced rate-dependent force-deflection trends and generated macroscopic crack paths comparable with the experiments. These are complementary observables: the global curve constrains overall resistance and dissipation, whereas the crack path tests localisation. Because the notch and specimen geometry restrict the fracture corridor, however, agreement does not uniquely identify the crystal-binder law or establish transferability to a different microstructure, loading mode or defect geometry.

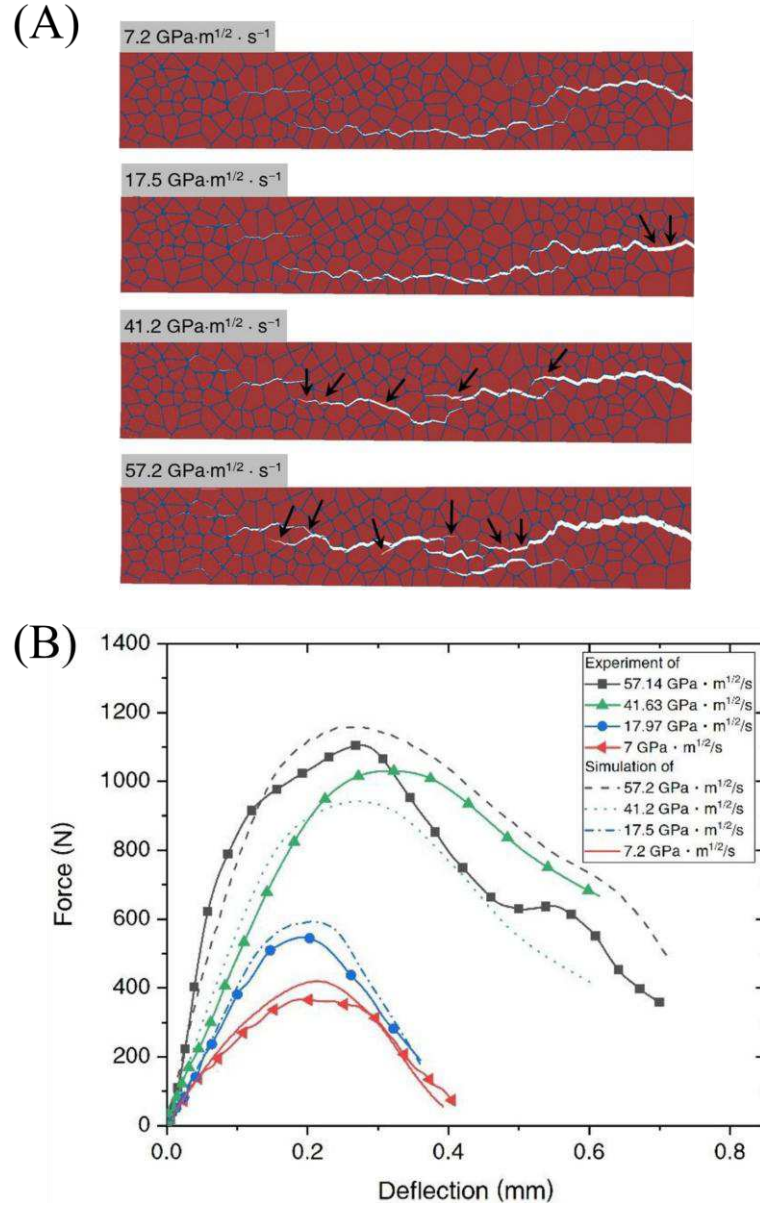


Fig. 3. CZM simulation of dynamic fracture in PBX-9001 [64]: (A) predicted crack paths at different loading rates and (B) comparison between measured and simulated force-deflection curves.

At the explicit-microstructure scale, Dai et al. [119] represented PBX-9501 using elastic HMX particles and a viscoelastic binder described by a Prony-series relaxation law. Bilinear cohesive elements were inserted at particle-binder boundaries and within both constituents, allowing interfacial debonding, binder rupture and particle fracture to compete. Fig. 4 shows that under simulated uniaxial tension, local debonding initiated at highly stressed particle boundaries and coalesced into a dominant crack approximately normal to the loading direction. This sequence illustrates the principal benefit of a mesoscale CZM: progressive loss of load transfer and its contribution to macroscopic localisation are directly observable in the calculation. The simulations identified interface debonding as the dominant tensile mechanism, whereas interface

shear failure and particle fracture became important under compression. Thus, the admissible fracture network included both interfacial and intraconstituent paths, although individual cohesive surfaces remained tied to the prescribed element boundaries.

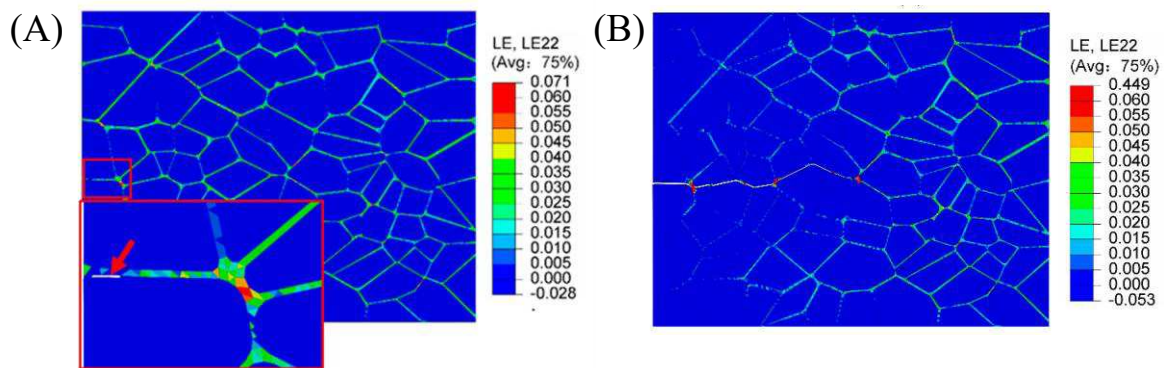


Fig. 4. Mesoscale CZM prediction of local strain and progressive interfacial failure in PBX-9501 under uniaxial tension [119]: (A) onset of a small debonded region and (B) subsequent growth and connection of interface damage.

For solid propellants, the central modelling problem is the interaction between time-dependent binder deformation and interface separation. Wubuliaisian et al. [8] incorporated a viscoelastic debonding criterion into a large-deformation propellant model, making the failure rule more consistent with the surrounding binder response. At the microstructural level, Hou et al. [120] used a piecewise cohesive law to represent debonding, nucleation and crack growth in HMX-modified double-base propellant, while Li [121] combined in situ tensile observations with cohesive simulations of composite-propellant microdamage. These studies support CZM as a mechanism-resolving description of progressive particle-binder separation, but the evidence is strongest for the tested two-dimensional microstructures and loading histories. When a macroscopic stress-strain curve is used to fit the cohesive law, agreement with that curve is calibration evidence and cannot determine whether the local partition between binder deformation and cohesive dissipation is unique. A distinct engineering application is propellant-insulation separation, for which the potential failure surface is manufactured and the normal and shear components can be defined explicitly. Cui and Ma [9] applied a mixed-mode cohesive formulation to this interface, aligning the model topology with the physical joint. When the target instead is a crack emerging through the propellant bulk, pre-inserting cohesive elements along all candidate paths can add artificial compliance. The distinction between intrinsic pre-insertion and extrinsic activation is illustrated in Fig. 5. Based on the latter strategy, Cui [122] used topology updates to insert a cohesive surface after an initiation criterion was met. Extrinsic insertion relaxes some path restrictions and avoids pre-damage compliance, but its predictions depend on the insertion criterion, crack-direction rule, contact treatment and the robustness of topology updates, particularly in three dimensions.

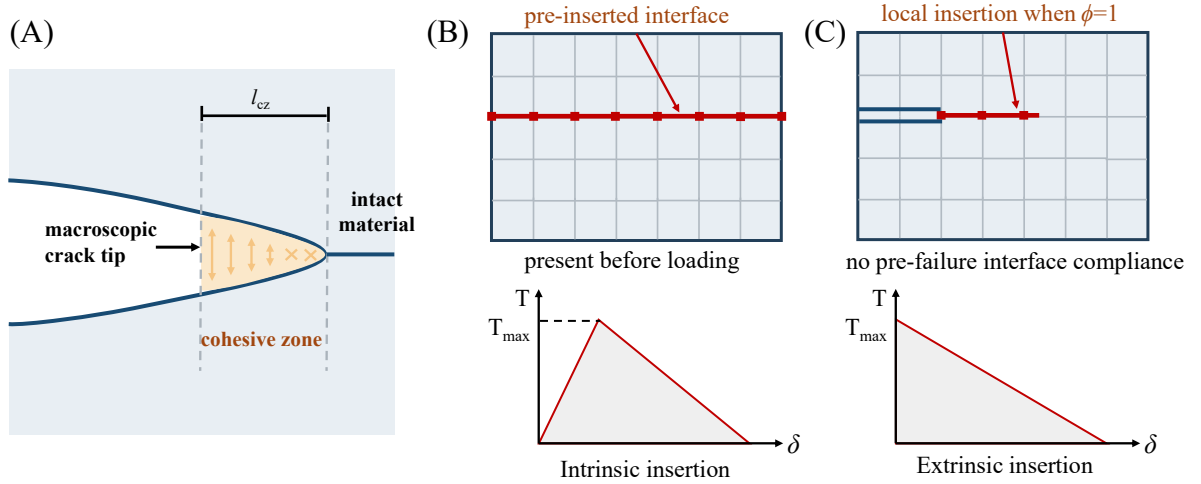


Fig. 5. Schematic diagram of intrinsic and extrinsic CZM [122]: (A) Cohesive zone; (B) Intrinsic CZM; (C) Extrinsic CZM.

Temperature-dependent fracture introduces an additional separation problem between bulk and interface effects. Wang et al. [123] combined thermo-viscoelastic behaviour with cohesive crack growth in HTPB propellant, while their related experimental–numerical study examined crack velocity and fracture toughness [124]. As shown in Fig. 6, their study also compared XFEM and CZM under one tensile configuration. Under this configuration, XFEM represented a discontinuity independently of element interfaces, whereas CZM resolved progressive traction loss and crack-tip blunting. This comparison is useful as a mechanism-specific example, not as a universal ranking: the outcome also depends on the bulk constitutive law, initiation criterion, fracture resistance, mesh, regularisation and parameter-identification procedure assigned to each method.

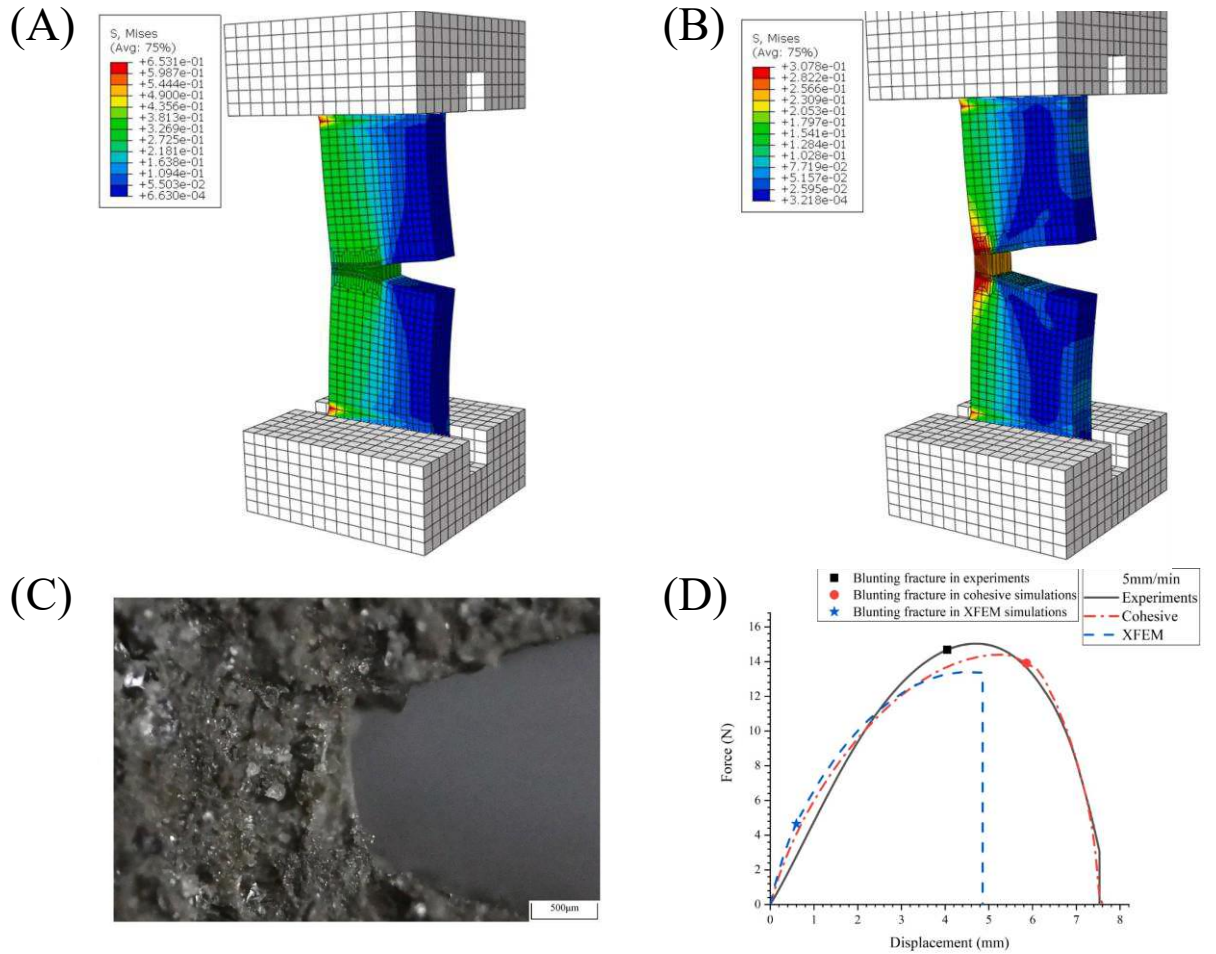


Fig. 6. Comparison of XFEM and CZM for HTPB-propellant tensile fracture at 5 mm min⁻¹ [124]: (A) XFEM result at 62.77 s; (B) CZM result at 84.30 s; (C) crack-tip blunting during cohesive-zone evolution at 52.030 s; and (D) comparison of experimental and simulated responses. The comparison is specific to the constitutive laws, fracture criteria and calibration used in the cited study.

4.3 Capabilities and limitations of CZM for PBXs and solid propellants

For PBXs and solid propellants, the principal capability of CZM is to represent progressive loss of load transfer across a known or explicitly resolved interface while retaining the finite-element framework for constitutive response and structural loading. The studies reviewed above directly demonstrate its use for crystal-binder and particle-binder debonding, propellant-insulation separation and dominant cracks constrained to physically defensible surfaces [8,64, 119-124]. In this regime, the traction-separation law separates initiation strength from dissipated fracture energy and can incorporate mixed-mode, rate- or temperature-dependent response when corresponding data are available. This energetic transparency should not, however, be interpreted as a general ability to predict fracture topology. The cohesive law governs separation on an admissible surface; nucleation away from that surface, competition with crystal or binder failure, crack closure and parameter transferability are

determined by additional modelling choices. Thus, interface-controlled separation has been demonstrated for specific PBX and propellant configurations, whereas transferable prediction of arbitrary bulk cracking, unconstrained multi-crack evolution and fragmentation has not.

The principal limitations of CZM are coupled through the assumed fracture topology, parameter identifiability and numerical regularisation. In intrinsic formulations, distributing cohesive surfaces across candidate interfaces alters the pre-damage compliance and may favour mesh-aligned crack trajectories. Extrinsic insertion avoids this built-in compliance, but transfers the uncertainty to the nucleation criterion, propagation direction, crack branching, contact treatment and topology-update algorithm. This trade-off becomes particularly consequential in PBXs and solid propellants, where interfacial debonding competes with binder tearing, crystal or particle fracture, and the formation of a macroscopic crack. Cohesive parameters inferred from a single global response are likewise rarely unique, because the initial stiffness, cohesive strength, fracture energy and bulk constitutive response can compensate for one another. Their dependence on particle-surface condition, binder formulation, porosity, loading rate, temperature and ageing further limits transferability across formulations and service conditions. Since the cohesive-zone length introduces an additional numerical scale, solution verification cannot be based on peak-load convergence alone. Resolution should therefore be reported as h/ℓ_{cz} , or equivalently $N_{cz} = \ell_{cz}/h$, where h is the characteristic interface-element length along the propagation direction and ℓ_{cz} is the characteristic cohesive-zone length for the adopted traction-separation law and loading mode. The predicted initiation site, debonded area, crack-growth history and cohesive dissipation must also converge with respect to interface discretisation, penalty stiffness, viscous regularisation and time increment. Moreover, the current evidence base remains dominated by two-dimensional, monotonic and mechanically driven problems, whereas three-dimensional particle networks, cyclic histories, confinement, crack closure and friction are substantially less validated. A mechanical traction-separation law provides interface opening and dissipated energy, but does not define how that energy is partitioned into heat or coupled to reaction kinetics. Predictive hot-spot, ignition or combustion simulations therefore require independently calibrated heat-generation, transport and chemical-reaction models, together with local thermal validation.

Accordingly, CZM should be selected when the target observable is progressive separation along a known or explicitly resolved interface and when cohesive parameters can be constrained independently of the bulk response. It is conditionally applicable to distributed particle-scale damage if all relevant interfaces and competing crystal or binder failure mechanisms are represented, and if solution verification establishes discretisation objectivity and independent local validation is demonstrated. It is not yet established as a stand-alone predictive framework for spontaneous bulk crack nucleation, unconstrained multi-crack growth, fragmentation or fracture-to-ignition coupling. Those regimes require an alternative crack representation or a carefully validated hybrid formulation, together with explicit

transition rules and additional parameters. Within this bounded domain, CZM offers a direct link between interface mechanics and observable damage evolution; outside it, a well-fitted traction-separation law can conceal stronger assumptions about crack topology, parameter identifiability and transferability.

5. Phase-field modelling: diffuse representation of interacting cracks

Phase-field modelling (PFM) is most compelling when the crack topology is not known in advance and when nucleation, branching or coalescence makes explicit crack tracking impractical [39,40]. These conditions can arise during distributed failure of PBXs and solid propellants, but topological flexibility alone does not make a phase-field model material-specific. Crystal-binder or particle-binder separation, binder tearing and crystal fracture are distinct dissipative processes. A predictive formulation must therefore identify which process the phase field represents and couple it to constitutive laws appropriate to the constituent, interface and loading regime.

5.1 Variational formulation and material-specific parameterisation

In variational fracture, a sharp crack surface is regularised by a scalar field d distributed over a regularisation length ℓ , with $d = 0$ denoting intact material and $d = 1$ denoting fully fractured material, as illustrated in Fig. 9. A representative total-energy functional is [125,126]

$$\Pi(\mathbf{u}, d) = \int_{\Omega} \psi(\boldsymbol{\varepsilon}(\mathbf{u}), d) d\Omega + \int_{\Omega} G_c \gamma(d, \nabla d) d\Omega \quad (7)$$

where $\mathbf{u}$ is the displacement field, and $\boldsymbol{\varepsilon}(\mathbf{u})$ denotes the linear strain tensor under the infinitesimal-strain assumption. Moreover, ψ is the stored-energy density, G_c is the critical energy-release rate and γ is the regularised crack-surface density. Minimisation with respect to $\mathbf{u}$ and d , together with an irreversibility constraint, produces coupled mechanical and phase-field equations without prescribing a crack path [127-131]. The formulation replaces a displacement discontinuity by a finite damage band of width $O(\ell)$; consequently, the degradation function, crack-density function, residual stiffness and solution of the irreversibility constraint are constitutive and numerical choices rather than implementation details.

The functional combines the degraded bulk-energy contribution with the regularised crack-surface energy. As d increases, the degradation function reduces the crack-driving part of the stored energy, whereas $\gamma(d, \nabla d)$ combines a local damage penalty with a gradient contribution governed by ℓ . The latter penalises sharp spatial variations in d , producing the finite-width crack profile illustrated in Fig. 7. When body forces or prescribed tractions are present, Π must additionally include the corresponding external potential. Incremental minimisation with respect to $\mathbf{u}$ and d ,

subject to the irreversibility constraint, yields the coupled mechanical and phase-field problem. A small residual stiffness is commonly retained to maintain algebraic solvability in fully degraded regions, and the coupled equations may be solved monolithically or by a staggered scheme [129].

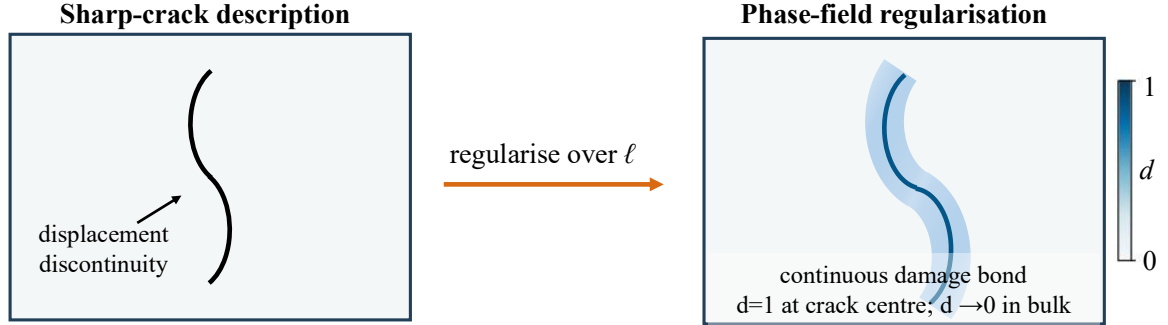


Fig. 7. Variational phase-field regularisation of fracture: replacement of a sharp displacement discontinuity by a continuous damage band [37,44,128].

Within the regularised Griffith family, the crack-density function distinguishes AT1 from AT2. For $d = 0$ in intact material and $d = 1$ in fully fractured material, AT1 uses $w(d) = d$ and AT2 uses $w(d) = d^2$. With the commonly adopted quadratic degradation function, AT1 retains an initial elastic domain and a finite homogeneous damage-initiation threshold, whereas AT2 admits damage evolution from arbitrarily small strain in the homogeneous one-dimensional setting. The selection therefore changes the relation among G_c , ℓ , elastic stiffness and apparent strength; cohesive phase-field variants permit strength and fracture energy to be specified more independently [39,40,43].

The same framework extends beyond quasi-static brittle fracture by adding the governing balances and internal variables required by the coupled physics. Dynamic and thermomechanical formulations introduce inertia, temperature-dependent free energy, thermal strain and heat balance, with damage-dependent transport or heat generation defined as separate constitutive couplings [130,132]. Ductile and fatigue formulations likewise couple the phase field d to plastic or accumulated cyclic variables rather than treating these processes as intrinsic to the phase field [133,134]. Validation of an AT2 model calibrated from one mode-I test against mixed-mode geometries, together with adaptive spatial and temporal strategies for heterogeneous domains, further illustrates predictive transfer and computational tractability [135,136]. These extensions broaden the PFM framework without replacing material-specific parameterisation, numerical verification or independent validation.

For PBXs and solid propellants, the crack-driving energy requires particular care. A tension-compression split is needed to prevent unphysical degradation under compression, but the selected split also controls shear-dominated cracking and the response under confinement. Crystal anisotropy, binder viscoelasticity or

viscoplasticity, and interfacial separation must likewise be represented at their respective scales. A single scalar field with one G_c cannot, without additional assumptions, distinguish interfacial debonding from binder tearing or transgranular fracture. Spatially varying resistance, separate bulk and interfacial fields, or a diffuse-interphase construction can represent that competition, provided that the assigned interface thickness and fracture properties are not numerical substitutes for unresolved microstructure [137-139].

The regularisation length ℓ introduced by the diffuse-crack approximation must be distinguished from an independently measurable material length, such as particle size, interface thickness or fracture-process-zone width. Its primary mathematical role is to control the width of the regularised crack and the approximation of a sharp discontinuity; its influence on strength and its physical interpretation depend on the phase-field model class. In AT1/AT2-type brittle formulations, ℓ enters the relation among G_c , elastic stiffness and nucleation strength, so fitting ℓ may reproduce a measured peak load without establishing that it equals a physical material length. Mandal et al. showed that values inferred from one-dimensional strength relations can be too large relative to the structural dimensions and can yield erroneous responses, whereas a cohesive phase-field/PF-CZM formulation can make the global response comparatively insensitive to ℓ when strength and G_c are independently parameterised and ℓ is sufficiently small and adequately resolved. Accordingly, ℓ should be assigned physical meaning only when an independently measured localisation-band or fracture-process-zone width is mapped to ℓ and that mapping is shown to remain transferable across geometry, loading mode, rate and temperature [140].

Moreover, mesh refinement alone does not constitute solution verification: ℓ must remain fixed while h/ℓ (h denotes the characteristic element size of the phase-field discretisation), the time increment and nonlinear-solver tolerances are varied. Convergence should then be demonstrated for the initiation load, crack topology and fracture dissipation, rather than inferred from a visually similar final phase-field contour.

5.2 Applications of PFM to PBXs and solid propellants

Applications of PFM to PBXs have mainly examined quasi-static fracture under stress states for which tension-compression asymmetry is decisive. Cao et al. [81] developed an asymmetric phase-field formulation for PBX cracking under combined tensile and compressive states, while Yuan et al. [141] applied PFM to arc-shaped Brazilian-disc specimens and reported close agreement in failure load for the tested configuration. These studies show that the crack-driving energy can be tailored to the pronounced strength asymmetry of PBXs. Their validation remains configuration-specific, however: agreement in peak load and macroscopic crack path does not by itself determine whether local failure occurred by crystal-binder debonding, binder cracking or crystal fracture, nor does it establish transfer across confinement, loading rate or temperature.

For solid propellants, the central advance has been the integration of fracture with time-dependent binder behaviour and explicit material interfaces. Wang et al. [142] coupled viscoelastic deformation with a fracture phase field and an auxiliary interphase field in a mesoscale HTPB-propellant model. The auxiliary field describes the particle–binder geometry, while the evolving fracture field represents damage across the interphase and the surrounding material. Fig. 8 combines two complementary descriptions of the failure process for a single AP particle embedded in an HTPB matrix. The successive damage-field snapshots in Fig. 8(A) show AP-HTPB interfacial damage developing before a crack traverses the surrounding matrix, whereas Fig. 8(B) presents the associated double-peaked force-displacement response. The characteristic points N, L and M denote the first force maximum, the force minimum following the loss of interfacial load-carrying capacity and the second force maximum, respectively. The study directly demonstrates that PFM can represent the simulated transition from particle-binder debonding to matrix cracking in a propellant mesostructure. The result remains specific to the adopted two-dimensional geometry, constitutive description and calibration, and should not be interpreted as validation across particle populations, loading modes or propellant formulations.

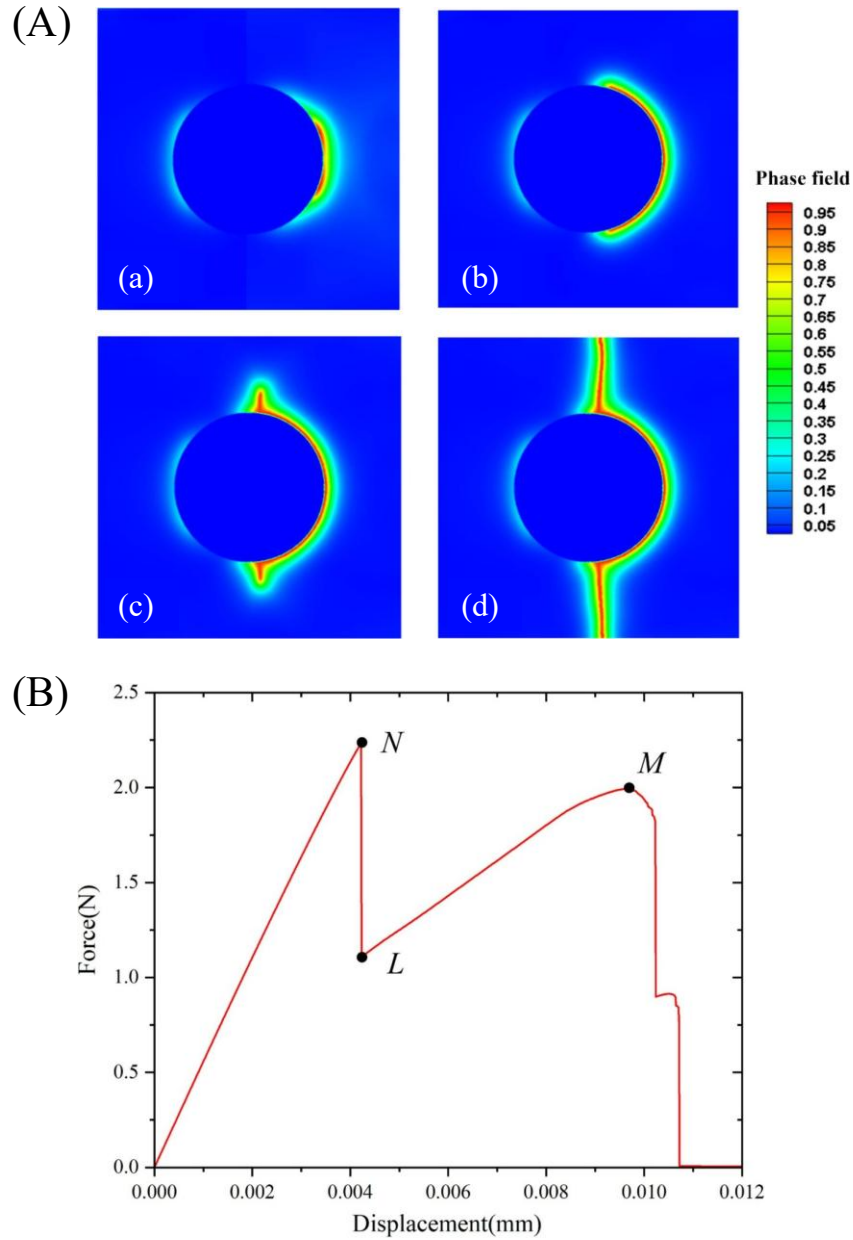


Fig. 8. Phase-field simulation of a single AP particle embedded in an HTPB matrix under tension [142]: (A) successive phase-field damage contours (a)-(d), showing the evolution from AP-HTPB interfacial damage to matrix cracking; and (B) the accompanying global force-displacement response, in which N, L and M denote the first force maximum, the force minimum after the loss of interfacial load-carrying capacity and the second force maximum, respectively.

Recent propellant studies have extended this constitutive coupling rather than merely changing the crack solver. Mei et al. [143] coupled viscoelasticity to fracture and used adaptive time stepping to analyse cyclic, relaxation and tensile responses, with model parameters identified from experimental data. Their subsequent viscoelastic-plastic formulation [63] incorporated confinement- and rate-dependent energy storage and was assessed against tensile and compressive force-displacement

curves and fracture morphologies. These results demonstrate that the predicted phase-field evolution depends on how recoverable, viscous and plastic energies enter the crack-driving force. They also leave a demanding transfer test: parameters calibrated over one set of histories should predict other rates, confinement levels, temperatures and geometries without retuning. Taken together, direct PBX and solid-propellant applications demonstrate PFM for two-dimensional specimen- and mesoscale fracture under the investigated loading conditions; anisotropic polycrystalline fracture, engineering-scale three-dimensional grain failure and crack-to-reaction coupling have not yet been demonstrated for these material systems.

5.3 Capabilities and limitations of PFM for PBXs and solid propellants

The main capability of PFM is the representation of nucleation and interacting crack topologies within a continuum discretisation. Direct applications to PBXs and solid propellants demonstrate tension-compression-asymmetric cracking, viscoelastic or viscoplastic fracture, and diffuse descriptions of particle-binder interfaces [63,142,143]. These features are supplied by the selected free energy and evolution laws; they are not inherent consequences of using a phase field. The demonstrated energetic-material scope is currently concentrated on two-dimensional mesoscale or specimen-scale calculations evaluated using global responses and selected crack morphologies. Thermo-mechanical PFM of HMX single crystals [67] provides constituent-scale energetic-material evidence, whereas anisotropic polycrystalline formulations developed for generic non-energetic materials [144] remain potential extensions to PBXs and solid propellants.

At finite ℓ , the diffuse degradation zone replaces the mathematically sharp crack tip and modifies the pointwise Williams field within the regularised region. The classical $r^{-1/2}$ LEFM asymptotics may be interpreted in an outer annulus satisfying $\ell \ll r \ll L$, where r is the distance from the crack tip and L is a relevant structural length, provided that such scale separation exists. Stress-intensity factors are consequently not intrinsic phase-field variables; meaningful K_I , K_{II} or K_{III} values require a separate interaction-integral, domain-integral or asymptotic-extrapolation procedure evaluated outside the diffuse zone and checked for sensitivity to both discretisation and regularisation length [145,146].

The diffuse representation removes explicit topology updates but introduces an internal length and a tightly coupled nonlinear problem. Because the mesh must resolve ℓ , three-dimensional particle-resolved calculations become expensive, while insufficient resolution can alter the initiation load, crack path and dissipation. More fundamentally, G_c , ℓ , the degradation law and the tension-compression split can compensate for one another when inferred from a single global response. Consequently, G_c fitted jointly with these quantities to a single structural response is a formulation-dependent effective resistance; interpreting it as transferable fracture

toughness requires independent fracture-resistance data and confirmation across geometries, loading modes, rates and temperatures. A visually plausible damage field may therefore conceal non-unique parameters or an incorrect partition among interface failure, binder dissipation and crystal fracture. Crack closure, friction and cyclic reopening also require additional treatment because standard irreversibility prevents healing but does not supply contact tractions. The experimental base remains limited for three-dimensional microstructures, long-term cyclic or ageing histories, high-rate confinement and local thermo-chemical feedback. In particular, a phase-field damage variable is not a temperature or reaction-progress variable; hot-spot and ignition predictions require independent energy-partition, transport and kinetic models with local thermal validation.

Accordingly, PFM is conditionally applicable to particle–binder debonding when the diffuse-interface representation is independently calibrated and competing bulk failure modes are included. Its demonstrated use is currently confined to mechanism-oriented PBX and solid-propellant calculations at the mesoscale and specimen scale; engineering-scale lifetime assessment, three-dimensional grain fracture, and hot-spot or ignition prediction remain prospective applications contingent on numerical verification, parameter transfer without retuning, and multiphysics validation.

6. Peridynamics: nonlocal continuum simulation of spontaneous fracture and fragmentation

PD is attractive when a fracture problem involves multiple initiation sites, rapid branching, fragmentation or large displacement, for which repeated updates of a sharp-crack topology become cumbersome. The method replaces the local stress-divergence operator with finite-range integral interactions, so displacement discontinuities can develop within the governing equation rather than through an external tracking algorithm [45,79,147]. For PBXs and solid propellants, however, this topological flexibility is useful only when the nonlocal constitutive description preserves the relevant binder, crystal and interface responses. The central issue is therefore not simply whether PD can generate a crack, but whether its horizon-scale parameters, failure law and multiphysics source terms can be identified and transferred across loading conditions.

6.1 Nonlocal formulation and material-specific parameterisation

In PD, a material point $\mathbf{x}$ interacts with every point $\mathbf{x}'$ in the family H defined by a finite horizon δ . Introducing the reference bond $\xi = \mathbf{x}' - \mathbf{x}$ and the relative displacement $\eta = \mathbf{u}(\mathbf{x}', t) - \mathbf{u}(\mathbf{x}, t)$, the equation of motion may be written as

$$\rho \ddot{\mathbf{u}}(\mathbf{x}, t) = \int_H \mathbf{f}(\mathbf{u}(\mathbf{x}, t), \mathbf{u}'(\mathbf{x}', t), \mathbf{x}, \mathbf{x}', t) dV_{\mathbf{x}'} + \mathbf{b}(\mathbf{x}, t) \quad (8)$$

where ρ is the mass density, $\mathbf{f}$ is the pairwise force density and $\mathbf{b}$ is the body-force density [79,148]. A common microelastic-brittle model characterises bond deformation by the stretch $s = (\|\boldsymbol{\xi} + \boldsymbol{\eta}\| - \|\boldsymbol{\xi}\|) / \|\boldsymbol{\xi}\|$ and irreversibly deletes the interaction when s reaches a critical value s_c . The local damage variable ψ is then evaluated from the fraction of broken bonds within the horizon. As illustrated in Fig. 9, intact and failed interactions can coexist in the same neighbourhood, allowing a connected discontinuity to emerge from progressive bond loss without prescribing a crack path.

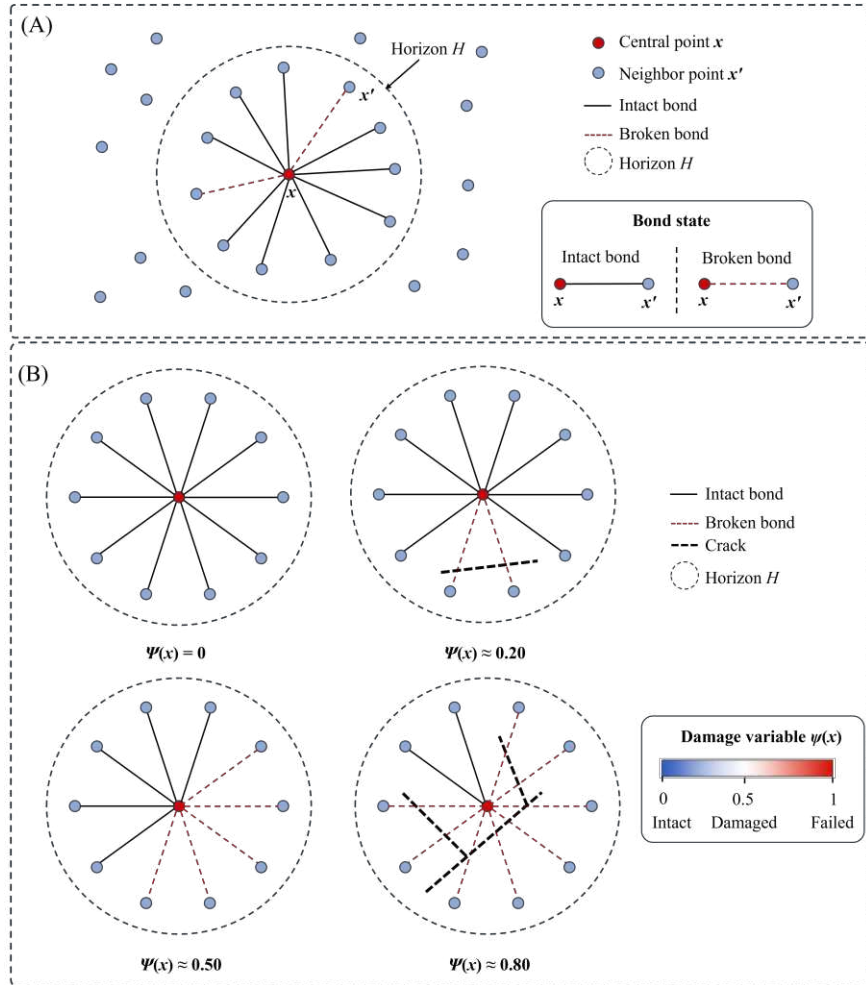


Fig. 9. Peridynamic representation of nonlocal interaction and damage: (A) The central material point $\mathbf{x}$ interacts with neighbouring points $\mathbf{x}'$ within the horizon δ ; (B) Schematic evaluation of the pointwise damage variable $\psi(\mathbf{x})$ from the statistics of bond states within H .

The bond-based formulation provides a transparent connection between bond failure and crack formation, but isotropic linear elasticity is restricted to fixed Poisson ratios— $\nu=1/4$ in three dimensions and $\nu=1/3$ in the usual two-dimensional plane-stress

setting. Ordinary state-based PD permits independent volumetric and shear responses by allowing each bond force to depend on the deformation of the whole family while remaining parallel to the deformed bond. Non-ordinary state-based and correspondence formulations can further incorporate classical viscoelastic, plastic or anisotropic constitutive laws [149-151]; for example, Lai et al. related the state-based nonlocal integral operator to its local differential counterpart and implemented finite-strain Drucker–Prager plasticity for geomaterial fragmentation [152]. Constitutive-correspondence formulations can incorporate conventional constitutive laws, but their particle discretisations may admit zero-energy deformation modes that produce spurious oscillations and non-physical damage. Stabilisation or sub-horizon treatments are therefore required, although their effects on energy consistency and crack evolution must be assessed [153]. This capability is relevant to rate-dependent binders and energetic crystals, although the imported bulk law does not automatically determine an appropriate nonlocal failure law; treatment of interfaces and the energy dissipated by bond degradation must still be established independently.

Tensorial stress and strain measures provide a further connection between interaction-based PD and local continuum descriptions. The peridynamic stress generated by pairwise forces can be expressed as a weighted static first Piola–Kirchhoff Virial stress, providing a directly computable tensor for evaluating stress concentrations within bond-based PD [154]. A complementary three-dimensional micro-potential formulation constructs a nonlocal strain measure that separates volumetric and deviatoric deformation, defines the force–deformation response through a Xu–Needleman micro-potential and governs irreversible bond failure using an energy-release-rate criterion; its deformation and fracture response has been assessed under mode I, mode II and mode III loading [155]. These constructions strengthen the relationship between finite-range interactions and continuum tensor measures, while the resulting fields and fracture predictions remain dependent on the horizon, spatial integration and material-specific parameter identification.

The horizon δ is both a constitutive length and a numerical support, and its effect cannot be assessed independently of the material-point spacing Δx . Relations derived for a homogeneous microelastic solid are therefore insufficient for a PBX or propellant mesostructure containing crystal–binder, particle–binder and binder–binder interactions. These bond families may require distinct elastic, rate-dependent and failure parameters constrained by constituent tests, interface experiments and notched-fracture data. Numerical verification should keep the intended physical horizon fixed while refining Δx , and should examine crack path, initiation time, dissipated energy and fragment statistics in addition to the peak load. Surface correction, partial-volume integration, imposed boundary layers and the time increment must also be reported because truncated neighbourhoods and discrete point layouts can otherwise change the apparent stiffness or preferred crack direction [44,45].

The discussion above already touches on two distinct convergence notions that must not be confused. At fixed δ , m -convergence tests the spatial discretisation of a given nonlocal problem; convergence towards local elasticity is a different limit. For sufficiently smooth elastic fields, the PD operator approaches its local counterpart as $\delta \rightarrow 0$ when the spatial discretisation, quadrature and nonlocal boundary conditions remain consistent with the shrinking horizon. A discretisation is asymptotically compatible only if it preserves this limit along the coupled δ - Δx refinement path. This elastic limit does not by itself establish convergence of fracture predictions, because the failure law and the mapping of interaction work to G_c can depend on δ [156].

6.2 Applications of PD to PBXs and solid propellants

Peridynamic applications to PBXs encompass mechanical damage and fracture and, in explicitly coupled formulations, the thermal and chemical fields governing hot-spot formation and ignition. Hou and Zhang [10] used PD to examine laser ignition in a cracked energetic material, linking the pre-existing discontinuity to heat transfer and reaction kinetics. For confined impact, Deng et al. [68] constructed a mechanical-thermal-chemical PD model incorporating inelastic deformation, frictional heating, heat conduction and Arrhenius kinetics. As shown in Fig. 10, the calculation resolved strong spatial differences in temperature at an impact velocity of 120 m s^{-1} . The study demonstrates how the peridynamic damage field can provide an evolving geometry for thermal and reaction calculations; nevertheless, agreement in an ignition time or a global damage pattern does not independently validate the partition of plastic, frictional and fracture work into heat, nor the local hot-spot temperature.

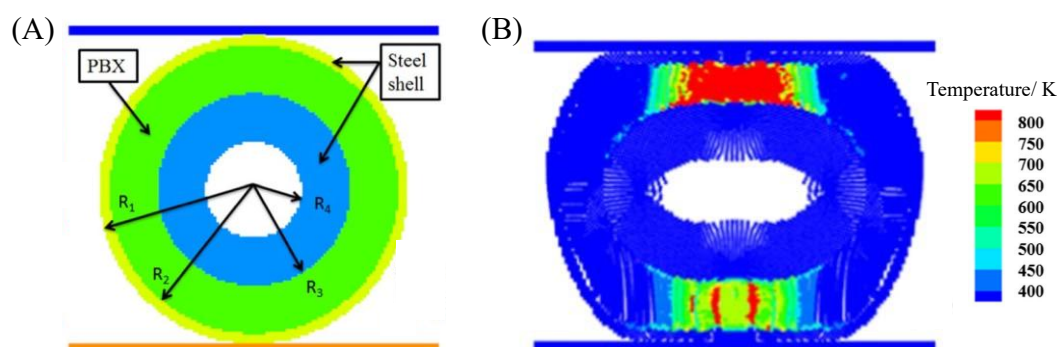


Fig. 10. Coupled peridynamic simulation of a confined PBX under impact: (A) partition of the monitored regions and (B) predicted temperature field at $t = 120 \mu\text{s}$ for an impact velocity of 120 m s^{-1} [68].

At specimen and mesostructural scales, the modelling objective shifts from ignition to the competition among interface separation, binder damage and crystal fracture. Li et al. [157] applied non-ordinary state-based PD to Brazilian-disc fracture and modified the influence function to reduce loss of accuracy in strongly damaged

neighbourhoods. Huang et al. [158] combined bond-based PD with Voronoi mesostructures to compare single- and double-layer coatings around HMX crystals. Fig. 11 shows that changing the coating architecture altered both the extent of crystal damage and the balance between transgranular and intergranular failure. This result is mechanistically informative, but its predictive use depends on whether the coating and interface bonds are calibrated independently.

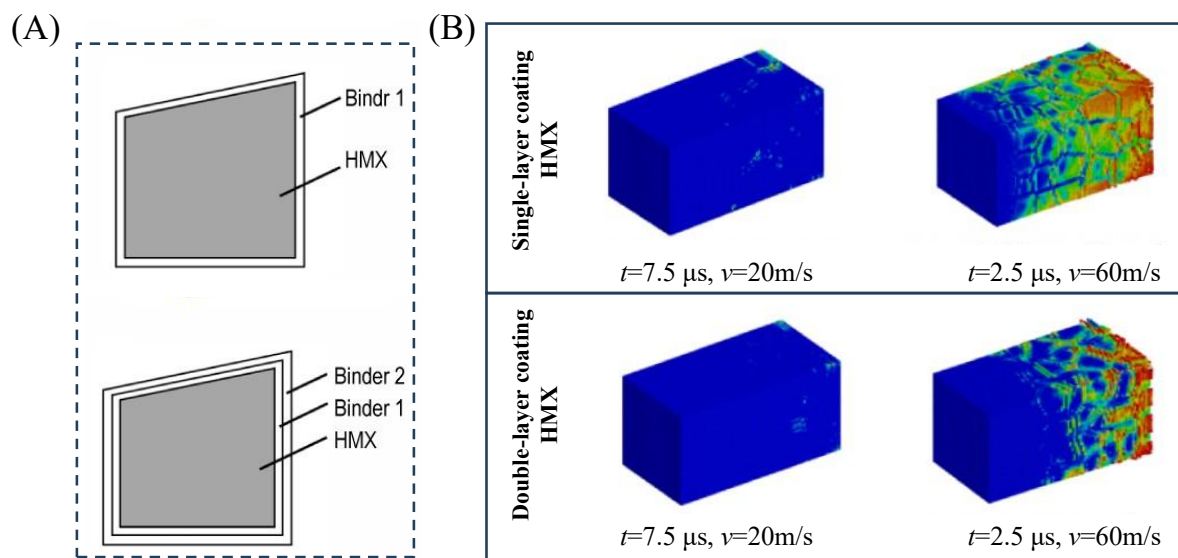


Fig. 11. Peridynamic comparison of coated HMX mesostructures under the same imposed displacement: (A) single- and double-layer coating geometries and (B) predicted damage distributions [158].

PD has also been used as a carrier for time-dependent constitutive behaviour. Li et al. [159] embedded a Burgers-type viscoelastic response and time-stress equivalence into a peridynamic force law for PBX 9502, obtaining creep curves consistent with measurements over the investigated temperatures and stresses. This supports the representation of viscoelastic deformation within a nonlocal peridynamic formulation, but creep agreement alone does not validate a fracture criterion: transfer to crack initiation and growth requires independent fracture data and a demonstration that bulk viscous dissipation is not absorbed into fitted bond-failure parameters.

Direct applications of PD to solid propellants are limited in number. Liu et al. [66,160,161] developed a sequence of bond-based PD studies for NEPE propellant covering single-edge-notched tension, mixed-mode I/II loading and rate-dependent fracture. Throughout this series, the time-dependent material response was described using a generalised Maxwell model in Prony-series form, while fracture was represented by irreversible bond failure governed by a critical-stretch criterion. Fig. 12 illustrates that the model reproduced the experimentally observed crack-tip blunting and the accompanying evolution of the damage field. Their mixed-mode calculations

further captured the change in crack trajectory with the initial notch inclination; the simulated local fracture process and corresponding load-displacement curve for $\beta=60^\circ$ are presented in Fig. 13. Comparisons with load-displacement curves and observed crack morphologies provide stronger validation than a final damage contour alone, and the reported errors for the mixed-mode global response remained below 9.3% [66]. The demonstrated scope nevertheless comes predominantly from two-dimensional, monotonic tests on one propellant family, so transfer to other binder chemistries, particle gradations, temperatures, confinement levels and cyclic histories remains unestablished.

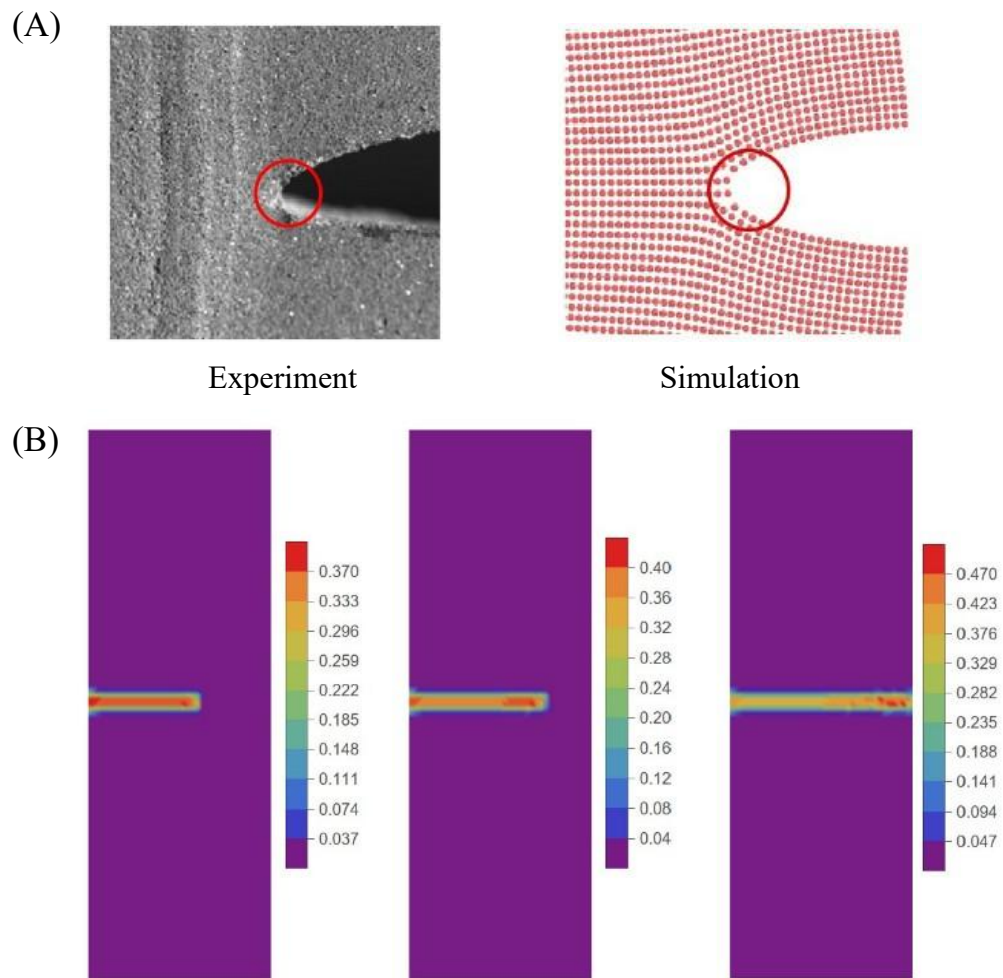


Fig. 12. BBPD simulation of a single-edge-notched NEPE propellant under tension: (A) crack-tip blunting observed experimentally and numerically and (B) evolution of the predicted damage field [161].

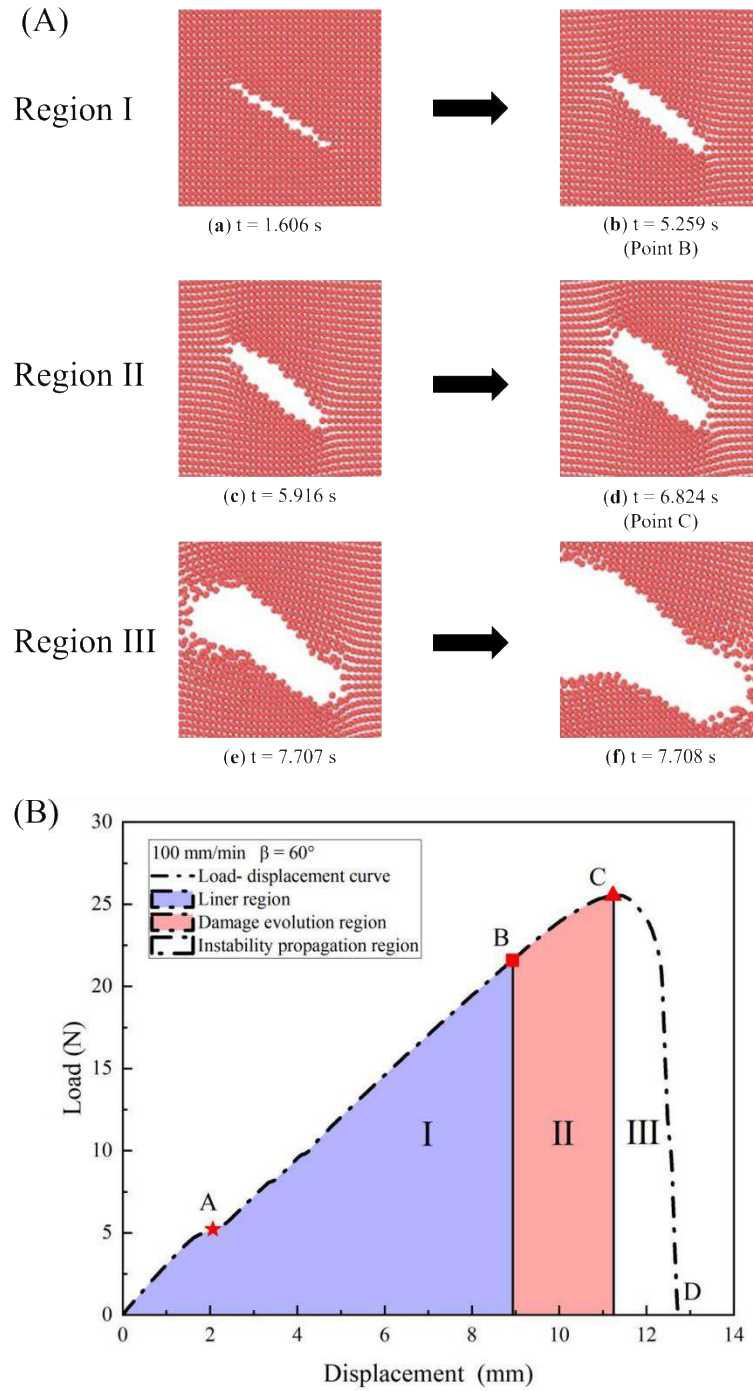


Fig. 13. Peridynamic prediction of mixed-mode crack growth in NEPE propellant for an initial crack inclination of $\beta=60^\circ$ [66]: (A) representative local fracture patterns within three successive response regimes; and (B) the corresponding load-displacement response.

Taken together, these studies demonstrate the direct application of PD to cracked-PBX laser ignition, PBX impact damage and NEPE-propellant crack growth. Although mechanical–thermal–chemical PD has also been implemented for confined PBX impact [68], the available comparisons do not independently validate local

heat-source partitioning, hot-spot temperature or reaction evolution. The demonstrated mechanical and multiphysics capabilities of PD should therefore be distinguished from the still limited predictive qualification of coupled ignition calculations.

6.3 Capabilities and limitations of PD for PBXs and solid propellants

PD is most distinctive when fracture topology is an output of the calculation: interacting microcracks, rapid branching, fragmentation and large relative motion can be represented without enrichment functions or remeshing. Direct PBX and solid-propellant studies demonstrate its use for cracked-PBX laser ignition, specimen-scale crack growth, mesostructure-dependent damage, rate-dependent NEPE fracture and impact-driven PBX response [10,157-159]. Its integral form also provides a common computational setting for mechanics, heat transfer and reaction, which is attractive for impact-damaged PBXs. These advantages do not make PD universally preferable. For quasi-static networks of interacting cracks, the choice between PD and PFM should be based on the available constitutive calibration, required treatment of contact and fragmentation, and computational scale rather than on crack-path visualisation alone [162,163].

The same nonlocality that enables spontaneous discontinuities introduces a coupled resolution problem. Crack initiation and dissipation depend on δ , Δx , neighbourhood integration, bond or force-state law and surface treatment. Regular point layouts may bias propagation directions [44], while incomplete horizons near external boundaries, pores and material interfaces can create artificial compliance unless corrected consistently. The resulting discretisation sensitivity should be assessed through m -convergence, where $m = \delta/\Delta x$ is the horizon-to-point-spacing ratio and Δx is reduced while δ and the model parameters are held fixed; reducing δ with resolution-dependent recalibration, or refining Δx at fixed m so that δ changes simultaneously, does not isolate numerical convergence. Credible studies should therefore state which length is regarded as physical, demonstrate convergence at fixed material parameters, and test the calibrated model on geometries or loading histories not used for fitting. The cost of evaluating many neighbours, together with the small stable time increment commonly required in explicit dynamics, remains a major obstacle to three-dimensional particle-resolved and engineering-scale calculations.

For energetic composites, the interpretation of damage and heat deserves equal caution. The bond-damage variable ψ is a neighbourhood statistic, not a direct measure of crack opening, porosity or temperature. In a thermo-mechanical–chemical model, plastic work, viscoelastic loss, frictional slip and fracture dissipation must be converted into heat through separately defined efficiencies; heat transport and kinetics must then evolve with damage, reaction-induced volume change and changing material properties. Without spatially and temporally resolved measurements—such as high-speed imaging

or DIC for cracks, X-ray tomography for internal damage and infrared diagnostics for temperature—different source-term choices may reproduce the same ignition delay. Current PD studies therefore support qualitative-to-semiquantitative mechanism assessment for PBX impact and specimen-scale fracture prediction for NEPE propellant, but engineering use requires transferable constituent and interface parameters, three-dimensional horizon/discretisation studies and validation of local mechanical and thermal observables under withheld conditions.

Cross-scale studies place an important boundary on this interpretation. Mesoscale reactive simulations, statistical crack mechanics, surface-defect studies and atomistic–continuum pore-collapse calculations show that defect population and dissipation mechanism can alter initiation independently of a scalar bond-damage field [164-167]. Atomistic studies may inform trends in propellant constituents and interfaces [168,169], but conversion to peridynamic bulk and failure parameters requires an explicit scale-bridging relation.

7. Discrete element method: particle-resolved contact, debonding and fragmentation

The DEM is most informative when particle rearrangement, contact-force transmission, interfacial bond loss or fragmentation is itself the target of prediction. Unlike continuum fracture methods, DEM represents the material as interacting discrete bodies and obtains the macroscopic response from their translation, rotation and contact evolution [49,51,52]. This description is physically natural for loose powders and fragmented material. For consolidated PBXs and solid propellants, the discrete particles may represent actual energetic grains, binder domains or coarser computational units; the meaning of a contact and a broken bond must therefore be defined before the resulting crack pattern can be interpreted physically.

7.1 Particle dynamics, contact laws and material-specific parameterisation

A DEM domain is assembled from spheres, clumps, polyhedra or deformable particle clusters. For particle i , the translational and rotational equations of motion are advanced from the contact forces and moments acting over its current neighbour set [52,170]:

$$m_i \ddot{\mathbf{u}}_i = \sum_j \mathbf{F}_{ij} + \mathbf{F}_i^{ext} \quad (9)$$

$$I_i \dot{\boldsymbol{\omega}}_i = \sum_j \mathbf{M}_{ij} \quad (10)$$

where m_i and I_i are the particle mass and moment of inertia, $\mathbf{u}_i$ and $\boldsymbol{\omega}_i$ denote the translational displacement and angular velocity, respectively. $\mathbf{F}_{ij}$ and $\mathbf{M}_{ij}$ are the contact force and moment, and $\mathbf{F}_i^{ext}$ is the external force. The scalar-inertia form of Eq. (10) applies to spherical particles or planar rotation; general three-dimensional non-spherical bodies require a tensorial angular-momentum balance [54]. Contact detection updates the neighbour list, a force-displacement law supplies the normal and tangential interaction, and an explicit integrator advances the particle state. The stable time increment is consequently governed by the smallest effective mass and the largest contact stiffness, rather than by the specimen dimensions alone [171].

At contact level, the relative motion is decomposed into normal overlap and tangential slip. Linear spring-dashpot, Hertzian, elastoplastic and frictional laws provide different representations of compression, restitution and sliding [172]. Consolidated energetic composites additionally require bonded contacts capable of carrying tension, shear and, in some formulations, bending moment. Once a tensile, shear or mixed failure criterion is reached, the cohesive contribution is removed and the post-failure pair may separate or transmit compressive and frictional forces [170,173,174]. As illustrated in Fig. 14, the macroscopic crack is therefore not an inserted surface but a spatially connected path of failed contacts embedded in an evolving force network.

In a basic frictional contact law, normal force depends on overlap and contact stiffness, while tangential elastic force accumulates with relative tangential displacement until a Coulomb limit initiates sliding [51]. A contact bond transmits forces across a bonded pair; a parallel bond additionally represents a finite bonded cross-section and can transmit moments [170]. Consequently, debonding between distinct particles and fracture within a particle require different assignments of breakable contacts. An unbreakable rigid body representing one energetic crystal cannot resolve cracking within that crystal.

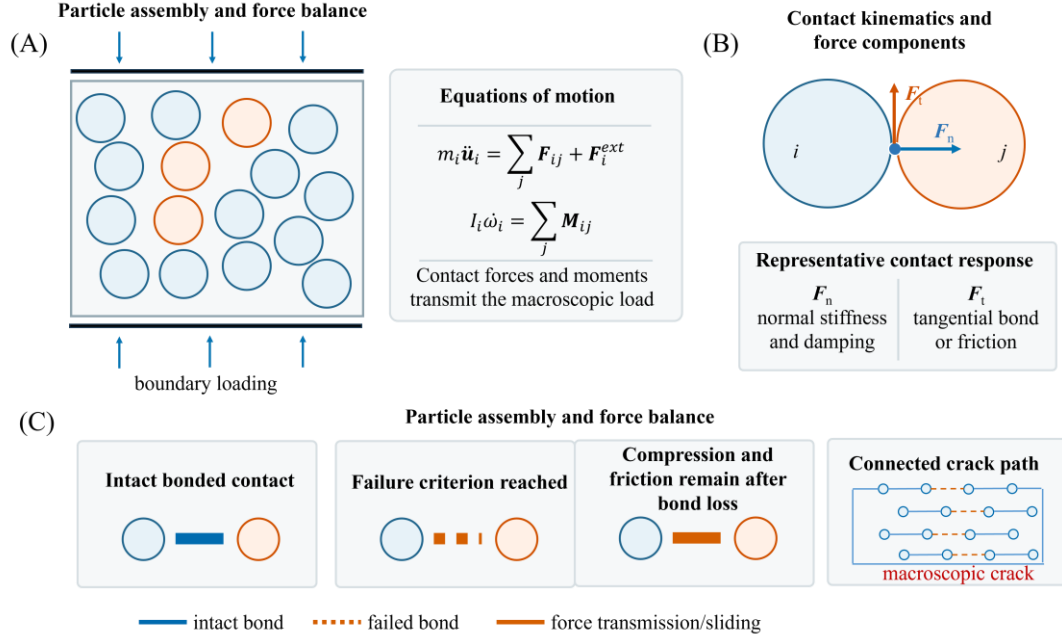


Fig. 14. Discrete-element representation of deformation and fracture [172-174]: (A) particle assembly and translational-rotational force balance; (B) contact-level kinematics and decomposition into normal and tangential force components; and (C) transition from an intact bonded contact to post-failure friction or separation, followed by coalescence of failed contacts into a macroscopic crack.

For PBXs and solid propellants, the apparent simplicity of a bonded contact conceals a scale-dependent constitutive choice. Crystal morphology, size distribution, phase fraction and initial porosity determine the packing and coordination network; contact stiffness, friction, rolling resistance and damping govern rearrangement and dissipation; bond stiffness, strength and failure envelope control the onset and topology of cracking. If one DEM particle represents an actual HMX, RDX or AP grain, crystal-crystal, crystal-binder and binder-binder contacts should be distinguished. If particles are coarse-grained computational units, the same parameters are effective quantities and cannot be interpreted as measured interface properties.

A single stress-strain curve cannot uniquely identify this parameter set because packing, stiffness, friction, bond strength and damping can compensate for one another [62]. Microstructural information should first constrain particle shape, gradation, phase fraction and porosity. Small-strain loading and unloading then provide information on recoverable contact stiffness, whereas compaction, shear and notched-fracture tests constrain friction, irreversible rearrangement and bond failure. Time-dependent and thermal parameters require additional creep, relaxation, rate and temperature data. Numerical credibility also depends on particle-size or coarse-graining sensitivity, specimen-to-particle size ratio, boundary friction, contact-search tolerance and time-step stability. Convergence should be evaluated in coordination number,

force-chain statistics, dissipated energy, crack topology and fragment distribution as well as in the global load response. For cross-resolution comparison, these dependencies should be expressed through d_p/L and, for coarse-grained particles, d_p/d_g , where d_p , d_g and L denote the computational-particle size, physical-grain size and characteristic problem dimension, respectively. When particles reproduce measured grains directly, varying d_p changes the material architecture rather than only the numerical discretisation; objectivity should then be assessed over statistically equivalent realisations and increasing representative volumes.

7.2 Applications of DEM to PBXs and solid propellants

Existing DEM applications and constituent-scale energetic-material studies relevant to PBXs and solid propellants address four physical processes: powder compaction and contact-network formation, deformation-induced debonding and cracking, time-dependent mechanical response, and impact-related energy dissipation.

For PBX processing, Sun et al. [175] reconstructed HMX particle morphologies from microscopy and represented the binder using deformable particles to investigate heterogeneous densification during compression moulding. Guo et al. [19] subsequently employed flexible particle clusters to examine the influence of crystal size on die-pressing behaviour. These studies demonstrate that DEM can relate particle morphology, size distribution and coordination evolution to local stress heterogeneity and macroscopic densification, thereby providing a particle-scale description of the processing-induced structure inherited by the consolidated PBX. The development of damage after consolidation was investigated more directly by Xiao et al. [20], who combined image-informed HMX geometries with phase-dependent contact laws to simulate PBX deformation under quasi-static compression and tension. As shown in Fig. 15, initially isolated contact failures progressively developed into distributed microcrack networks as the compressive strain increased. Analysis of contact forces and energy dissipation links the growing failed-bond network to the macroscopic response, which is a principal advantage of DEM. The red contact failures in such a calculation remain model-defined microcracks, however; establishing their physical fidelity requires independent spatial comparison with internal or surface crack measurements rather than agreement with the global curve alone.

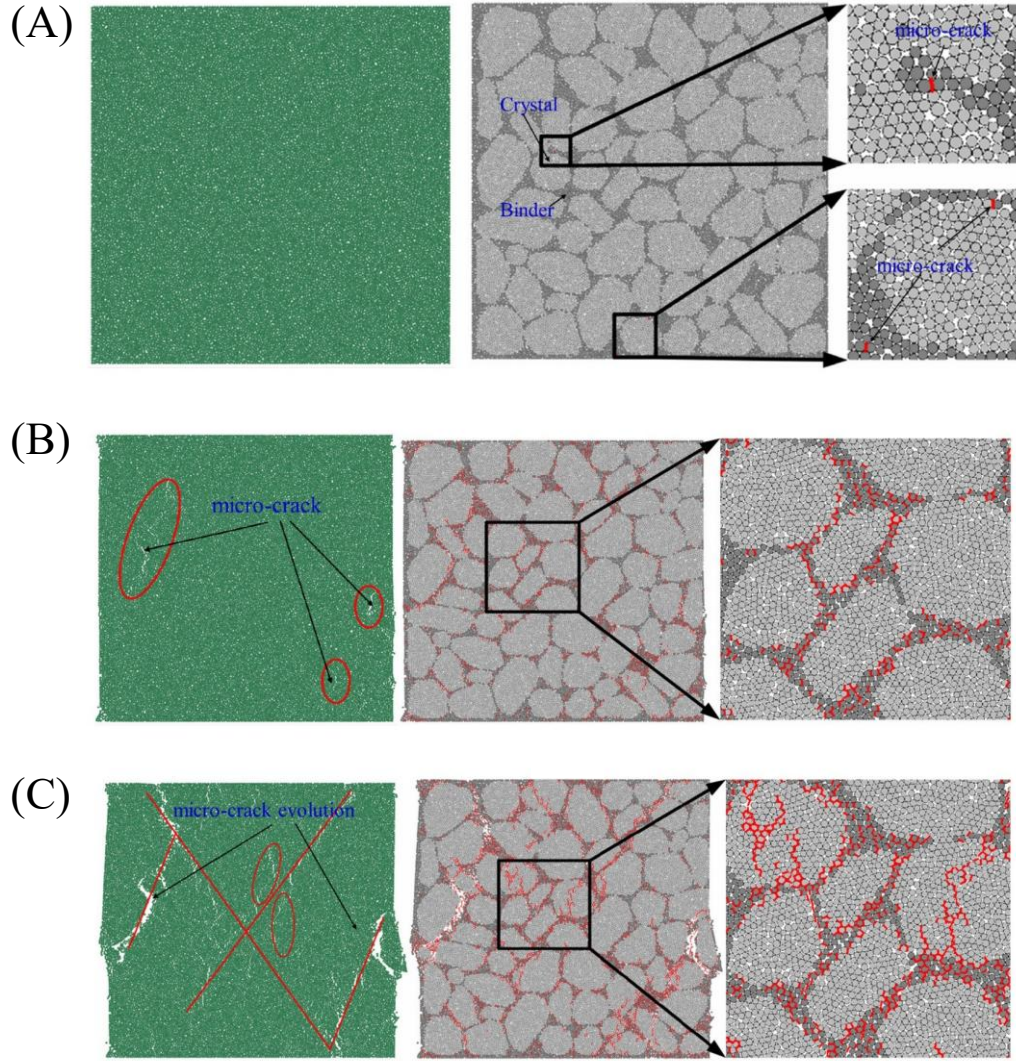


Fig. 15. DEM-predicted damage evolution of PBX under compression at a strain rate of 0.1 s^{-1} [20]: (A) $\varepsilon = 0.32\%$, (B) $\varepsilon = 1.27\%$, and (C) $\varepsilon = 1.60\%$. Each stage combines specimen-scale damage with crystal–binder and contact-level views.

Time-dependent propellant behaviour introduces a different requirement for the contact formulation. Pan et al. [21] implemented a modified soft-bond contact model based on rate-process theory within DEM to describe primary, secondary and tertiary creep as well as stress relaxation in HTPB and NEPE propellants. Fig. 16 presents the corresponding three-dimensional particle representations and comparisons between the simulated and measured tensile stress-strain responses. The results demonstrate that time-dependent contact laws can reproduce the pronounced nonlinearity and formulation dependence of particulate propellants within a common discrete framework.

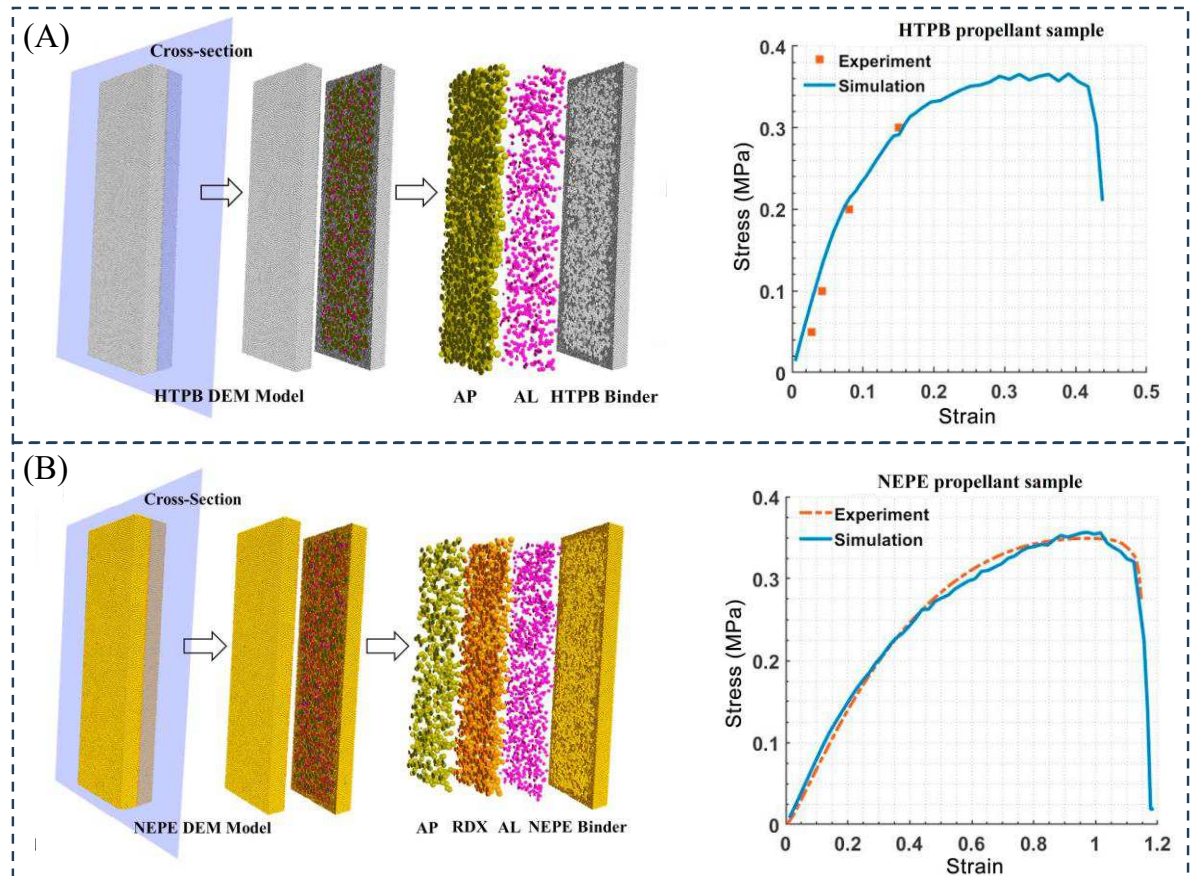


Fig. 16. Three-dimensional DEM representations and comparison of simulated and measured tensile stress-strain responses for (A) HTPB and (B) NEPE propellants [21].

Impact calculations extend DEM from deformation and fracture to local dissipation. At the energetic-constituent scale, Sun et al. [176] incorporated an elastoplastic contact law and evaluated plastic, sliding-friction and rolling-friction contributions during drop-weight impact of HMX explosives particles. This study provides direct constituent-scale evidence that DEM can resolve model-defined energy-dissipation pathways during HMX particle impact. The predicted dominance of rolling-friction dissipation is nevertheless sensitive to particle shape, rolling resistance, damping and the selected contact law. Because the simulated assembly contains HMX particles but no polymer binder, the result should be interpreted as constituent-scale evidence relevant to PBXs rather than validation of PBX composite response. Dissipated mechanical energy is not itself a hot-spot temperature: thermal contact conductance, heat capacity, conversion efficiency, conduction and reaction kinetics must be added and validated before the model can support ignition prediction.

The studies reviewed above demonstrate DEM applications to PBX powder compaction and contact-network evolution, to the global mechanical response of PBXs and propellants, and to time-dependent propellant deformation. Distributed

failed-contact patterns have also been computed for PBXs [20], while constituent-scale HMX impact calculations provide access to contact-level energy partition [176]. Their local correspondence to measured three-dimensional crack networks, particle-binder separation, fragment statistics and temperature fields remains insufficiently validated. Thus, demonstrated agreement in density or stress-strain response, or constituent-scale energy partition, should not be extended to PBX fracture or hot-spot prediction without independent local measurements and parameter-transfer tests.

7.3 Capabilities and limitations of DEM for PBXs and solid propellants

The principal advantage of DEM is its explicit representation of the evolving contact network between particles. PBX and solid-propellant studies demonstrate that this representation can relate particle morphology and packing to force-chain redistribution, densification, global deformation and model-defined bond failure [19-21]. Constituent-scale HMX particle calculations further demonstrate access to plastic and frictional dissipation during impact [176], but this evidence should not be treated as composite-scale PBX validation. Contact forces, coordination evolution, frictional sliding, particle rearrangement and post-failure interaction are therefore direct simulation outputs. Their physical interpretation remains conditional on the meaning and calibration of the discrete particles, contacts and bonds. Local continuum formulations based on conventional finite-element discretisations are generally more computationally efficient when deformation remains predominantly continuous and only a limited number of macroscopic cracks need to be predicted. DEM is consequently most defensible when particle-scale contact and rearrangement observables are required; predictive three-dimensional fracture, fragment interaction and thermo-chemical response remain limited by parameter identifiability, scale translation and local validation.

Predictive use is limited chiefly by scale translation and parameter identifiability. Particle shape and coarse-graining change coordination, fabric and force transmission; contact stiffness and bond density determine the effective modulus; friction, damping and bond failure jointly control dissipation and post-peak response. Several parameter combinations can reproduce one loading path, especially when only global data are available. Calibration requires independent constraints on packing, elastic recovery, interface or bond strength, frictional response and rate-temperature dependence, whereas validation requires tests on geometries and histories excluded from fitting. The required particle count rises rapidly when real grain sizes are resolved in three dimensions, while contact detection and the stiffness-controlled explicit time increment make component-scale simulations expensive. Representative-volume and particle-size effects must consequently be demonstrated rather than assumed.

Thermo-mechanical extensions require additional qualification. Recent particle-scale modelling of porous propellant has linked impact fracture to thermal and combustion response [177], but contact or bond dissipation is not itself a temperature model; conversion efficiencies, thermal contact, heat transport and kinetics must be independently calibrated and validated.

8. Prospective multimethod coupling and data-enabled modelling for PBXs and solid propellants

The methods reviewed in Sections 3-7 resolve different parts of the fracture process: local continuum formulations represent the rate- and temperature-dependent deformation of an intact binder-dominated body; interface formulations describe particle-binder separation; the nonlocal continuum theory of PD accommodates crack nucleation and branching; and DEM, as a discrete particle method, directly resolves post-separation contact and fragmentation. Because each method resolves only part of the fracture process, a more productive direction is to couple complementary descriptions so that each is used only where its kinematics and constitutive assumptions remain physically appropriate. Although such frameworks have been primarily developed for composites, metals, and geomaterials, their potential for energetic material applications is substantial.

8.1 Coupling principles and model architecture

A hybrid model should be constructed around a physical transition that cannot be represented adequately by one method. Relevant transitions include intact viscoelastic deformation to fragment interaction, localised crack nucleation to structural-scale response, and competition between bulk cracking and particle–binder debonding. This mechanism-centred view is more useful than combining solvers solely to offset their individual numerical limitations. It also determines whether the coupling should be concurrent, with two descriptions active in adjacent or overlapping domains, or hierarchical, with information passed between scales or with one representation replacing another after a transition criterion is satisfied.

As shown in Fig. 17, the proposed workflow begins with material architecture and loading conditions, identifies the unresolved physical transition, and then selects the least complex coupling capable of resolving it. FEM-DEM is directed towards continuum-to-fragment evolution; PD-FEM provides nonlocal-to-local continuum coupling between a fracture-critical PD subdomain and a surrounding classical finite-element domain; XFEM-CZM and PFM-CZM represent interactions between bulk cracks and weak interfaces; and machine learning assists parameter inference, surrogate evaluation and adaptive model allocation. These routes are complementary rather than cumulative. In particular, a model containing more fracture formulations is

not necessarily more physical if the same dissipation process is represented more than once.

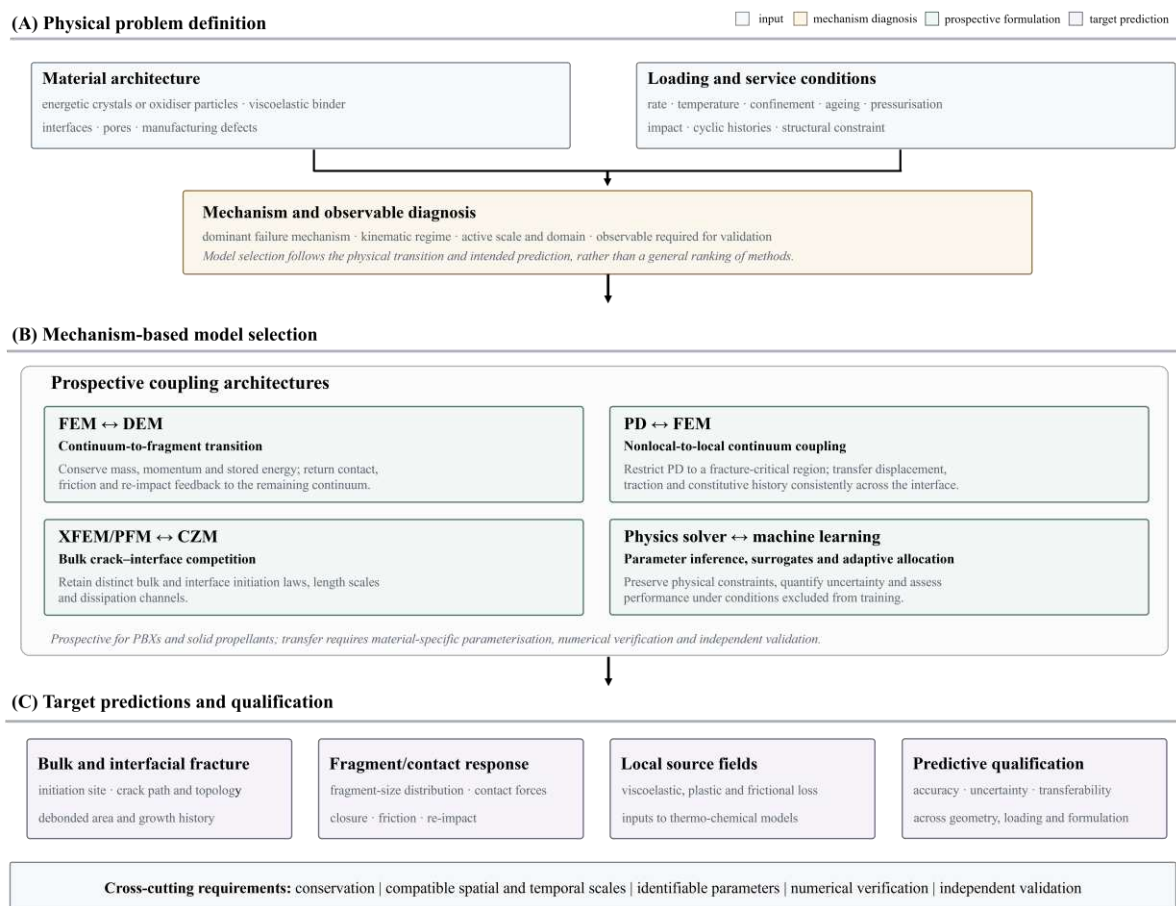


Fig. 17. Mechanism-centred workflow for selecting and qualifying prospective coupled fracture-modelling frameworks for PBXs and solid propellants. Colours distinguish problem inputs, mechanism diagnosis, prospective formulations and target predictions.

The principal difficulty is not exchanging numerical fields but preserving their physical consistency. Displacement and traction must remain compatible across interfaces, mass and momentum must be conserved during continuum-to-discrete conversion, and energy dissipated by one description must not reappear as damage or heat in another. Spatial resolution must be sufficient for the smallest active fracture or cohesive length, while temporal coupling must accommodate the different stability limits of local continuum discretisations, nonlocal continuum discretisations, discrete-particle dynamics and contact algorithms. Switching criteria should depend on a physically interpretable state variable—such as loss of load-carrying capacity, accumulated fracture energy or contact formation—rather than on mesh-dependent damage alone. Verification must consequently examine interface reflections, energy balance and path independence before the coupled model is calibrated against material tests.

8.2 Coupling continuous and discontinuous descriptions

FEM-DEM coupling is a natural candidate when an initially continuous body evolves into fragments whose collision, friction, closure or re-impact alters the subsequent response. Continuum-to-discrete conversion techniques developed for geomaterials and structural fracture provide the basic algorithmic architecture [178,179]. In a solid-propellant grain, FEM could represent bulk finite viscoelastic deformation during pressurisation, while DEM would be activated only after intersecting cracks create blocks that separate and interact. At the PBX mesoscale, the same strategy could describe the transition from distributed particle-binder damage to granular flow under severe compression or impact. Its use is less compelling when the material remains kinematically continuous and only one dominant crack is required, because the additional contact parameters would not correspond to a new physical observable.

Transfer to energetic composites requires an energetically consistent conversion rule. The mass, momentum and stored energy of the deleted or converted finite elements must be assigned to the discrete entities, while the fracture energy expended during conversion must remain distinct from later frictional and collisional dissipation. Contact stiffness, damping, friction and residual bonding should be linked to constituent and interface behaviour rather than calibrated collectively against one global load curve. Large contrasts between the continuum and contact time scales may require subcycling or asynchronous integration, but these procedures should not introduce artificial wave reflection or numerical damping at the coupling boundary. Fragment-size distributions, contact-force histories and reclosure behaviour are therefore as important as the external force response when assessing such a model.

PD-FEM coupling addresses a different problem: complex crack topology is required only within a small portion of a much larger component. Coupling schemes based on overlapping, constrained or blended subdomains [60,180] suggest a route in which PD is assigned to defects, notches, particle clusters or locally heated regions, whereas the surrounding grain is solved by FEM. An adaptive implementation could relocate or enlarge the PD domain as the damage front advances, thereby retaining the PD representation of crack nucleation and branching without applying the associated computational cost throughout the structure.

Direct nonlocal-to-local continuum coupling formulations provide concrete implementations of this strategy. An OSPD-NS-FEM coupling partitions fracture-critical and surrounding regions without a transition zone, and its implicit dual-based extension (DB-CA) transmits information through coupling elements for static crack-growth analysis [181,182]. In Abaqus, dual peridynamics has been implemented through UEL/VUEL and UMAT/VUMAT subroutines for implicit and

explicit PDFEM analyses, with a dual-based coupling strategy used to connect a nonlocal PDFEM subdomain and a classical FEM subdomain governed by local continuum mechanics [183]. Dual-horizon formulations additionally support variable horizons, nonuniform discretisations and implicit thermo-mechanical or chemo-mechanical fracture, while a recent DHPD-FEM implementation provides Abaqus UEL/VUEL routes for two- and three-dimensional coupled calculations [184-186]. Collectively, these developments can substantially reduce computational cost relative to an equivalently resolved full-domain PD model by confining nonlocal interactions to fracture-critical regions, while implementation within established finite-element platforms enables the use of mature solvers, parallel-computing infrastructure and post-processing tools for large-scale three-dimensional analyses.

The usefulness of this strategy depends on a transparent interface treatment. Truncated horizons and inconsistent quadrature can generate ghost forces; a crack crossing the PD-FEM boundary may experience an artificial change in resistance; and viscoelastic history variables must be transferred without resetting the local material state. The criterion used to activate PD must also precede, rather than follow, the loss of localisation information in the solution of the local continuum subdomain. FEM-DEM and PD-FEM should therefore not be treated as interchangeable acceleration techniques: the former is appropriate when separated fragments and contact become part of the physics, whereas the latter is appropriate when discontinuous evolution remains spatially localised within an otherwise continuous body. Although these formulations provide a general framework for large-scale PD analyses, their applicability to PBXs and solid propellants remains to be demonstrated. Transfer to these materials requires constituent- and interface-specific constitutive laws, verification of coupling consistency and discretisation convergence with respect to point spacing and horizon size, independent validation against local fracture measurements, and quantitative assessment of accuracy and computational performance.

8.3 Coupled formulations for bulk crack–interface competition

Mesoscale failure in PBXs and solid propellants commonly involves competition among particle-binder debonding, tearing of the binder-rich phase and fracture of energetic crystals. A single bulk-fracture formulation cannot represent the distinct strength, mode mixity and rate dependence of these paths without homogenising the mechanism that controls crack selection. The modelling challenge is therefore to construct coupled formulations that resolve competition between bulk cracking and interfacial debonding without conflating their initiation and dissipation mechanisms. Three prospective architectures are considered here: XFEM-CZM, PFM-CZM and interface PFM. In each case, the bulk and interface contributions to dissipation must remain separately identifiable.

XFEM-CZM is best suited to problems in which one or a few sharp bulk cracks interact with known weak interfaces. The approach has been used in fibre composites to combine intralaminar cracking with interfacial separation [187], and the corresponding energetic-material problem is the deflection, penetration or arrest of a crack at a crystal-binder boundary. A future formulation would require a crack-transfer rule between the enriched bulk and the cohesive interface, consistent mixed-mode dissipation, and contact or friction after complete separation [188]. The cohesive law should inherit the rate-temperature dependence and ageing sensitivity of the binder-particle interface; otherwise, the predicted competition between interfacial and bulk failure would change for numerical rather than physical reasons.

PFM-CZM is more attractive when bulk cracks nucleate at multiple sites, branch or coalesce while interface debonding remains explicitly distinguishable. Cohesive-type phase-field formulations such as PF-CZM [189] should be distinguished from a true domain combination in which PFM governs bulk cracking and interface elements govern separation. The latter architecture has been demonstrated for layered rubber-like materials [61] and provides a transferable concept for particulate energetic composites. Its implementation must reconcile the phase-field regularisation length, cohesive-zone length and interface discretisation, while maintaining separate bulk fracture energy and interfacial work of separation. If these length and energy scales are calibrated simultaneously against one structural response, the apparent agreement is calibration evidence and may conceal non-unique partitions of bulk cracking and debonding.

Interface PFM provides a third architecture in which an auxiliary phase field regularises a known material interface and interpolates its strength and fracture properties over a finite width, whereas a separate crack phase field evolves during loading. The interface field is therefore a geometric descriptor rather than an interfacial damage variable; debonding is represented by the crack field within the regularised interface region. Two-field formulations have captured matrix cracking, interface debonding and crack deflection in heterogeneous composites, including a cohesive phase-field formulation validated against observed microcrack trajectories in fibre-reinforced cement [190,191]. A finite-deformation extension has further coupled crack and interface phase fields with elasto-viscoplasticity to resolve creep-assisted bulk cracking and interface delamination in thermal barrier coatings [192]. For PBXs and solid propellants, interface PFM is therefore a potential route for complex crystal-binder networks. Its transfer requires independently identified bulk and interfacial strength and fracture energy, adequate resolution of both crack and interface regularisation lengths, preservation of interfacial strength and work of separation under regularisation, and validation against local debonding and crack-path measurements over the relevant rates and temperatures.

Method selection should follow both the expected crack morphology and the required representation of the material interface. XFEM-CZM offers a compact description when one or a few sharp cracks interact with discrete, known interfaces; PFM-CZM retains an explicit traction-separation law when distributed bulk cracking coexists with resolved interfaces; and interface PFM provides a common volumetric representation when complex interface geometry and bulk-interface crack competition must be treated without discrete interface elements. A triple XFEM-CZM-PFM formulation is not an obvious next step unless experiments identify three distinct fracture processes that require all three kinematic descriptions. The more defensible objective is the minimum mechanism-complete model, because every added formulation introduces another length scale, initiation rule and dissipation channel that must be independently constrained.

8.4 Machine-learning-assisted and multiphysics modelling

Machine learning should not be presented as a replacement for fracture mechanics. Its most credible role is to augment a physics-based model where parameter identification, repeated high-fidelity calculation or adaptive allocation of numerical resolution becomes prohibitive. Three uses are particularly relevant: inverse identification of constitutive and interfacial parameters; surrogates for computationally expensive PD, DEM or microstructure-resolved calculations; and decision models that determine where a PD subdomain governed by nonlocal continuum mechanics, a discrete-particle DEM subdomain or a locally refined subdomain should be activated.

Data-assisted constitutive modelling of hydroxyl-terminated polyether propellants [193] indicates how nonlinear rate-dependent response can be represented when a sufficiently structured dataset is available. The same principle could be extended to joint identification of viscoelastic spectra, cohesive parameters and damage kinetics using unnotched, notched and full-field tests rather than fitting each component independently. Regression and Bayesian strategies developed for cohesive-parameter inference and uncertainty propagation [62,194], together with learning-assisted DEM calibration [195], provide useful starting points. For energetic composites, the learned parameter map must retain formulation descriptors, particle statistics, porosity, temperature, loading rate, confinement and ageing state.

Surrogate modelling could substantially expand the feasible design and uncertainty space. Neural-network and micromechanics-assisted surrogates have accelerated progressive-damage and multiscale calculations in other heterogeneous materials [196-200]. For PBXs and propellants, a surrogate could replace repeated spatially restricted PD or DEM solves within a macroscale simulation, approximate a microstructure-sensitive constitutive closure, or support active selection of the next experiment. Multi-fidelity training is preferable to reliance on a single numerical

generator: inexpensive local continuum calculations can cover broad parameter ranges, while a smaller set of microstructure-resolved simulations and experiments corrects the response in fracture-critical regions.

Physics-informed learning offers an additional route for combining sparse measurements with field equations [201-203]. Potential uses include reconstructing stress or damage fields from DIC data, inferring spatially varying interface properties, and assimilating high-speed thermal measurements into a coupled fracture calculation. Domain decomposition, discontinuity-aware enrichment and adaptive sampling near evolving cracks are more appropriate than applying a generic physics-informed network to the entire specimen. The small, hazardous and formulation-dependent datasets available for energetic materials require a physical-validation strategy distinct from internal machine-learning train/validation/test partitioning. Specimens, formulations and loading regimes should be separated between model training or calibration and independent physical validation; uncertainty and out-of-distribution indicators should accompany every prediction; and physical constraints should enforce material symmetry, objectivity, irreversibility and non-negative dissipation. Synthetic data can reduce the number of dangerous experiments, but they cannot correct an omitted mechanism and will reproduce the assumptions of the generating model. Machine learning is consequently most valuable when it exposes parameter uncertainty, guides acquisition of informative measurements and accelerates a model whose conservation laws remain explicit.

Coupled peridynamics–smoothed particle hydrodynamics (PD–SPH) formulations provide a complementary architecture for blast-driven solid–fluid interaction: PD resolves deformation and fragmentation of the solid, whereas SPH represents the shock-loaded fluid or gas, with coupling established across the peridynamic horizon and SPH kernel support. Applications to soil fragmentation induced by buried explosives provide a methodological basis for potential extension to fracture-driven solid–gas interaction in PBXs and solid propellants [204,205]. Beyond solid–fluid interaction, future hybrid frameworks should also connect fracture to thermal and chemical response without treating all mechanical dissipation as heat. Viscoelastic loss, plastic work, frictional sliding, pore collapse and fracture-surface formation contribute differently to local heating; their partition and conversion efficiency must be defined before they are supplied to heat conduction and reaction kinetics. The thermal–chemical solution should then feed back through temperature-dependent stiffness, interfacial strength, thermal expansion, reaction-induced gas pressure and evolving contact. A mechanically coupled model may predict crack opening or dissipated work, but ignition prediction additionally requires spatially resolved temperature and reaction variables. High-speed infrared thermography, in situ imaging and ignition-delay measurements are therefore essential

for constraining this feedback rather than merely confirming the final macroscopic failure.

The most promising direction is thus an adaptive, hierarchical framework rather than a monolithic combination of every available method. A local continuum model would govern the intact structure; spatially restricted PFM, PD or CZM descriptions would be activated by mechanism-based indicators; DEM would take over only where separation creates contact-dominated motion; and data-assisted components would support calibration, surrogate evaluation and uncertainty control. Such a framework would advance fracture modelling of PBXs and solid propellants only if information transfer remains conservative, each dissipation mechanism is identifiable and validation progresses from constituent response to crack topology, fragment interaction, local temperature and, ultimately, ignition-related observables.

9. Comparative capability, validation and method-selection framework

The preceding sections show that XFEM, CZM, PFM, PD and DEM are not successive levels of numerical sophistication. All are embedded in governing frameworks subject to the relevant balance laws, but they differ in their kinematic representations of discontinuity, damage evolution and post-failure interaction. Their relative suitability therefore depends on the dominant fracture or fragmentation mechanism, the operative spatial and temporal scales, the expected crack topology and the target observables, rather than on any universal hierarchy of numerical sophistication. A meaningful comparison must distinguish the fracture representation supplied by the method from the constitutive, contact, thermal and chemical laws coupled to it. It must also distinguish numerical feasibility from predictive qualification: the ability to produce a crack pattern does not establish that the governing parameters are identifiable or that the same model will predict another geometry, loading history or material formulation.

9.1 Mechanism compatibility and computational scale

Table 2 compares XFEM, CZM, PFM, PD and DEM against the fracture processes most relevant to PBXs and solid propellants. The matrix evaluates the correspondence between each method's kinematic representation and the process to be resolved. It does not assign a universal ranking: a direct representation may still be poorly predictive when its constitutive parameters, spatial resolution or validation data are inadequate. The capability assignments are based on applications to PBXs, solid propellants and explicitly identified energetic constituents reviewed in Sections 3-7; potential extensions discussed in Section 8 are not included.

Table 2. Compact capability matrix for fracture modelling of PBXs and solid

propellants.

Fracture-modelling requirement	XFEM	CZM	PFM	PD	DEM
Resolved interface debonding	◐	•	◐	•	•
Representation of one or a few dominant crack paths	•	◐	◐	◐	○
Distributed nucleation, branching and coalescence	○	◐	•	•	•
Fragmentation and large separation	○	◐	◐	•	•
Closure, friction and rearrangement	◐	◐	○	◐	•
Coupling to continuum multiphysics fields	•	•	•	•	◐
Three-dimensional engineering-scale application	•	•	◐	○	○

Note: The classifications are based on applications to PBXs, solid propellants and explicitly identified energetic constituents reviewed in Sections 3-7. • indicates direct application evidence for the stated process; ◐ indicates application evidence limited by material scope, dimensionality, process coverage or local validation; and ○ indicates little or no direct evidence in the reviewed energetic-material literature. The symbols describe the application-supported scope of each method rather than a universal ranking of intrinsic capability, predictive accuracy or computational efficiency.

The matrix exposes two distinctions that are easily obscured by generic lists of advantages and disadvantages. The first is localisation density, which determines whether the model must resolve isolated cracks or interfaces or an interacting crack network. The second is post-failure kinematics. DEM is warranted when contact-network evolution, rearrangement or fragment interaction is itself an intended observable; if the body remains continuous apart from one dominant crack, replacing it with a particle assembly introduces additional parameters without resolving additional physics. These kinematic tendencies do not determine the constitutive damage law, heat transport or reaction kinetics; each remains a separate model component with its own parameters and validation observables.

Calibration and solution verification remain method-specific: XFEM requires independently constrained initiation and propagation laws together with control of enrichment, quadrature and crack increments; CZM requires identifiable strength and separation energy together with cohesive-zone resolution; PFM requires separation of fracture energy from the regularisation length together with convergence in h/ℓ at fixed

ℓ ; PD requires failure-law calibration together with independent assessment of point spacing, horizon and surface correction; and DEM requires contact-law calibration together with particle-scale, coarse-graining and representative-volume assessment.

Computational tractability depends on problem dimensionality and physical scale, the discretisation and resolution required to represent the fracture process, and the resulting algebraic or particle-system size. Table 3 summarises these attributes for PBX and solid-propellant applications and indicates the corresponding method-specific cost tendencies.

Table 3. Numerical scale and computational characteristics of fracture modelling for PBXs and solid propellants.

Method	Dimensionality and scale	Discretisation and resolution	Conditional cost tendency
XFEM	2D specimens and 3D structural-scale propellant-grain models [3,13,16,26,94,95].	FE mesh with local enrichment; the classical four-function basis adds n_{dim} Heaviside or $4n_{\text{dim}}$ crack-tip DOFs per enriched node. Key controls: h , quadrature and enriched-node count.	Favourable for sparse cracks; cost rises with multiple fronts, branching, contact and 3D tracking [206].
		FE mesh with cohesive interfaces; h must resolve the cohesive zone. Example: 1.0×0.8 mm, 98 HMX particles (25–98 μm) and 118,377 bulk/cohesive elements [119].	Favourable for a limited set of known interfaces; dense interface networks increase DOFs and stiffness constraints.
PFM	Predominantly 2D PBX/propellant mesoscale and specimen models; 3D HMX single-crystal evidence [63,67,81,141-143].	FE displacement–phase-field system; one scalar phase-field DOF per node. Key controls: h/ℓ , refined-zone extent and nonlinear iterations.	Uniform 3D resolution is costly; adaptivity is advantageous when fracture remains localised.
PD	Mainly 2D PBX/propellant mesoscale and specimen models; limited 3D engineering-scale evidence [10,66,68,157-159].	Meshfree material points with n_{dim} mechanical DOFs per point. Example: $60 \times 20 \times 5$ mm, 4,961 points, $\Delta x = 0.5$ mm and $\delta/\Delta x = 3.134$ [161].	Cost scales with point count, neighbour count and explicit time-step restriction; full-domain 3D analyses remain expensive.
DEM	2D PBX damage	Rigid-particle DEM; 3	Cost scales with

models; 3D HTPB/NEPE particle assemblies for deformation and time-dependent response [19– 21,175,176].	DOFs per particle in 2D and 6 in 3D. Key controls: N_p , coarse-graining and contact time step.	particle/contact count and the stiffness-controlled time step; most useful when contact and rearrangement are target observables.
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Note: n_{dim} , spatial dimension; h , FE size; ℓ , phase-field length; Δx , PD point spacing; δ , PD horizon; and N_p , point/particle count. Cost tendencies are conditional on accuracy, implementation, solver and hardware.

Mechanism compatibility and numerical tractability jointly govern the practical applicability of each formulation. XFEM and CZM concentrate additional resolution around enriched crack fronts or represented interfaces, favouring problems with sparse cracks or a limited set of candidate interfaces. In conventional full-domain implementations, PFM, PD and DEM distribute phase-field degrees of freedom, finite-horizon interactions or particle-contact calculations over larger portions of the domain, making computational demand more sensitive to spatial dimensionality and resolution. Method selection must therefore balance the representation required by the governing fracture mechanism and target observables against the resulting algebraic or particle-system size, with realised efficiency further dependent on discretisation, implementation, solver strategy, hardware and problem size.

9.2 Mechanism-based method selection

Method selection begins with the intended prediction rather than with a preferred solver. Material architecture, loading regime, spatial scale and target observable should identify the dominant kinematic event and the minimum fracture representation required to resolve it; the method-specific correspondence is summarised in Table 2.

The primary method supplies only the fracture kinematics. Bulk viscoelasticity or viscoplasticity, rate-temperature dependence, ageing, crystal anisotropy, crack-face contact, heat transport and reaction kinetics must be attached according to the material and loading problem. When mechanisms compete or occur sequentially, the minimum mechanism-complete coupling identified in Section 8 should be used: XFEM-CZM or PFM-CZM for bulk-interface competition, PD-FEM for a fracture-critical PD subdomain embedded within a larger continuum structure, and FEM-DEM for transition from an intact continuum to interacting fragments. These combinations are proposed from mechanism compatibility; they have not yet been demonstrated as integrated PBX or solid-propellant fracture frameworks. Additional formulations are justified only when they represent a distinct process required by the target observable.

Regardless of method, model credibility requires compatible measurements for deformation, initiation, propagation and post-failure response; sufficient resolution of

the relevant cohesive, phase-field, peridynamic or particle scale; and independent assessment of the local or coupled-field observable supporting the conclusion. Where these conditions cannot be met, the scope of interpretation should be narrowed or the experimental and model design revised, rather than parameters retuned against the same response.

In each case, the least complex formulation satisfying the required physics and supported by solution verification and independent validation should be preferred.

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10. Conclusions

This review has compared local and nonlocal continuum formulations and discrete particle approaches for fracture modelling of PBXs and solid propellants within a common material-mechanism-method framework. The central conclusion is that method selection should begin with the physical transition and observable to be predicted, rather than with a preferred numerical formulation. PBXs and solid propellants share a highly filled particle-binder architecture, but their fracture problems are not interchangeable. PBX failure is commonly governed by competition among crystal-binder debonding, binder-ligament failure, crystal fracture and microcrack coalescence, whereas solid-propellant integrity is more strongly conditioned by binder viscoelasticity, particle dewetting, large deformation, ageing and grain-scale constraint. These common balance-law and dissipation requirements coexist with method-specific representations of sharp cracks, cohesive process zones, diffuse crack fields, finite-horizon interactions and particle contacts. A method well suited to one class of observables may be unnecessarily expensive or miss a key deformation mode for another.

The comparative assessment identifies distinct domains in which each method is most defensible. XFEM provides an enriched finite-element representation of one or a few sharp cracks whose paths need not conform to the background mesh, particularly when they emanate from a resolved cavity, notch or pre-existing flaw. CZM offers the most direct description of progressive separation along crystal-binder, particle-binder or propellant-insulation interfaces when the admissible surface and traction-separation parameters can be constrained. PFM is preferable when distributed nucleation, branching and coalescence make crack topology an unknown of the problem. PD provides a nonlocal continuum formulation for rapid fracture evolution, interacting cracks and fragmentation, while DEM is justified when force chains, rearrangement, frictional sliding, bond failure and post-fracture contact are themselves required outputs. These domains overlap, but overlap does not imply interchangeability: the least complex method that resolves the required kinematics should normally be preferred.

Across all five formulations, predictive qualification is limited less by the ability to generate a crack pattern than by constitutive fidelity, parameter identifiability, numerical verification and validation for the intended use. Agreement with a single global stress-strain or force-displacement curve cannot uniquely determine bulk, interface and fracture parameters or establish transfer to another geometry, loading history, temperature or formulation. Such agreement is calibration evidence when the curve was used to identify parameters; it becomes validation evidence only when the curve was withheld from calibration, and even then it tests only that global observable under the stated conditions. Verification should first establish correct implementation and quantify numerical error for the scale specific to each method, including enrichment and crack increments in XFEM, cohesive-zone resolution in CZM, h/ℓ convergence at fixed ℓ in PFM, point-spacing refinement Δx at fixed physical horizon δ in PD, and time-step, particle-size, coarse-graining and representative-volume effects in DEM. Validation should then compare the calibrated and verified model with independent global and local observables, progressing from constitutive response to initiation and propagation quantities such as crack path, debonded area, crack-growth history, fragment interaction and dissipated energy. Cross-geometry or withheld-condition validation without retuning is essential if the model is to be regarded as predictive within its stated domain rather than merely calibrated.

Predictive ignition modelling requires mechanical damage and fracture evolution to be coupled explicitly to heat generation, thermal transport and reaction kinetics. Viscoelastic loss, plastic work, frictional slip, pore collapse and fracture-surface formation contribute differently to heat generation; their conversion into temperature therefore requires independently constrained energy-partition parameters. Damage contours or total dissipated energy cannot substitute for spatially and temporally resolved validation of deformation, crack evolution, temperature and ignition delay.

Future progress may come from minimal, mechanism-complete, adaptive frameworks rather than from monolithic combinations of all available methods. XFEM-CZM, PFM-CZM, PD-FEM and FEM-DEM provide transferable architectures from non-energetic material systems, but their integrated application to PBX and solid-propellant fracture remains prospective. Such couplings must conserve mass, momentum and energy, prevent duplicate dissipation and transfer history variables without artificial changes in fracture resistance. Machine learning has been applied directly to propellant constitutive characterisation, whereas its use for fracture-parameter identification, surrogate fracture simulation, uncertainty quantification and adaptive allocation of high-fidelity models remains a potential extension. Three-dimensional microstructure-resolved experiments, rate-temperature-ageing datasets and validation under conditions excluded from calibration are therefore the key requirements for converting current mechanism-oriented simulations into transferable engineering tools.

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