

Comparative Assessment of Discrete Element Approaches for Non-Spherical Fuel Debris in Nuclear Severe Accidents

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1. Introduction

During a severe accident in a pressurized water reactor (PWR), core degradation may produce a molten corium pool. If in-vessel retention is not achieved, continued thermal attack may cause the lower head of the reactor pressure vessel to fail, resulting in the discharge of molten corium into the reactor cavity. For Korean PWRs employing a cavity-flooding strategy, the high-temperature melt discharged into a water-filled cavity experiences fuel-coolant interaction, and depending on the cavity depth, the jet velocity and other flow and geometrical conditions, the melt jet can break up and fragment [1]. The melt fragments may be quenched and solidified to form particulate debris. The debris particles then undergo sedimentation and accumulate on the cavity floor to form a porous debris bed. Depending on the internal thermal-hydraulic conditions, the bed may subsequently undergo granular rearrangement and self-leveling, while insufficient heat removal may cause portions of the debris to remelt and re-agglomerate. Since the coolability of this bed determines whether molten core-concrete interaction (MCCI) is arrested, the configuration of the bed - its height, porosity, particle size distribution and repose angle - is a first-order safety parameter [1].

As in other reactor system analyses, severe accident progression is evaluated mainly with lumped-parameter (LP) integral codes such as MAAP and MELCOR. By representing the plant as a network of control volumes and typically modeling the debris bed as an equivalent porous medium characterized by bulk parameters such as bed geometry, porosity, and representative particle diameter, these codes enable rapid and computationally efficient simulations of the entire accident sequence. They are therefore widely used in probabilistic safety assessments and licensing analyses.

Precisely because they are lumped-parameter tools, however, their predictive accuracy depends strongly on the constitutive correlations and modeling assumptions employed: dryout heat flux correlations, debris size correlations, pressure-drop laws for the porous layer, and conservative assumptions imposed on the bed shape and void distribution [1].

Severe accident phenomena are intrinsically difficult to reproduce experimentally. Prototypic-material tests and simulant-material tests have been carried out only over a narrow range of conditions because of the high temperature, the radiological hazard and scale limitations, so that a number of correlations are either unavailable or in need of improvement, and their extrapolation to reactor-scale conditions introduces significant epistemic uncertainty [1].

Detailed three-dimensional computational analysis is therefore needed to complement the limited experimental database and provide mechanistic insights and high-resolution data for improving the correlations used in integral severe accident codes. In particular, the behavior of fuel debris in the late phase of a severe accident is intrinsically discrete: it is governed by individual particle collisions, friction, interlocking and granular rearrangement, and it takes place inside a boiling coolant pool. To resolve these particle-scale mechanisms and their interactions with the surrounding fluid, a discrete solid-particle model should be coupled with a description of the continuous fluid phases. For this purpose, the discrete element method (DEM) has been coupled with either grid-based computational fluid dynamics (CFD) or mesh-free particle methods such as smoothed particle hydrodynamics (SPH) and the moving particle semi-implicit (MPS) method [2,3].

The present paper compares three DEM-based representations for the late-phase corium debris problem: conventional DEM with spherical particles, rigid multi-sphere DEM for representing non-spherical debris, and bonded-particle DEM using breakable bonds between spherical elements to represent aggregation and fragmentation. These approaches are compared in terms of their modeling capabilities, coupling requirements for the continuous fluid phases, computational costs, and parallelization characteristics. Based on this comparison, the paper discusses the suitability of each approach and identifies priorities for future development.

2. Basic Discrete Element Method

2.1. Soft-sphere contact modeling

The DEM predicts the collective behavior of a granular system by integrating the Newton-Euler equations of every individual particle,

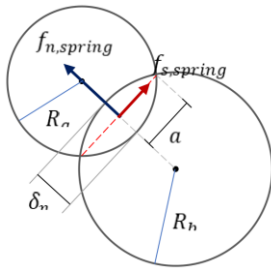
$$m_i \, dv_i/dt = \sum_j f_{ij} + m_i g + f_i^f \quad (1)$$

$$I_i \, d\omega_i/dt = \sum_j r_{ij} \times f_{ij} \quad (2)$$

where m_i , v_i , ω_i and I_i are the mass, translational velocity, angular velocity and moment of inertia of particle i , f_{ij} is the contact force exerted by a colliding particle j , r_{ij} is the branch vector from the particle center to the contact point, and f_i^f is the force transmitted by the surrounding fluid. In the soft-sphere formulation adopted by most DEM codes, a small overlap δ_n is allowed at the contact and the contact force is decomposed into normal and tangential components, each of which is represented by a spring-dashpot system (Fig. 1). Using the widely used Hertz-Mindlin law,

$$f_n = (4/3)E^*\sqrt{R^*} \, \delta_n^{3/2} - \gamma_n v_n \quad (3)$$

$$f_t = 8G^*\sqrt{(R^*\delta_n)} \, \delta_t - \gamma_t v_t \quad (4)$$



Hertz-Mindlin Model

$$f_n = \frac{4}{3}E^*\sqrt{R^*} \, \delta_n^{3/2}$$

$$f_t = 8G^*\sqrt{R^*\delta_n} \, \delta_s$$

Fig. 1. Overlap of two solid particles in the soft-sphere model and the Hertz-Mindlin contact force law.

where E^* and G^* are the equivalent Young's and shear moduli, R^* the equivalent radius, γ the damping coefficient, and v_n , v_t the relative velocities at the contact point. Because soft-sphere DEM explicitly resolves short-duration contacts governed by the particle mass and contact stiffness, stable time integration requires a time step smaller than the critical contact time. Contact detection can be accelerated using a cell-based neighbor-search algorithm. On the other hand, exactly the same sequence of operations is applied to every particle, so that assigning one GPU thread per particle gives an almost ideal parallelization, and large speedups have been demonstrated for reactor-scale particulate problems [3].

2.2. Unresolved coupling with the continuous phases

A reactor-scale debris bed consists of an enormous number of particles, and resolving the flow field around each of them would require a grid or kernel much finer than the particle diameter. At reactor scale, such a fully

resolved treatment is generally computationally prohibitive. Consequently, unresolved (volume-averaged) coupling is commonly adopted in debris-bed simulations, with the fluid phases described by locally averaged conservation equations of the form

$$D(\varepsilon \rho u)/Dt = -\varepsilon \nabla p + \nabla \cdot (\varepsilon \tau) + \varepsilon \rho g - f_{pf} \quad (5)$$

where D/Dt is the averaged material derivative, ε the local fluid volume fraction and f_{pf} the volumetric fluid-particle interaction force, which is evaluated from empirical drag correlations expressed in terms of the particle diameter, the local void fraction and the slip velocity. The same principle applies whether the fluid solver is grid-based (CFD-DEM) or particle-based (SPH-DEM, MPS-DEM) [2,3]; in either case the fluid resolution must remain considerably coarser than the solid particles so that a meaningful local average exists. This is the practical framework within which debris bed formation, sedimentation and self-leveling have so far been simulated.

2.3. Limitation of a spherical debris representation

The angle of repose of the debris bed controls its peak height, its lateral extent and its porosity distribution, and therefore directly affects the dryout heat flux and the long-term coolability that are evaluated in a safety analysis. Real fuel debris produced by fuel-coolant interaction, however, is highly irregular; the fragments are angular, elongated or dendritic, and the behavior of a bed formed by such particles is fundamentally different from that of a sphere assembly [1]. When irregular fragments are replaced by single spheres, the interlocking and the rolling resistance between the grains are lost, and the bed is predicted to be flatter than it actually is.

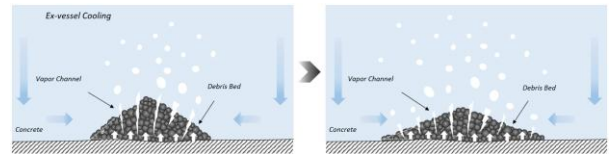


Fig. 2. Self-leveling of a debris bed under decay-heat-driven boiling in a flooded cavity (left: initial bed, right: leveled bed).

This is not a conservative simplification. As illustrated in Fig. 2, the decay heat generated inside the bed drives a two-phase natural circulation that flattens the debris layer, a process known as debris bed self-leveling. When the central part of the bed becomes lower, the length of the upward boiling channel in the central region is reduced and the thermal margin to dryout is increased. Consequently, modeling the debris as spheres yields a bed that is flatter, and hence apparently safer with respect to dryout, than the real configuration. From the conservative standpoint required in a safety analysis, this

is an undesirable direction of error, and it constitutes the fundamental limitation of the basic spherical DEM.

3. Non-Spherical Discrete Element Method

3.1. Shape representation strategies

Non-spherical DEM shares the entire philosophy of the basic method - the soft-sphere assumption, the spring-dashpot contact force model and the explicit integration of Eqs. (1) and (2) - but generalizes the geometry of the element so that the irregular shape of a real grain can be reflected. Two families of shape representation are commonly distinguished [5,6].

The first family describes the particle surface directly by a single mathematical body: ellipsoids, superquadrics and poly-superquadrics, polyhedra and dilated polyhedra, spherical-harmonic particles, and level-set particles. These representations reproduce sharp edges, corners and flat faces faithfully, but the contact detection is no longer analytic. For each candidate pair, an iterative optimization problem must be solved to locate the contact point and to evaluate the overlap and the contact normal (Fig. 3(a)), which increases the cost per contact by one to two orders of magnitude relative to a sphere pair, and the contact point may become ill-defined for face-edge or edge-edge configurations of polyhedra. Multiple contact points between a single pair must also be handled explicitly.

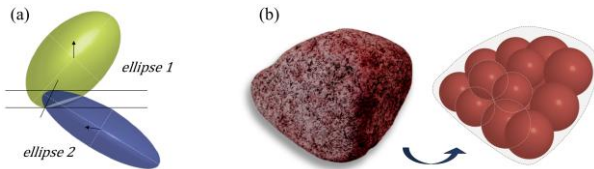


Fig. 3. Non-spherical particle representation: (a) contact detection between two surface-based (ellipsoidal) particles, and (b) multi-sphere representation of an irregular debris fragment.

The second family, and the one most widely used in practice, is the multi-sphere (also called composite particle or clumped particle) approach, in which an irregular grain is approximated by a rigid assembly of overlapping spheres (Fig. 3(b)). Its principal merit is reliability: both the contact detection and the contact force evaluation reduce to the well-validated sphere-sphere case, so an existing and verified spherical DEM kernel can be reused almost without modification. The drawbacks are that sharp edges and corners are poorly reproduced, that the artificially bumpy surface introduces a rolling resistance which depends on the number and size of the constituent spheres, and that the computational cost grows with the number of spheres used per grain.

3.2. Multi-sphere formulation and validation

In the multi-sphere formulation each rigid body a is defined by the arrangement of its constituent spheres k . The center of mass and the inertia tensor must be constructed explicitly from that arrangement,

$$X_{cm} = \sum_k m_k x_k / \sum_k m_k \quad (6)$$

$$I_a = \sum_k m_k (|r_k|^2 \delta - r_k \otimes r_k) \quad (7)$$

where $r_k = x_k - X_{cm}$, parallel-axis theorem is used to transform I_a into the global frame. The net force and the net torque about the center of mass are then obtained by summing the contact contributions of all constituent spheres, and the translational and rotational motion of the rigid body is integrated from Eqs. (1) and (2) with the full inertia tensor.

The formulation has been verified against the conservation of linear momentum, angular momentum and kinetic energy before and after a single collision between two composite bodies, with maximum errors of 0.003 %, 1.13 % and 3.41 %, respectively. A system-level validation was performed against an angle-of-repose experiment with ellipsoidal seeds [4]. As shown in Fig. 4, the multi-sphere model reproduces the measured repose angle of about 34.1° within 1 % (33.8°), whereas a single-sphere model of the same particle volume yields only about 29.2°, i.e. the repose angle is under-predicted by more than 13 % and the heap is correspondingly flattened. This quantitatively confirms the concern raised in Section 2.3.

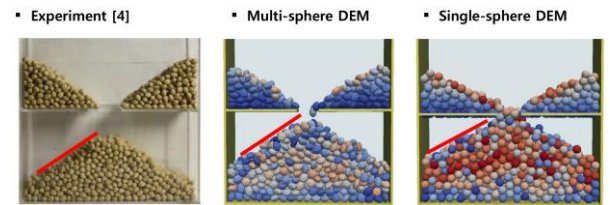


Fig. 4. Angle-of-repose benchmark: experiment [4] (~34.1°), multi-sphere DEM (~33.8°) and single-sphere DEM (~29.2°).

3.3. Computational and coupling difficulties

Introducing a non-spherical element, however, is not free. Three difficulties are worth emphasizing for the debris application.

First, the per-body bookkeeping breaks the regular data structure of a spherical DEM code. As summarized in Fig. 5, the contact detection and the contact force calculation are still performed sphere by sphere and can be parallelized as before, but an additional step is required at every time step in which the forces, torques and inertia tensor components of all spheres belonging to the same rigid body are summed. On a GPU this cross-

thread summation is precisely the operation that one-thread-per-particle parallelism does not support: it must be realized either with atomic operations, which serialize part of the calculation, or with an index-based sorting and reduction, which adds extra passes over the whole particle array. The relative merit of the two strategies depends on the number of rigid bodies and on the number of spheres per body, and in either case the total cost increases with the resolution used to describe the particle shape.

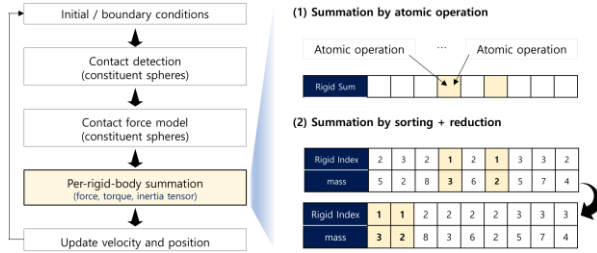


Fig. 5. Multi-sphere DEM algorithm and the additional per-rigid-body data summation required on a GPU (atomic operation versus sorting and reduction).

Second, the rotational dynamics of a general rigid body is considerably more expensive and more delicate than that of a sphere. The scalar moment of inertia is replaced by a full tensor that has to be rotated into the global frame at every step, the Euler equations become non-linear through the gyroscopic term, and the orientation has to be tracked with quaternions or rotation matrices to avoid singularities and drift.

Third, and most important for the present discussion, the coupling with the continuous phases becomes considerably harder. For computationally tractable reactor-scale simulations, debris beds are generally treated using the unresolved framework of Eq. (5), in which fluid-particle interactions are represented by closure laws. For non-spherical particles, the drag, lift, and hydrodynamic torque may depend on the particle orientation relative to the local flow, as well as on the aspect ratio, sphericity, and Reynolds number. A hydrodynamic-torque model may be required when fluid-induced torque has a significant influence on particle orientation, but its importance depends on the particle shape and flow regime. Orientation-dependent correlations have been derived only for a limited set of canonical shapes and Reynolds number ranges, mostly for isolated particles [7], so that their extension to a dense, polydisperse and thermally active three-phase debris bed remains uncertain. Additional practical issues arise in evaluating the local void fraction when an elongated body spans several fluid cells, and in distributing the resulting fluid force over the constituent spheres of a clump [6].

Finally, a non-spherical element defined as a rigid body cannot break or merge by construction, so that neither the fragmentation of debris under impact nor its

re-agglomeration after partial re-melting can be represented.

Nevertheless, within the unresolved coupling framework, non-spherical DEM provides a practical means of accounting for debris irregularity and therefore represents a valuable intermediate step toward higher-fidelity debris simulations.

4. Particle Bonding Approach

4.1. Bonded-particle formulation

In the particle bonding approach, originally proposed to represent rock as a cemented assembly of grains [8], an irregular solid body is described not as a rigid clump but as an assembly of individual DEM particles connected to their neighbours by finite-sized elastic bonds. As shown in Fig. 6, a bond of length l_b and radius R_b behaves as a set of elastic springs uniformly distributed over the bond cross-section, so that it transmits not only normal and tangential forces but also twisting and bending moments. The bond force and moment are accumulated incrementally at each time step,

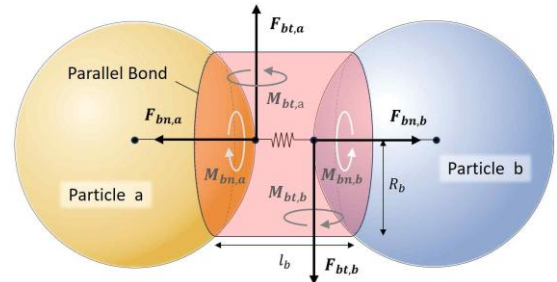


Fig. 6. Parallel bond model between two DEM particles: normal and tangential bond forces and the associated twisting and bending moments.

$$\Delta F_n = -k_n A \Delta \delta_n, \Delta F_t = -k_t A \Delta \delta_t \quad (8)$$

$$\Delta M_n = -k_t J \Delta \theta_n, \Delta M_t = -k_n I_b \Delta \theta_t \quad (9)$$

where $A = \pi R_b^2$ is the bond cross-sectional area, I_b and J are the second and polar second moments of area, respectively, and k_n and k_t are normal and shear bond stiffnesses per unit area, and $\Delta \delta$ and $\Delta \theta$ are the incremental relative displacement and rotation of the bonded pair. A viscous damping term proportional to the relative velocity is added to both the force and the moment so that the bending or twisting motion excited by an external load is dissipated instead of oscillating indefinitely. The bond is broken when the maximum tensile or shear stress acting on the bond section exceeds the corresponding bond strength,

$$\sigma_{max} = -F_n/A + |M_t| R_b/I_b \geq \sigma_c \quad (10)$$

and an equivalent criterion is applied to the shear stress [8,9]. Once a bond has failed it is removed and the pair

reverts to the ordinary contact law of Eqs. (3) and (4), whereas a pair that later satisfies the bonding criterion can be bonded again. The bond is usually established when two particles lie within a prescribed separation, with a bond radius of about 0.9-1.0 times the mean particle radius.

4.2. Verification

Because the bond force and moment act as internal action-reaction pairs, the linear and angular momentum of a bonded system are conserved exactly, and in the absence of the damping terms the kinetic energy is conserved as well. As a system-level verification, the bending of a three-dimensional cantilever beam was simulated: a beam 1.94 m long with a 0.2 m × 0.2 m square cross-section was discretized into bonded DEM particles, one end was fixed and a transverse load of 20 kN was applied at the free end, for Young's moduli between 10 and 100 GPa. The computed deflection along the beam agrees closely with the analytic beam solution (Fig. 7), and the maximum tip deflection agrees within 4.03 % over the whole range of Young's modulus considered.

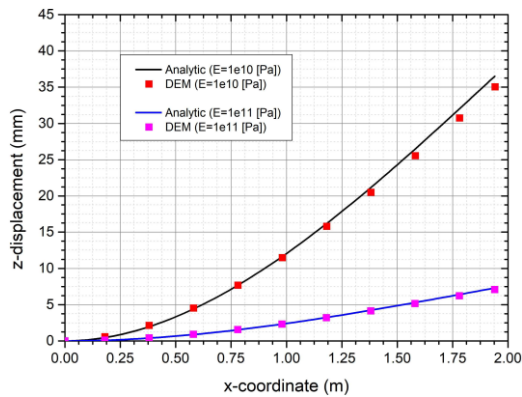


Fig. 7. Verification of the bond model: deflection of a bonded-DEM cantilever beam compared with the analytic solution.

4.3. Advantages for late-phase debris analysis

The first advantage is the uniformity of the data structure. In a bonded framework every state variable is stored on a single particle, and the collective translation and rotation of an aggregate emerge from the internal bond forces between its constituent particles. Consequently the center of mass, the inertia tensor and the net torque of the aggregate never have to be evaluated, and the orientation of a composite rigid body never has to be integrated. If the force acting on one constituent particle is known, the collective behavior of the whole aggregate follows automatically. Every particle is therefore subject to exactly the same set of operations, the existing one-thread-per-particle GPU parallelization can be used without modification, and the additional

reduction step of Fig. 5 disappears. This makes it practical to run systems composed of millions of constituent particles.

The second advantage is that fracture and re-agglomeration are represented naturally. Because bonds can break according to Eq. (10) and can be re-established, the model reproduces phenomena that a rigid non-spherical element cannot: the fragmentation of debris under impact or under strong pressure and flow loading, and the re-agglomeration or crust formation that occurs when partially re-melted debris solidifies again while in contact. Fig. 8 shows two large bonded aggregates that first move as rigid bodies and then break up into secondary fragments and loose particles once the bond strength criterion is exceeded during the impact. These are exactly the processes - fragmentation, quenching, re-melting and re-solidification - that occur sequentially or simultaneously in the late phase of a severe accident.

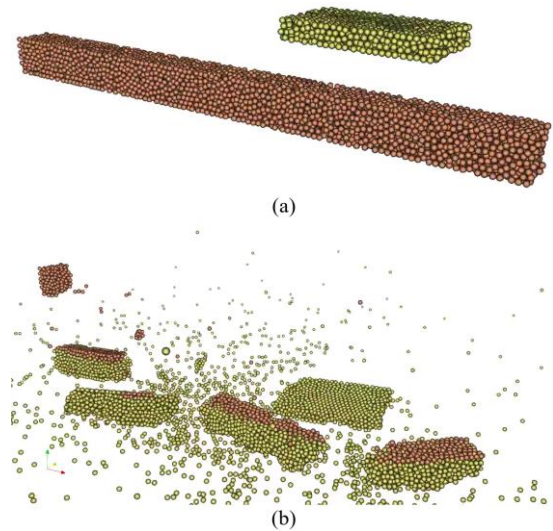


Fig. 8. Impact-induced fragmentation of bonded aggregates: (a) initial bonded bodies, and (b) bond failure producing secondary fragments and loose debris during impact.

The third and most far-reaching advantage appears when the surrounding coolant and the boiling vapour are also solved by a Lagrangian particle method such as SPH or MPS. If the size of the constituent DEM particles is chosen comparable to the fluid particle spacing, the fluid-solid interface of an irregular fragment is geometrically resolved, and the hydrodynamic force acting on the aggregate is obtained simply by summing the resolved interactions on its constituent particles. In this limit the locally averaged equations of Eq. (5) and the shape- and orientation-dependent closure laws discussed in Section 3.3 are no longer required: the orientation-dependent drag, the lift, the hydrodynamic torque and the flow through the interstices of the debris bed emerge from the calculation itself. This is the realistic modeling that severe accident research ultimately needs, and it is attainable within a single fully Lagrangian, GPU-parallel framework. The price is the

number of degrees of freedom and therefore the GPU resources required, but the algorithm remains regular and its cost scales essentially with the particle count alone.

Two issues remain to be resolved before the approach can be applied to prototypic conditions. The micro-parameters of the bond, namely its stiffness and its strength, must be calibrated so that the assembly reproduces the macroscopic elastic modulus and strength of the debris material, and a physically based criterion linking bond formation and failure to the local thermal state is needed if re-melting and re-solidification are to be represented quantitatively.

5. Conclusions

Discrete solid-particle methodologies applicable to the behavior of fuel debris in the late phase of a severe accident have been compared. Under the test conditions considered in the present study, the conventional spherical DEM is computationally efficient and fits the unresolved coupling framework naturally, but because it cannot reproduce the interlocking of irregular fragments it under-predicts the angle of repose by more than 13 % and yields a flatter debris bed. Since a flatter bed shortens the central boiling channel and thereby increases the apparent thermal margin to dryout, this is an undesirable direction of error from the conservative standpoint of a safety analysis.

Non-spherical DEM, whether based on a direct surface description or on the multi-sphere approach, restores the effect of particle shape and reproduces the measured repose angle within 1 %. It does so, however, at the price of constructing the center of mass and the inertia tensor of every rigid body, of integrating a non-linear rigid-body rotation, and of performing an additional per-body reduction that does not map cleanly onto per-particle GPU parallelism. For reactor-scale simulations involving large numbers of debris particles, unresolved coupling currently remains the more practical option for coupling non-spherical DEM with the continuous fluid phases. Nevertheless, within the unresolved coupling framework, non-spherical DEM provides a practical means of accounting for debris irregularity and therefore represents a valuable intermediate step toward higher-fidelity debris simulations.

The particle bonding approach is judged to be the most desirable long-term direction. Representing an irregular fragment as an assembly of small particles connected by parallel bonds keeps all state variables on individual particles, so that the collective motion of an aggregate is obtained without any center-of-mass or inertia-tensor computation and the method maps directly onto massively parallel GPU architectures. It additionally allows impact-induced fragmentation and the re-agglomeration of partially re-melted debris to be treated,

and, when combined with a particle-based fluid solver using a sufficiently fine fluid resolution and an appropriate fluid–solid interface treatment, the approach offers a pathway toward spatially resolved three-dimensional three-phase simulations, thereby reducing dependence on locally averaged governing equations and empirical interaction closures.

Because full-scale experiments under prototypic severe-accident conditions are severely constrained, high-fidelity computational analysis can provide valuable mechanistic information that complements the limited experimental database. Continued advances in GPU hardware and parallel algorithms are expected to further improve the computational feasibility of this approach, making it a promising direction for long-term development. Future work will focus on the calibration of the bond micro-parameters for prototypic debris materials and on the coupling of the bonded DEM framework with a GPU-based SPH solver for a boiling coolant pool.

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