

## Particle-Based Numerical Approaches for Multi-Physics Modeling of Severe Accidents

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### 1. Introduction

The late phase of a nuclear reactor severe accident involves highly complex multi-physics and multi-disciplinary phenomena. After core degradation and melt relocation, molten corium interacts with coolant, fragments, solidifies, spreads, and accumulates as debris beds. These processes strongly couple thermal-hydraulics, phase change, and structural response, and directly determine the feasibility of in-vessel retention (IVR) and long-term coolability. In sodium-cooled fast reactors, debris discharge and accumulation during core disruptive accidents further emphasize the importance of accurately predicting debris bed configuration and behavior.

however, often involve multi-phase flow, evolving interfaces, and interactions among fragmented materials, which require flexible and robust numerical treatment. In this context, particle-based numerical methods provide an alternative Lagrangian framework that can complement conventional mesh-based approaches in representing highly dynamic and multi-material systems. Although their application was historically constrained by computational cost, recent advances in GPU-based parallelization have substantially improved their practicality for large-scale nuclear safety simulations.

This study discusses the role and future direction of particle-based numerical approaches for multi-physics modeling of severe accidents.

### 2. Particle-based Numerical Methods

#### 2.1. Particle-based Continuum Modeling

Particle-based continuum methods, such as the Moving Particle Semi-implicit (MPS) method and Smoothed Particle Hydrodynamics (SPH), provide an alternative Lagrangian framework. In these methods, governing equations are discretized through particle-particle interactions using distance-weighted kernel functions.

In SPH, a field variable is expressed in integral form using the Dirac delta function as

$$f(\mathbf{r}) = \int_{\Omega} f(\mathbf{r}') \delta(\mathbf{r} - \mathbf{r}') d\mathbf{r}' \quad (1)$$

To obtain a numerically tractable formulation, the delta function is replaced by a smoothing kernel function with compact support and smoothing length  $h$ . The integral representation is then discretized over neighboring particles as

$$f(\mathbf{r}_i) = \sum_j \frac{m_j}{\rho_j} f(\mathbf{r}_j) W(\mathbf{r}_i - \mathbf{r}_j, h) \quad (2)$$

where  $m_j$  and  $\rho_j$  denote the mass and density of particle  $j$ , respectively.

Similarly, spatial derivatives required to solve continuum conservation equations are obtained by differentiating the kernel function. The gradient,

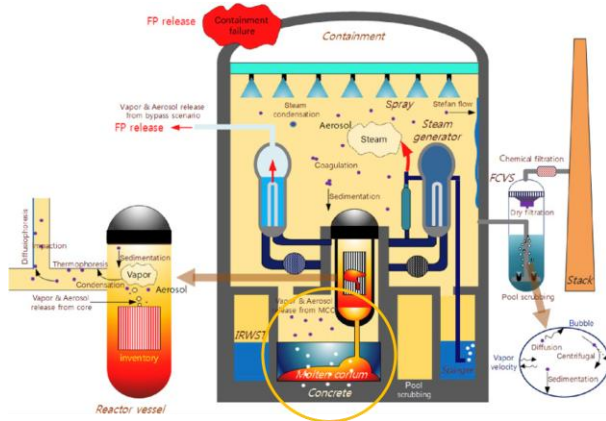


Fig. 1. Major phenomena during severe accident progression [1].

Conventional system-level severe accident codes have provided macroscopic predictions of fuel-coolant interaction and accident progression. However, these continuum-based approaches have limited capability in resolving detailed fluid-solid interaction, solid-solid collision, and morphology evolution during debris formation. Since debris bed shape and internal structure significantly influence coolability, higher-fidelity numerical approaches are required.

CFD-level simulations have therefore been increasingly incorporated into severe accident analysis to enhance mechanistic understanding of complex thermo-fluid behavior. Grid-based methods remain highly mature and effective for a wide range of thermal-hydraulic applications. Severe accident phenomena,

divergence, and Laplacian operators are approximated as

$$\nabla f(\mathbf{r}_i) = \sum_j \frac{m_j}{\rho_j} f(\mathbf{r}_j) \nabla W(\mathbf{r}_i - \mathbf{r}_j, h) \quad (3)$$

$$\nabla \cdot f(\mathbf{r}_i) = \sum_j \frac{m_j}{\rho_j} f(\mathbf{r}_j) \nabla \cdot W(\mathbf{r}_i - \mathbf{r}_j, h) \quad (4)$$

$$\nabla^2 f(\mathbf{r}_i) = \sum_j \frac{m_j}{\rho_j} f(\mathbf{r}_j) \nabla^2 W(\mathbf{r}_i - \mathbf{r}_j, h) \quad (5)$$

Through these kernel-based approximations, partial differential equations governing mass, momentum, and energy conservation are transformed into particle interaction summations over neighboring particles.

Although algorithmic differences exist between MPS and SPH, both solve continuum conservation equations by evaluating interactions among neighboring particles. Such approaches naturally capture free-surface motion, large deformation, and multi-phase flow without explicit interface tracking, and these characteristics have enabled their application to jet breakup, FCI phenomena, and corium spreading under severe accident conditions.

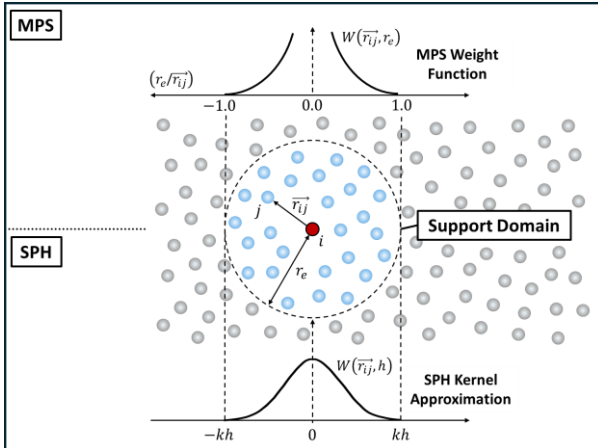


Fig. 2. Concept of particle-based continuum modeling using kernel approximation.

## 2.2. Particle-based Discrete Modeling

Severe accidents may generate fragmented fuel debris whose motion and accumulation significantly affect long-term cooling performance. Since debris sedimentation and bed formation depend on individual particle interactions, a methodology capable of resolving particle-scale mechanics is required.

The Discrete Element Method (DEM) provides a Lagrangian framework to compute translational and rotational motion of individual particles based on Newton's second law and contact mechanics. Solid–solid and solid–wall collisions are typically modeled

using spring–dashpot formulations derived from Hertzian contact theory.

The translational and rotational motion of each DEM particle can be determined according to Newton's second law:

$$m_a \frac{v_a}{dt} = \sum_b \mathbf{F}_{ba} + m_a \mathbf{g} \quad (6)$$

$$I_a \frac{\omega_a}{dt} = \sum_b (\mathbf{r}_{ac} \times \mathbf{F}_{ba}^t) \quad (7)$$

where  $m_a$  and  $I_a$  denote the mass and rotational inertia of particle a, respectively, and  $\mathbf{r}_{ac}$  is the position vector from the center of particle a toward the contact point c.

the collision force between the particles is divided into the normal and tangential components, which are further divided into the elastic and damping terms:

$$\begin{aligned} \mathbf{F}_{ab} &= f_{ab}^n \hat{n} + f_{ab}^t \hat{t} \\ &= (f_s^n + f_d^n) \hat{n} + (f_s^t + f_d^t) \hat{t} \end{aligned} \quad (8)$$

where the unit vector  $n$  and  $t$  respectively denote the normal and tangential components between particles a and b.  $f_{ab}^n$  and  $f_{ab}^t$  represent the magnitude of the normal and tangential components of the contact force, respectively. Subscripts s and d indicate the spring and damper, respectively.

In the Hertz-Mindlin contact model, each term on the RHS of Eq. (8) can be defined as follows:

$$f_s^n = \frac{4}{3} E_{ab}^* \sqrt{R_{ab}^*} \delta^{3/2} \quad (9)$$

$$f_d^n = -\sqrt{\frac{10}{3}} \frac{\ln(e)}{\sqrt{\ln(e)^2 + \pi^2}} \sqrt{M_{ab}^* K_n'} v_n \quad (10)$$

$$f_s^t = 8 G_{ab}^* \sqrt{R_{ab}^*} \delta_t \quad (11)$$

$$f_d^t = -\sqrt{\frac{10}{3}} \frac{\ln(e)}{\sqrt{\ln(e)^2 + \pi^2}} \sqrt{M_{ab}^* k_t} v_t \quad (12)$$

where  $e$  is the restitution coefficient between particles a and b,  $\delta_n$  and  $\delta_t$  denote the interparticle overlap in the normal and tangential directions, respectively, and  $v_n$  and  $v_t$  indicate the relative velocity components in the corresponding directions.  $M_{ab}^*$ ,  $R_{ab}^*$ ,  $E_{ab}^*$ , and  $G_{ab}^*$  represent the equivalent properties for the mass, radius, Young's modulus, and shear modulus, respectively.

DEM has been widely applied to debris bed formation and granular systems in nuclear engineering, enabling

prediction of bed morphology, porosity distribution, and particle mixing behavior.

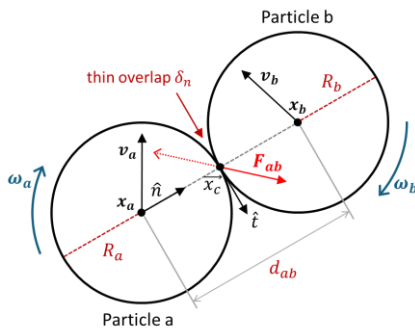


Fig. 3. Concept of Discrete Element Method for particle-particle contact approximation.

### 2.3. Coupled Approaches

In severe accident conditions, discrete debris particles do not move independently but interact strongly with surrounding fluid. Therefore, coupled fluid-particle approaches are essential. DEM is typically combined with CFD solvers using either resolved or unresolved coupling strategies. In practical severe accident simulations involving numerous particles, unresolved coupling is frequently adopted to reduce computational cost while capturing momentum exchange effects.

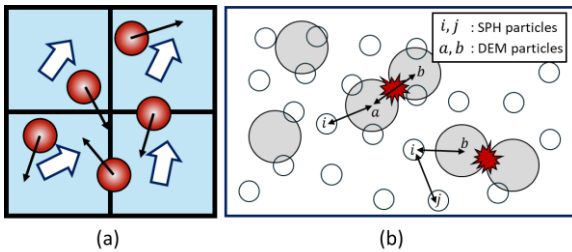


Fig. 4. Schematic of fluid-particle coupling approaches: grid-based CFD-DEM and particle-based SPH/MPS-DEM.

Moreover, particle-based continuum solvers such as SPH or MPS can be coupled with DEM within a unified Lagrangian framework, facilitating fluid-solid interaction modeling without complex mesh handling. Recent GPU-based parallelization has significantly improved the computational efficiency of such coupled approaches, enhancing their applicability to large-scale severe accident simulations

## 3. Particle-based Modeling of SA

The late phase of severe accidents is characterized by complex multiphase and multi-physics flow behavior. The following subsections briefly review representative studies demonstrating the contributions of particle-based approaches to these phenomena.

### 3.1. IVR-ERVC

Particle-based continuum methods, particularly SPH, have been applied to simulate molten pool behavior under in-vessel retention (IVR) conditions with external reactor vessel cooling (ERVC). These studies modeled stratified molten pools consisting of metallic and oxide layers and resolved internal natural convection and heat transfer within the RPV lower head.

Numerical results reproduced multi-layer thermal stratification and the time-dependent evolution of temperature fields within the melt pool. The interaction between buoyancy-driven flow and phase distribution was shown to significantly affect heat flux distribution along the vessel wall. In addition, coupled analyses integrating SPH-based molten pool modeling with system-level boundary conditions were performed to evaluate vessel cooling performance under ERVC scenarios.

These studies demonstrated the capability of particle-based continuum solvers to handle large deformation, multi-layer stratification, and conjugate heat transfer in IVR configurations.

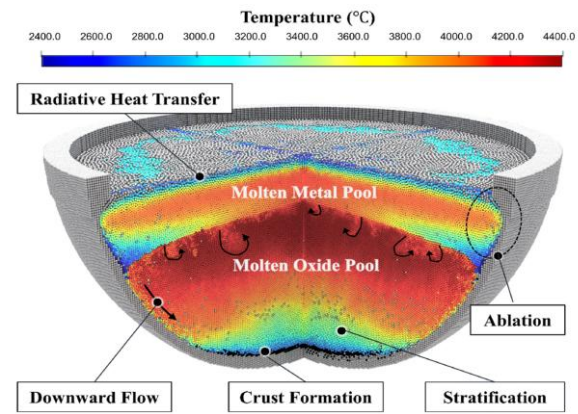


Fig. 5. SPH simulation of IVR-ERVC showing stratified molten pool and vessel wall heat transfer [2].

### 3.2. Molten Corium Spreading

Molten corium spreading after vessel failure or core catcher activation involves free-surface flow, strong temperature gradients, and solidification. Particle-based methods such as MPS and SPH have been employed to simulate spreading dynamics and crust formation without requiring explicit interface tracking.

MPS simulations validated against VULCANO experiments reproduced spreading radius, front velocity, and solidification-induced viscosity variation[3]. These analyses incorporated temperature-dependent material properties and phase change models to capture the transition from liquid flow to partially solidified crust.

Large-scale GPU-parallelized SPH simulations were also performed for corium spreading benchmarks, demonstrating stable prediction of transient free-surface evolution and thermal fields. The numerical results showed reasonable agreement with experimental spreading behavior and confirmed the applicability of particle-based approaches to high-temperature multiphase flow problems.

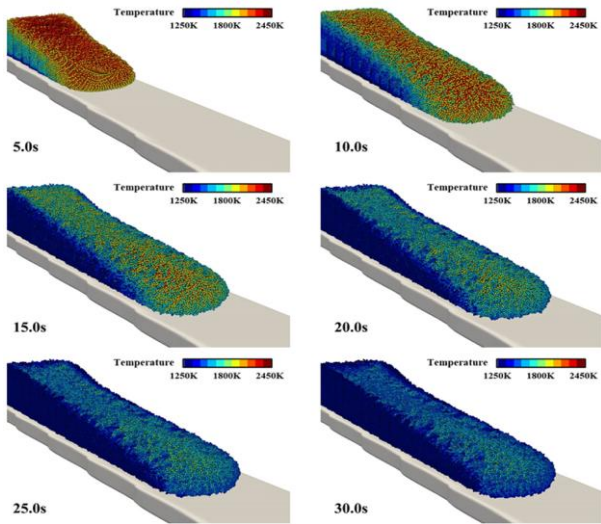


Fig. 6. Corium spreading simulation for VULCANO VE-U7 benchmark [4].

### 3.3. MCCI

Molten core–concrete interaction (MCCI) involves complex coupling between molten corium, concrete ablation, gas generation, and melt penetration. Particle-based approaches have been introduced to simulate melt penetration and concrete erosion processes.

MPS-based models incorporating phase change and multi-material interaction were used to investigate melt penetration behavior and surface regression[5]. These simulations reproduced the interaction between high-temperature melt and structural materials while resolving deformation and interface evolution. The analyses focused on melt front progression, material removal rate, and temperature distribution in the concrete domain. Such studies demonstrated the feasibility of particle-based modeling for capturing moving boundaries and strong thermo-mechanical coupling during MCCI.

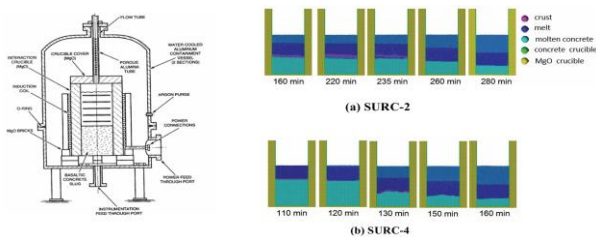


Fig. 7. MPS simulation MCCI showing melt penetration and concrete ablation [5].

### 3.4. Debris Bed Behavior

Debris bed formation and relocation are governed by sedimentation, solid–solid collision, and fluid–particle interaction. DEM-based and coupled CFD-DEM or MPS-DEM approaches have been widely applied to simulate debris bed formation under severe accident conditions.

MPS-DEM coupling models were developed to resolve both fluid–solid interaction and solid–solid collision during debris sedimentation. These models were validated against experimental tests and reproduced particle collapse, drafting–kissing–tumbling behavior, and debris bed accumulation patterns.

CFD-DEM approaches were also used to simulate debris bed formation and predict final bed geometry, porosity, and static angle under different particle properties. In sodium-cooled fast reactor scenarios, least-square MPS-DEM methods were applied to investigate debris bed formation behavior under sodium coolant conditions. The simulations showed that debris size, density, and coolant properties significantly influence sedimentation dynamics and final bed configuration.

In addition, GPU-based SPH-DEM solvers were developed to simulate three-phase flow and gas-driven leveling behavior of particulate beds, improving computational efficiency for large-scale particulate systems.

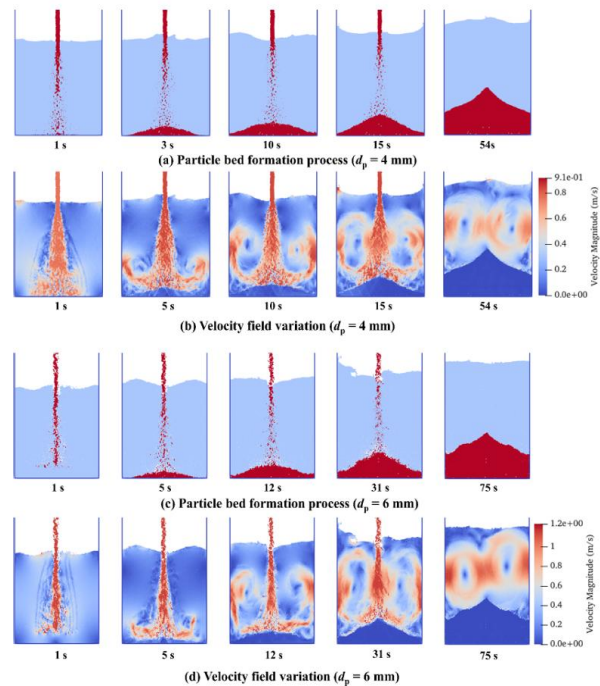


Fig. 8. LSMPS-DEM simulation of debris bed formation in liquid sodium pool [6].

#### 4. Discussion: Role of Particle-Based Modeling

##### 4.1. Providing Physical Insight into SA Phenomena

Particle-based modeling in severe accident analysis provides high-fidelity, multi-physics simulations that enable detailed observation of complex multi-phase and multi-material phenomena. By directly tracking the motion of Lagrangian nodes governed by fundamental conservation equations, these methods allow mechanistic visualization and local-scale analysis of transient processes involving interface deformation, particle rearrangement, and phase change in a physically consistent manner. Such analyses offer insight into the underlying behavior of the phenomena themselves and complement conventional grid-based CFD approaches. Moreover, the insight obtained from these simulations can support the assessment of the applicability and consistency of empirical correlations used in system-level severe accident codes, thereby contributing to the evaluation and potential improvement of reduced-order safety models. These capabilities have been demonstrated across various SA phenomena, where particle-based approaches have revealed detailed local mechanisms that are difficult to capture using conventional modeling frameworks.

In IVR-ERVC simulations using SPH, the internal convection structure of stratified molten pools was resolved without predefined flow patterns [7]. Beyond capturing buoyancy-driven circulation and inter-layer interaction, the simulations enabled detailed evaluation of angular heat flux distribution along the vessel wall, revealing peak thermal loading near the oxide-metal interface and its dependence on stratification dynamics. The analyses further provided spatial prediction of vessel wall thinning and crust thickness formation, showing that thermal concentration and solidification behavior vary systematically with melt configuration. By directly visualizing melt motion and evolving temperature fields while linking them to local heat transfer and structural response, particle-based simulations offer mechanistic insight beyond averaged heat transfer correlations.

In debris remelting studies using coupled MPS-DEM frameworks, the interaction between remelting debris and surrounding fluid was simulated at the particle scale. These simulations demonstrated that the remelting process is strongly influenced by local debris configuration and flow-induced rearrangement. In particular, large debris fragments may remain in stable positions during partial melting, potentially affecting local thermal loading and vessel integrity. Such localized behavior is difficult to capture with homogenized models.

Similarly, in SFR debris bed formation simulations using LSMPS-DEM, it was observed that the interplay between particle inertia and coolant-induced convection governs the final bed shape. Different coolant properties

(e.g., sodium versus water) led to distinct sedimentation and accumulation patterns, indicating that debris bed morphology cannot be universally represented by simplified geometric assumptions.

In addition, SPH simulations of jet breakup and multiphase interaction resolved the growth of hydrodynamic instabilities and fragmentation dynamics during FCI-like conditions[8]. By directly tracking interface deformation and instability development, particle-based methods provide detailed flow visualization and temporal evolution that enhance physical understanding of breakup mechanisms.

Overall, particle-based approaches enable fact-based modeling grounded in first principles. Their Lagrangian representation naturally supports intuitive visualization of particle motion, interface deformation, and phase interaction, thereby offering direct physical insight into severe accident phenomena.

##### 4.2. Strengthening the Role of CFD in SA Modeling

Beyond providing insight, particle-based modeling expands and strengthens the role of CFD in severe accident analysis by offering an alternative numerical framework for highly deformable and multiphase conditions. Severe accident phenomena frequently involve large deformation, free-surface motion, fragmentation, and multi-material interaction. In such contexts, particle-based continuum methods such as SPH and MPS provide a Lagrangian description that naturally accommodates moving interfaces and evolving geometries without explicit mesh reconstruction [9]. These particle-based approaches can complement conventional CFD methods by enabling additional flexibility in situations where complex interface dynamics and material fragmentation need to be resolved in a physically consistent manner.

In fuel-coolant interaction simulations, particle-based multiphase solvers demonstrated that neglecting certain phases (e.g., gas phase) may distort jet dispersion behavior. By explicitly resolving multi-phase flow without relying solely on averaged interface models, particle-based CFD enhances predictive capability for complex FCI conditions.

For corium spreading, particle-based simulations captured coupled thermal-hydrodynamic behavior, including viscosity variation due to solidification and free-surface evolution. These results highlight that spreading dynamics are governed by strongly coupled temperature-dependent material properties, which can be difficult to treat consistently in traditional mesh-based frameworks when large deformation occurs.

In debris bed problems, unresolved CFD-DEM and MPS-DEM coupling strategies provide a practical

balance between fidelity and computational cost [10]. While fully resolved approaches are computationally expensive for large particle numbers, locally averaged coupling enables simulation of macroscopic debris behavior while retaining particle-scale mechanics. This hybrid strategy extends CFD applicability to particle-laden multiphase flows characteristic of severe accidents.

Importantly, recent multi-GPU parallelization techniques have significantly reduced computational limitations traditionally associated with particle-based methods. The scalability demonstrated in large-scale SPH-DEM solvers suggests that high-resolution multiphase simulations are becoming increasingly feasible for engineering-scale severe accident problems.

From a regulatory and safety analysis perspective, high-fidelity particle-based simulations can serve as a database-generation tool. Detailed local simulations may support the development of improved correlations or reduced-order models that can be integrated into system-level severe accident codes. In this way, particle-based CFD does not replace system codes but reinforces them by providing mechanistic foundations and reducing model-form uncertainty.

## 5. Conclusion

The late phase of severe accidents involves strongly coupled multi-physics phenomena, including multiphase flow, phase change, structural interaction, and discrete debris behavior. While conventional system-level codes enable integral accident progression analysis, their capability to resolve detailed fluid–solid interaction, debris morphology evolution, and large deformation is limited. This study reviewed particle-based numerical approaches—including SPH, MPS, DEM, and their coupled frameworks—and their applications to IVR-ERVC, corium spreading, MCCI, and debris bed behavior. These methods demonstrate stable handling of free surfaces, stratified melts, solidification, and particle-scale sedimentation under severe accident conditions.

Particle-based modeling enhances physical fidelity and extends the role of CFD in highly deformable, particle-laden multiphase systems. High-resolution simulations provide mechanistic understanding and can support the development of improved correlations for system-level codes. With continued advancement in GPU-based parallelization and coupling strategies, particle-based multi-physics modeling is expected to become an increasingly important tool in severe accident safety analysis and regulatory evaluation.

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