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Topic C: Computational Multi-Physics

A MULTISCALE MULTIPHYSICS COMPUTATIONAL FRAMEWORK FOR MONTECARLO SIMULATION OF BLAST INDUCED PERVASIVE FAILURE

Background, Motivations, and Research Needs

Within the weapons of mass destruction (WMD) counter-proliferation policy of the Department of Defense, the Defense Threat Reduction Agency (DTRA) seeks innovative approaches to advance current knowledge on *Science for Protection* and *Science to Defeat WMD*. Of extreme interest is, for example, the formulation of theories and computational algorithms that would enable the accurate assessment of the effect of blasts on structures or the effect of over-ground explosions on underground structures (often used to produce and store WMD).

A necessary tool for reliable vulnerability assessments and weapons effects analyses is the accurate modeling of (1) the failure response of structures, and (2) the interaction between the structure and the surrounding fluid (air, water, or both). These phenomena are extremely complex and are relevant to a wide range of time and length scales.

Structural failures resulting from blast loads are highly nonlinear processes involving complex material constitutive behavior, post-peak material softening, localization, new surface generation via dynamic crack propagation, and ubiquitous contact. The extent of material fracturing is pervasive in the sense that a multitude of cracks are dynamically active, propagating in arbitrary directions, branching, and coalescing. An additional challenge for modeling blast induced pervasive failure is the two-way coupling between the fluid and the structure. This two-way coupling is essential for accurately simulating confined blasts as well as the flow of structural debris within the blast. Currently, there is a very limited set of computational tools that can attempt to simulate accurately and reliably blast induced pervasive failures. On the solid side, common and often unsatisfactory techniques include 'element death' in Lagrangian finite element codes and 'void insertion' in hydrocodes. The extended finite element methods have had success in modeling dilute fracture problems, but once crack branching and crack coalescence phenomena appear, the prospect of modeling a multitude of arbitrary three-dimensional intersecting cracks quickly becomes untenable. 'Element to sphere' conversion methods, while not as crude as element death, are still lacking in many respects. As far as fluid-structure interaction is concerned, various theories and computational tools are indeed available nowadays. However, none of them are able to naturally transition between the different physics relevant to the fluid interaction with the entire structure (length scale of meters) as opposed to structural debris (length scale of millimeters or less).

Proposed Research

The goal of the proposed research effort is to formulate a probabilistic multiscale multiphysics computational approach for the accurate simulation of the blast induced failure response of structures, including generated debris flow and the accurate assessment of debris inflicted secondary damage. The structural domain will be modeled using a multiscale pure Lagrangian approach whereas the fluid domain will be modeled using a fluid dynamic framework. The proposed research will consist of four key components: (1) a mesoscale Lattice Discrete Particle Model (LDPM) containing aleatory material uncertainty for modeling arbitrary crack growth and fragmentation, (2) a macroscale Randomly Close-Packed Voronoi Model (RCPVM) for modeling semi-arbitrary crack growth and fragmentation, (3) a multiscale coupling of components 1 and 2, and (4) a two way coupling between the solid and fluid domains at various length scales.

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1. Probabilistic LDPM Framework. The Lattice Discrete Particle Model (LDPM) is a meso-scale model that was first developed for concrete and lately generalized to simulate other quasi-brittle materials such as rocks, frozen soils, and brittle matrix composites. LDPM replaces the actual mesostructure of the material by an assemblage of discrete cells interacting through their exterior surfaces. Discrete compatibility and equilibrium equations along with vectorial constitutive laws are formulated to describe linear, nonlinear and fracturing behavior. LDPM has shown superior capabilities of modeling and predicting material and structural behavior under severe loading conditions. Its unique feature is the ability to transition seamlessly from the continuous representation of solids to complete fragmentation. This makes LDPM the best candidate for the characterization of air blast generated debris. Generation and dynamics of debris and its interaction with fluid, however, is a stochastic phenomenon that calls for probabilistic computational simulations. Currently, LDPM implements the randomness associated with the geometrical description of the mesostructrure but does not implement randomness of material parameters. The latter is crucial if one wants to capture with accuracy the statistical distribution of the response and not only the mean and the coefficient of variation of the response distribution. This is important to be able to capture the shape of the probability density function (pdf) of the response, and especially the far-out tail, which, in turn, is crucial for the assessment of the effect of low probability events like blasts (as well as other man-made and natural hazards). It is proposed here to develop a fully probabilistic LDPM (p-LDPM) by randomizing the material parameters through auto-correlated random fields. Various pdfs (Gaussian, Weibull, etc.) will be adopted and both autocorrelation among material parameters and auto-correlation in space will be explored. In particular, spatial autocorrelation will be analyzed carefully in order to investigate the (so far unknown) physical meaning of the so-called "auto-correlation length". The relationship between the auto-correlation length and the material characteristic length (associated with meso-scale heterogeneity) will be investigated in details. p-LDPM will be implemented in an explicit dynamic computer code and it will be calibrated and validated against experimental data relevant to failure and fragmentation of quasi-brittle materials. In particular it will be important to assess the capability of the model to reproduce typical statistical scatters shown by experiments and to simulate the so-called "statistical size effect" (reduction of structural strength with structural size in absence of significant stress redistribution prior to failure).

2. Three-Dimensional RCPVM Framework. The Randomly Close-Packed Voronoi Model (RCPVM), recently developed at Sandia National Laboratories (Sandia), is a *macroscale* finite-element method for simulating the progression of a continuum to a discontinuum. Fracture surfaces are allowed to nucleate and propagate only at interelement faces of the domain mesh. At the inception of material softening and localization the mesh connectivity is modified to reflect the new surface and a cohesive traction with a softening constitutive behavior is *dynamically* inserted. Allowing new surfaces to form only at interelement faces results in a time varying domain whose volume is continuous in time. The use of conventional finite-element meshes, albeit unstructured, is inherently biased with respect to edge and face orientation. Instead, randomly close packed (RCP) Voronoi tessellations of the domain are used. The resulting random face network provides an unbiased computational basis for representing fracture surfaces in a homogenous isotropic continuum. The polyhedral cells of the RCP Voronoi tessellation are formulated as finite elements using the reproducing kernel method. The resulting polyhedral elements have a number of desirable properties including convexity and relatively large included angles. The current RCPVM version is two dimensional. It is proposed here to formulate and validate a three-dimensional RCPVM suitable for the multiscale coupling with LDPM discussed in the next section. The 3D RCPVM will be implemented in an explicit dynamic computer code. Extensive numerical analyses will be carried out in order to study mesh sensitivity and convergence properties of the method during fragmentation. In particular, new notions of convergence will be explored since classical definitions of convergence with mesh refinement are inappropriate during fragmentation in which engineering quantities of interest can exhibit stochastic like response even though the governing equations are completely deterministic. More general notions of convergence will be considered, ones based on statistical theory or measure theory in analysis. The following three definitions of convergence will be considered: (1) *convergence in distribution*, (2) *convergence in probability*, (3) *convergence in r-th mean*. They are given in order of increasing 'strength' in the sense that if a sequence of probability distributions converge in probability then it also converges in distribution, and if a sequence of probability distributions converge in *r*-th mean then in also converges in probability. Convergence studies of various quantities of interest including, but not limited to, moments of fragment distributions (in terms of size, mass, velocity, kinetic energy, etc.) will be carried out.

3. Multiscale Coupling of LDPM and RCPVM. At the macroscopic scale (length scale of several meters), random heterogeneous materials can be modeled as statistically homogeneous materials. However, their fracturing and fragmentation behavior is strongly influenced by meso-scale material heterogeneity which needs to be taken into account in order to define meaningful macroscopic material properties and macroscopic constitutive laws. The possibility of using meso-scale models, like LDPM, for the macro-scale simulation of fragmentation is hampered by their computational cost. A typical LDPM simulation of a 100 mm side concrete cube requires about 10,000 degrees of freedom. As a consequence, one would need to run a system of millions of degrees of freedom to simulate a typical reinforced concrete beam and billions of degrees of freedom to simulate a high-rise building. These numbers show clearly that direct numerical simulation, i.e. mesoscale modeling of entire structures, is not feasible. In the present research, it is proposed to overcome this limitation by formulating a multiscale technique suitable for fragmentation. The adopted meso-scale framework will be LDPM whereas the macroscopic framework will be the Sandia RCPVM.

Multiscale coupling of mesoscale and macroscale frameworks will be done without the need of macroscopic tensorial constitutive laws. The macroscale finite element mesh will be superimposed to the LDPM system and the macroscoscale displacement field projected into the mesoscale. Various projection strategies will be formulated and explored. The projected mesoscale nodal displacements and rotations will be used to compute LDPM nodal forces (mesoscale response) which will be eventually averaged to compute macroscale nodal forces. The averaging technique will be based on the principle of virtual power in order to ensure correct energy conservation. The macroscale RCPVM kinematics will be equipped "on-the-fly" with displacement discontinuities at the interface of the Voronoi cells when the mesoscale response transmitted across that interface starts to soften. The formulated multiscale framework will be implemented in an explicit dynamic computer code. Numerical simulations of benchmark problems will be carried out to study accuracy and computational cost of the method by comparing the multiscale response to the reference full mesoscale response. Mesh sensitivity and convergence properties will be also studied as per the discussion in the previous section.

4. Multiscale Fluid-Solid Interaction. The multiscale framework developed above will then be coupled with a fluid-dynamic framework in order to study the fundamental physics of fluid-solid interaction during blast induced pervasive failure and fragmentation. The physics of the interaction largely depends on the size of the solid object interacting with the fluid. In order to account for the high speeds of the fragments the fluid will be modeled by solving the *compressible* Navier-Stokes equations. For both LPDM and RCPVM descriptions of the solid, fluid-structure interaction will be modeled using the Immersed Boundary method. In this method the fluid is represented using an Eulerian description and the fluid equations are solved on a grid that does not change with the motion of the solid. This eliminates the need for remeshing with large scale solid motion. For the mesoscale LPDM description, the fluid grid will be very fine with mesh sizes in the order of millimeters so as to accurately model the effect of tiny fragments. For the coarse scale RCPVM description this grid will be much coarser. In either case dirac-delta forces that will act on the fluid-solid interface will represent the effect of the solid on the fluid. Both the LPDM and the RCPVM methods naturally involve the evaluation of internal forces at interfaces, and will be easily implemented within this framework. The location and the strength of dirac-forces will change as the solid moves with respect to the fluid. Within this approach all fragments will interact with each-other and the structure through the fluid (reword). An adaptive strategy will also be formulated in order to refine the fluid mesh as the fragmentation process takes place.

In order to maximize the efficiency of the coupled computational framework a “weak” coupling will be adopted. The solid and the fluid platforms will perform their own independent time step solution using boundary data from other code. For the fluids code this boundary data will consist of a time-interpolated surface mesh (position and velocity) from the finite element mesh. For the fluids code this boundary data will consist of a time-averaged surface pressure from the fluids code. An interface agent will negotiate the time-interpolation, time-averaging, and exchange of surface data during coupled execution.

Finally, with the entire solid-fluid computational framework in place, Montecarlo simulations of the blast induced fragmentation will be carried out. Debris dynamics will be investigated with the goal of assessing blast induced secondary damage.

Research Impact

The proposed research will eventually lead to the development of advanced computational tools that will impact significantly the ability of DoD Agencies to assess primary and secondary damage caused by blast loading. This, in turn, will lead to more effective design of protective structures and to more effective strategies for WMD defeat.

Team and Management Plan

The Research Team is composed by individuals from Rensselaer (Dr. G. Cusatis, Dr. A. Oberai, and two research assistants), Sandia (Dr. J. Bishop), and ES3 (Dr. D. Pelessone). The Rensselaer Polytechnic Institute will lead the research effort and Dr. Cusatis will serve as Principal Investigator. The duration of the project will be three years. At Rensselaer, the project will be conducted within the Multiscale Science and Engineering Center (MSEC), which features state-of-art technologies and computing facilities for multiscale and multiphysics simulations. At Sandia, research and development will be conducted within the Engineering Sciences Center which has extensive computational resources and experimental facilities. ES3 (San Diego, CA) will assist Rensselaer and Sandia in the implementation of the developed theories and algorithms into computer codes.

Estimated Costs

Under this project, two graduate students will be fully supported (tuition and stipend) as graduate Research Assistants for the duration of the project. Partial summer and academic salary will be provided for Dr. Cusatis and Dr. Oberai. Support for Dr. Bishop and Dr. Pelessone will be provided according to their share of the effort. Travel to national and international conferences, as well as travel to DTRA meetings and workshops will be budgeted. The estimated total cost of the project is $350,000/year per three (3) years.