

Particle Interaction Physics Model Formulation for Plume-Surface Interaction Erosion and Cratering

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The Predictive Simulation Capability development team of the STMD Game Changing Development sponsored PSI project is implementing computational simulation capability for the efficient and accurate prediction of Plume-Surface Interaction induced surface erosion and cratering in Martian and Lunar environments. The status of the Focus Area 3 of the PSI project in the generation and efficient application of accurate soil particle composition modeling in the Gas-Granular Flow Solver (GGFS) computational framework is presented. The process of constitutive closure model database generation using DEM particle interaction modeling for capturing the effects of irregular particle shape and poly-disperse mixture distribution effects is outlined. This capability has now been ported to NASA supercomputer assets and NASA engineers successfully demonstrated technology and skillset transfer in model generation for spherical and irregularly shaped, mono-disperse and bi-disperse mixture compositions. Assessment of the computational efficiency and practicality of the academic serially executed DEM tools on NASA supercomputers identified the need to migrate to a DEM framework capable of performing parallel simulations in a simultaneous process orchestrated in an automated setup, execution, database extraction, and dataset delivery ready for application simulations. The LIGGGHTS DEM toolset has been selected as the most suitable tool to migrate the DEM simulations. Once the soil model generation process is implemented, models capturing the shape and poly-dispersity effects will be generated to perform much refined validation simulations against the experiments performed under the PSI project. The application readiness of the soil models currently operational in GGFS was presented for the example of a full scale, 3-D simulation of the plume induced erosion and crater formation of the Apollo LM at an elevation of 5m above ground in a low pressure, near vacuum background.

I. Nomenclature

N	= particle size species
s	= particle species mixture fraction
γ	= collisional dissipation rate
AR	= particle aspect ratio
h	= particle shape height
d	= particle shape diameter

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II. Introduction

The development of simulation capability for the prediction of extra-terrestrial Plume Surface Interaction (PSI) environments is undertaken by the Fluid Dynamics Branch at NASA/MSFC under the Game Changing Development (GCD) Program, funded by NASA's Space Technology Mission Directorate (STMD). The Predictive Simulation Capability (PSC) Element of this PSI project is focused on creating simulation capability for the reliable and accurate prediction of PSI induced surface erosion and cratering in Martian (low atmospheric pressure) and Lunar (vacuum) environments.

Gas-particle multi-phase interaction modeling of plume impingement flow on the extra-terrestrial soil material is performed with the Gas-Granular Flow Solver (GGFS). The GGFS multi-phase flow solver features an Eulerian-Eulerian modeling approach, treating both the gas and granular material as continuum phases, to directly compute the interaction of the gas and granular phases at the surface and to directly simulate erosion, cratering and transport processes. The computational cost of discrete particle modeling methods becomes prohibitive for dense granular flows where a simulation would have to track hundreds of billions of particles individually. The Eulerian-Eulerian modeling approach allows simulation of dense as well as dilute granular flows with much lower computational cost. To enable the simulation of gas-solid flows with the Eulerian multi-phase solver, an Eulerian granular mechanics model was implemented. Details of the gas-granular modeling approach and the development of the GGFS simulation tool can be found in [1], [2].

The simulation of granular material as Eulerian continuum relies on closure models for the Eulerian granular mechanics models that describe particle-particle and particle-fluid interactions. The particle-particle interactions that govern granular kinetic theory models are the solid stresses, collisional dissipation rate, and solid conductivity. The particle-fluid interactions are represented by a drag model that exchanges energy between the phases. These model closure terms feature dominantly in the granular energy balance equation with the 'granular temperature' representing the particle kinetic energy state. Constitutive closure models for mono-disperse spherical particles can be formulated directly from particle kinetics theory. Closure models for spherical particle mixtures can be derived from kinetic energy formulations in combination with a particle mixture model introduced by Garzo, Hrenya & Dufty, abbreviated as the GHD model, which models the poly-disperse mixture as a finite set of distinct particle size bins [3], [4], [5], [6].

Realistic soil compositions are neither simply spherical nor mono-disperse. The lunar regolith, as the extreme example, is poorly sorted with broad particle size distributions and large fines content. It has significant cohesion due to interlocking particle shapes for the very jagged particles. The combination of particle shape and size distribution has been identified as major drivers in the complex particle flow response and resulting crater shape characteristics of extra-terrestrial granular material. Constitutive models for complex particle shapes cannot be directly formulated from kinetic theory. The particles are instead modeled as analytical shapes such as cylinders, ellipsoids, super-quadratics and others, or in the most general and practical way, by gluing together elemental spherical shapes into composite particles and performing Discrete Element Model (DEM) particle kinetics simulations to extract data and formulate constitutive closure models. The required non-spherical particle mixture granular material response closure models are obtained through these small-scale unit physics DEM simulations for the range of particle shapes, mixture species fraction compositions, and packing densities. Dataset at finite intervals over the volume fraction range are assembled in a tabular form for interpolation during GGFS execution.

This DEM-based constituent model generation process and formulation of poly-disperse particle mixtures has been successfully implemented during the initial development of the Gas-Granular Flow Solver (GGFS) simulation framework with NASA SBIR/STTR program support. Under one of the prime tasks of the PSI project, "*PSC Task 3 – Regolith Particle Phase Modeling*", this soil model formulation and database generation process is being further developed, transferred to NASA analysts, and matured towards project support application readiness. The outcome will be the validated capability to simulate complex particle shapes and mixtures in production predictive simulation tool such as the GGFS. This capability is critical for lunar PSI because of the complex lunar regolith soil composition.

Recent accomplishments towards this goal involved the porting of the academic simulation tools used in the GGFS development to NASA HPC asset, transferring the skillsets to NASA engineers, and assessing the production readiness and computational speed efficiency for timely support of NASA project applications. The NASA team has successfully replicated the generation of databases currently implemented in the GGFS model base, performed on

NASA supercomputing assets by NASA analysts. Identification of computational efficiency bottle necks due to the academic DEM tools being limited to sequential execution without the ability to take advantage of NASA massively parallel HPC assets is now leading to the migration of the academic DEM tools to a HPC capable open source tool.

This paper presents an overview of the particle phase model generation approach and the status of migrating the capability to NASA analyst teams. Application testing examples for the case of Apollo LM plume-induced crater formation simulations demonstrate the applications readiness of the currently implemented production ready models for mono-disperse spheres, irregular particle shapes, and bi-disperse sphere mixtures. Distinct differences in the predicted crater features demonstrate the effects and importance of modeling both particle shape and mixture effects.

III. Influence of Shape and Mixture on Erosion and Cratering

The regolith particle flow induced by lander PSI requires accurate representation of the regolith granular material fluidic behavior and gas-granular interactions. The lunar regolith, as the extreme example, is poorly sorted with broad particle size distributions and large fines content [7], [15]. It has significant cohesion, due to interlocking particle shapes for the very jagged particles. The combination of particle shape and size distribution has been identified as major drivers in the complex particle flow response and resulting crater shape characteristics of extra-terrestrial granular material (see Figure 1). Lab experiments of gas jets impinging on soil beds composed of a range of particle shapes and mixtures clearly demonstrates that particle shape and size distribution greatly influences particle liberation and cratering [8], [9]. For mono-disperse sphere particles, a distinctly separate shallow outer crater and deep center bowl form. For mono-disperse irregular particle composition of JSC-1A lunar simulant sieved to a narrow size range, the crater becomes narrower and deeper due to increased friction and interlocking effects. The effects of poly-disperse particle mixtures for full size range of JSC-1A and Chenobi lunar simulants result in deep, compact craters with steep walls and without a shallow secondary crater perimeter. The wide particle size range results in increased collisional/frictional contact and reduced particle bed porosity. It is therefore essential that particle phase modeling accounts for both: irregular shape effects AND poly-disperse mixture effects.

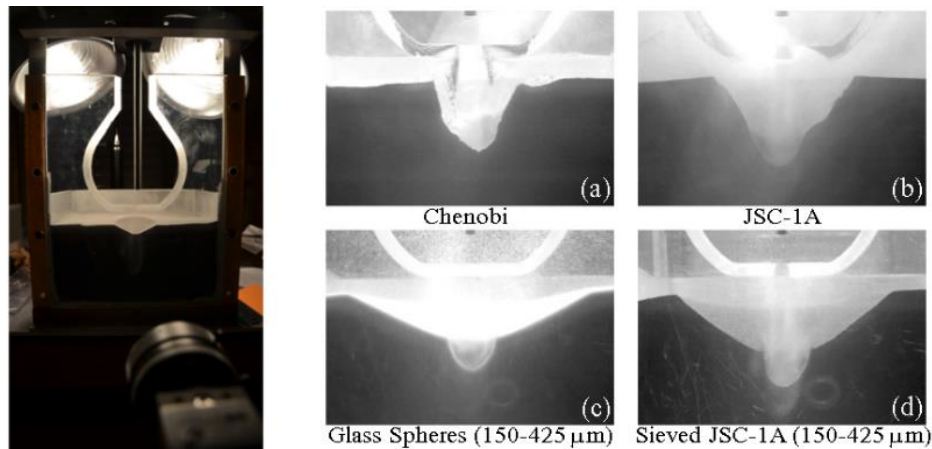


Fig. 1: Strong Influence of Particle Shape And Polydispersity In Lab Scale Jet Cratering Experiments. (Lamarche, 2013)

IV. Modeling Particle Irregular Shape and Mixture Poly-Dispersity Effects

A. Modeling Irregular Particle Shapes

The granular phase constituent model definition for implementation irregular shaped particle effects into a granular continuum flow simulation format applies an innovative use of the DEM technique: Generating non-spherical particle shapes from linked and overlapping elemental spheres and retain the efficient fundamental DEM collision kinetics modeling approach. In ground breaking work by academic partners in the NASA STTR project that developed the GGFS simulation tool and current collaborators under the PSI project led by Prof. Jennifer S. Curtis, previously at the

University of Florida, now residing at UC Davis, novel granular models for the particle phase stress describing the effects of non-spherical particle shapes have been developed employing DEM simulations [12].

Figure 2 shows examples of DEM particle compositions for spherical and irregular shapes, as well as mixtures of different shapes in a poly-disperse mixture analysis [10], [11], [12], [13]. DEM unit physics simulations of shear flow and granular temperature dissipation are then performed with these particle models. The resulting formulations for particle phase constituent models are then applied as closure models in the Eulerian granular phase kinetic energy equations.

B. Modeling Poly-disperse Mixtures (Garzo-Hrenya-Duffy Model)

To account for the effect of particle size distribution in regolith, Garzo, Hrenya & Duffy, with corrections by Murray et al., have extended mono-disperse granular kinetic theory to account for a discrete number of species [3], [4], [5]. Here, a species is a bin of particles of a certain size range, i.e., 10 micron, 100 micron, etc. This work originates from and extends the GGFS mono-disperse model development. In the GHD modeling framework, only one solid momentum equation and one granular energy balance are required; these incorporate a mass-based mixture velocity and a number-based mixture granular temperature. These two equations (momentum and granular energy) require constitutive relations for the dissipation rate of granular energy, the granular energy flux vector, the solid stress tensor, and the mass flux of species which depend on the species number density as well as various transport coefficients (e.g. granular conductivity, pressure, shear and bulk viscosity, etc.). These transport coefficients, in turn, depend on the specific properties of the local particle mixture composition, as well as the flow variables.

Given the wide particle size distribution of regolith, the challenge is to determine the number of species ‘s’ in the granular model needed to sufficiently represent the full, continuous distribution. Since the number of governing differential equations increases with increasing number of species - the number that needs to be solved is equal to $N + 2$ (1 momentum equation, 1 granular energy equation and ‘N’ species balances) - the computational complexity increases with increasing number of species ‘N’. Hence, it is desirable to determine the minimum number of species s balances which yield sufficient accuracy. Murray et al. [6] recommended that for lunar soil simulants, such as OB-1, JSC-1A, and BP-1, eight species are sufficient to describe the wide particle size distribution of regolith. For NASA production application efficiency, it will be desirable to limit the number of soil species bins, and thus the number of equations to be solve and the number of soil species DEM database generation runs, to a level that is acceptable for ‘engineering accuracy’ at various phases of a project.

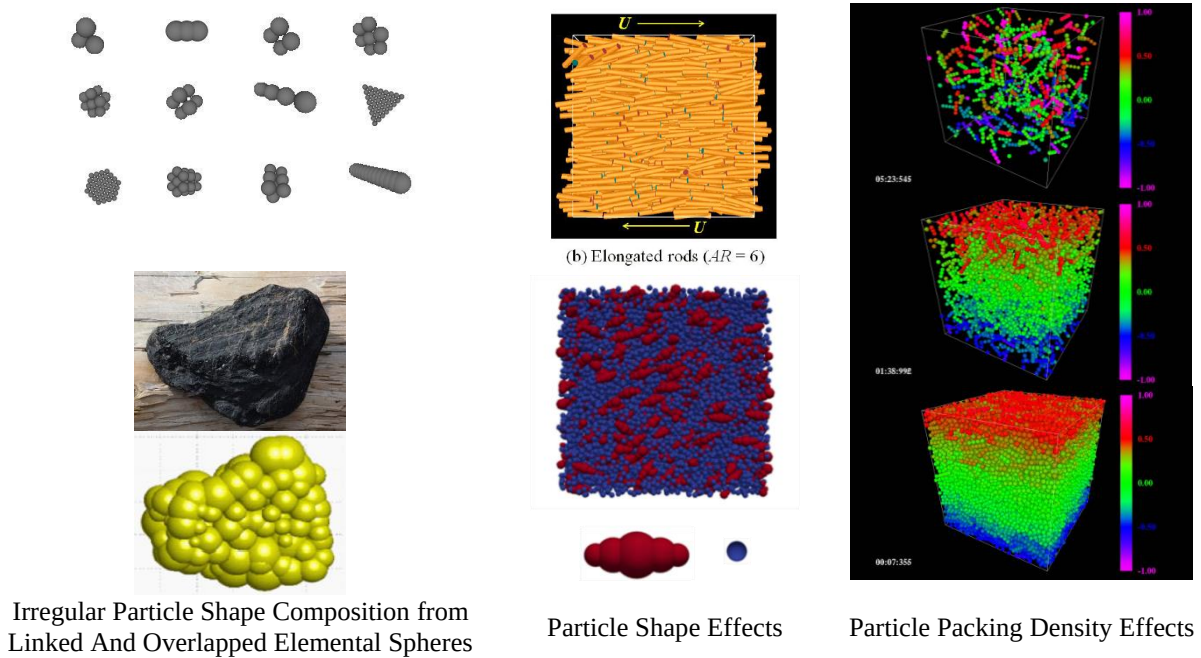


Fig. 2. Irregular Shaped Particle Interaction Modeling Approach.

C. Discrete GHD Databases Generation and Run-Time Database Interpolation

For large, production-level cases, the GHD model is prohibitively expensive to use in its direct analytical form for large number of species bins representing a poly-disperse composition. The major reasons for this large simulation overhead just from computing coefficients which require the solution of seven linear systems of equations of the size of number of species squared at each computational cell. The main driver with the analytical GHD is the computational cost associated with the numerous local matrix inversions. Since the analytical form of GHD is only suitable for spheres and DEM generated tabular databases will be required for all realistic compositions, the decision was made during GGFS development to implement a discrete database GHD model featuring adaptive tabular database interpolation methods. To alleviate the cost, a discrete-coefficient algorithm was developed where each of the closure model coefficients is generated as a function of the solid-volume fraction state of the mixture and tabulated prior to the start of a simulation.

The database for a mono-disperse particle results in a one-dimensional database, such as shear stress as a function of volume fraction in Figure 3. For a bi-disperse mixture the dataset becomes two-dimensional with the volume fraction and the particle mixture fraction becoming independent variables. the shear stress distribution of the bi-disperse mixture shown in Figure 5. Whereas the mono-disperse curve in Figure 3 is resolved by eight distinct datapoints, the bi-disperse dataset is discretized with eight volume fraction datapoints and five mixture fraction datapoints, with $s=0$ being all irregular particles and $s=1.0$ being all spheres. Thus, the dataset now has a dimension of 8×5 and requires a two-dimensional interpolation. For poly-disperse mixtures with N greater than two, the size of the database discrete point goes up by the datapoints to the power of N and an N -dimensional search and interpolation algorithm is required.

D. Current Capability: Bi-Disperse Database Interpolation

The initial implementation of the discrete GHD model implementation was performed for a bi-disperse mixture. Two-dimensional computationally efficient database interpolation algorithms were readily available in the Loci computational framework which developed efficient, two-dimensional, adaptive, tabular representations for complex equations of state. A general N -dimensional interpolation module for N -dimensional database interpolations was not available in the Loci computational framework. The required N -dimensional interpolation capability in the Loci framework is in development by the developers of the Loci framework and is currently being integrated by the GGFS development team. This bi-disperse discrete GHD model with a-priori tabular dataset generation and runtime access by dataset interpolation is the current operational status of GGFS.

V. First-principle DEM Simulations to Capture Constitutive Closure Models

The Discrete Element Model (DEM) approach is applied as a first principles particle kinetics simulation method to extract and formulate the granular material physics constituent models from unit physics simulations. Two DEM models are applied: a shear flow simulation to extract normal and shear stresses between particles, and a granular temperature dissipation (“cooling”) simulation to extract kinetic dissipation rate models.

A. Shear Flow DEM

A simple shear simulation is set up where a particle volume is exposed to shear flow by top and bottom walls moving in opposite direction to impose a shear on the particles. The resulting shear for each particle is averaged over a suitable time interval after a quasi-steady shear level state has been reached. Closure models for the kinetic + collisional pressure are formulated from the normal stresses. Shear viscosity is extracted from the shear stresses. Figure 3 shows a comparison of the shear stress for spheres extracted from DEM simulations compared to kinetic energy formulations. Results from DEM simulations performed with the LIGGGHTS code are also shown, to be discussed later. The DEM results agree very well with the kinetic theory at dilute and intermediate volume fractions. DEM results for dense packing ratios increase to higher levels than predicted by Kinetic theory. Kinetic theory is not well suited for capturing the frictional stresses that dominate at larger packing levels. DEM simulations are more credible in this range.

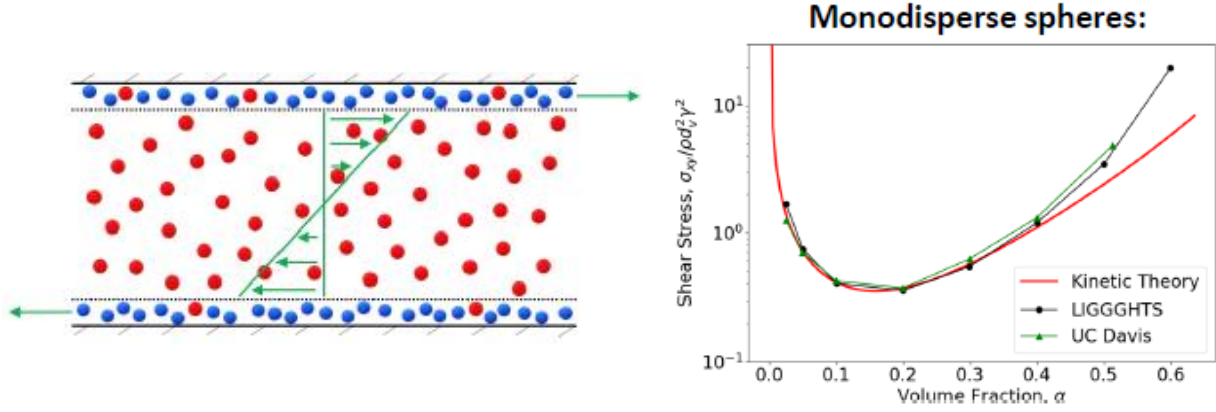


Fig. 3. Unit Physics DEM Simulation to Predict Particle Interaction Stresses.

B. Granular temperature dissipation (cooling)

First principle DEM simulations to extract the particle kinetic energy dissipation characteristics are performed by initializing a volume of particles inside a periodic volume with an initial granular temperature but zero bulk velocity. The process is depicted in Figure 4. The dissipation rate of the kinetic energy is recorded after a quasi-steady homogeneous cooling rate state has been reached indicated by a constant slope of the granular temperature dissipation. Figure 4 shows the DEM granular temperature dissipation ('cooling') simulation setup and a comparison of the DEM generated collisional dissipation rate (γ) results with Kinetic theory. Excellent agreement is also seen with the results replicated by the NASA team.

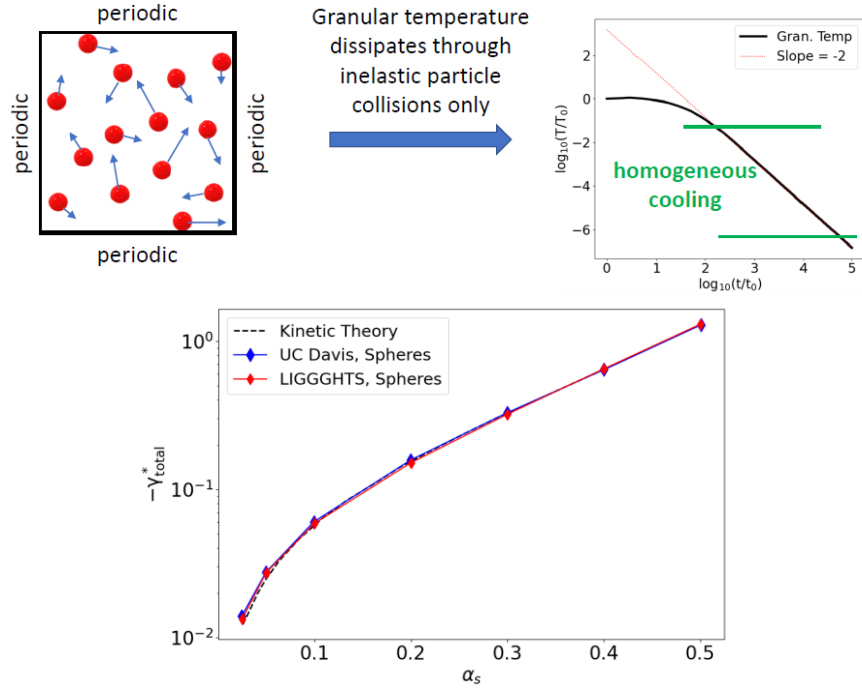


Fig. 4. Unit Physics DEM Simulation to Predict Particle Granular Temperature Dissipation.

C. DEM Modeling and database generation of poly-disperse mixtures

In realistic, naturally occurring sand or regolith mixtures, particles sizes are present over a wide range from micron size to millimeter size particles and beyond. A particle bed composed of such a range of particle sizes will result in a significantly altered packing distribution, where the smaller particles begin to fill voids between larger particles. The end result is reduced porosity of the granular bed combined with increased particle-particle contact. The kinetic/collisional/frictional/ interaction of single size particles is considerably altered when a range of particles

interact. It is therefore important to capture the poly-dispersity effects resulting from Figure 5 shows the shear stress predicted in DEM simulations of a bi-disperse mixture of a larger irregularly shaped (near oval with aspect ratio $AR=2.25$) particle embedded in small spheres. The shear stresses first decrease and then increase with total solid volume fraction. In addition, the shear stresses increase with the increasing solid fraction ratio of large particles. The same conclusion can be made with regards to normal stress. There is considerable spread in stress levels between the bounds of spheres only ($s=1.0$) and large oval shapes only ($s=0.0$).

The generation of the bi-disperse mixture of an irregular particle and a small sphere databases shown in Figure 5 was performed during the implementation of the poly-disperse in the GGFS framework before The replication of this database generation process was again undertaken under the PSI project by NASA personnel. This served again the purposed of skill-set transfer to NASA and to establish an assessment of the computational expense and time required to generate a DEM based dataset on NASA supercomputers. As for the mono-disperse process, the limitations of the academic tools to sequential execution resulted in unacceptable execution time of weeks for high particle count simulation in the dense regime. This insight again strengthened the case for migrating this capability to a parallel simulation tool capable of utilizing supercomputer asset scalability and concurrent execution.

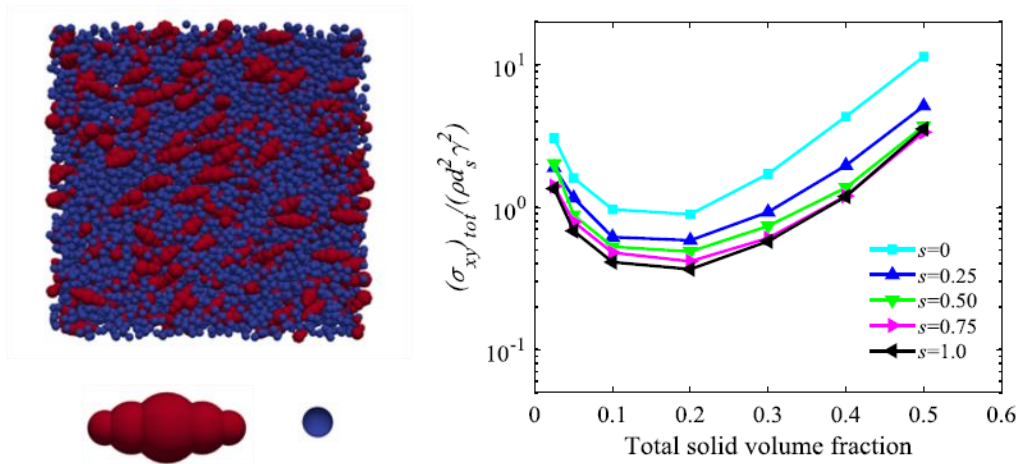


Fig. 5. Total Shear Stress for a Binary Non-Spherical Mixture for Various Solid Volume Fraction Ratios.

VI. Migration of DEM based database generation to NASA

A. Migration of DEM tools from Small Business/Academic Partners to NASA

NASA production applications require fast and automated model generation on demand of a soil particle shape and mixture composition tailored for each customer application. An efficient and automated process of performing large number of DEM simulations required for poly-disperse modeling, extracting and packaging required databases in format for application in GGFS must be instituted.

As a first step, the DEM tools and process application knowledge that were instrumental in establishing the DEM based database generation were transferred from the academic partners at UC Davis to NASA. The DEM tools and processes were installed on NAS supercomputer. Application examples published by the UC Davis team over the last decade were then replicated by the NASA team. Sample simulations were performed for mono-disperse sphere cases (Guo, 2012) and for bi-disperse irregular particle shapes formed by glued spheres interacting with small spheres [13]. Results shown in Figures 3, 4, and 5 were successfully replicated by NASA personnel on NASA supercomputers. This exercise established NASA application engineer knowledge pool of process. Processing times required for representative NASA applications expected for current and future customers. The conclusion was that the speed requirements could not be satisfied with academic tools. In the dilute regime, each DEM simulations require a matter of hours in a single core, but for the dense regime where tens of thousands of particles need to be modeled, the UC Davis DEM tools require weeks of simulation time. For NASA to be able to develop accurate material models to specification for different applications, this procedure needs to be significantly improved such that material models can be generated in a matter of hours or days instead of weeks or months. An alternate DEM simulation tool was

required that allows parallel multi-core execution of each simulation for dramatic speed-up and simultaneous execution of the hundreds or thousands datapoints required to populate a poly-disperse mixture database. The DEM tool must therefore be ready for application on NASA supercomputer architectures.

B. Migration of DEM process to HPC-Capable DEM Framework: LIGGGHTS

The requirements, as desired by NASA, for a higher performance DEM tool for this project are: (1) runs in parallel in a memory-distributed manner (MPI) on NASA HPC assets, (2) extendibility by NASA personnel, and (3) offer a framework of large range of features for future refinement of particle features and physics representations, (3) be freely available as open source software. The CFDEM package contains all the desired features to be of direct use in the granular model generation process. It contains a DEM package for public use, LIGGGHTS-PUBLIC, that is designed for large-scale DEM simulations [14]. It is GPL open source, written in C++, and uses MPI for scalability on distributed or shared-memory parallel machines. The main DEM algorithms are based on LAMMPS, a classical molecular dynamics simulation code designed to run efficiently on parallel computers that was developed at Sandia National Laboratories. The LIGGGHTS package is currently in use by a variety of institutions in the fields of chemical, pharmaceutical, agricultural engineering, food production, and mining production as it can model systems with only a few particles up to millions or billions and is designed to be easy to modify or extend with new capabilities.

The process of migrating to the LIGGGHTS software package began with certifying its capabilities to generate the well validated models previously generated in the DEM software developed by the UC Davis team. LIGGGHTS simulations with monodisperse spheres have reproduced results of UC Davis code for simple shear and cooling simulations. Direct comparison of shear stress simulations and collisional cooling dissipation generated with the UC Davis DEM code and LIGGGHTS against kinetic theory demonstrated both tools results in same outcome and agree well with kinetic theory (see Figure 3 and Figure 4).

VII. Automated DEM Database Execution and Constitutive Model Delivery

The requirements for timely generation of DEM based soil models for any new-customer application requires to automate most of the process. As part of the migration to the LIGGGHTS simulation process, the process will be Python scripted to automatically generate LIGGGHTS input files, perform the simulations, and extract the output data in the database form expected by GGFS. Installation of the LIGGGHTS DEM database simulation capability on the NASA supercomputers and enabling execution in this scripted automation process has been spearheaded by the GGFS development team and nears completion. Application testing of the automation framework by NASA PSC team members will commence in the near future.

An automated database generation process tailored to take advantage of the NASA HPC resources will be implemented around the LIGGGHTS DEM framework. The resulting process will aid NASA in generating granular models for the Eulerian-Eulerian method significantly faster, allowing NASA to target specific mixture compositions as needed in an efficient manner. This constitutes a major milestone towards achieving the goal of the PSC Task 3, the accurate and efficient regolith particle phase model generation.

VIII. Demonstration of GGFS Current Production Capabilities for Apollo LM Crater Prediction

This section presents the evaluation of GGFS predictive capabilities achieved during the FY2021 of the multi-year PSI project. The purpose was two-fold: to evaluate GGFS performance for plume flow simulations in near vacuum conditions, and to evaluate the available modeling for realistic particle shape and mixture effects. Similar assessments were performed for Martian and terrestrial conditions and will be reported separately. At that point in the GGFS development cycle, the framework had operational capabilities for mono-disperse spherical and for cylindrical particles with aspect ratios of $h/d = 1, 2, 4, 6$, and the ability to perform bi-disperse mixtures of spherical particles using the GHD tabular database approach. Lunar plume cratering simulations were therefore performed for mono-disperse spheres with 30mi and 100mi diameters, a bi-disperse mixture of the 30mi+100mi spheres with a solid volume fraction of 50% for each, and a mono-disperse cylindrical particle with an aspect ratio of $AR=4$. The particles are shown in Figure 6. These particle variations allowed the check-out of GGFS for all available options and assessment of the effects of the variations in shape and mixture and the operational maturity status of those modeling options.

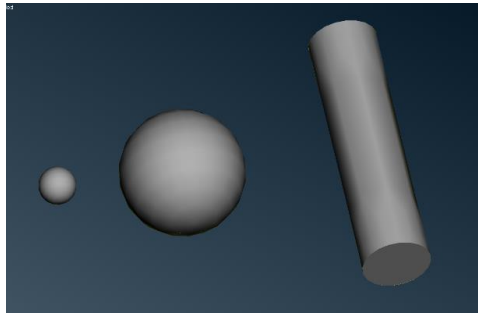


Fig. 6. Particle Shapes and Sizes Evaluated: 30micron Sphere, 100micron Sphere, Aspect Ratio AR=4 Cylinder With 100micron Sphere Equivalent Volume

A demonstration of the current capabilities was performed for a 3D cratering simulation of Apollo LM at an altitude of 5 meter of the nozzle exit above the Lunar surface. The LM nozzle has an exit diameter of 1.457m. By simulating cratering from Apollo LM, current capabilities for a set of realistic conditions can be assessed with respect to a representative human lander landing on the Moon. The Loci/GGFS tool is used to simulate the 3D geometry shown in Figure 7 below. The domain has a radial extend of 25m and a total height of 25m. A regolith layer 3m deep below the surface is comprised of particle mixtures of the four compositions evaluated.

The simulation is performed with the entire domain set to an initial ambient pressure of 0.1 Pa, a relatively low but non-zero pressure to demonstrates the ability of the currently continuum-only solver to perform in the vacuum environment on the Moon. Extension of the GGFS capabilities to mixed continuum-rarefied flow physics is in early development. The plume flow is composed of a Hydrazine combustion product surrogate gas and initiated from the engine chamber inflow conditions at 23 psi chamber pressure. This corresponds to Apollo LM terminal descent thrust levels of approximately 2200 lbf. The plume flow is initiated impulsively through the nozzle into the initial quiescent domain and impinges on the regolith surface to quickly progress into a fully developed plume flow field. At the low elevation of 5m, the plume flow expands to a supersonic outflow in both outward and upward directions, as shown in Figure 8. Note how the plume flow escapes from the stagnation region forming inside the developing crater in an outward supersonic, high shear flow pattern along the crater walls and the lunar surface as the main erosion mechanism.

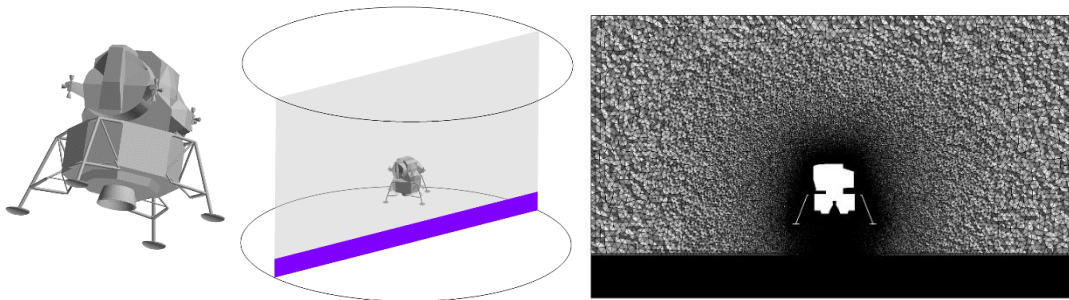


Fig. 7: Computational Geometry of For Apollo LM Crater Formation Simulation For 5m Nozzle Exit Elevation Above a 3m Deep Soil Layer.

The resulting particle ejecta patterns can be observed from contours of solid volume fraction shown in Figure 8 below. As the plume initially impinges on the lunar surface below, regolith is lofted and slowly ascends upward with the farfield plume flow. Once the quasi-steady plume field has settled, the ground regolith begins to be eroded steadily and is ejected radially outwards at low angles in the 5- to 10-degree range and with a streaking pattern similar to those observed in actual landing footing. The crater forms under the central portions of the plume where the highest impingement pressure and shear layer levels occur.

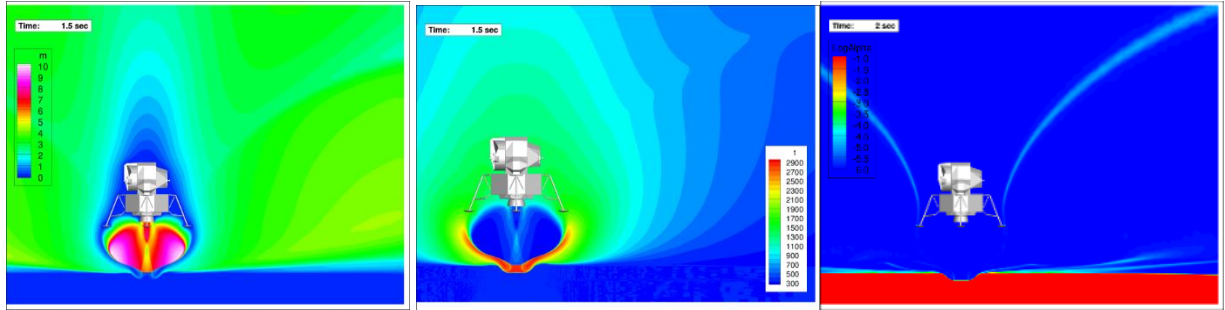


Fig. 8: Flowfield details of Apollo LM crater formation simulation for 5m nozzle exit elevation. Left: Mach number; Middle: Gas Temperature; Right: Contours of solid phase volume fraction (log10) indicating formation of crater and shallow angle near-surface ejecta sheets

A total of two seconds of flow time was simulated, resulting in a relatively wide but shallow crater of approximately 0.75m depth and diameter approaching 4.0m, as shown in Figure 9 below. Such crater dimensions are obviously much larger than actual craters observed for the actual lunar regolith composition. The regolith simulant model applied here used a simple mono-disperse spherical shape model, all be it with a more realistic internal friction angle of 45 degrees. Loci/GGFS is designed to perform particle composition modeling of more realistic irregular, jagged, non-spherical particle shapes and poly-disperse mixtures composed of a wide range of particle sizes. This more realistic particle phase modeling will be applied in follow-on work to improve the initial demonstration results reported here. The purpose of the current simulation was to demonstrate the ability of Loci/GGFS to perform practical full resolution, 3D, production level simulations for a representative Lunar lander for high Mach plume flow expansion under lunar near-vacuum external conditions. The accuracy of both predictions under relevant conditions is to be assessed with respect to validation cases, and this is the focus of the next section.

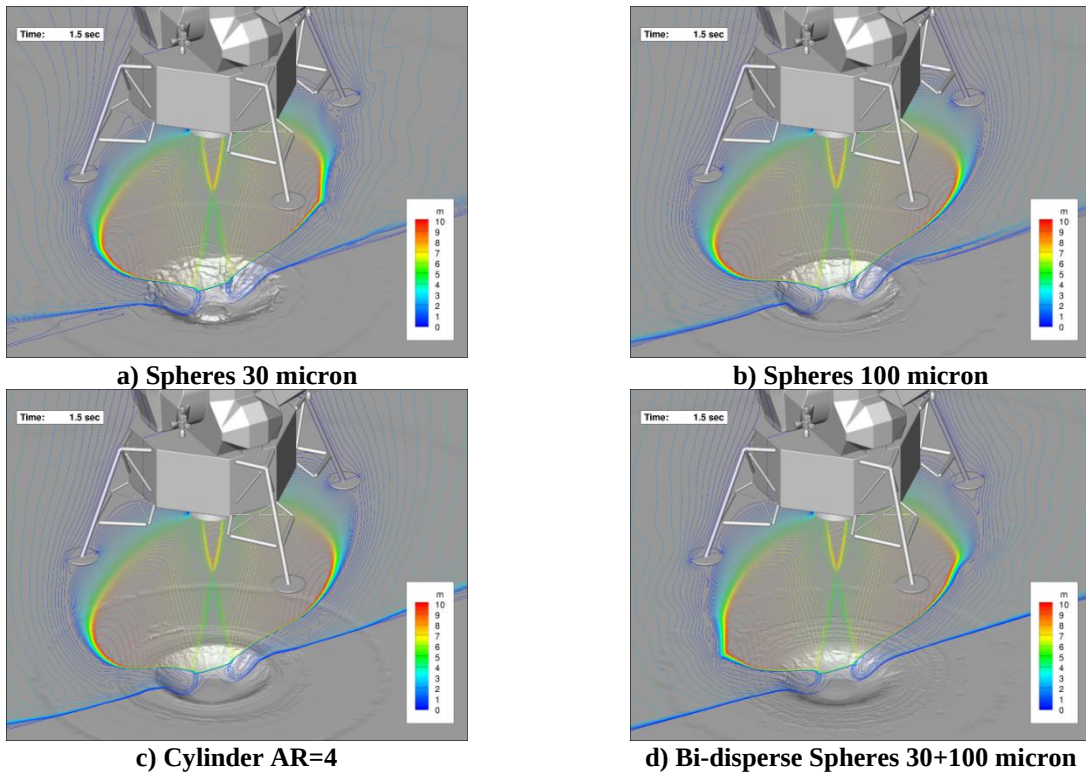


Fig. 9: Comparison of Crater Shapes at $t=1.5$ seconds For Four Composition Modeled

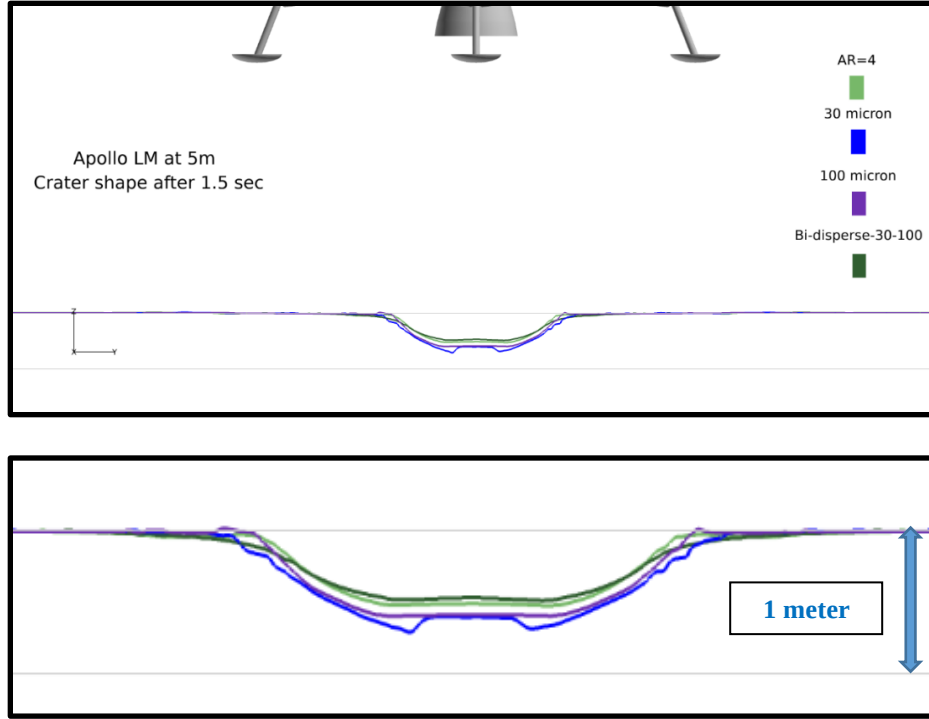


Fig. 10: Profile of Crater Outline in Cross Section at $t=1.5$ seconds For The Four Compositions Modeled. Close-Up View Shown at Bottom.

IX. Future work

Implementation of the automated database generation process with the LIGGGHTS DEM program as the compute engine is the essential precursor to the generation of databases for user specified soil composition. The ultimate application will be the generation of Martian and lunar models. The immediate application at hand will be the generation of models of the six simulants tested in the PSI project validation experiments. The so-called Physics Focused Ground Test 1, PFGT-1, performed scaled supersonic nozzle impingement experiments in a vacuum chamber at Martian and near-lunar background conditions. This experimental campaign is presented in detail in companion publications. The simulant mixtures included mono-dispersed spheres, mono-disperse quartz sand, bi-disperse quartz sand, mono-disperse sieved BP-1, a tri-disperse mixture of the quartz sand and sieved BP-1, and the full range BP-1. Mono-disperse in this context refers to the simulants sieved to a narrow size range. Except for the spheres, all simulants feature irregular shapes and the bi-disperse, tri-disperse and full range mixtures were selected with the distinct purpose to validate the DEM based soil model generation process. Generation of these irregular shaped particle mixtures is the essential next step towards validation and maturations of the GGFS modeling capabilities with realistic soil models against the PFGT-1 experiments. Other applications include revisiting and refining the previously undertaken validation simulations against the PSI experiments performed by Metzger at Martian conditions [16]. All validation simulations to date have been performed with the sphere-based soil models.

X. Conclusion

The Predictive Simulation Capability development team of the PSI project is creating computational simulation capability for the efficient and accurate prediction of PSI induced surface erosion and cratering in Martian and Lunar environments. The status of the Focus Area 3 of the PSI project in the generation and efficient application of accurate soil particle composition in the Gas-Granular Flow Solver computational framework was presented. The process of constitutive closure model database generation using DEM particle interaction modeling was presented. The process for capturing the effects of irregular particle shape and poly-disperse mixture distribution effects was outlined. This capability has now been ported to NASA supercomputer assets and NASA engineers successfully demonstrated technology and skillset transfer by replicating model generation for spherical and irregularly shaped, mono-disperse

and bi-disperse mixture compositions. Assessment of the computational efficiency and practicality of the academic serially executed DEM tools on NASA supercomputers identified the need to migrate to a DEM framework capable of performing parallel simulations in a simultaneous process orchestrated in an automated setup, execution, database extraction, and dataset delivery ready for application if GGFS simulations. The LIGGGHTS DEM toolset has been selected as the most suitable tool to migrate the DEM simulations to. Code-to-code comparison demonstrated the equivalent accuracy of the DEM tools. Implementation of an automated database generation process will proceed in the next project phase. The application readiness of the soil models currently operational in GGFS was presented for the example of a full scale, 3-D simulation of the plume induced erosion and crater formation of the Apollo LM at an elevation of 5m above ground in a low pressure, near vacuum background. Comparison of the predicted crater shape differences between soil models with spheres, irregular cylindrical particles, and a bi-disperse sphere mixture confirmed the significance of the irregular shape and mixture effects. Once the implementation of the automated database generation process with the LIGGGHTS DEM program as the compute engine is operational, the capability will be applied to generate realistic particle shape and mixture models for the simulants that were tested in the PSI projects PFGT-1 experiments and other validation experiments that so far could only be simulated with spherical particle models. This will enable a much more accurate validation of the soil models and the overall simulation capability of the GGFS predictive capability against the experiments that have now become available.

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