



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

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2022 AIAA SciTech Forum, Jan. 3–7, 2022

Outline



- Introduction: Focus of PSI project Task 3 – efficient realistic regolith model generation
- Drivers: Influence of Shape and Mixture on Erosion and Cratering
- Modeling Particle Irregular Shape and Mixture Poly-Dispersity Effects for Eulerian-Eulerian flow Constitutive closure models
- Generating DEM based closure model databases
- Migration of DEM database generation with academic research tools to NASA production environment
- Improvements towards NASA application effectiveness
- Demonstration of GGFS Current Production Capabilities: Apollo LM Crater Prediction
- Future Work
- Conclusions

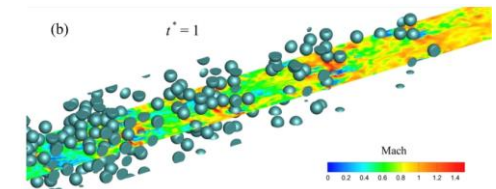
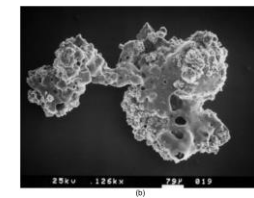
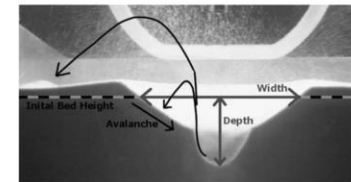
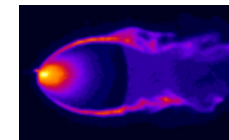
PSI – A “New Start” STMD GCD Project – 5-Year Program



Objective: Develop an integrated modeling, simulation, instrumentation capability, and testing approach to predict propulsive landing Plume-Surface Interaction (PSI) effects

FOUR SPECIFIC TASKS were defined for the Predictive Simulation Capability project component.

- **Task 1 – Plume Flow in Low-Pressure/Vacuum Environments**
 - Accurately model plume expansion, dynamics, and impingement in Martian and Lunar low-pressure/vacuum environments
- **Task 2 – Effect of Plume Flow on Crater Development and Ejecta Sheets**
 - Simulate complete range of soil material erosion and fluidization mechanism with gas-particle two-phase simulations to accurately predict crater shape and size
- **Task 3 – Regolith Particle Phase Modeling**
 - Refine soil mixture particle-particle interaction modeling to capture extreme cohesiveness of irregular shape, poly-disperse lunar regolith
- **Task 4 – Gas-Particle Interaction Modeling**
 - Close fundamental modeling gaps for gas-particle interaction in supersonic ejecta streams and clouds



Focus Area 2

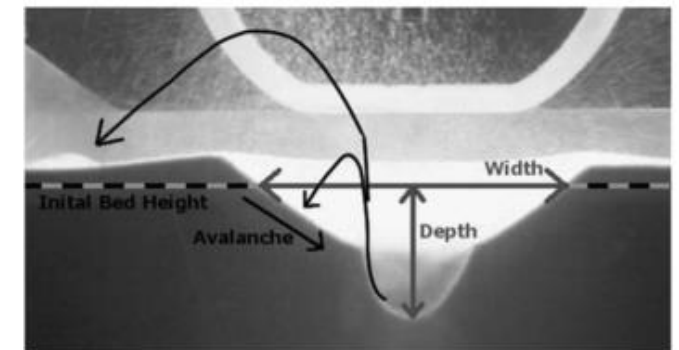
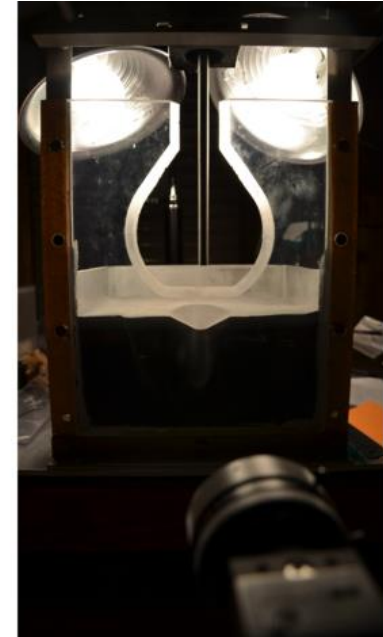
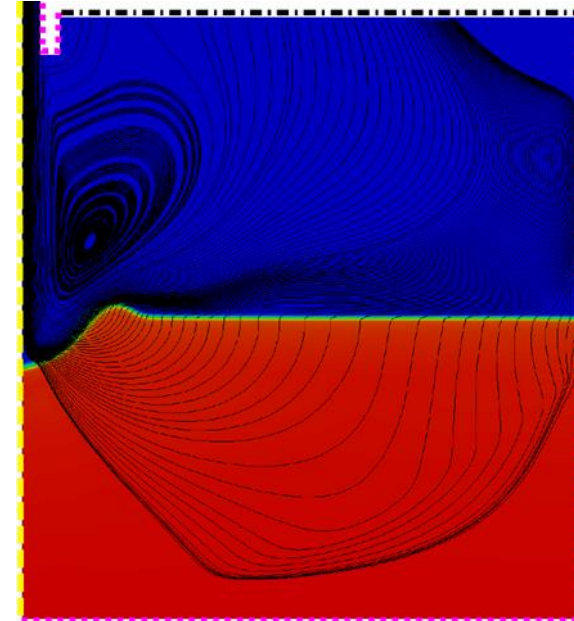
Effect of PSI Flow on Crater Development and Ejecta Sheets



Gas-Granular Flow Solver (GGFS): Gas-Particle Two-Phase Simulations

- **GGFS** features Eulerian-Eulerian modeling approach, treating both gas and granular material as mixing continuum phases. Directly compute the interaction of gas and granular phases and simulate erosion, cratering and transport processes.
- Eulerian granular material flow modeling approach with proper granular material constitutive closure models (stress, cohesion, etc.) allows simulation across dense to dilute granular flows with lower computational cost.
- The granular material response closure models for non-spherical particles are extracted from small-scale detailed DEM simulations and implemented in the Eulerian granular flow formulation.
- The Eulerian-Eulerian gas/granular flow solution framework is then applied to efficiently simulate the gas-granular multi-phase flow.

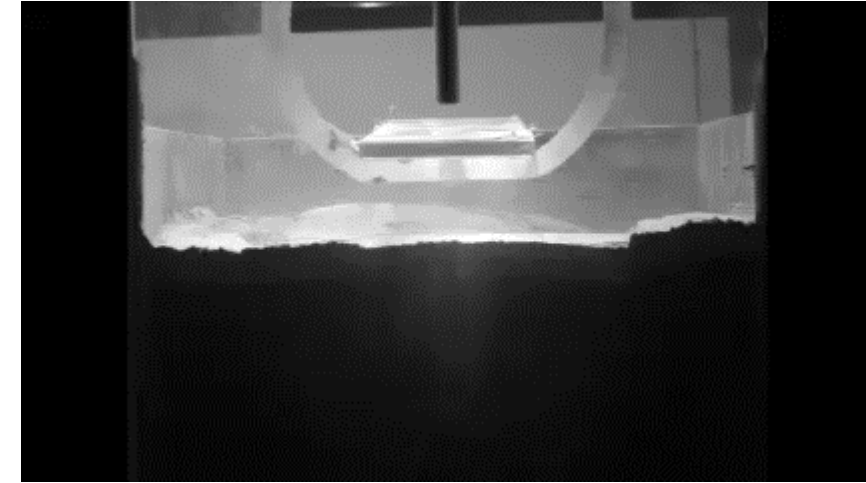
Focus Area 3 will deliver the soil particle composition effects constitutive models database generation



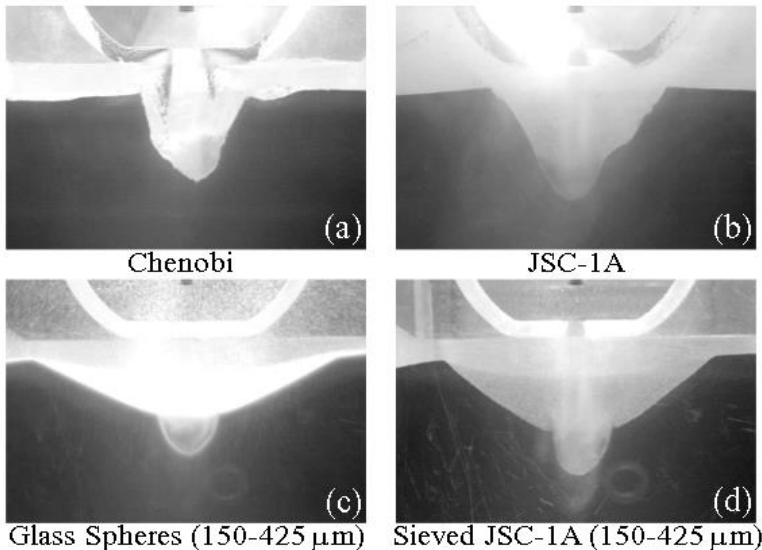
Realistic Regolith Granular Material Model Is Crucial



- Particle shape and size distribution greatly influences particle liberation and cratering
- Sphere particles: distinctly separate shallow outer crater and deep center bowl
- Effects of irregular, non-spherical shape: crater narrower and deeper
- Effects of poly-disperse particle mix: deep, compact crater, no shallow perimeter
- Combined effect: poly-disperse irregular regolith results in deep compact crater
- **Granular models must account for both: Irregular shape effects AND poly-disperse mix**

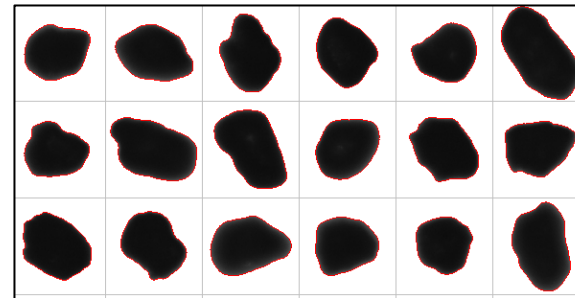


BP-1 regolith simulant cratering experiment Movie

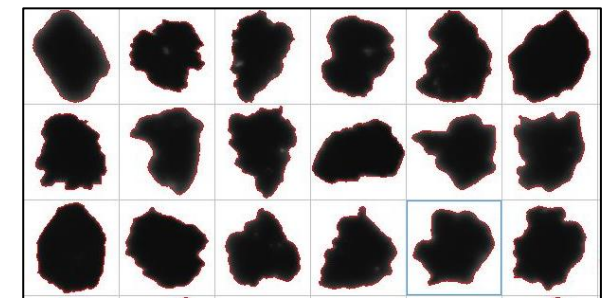


*Crater shape after 50 seconds of 25 m/s
air jet impingement*

PFGT-1 Simulant Pre-Test Simulant Particle Scanning



PFGT-1 Simulant: Quartz Sand
Irregular, sub-rounded/sub-angular

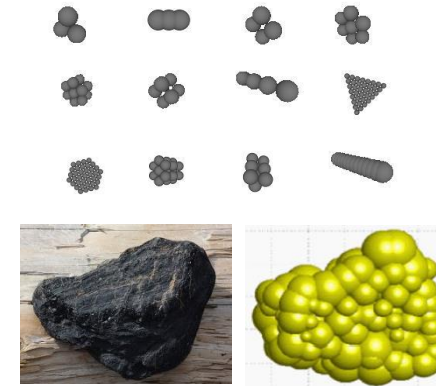


PFGT-1 Simulant: BP-1
Irregular, sub-angular/angular

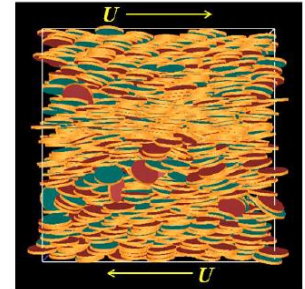
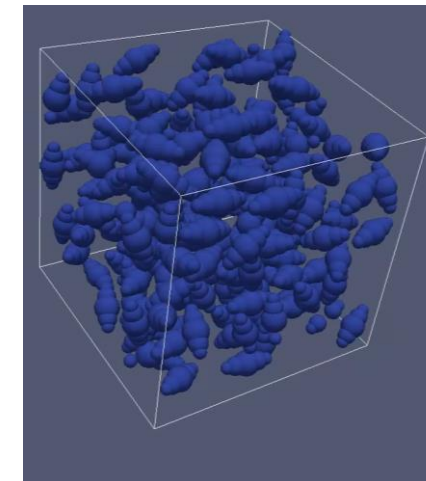
Academic Partners Contributed Realistic Regolith Particle Model Formulation And DEM Based Constitutive Model Database Generation



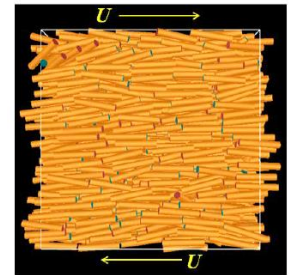
- Academic partners in GGFS development team under Prof. J. S. Curtis (UC Davis) are recognized authority in formulating particle mixture computational algorithms and DEM based constitutive closure model generation process for Eulerian flow modeling implementation.
- The process for capturing the effects of irregular particle shape and poly-disperse mixture distribution effects is well documented and published.
- Non-spherical granular material response closure models obtained through small-scale detailed DEM simulations for variety of particle shapes, mixtures and packing densities
- Development of additional important shaped and mixture effects (e.g., particle surface angularity, particle interlocking) continues by academic team under PSI project.



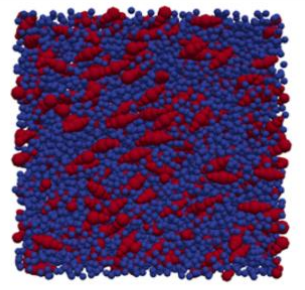
Irregular Particle Shape
Composition from Linked And
Overlapped Elemental Spheres



(a) Flat disks ($AR = 0.1$)



(b) Elongated rods ($AR = 6$)



Poly-disperse composition

Particle Modeling Capabilities in Current GGFS Release



- GGFS Particle modeling framework designed to accommodate mono-disperse and poly-disperse mixtures of ideal (spherical) and irregular particle shapes
- **Mono-disperse mixture**
 - Spherical shape using kinetic theory analytical formulations – Baseline implementation
 - Irregular (non-spherical) analytical particle shapes utilize shape specific databases generated with DEM simulations
 - Academic partners generated databases for range of analytical shapes (cylinders, ellipsoids, superquadrics, etc.) and glued spheres composite shapes. Currently implemented in GGFS: Cylinder shape with AR=1,2,4,6
 - Extension to generalized irregular shape database generation with DEM and practical application readiness is focus of PSC Task 3
- **Poly-disperse mixture algorithm: Garzo-Hrenya-Duffy (GHD) model**
 - General N-disperse spheres GHD analytical formulation implemented for direct computation. Initial implementation in GGFS prototype proved computationally too expensive – Redirected efforts to tabular database interpolation approach; tabular databases approach is required anyway for irregular shape databases
 - Bi-disperse tabular data set: operational for bi-disperse spherical shape using GHD; requires pre-processing to generate tabular datasets accessed by GGFS during execution. Efficient 2-D interpolation schemes readily available.
 - N-disperse tabular dataset application required development of efficient N-dimensional interpolation algorithms in Loci framework. Development ongoing under supplemental STTR project funding.

Garzo, V., J. Dufty, C. Hrenya, "Enskog theory for polydisperse granular mixtures I: Navier-Stokes order transport", Phys. Rev. E. 76 (2007)
Garzo, V., C. Hrenya, J. Dufty, "Enskog theory for polydisperse granular mixtures II: Sonine polynomial approximation", Phys. Rev. E. 76 (2007)
Murray, J.A., Benyahia, S., Metzger, P., Hrenya, C. M., "Continuum representation of a continuous size distribution of particles engaged in rapid granular flow", Physics of Fluids 24, (2012).



DEM Technology and Application Skill Transfer To NASA

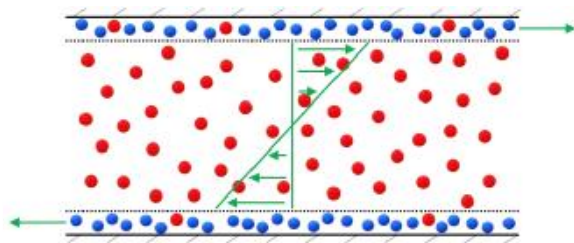
Migration to HPC Capable DEM Tools and Process Automation

- Academic research DEM tools and procedures have now been transferred to NASA Predictive Simulation Development team under the PSI project with goal of establishing application readiness for NASA project applications.
- Ported tools to NASA supercomputer assets and NASA engineers successfully replicated model generation for spherical and irregularly shaped, mono-disperse and bi-disperse mixture compositions previously published by academic team.
- Application of DEM tools on NASA supercomputer clearly identified scalability of academic sequential single-processor tool architecture insufficient for timely highly-parallelized model generation making use of NASA HPC capabilities.
- Migration of DEM simulations is now underway to the LIGGGHTS framework DEM tool chosen as best tool to deliver the speed-up and efficiency required for NASA project work. Enables parallel execution in a memory-distributed manner (MPI) on NASA HPC assets.
- Simultaneous, an automated python-based DEM database execution process followed by assembly of simulation data into a constitutive model dataset for delivery to GGFS simulations is being implemented.
- Replication of the database generation with the LIGGGHTS tools confirmed the UC Davis DEM tool and LIGGGHTS both delivered excellent agreement with Kinetic Theory validations.

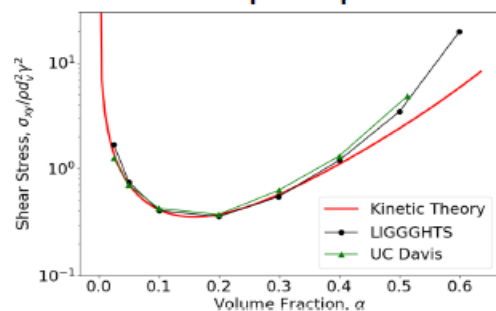
DEM Application Demonstration by NASA Engineers



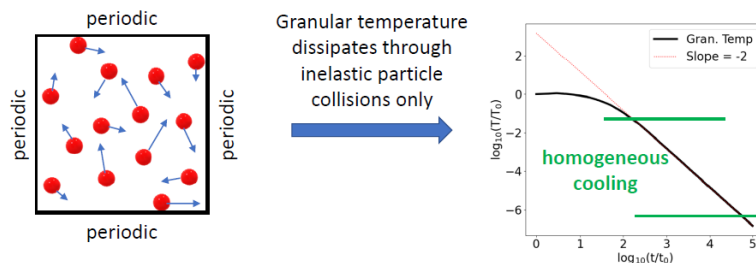
Unit Physics DEM simulation to predict particle interaction stresses.



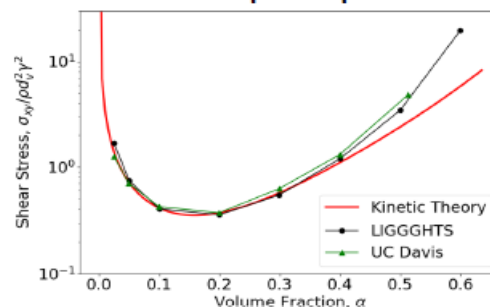
Monodisperse spheres:



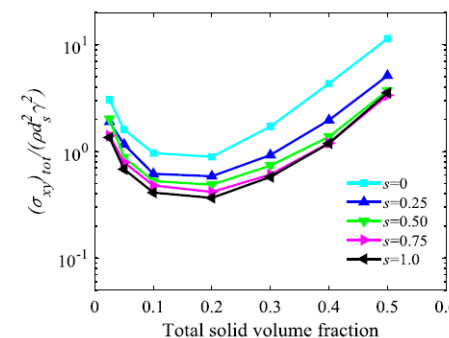
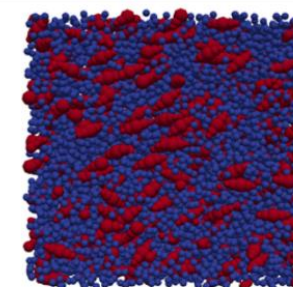
Unit Physics DEM simulation to predict particle granular temperature dissipation.



Monodisperse spheres:



Total shear stress for binary non-spherical mixture fraction ratios.



- Excellent agreement between UC Davis DEM code and LIGGGHTS predictions
- Both DEM predictions agree very well with Kinetic Theory in dilute and intermediate volume fraction regime
- Kinetic Theory known to be inadequate in dense volume fraction regime
- DEM-generated databases offer accurate physics modeling across all regimes

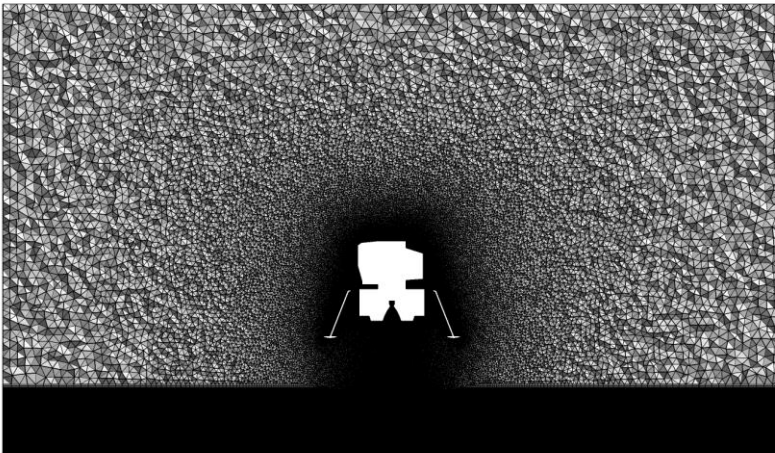
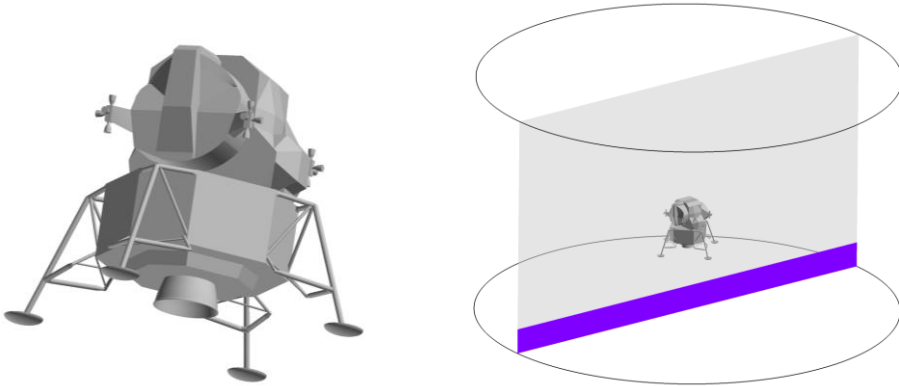


- An Application Demonstration of Loci-GGFS was performed of Apollo Lunar Module PSI surface cratering.
- These simulations served to assess and demonstrate the capabilities and robustness of the currently available particle models in the GGFS simulation arsenal, and in particular to assess simulation robustness in the stressing lunar low pressure background environments.
- The simulations were performed with Loci/GGFS Release 0.7, March 2021. Release 0.7 features mature capabilities for spherical and select irregular (non-spherical) shapes and bi-disperse spherical mixture modeling.
- The framework is readily set up to perform more general irregular shape simulations and bi-disperse irregular shape simulations as soon as the progress under this Task 3 enables the delivery of such databases.
- The effects of particle shape and mixture were assessed with four models:
 1. Single size spherical particle shape, $D=30$ micron
 2. Single size spherical particle shape, $D=100$ micron
 3. Bi-disperse spherical particle shape, $D=30+100$ micron
 4. Single size irregular particle shape, Cylinder $AR=4$ with volume equivalent to 100 micron
- The influence of the various composition models on the crater depth and shape and the resulting ejecta stream patterns is presented

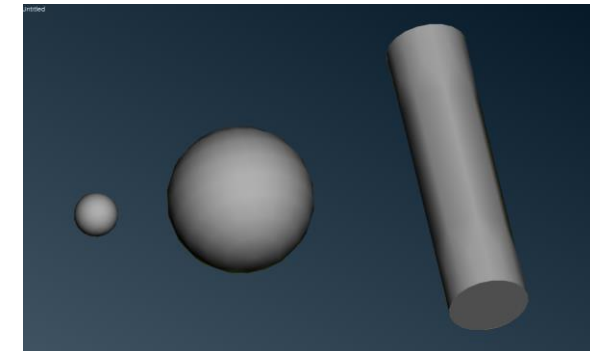
Apollo LM Crater Simulation



- Apollo Lunar Module full scale geometry model
- Domain modeled out to 25m radial distance, 20m height
- Elevation 5m from soil surface to engine exit plane
- Soil bed subdomain to 3m depth



- Assessed particle shape and mixture effects with four models:
 - Single size spherical particle shape, $D=30$ micron
 - Single size spherical particle shape, $D=100$ micron
 - Bi-disperse spherical particle shape, $D=30+100$ micron
 - Single size irregular particle shape, Cylinder $AR=4$ with volume equivalent to 100 micron
- Regolith phase soil model inputs
 - Lunar regolith density 3000 kg/m^3 (assumed solid particle, no internal voids/porosity)
 - Elastic solid model: Internal friction angle 45° , Coefficient of Restitution 0.95

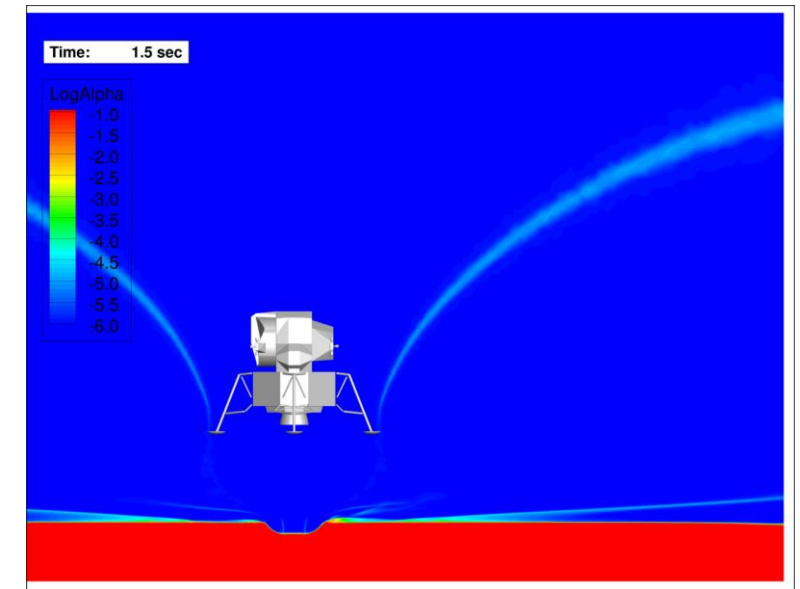
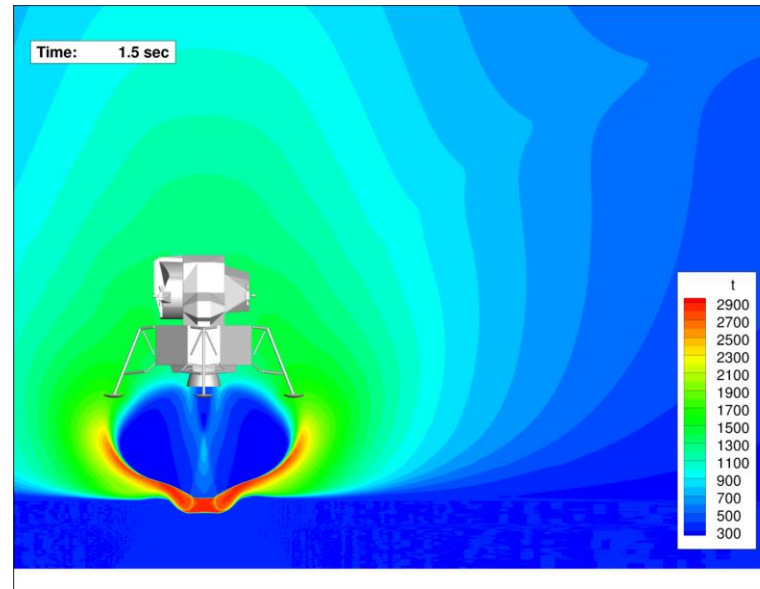
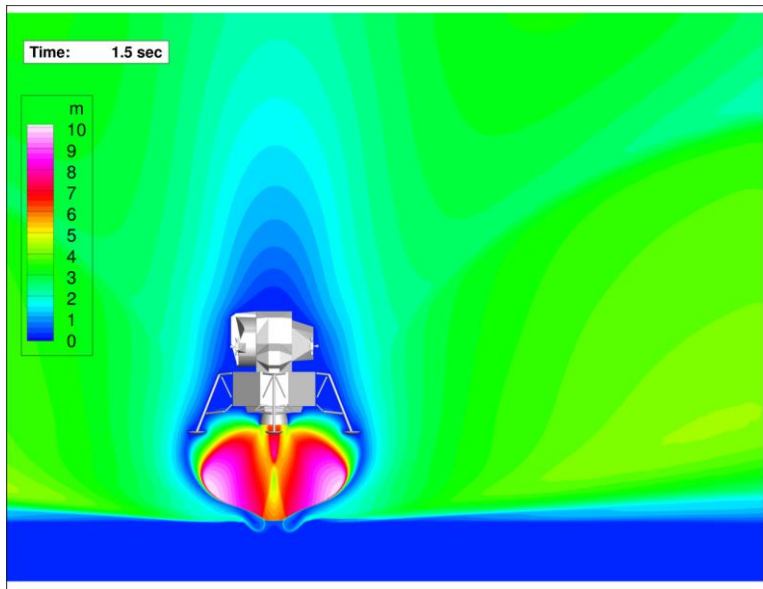


Sphere $D=30$ micron, Sphere $D=100$ micron, Cylinder $AR=4$

Apollo LM at 5m: Spheres 100micron



- Simulation with 100micron spheres shown as example
- Rapid expansion of plume flow results in supersonic outflow outward and upward
- Initial stir-up of particles from impulsive plume startup and impingement on soil slowly rising up with
- Near surface ejecta sheet forming from soil surface outside of crater ; ejecta sheet angle $\sim 5-10\text{deg}$
- Secondary ejecta stream ejected from crater edge

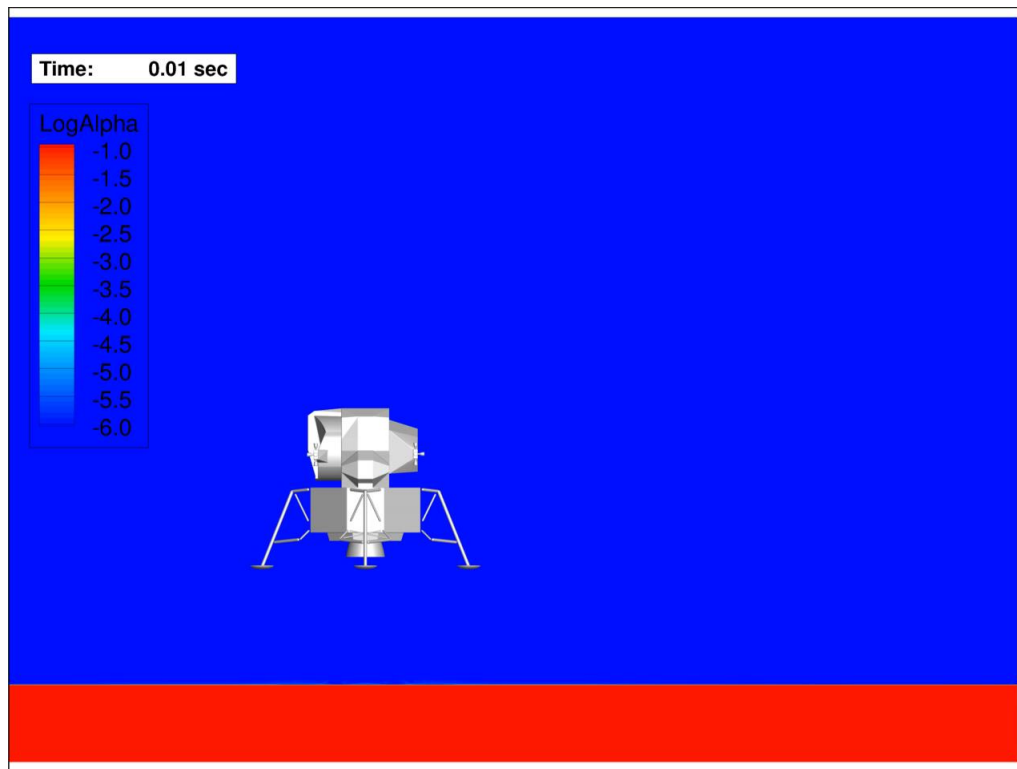


Ejecta Sheet Evolution: Effects of Poly-dispersity

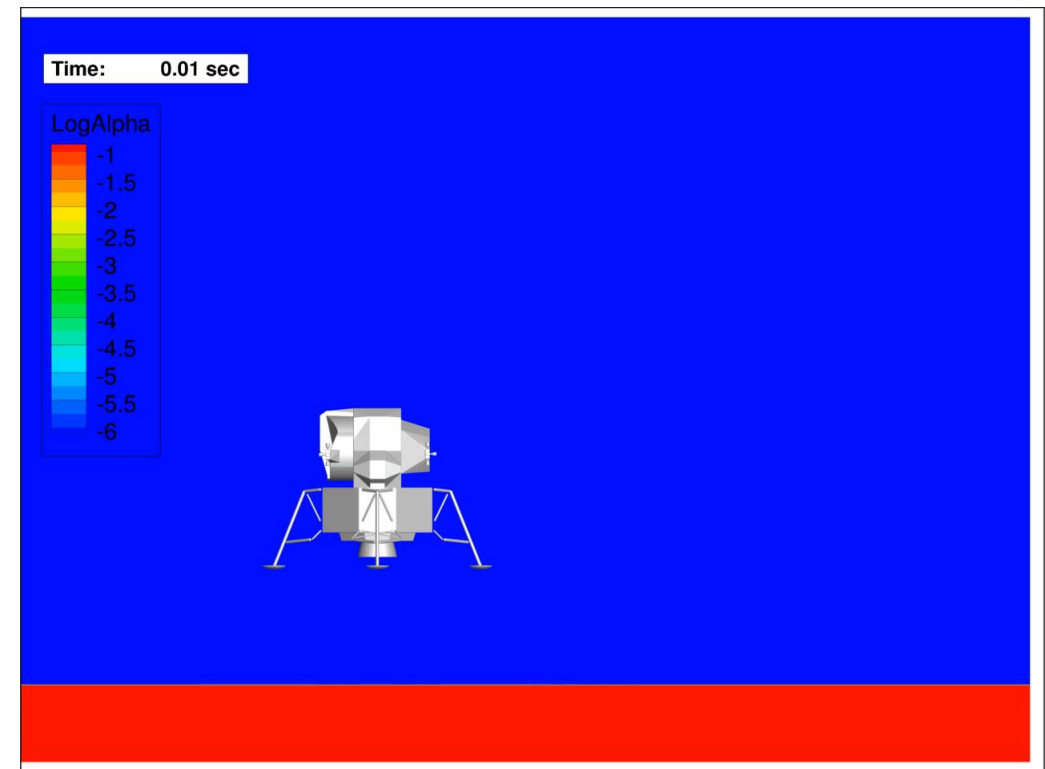


- Initial stir-up of particles from impulsive plume startup and impingement on soil slowly rising as quasi-steady plume field establishes

Mono-disperse 30mi spheres



Bi-disperse 30-100mi spheres

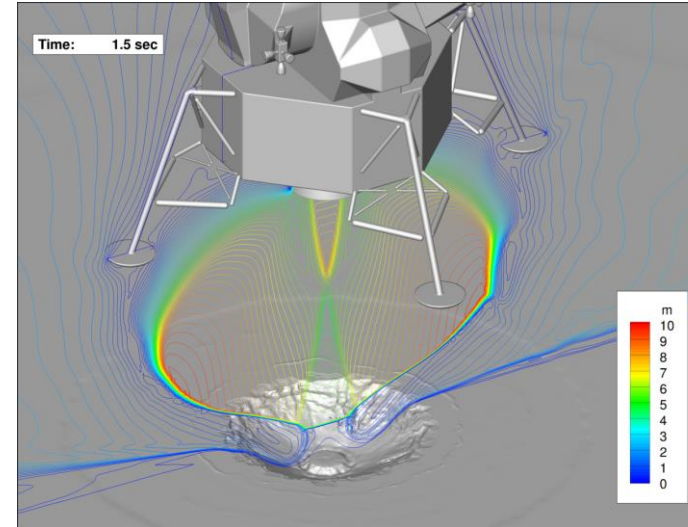


Animations

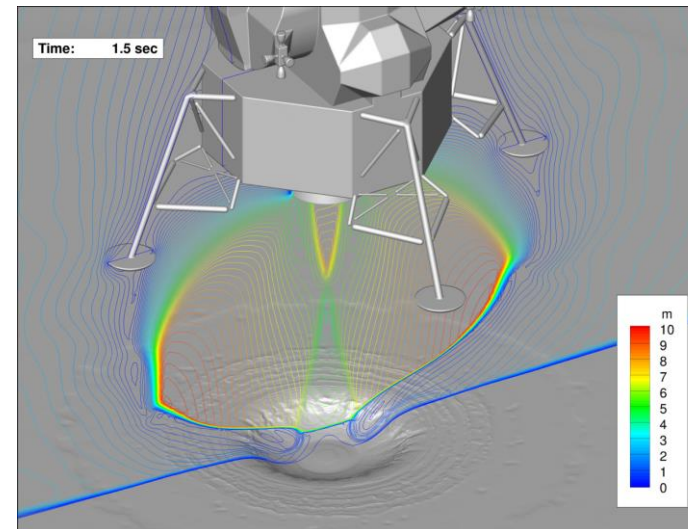
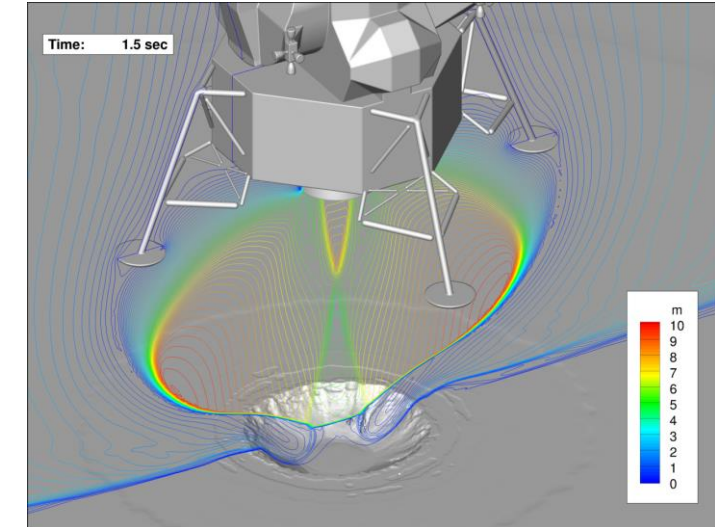
Effect of Particle Shape/Mixture on Crater Shape/Depth

- Comparison of crater shape shown at $t=1.5$ sec
- Crater walls show more pocketed appearance for small spheres
- Non-spherical elongated shape (cylinder AR=4) results in reduced crater depth compared to spheres
- Bi-disperse mixture results in highest reduction in crater depth and shallow crater

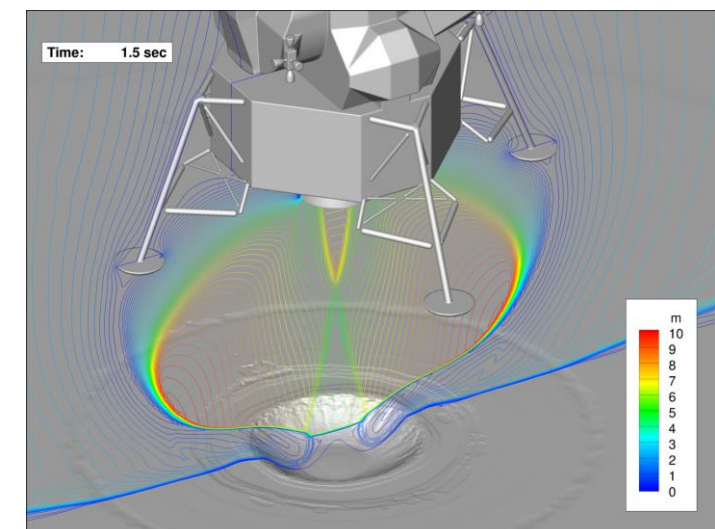
30mi spheres



100mi spheres



Bi-disperse 30-100mi spheres

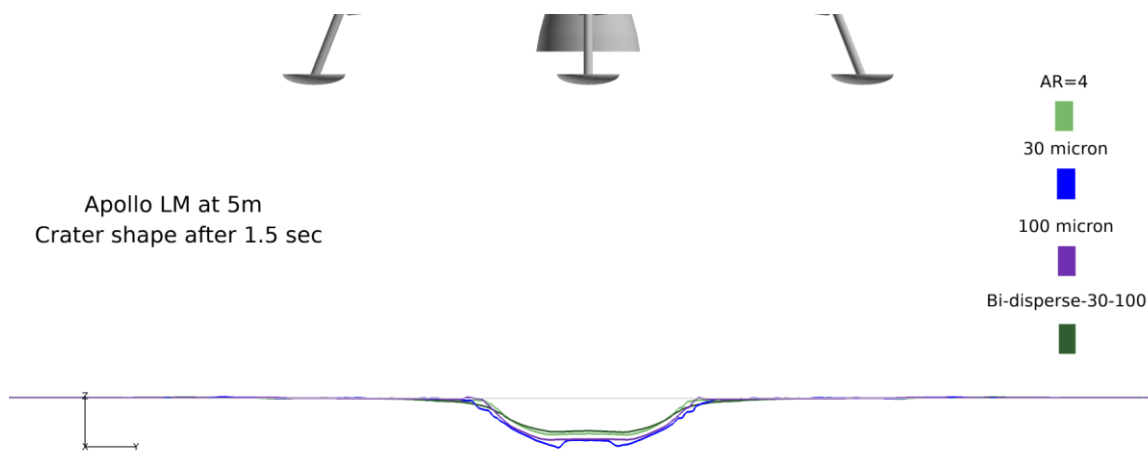


Non-Spherical AR=4

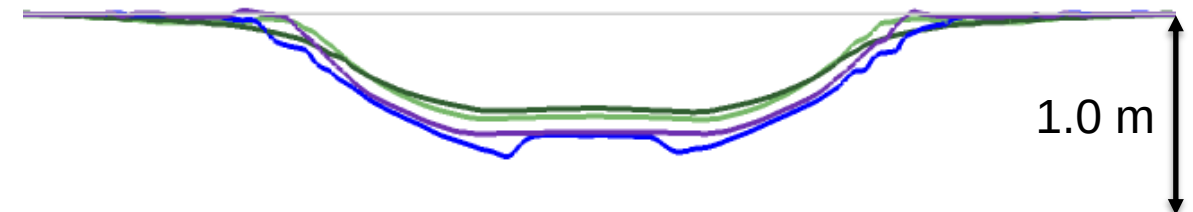
Effect of Particle Shape/Mixture on Crater Depth



- Crater depth profile comparison shown at $t=1.5$ sec
- Smaller 30mi spheres show erosion gouges in outer region of crater floor compared to 100mi; forms distinct plateau under central post-shock region;
- Non-spherical elongated shape (smooth cylinder $AR=4$) results in reduced crater depth compared to spheres; stress models from DEM predict elongated smooth cylinder shapes align with particle and gas flow direction and result in reduced stress
- Bi-disperse mixture 30mi+100mi results in reduced crater depth compared to either 30mi or 100mi mono-disperse
- At final simulation time $t=2.0$ sec, crater depth is approximately 0.75m and diameter approaching 4.0m. The particle compositions modeled here are more mono-disperse like sand than lunar regolith. Quick-look comparison of PFGT-1 craters between mono-disperse sand and poly-disperse BP-1 appears to indicate this tendency.



Accounting for irregular shape and poly-dispersity effects matters!



Future work



- Fully migrate DEM database simulation to LIGGGHTS execution on NASA Pleiades supercomputer
- The LIGGGHTS database generation process will be Python scripted to automatically generate LIGGGHTS input files, perform the simulations, and extract the output data in the database format expected by GGFS.
- Installation of the LIGGGHTS DEM automated database simulation capability on the NASA supercomputers and enabling execution in this scripted automation process has been spearheaded by the GGFS development team and will be executed in near future.
- Extend GGFS run-time database access to general poly-disperse bin numbers through multi-dimensional database interpolation capability in Loci/GGFS framework for supercomputer. This capability has been pursued by GGFS developers in cooperation with Loci computational framework developers.
- Once automated database generation process is operational, generate regolith particle and mixture models for simulants tested in PFTG-1 experimental campaign to enable validation of GGFS capabilities with more realistic particle effects resolution. All validation exercises to date have been performed with spherical particles.

Conclusions



- The status of Focus Area 3 of the PSI project was presented: Efficient generation of accurate soil particle composition constitutive closure model databases for application in the Gas-Granular Flow Solver computational process.
- The process of particle interaction constitutive closure model database generation using DEM particle interaction modeling was presented.
- 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. The LIGGGHTS DEM toolset has been selected as the most suitable tool to migrate the DEM simulations to.
- Implementation of an automated process of setup, execution, database extraction, and dataset delivery ready for application if GGFS simulations is in progress.
- This new capability will facilitate generation of higher fidelity regolith particle and mixture models for the simulants tested in PFTG-1 experimental campaign to enable validation of GGFS capabilities.
- The application readiness of the soil models currently operational in GGFS was demonstrated with the example of a full scale, 3-D simulation of the plume induced erosion and crater formation of the Apollo LM in a low pressure, near vacuum background.