A NUMERICAL APPROACH TO STUDYING THE EFFECTS OF PARTICLE SHAPE ON RUBBLE-PILE DYNAMICS. J.C. Marohnic[1,2], J.V. DeMartini[1], and D.C. Richardson[1], [1]Department of Astronomy, University of Maryland, College Park, MD 20742, [2]Email: jmarohni@umd.edu

Introduction: Most small solar system bodies are thought to be loose, gravitationally bound aggregates of material ("rubble piles"), rather than solid, monolithic objects [1]. To better understand these bodies, a great deal of prior work has used numerical techniques to model them. While there are a variety of viable approaches, ours uses the discrete element method (DEM), which allows us to consider how the shapes of individual particles affect our simulations and the physical processes they represent. Though it has long been accepted that particle shape plays an important role in granular processes like those present in rubble-pile bodies [2,3], most DEM codes have used spherical particles for the simplicity and computational efficiency they afford. Other codes include implementations of non-spherical particles [4] but their complexity can limit the numbers of particles that can be used in a simulation. We present a scheme for constructing rigid, non-spherical shapes out of spheres that leverages our code's existing ability to quickly compute gravity and contact interactions between large numbers of particles.

Method: We use the *N*-body code pkdgrav, which is highly optimized for calculating gravitational interactions between very large numbers of particles efficiently [5]. pkdgrav uses a hierarchical tree algorithm that reduces the cost of finding particle neighbors and calculating interparticle gravitational forces. The code is also parallelized.

The pkdgrav code uses a soft-sphere discrete element method (SSDEM) scheme for handling particle collisions (for other examples of SSDEM see [6,7]). Particles are spherical, and colliding particles are allowed to interpenetrate slightly as a proxy for surface deformation. Contacts are resolved using a spring-dashpot model in which overlaps are detected and result in normal and tangential restoring forces. These forces are modeled as damped springs with user-adjustable spring and damping constants. We also use this approach to calculate forces and torques from static, rolling, and twisting friction. Overlaps are tracked for the duration of particle contacts, and interparticle forces depend on the contact history in addition to the immediate overlap state. For a more detailed description of the SSDEM implementation in pkdgrav, see [8,9].

Non-spherical particles. To address the question of particle shape in rubble-pile bodies, we naturally need the ability to simulate non-spherical particles. While pkdgrav already had this functionality for hard-sphere aggregates [10], a different model is required here because contacts can persist across multiple time steps.

Instead of constructing polyhedral particles with flat faces and edges, we make use of the existing capabilities of pkdgrav and model non-spherical particles using a "glued-sphere" approach. We arrange arbitrary numbers of spherical particles in any desired shape and then fix their relative positions so that they behave as a unit, creating rigid, non-spherical aggregates. Since we already track the positions and velocities of the constituent spheres, we can easily calculate the total mass and center of mass position and velocity of these rigid aggregates. They can then be treated as "pseudo-particles."

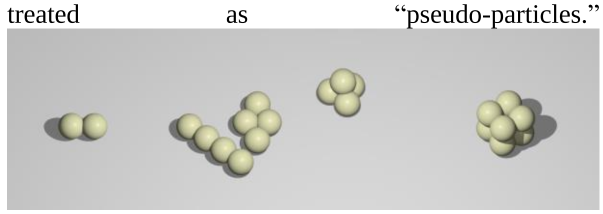

Figure 1. Examples of some simple rigid aggregates in pkdgrav. From left to right: a dumbbell-like shape, a 4-particle rod, a planar diamond, a tetrahedron, and a cube.

Forces and Torques. One of the primary advantages of constructing non-spherical particles in this way is that computing forces and torques is relatively straightforward. We can further divide these calculations into gravitational and contact interactions.

Gravity. Gravitational interactions are already calculated for each individual sphere in pkdgrav, so to find the net acceleration due to gravity on a rigid aggregate we only need the vector sum of the gravitational forces on each particle in the aggregate. On the other hand, individual spheres feel no net torque from gravity, so here we record the position of each sphere relative to the center of mass of the aggregate it belongs to. The gravitational torque contribution is the force of gravity acting on that sphere with a lever arm stretching from the aggregate center of mass to the center of the sphere. The vector sum of the torque contributions from each constituent sphere in an aggregate is the net gravitational torque on the aggregate.

Contacts. Resolving contact forces requires a bit more care. In pkdgrav, particle contacts result in both a force and a torque on each particle. While in gravitational interactions forces act on particle centers, contact forces must be applied *at the contact point*. Each particle feels a normal restoring force that depends on the extent of the overlap. If the particles have non-zero friction, they may also experience a tangential surface force. Contact forces between particles are then referred to their containing aggregate, and the net center-of-mass acceleration on the aggregate due to contact forces is calculated. In the case of individual spheres, tangential surface forces will give rise to torques as well as accelerations, while normal contact forces cannot. For aggregates, both types of forces will in general result in net torques. The contact torque contribution from a particle is calculated by considering the normal and tangential contact forces felt by that particle acting on a lever arm connecting the aggregate center of mass and the contact point on the particle, instead of the particle center as in the case of gravity. The vector sum of these torque contributions gives the net torque due to contact forces on a rigid aggregate in pkdgrav. For all the above calculations, we discount contributions from forces acting between two particles in the same aggregate.

We note here that the careful approach to applying gravity and contact forces described above is necessary for achieving proper physical behavior. In the case of large rubble piles, angular momentum conservation in particular suffers if torques are not applied at the contact points.

Summary and Future Work: As far as we are aware, pkdgrav is the only code that combines an *N*-body gravity solver and a soft-sphere contact model with an efficient “glued-sphere” approach to constructing non-spherical particles. This allows us to conduct high-resolution simulations of self-gravitating aggregates of non-spherical grains. Currently, complete rolling and twisting friction implementations are not part of our model for rigid aggregates. In the context of rubble-pile dynamics, we expect that these forces are less significant than the additional shear strength that arises from particle shape. However, work on these features is ongoing and should be completed soon. pkdgrav also has the capability to apply finely controlled spin-ups to rubble piles [11]. After some modifications, this feature can now also be used to spin up rubble piles composed of the non-spherical particles described here. See Fig. 2.

While this technique has broad relevance to the study of small solar system bodies, we plan to use it to study spin-up and tidal effects. For example, what role does particle shape play in setting the critical spin limit for rubble piles, and to what extent? How does particle shape affect binary formation under tidal stresses? Given the resolution and efficiency we can now achieve with non-spherical particles in pkdgrav, these are questions we can begin to answer. Preliminary results of these investigations will be presented.

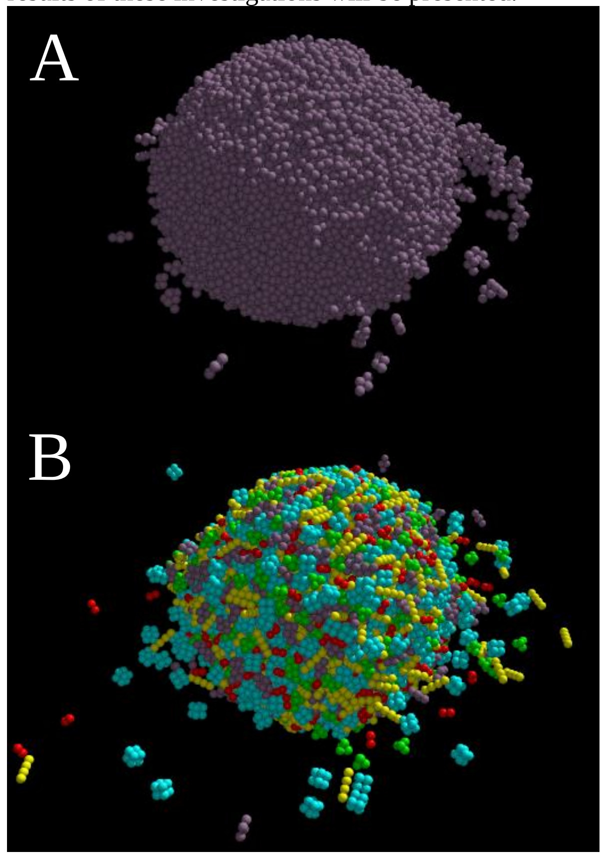

Figure 2. Rubble piles composed of rigid aggregates shedding material during spin-up. Object A is composed entirely of planar diamond-shaped aggregates. Object B is composed of a mix of different shapes. Aggregates are color-coded by shape.

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References: [1] Walsh, K. J. (2018) *Ann. Rev. Astron. Astr.*, *56*, 593-624. [2] Robinson, D. A. and Friedman, S. P. (2002) *Physica A*, *311(1-2)*, 97-110. [3] Wegner, S et al. (2014) *Soft Matter*, *10.28*, 5157-5167. [4] Ferrari, F. and Tanga, P. (2020) *Icarus*, *350*, 113871. [5] Stadel, J. G. (2001) *PhD Thesis*, *Univ. of Washington.* [6] Cundall, P. A. and Strack, O. D. (1979) *Geotechnique*, *29.1*, 47-65. [7] Sánchez, P and Scheeres, D. J. (2011) *Astrophys. J.*, *727.2* 120. [8] Schwartz, S. R. et al. (2012) *Granul. Matter*, *14.3*, 363-380. [9] Zhang, Y. (2017) *Icarus*, *394*, 98-123. [10] Richardson, D. C. et al. (2008) *Plan. Space Sci.*, *57*, 183-192. [11] Zhang, Y. (2018) *Astrophys. J.*, *857.1*, 15.