Granular Flow in a Rough Annular Shear

Validating DEM Simulations with Experiments

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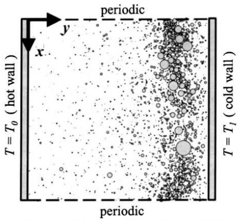
April, 2009

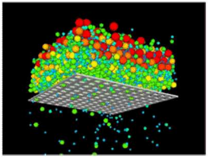
Outline

DEM: the Gold Standard

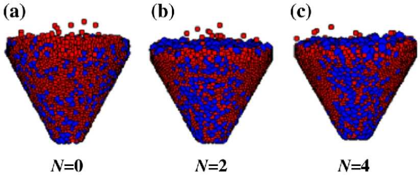
- Model diverse particles and properties
- Measure relevant quantities
- Control material properties
- "Combinatorial" experiments



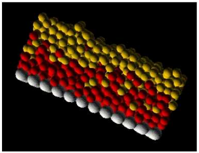
Dahl and Hrenya, Phys. Fluids, 2004.



Clear and Sawley, Appl. Math. Mod., 2002.

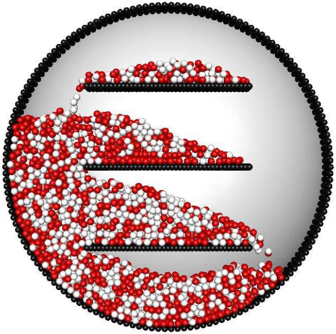


Arratia et al., Pow. technol., 2006.



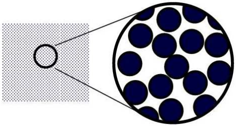
Khakhar et al., Phys. Fluids, 1997.

DEM: the Gold Standard (cont.)

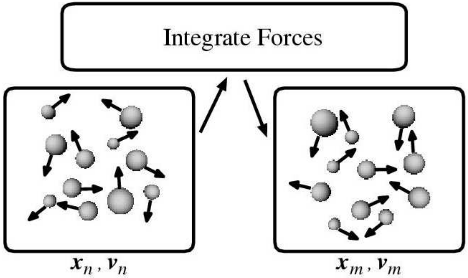


- Remarkable qualitative agreement
- Good mascroscopic quantitative agreement (IS, etc.)

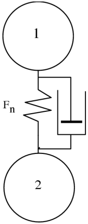
Discrete Element Method



- Goal: gain *macro*scopic insight from *micro*scopic considerations
- Method: Model interaction forces
- Specifics: Newton's Law ($\mathbf{F} = m\mathbf{a}$)



Contact Mechanics – Normal Force Models



- Simple spring-dashpot model schematic (shown)
- Force models vary in both accuracy and computational difficulty.

Model	Restitution Coefficient (RC)	Mathematical Form	Comments
Purely Viscous (PV : Lee and Herrmann 1993)	Increases with velocity	$k_n\alpha^{3/2} - k_d v_n$	Computationally simple, yet poor RC, discontinuous force vs. approach
Oden-Martins (OM : 1984)	agrees w/experiment	$k_n\alpha^{3/2} - k_d v_n \alpha$	More computationally complex, realistic RC and force vs. approach
Tsuji (T : 1993)	Constant	$k_n\alpha^{3/2} - \tilde{k}_d(\sqrt{mk_n})v_n\sqrt[4]{\alpha}$	More computationally complex, yet yields constant RC and unrealistic force at small unloading
Walton-Braun dependent (WB-d : 1986)	agrees w/experiment	$k_1\alpha$ $k_2(\alpha-\alpha_o)$ $k_u=\mathcal{F}(f_n)$	Computationally simple, realistic RC and force vs. approach
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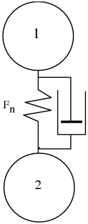

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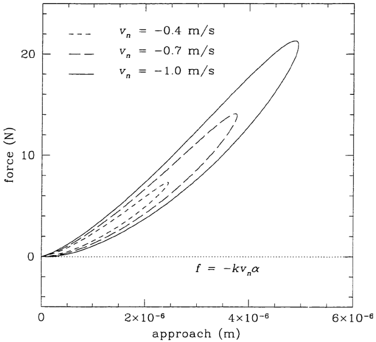
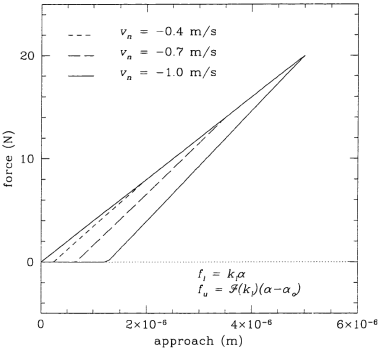
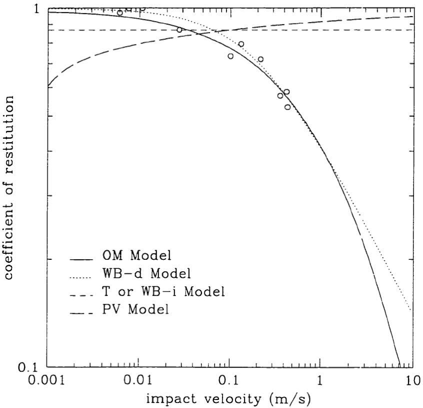
Force versus Approach





- A simple test of a model's accuracy
- Area "under" the curve represents energy dissipation.

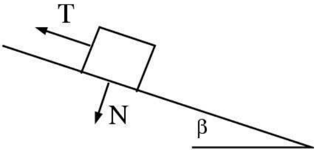
Coefficient of Restitution



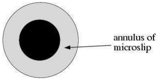
- A useful test of model's dynamic response (typically **only** test)
- Note that CR accuracy is not necessary for obtaining correct kinematics!

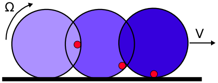
Coulomb limit applies after (macro-)sliding occurs:

$$T = \mu N$$



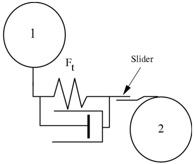
Sliding onset is more complicated (Mindlin, 1949):





- Friction has a "memory": $T = T_{old} + k_T s$
- Watch out for rolling on perfectly smooth surface! (rolling friction?).

Friction Force Models



- Key issue is incremental friction (proportional to displacement, not velocity → creep!)
- Capturing microslip not generally considered critical.

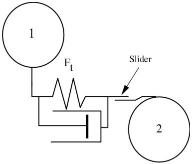
Model	Form	Displacement	k_t	Comments
Zero Model (Tsuji 1993)	$-k_t s$	$s = v_t \Delta t$	constant	Computationally simple, yet allows particle creep
One Model (Cundall and Strack 1979)	$-k_t s$	$s = \int_0^t v_t(\xi) d\xi$	constant	More computationally complex, realistic collisions, no particle creep (save s_o)
Two Model (Walton and Braun 1986)	$-k_t s$	$s = \int_0^t v_t(\xi) d\xi$	$k_t = \mathcal{F}(f_t)$	More computationally complex, realistic collisions, no particle creep, dissipates energy through microslip (save s_o, f_t)

Walton-Braun (Two Model):

$$k_t = k_{to}\left(1 - \frac{f_t{}' - f_t{}^*}{\mu f_n - f_t{}^*}\right)^n \; for\ loading$$

$$k_t = k_{to}\left(1 - \frac{f_t{}^* - f_t{}'}{\mu f_n + f_t{}^*}\right)^n \; for\ unloading$$

Friction Force Models



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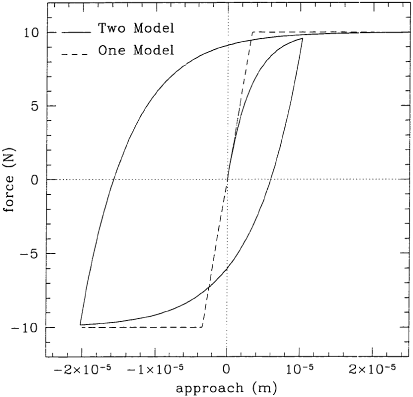
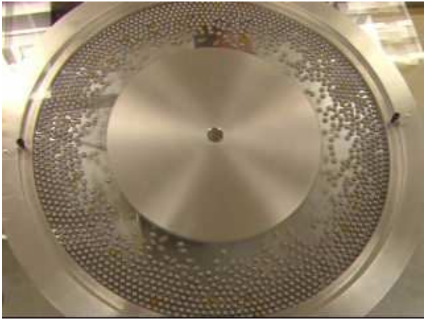
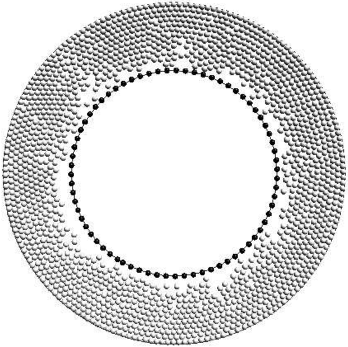


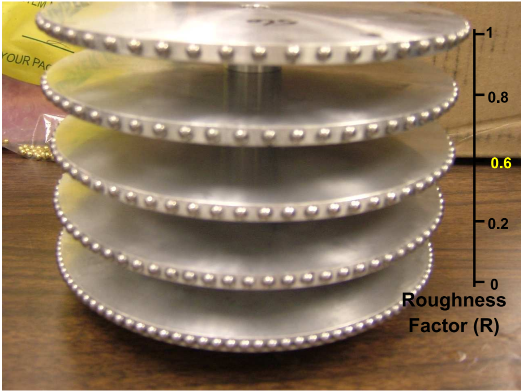
- Note the asymptote to Coulomb sliding
- Zero model not shown since force is not a function of displacement

Model System



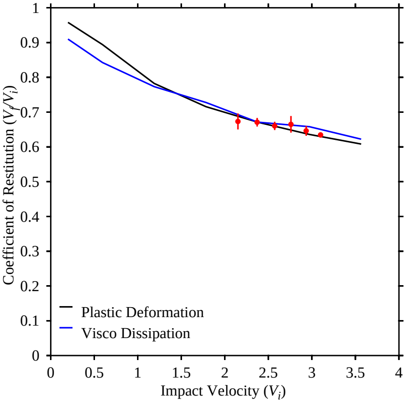


- Roughened inner cylinder rotates
- Experimentally extract f, v, T profiles



- Roughness varies from 0→1
- Ω varies from 220RPM→270RPM
- “Base case”: Ω = 240RPM, R = 0.6

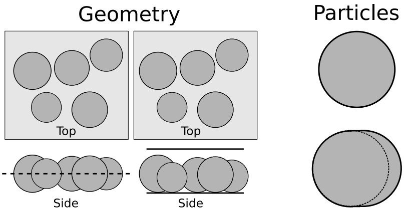
Match Properties



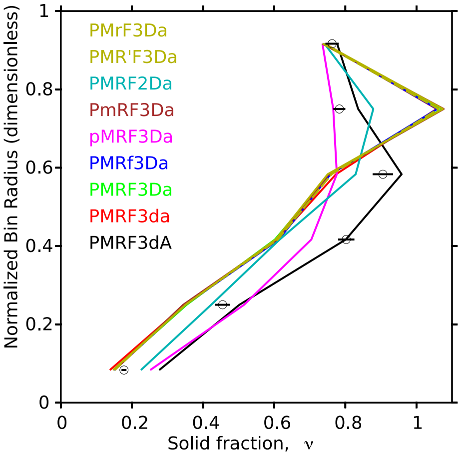
- Match dissipation for both plastic and visco
- Some simulations in 2d, others with varying gaps

Geometry and Models

Model variation	Version 1	Version 2+
Normal force model	Plastic [P]	Spring-Dashpot [p]
Friction force model	Mindlin [M]	Cundall [m]
Rolling friction	Large [R′]	Present [R] Absent [r]
Dissipation	Fit to experiment [F]	Larger than physical [f]
Geometry	Fit to experiment [3d]	Larger head space [3D] Ideal two dimensional [2D]
Particle Geometry	Aspherical [A]	Perfect spheres [a]



Solid Fraction by Model



Plastic Dissipation [P]	Spring-Dashpot [p]
Two Model Friction [M]	One Model [m]
Rolling friction [R′/R]	Absent [r]
Dissipation Fit [F]	Larger [f]
Geometry Fit [3d/3D]	Planar [2D]
Particles Aspherical [A]	Spheres [a]

- In 2d, max packing 0.91; 3d systems overlap so f above 1
- Particle geometry is important; little else matters

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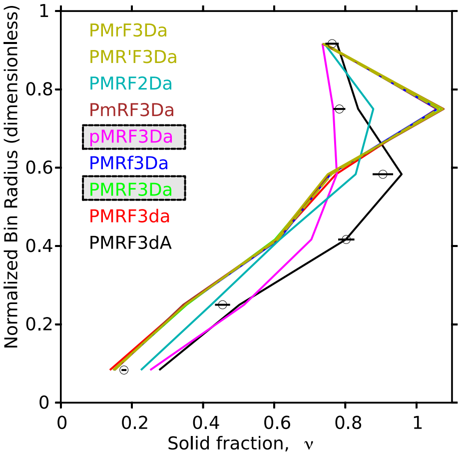

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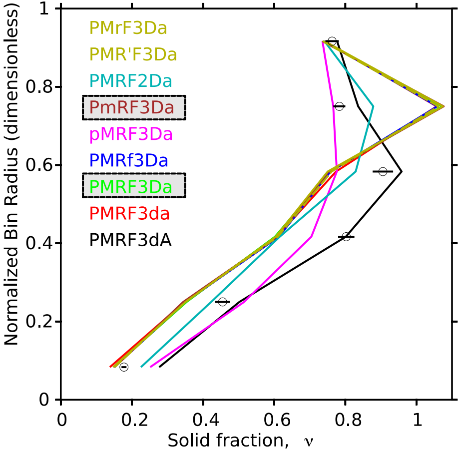

Plastic Dissipation [P] — Spring-Dashpot [p]
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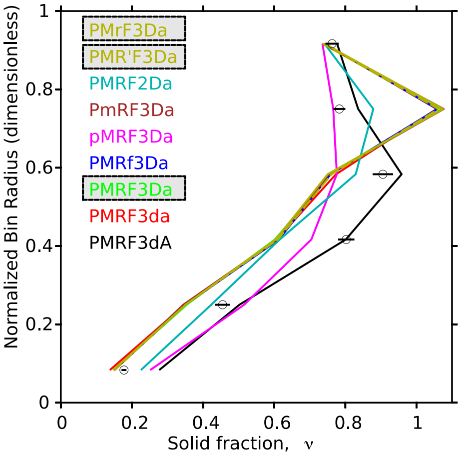

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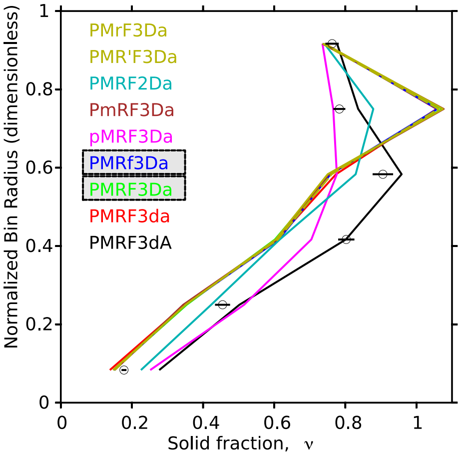

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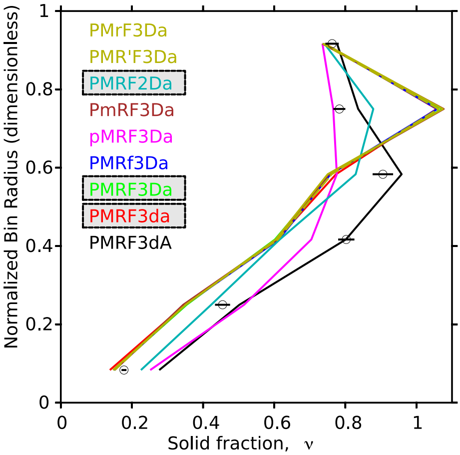

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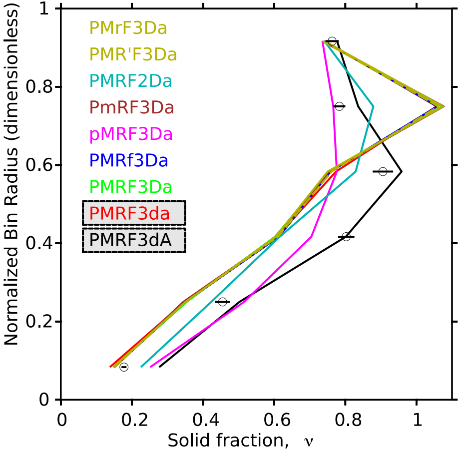

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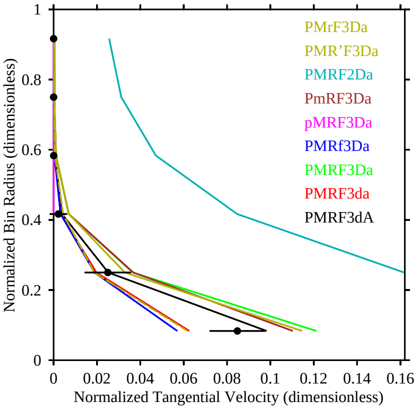
Velocity Profile by Model



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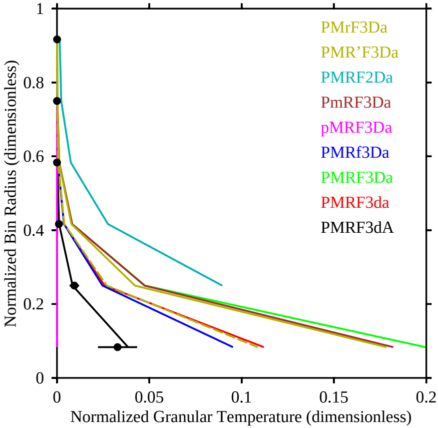
Particles Aspherical [A]	Spheres [a]

- System geometry match is *critical* (2D qualitatively wrong)!
- Rolling friction and/or dissipation may be tuned (to mimic asphericity?)
- Visco is way off

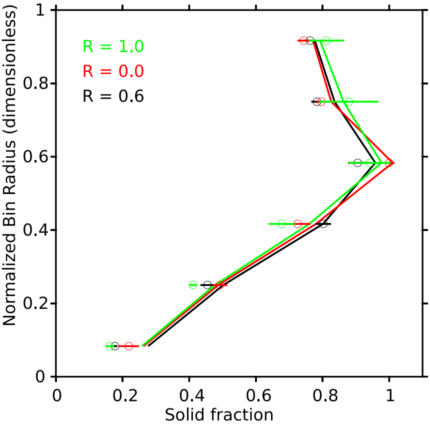
Granular Temperature by Model

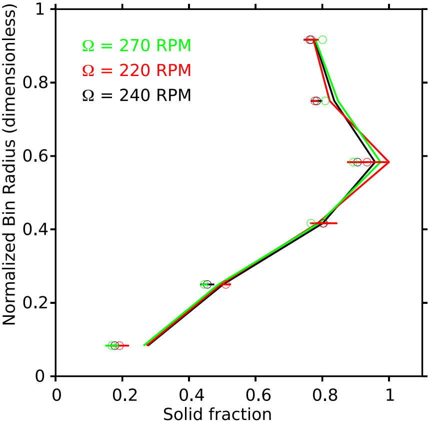


Plastic Dissipation [P]	Spring-Dashpot [p]
Two Model Friction [M]	One Model [m]
Rolling friction [R′/R]	Absent [r]
Dissipation Fit [F]	Larger [f]
Geometry Fit [3d/3D]	Planar [2D]
Particles Aspherical [A]	Spheres [a]

- “Extra” dissipation may work (but may create more errors)
- Rolling friction *cannot be tuned* properly
- Visco is way off

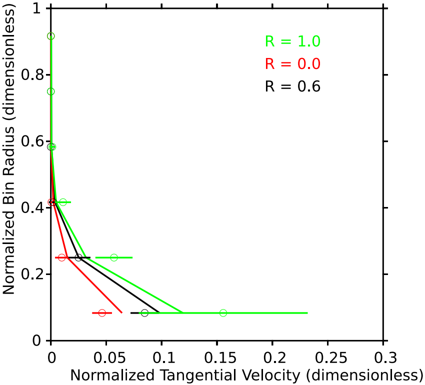
Varying Roughness/Rotation Rate (f Profile)

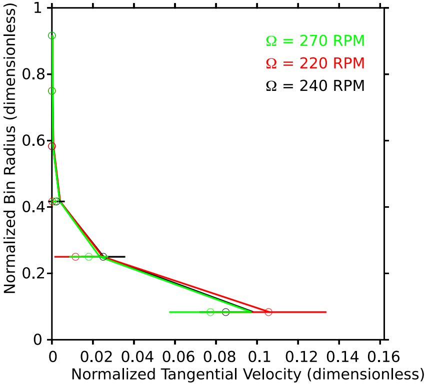




- Max location is very robust
- Roughness simulations captures trends properly (even cross-over)
- Rotation rate is very slightly off

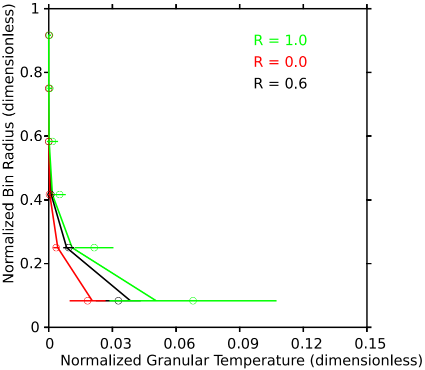
Varying Roughness/Rotation Rate (Velocity)

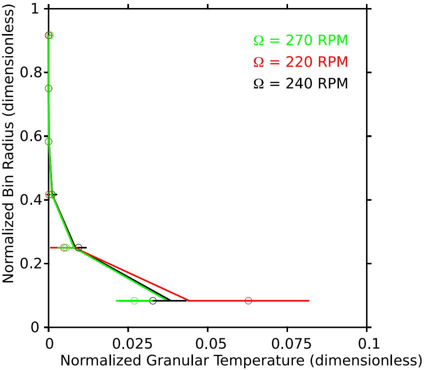




- Roughness trend is captured
- Rotation trend is captured

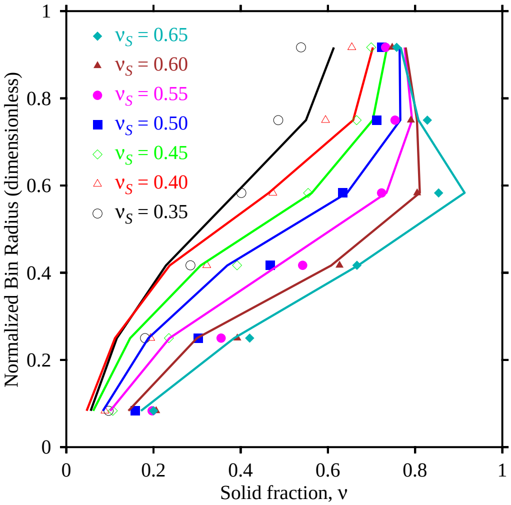
Varying Roughness/Rotation Rate (Granular Temp)





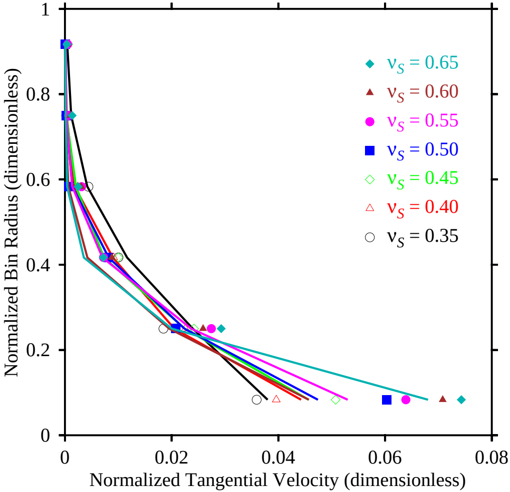
- Roughness trend is captured
- Rotation rate trend is captured

Parametric Study, f_{tot} (Solid Fraction Profile)



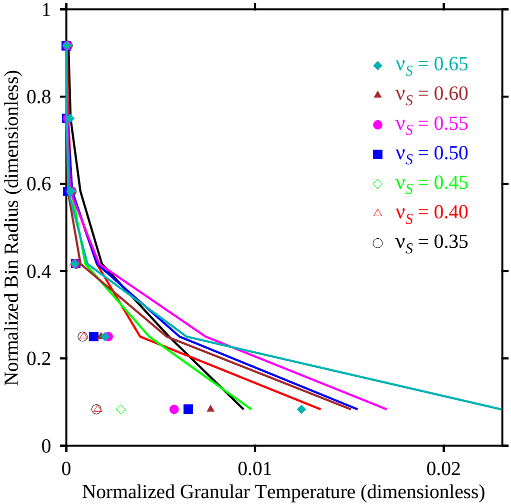
- Surprising agreement both qualitative and quantitative

Parametric Study, f_{tot} (Velocity Profile)



- Qualitative trends are captured
- Slightly off quantitatively (perhaps)

Parametric Study, f_{tot} (Granular Temp Profile)



- Qualitative trend is decent
- Consistently overpredict T

Outlook

- DEM "gold standard" – good quantitative
- Modeling **exact** physical geometry is critical
- Modeling of normal force/dissipation is important for v profile
- Modeling friction is more flexible (likely **not viscous**)
- Rolling friction can compensate for shape for v *or* T, not both
- Particle shape itself needed to capture both v and T
- Looking at f, v, and T is surprisingly discriminatory
- Single-particle tests may not tell whole story ...
- Acknowledgment: National Energy Technology Lab, Department of Energy