IFPRI BRIEF TEMPLATE

Check One: ☐**Project** ☐**Review** ☐**Collaboration** ☐**Workshop** ☒**Other**

Descriptive Title	Implementation powder rheology in grid-free methods and testing on Industrial challenges
Working Title[1]	Industrial implementation powder flow continuous models
Technical Area[2]	Dry Powder Flow
Date	June 13th, 2023
Short Description	General continuum solvers for particle flows, suitable for use in industry with adjustable boundary conditions and adjustable friction parameters, including a recipe for determining simulation (e.g., friction, restitution, continuum rheology) parameters from real powders.
Objectives	Obtain, test, and verify an open-source package for dense powder flows and apply in industry, including procedures to determine relevant parameters for real powders. Make package available to all IFPRI members, including standard flow simulations such as silo flow, chute flow and rotating drum flow.
Scope	Open-source, basic continuum solver for dense dry media, including an adjustable friction coefficient, wall friction coefficient, arbitrary geometries, and capability of forming new free surfaces, options for rapid flow effects on friction and the dependence of friction on evolving packing fraction. Make available to IFPRI members, documentation, and updates and examples.

Recommended Contractors (2 or 3)		
Name	**Institution**	**Email Address**
Ken Kamrin	MIT, Cambridge, MA, USA	kkamrin@mit.edu
Nico Gray	U Manchester, UK	

Submitted By:	
Name	**Organization**
Eric Grolman, Pieter Vonk	Envalior (DSM)
Jeremy Leachman	Sandia
Alex Fry	P&G
Subash Thakur	Vertex Pharmaceuticals

[1] Title used in meeting agendas and file archives

[2] One or more from the following list: W = wet systems; D = dry systems; F = particle formation; SR = size reduction; M = modeling; SE = systems engineering

1 Background and objectives

IFPRI AGM 2022 presentations and the powder flow workshop 2023 have shown that industry has a long-felt need for simulation of large-scale powder flows. Continuum approaches have the potential to allow such large-scale simulations and have sufficiently developed in academia over the past decade to merit application in industry. However, there exists a significant entry barrier, i.e. in expertise and hours required, that needs to be significantly lowered to enable their widespread use in industry.
The aim of the project is to bring the capability of continuum powder flow simulation to the hands of industry via open-source implementation of μ-f(I) rheology in a meshless simulation package with particular attention to ease of use. After a minimum viable implementation and testing, extensions of the implemented rheology with models for segregation, cohesion and non-local rheology become in scope. The selected modeling framework will be examined for suitability for reaching the end-goals from the start. Maintainability will also be an important selection criterium.

2 Deliverables

Phase 1

- Continuum implementation of relevant, adjustable μ-f(I) rheology calibrated with DEM simulations in the MPM/SPH framework in the open-source LAMMPS package, enabling the use in industry and continued support in the future.
- Testing of LAMMPS-MPM/SPH framework on industrial scale problems.
- Assessment of feasibility of application of MPM/SPH framework for industrial scale problems.
- Gap analysis & definition of the way forward on MPM modeling of powder flow.

Phase 2

- Include segregation
- Include non-local effects

3 Project steps & resources

- Implementation MPM framework in LAMMPS. This requires the collaboration between the academic researcher developing the MPM method with the software developers of Sandia Laboratories for implementation within the LAMMPS package.
- Definition of a calibration protocol for the rheology parameters within the continuous model used in the implementation. This requires the collaboration between the academic researchers and the industrial participant, in view of their experimental capabilities.
- Implementation of LAMMPS MPM tool within industry. This requires the collaboration between the software developers of Sandia Laboratories and the industrial collaborators.

- Testing of the LAMMPS package on industrial scale problems. This requires the collaboration between the academic researchers, software developers and industrial participants.
- Assessment of the simulation results in relation to the applicability of the continuum modeling in industry. This requires the collaboration between the academic researchers and industrial partners.
- Assessment of the simulation results in relation to the scientific gap within the continuum modeling of powder flows and definition of follow-up research to be conducted. This is a task for the academic researchers.

The funding of IFPRI (one year) is required for supporting the academic researchers to collaborate with the industrial partners (including Sandia). The industrial partners will perform their contribution as an in-kind contribution.

PHASING
First year
A continuum implementation of granular flow with adjustable rheology
Check capabilities of currently envisioned implementation in LAMMPS, including

- Parameterized process boundaries
- Capability to define topology of the equipment, e.g. via importing STL files
- Ability to adjust rheology parameters to mimic real materials
- Visualization of results
- Special attention for achieving a low entry barrier for industry users

Validation of simulation results
First minimum viable implementation
Testing and feedback from industry members

Second year
Simulation of standard test equipment (rotating drum, angle of repose, shear cell, FT4) as derived from DEM Round Robin to calibrate rheology
Optimized method to translate DEM results into the LAMMPS rheology
Add segregation due to size to the model framework

Third year
Add non-local rheology to the package, so that it can be used when required
Add adhesion to the model