IFPRI BRIEF TEMPLATE

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

Descriptive Title	High Performance Simulation Modeling of Particle Suspensions
Working Title[1]	Simulating Particle Suspensions
Technical Area[2]	W, M
Date	13/6/2023
Short Description	New state-of-the-art simulations incorporate hydrodynamic interactions to generate large-scale (~10^6 or more) particle simulations that *quantitatively* capture macroscopic properties. With two excellent experiment projects currently in the wet systems portfolio (SIFs, Slurries and Pastes), maximum benefit can be extracted from that work with computational support to give further insights to properties that cannot be disentangled experimentally. The goal of this collaboration is to bring insights to the experimental work by comparing with state of the art simulations. The simulations have the ability to systematically add and remove physics (interactions, concentrations, hydrodynamics, gravity, walls / surfaces) to identify key drivers to sedimentation/stability, processability, dispersibility, flowability and microstructural changes over time and in flows. This collaboration will seed an interaction between the established experimental group and innovator in the simulation and modeling space. A long-term goal of this work is towards computer simulations that can be used to design processes (e.g. formulations) and explore large design spaces as the complexity of systems increases through the incorporation of multiple aspects of shape, roughness, polydispersity, heterogeneity, etc.
Objectives	Develop a simulation with hydrodynamic interactions of rough and anisotropic particles in the "building up" part of the SIF project.

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[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

Scope	In:
	- Analyze the structure of simulated suspensions and compare with experiments
	Out:
	- Freely draining hard spheres (oversimplified system)

Recommended Contractors (2 or 3)		
Name	**Institution**	**Email Address**
Sho Takatori	UCSB	
Michael Howard	Auburn University	
Zachary Sherman	University of Washington	

Submitted By:	
Name	**Organization**
John Hone	Syngenta
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