**Check One:** [ ] **Project** [x] **Review** [ ] **Collaboration**

[ ] **Workshop** [ ] **Other**

|  |  |
| --- | --- |
| **Descriptive Title** | Simulation Methods for Colloidal Dispersions |
| **Working Title[[1]](#footnote-1)** | Simulation Methods for Colloidal Dispersions |
| **Technical Area[[2]](#footnote-2)** | W |
| **Date** | 17 June 2025 |
| **Short Description** | Hydrodynamic interactions between dispersed particles are important in processes such as reconstitution, mixing, and gelation. Multiple methods for simulating hydrodynamic interactions are being used in IFPRI-funded work, but there is lack of guidance about how to select between them for different systems. This review will compare the accuracy and computational efficiency of methods for simulating hydrodynamic interactions, including Rotne–Prager–Yamakawa far-field hydrodynamics, lubrication dynamics, Stokesian dynamics, and multiparticle collision dynamics, for a representative set of colloidal dispersions. It complements a review previously conducted for dry systems. |
| **Objectives** | 1. Identify a set of colloidal dispersions with interactions, concentrations, and microstructures that are representative of IFPRI-relevant work.
2. Identify processes that can be simulated and properties that can be measured for the selected dispersions using all methods.
3. Compare accuracy of methods for simulating hydrodynamic interactions in selected colloidal dispersions and properties.
4. Compare performance of methods using representative computing hardware.
 |
| **Scope** | Dispersions must go beyond monodisperse hard-sphere suspensions. |

|  |
| --- |
| **Recommended Contractors (2 or 3)** |
| **Name** | **Institution** | **Email Address** |
| Joost de Graaf | Utrecht | j.degraaf@uu.nl |
|  |  |  |
|  |  |  |

|  |
| --- |
| **Submitted By:** |
| **Name** | **Organization** |
| Jim Michaels | IFPRI |
|  |  |
|  |  |

1. Title used in meeting agendas and file archives [↑](#footnote-ref-1)
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 [↑](#footnote-ref-2)