Development of a Two-Fluid Drag Law for Clustered Particles using Direct Numerical Simulation and Validation through Experiments

HBCU/MI Award DE-FE0007260 Review Meeting

Program Manager: Vito Cedro

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May 31, 2012

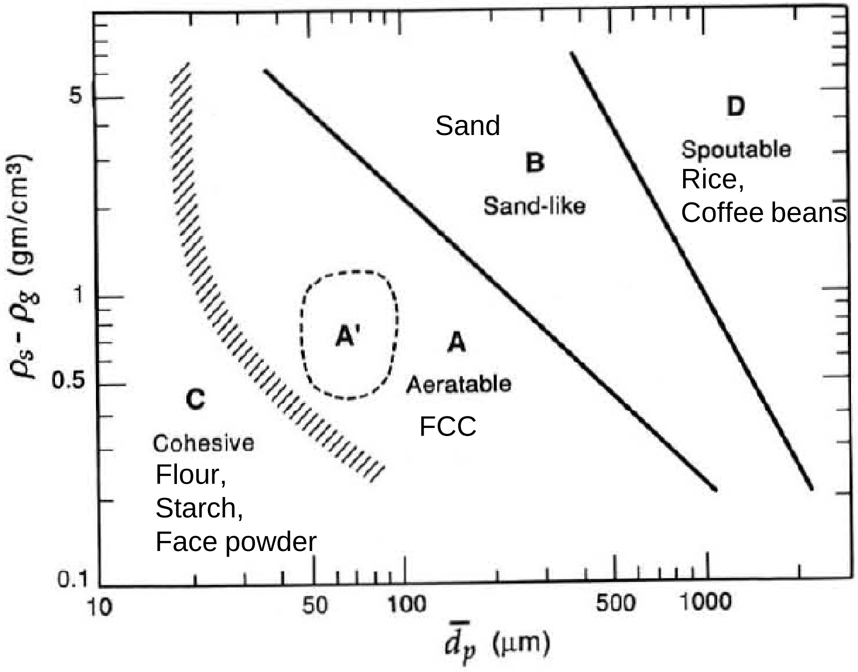
Technical Background

- Developers of gasifiers, combustors, chemical reactors, and owners of energy power plants are incorporating simulation in their design and evaluation processes to enhance process control and increase efficiency yield and selectivity.
- Several computational fluid dynamics (CFD) codes have been developed to simulate the hydrodynamics, heat transfer, and chemical reactions in fluidized bed reactors (MFIX, CFDLIB, etc.).
- Closure laws are required in the CFD simulations in order to capture the interaction between the gas and the solid phases in the system. For large scale simulations, a drag law is used in order to model the average interphase momentum transfer.
- Empirical correlations based on experiments by Ergun[1] and Wen-Yu[2] have been used frequently to calculate the drag force in dense and dilute flow regimes.

(1) Ergun, Chemical Engineering Progress, vol. 48, pp. 89-94, 1952.
(2) Wen and Yu, Chemical Engineering Progress Symposium Series, vol. 62, pp. 100-111, 1966.

Technical Background

- ❑ Particle-resolved direct numerical simulation (DNS) of flow past fixed particle assemblies[3,4,5] yielded a drag relation that is more accurate than the Ergun and Wen-Yu correlations.
- ❑ These drag laws are applicable to suspensions where particles do not form clusters, and they have been useful in modeling the hydrodynamics of fluidized beds for Geldart B and D particles[6].
- ❑ CFD simulation of fluidized beds with Geldart A particles remains a challenge because they fail to reproduce the pressure drop and bed expansion that are observed in experiments[7,8].
  - ➢ Formation of particle clusters significantly reduces the drag force.
  - ➢ The drag force is overestimated by standard drag laws.



(3) Hill et al., Journal of Fluid Mechanics, vol. 448, pp. 243-278, 2001.
(4) Beetstra et al., AIChEJ, vol. 53, pp. 489, 2007.
(5) Tenneti et al., International Journal of Multiphase Flow, 37, 1072-1092, 2011.
(6) van der Hoef et al., Annual Review of Fluid Mechanics, vol. 40, pp. 47-70, 2008.
(7) Wang et al. Chemical Engineering Science, vol. 64, no. 3, pp. 622-625, 2009.
(8) Wang, Ind. Eng. Res., vol. 48, no. 12, pp. 5567-5577, 2009.

Technical Background

- ❑ Ad hoc approaches to account for the presence of particle clusters have been proposed (e.g., the Energy-minimizing Multi-Scale model) to modify the standard drag laws and these give improved simulation results in a limited fluidization regime.
- ❑ However, these ad hoc modifications do not have any predictive capability over the parameter range that is necessary for design optimization, nor do they provide insight into the fundamental multiphase flow physics.
- ❑ Therefore, a first-principles based approach is needed to quantify the mechanisms underlying particle clustering and their effect on the drag force.

Technical Background

- ❑ The current research includes utilization of a combination of numerical and experimental approaches to provide detailed data necessary for validation and optimization purposes.
  - ➢ Experimental evaluation of particle clusters will be investigated using high speed imaging.
  - ➢ The drag law applicable to particle clustering in fluidized beds will be developed using direct numerical simulations.
  - ➢ Finally the developed drag law will be implemented in the MFIX software and the results will be validated against experimental data.

Significance of the results of the work

- ❑ Supports the vision of the NETL 2006 Workshop on Multiphase Flow Research[9]:
  - ➢ "*To ensure that by 2015 multiphase science based computer simulations play a significant role in the design, operation, and troubleshooting of multiphase flow devices in fossil fuel processing plants*."
- ❑ Will develop missing critical constitutive relations to increase the fidelity of CFD models.
- ❑ Accurate drag law will result in improved modeling of multiphase flow systems such as fluidized beds and risers.
- ❑ Computational advances will be provided to NETL's open-source CFD tool MFIX and validation cases will be provided.

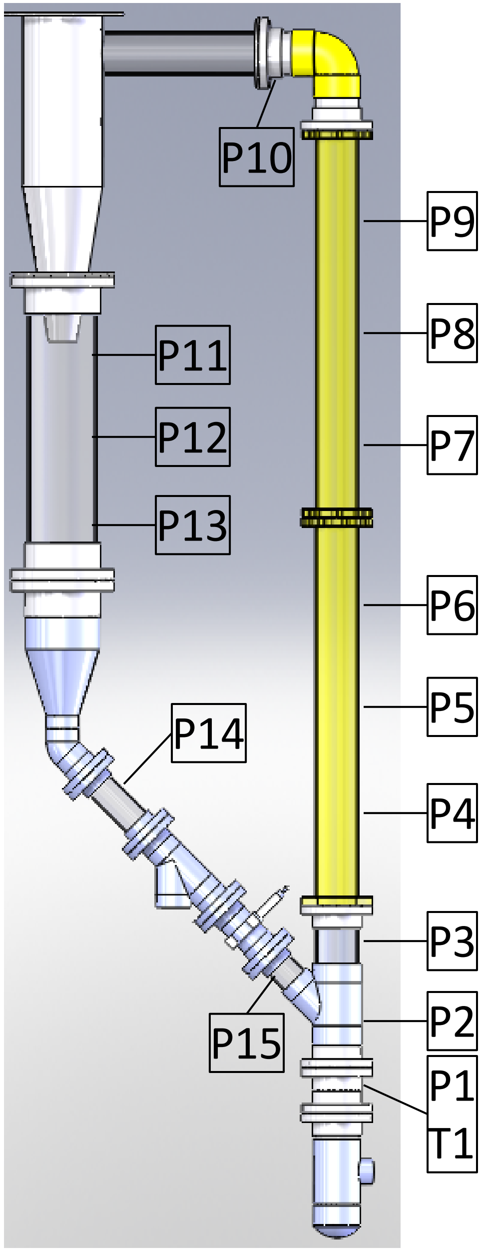
(9) Report on Workshop on Multiphase Flow Research, Morgantown, WV, Ed. M. Syamlal, DOE/NETL-2007/1259, 2006.

Statement of project objectives

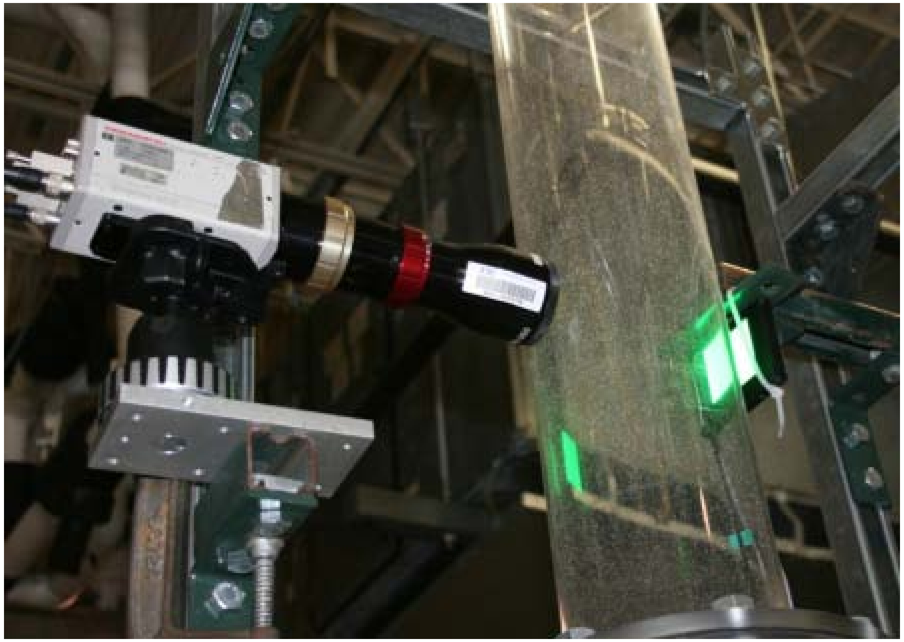
☐ To develop a two-fluid drag-law for clustered particles using direct numerical simulations with experimental validation.

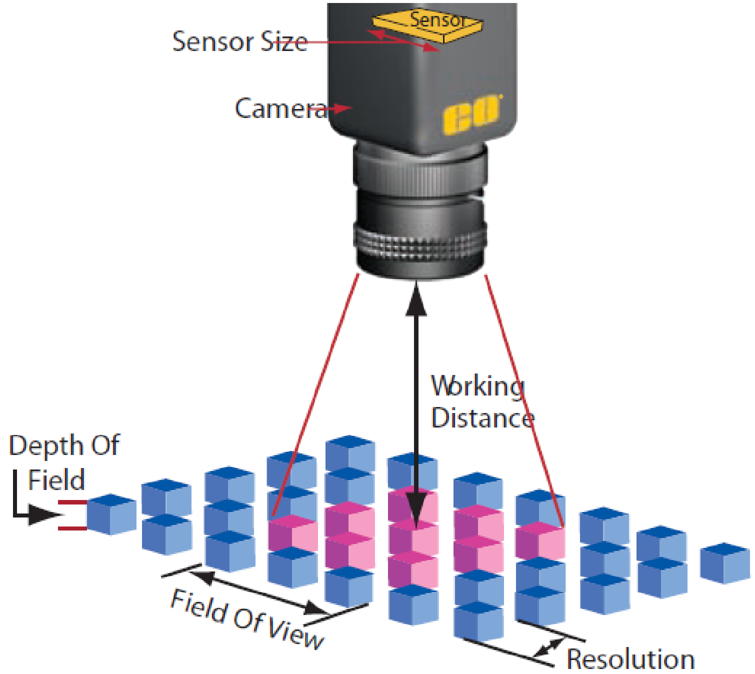
- Fluidization experiments at the FIU CFB facility:
  - ✓ Geldart A type particles to observe clustering of particles,
  - ✓ High speed imaging to capture the instantaneous distribution of particles,
  - ✓ Convert the images of particle clusters into particle configurations to be used in the DNS.
- Conduct DNS simulations at ISU:
  - ✓ Use the outcome of the DNS for pressure field, velocities of the gas phase and solid particles to calculate the actual drag force on the system of particles.
- Develop a new drag correlation in the presence of particle clustering and implement in the MFIX computer code. (ISU and FIU)
  - ✓ Integrate the new drag-law with MFIX,
  - ✓ Simulate the experimental test cases using MFIX with the new drag correlation,
  - ✓ Compare the results against the experimental data for pressure drop in the riser.
- Raise FIU's competitiveness with other institutions in the fields of conversion and utilization of fossil energy research.

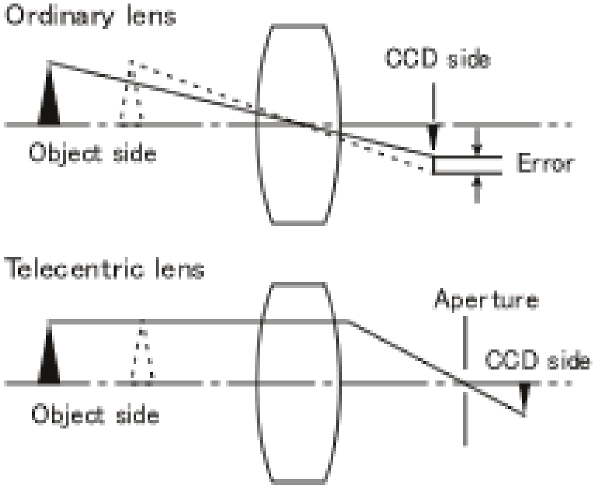
Experimental Approach



Experimental Approach



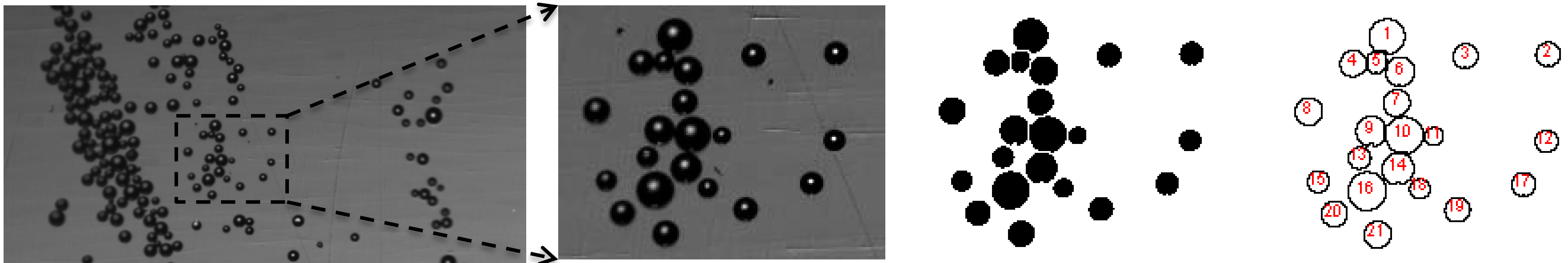




(11) S. Gokaltun, et al., Powder Technology, 220, pp. 98 –103, 2012.

Telecentric Lens	Edmund Optics 55-350
Primary magnification	1X
Horizontal field of view	8.8 mm
Working distance	98 mm – 123 mm
Resolution (MTF Image Space @ F6)	>45% @ 40 lp/mm
Telecentricity	<.1°
Distortion	.5% Max
Depth of field (20% @ 20 lp/mm)	± 0.6mm at F12
Aperture (f/#)	F6 – F25

Image processing (NI ImageJ)



Region of interest

Binary > Fill holes > Watershed

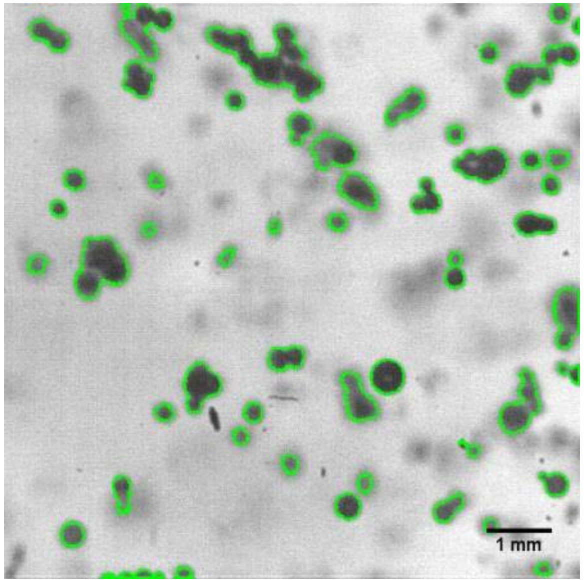
Particle analyzer

$$\varepsilon_s = \frac{\sum_{i}^{n} V_i}{Ah}$$

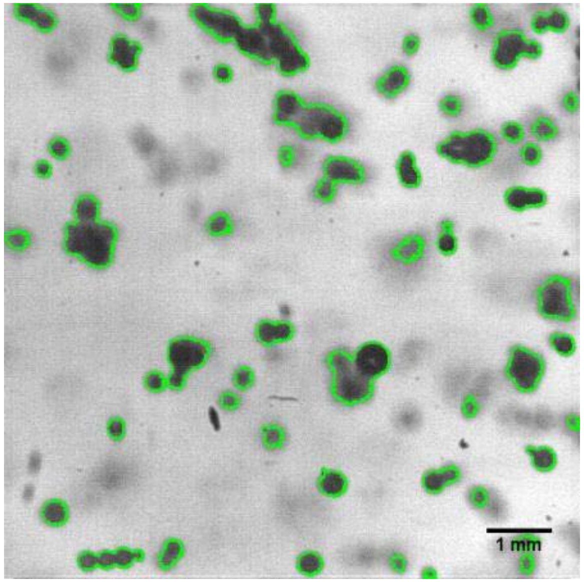
- Polystyrene particles:
  - $d_m = 350 \mu m$, $\rho_b = 650$ kg/m^3
- Vision Research Phantom v5.0 (1024x1024 Sensor, 10 μs exposure time):
  - 3,800 pps @ 512 × 512 pixels
  - 60,000 pps @ 256x32 pixels
  - 1024MB memory (1s of 1024 frames)

Solid volume calculation

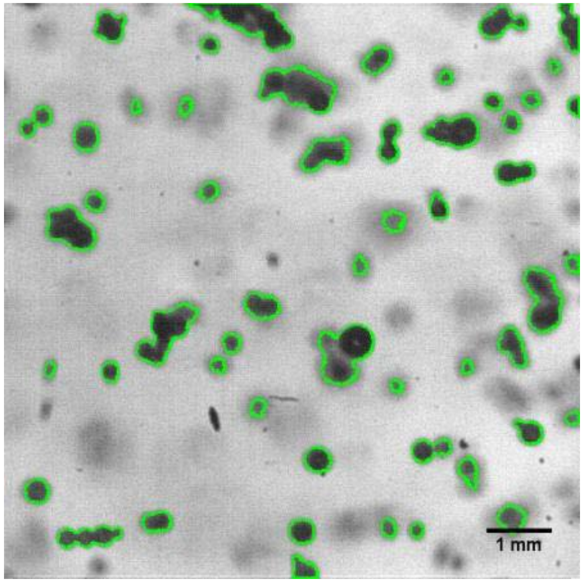
Frame 1



Frame 2



Frame 3

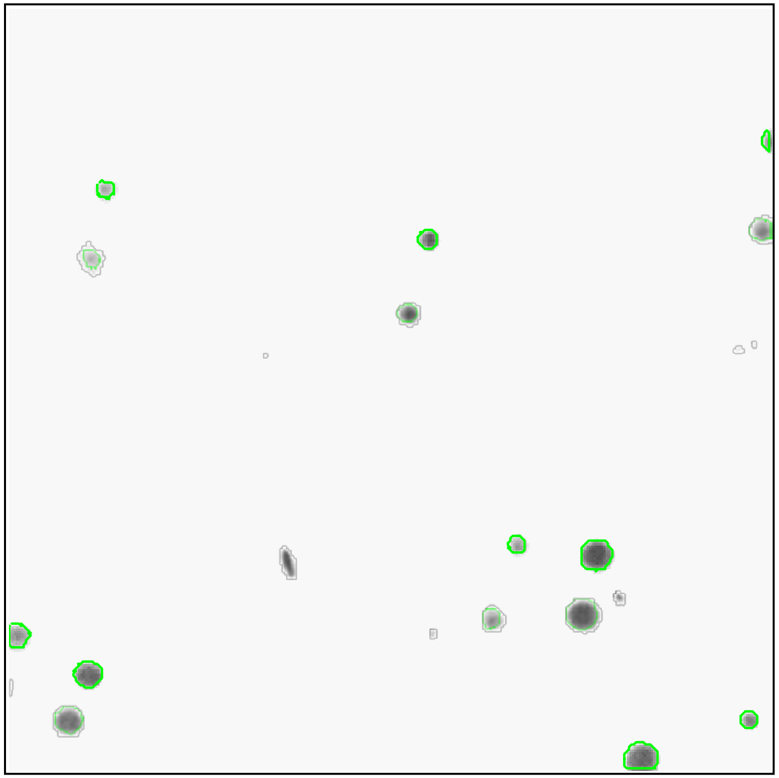


- Matlab Image Processing Toolkit used for frame by frame analysis.

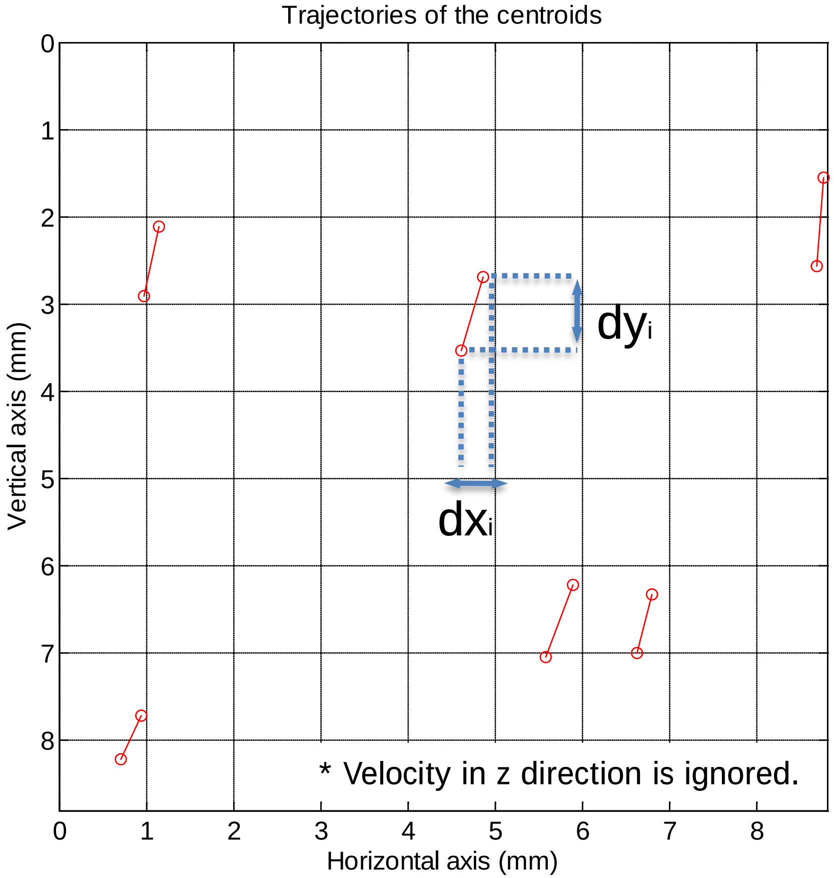
- Telecentric lens (Edmund Optics Inc. 55 – 350)
  - horizontal field of view of 8.8mm
  - depth of field of 1mm

Velocity calculation from trajectories

Tracking algorithm → trajectories → particle velocities[12]



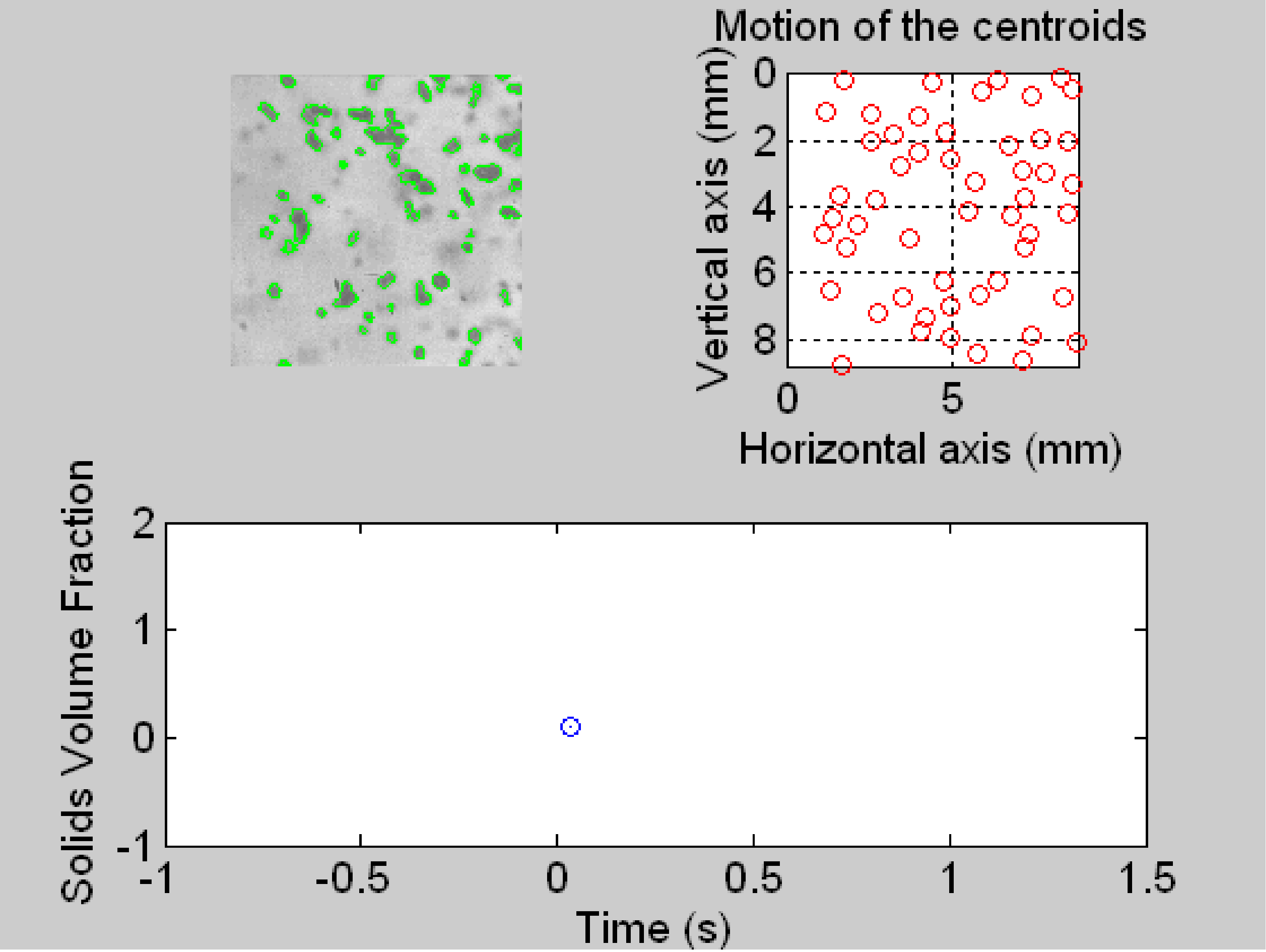
Frame 2 imposed on Frame 1



* Velocity in z direction is ignored.

(12) Crocker and Grier, Journal of Colloid and Interface Science, 179, pp. 298–310, 1996.

Particle Tracking

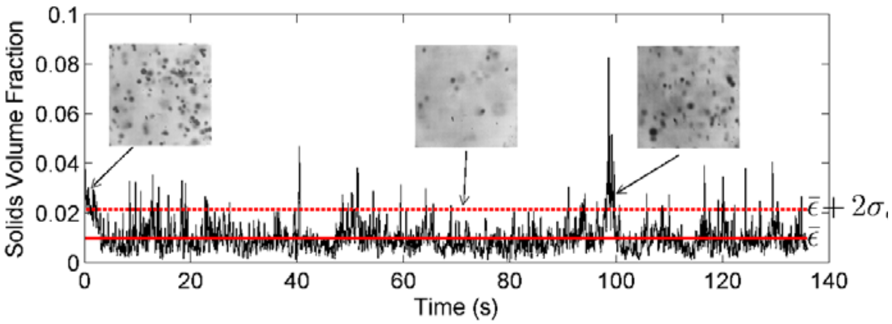


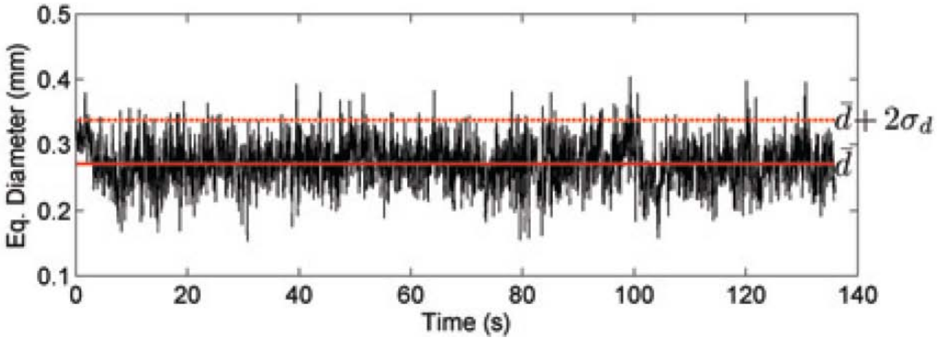
Boundary identification issues

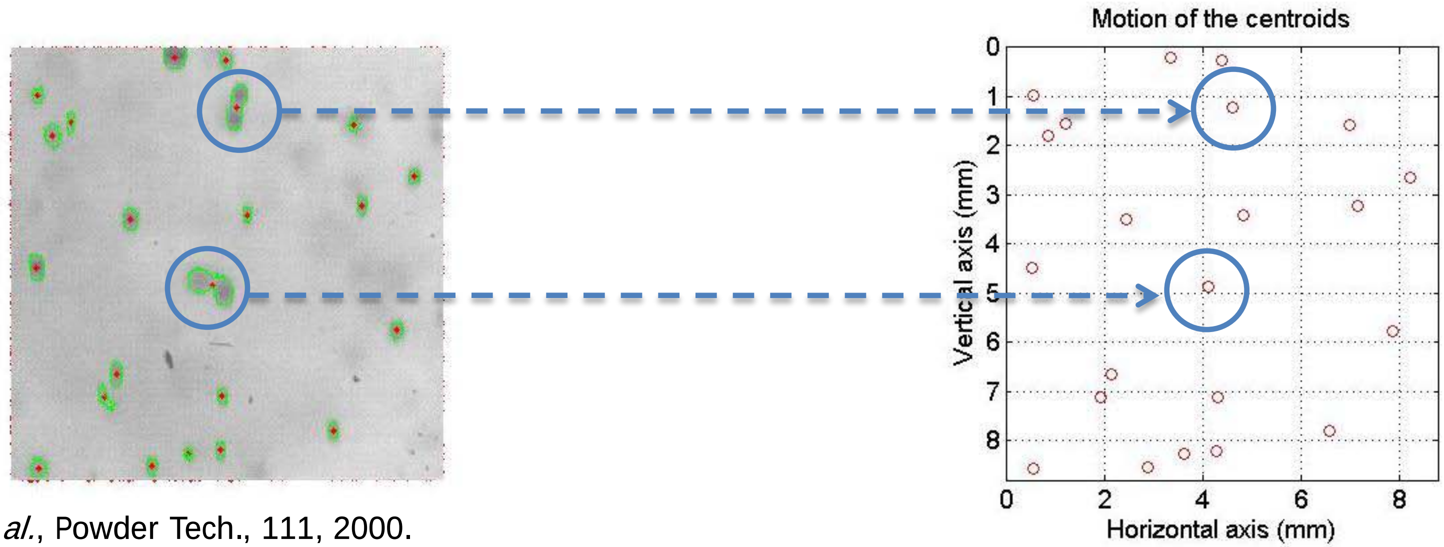
Mean-referenced criterion: time-mean + 2 x SD [13]

$$\epsilon = \sum_{i}^{n} \frac{2A_i d_i}{3hA_f}$$

$$d_i = \sqrt{\frac{4A_i}{\pi}}$$



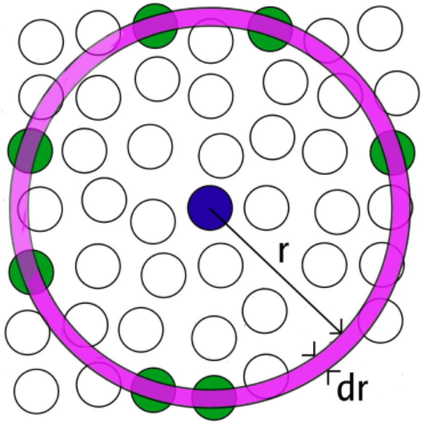


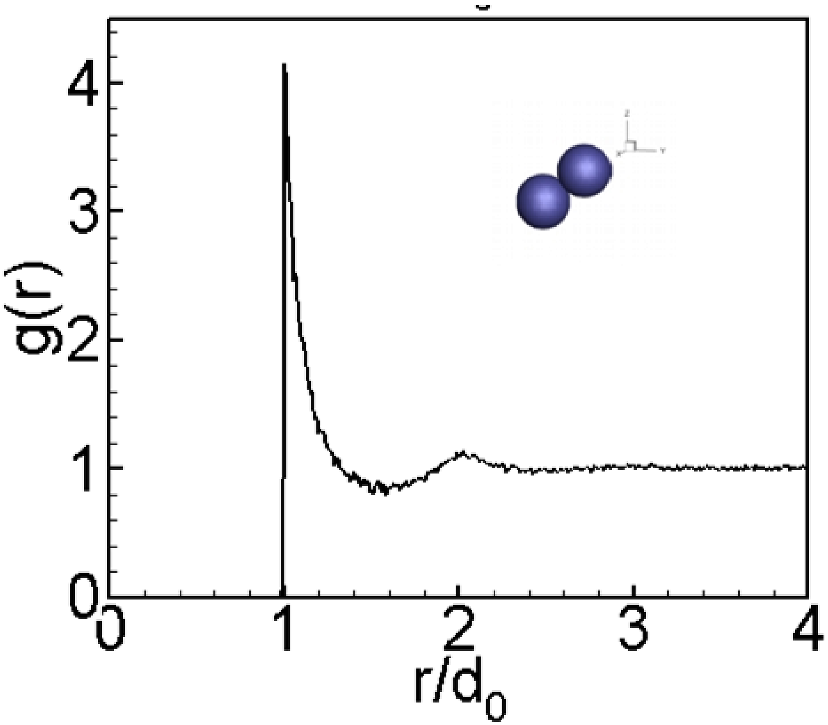


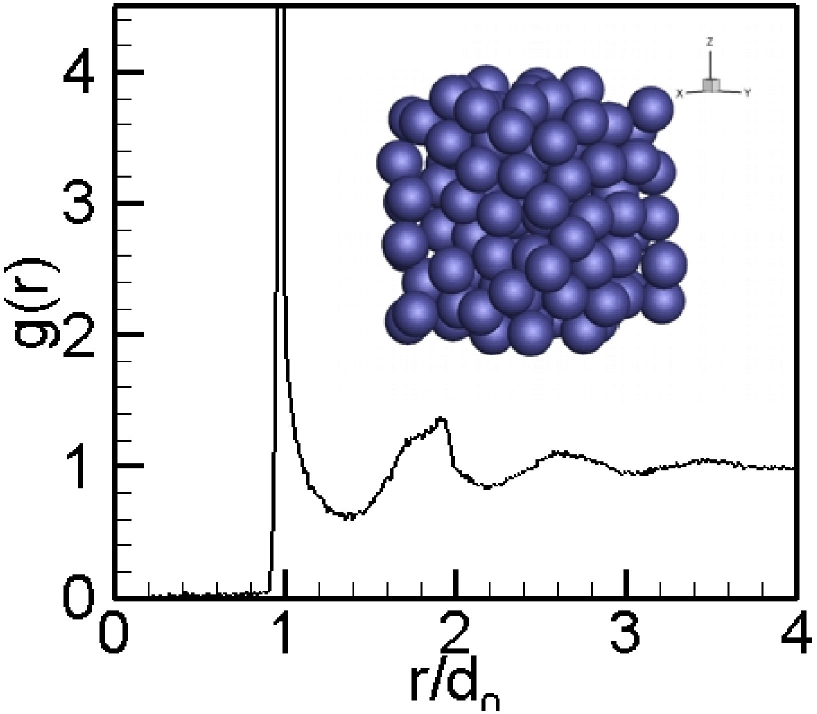
(13) Sharma *et al.*, Powder Tech., 111, 2000.

Particle configurations from images

- Shadow sizing
  - Generating 2D images of the field
  - Measuring the projected area fraction
  - Measuring the 2-D pair-correlation function (statistical representation of neighbor particles)



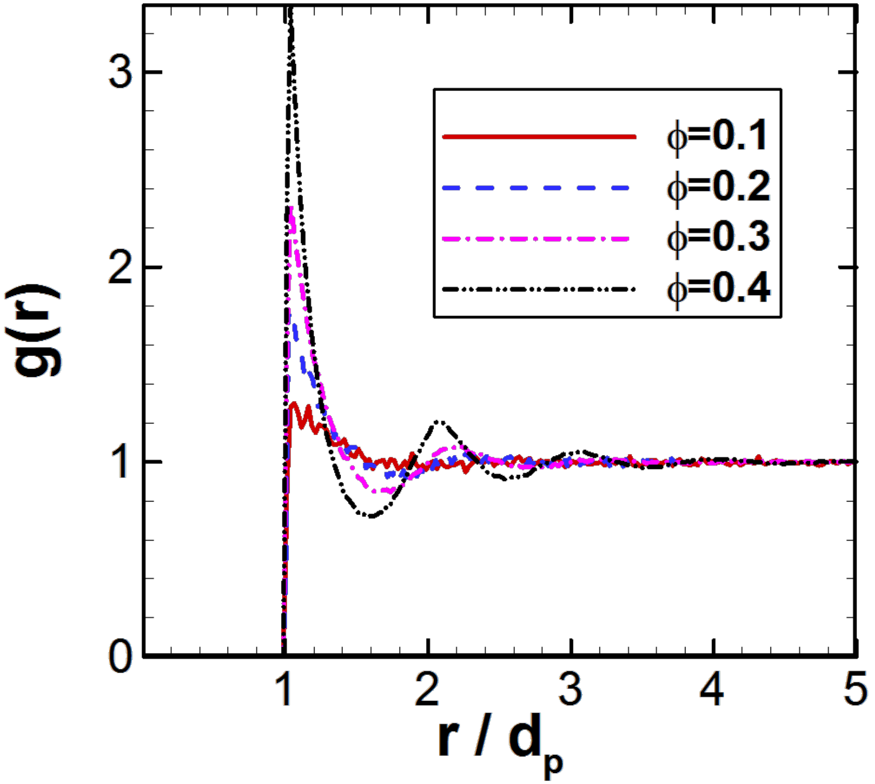


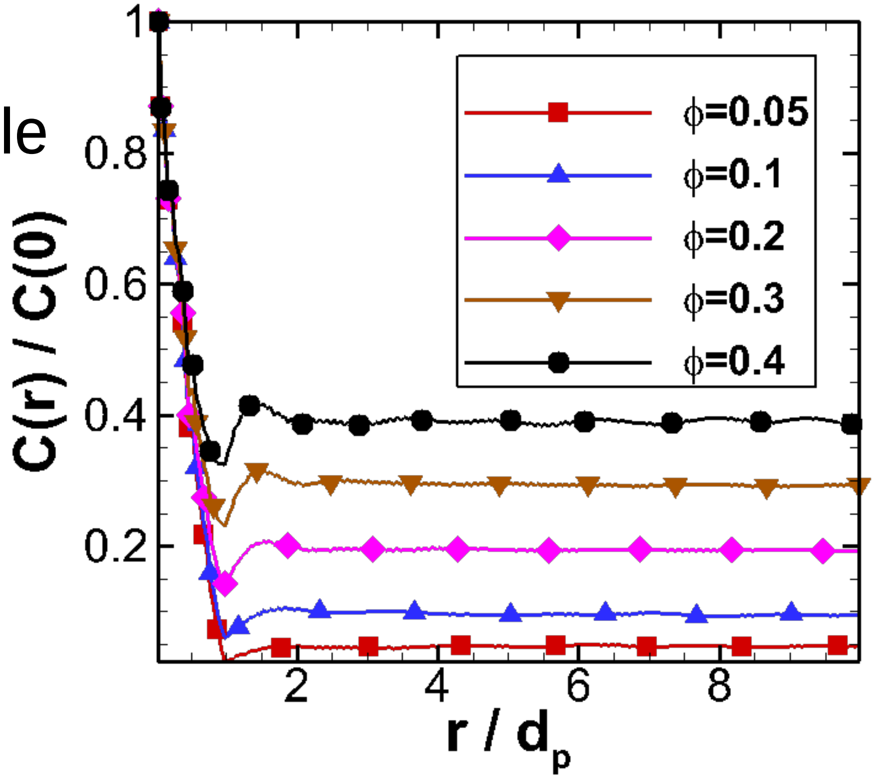


Characteristics of Particle Configurations

- Radial distribution function
  - Probability of finding a particle at separation

$$g(r) \equiv \frac{1}{N_p/2} \frac{N_r}{4\pi r^2 \delta r} \frac{V}{N_p}$$





- Covariance of indicator field
  - local solid volume fraction at separation *r*

$$C(r) = \left\langle I^{(p)}(x) I^{(p)}(x+r) \right\rangle$$

Approaches

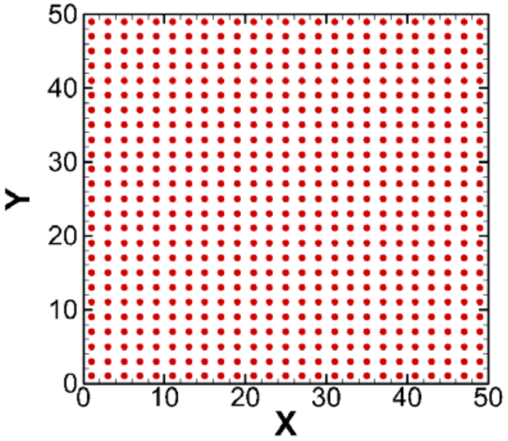
- ☐ Experimental approach
  - ➢ Shadow sizing technique
  - ➢ 2D projections of 3D particle configurations at a particular plane
- ☐ Numerical approach
  - ➢ Regeneration of particle configuration is non-trivial
  - ➢ Consistent with experimental measurements
    - ✓ Producing 2D planar projections of numerical particle configuration
    - ✓ computing $g_{2D}(r)$ and $C_{2D}(r)$ for each projection
    - ✓ computing ensemble averages
    - ✓ Minimizing the difference between experimental and numerical measurements

Optimization process

Simulated Annealing[14]

- From analogy to annealing process in metallurgy
  - Heating, and then controlled cooling of a material
  - Objective function

$$F(r) \equiv \alpha \left\| g_{2D}^{E}(r) - g_{2D}^{N}(r) \right\|_2 + \beta \left\| C_{2D}^{E}(r) - C_{2D}^{N}(r) \right\|_2$$

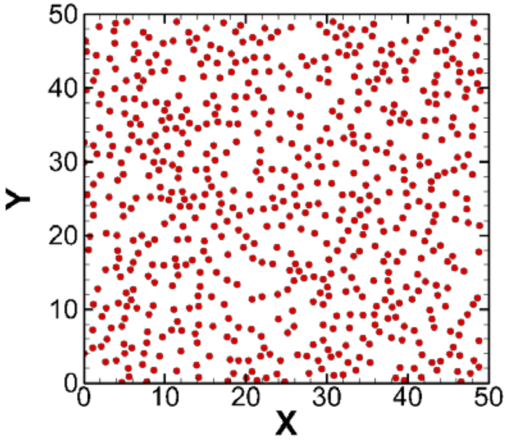


  - Generating a new solution by a local transformation

$$T^{n+1} = \alpha T^{n} \qquad \mathbf{x}^{n+1} = \mathbf{x}^{n} + \beta d_p \mathbf{r}$$

  - The probability of accepting a new solution

$$P = \begin{cases} 1, & \Delta F \leq 0 \\ e^{-\Delta F/T}, & \Delta F > 0 \end{cases}$$



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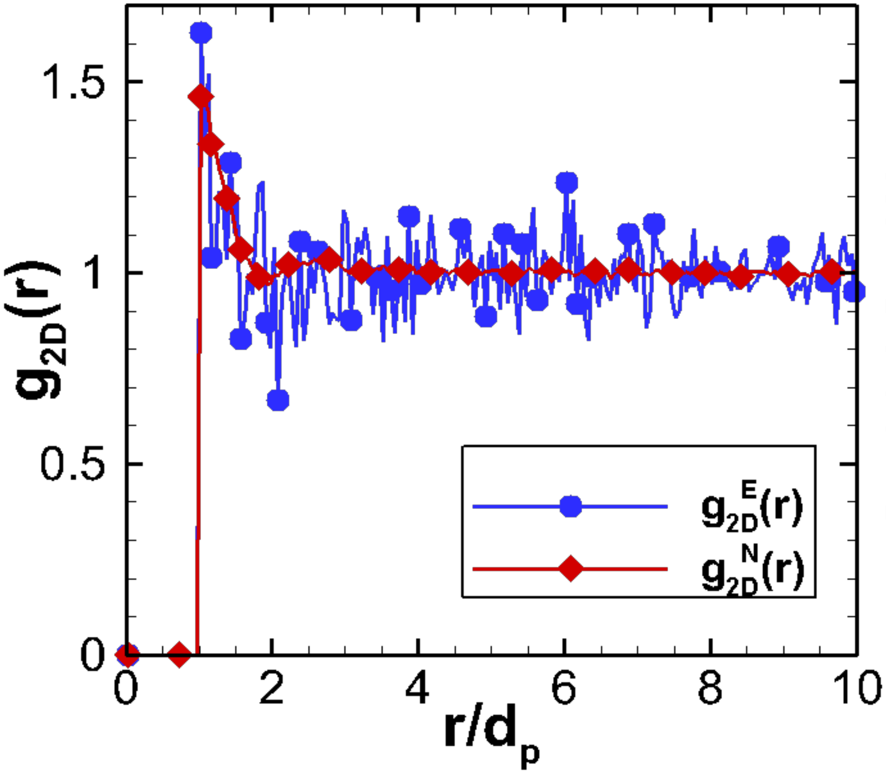
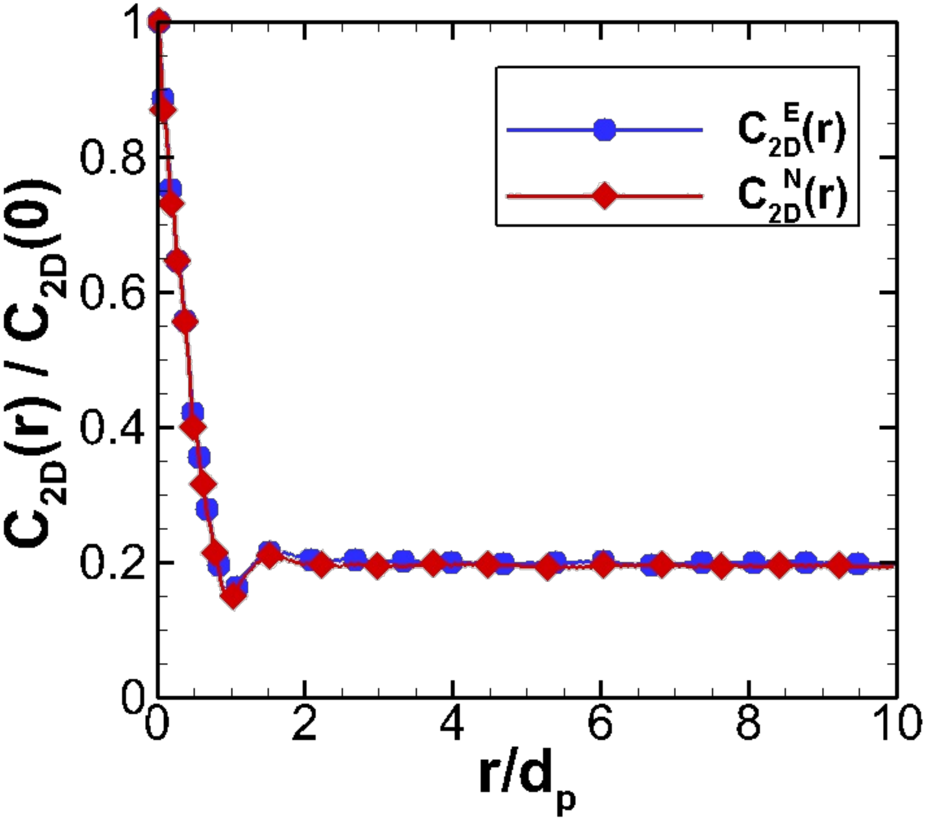
(14) Kirkpatrick, S., Gelatt, C.D., Vecchi, M.P., Science, 220 (4598) pp. 671-680, 1983.

Simulated Annealing

- ☐ Ensemble averages of $g_{2D}(r)$ and $C_{2D}(r)$ for 200 realizations used as our benchmark

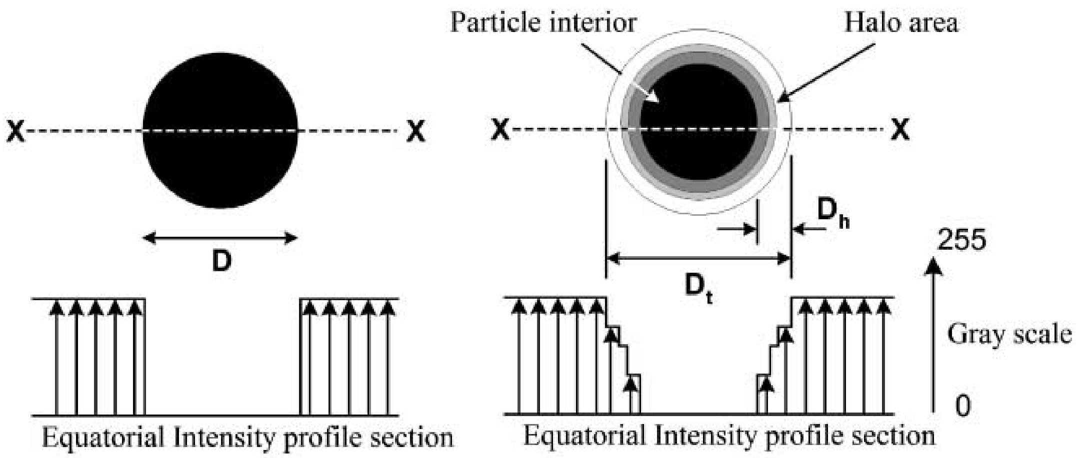
$\phi=0.2$

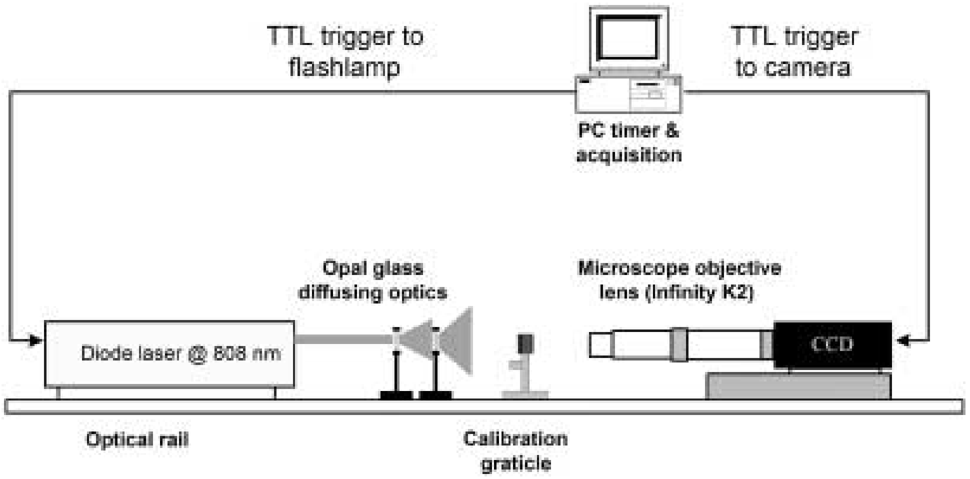




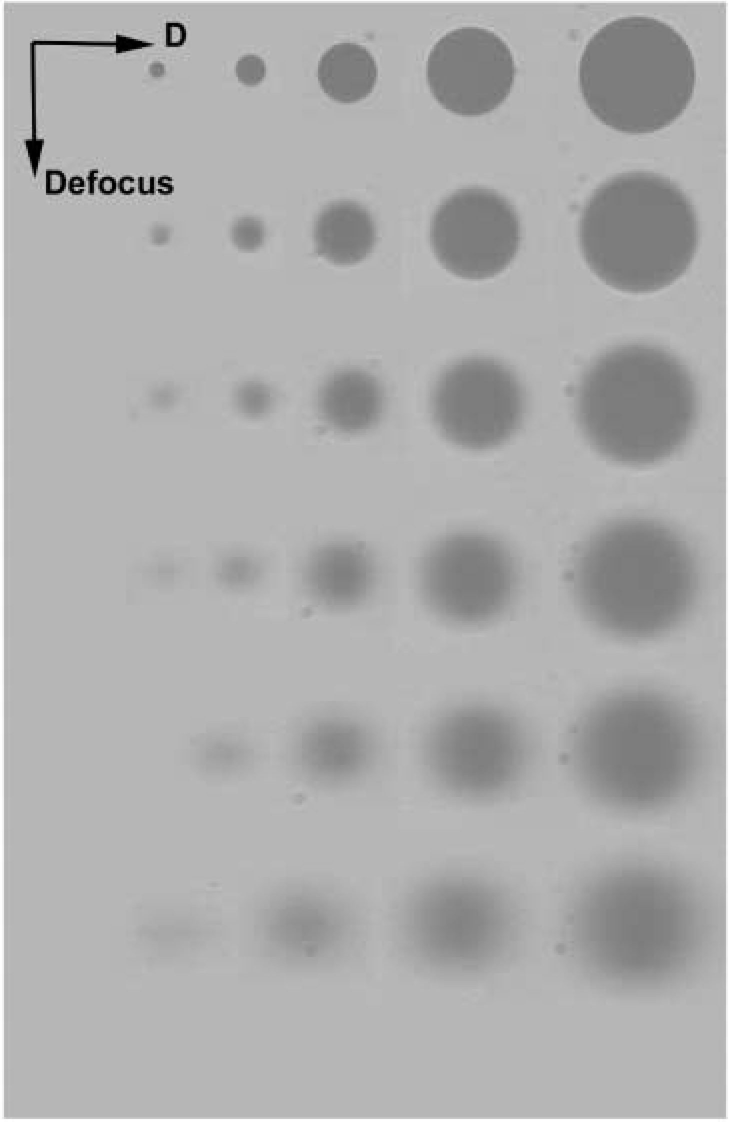
Fluctuations will be removed by generating more realizations

Shadow Intensity profile calibration[15]





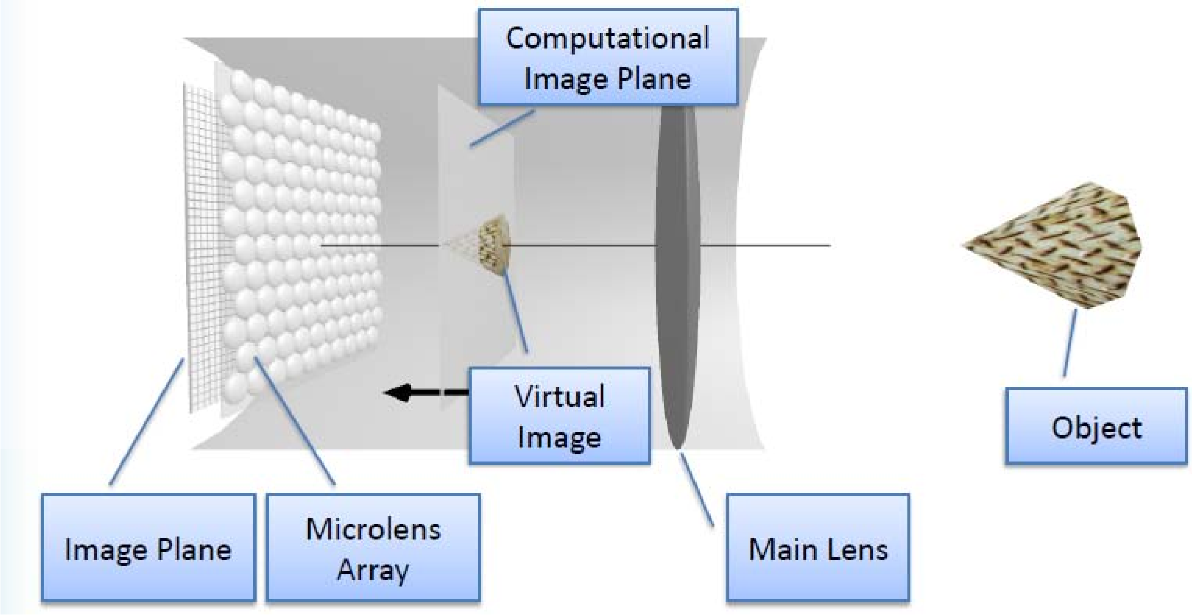
Calibration set-up [15].



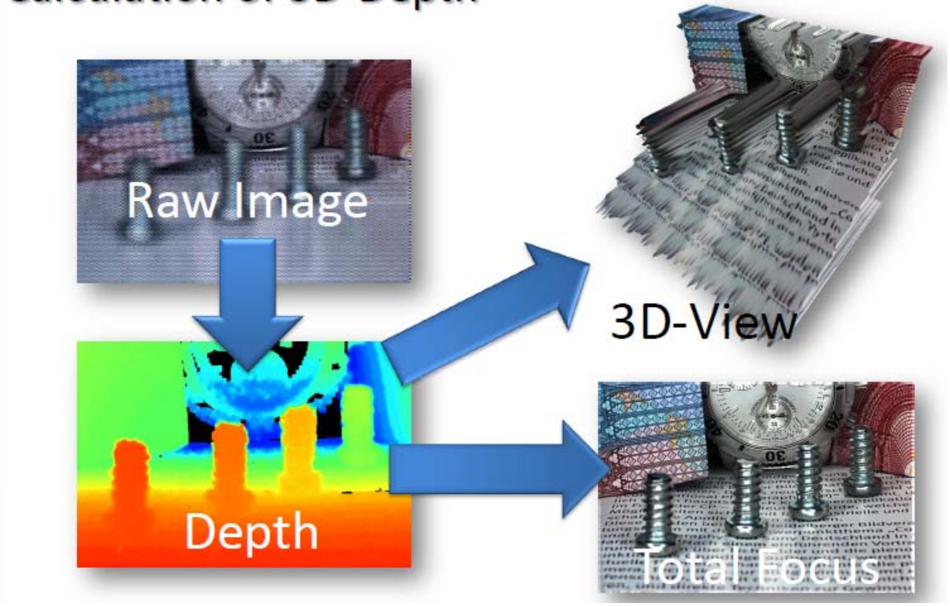
Patterson globe calibration graticle at increasing defocus distances[15].

(15) Kashdan *et al.*, Part. Part. Syst. Charact., 20, pp. 387 – 397, 2003.

Light field photography



Calculation of 3D-Depth



Professional light-field camera (7 MP, 3D reconstruction software) www.raytrix.de

Consumer level light-field camera
Ren Ng (1.2 MP, $400-$500)
www.lytro.com

Technical Approach to Achieving the goals

- ❑ DNS part
  - ➢ Regeneration of 3D particle configuration using the experimental images
    - ✓ Simulated annealing approach
  - ➢ Quantification of drag force from simulations
  - ➢ Proposing a drag law that includes the clustering effects

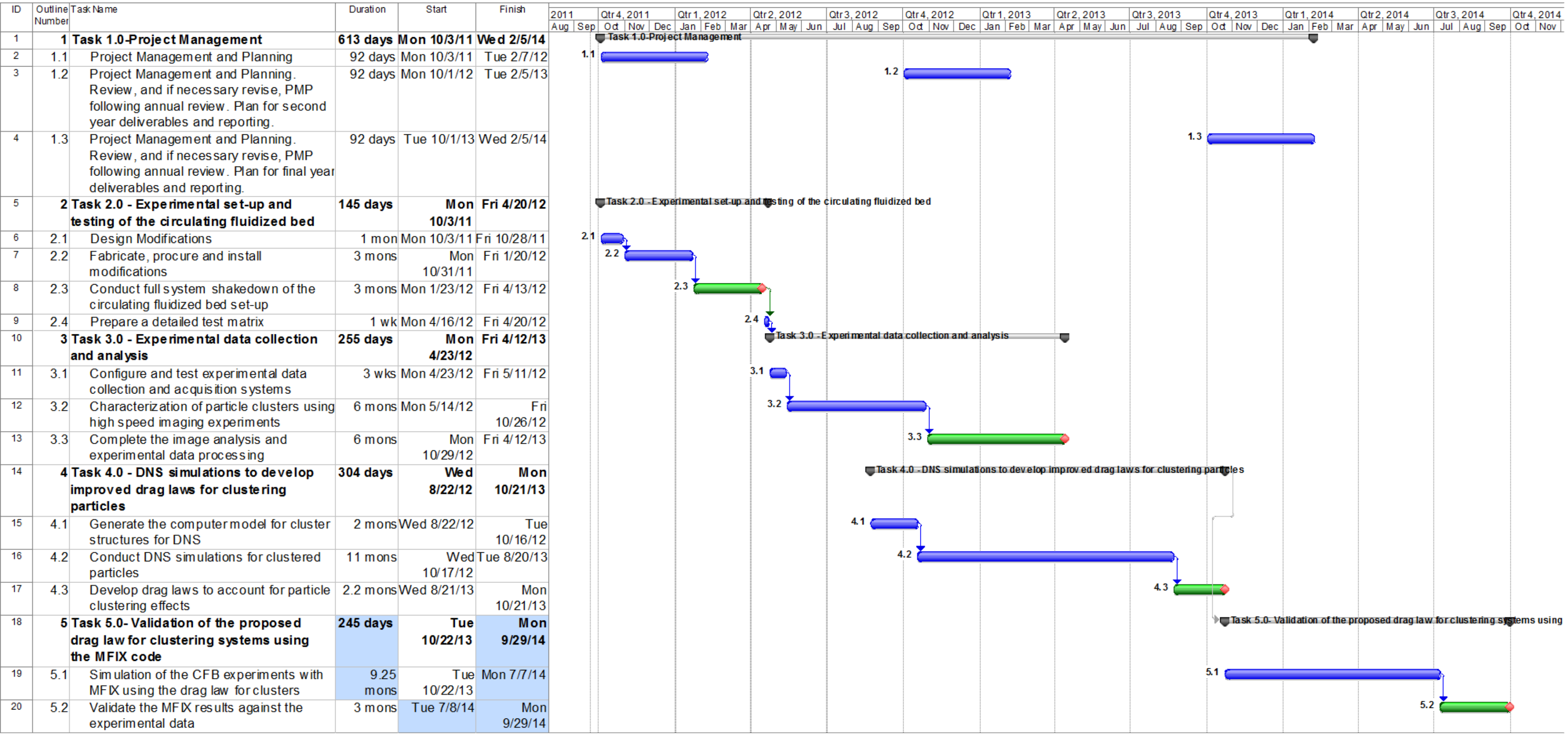
$$F(\phi, Re_m, \sigma_\phi)$$

- ❑ Validation
  - ➢ Implement the model in MFIX
  - ➢ Simulating a CFB configuration (setup from NETL)
  - ➢ Validating the results with experiment

Project milestones and schedule

Technical Milestones:

Milestone #	Description	Completion Date
1	Conduct full system shakedown of the circulating fluidized bed set-up	~~04/13/12~~ **07/01/12**
2	Complete the image analysis and experimental data processing	04/12/13
3	Develop drag laws to account for particle clustering effects	10/21/13
4	Validate the MFIX results against the experimental data	09/29/14

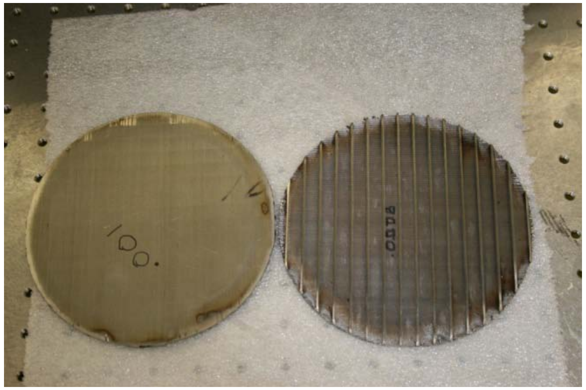


ID	Outline Number	Task Name	Duration	Start	Finish
1	1	**Task 1.0-Project Management**	**613 days**	**Mon 10/3/11**	**Wed 2/5/14**
2	1.1	Project Management and Planning	92 days	Mon 10/3/11	Tue 2/7/12
3	1.2	Project Management and Planning. Review, and if necessary revise, PMP following annual review. Plan for second year deliverables and reporting.	92 days	Mon 10/1/12	Tue 2/5/13
4	1.3	Project Management and Planning. Review, and if necessary revise, PMP following annual review. Plan for final year deliverables and reporting.	92 days	Tue 10/1/13	Wed 2/5/14
5	2	**Task 2.0 - Experimental set-up and testing of the circulating fluidized bed**	**145 days**	**Mon 10/3/11**	**Fri 4/20/12**
6	2.1	Design Modifications	1 mon	Mon 10/3/11	Fri 10/28/11
7	2.2	Fabricate, procure and install modifications	3 mons	Mon 10/31/11	Fri 1/20/12
8	2.3	Conduct full system shakedown of the circulating fluidized bed set-up	3 mons	Mon 1/23/12	Fri 4/13/12
9	2.4	Prepare a detailed test matrix	1 wk	Mon 4/16/12	Fri 4/20/12
10	3	**Task 3.0 - Experimental data collection and analysis**	**255 days**	**Mon 4/23/12**	**Fri 4/12/13**
11	3.1	Configure and test experimental data collection and acquisition systems	3 wks	Mon 4/23/12	Fri 5/11/12
12	3.2	Characterization of particle clusters using high speed imaging experiments	6 mons	Mon 5/14/12	Fri 10/26/12
13	3.3	Complete the image analysis and experimental data processing	6 mons	Mon 10/29/12	Fri 4/12/13
14	4	**Task 4.0 - DNS simulations to develop improved drag laws for clustering particles**	**304 days**	**Wed 8/22/12**	**Mon 10/21/13**
15	4.1	Generate the computer model for cluster structures for DNS	2 mons	Wed 8/22/12	Tue 10/16/12
16	4.2	Conduct DNS simulations for clustered particles	11 mons	Wed 10/17/12	Tue 8/20/13
17	4.3	Develop drag laws to account for particle clustering effects	2.2 mons	Wed 8/21/13	Mon 10/21/13
18	5	**Task 5.0- Validation of the proposed drag law for clustering systems using the MFIX code**	**245 days**	**Tue 10/22/13**	**Mon 9/29/14**
19	5.1	Simulation of the CFB experiments with MFIX using the drag law for clusters	9.25 mons	Tue 10/22/13	Mon 7/7/14
20	5.2	Validate the MFIX results against the experimental data	3 mons	Tue 7/8/14	Mon 9/29/14

Project status

- FIU:
  - All CFB parts procured. FCC particles obtained. Blower identified.
  - Graduate student candidates identified, Ph.D. admission process started
    - ✓ expected start date: Fall 2012.
  - MFIX user account obtained. Software installation in FIU cluster in progress.
- ISU:
  - Graduate student recruited (Mohammad Mehrabadi).
  - Preliminary analysis of generation of particle configurations in DNS.

Distributor plate using a porous plate (Mott Corp.)



20 and 25 micron screens received from Johnson Screens

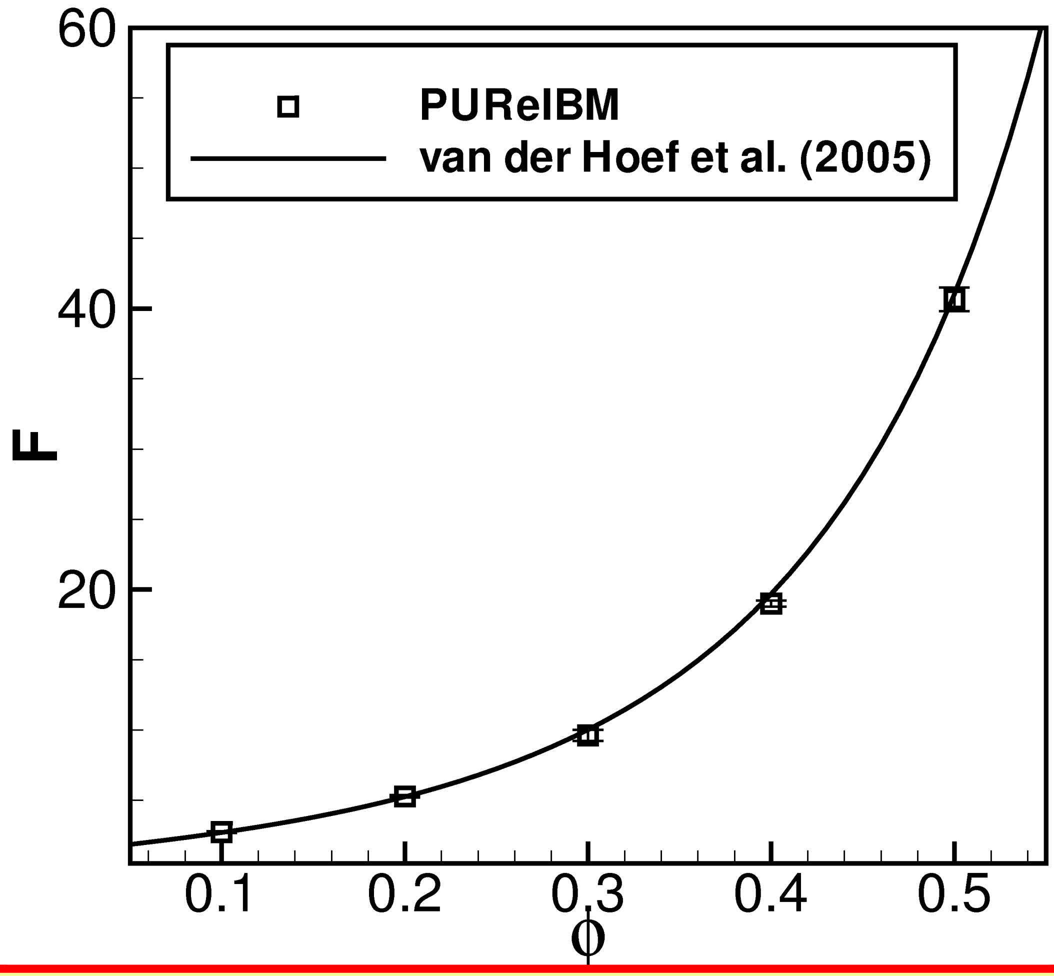
Windbox section manufactured

Questions and feedback?

Backup Slides

- ❑ Backup Slides

Validation Tests

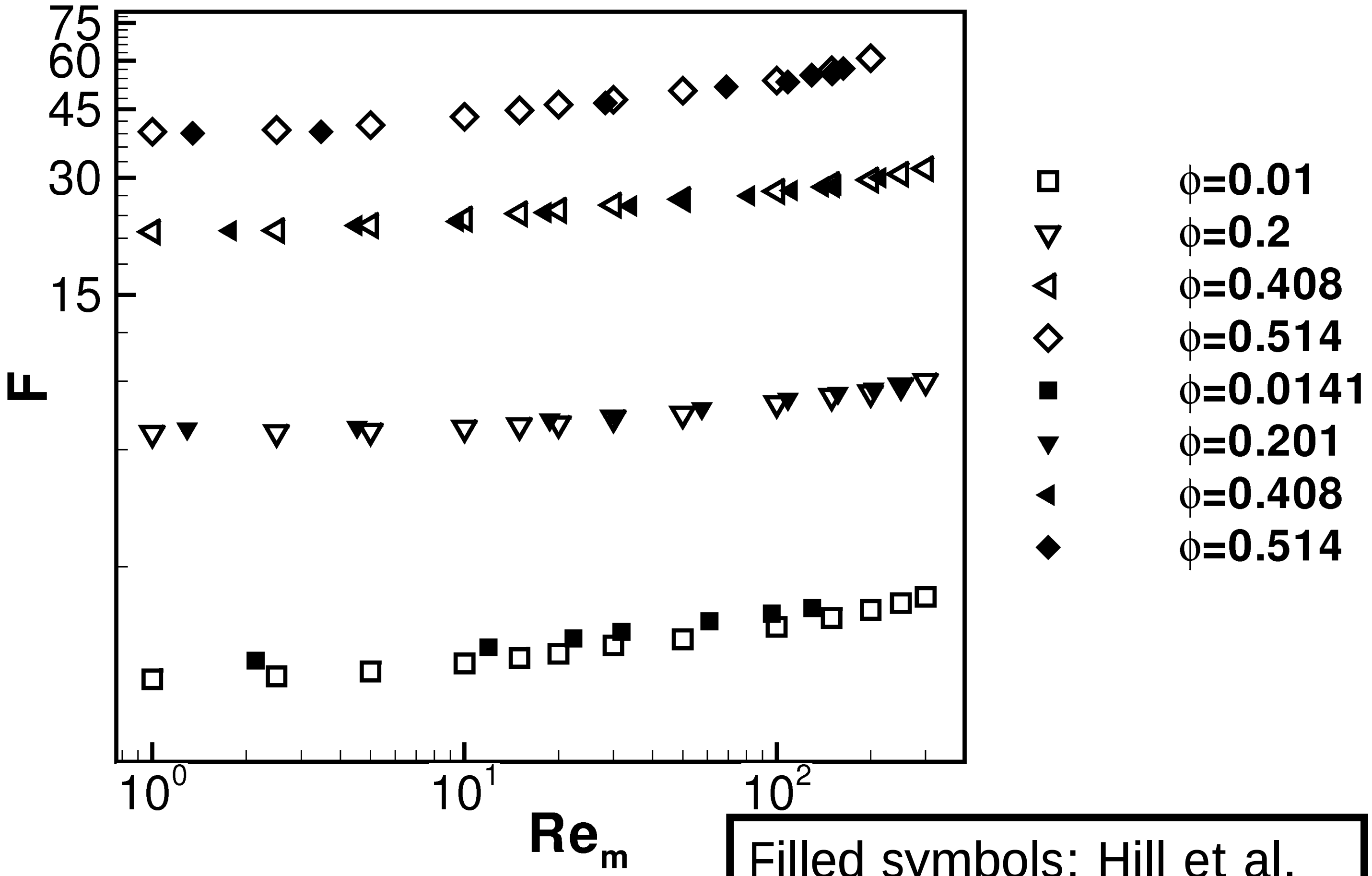


van der Hoef, M. A., Beetstra, R. & Kuipers, J. A. M. 2005 "*Lattice-Boltzmann simulations of low-Reynolds-number flow past mono- and bidisperse arrays of sphere: results for the permeability and drag force*." JFM 528.

Stokes flow past random arrangement of monodisperse spheres

Validation Tests

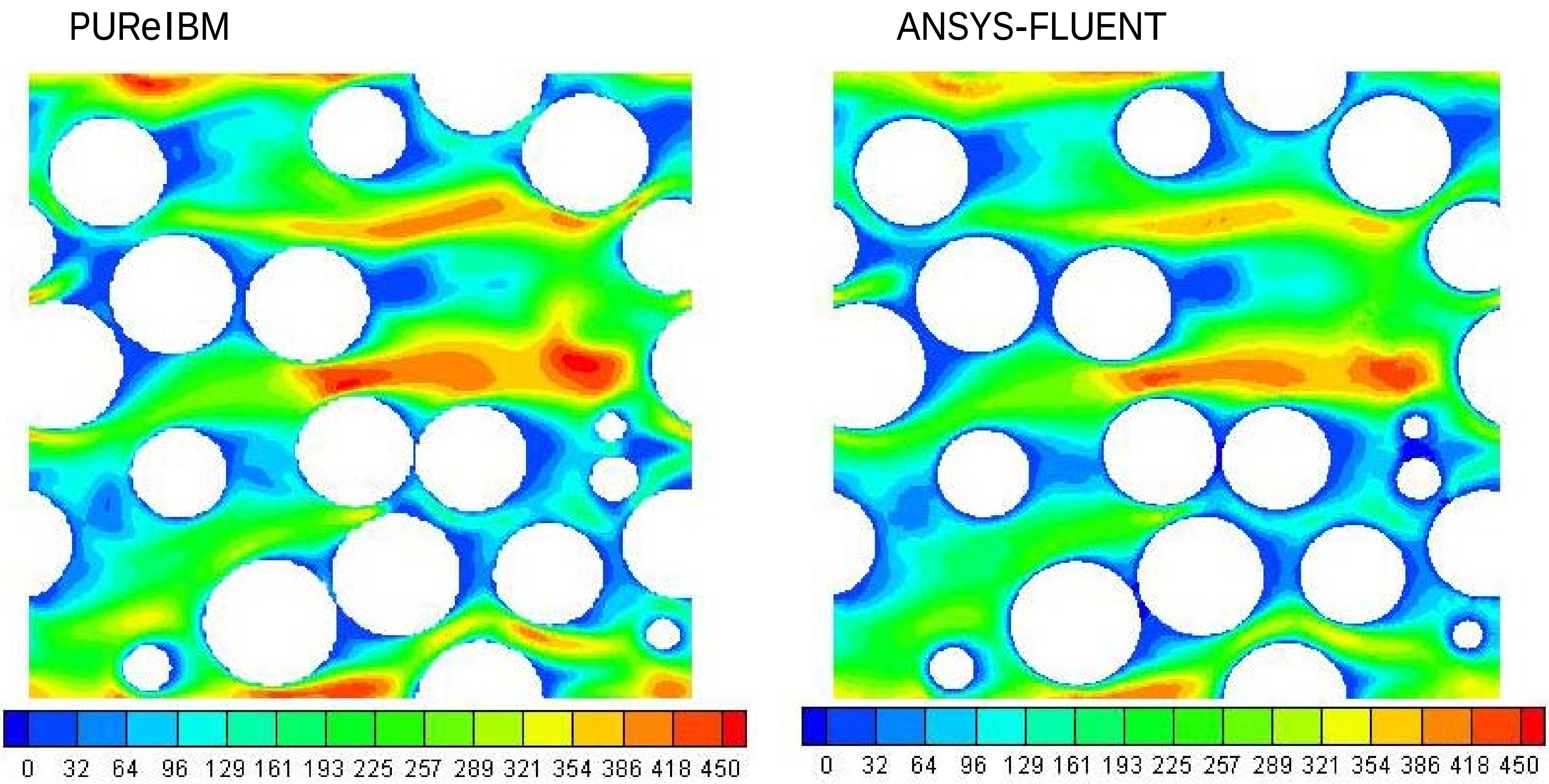
Hill, R. J., Koch, D. L. & Ladd, A. J. C. 2001*b* *"Moderate Reynolds number flows in ordered and random arrays of spheres*." JFM 448



Filled symbols: Hill et al.
Open symbols: PUReIBM

Moderate Reynolds number flow past simple cubic arrays of monodisperse spheres

Validation Tests



PUReIBM

ANSYS-FLUENT

Volume fraction: 0.4; Reynolds number: 100

High Reynolds number flow past random arrangement of monodisperse spheres