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Project acronym: NanoSim

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WP N°	Del. N°	Title	Contributors	Version	Lead beneficiary	Nature	Dissemin. level	Delivery date from Annex I	Actual delivery date dd/mm/yyyy
4	D4.3	Models on Heat and Mass Transfer	Authors: Stefan Radl, Federico Municchi Checked by: Stefan Radl	1.0	TUG	Other	PU	31/10/2015	30/12/2015

1 Introduction

This document summarizes the developments (i.e., code, documentation, test cases, standard parameters) for

- the generation of data from filtered DNS of heat/mass transfer in fluid-particle beds using CPPPO
- the establishment of a work-flow for generating heat/mass transfer closures (i.e., »material relations«) from filtered DNS data.

1.1 Document identification

Document Identification	MODELS_HEAT_MASS
Author(s)	Stefan Radl, Federico Municchi
Reviewers	Stefan Radl
Manager	Stefan Radl (TUG)
Version of the Product	1.0
Version of "ParScale"	1.1.1-beta
Version of "CPPPO"	1.0.1-beta
Version of "CFDEM"	2.9.0 (branch CFDEMcoupling-RADL/master)

1.2 Scope

CPPPO is used to filter DNS data from the generic particle/fluid solver. Filtered data are then used to develop closure models for heat and mass transfer to be used in CFD-DEM simulations. These models are in the form of a particle-based dimensionless transfer coefficient, e.g. Nusselt or Sherwood number. The existing CFDEM immersed boundary solver is upgraded to include heat and mass transport and a work-flow for computing coefficients for heat/mass transfer closure models from produced data is established.

As specified in task 4.4 of the DOW, these models have to be based on key dimensionless parameters, and cover a wide range of process parameters in order to facilitate model re-use.

1.3 References

Acronym	Name
DOW	Description of Work (Work Package 4)
OPH-PRIV	Online Project Hosting – Private (available to the consortium only)
OPH-PU	Online Project Hosting – https://github.com/CFDEMproject/CFDEMcoupling-PUBLIC for CPPPO)
CPPPO	Compilation of fluid/Particle Post Processing routines

1.4 System Overview

The CFDEM Immersed Boundary solver has been extended in order to solve a scalar transport equation ($CFDEM_SOLVER_DIR/cfdemSolverForcingIBScalar). Also, a utility was developed to simulate fully periodic computational domains. This utilities is located in $CFDEM_SRC_DIR/eulerian/fvOptionsCFDEM/constraints/derived/fixedBulkConstraint.

Unfortunately, the original "cfdemSolverForcingIBScalar" solver proofed to be rather inefficient and inaccurate, thus requiring the development of a different approach. Consequently, a Hybrid Fictitious Domain Immersed Boundary Method (HFD-IBM) was implemented (solver "cfdemSolverHFDIBMScalar"). Indeed, the HFD-IBM showed a much better performance in initial tests, and hence has been used to establish the heat and mass transfer model provided in this deliverable report.

In order to derive a closure for heat and mass transfer rates, a "functional form" for the dimensionless heat/mass transfer coefficient was selected accordingly to current literature. This functional form was implemented in the software tool octave to realize a workflow for the automatic fitting of parameters (of this functional form) using octave. The workflow is available to the consortium via the OPH-PRIV repository (sub-directory: tutorials/octave), and can be seen as a generalized workflow to derive closures from any source of data.

1.5 Overview of the Use Cases

In order to generate reliable date for the development of the heat and mass transfer model, a set of verification and validation cases has been defined (see Table 1).

Use Case Name	Key Feature
1 - Cooling of a sphere	Verification: allows to assess the accuracy of enforcing the temperature at the particle boundary (only conduction is considered, no flow)
2 - Forced convection around a sphere	Verification: allows to evaluate the solver accuracy in predicting the Nusselt number for different Reynolds numbers
3 - Forced convection around three spheres (parallel to main flow)	Validation: allows to evaluate the solver performance in predicting the Nusselt number and drag coefficient for different Reynolds numbers for three particles at a relatively large distance
4 - Forced convection around two spheres (perpendicular to main flow)	Validation: allows to evaluate the solver performance in predicting the Nusselt number and drag coefficient for different Reynolds numbers for two particles at a relatively small distance
5 - Heat transfer in a fixed periodic particle bed (monodisperse)	Validation: evaluation of the particle based Nusselt number as a function of the fraction of solid and the Reynolds number using different realizations

Table 1: Overview of verification and validation cases for the IB solver.

1.6 Organization and Responsibilities

TUG was responsible for implementation, documentation, testing and analysis work, while DCS contributed with respect to the code architecture, reviewing activities and test harness integration.

1.7 Applied Workflow

The following workflow was followed during the development process of the model:

- Documentation of the theoretical framework.
- Implementation of new functionalities into the "CPPPO" framework.
- Test runs involving definition of new verification/example cases based on the DOW.
- Establishment and update of the user documentation.
- Backward compatibility checks based on already defined verification/example cases (see DOW report of WP4-D4.1).
- Implementation of the new hybrid fictitious domain – immersed boundary method solver.

- Data and model generation

2 Results obtained with the HFD-IBM Solver

2.1 Use Case 1 – Cooling of a Sphere

The modified CFDEM Immersed Boundary Method solver "cfdemSolverForcingIBScalar" is used to evaluate the heat conduction (no flow) from a steady sphere into a static fluid. In addition, the novel solver (HFD-IBM, i.e. Hybrid Fictitious Domain Immerse Boundary Method) is compared against the old solver.

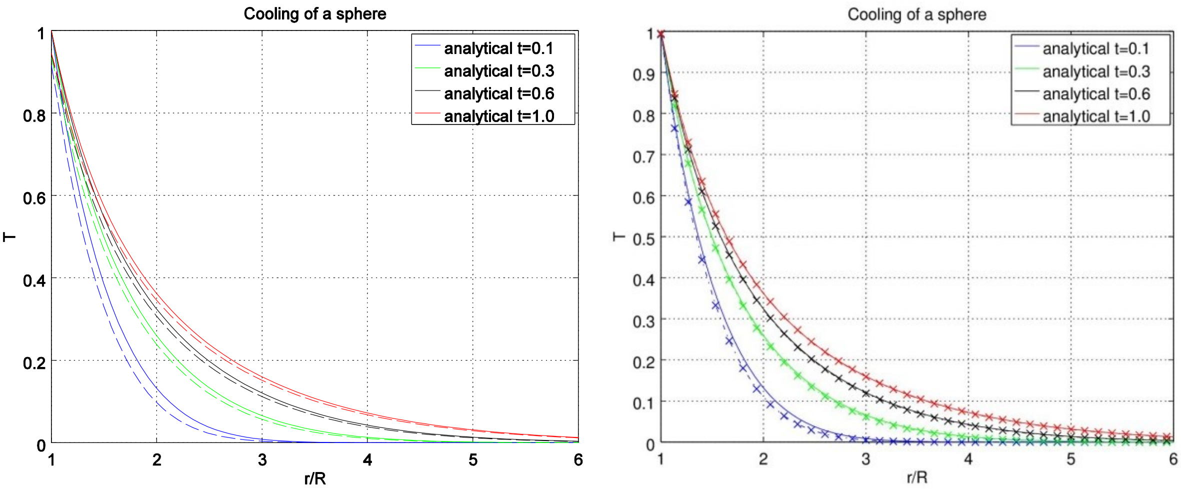

Figure 1: Cooling of a sphere - CFDEM IB (left panel, 30 cells per particle diameter) vs. HFD-IBM (right panel, 10 cells per particle diameter).

Figure 1 shows that the new algorithm (right panel) is in better agreement with the analytical solutions, and most important, it is able to exactly impose the particle surface temperature at the particle surface. In addition, the mesh resolution required by the HFD-IBM is much smaller than that required by the IB solver "cfdemSolverForcingIBScalar" (i.e., 10 cells per particle diameter vs. 30 cells per particle diameter). This test is also showing that the IB requires a high mesh resolution (with respect to the resolution used in the current literature, i.e., Tavassoli et al., 2015 or Tenneti et al., 2013) and, thus, high computational resources.

2.2 Use Case 2 – Forced convection around a sphere

The two solvers are compared, in terms of performance and accuracy, for the case of forced convection around a single sphere.

Figure 2 shows that the old CFDEM solver (CFDEM-FD) tends to over predict the Nusselt number, while the HFD-IBM predicts a Nusselt number in the range of the correlations found in literature. It is noteworthy that the new HFD-IBM solver uses a significantly coarser mesh than the old CFDEM solver.

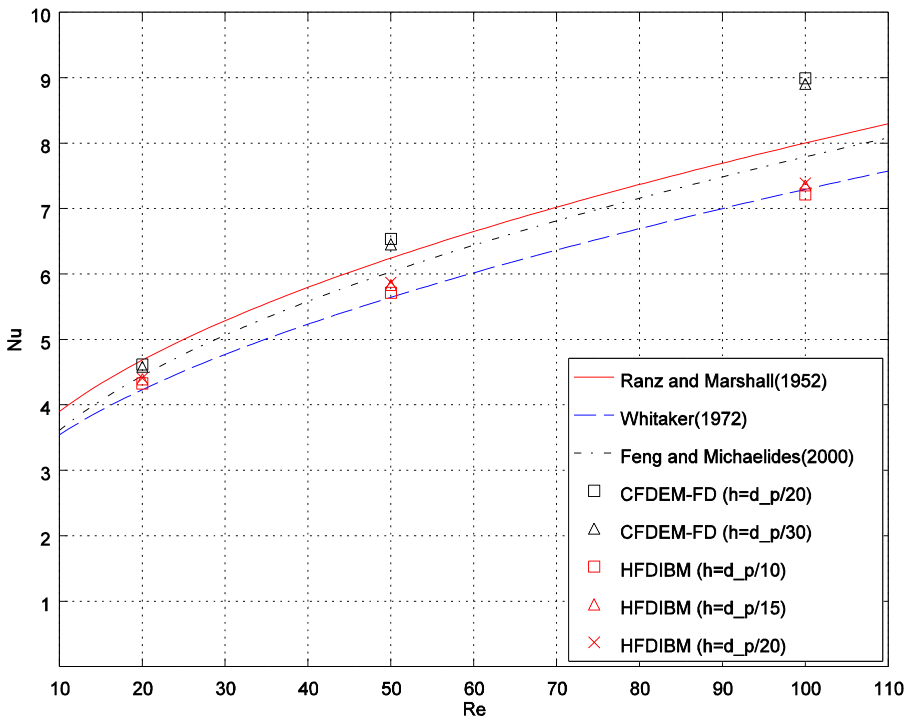

Figure 2: Comparison of the current IB (denoted here as “FD” for fictitious domain) and the HFD-IBM in the case of forced convection.

2.3 Use Case 3 – Heat transfer from three particles

This use case has been selected to test the solver’s ability to model multiple particles that are separated by a comparably large distance (see Figure 3). Also, for this specific flow configuration, reference data from literature was available. As can be seen from Figure 4, the agreement with both sources of literature data agree very well with our predictions for the force and heat flux experienced by the individual particles.

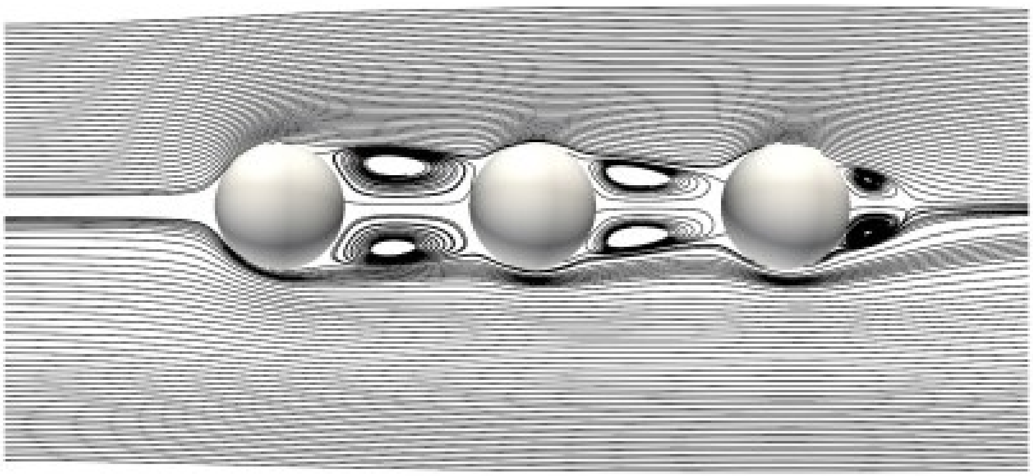

Figure 3: Streamlines predicted using the new HFD-IBM for flow around three spheres aligned with the main flow direction.

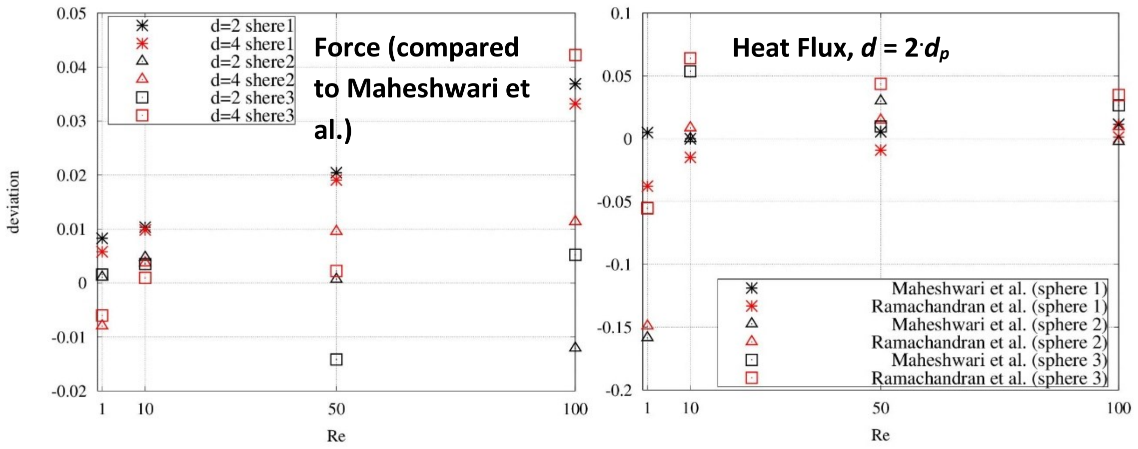

Figure 4: Relative deviations of the predicted force (left panel) and heat flux (right panel) when using the HFD-IBM solver from literature data.

2.4 Use Case 4 – Heat transfer from two particles

The three-particle test case discussed in Chapter 2.3 contains particles that are located at relatively large distance. However, for a typical situation (i.e., a randomly-oriented particle ensemble), particles may often be located very close to each other. Initial test runs showed that this situation is especially difficult to handle for Immersed Boundary Method-based solvers. Hence, we have included a use case that considers two particles (with their connecting axis perpendicular to the main flow) at a relatively small distance to each other (see Figure 5). Fortunately, this setup is simple enough to allow us to obtain a reference solution using a body-fitted mesh (the mesh is fine enough to fully resolve all details of the flow, data not shown). Our analysis of the force and heat flux data indicates, that the predictions of the new HFD-IBM solver is within ca. 6 % of the solution obtained with a body-fitted mesh. This suggests that our HFD-IBM solver is indeed able to correctly predict the flow and the temperature (or other scalar) fields in dense fluid-particle suspensions.

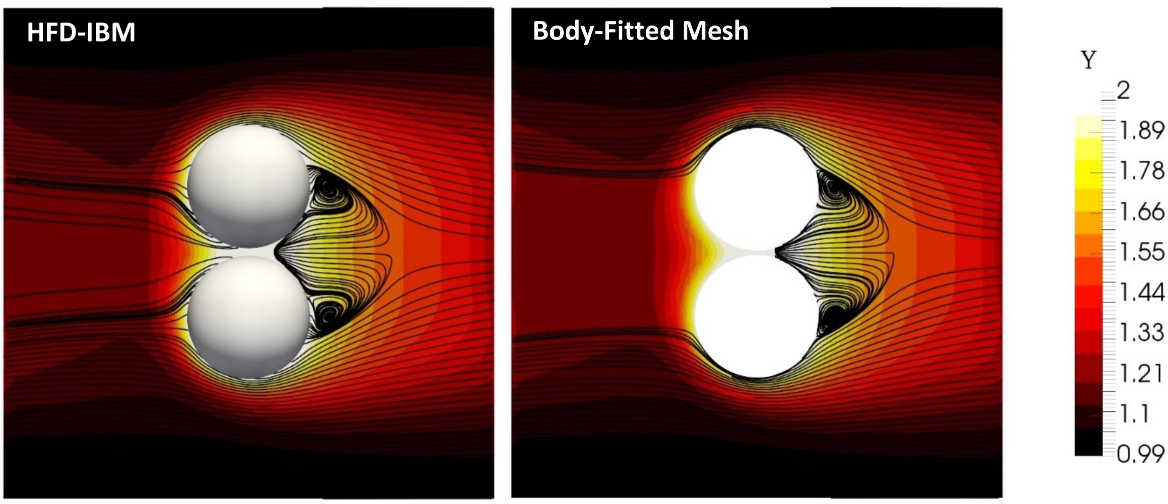

Figure 5: Comparison the dimensionless temperature field (color contours), as well as the streamlines (black lines) for the new HFD-IBM solver (left panel), and a solution obtained with a body-fitted mesh (right panel, flow is from left to right).

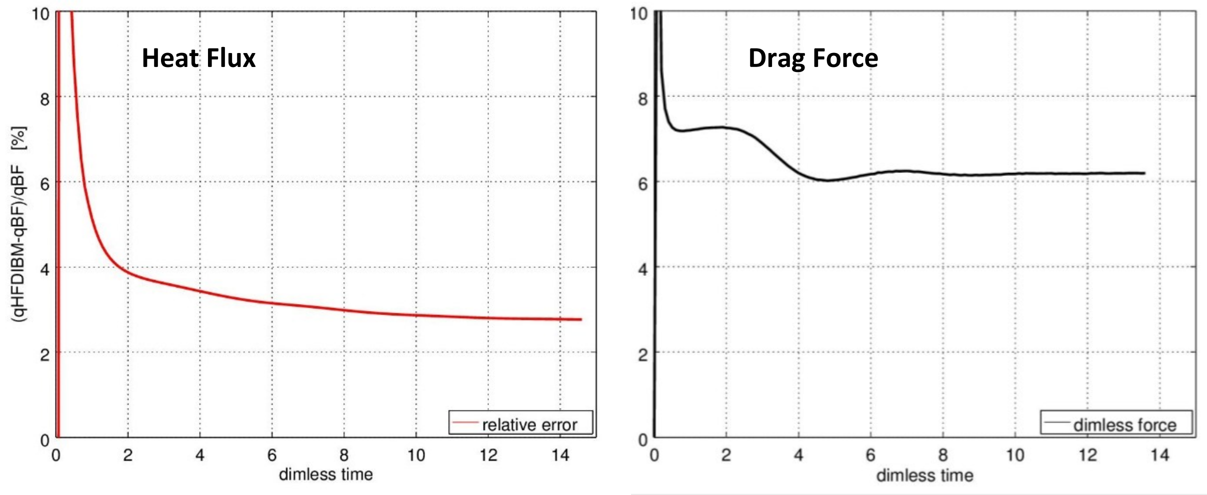

Figure 6: Relative error of the heat flux (left panel), as well as the force (right panel) when using the HFD-IBM solver (the reference is the solution obtained with the body-fitted mesh).

2.5 Use Case 5 – Heat transfer in a fixed periodic particle bed

This case is the most relevant one, since it is closest to the final application of the DNS solver, i.e., the prediction of heat and mass transfer in a randomly-arranged particle bed (mono-sized particles). Unfortunately, for this situation, it was very challenging to generate a body-fitted mesh. Hence, the results are only compared to literature data (see Figure 7). As can be seen, the agreement with the results of Gunn is excellent, whereas the more recent results of Deen et al. are somewhat below our predictions.

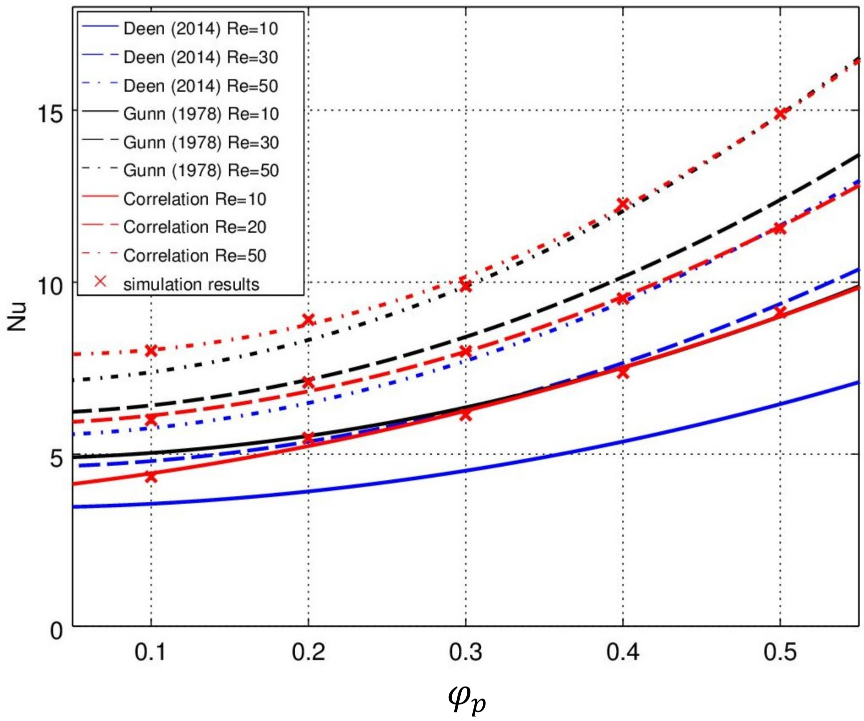

Figure 7: Comparison of the predicted Nusselt number (red crosses, each data points represents the mean value obtained from multiple realizations for identical system parameters), as well as the newly developed correlation (red lines) with literature data (black and blue lines).

Also, the newly developed correlation (see next Chapter for details) approximates the predicted Nusselt numbers reasonably well, indicating that the chosen functional form for the Nusselt numbers seems to be appropriate.

3 Workflow and Model Parameters

3.1 Fitting a Correlation

The closure model is formulated in the form of a correlation for the particle-based Nusselt number. This correlation is derived from a refitting of the widely used Gunn correlation (Gunn, 1978), which is valid for a mono-disperse bed of particles. The refitting is done by changing three coefficients of the Gunn correlation, similar to the approach chosen by Deen et al. (2014). Thus, the original Gunn correlation is re-written in the form:

$$\frac{Nu - \left(7 - 10\varphi_p + 5\varphi_p^2\right)}{Pr^{1/3}} = C_0 Re^{0.2}\left(7 - 10\varphi_p + 5\varphi_p^2\right) + Re^{0.7}\left(1.33 - C_1\varphi_p + C_2\varphi_p^2\right)$$

The three coefficients (C_0, C_1, C_2) are obtained by fitting the particle-based Nusselt number calculated from fully resolved simulations.

For the data shown in Figure 7, we obtain

$$C_0 = 1.118 \quad C_1 = -2.066 \quad C_2 = 1.197$$

It is worth to notice that Gunn (1978) obtained the following coefficients instead:

$$C_0 = 0.7 \quad C_1 = -2.4 \quad C_2 = 1.2,$$

while Deen et al. (2014) obtained the coefficients:

$$C_0 = 0.17 \quad C_1 = -2.31 \quad C_2 = 1.16$$

3.2 Integration with Porto

The integration of the developed workflow with any data management tool run is straight forward, since the workflow is fully controlled by scripts. For the integration within the NanoSim project, the Porto tool must provide an appropriate data file containing the data to be fitted. Then, the appropriate octave script must be run to actually fit the data, and determine the coefficients in the closure. This closure is then saved in the form of a JSON file where the functional form (i.e. Gunn) is specified together with the coefficients. This file is then committed to a database (e.g., MongoDB) via Porto. The example case to highlight the integration with Porto is available here:

$CFDEM_SRC_DIR/../tutorials/octave/correlationNusselt

4 Appendix

4.1 Glossary

See List of definitions and abbreviations in Section 1.3

4.2 Document Change Log

Date	Description	Author(s)	Comments
18.12.2015	Preliminary version (0.1)	F. Municchi	Contained data with old solver for particle bed.
30.12.2015	First complete version (1.0)	F. Municchi, S. Radl	