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Coupling of particle and continuum methods

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Abstract
Particle methods are the method of choice for flow conditions at high altitude, particle-laden flows or radiative heat transfer. One big challenge is to provide an efficient coupling interface to established numerical methods for the continuum regime to be able to use a generalized user interface for all flow regimes. The chosen unified approach based on a plugin to the coupling software FlowSimulator provides a general python-based coupling interface. This allows the straightforward combination and data exchange between the numerical solvers, e. g. for the rarefied and continuum regions. The two-way particle coupling approach is demonstrated using Lagrangian particle test cases.

Nomenclature

Roman	**Symbols**
C_D	particle drag coefficient
d	diameter
$\mathbf{F}$	force coefficient
$\mathbf{v}$	velocity vector
$\dot{m}$	mass flow rate
n	mean free path
m	mass
N	number
p	pressure
S	Eulerian source term
T	temperature
w	particle weight

Greek symbols

ρ	density
λ	backward facing step expansion ratio

Subscripts

0	stagnation conditions
c	continuous phase
p	discrete particle phase

Non-dimensional numbers

Re	Reynolds number

1. Introduction

For simulation of flow conditions at high altitude, of particle-laden flows or of radiative heat transfer,[13] particle-based methods are the numerical method of choice. Depending on the flow regimes of interest the appropriate numerical method has to be chosen depending on the local Knudsen number Kn. This non-dimensional number is defined as ratio of the molecular mean free path n to a length scale l

$$\mathrm{Kn} = \frac{n}{l}\,.$$

At altitudes above approx. 80 km, the continuum hipothesis does not hold and effects of the rarefied gases have to be considered that are typically computed using the Direct Simulation Monte Carlo (DSMC[2]) methods or Fokker-Planck methods.[6] Both numerical methods are based on particle methods such that a general coupling interface between continuum and particle-based methods is needed to provide a general numerical design tool suitable for all flow regimes. Another application is the solution of particle-laden flows, in which macro-style particles are moved within an Eulerian flow field.

To cover all these applications a general numerical tool-chain is needed that allows the coupling of particle-based methods to commonly used contiuum methods based on a unified coupling interface. Ideally, this coupling

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is performed without the need to rely on file input and output (IO) operations as the file IO limits constitutes a key limiting factor on current high performance computing (HPC) systems. This contribution demonstrates an in-memory coupling interface of a state-of-the-art DSMC solver based on the open source code SPARTA[5, 19] (Stochastic PArallel Rarefied-gas Time-accurate Analyzer) to the coupling software FlowSimulator DataManager (FSDM).[17] The interface provides data handling as well as interpolation methods to couple different numerical solvers with a centralized data handling removing the need to do expensive file-IO operations. One popular application is the coupled simulation of flow and structural solvers to account for deformations or heat transfer into the structure.

In this contribution the extension FlowSimulator Coupling Application Layer for SPARTA (FSClappSPARTA) is described which allows the direct coupling of the particle properties, as present in the SPARTA code, to the cell-based continuum solver FSDM ecosystem by means of in-memory coupling using the SPARTA library interface. This extends the applicability of the FSDM-based tool-chains to applications for which particle-based methods are required, e. g. particle-laden flows or radiation simulations based on a Photon Monte Carlo method.[18] We describe the coupling process of the DSMC solver SPARTA to the CFD solvers CODA/HyperCODA[7, 10, 15] and vice versa. This method allows the two-way coupled simulation of particle-laden flows. The corresponding data fields can be exchanged between the different solvers providing input for the particle acceleration in SPARTA as well as providing source terms for the flow solver due to the presence of particles. In this first contribution we validate the data exchange between the solvers based on test cases that use particles within an Eulerian flow field. Application of this type of simulations in the space-sector for the described two-way Lagrangian-Eulerian coupling include the modeling of solid rocket motors in which aluminium particles[3] need to be considered in the simulation chain.

The paper is structured in the following: first we introduce shortly both flow solvers as well as the general coupling software FlowSimulator. Then we describe the two-way coupling of the particles with a compressible flow using a particle drag model on the Lagrangian solver and source terms in the Eulerian solver. The here described coupling layer FSClappSPARTA is not solely capable for the solution of two-way coupled Euler-Lagrangian particle flows but as well provides a generic Python-based interface for the coupling of particle and continuum based methods via a generic coupling interface. Results of the first two-way coupled simulations will be presented as well as ideas for further development of the coupling interface. The paper is closed with a summary and an outlook onto further applications.

2. Methodology

2.1 Euler-Lagrangian method

We rely on the following baseline software that we need to achieve a two-way coupling of particle and continuum methods. The corresponding software can be controlled using a Python scripting layer that facilitates the setup of coupled simulations. In the past this coupling has been demonstrated for many applications, see e. g. Meinel et al.[17] The focus of the application is here to be able to compute the particle transport within an Eulerian flow field, an application for which typically particle drag models are applied to compute the particle acceleration.

In the following the different numerical tools are introduced:

Lagrangian particle solver The open source DSMC solver Sparta[5, 19] developed by Sandia National Laboratories is chosen here to solve all particle motion related tasks. The choice of SPARTA as Lagrangian solver is motivated by the following criteria:

- it was specifically designed for particle based simulations including all relevant data structures and algorithms for particle tracking and is available as open source software.
- it has MPI support and good scaling[19] as well as support for the KOKKOS API[4]
- it has an existing library interface to couple external codes to SPARTA as well as an Python control interface.
- the orthogonal Cartesian grids with adaptive grid refinement are well suited for efficient particle transport.
- it is widely used in academia and research for DSMC applications.
- it is used at German Aerospace Center (DLR) for the hybrid Fokker-Planck/DSMC approach for plume impingement simulations.[1, 9, 12]
- it is used as Photon Monte Carlo method for radiation simulations.[18]

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To further improve the synergies within DLR spacecraft department, the DSMC solver SPARTA was chosen as Lagrangian particle solver for the Euler-Lagrangian particle coupling.

Being developed as DSMC solver the SPARTA solver contains models for particle transport, collisions and reactions. It has an external force interface for the interference of particles with electro-magnetic forces. This interface is used to modify the particle trajectories in combination with an Eulerian flow field. For coupled Euler-Lagrangian simulations typically particle drag models are used to compute the acceleration of the generic particles. All collision and wall interactions that are already present in the DSMC solver can be applied for this generic particle transport as well, limiting the amount of new models that have to be integrated in the Lagrangian solver. It would be far too expensive to model all particle interactions in a continuum (as we would do in DSMC).

The DSMC solver SPARTA is written in C++ and has a Python interface to allow for code-to-code in-memory coupling. The solver is based on hierarchical grids with automatic grid refinement at surfaces by means of cut-cells. In the coupling framework we rely on the SPARTA library interface that facilitates the in-memory data exchange using the particle and grid based variables.

Coupling layer FlowSimulator The coupling software FlowSimulator DataManager[17] is an open source framework for multi-disciplinary simulations, i. e. problems for which different solvers are needed. It is used to share data between different solvers, e. g. between a flow solver and a structural solver without the need for a huge amount of file IO.

The software has a common distributed memory data format for an efficient data exchange between the different FSDM plugins that handle the interfaces to the different solvers. The general software core handles all common data fields and has various data import and export filters. It provides a Python scripting layer for the user interaction that allows the design of coupling scripts.

Eulerian flow solver For the continuum solver part we rely on the (modular) compressible flow solver framework HyperCODA[10] that is based on the flow solver CODA.[7,15] The flow solver is fully integrated as FSDM plugin and handles all data input and output using the FSDM export filters. Thus, data fields that are present in FSDM can be directly used in the flow solver without the need for file-IO. The extension HyperCODA handles as additional modularized layer of CODA all mixture related flow effects, i. e. as well any particle source terms in a flow.

FSClappSPARTA The FSDM plugin FSClappSPARTA provides a Python steering layer for the particle two-way coupling. It handles the data transfer from the particle tracer (e. g. the particle masses, particle velocities, . . .) to the flow solver. Vice versa the particle acceleration is transferred (e. g. as computed by a particle drag model) to the particle solver via an external field formulation (two-way coupled particles). That way the DSMC solver SPARTA can be used as for Langragian particle tracking (including all particle collisions and reactions) combined with an continuum flow solver CODA/HyperCODA. The complete workflow and data handling is summarized in Figure 1.

Due to the limitation of using two different tools for the Eulerian and Lagrangian phases, the data has to be transfered from one tool to another including a different mesh structure. Another limitation is that since SPARTA works solely on hierarchical grids with grid refinement, mesh interpolation operators are needed to interpolate the Eulerian field data at the particle positions.

2.2 Computation of particle acceleration

For the coupling of Lagrangian particles within an Eulerian flow field, the approach that was already used in the TAU Particle Tracer (see e. g. Widhalm et al.[20] and its extension for mixture flows in Ecker et al.[3]) is applied. The Lagrangian velocities gradient for a single particle (considering solely the drag force of the particles) in a flow field is given by

$$\frac{\partial v}{\partial t} = m_p \mathbf{F}_D = \frac{3}{4}\frac{C_D}{d_p}\frac{\rho_c}{\rho_p}(v_c - v_p)|v_c - v_p| \tag{1}$$

with the subscript p referring to particle quantities and c to the continuum flow field values evaluated at the particle positions. The particle Reynolds number is estimated to

$$\mathrm{Re_p} = \frac{\rho_p |v_c - v_p| d_p}{\mu_c} \tag{2}$$

using the viscosity μ_c of the surrounding fluid. Its physical significance is the ratio of the inertial forces to the vicous forces. C_D is the particle drag coefficient that is estimated as in Ecker et al.[3,8] using the simple Stokes drag model

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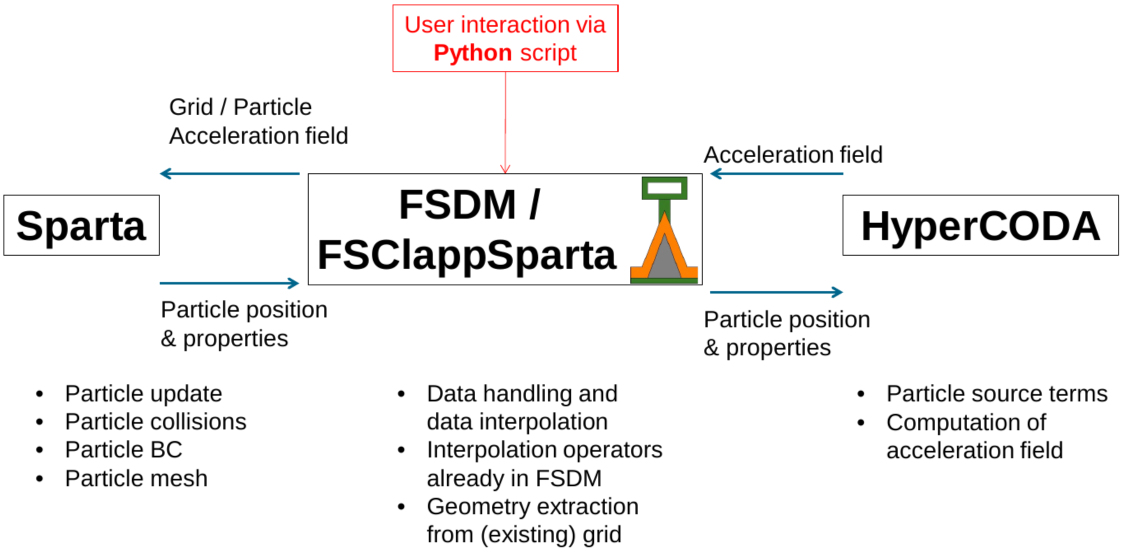

Figure 1: Coupling and data exchange flowchart between the continuum solver HyperCODA and the DSMC particle method SPARTA. The coupling interface is provided by the FSDM plugin FSClappSPARTA that handles all data exchange between the solvers that is needed for the source term computation or the computation of the (external) particle acceleration.

based on the particle Reynolds number

$$C_D = \begin{cases} 24/\mathrm{Re_p}, & 0 < \mathrm{Re_p} < 0.34 \\ 0.48 + 28\mathrm{Re_p}^{-0.85} & 0.34 < \mathrm{Re_p} < 10^5 \end{cases} \tag{3}$$

More sophisticated particle drag models exist in literature that take more physics, i. e. compressibility and temperature effects, into account. Worth to mention is the more sophisticated Nickerson drag model as described in Hwang and Chang[11] that was applied to high speed nozzle flows.

2.3 Two-way coupling approach

To account for the mass, momentum, and energy of the particles a source term to be applied in the Eulerian flow solver has to be computed. Two different methods exist for tracking particles in a flow field: the trajectory method and the discrete particle method. In the trajectory method the flight path of particles is tracked from which then in a second step representative source terms are computed in these cells that are traversed by the particle trajectory. In this approach the particle and flow field are decoupled and, thus, only suitable for steady-state simulations. In the discrete particle method all particles in the flow field are tracked in space and time. Physical effects like particle collisions and reflections at boundary conditions are resolved. Thus, the particle transport and the flow solution are coupled as the particles influence the flow field and the flow field the acceleration of the particles.

Each Lagrangian particle within a Eulerian cell generates a source term in the mass, momentum and energy equation that accounts for the interaction between Eulerian and Lagrangian phases. Here we consider the simple case without any inter-phase mass transfer effects. Thus, the Eulerian source terms can be described as follows:

The mass source term accounts for the particle mass in the cell

$$\mathcal{S}_{\text{mass}} = \mathcal{P}\left\{w_i m_{p,i}, \mathbf{x}\right\} \tag{4}$$

using the particle position $\mathbf{x}$, particle weight factor w_i that represents the ratio between real and computational particles. This particle weight factor is introduced to increase computational efficiency and is usually chosen larger than one.

The momentum source term accounts for the momentum change due to drag or lift forces onto the particles. Forces due to shear stresses, pressure gradients, or body forces are not included in the model.

$$\mathcal{S}_{\text{momentum}} = \mathcal{P}\left\{\left(F_D + \frac{m_c}{2}\left(\frac{D\mathbf{u}_c}{Dt} - \frac{d\mathbf{v}_p}{dt}\right)\right), \mathbf{x}\right\} \tag{5}$$

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air flow			seeding particles		
density	ρ_c	$1.225\ \frac{kg}{m^3}$	density	ρ_p	$1000\ \frac{kg}{m^3}$
velocity	v_c	$5.5\ \frac{m}{s}$	diameter	d_p	$[1\,\mu m, 10\,\mu m, 50\,\mu m]$
Reynolds number	Re	7534			
dynamic viscosity	μ	$1.78910^{-5}\ \frac{kg}{ms}$			

Table 1: Simulation parameters for the channel and the backward facing step test cases with particle seeding

The energy source term accounts for the convective heat flux between Eulerian and Lagrangian phase as well as the energy change due to the particle drag and lift force. Enthalpy changes due to reactions and interphase mass transfers are not included.

$$\mathcal{S}_{\text{energy}} = \mathcal{P}\left\{\mathcal{S}_{\text{momentum}} \cdot \mathbf{v}_p, \mathbf{x}\right\} \tag{6}$$

using the projection operator $\mathcal{P}$ that is used to project the particle source term onto the computational fluid grid. In the current case using a Finite-Volume discretization the influence of the particle source term is restricted only to the cell that particle is located in. Thus, the projection operator for a general variable a is $\mathcal{P}(a, \mathbf{x}) = \frac{a}{V_{\text{cell}}}$.

The direct Euler-Lagrangian coupling approach is visualized in Figure 1. For the Eulerian part the CFD solver CODA/HyperCODA is used that is coupled to the particle tracer via the computation of particle source terms. In the Lagrangian part the particles are tracked and managed in the DSMC solver SPARTA that provide methods for colliding and reacting particles. Both codes are coupled using the FSDM plugin FSClappSPARTA that provide generic data exchange and interpolation routines. By means of a Python coupling layer both codes are in-memory coupled allowing for an efficient data exchange between the different codes.

3. Coupling of particles in air flow stream

Inspired by the test case described by Lu & Zhang[16] for particle deposition the following test cases are defined to demonstrate the coupling of particles with the flow field: the first one is the a turbulent channel geometry (shown in Figure 2) as well as in a backward facing step geometry (see Figure 4). The particle seeding is done at the channel inlet and the particles are tracked throughout the flow field. The parameters for the air flow and the particles are summarized in Table 1. The duct inlet was chosen to $D_u = 0.02$ and the duct length to $L_u = 0.4$. For the backward facing step test case two expansion ratios $\lambda = {}^{D_b}/_{H_b}$ with 4:3 and 6:3. Similar to the duct test case the inlet was chosen to $D_u = 0.02$ and the lengths $L_{b1} = L_{b2} = 0.2$. The upper and lower channel wall boundary conditions were considered to nonslip adiabatic walls.

For both test cases, a structured mesh was created. For the backward facing step test case it is shown in Figure 5. The mesh wall distance was set to a y^+-value of 1 to resolve the turbulent boundary layer. The final two-dimensional mesh has about 40000 cells.

3.1 Particles in channel flow

A generic validation test case is the channel flow with the geometry defined in Figure 2. As a first step, the steady flow solution without the influence of the particles was computed with CODA assuming a standard air flow. The Spalart-Alamaras turbulence model in negative formulation is applied to resolve the turbulence effects on the flow field.

For the coupled simulation we combine the DSMC particle solver SPARTA with the CODA flow solver using the FlowSimulator. The particles of $1\,\mu$m size are injected with a random velocity at the inlet. With the particle drag model, that is described in Section 2.2, the injected particles are accelerated o decelerated to the flow velocity. Due to the inert mass of particles the particles do not react immediately onto changes of the flow velocity.

The results for the turbulent channel flow are visualized in Figure 3 using a RANS Spalart-Alamaras turbulence model in negative formulation. A distribution of the ratio of the turbulent to molecular viscosity as well as the particle positions for the smallest particle size of $1\,\mu$m are plotted including the vleocity streamlines. Investigating carefully the final velocity distribution of the particles at the exit plane, the velocity profile of the air flow can be recovered. Thus, the used particle drag formulation works in that sense that the (small) particles here are just accelerated until the flow velocity is reached.

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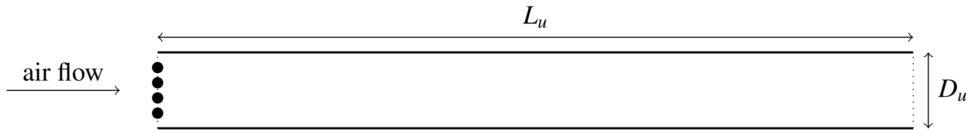
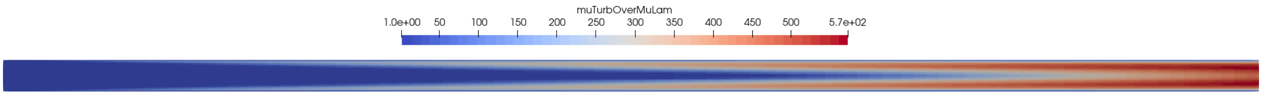
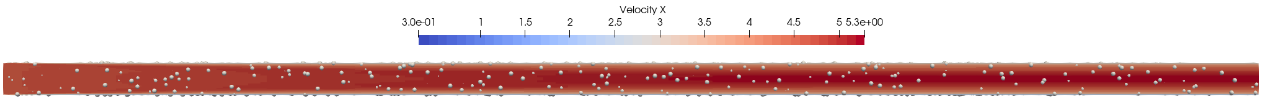


Figure 2: Schematic of the particle deposition in uniform channel flow with the particle seeding at the inflow (marked by the dots). The particles and the air flow leave the channel on the right at the exit.



(a) Ratio of turbulent viscosity to molecular viscosity with streamlines of air flow.



(b) Particle positions for $d_p = 1\,\mu$m.

Figure 3: Particles in the turbulent channel flow

3.2 Particles in a backward facing step flow

Validation of the air flow The air flow velocity is validated using the measurements of Kim et al.[14] for the here considered Backward Facing Step (BFS) geometries (see geometry in Figure 4 and mesh in Figure 5). The validation is shown in Figure 6 for a Reynolds number of 18400 based on the duct height. The numerical results are in agreement with the results obtained by Lu & Zhang[16] evaluated at different slices in the BFS domain and recover the experimental measurements of Kim et al.[14]

Backward facing step with particle seeding The second test case is the backward facing step with seeded particles. Two different configurations are compared in detail with a expansion ratios of λ equal to 4:3 and 6:3 with 3 different particle sizes each. The flow conditions as well as the particle characteristics are summarized in Table 1.

The distribution of the ratio between the turbulent viscosity to the molecular one as well as instantaneous snapshots of the particle distributions are visualized for 3 different particles sizes in Figure 7 and 8 for two BFS expansion ratios of 4:3 and 6:3. The particle streams in the BFS test case are expanding because of the flow expansion after the step. The particle deposition length is increased as the expansion ratio is increased.

Small particles are more likely to be affected by the small-scale turbulent velocity structures due to their small mass. Due to the large inertia of the large particles the particle flow path is nearly unchanged resulting in a particle free zone behind the BFS, the "particle free zone". Small particles are more likely to fill the zone behind the step, something that was not observed in the test case here. This might be related to the neglection of the gravity source term that forces the particles towards the lower wall.

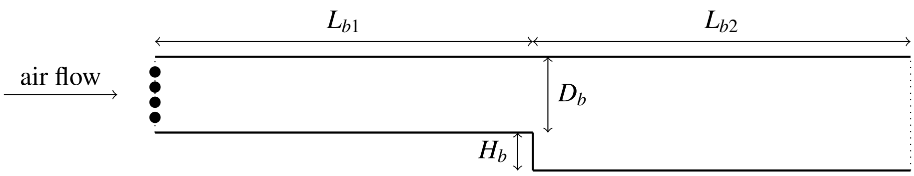


Figure 4: Schematic of the particle deposition in backward facing step geometry with the particle seeding at the inflow (marked by the dots). The particles and the air flow leave the channel on the right at the exit.

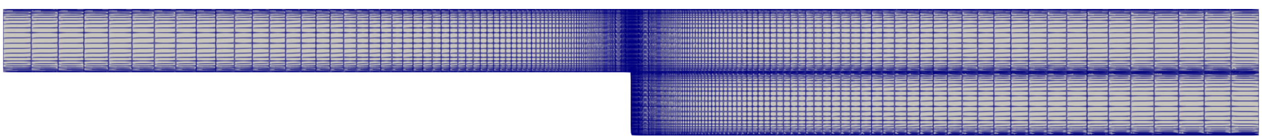


Figure 5: Computational mesh for the backward facing step test case with expansion ratio of λ=6:3.

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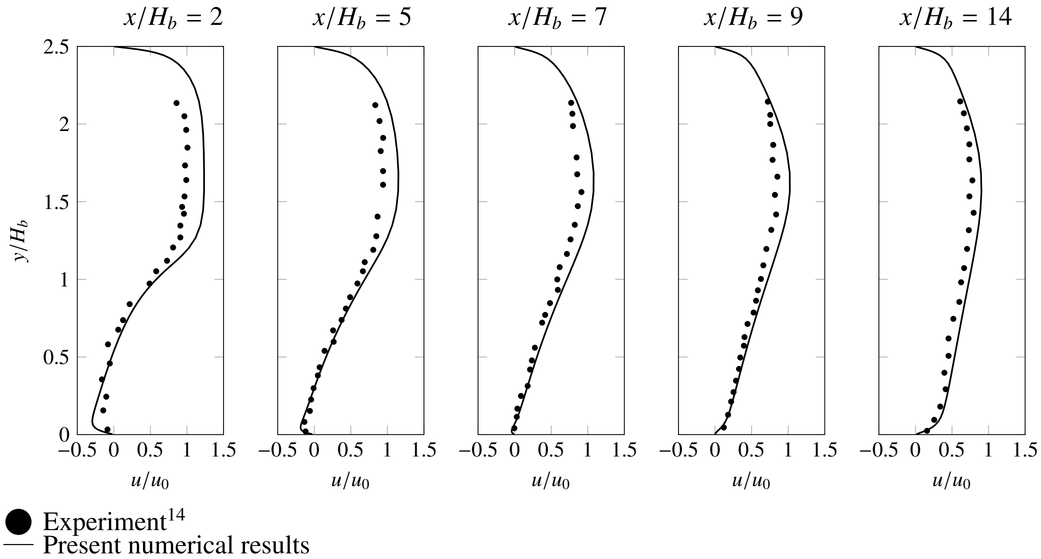

Figure 6: Air flow velocity profiles in the backward facing step duct with expansion ratio of λ = 5:3 in comparison to experimental measurements by Kim et al.[14]

4. Summary and Outlook

In this publication we presented a general coupling layer to couple the DSMC solver SPARTA with the fluid solver CODA using a two-way coupled approach. Basis for the efficient coupling procedure is the software FSDM that is designed for multi-physics simulation problems by coupling different numerical solvers. In this framework we presented the new FSDM plugin FSClappSPARTA that provides the interface to couple SPARTA to the FSDM data structures enabling the exchange of coupling data between the solvers. In a first step the approach was designed to provide a workflow for two-way coupled particle flows in Eulerian flow fields. For now the particles are kept static and did not change their particle properties (e. g. particle mass and charge) but being allowed to interact between each other. We demonstrated the particle transport within a turbulent channel flow as well as a backward facing step. The results are in agreement with available literature data for the particle transport.

In the future this approach the generic coupling interface defined in FSClappSPARTA can be extended for several other applications, including the input and output of data fields for the Photonsparta method by Oblapenko et al.[18] This facilitates the data exchange of absorption and emission spectrographic data to and from SPARTA-based tool-chain for radiation. Another extension would cover vaporizing particles within the flow field, one approach needed for the modeling of solid rockets.

Acknowledgments

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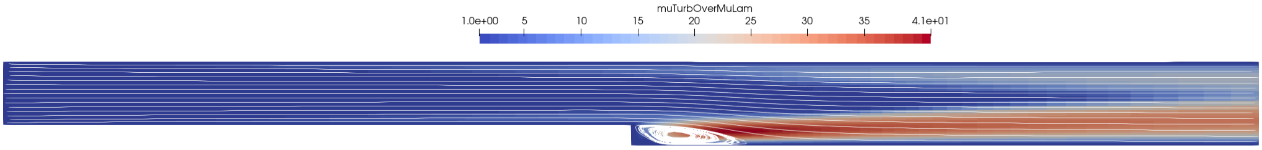
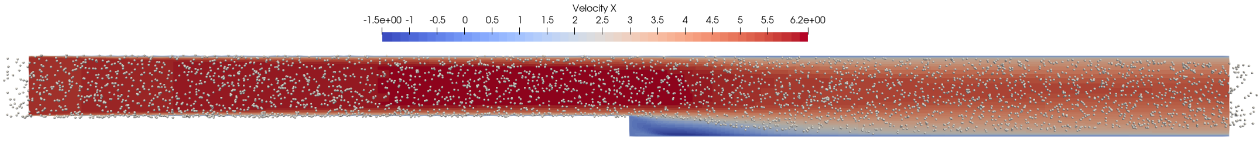
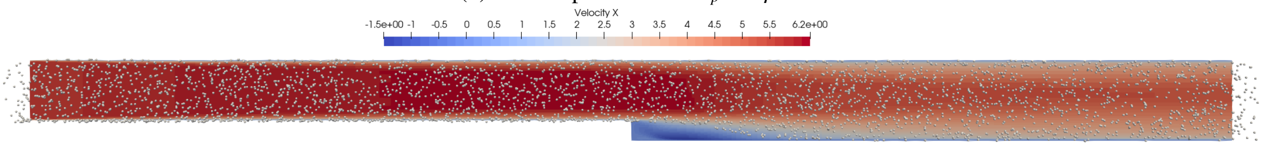


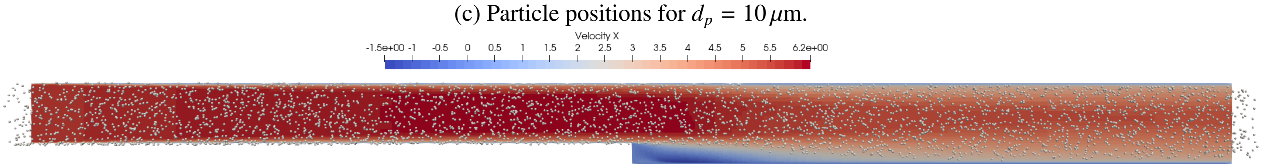
(a) Ratio of turbulent viscosity to molecular viscosity with streamlines of air flow.



(b) Particle positions for $d_p = 1\,\mu$m.

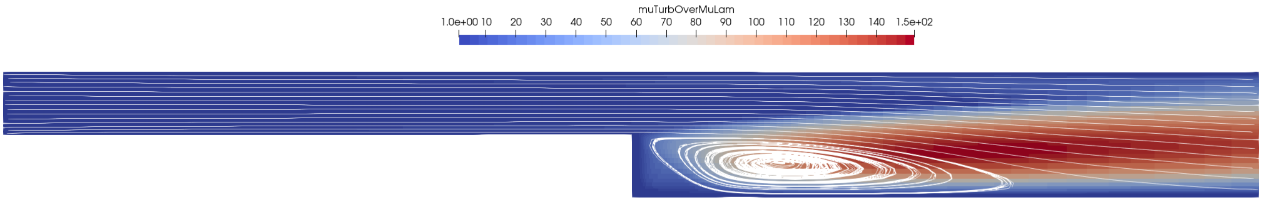


(c) Particle positions for $d_p = 10\,\mu$m.

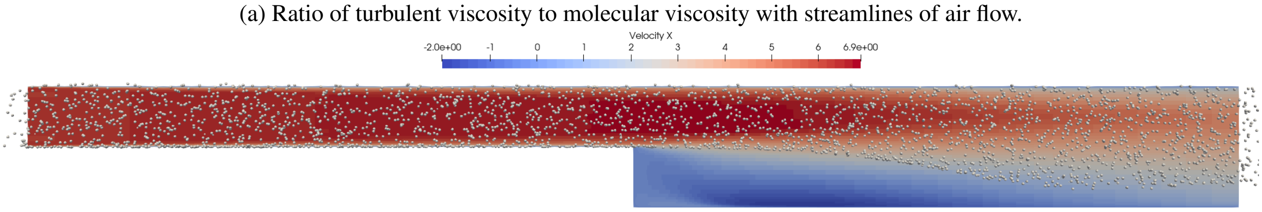


(d) Particle positions for $d_p = 50\,\mu$m.

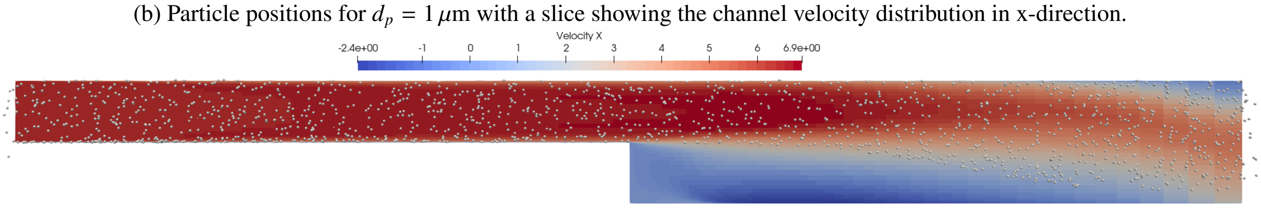
Figure 7: Distribution of turbulent viscosity ratio and the particle positions in the backward facing step duct with expansion ratio of $\lambda = 4 : 3$



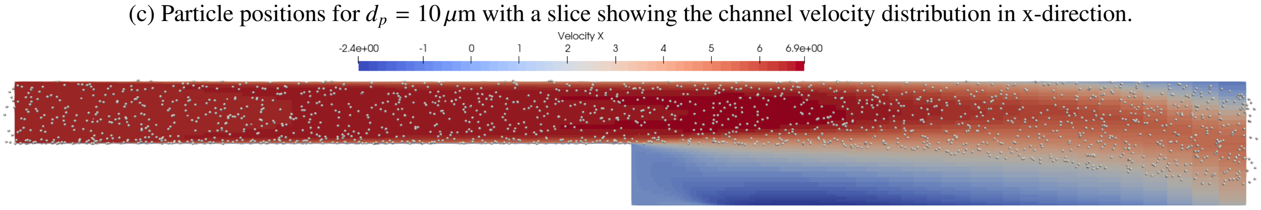
(a) Ratio of turbulent viscosity to molecular viscosity with streamlines of air flow.



(b) Particle positions for $d_p = 1\,\mu$m with a slice showing the channel velocity distribution in x-direction.



(c) Particle positions for $d_p = 10\,\mu$m with a slice showing the channel velocity distribution in x-direction.



(d) Particle positions for $d_p = 50\,\mu$m with a slice showing the channel velocity distribution in x-direction.

Figure 8: Distribution of turbulent viscosity ratio and the particle positions in the backward facing step duct with expansion ratio of $\lambda = 6 : 3$

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