

# High-order overset grid method for detecting particle impaction on a cylinder in a cross flow

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## Abstract

An overset grid method is used to investigate the interaction between a particle-laden flow and a circular cylinder. The overset grid method is implemented in the Pencil code, a high-order finite-difference code for compressible flow simulations. High-order summation-by-part operators are used at the cylinder boundary and both bi-linear Lagrangian and bi-quadratic spline interpolation is used for communication between the background grid and the body-conformal cylindrical grid. The performance of the overset grid method is assessed for benchmarking cases of steady and unsteady flows past a cylinder. For steady flow at low Reynolds number, high-order accuracy is achieved for velocity components. Results for flow in the vortex shedding regime is compared with literature, and show good agreement. Following this, the method is applied to particle-laden flow simulations, where spherical point particles are inserted in the flow upstream of the cylinder. These inertial particles are convected downstream towards and (possibly) past the cylinder. The simulations reproduce data from literature at a significantly reduced cost, and reveal that the previously published DNS data is less accurate than assumed for particles with very small Stokes numbers.

*Key words:* overset grids, particle-laden flow, high-order, finite-difference, particle impaction, compressible fluid dynamics

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## 1. Introduction

A common flow problem in numerical simulations is flow past a bluff body. Obstructions in the flow include (but are not limited to) spheres, flat plates, circular, rectangular or elliptical cylinders, triangles and spheroids, and complex geometries made out of a combination of these. Particle-laden flows interacting with such obstacles are important for a range of applications. Whether the goal

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is to maximize the particle extraction from the flow, as for filter applications, or minimizing particle sticking on the object to avoid an insulating layer, as for biomass boilers, understanding the mechanics of inertial particles may help improve design, and hence efficiency, of said applications. Accurate predictions of particle behavior in the vicinity of the bluff bodies require highly accurate boundary layer representation in numerical simulations. Finding the numerical method best suited to this task is not trivial task, but can have a huge impact on both efficiency and accuracy of such simulations.

### *1.1. Representing solid objects in the flow*

For generic shapes (cylinders, spheres, plates, etc.) both body-fitted structured meshes are commonly used to accurately resolve the solid boundary. Such methods use grids that conform to the solid (or solids) immersed in the flow and to other the physical boundaries of the domain (inlet/outlet, walls, etc.). Depending on the flow domain, this may require some deformation of the grid to conform to the boundaries, in addition to the mapping of the flow domain into a simple computational domain. The result may be unnecessary local variations of the grid and time consuming grid generation [1]. Alternatively, one can use unstructured meshes in order to resolve the solid boundaries in the flow. Unstructured meshes provide the highest flexibility in adapting a mesh to the flow problem, and are a good alternative for complex geometries when finite-volume or finite-element formulations of the governing equations are used [2]. Among the disadvantages of such grids are much larger storage requirements than for structured grids [3] and the need for intricate mesh generation techniques [4].

An alternative to body-fitted grids are non-conforming (typically Cartesian) meshes, where a solid in the flow is represented by some change in the fluid equations in the vicinity of the solid boundary. One such method, that has gained vast popularity the last decades, is the immersed boundary method (IBM). This method (or rather, this class of methods) was originally developed to model flow around heart valves [5] by allowing for representation of bluff bodies in the flow without using body-conformal grids. A simple Cartesian grid can be used, where the boundary conditions (the sharp interface) of the bluff body are incorporated in the solver by a modification of the equations in the vicinity of the boundary (see review article by Mittal & Iaccarino [6] and references therein for details). This makes IBMs very flexible in representing bluff bodies, and particularly well suited for complex geometries where the use of body-fitted structured meshes are limited. A caveat of the IBM is the difficulty in achieving high-order accuracy near boundaries that do not conform to physical boundaries. For complex geometries this may be regarded as a necessary loss in order to be able to represent the boundary, but not so for simple geometric shapes. For flow past such bodies other methods may be more suitable, especially when the accuracy in the vicinity of the surface is a major concern.

Roughly ten years after the development of the IBM, a method of multiple grids overset one another was proposed to represent solids in a flow (see [7, 8, 9]). Overset grids, or Chimera methods, employ body-conformal grids

at the bluff bodies, but the body-conformal grids do not extend to the domain boundaries. Instead, a non-conforming background grid (typically uniform Cartesian) is used, and updated flow information of overlapping grid regions is communicated between grids at every time step. In this way, a flow simulation is split into multiple simulations, one for each grid, and the boundaries of one grid is updated with information from the other grids. The background grid is used to compute the general flow outside the smaller body-fitted grids, and the communication between the different grids is done by interpolation.

Overset grid methods have the advantages of being highly accurate at the solid-fluid interface. This is due to the use of body-fitted grids in these regions, and the flexibility in grid stretching made possible when several grids are used. At the same time, no grid deformation is necessary to conform to domain boundaries, due to the use of an appropriate non body-conformal background grid. If the domain is circular, a cylindrical grid can be used as a background grid, if rectangular, a Cartesian grid, etc.

The communication between the grids is the limiting factor in terms of accuracy of overset grid methods. As in fluid dynamic codes using IBM, interpolation of flow variables is detrimental to mass conservation (although conservative, mass correcting overset grid methods do exist for finite-volume codes, see e.g. [10, 11]). Using high-order interpolation between grids have proved beneficial in regards to the overall accuracy and stability of the overset grid method for both finite-difference and finite-volume implementations [12, 13, 14]. While advantageous in terms of accuracy, high-order interpolation techniques have the disadvantage of an increase in complexity, inter-processor communication and floating-point operations, as compared to low-order interpolation schemes. Furthermore, straightforward extension to high-order interpolation, typically from second-order to fourth-order Lagrangian interpolation, does not guarantee a better solution. Possible overshoots in the interpolation polynomials may have a devastating impact on the interpolation accuracy. The applied interpolation scheme should therefore be evaluated for the flow problem at hand. For overset grid implementations several interpolation schemes are available. In this study we compare two of these: bi-linear Lagrangian interpolation and bi-quadratic spline interpolation. Together with high-order low-pass filtering, the resulting computations are both stable and accurate. We will consider this topic further in Section 2.

If several body-fitted grids overlap, the overset grid computations will be increasingly difficult, particularly in regards to the communication of overlapping zones of the different grids. For our purpose, we limit the discussion to a single body-fitted grid on top of a Cartesian background grid. For a more general discussion on overset grids, see [15] or [16].

### *1.2. Particle impaction*

When considering particle deposition on a surface, two mechanisms are necessary for a particle to deposit. The particle must impact the surface, that is, it must get in physical contact with the surface, and it must stick to it. Only the first of these two mechanisms will be a focus of this study. Hence, all particles

that come in contact with the bluff body are absorbed by it. Further, only inertial impaction is considered, and other particle impaction mechanisms like Brownian motion, thermophoresis and turbulent diffusion are omitted. This is acceptable for inertial particles in laminar flows without temperature gradients [17].

The impaction efficiency  $\eta = N_{imp}/N_{ins}$  is a measure of the efficiency of a cylindrical object to capture the particles that initially is incident on the cylinder. The number of impacting particles is given by  $N_{imp}$ , while  $N_{ins}$  is a count of particles with a center of mass that is initially moving in the direction of the solid object. Note that following this convention may lead to  $\eta > 1$ , even if no forces act on the particles, since a particle may follow a path close enough to be intercepted by the object, due to its finite size, although the path of the center of mass does not hit the object.

A flow past a bluff body will be deflected by the object, and particles in the flow will experience a drag force. This force will accelerate the particles towards the fluid trajectory, leading particles away from the bluff body. The particle Stokes number,  $St = \tau_p/\tau_f$ , where  $\tau_p$  and  $\tau_f$  are particle and fluid time scales, respectively (details in Section 4), can be considered a measure of particle inertia. Hence, particles with a small Stokes number follow the flow to a larger extent than particles with a large Stokes number. By using potential flow theory to compute the flow past a circular cylinder, Israel & Rosner [18] found a curve fit for the impaction efficiency as a function of the Stokes number. The predictions by Israel & Rosner are useful, but they are inaccurate in predicting particle impactions for flows where the viscous boundary layer on the cylinder plays an important role (as potential flow theory assumes inviscid flow). In particular, the theory is insufficient in predicting particle impactions for particles with small Stokes number, and impaction in moderate Reynolds number flows. Here, the Reynolds number is defined as  $Re = U_0 D/\nu$ , where  $U_0$  is the mean flow velocity,  $D$  is the diameter of a cylinder (the bluff body in the flow) and  $\nu$  is the kinematic viscosity. Haugen & Kragset [19] performed simulations using the Pencil Code to compute inertial particle impaction on a cylinder in a crossflow for different Stokes and Reynolds numbers. Later, Haugen et al. [20] performed a similar study on a flow with multiple cylinders in order to emulate impaction on a super-heater tube bundle. The impaction efficiencies obtained by Haugen & Kragset [19] have been used as benchmarking results, but they are limited to moderate Reynolds numbers and two-dimensional flows. Part of the reason of this limitation is the use of an immersed boundary method that requires a very fine grid to achieve the accuracy necessary to get accurate results in such simulations.

### 1.3. Present

The purpose of this paper is to introduce an overset grid method applicable to compressible particle-laden flows past a circular cylinder, and to assess its performance for benchmarking cases and for a full blown particle-laden flow simulation. The method has been implemented in the open source compressible flow solver known as The Pencil Code [21, 22]. The aim is to improve the

accuracy of the flow in the vicinity of a cylinder and to reduce computational cost of these kinds of particle-laden flow simulations.

The structure of the paper is the following: In Section 2 the equations governing the flow and the bluff body representation is described. An assessment of the accuracy of the method for steady and unsteady flow past a cylinder is given in Section 3. In Section 4 the capabilities of the overset grid method is demonstrated by simulating particle-laden flow interacting with a bluff body at a moderate Reynolds number. The results and the computational costs are compared with those of Haugen & Kragset [19], before concluding remarks are given in Section 5.

## 2. Methodology

### 2.1. Governing equations

The governing equations of the flow are the continuity equation:

$$\frac{D\rho}{Dt} = -\rho \nabla \cdot \mathbf{u}, \quad (1)$$

and the momentum equation:

$$\rho \frac{D\mathbf{u}}{Dt} = -\nabla p + \nabla \cdot (2\mu \mathbf{S}), \quad (2)$$

where  $\rho$ ,  $t$ ,  $\mathbf{u}$  and  $p$  are the density, time, velocity vector and pressure, respectively, and  $\mu = \rho\nu$  is the dynamic viscosity. The compressible strain rate tensor  $\mathbf{S}$  is given by:

$$\mathbf{S} = \frac{1}{2} \left( \nabla \mathbf{u} + (\nabla \mathbf{u})^T \right) - \mathbf{I} \left( \frac{1}{3} \nabla \cdot \mathbf{u} \right), \quad (3)$$

where  $\mathbf{I}$  is the identity matrix. The pressure is computed by the isothermal ideal gas law,  $p = c_s^2 \rho$ , where  $c_s$  is the speed of sound. The flow is isothermal and weakly compressible, with the Mach number of  $\sim 0.1$  for all simulations. With a constant speed of sound (for the isothermal case) and a constant kinematic viscosity, the momentum equation solved on the overset grids is:

$$\frac{D\mathbf{u}}{Dt} = -c_s^2 \nabla (\ln \rho) + \nu \left( \nabla^2 \mathbf{u} + \frac{1}{3} \nabla (\nabla \cdot \mathbf{u}) + 2\mathbf{S} \cdot \nabla (\ln \rho) \right). \quad (4)$$

The governing equations are discretized with sixth-order finite-differences in space and a third-order memory efficient Runge-Kutta scheme in time [23]. The flow is simulated on a rectangular domain with inlet at the bottom and flow in the vertical direction. The circular cylinder is situated in the center of the domain, and has boundary conditions no-slip and impermeability for the velocity, and zero gradient in the radial direction for the density at its surface. The latter condition can be derived from the ideal gas law and the boundary layer approximation  $\left( \frac{\partial p}{\partial n} = 0, \text{ where } n \text{ is the wall normal direction} \right)$  for an isothermal flow. Navier-Stokes characteristic boundary conditions are

used both at the inlet and at the outlet of the flow domain. This boundary condition is a formulation that makes use of one-dimensional characteristic wave relations to allow acoustic waves to pass through the boundaries [24]. The remaining domain boundaries are periodic.

## 2.2. Overset grids

To resolve the flow domain with an overset grid method, a cylindrical coordinate grid is body-fitted to the cylinder, and a uniform Cartesian grid is used as the background grid (see Fig. 1a). Stretching in the radial direction is used for the cylindrical grid. It is beneficial that the grids have similar grid spacing in the region where fluid data is communicated between them. The stretching enables having similar grid spacing in the interpolation region and a much finer grid near the cylinder surface.

The compressibility of the flow leads to a strict stability limit for the Runge-Kutta method, imposing a very small time step in the simulations. As we are effectively solving two different flow problems, coupled only by the communications between the grids, some flexibility in the choice of time step is possible. Choosing a time step on the background grid small enough to guarantee stability for the Cartesian grid spacing, and a smaller time step on the cylindrical grid can reduce the overall computational cost significantly. The cylindrical grid time step must be a multiple of the background grid time step to ensure that the computations on each grid are synchronized. Another possibility, possibly beneficial if the grid spacing near the cylinder is several orders of magnitude smaller than that of the background grid, is to use an implicit solver on the cylindrical grid. Such a solver is beyond the scope of this study.

The communication of data between the grids in the overset grid simulation is done in two stages for each time step of the background grid. At each stage of the communication, the required flow properties are interpolated from donor-points to fringe-points. Each grid needs a zone of fringe-points at least three point deep, such that the seven point central difference stencil can be used without any special handling at points adjacent to the fringe-points. For a curvilinear grid, the fringe-points are simply the three outer points at each radial grid line (see Fig. 1b). For the Cartesian grid, the fringe-points need to be identified, typically during pre-processing, to include all grid points within a fixed area in the region covered by both the Cartesian and the cylindrical grid. This is set by an inner and outer radius defining the interpolation region, see red lines enclosing fringe-points on the Cartesian grid in Fig. 1c. Cartesian grid points that are closer to the solid than the inner radius of the fringe-point zone (or inside the solid), are hole-points. The hole-points are not used at all in the computations.

In the overset grid method implemented in the Pencil Code, there is no overlap between the two interpolation regions of Figs. 1b and 1c. That is, no fringe-points are used as donor points. Hence, the interpolation is explicit, not implicit [16]. Note that if the bluff body enclosed by the body-fitted grid is moving, the cost of inter-grid communication is significantly increased due to

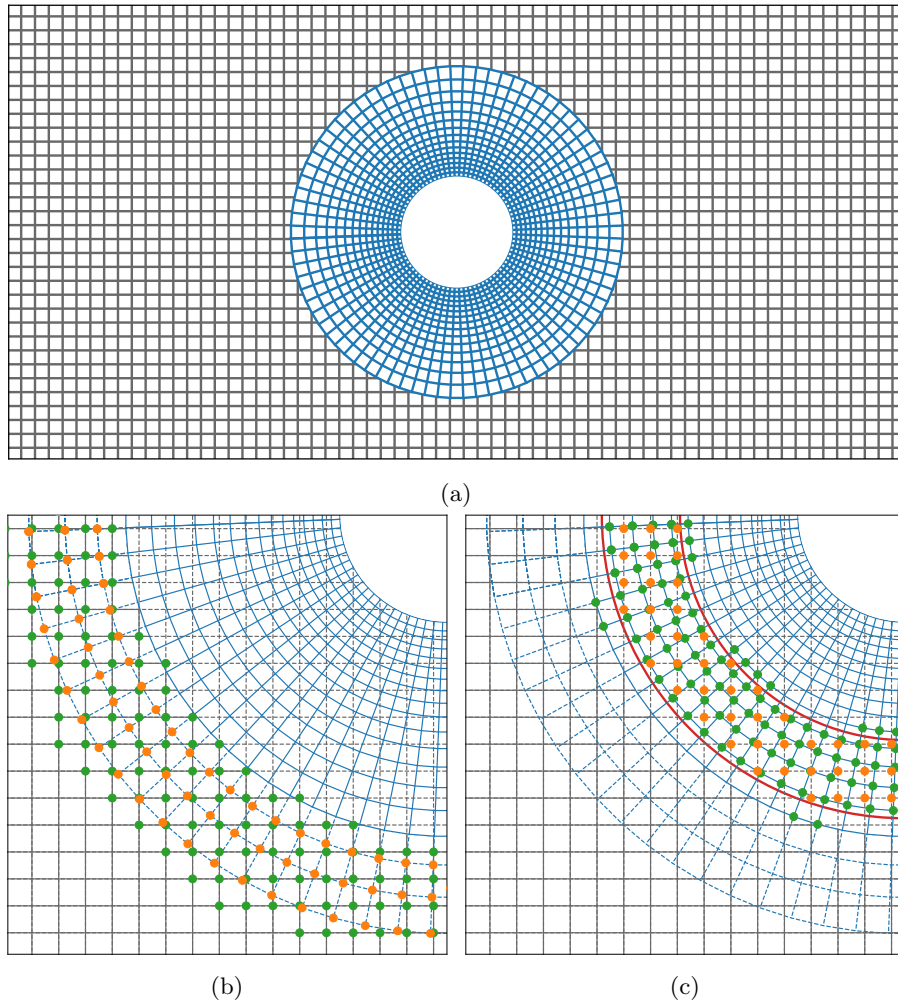


Figure 1: Overset grid method: (a) Cylinder grid on top of background grid (fringe-points of cylinder grid and background grid points within cylinder grid radius not shown). (b) Communication between grids, interpolation from Cartesian donor-points to cylindrical fringe-points. (c) Communication between grids, interpolation from cylindrical donor-points to Cartesian fringe-points. Four donor-points (green) surround each fringe-point (orange) in bi-linear interpolation. Dashed lines used for the part of the grid where variables are not computed by finite-differences (fringe-points and hole-points).

cost related to identifying new fringe and donor-points on the background grid at each new position of the bluff body.

At present, two types of interpolation are implemented for overset grid communication in the Pencil Code. These are bi-linear Lagrangian interpolation and bi-quadratic spline interpolation. Both methods have the advantage of avoiding oscillations in the interpolation interval, a common problem for high-order

interpolation. The Lagrangian interpolation is a second-order accurate scheme, while the spline interpolation is third-order accurate. The illustration of donor-points and fringe-points in Figs. 1b and 1c is for the Lagrangian interpolation, where each fringe-point on one grid is interpolated from the  $2 \times 2$  surrounding donor-points from the other grid. For the spline interpolation, a zone of the  $3 \times 3$  closest grid points are used as donor-points for interpolation of each fringe-point. Note that the interpolation is bi-linear or bi-quadratic in both two- and three-dimensions. This is due to the Cartesian and cylindrical grid having a shared  $z$ -plane, hence no interpolation is needed in the  $z$ -direction.

At the solid-fluid interface, summation-by-parts finite-difference operators are used to enhance stability for the unsteady flow problem (an unsteady wake develops for  $Re > 47$ ). The order of accuracy for such operators are third-order for the sixth-order centered finite-difference method. Details on these operators can be found in [25] (first derivatives) and [26] (second derivatives).

The centered finite-difference schemes are non-dissipative. This can cause problems due to the potential growth of high-frequency modes, leading to numerical instability. To some extent, the summation-by-parts boundary conditions suppress such instabilities that are due to boundary conditions, but these boundary stencils are not sufficient to suppress all oscillations in the solution on the curvilinear stretched grid. In particular, such oscillations are prominent in the density field. The detrimental effect of the high-frequency modes increase as the grid spacing decreases, and may lead to diverging solutions as the grid is refined. To suppress the high-frequency modes, a high-order low-pass filter is used on the curvilinear part of the overset grid. The filter is a 10th order Padé filter, with boundary stencils of 8th and 6th order. On the interior of the domain, the filter is given by:

$$\alpha_f \hat{\phi}_{i-1} + \hat{\phi}_i + \alpha_f \hat{\phi}_{i+1} = \sum_{n=0}^N \frac{\alpha_n}{2} (\phi_{i+n} + \phi_{i-n}), \quad (5)$$

where  $\hat{\phi}_k$  and  $\phi_k$  are components  $k$  of the filtered and unfiltered solution vectors, respectively,  $\alpha_f$  is a free parameter ( $|\alpha_f| \leq 0.5$ ) and  $\alpha_n$  are fixed parameters dependent only on  $\alpha_f$  [27]. Boundary stencils can be found in Gaitonde and Visbal [28]. The Padé filter is implicit, and requires us to solve a tri-diagonal linear system at grid point in the radial direction, and a cyclic tri-diagonal system at every grid point in the direction tangential to the surface. The free parameter  $\alpha_f$  is set to 0.1. With such a small value for  $\alpha_f$ , filtering the solution once per Cartesian time step is found sufficient to get a stable and accurate solution.

### 3. Performance

#### 3.1. Assessment of accuracy

The spatial accuracy of the overset grid method is examined by simulating a steady flow past a circular cylinder at Reynolds number 20. A domain of size



Table 1: Grid refinement levels used in the assessment of accuracy of the overset grid method.

Refinement level	Cylinder grid $N_r \times N_\theta$	Cartesian grid $N_x \times N_y$
0	$17 \times 80$	$80 \times 81$
1	$33 \times 160$	$160 \times 161$
2	$65 \times 320$	$320 \times 321$
3	$129 \times 640$	$640 \times 641$

$L_x \times L_y = 10D \times 10D$  is used. The diameter of the curvilinear, body-fitted grid (henceforth called the cylinder grid) is three times the cylinder diameter.

An indicative measure of the accuracy of the method can be found by computing solutions on several grid refinement levels, and using the finest grid as the “correct solution” when computing two-norm errors of the solution. The grids used in this accuracy assessment are listed in Tab. 1. An odd number of grid points is used in the directions that are not periodic, to get grid points that are aligned at each refinement level. A fixed (dimensionless) time step  $\Delta t = 0.25 \times 10^{-5}$  is used for the Cartesian grid computations at all refinement levels. The small time step ensures that there is no violation of diffusive or advective time step restrictions on any of the grids. These restrictions are  $\Delta \tau \leq C_\nu \Delta \chi_{min}^2 / \nu$  and  $\Delta \tau \leq C_u \Delta \chi_{min} / (|\mathbf{u}| + c_s)$ , respectively, where  $\Delta \tau$  is the dimensional time step,  $\Delta \chi_{min}$  the smallest grid spacing in any direction, and  $C_\nu$  and  $C_u$  are the diffusive and advective Courant numbers, respectively.

Hyperbolic sine functions are used for the stretching in the radial direction. The parameters in the grid stretching are set such that the ratio between the grid spacing normal and tangential to the cylinder surface is approximately one, both in the vicinity of the solid surface and in the interpolation region in the outer part of the cylinder grid. Furthermore, the number of grid points of the Cartesian and the cylindrical grids are chosen to have similar grid spacings in the region of inter-grid interpolation. The resulting local time step on the cylindrical grid is  $\Delta t_c = 0.2\Delta t$ .

The main concern of the method we describe here, is to compute a very accurate boundary layer around the cylinder. This is crucial for the application to particle impaction simulations that the code will be used for in Section 4 and in future studies. We therefore consider the  $L_2$ -error norms of flow variables along strips tangential to the cylinder surface as close as possible to the surface, to get an indication of the accuracy of the scheme in the boundary layer. Figure 2 depicts  $L_2$ -error norms of the density and the normal and tangential velocity components (with respect to the cylinder surface), computed with the two different interpolation methods. The norms are computed along a strip around the cylinder, at the grid point closest the cylinder for refinement level 0 (this corresponds to the 2nd point from the cylinder for refinement level 1, 4th for level 2, etc.).

For both interpolation methods the density computation is second-order and the computation of the radial velocity component is between third- and fourth-

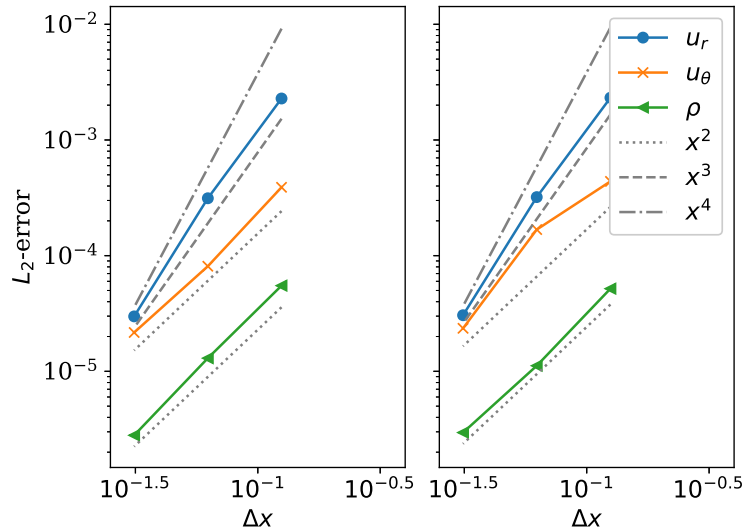


Figure 2:  $L_2$ -error norms of  $u_r$ ,  $u_\theta$  and  $\rho$  at varying refinement levels at the grid point closest to the cylinder surface (for the coarsest grid). Results are for the computations with bi-linear Lagrangian interpolation (left) and bi-quadratic spline interpolation (right), and  $\Delta x$  is the grid spacing on the Cartesian grid.

order accurate, at the grid point closest to the surface on the coarsest grid. Note that although the density computations are only second-order accurate, the  $L_2$ -error norms of density are approximately one order of magnitude smaller than those of the velocity components on the finest grid. Further, the fluctuations in density are very small compared to those in the velocity, in our low Mach number simulations. We therefore focus only on the velocity components in the further assessment of the order of accuracy.

The only noticeable difference between the results from simulations with different interpolation methods, as seen in Fig. 2, is the computation of the tangential velocity component. With the Lagrangian interpolation the accuracy is approximately second-order. With spline interpolation, on the other hand, the order is in-between first and second-order for the first grid refinement and improves to third-order for the second grid refinement. The results suggest that the communication between grids is less influential to the accuracy in the boundary layer when spline interpolation is used rather than second-order Lagrangian interpolation.

For a more detailed picture of the formal order of accuracy of the overset grid method, consider Fig. 3. The figure depicts the formal order of accuracy  $P$ , of the radial and tangential velocity components, computed along strips at increasing distance from the cylinder boundary (cylinder boundary at  $r_c = 0.5$ ). Based on the assumption that the  $L_2$ -error norm on a grid with grid spacing  $\Delta x$  can be expressed as  $L_2(\Delta x) \sim \Delta x^P$ , the order of accuracy  $P$  can be computed

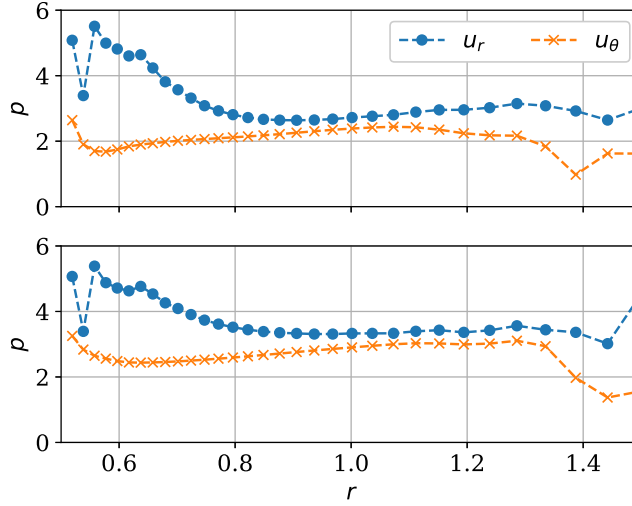


Figure 3: Formal order of accuracy of velocity components computed along strips tangential to the cylinder surface at non-dimensional radial position  $r$ , for upper refinement levels for flow with  $Re = 20$  with Lagrangian interpolation (upper) and spline interpolation (lower).

by:

$$P = \frac{\log(L_2(\Delta x)/L_2(\Delta x/2))}{\log 2}. \quad (6)$$

As expected, the interpolation between grids has a significant effect on the accuracy over the entire cylinder domain. In principle, the spline interpolation scheme is third-order accurate while the Lagrangian interpolation a second-order accurate method. The effect of using the different methods of interpolation can be seen in Fig. 3. We see that the interpolation alone is not enough to lower the accuracy by one order (there is approximately half an order of accuracy difference between the results obtained with the two methods). This may be due to a number of other properties that affect the accuracy, like grid stretching, boundary conditions, filtering, etc. The accuracy from the simulations using Lagrangian interpolation yields  $P \approx 3$  for  $u_r$  and  $P \geq 2$  for  $u_\theta$  on most of the cylinder grid. In the vicinity of the cylinder surface the difference between the Lagrangian and spline interpolation diminishes, particularly for the radial velocity component where both methods yield very high order of accuracy, with  $P \approx 5$ . This is significantly more accurate than the more conservative suggestion of radial velocity accuracy in-between third- and fourth-order, that we saw in Fig. 2 (the results in Fig. 2 correspond to the second point from the left in Fig. 3).

### 3.2. Unsteady flow

The  $L_2$ -error norms are suggestive of the formal accuracy of the numerical method, but do not reveal the in-use accuracy of the method for simulations in the unsteady flow regime. We therefore need to consider the performance

of the overset grid scheme for unsteady flow, before arriving at our goal of a full-blown simulation of a particle-laden flow interacting with a cylinder in this flow regime.

A grid refinement study is performed for  $Re = 100$ , where unsteady vortex shedding has developed in the cylinder wake. A domain with  $L_x \times L_y = 10D \times 20D$  is used, still with the cylinder in the center of the domain. The resulting mean drag coefficient ( $C_D$ ), root-mean-square lift coefficient ( $C'_L$ ) and Strouhal number ( $Str$ ) are computed, where the drag and lift coefficients are computed from the pressure and shear forces on the cylinder,  $\mathbf{F}_p$  and  $\mathbf{F}_s$ , respectively. These are given by:

$$\mathbf{F}_p = - \int p|_{r_c} \mathbf{dA} \approx -\hat{\mathbf{r}} h r_c \Delta\theta \sum_{i=1}^{N_\theta} p(r_c, \theta_i), \quad (7)$$

$$\mathbf{F}_s = \int \boldsymbol{\sigma}|_{r_c} dA \approx \hat{\boldsymbol{\theta}} \nu h r_c \Delta\theta \sum_{i=1}^{N_\theta} \rho(r_c, \theta_i) \left. \frac{\partial u}{\partial r} \right|_{(r_c, \theta_i)}, \quad (8)$$

where  $h$  is the height of the cylinder and  $\boldsymbol{\sigma}$  is the shear stress. With flow in the  $y$ -direction, the drag and lift forces,  $F_D$  and  $F_L$ , are found by taking the sum of the pressure and shear forces in  $y$ - and  $x$ -direction, respectively. These forces can be used to find the drag and lift coefficients by:

$$C_D = \frac{F_D}{\frac{1}{2} \rho_0 U_0^2 A}, \quad (9)$$

$$C_L = \frac{F_L}{\frac{1}{2} \rho_0 U_0^2 A}, \quad (10)$$

where  $\rho_0$  and  $U_0$  are free-stream values of the density and velocity, respectively, and  $A = 2hr_c$  is the projected frontal area of the cylinder. The Strouhal number is simply the shedding frequency, non-dimensionalized by the free-stream velocity and cylinder diameter.

The grid refinement study of the unsteady flow is performed with both Lagrangian and spline interpolation on two differently sized overset grids. One overset grid has a cylindrical grid with diameter  $3D$ , that is, the same size that was used in the assessment of accuracy for the  $Re = 20$ . The other has a size  $5D$ . Hence, there is a factor two difference in the radial length ( $L_r = r_{cg} - r_c$ , where  $r_{cg}$  is the outer cylinder grid radius) of the two cylindrical grids. At each refinement level, the smallest spacing in the radial direction is the same for the two different overset grids, and the properties of the stretching is the same as that in the  $Re = 20$  flow simulations (approximately quadratic cells in the vicinity of the surface and in the interpolation region, and approximately equal grid spacing on the Cartesian and curvilinear grid on the interpolation region). Hence, the outer grid spacing on the larger cylindrical grid will be larger than the outer grid spacing of the smaller cylindrical grid. Thus, a coarser Cartesian grid can be used for the overset grid with the larger cylinder grid. This, in turn, allows for a larger time step on the background grid, but requires more

Table 2: Grid refinement levels used in the grid refinement study for flow past a cylinder at  $Re = 100$  with two different sized cylindrical grids. Grid spacing  $\Delta r$  has been made non-dimensional by the cylinder diameter.

Refinement level	$\Delta r_{min} \times 10^{-2}$	$r_{cg} = 3r_c$		$r_{cg} = 5r_c$	
		$N_r \times N_\theta$	$N_x \times N_y$	$N_r \times N_\theta$	$N_x \times N_y$
0	4.1	$16 \times 80$	$80 \times 160$	$24 \times 80$	$50 \times 100$
1	2.7	$24 \times 120$	$120 \times 240$	$36 \times 120$	$76 \times 152$
2	2.0	$32 \times 160$	$160 \times 320$	$48 \times 160$	$100 \times 200$
3	1.6	$40 \times 200$	$200 \times 400$	$60 \times 200$	$128 \times 256$
4	1.3	$48 \times 240$	$240 \times 480$	$72 \times 240$	$150 \times 300$
5	0.97	$64 \times 320$	$320 \times 640$	$96 \times 320$	$200 \times 400$
6	0.77	$80 \times 400$	$400 \times 800$	$120 \times 400$	$256 \times 512$
7	0.64	$96 \times 480$	$480 \times 960$	$144 \times 480$	$306 \times 612$
8	0.48	$128 \times 640$	$640 \times 1280$	$192 \times 640$	$408 \times 816$

Table 3: Mean drag coefficient ( $C_D$ ), rms-lift coefficient ( $C'_L$ ) and Strouhal number ( $Str$ ) for  $Re = 100$  computed at a domain  $L_x \times L_y = 10D \times 20D$  with two different overset grids. The resolution is given by the finest refinement levels in Tab. 2, and both Lagrangian (LI) and spline interpolation (SI) cases are considered.

Coefficient	$r_{cg} = 3r_c$		$r_{cg} = 5r_c$	
	LI	SI	LI	SI
$C_D$	1.461	1.459	1.473	1.473
$C'_L$	0.2535	0.2492	0.2637	0.2633
$Str$	0.1721	0.1720	0.1724	0.1724

sub-cycles on the cylindrical grid for each Cartesian time step. Details on the grids used in this refinement study are listed in Tab. 2.

Results for the grid refinement at  $Re = 100$  can be seen in Fig. 4 and Tab. 3. In Fig. 4, the dimensionless drag and lift coefficients, and the Strouhal number have been normalized by the result computed at the finest grid. Hence, the plots depict the relative deviation from the result at grid refinement level eight from Tab. 2. The values of the coefficients computed at this refinement level, for each of the four cases, are given in Tab. 3.

We see that the dimensionless numbers converge quite rapidly for all but one of the cases tested. The exception is the rms lift coefficient computed at the smaller of the two cylindrical grids with spline interpolation, where the values at refinement levels five to seven deviate approximately one percent from the finest grid result. For the three remaining cases, the deviation from results at refinement levels four to seven from the finest grid result is less than 0.14% for all coefficients (if only drag and Strouhal number are considered, the deviation is less than 0.06% for these cases). Hence, a definite grid independent solution is achieved for three of the four cases considered.

The fact that one of the cases with a cylinder grid with radius  $r_{cg} = 3r_c$  gives

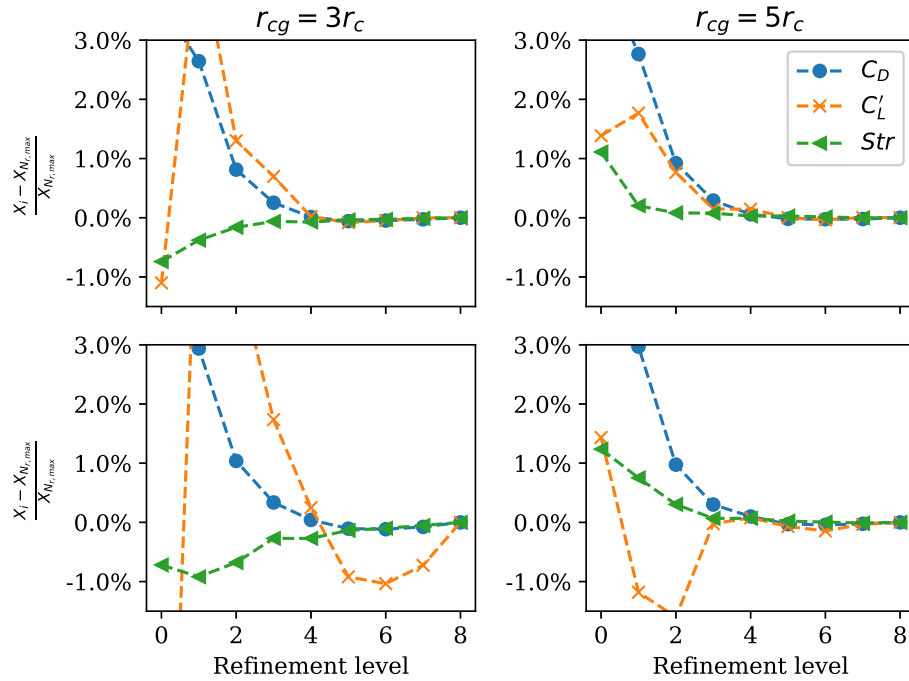


Figure 4: Normalized values for mean drag coefficient ( $C_D$ ), rms-lift coefficient ( $C'_L$ ) and Strouhal number ( $Str$ ) for  $Re = 100$  computed at different refinement levels (see Tab. 2) for overset grids with two sizes of the radii of the body-fitted cylindrical grid,  $r_{cg}$ . Results are given for computations with Lagrangian interpolation (upper) and spline interpolation (lower).

a sub-par solution for the unsteady flow is quite surprising. Especially as the case is the one using the high-order interpolation (quadratic spline interpolation), which had the best performance for the steady flow simulations. This is perhaps caused by a larger mass loss in the inter-grid communication for transient flow, when spline interpolation is used rather than Lagrangian interpolation. We will not speculate further on this, but note that the Lagrangian interpolation outperformed the spline interpolation on the smaller cylindrical grid.

By considering the grid independent solutions in Tab. 3, used to normalize the grid refinement results, two particular factors catch our attention. Firstly, by comparing the results with the two different interpolation schemes at the domain where the cylindrical grid has  $r_{cg} = 5r_c$ , we see that the computed drag, lift and Strouhal number appear to be independent of choice of inter-grid communication for these cases. This in contrast to the  $r_{cg} = 3r_c$  results, but in accordance with our intuitive understanding of the problem: the farther away from the cylinder boundary the interpolation is moved, the less it affects computation of quantities at the boundary. Note, however, that even though the drag and lift forces are computed at the boundary, the boundary layer variables that these coefficients are dependent on are dependent on the flow

upstream and downstream of the cylinder. The results therefore suggest that the flow surrounding the cylinder, not just the solution in its immediate vicinity, is affected little from the choice between the two interpolation methods when the larger  $r_{cg}$  is used for the cylinder grid.

Secondly, by comparing the results for  $C_D$  and  $C'_L$  on the different sized cylinder grids, computed with Lagrangian interpolation, we see that the values are somewhat higher for the larger cylinder grid. Although the results are grid independent, neither of the values are quantitatively accurate values for the drag or lift of a cylinder in a cross flow at  $Re = 100$ . The values are too large, which is due to the small domain sizes. The higher values computed for the case with the larger  $r_{cg}$  suggest that the blockage effect is largest for this case. Since the width of the domain is only  $10D$ , a cylinder grid with diameter  $5D$  covers up to half of the spanwise width. It is not unlikely that interpolation errors on the Cartesian grid, on one side of the cylinder grid can affect the flow on the other side of the cylinder grid, due to the periodic boundary. Further, a larger cylinder grid brings the interpolation region closer to the inlet and outlet, and a larger effect from the limited streamwise length may have a significant effect on the flow. The increased blockage effects may appear contradictory to the interpolation independent solution noted above, as it is farther from the interpolation region to the solid boundary, than from this region to the inlet, outlet or periodic boundary. But keep in mind that when moving from the interpolation region to the cylinder the solution is filtered, which has a smoothing effect on spurious errors that arise from interpolation, grid stretching, etc., while no filtering is used on the Cartesian grid.

To control that the grid independent solutions yield accurate flow predictions we also perform a simulation on a large domain,  $L_x \times L_y = 50D \times 50D$ , for each of the four flow cases, and compare the results with data from previous studies. The grid spacing corresponding to grid refinement level five in Tab. 2 is used on the large square domain. The computed flow quantities show good agreement with previous studies performed on similar domain sizes (see Tab. 4). Again we note that the results from the simulations with the larger cylinder grid is somewhat larger than the results with  $r_{cg} = 3r_c$ . The increased blockage effect on the larger cylindrical grid means that larger domains should be used when a larger cylinder grid radius is used. This will decrease the difference in the number of grid points required to resolve the flow for the two different grid sizes. Further, as more sub-cycles of the cylindrical grid are necessary for each time step for the  $5r_c$  case, and each sub-cycle is more expensive due to more cylindrical grid points than for the  $3r_c$  case, we stick to the smaller of the two cylindrical grids in the simulations with particle deposition.

#### 4. Particle deposition on a circular cylinder in a laminar cross flow

Direct numerical simulations with a large number of particles suspended in the flow have been performed. This has been done to assess the performance of the overset grids on a more complex and demanding simulation than the simple flow past a cylinder at low Reynolds numbers.

Table 4: Comparison with previous studies. The studies are performed on domains with streamwise length  $60 \leq L_x/D \leq 100$  and spanwise length  $40 \leq L_y/D \leq 100$ , and the present study has  $L_x = L_y = 50D$ . Results from the present study are listed for both Lagrangian interpolation (LI) and spline interpolation (SI) for two different sized overset grids. The asterisk on some values of  $C'_L$  denote a value where only the amplitude of the lift was given. The asterisk mark a lift amplitude scaled by  $1/\sqrt{2}$  to get the root-mean-square lift coefficient, a valid scaling for the sinusoidal-like lift coefficient (with mean value zero).

	$C_D$	$C'_L$	$St$
Li et al. [29]	1.336	–	0.164
Posdziech & Grundmann [30]	1.3504	0.234 <sup>(*)</sup>	0.1667
Pan [31]	1.32	0.23 <sup>(*)</sup>	0.16
Qu et. al. [32]	1.326	0.2191	0.1660
Present, $r_{cg} = 3r_c$ (LI)	1.3368	0.2352	0.1609
Present, $r_{cg} = 3r_c$ (SI)	1.3342	0.2292	0.1605
Present, $r_{cg} = 5r_c$ (LI)	1.3409	0.2428	0.1605
Present, $r_{cg} = 5r_c$ (SI)	1.3407	0.2423	0.1604

The particle deposition simulations are based on the study by Haugen & Kragset [19] where particle-laden flow simulations were performed on a range of Reynolds numbers on a moderate sized flow domain ( $6D \times 12D$ ). The analysis will not be repeated here, as a brief introduction to the method used for particle representation and deposition is sufficient for our present purpose. The particle-laden flow simulations have been performed on a domain of the same size as in Haugen & Kragset[19], for unsteady laminar flow with Reynolds number 100.

#### 4.1. Particle equations

The particles are point particles tracked using a Lagrangian formalism, where the particle velocity and position are described by:

$$\frac{d\mathbf{v}_p}{dt} = \frac{\mathbf{F}_{D,p}}{m_p}, \quad (11)$$

$$\frac{d\mathbf{x}_p}{dt} = \mathbf{v}_p, \quad (12)$$

where  $\mathbf{v}_p$ ,  $\mathbf{x}_p$  and  $m_p$  are the velocity, center of mass position and mass of the particle, respectively. The force  $\mathbf{F}_{D,p}$  acting upon a spherical particle is the drag force:

$$\mathbf{F}_{D,p} = \frac{1}{2C_c} \rho C_{D,p} A_p |\mathbf{u} - \mathbf{v}_p| (\mathbf{u} - \mathbf{v}_p), \quad (13)$$

where  $A_p = \pi d_p^2/4$  is the cross sectional area of the particle and

$$C_c = 1 + \frac{2\lambda}{d_p} \left( 1.257 + 0.4e^{(-1.1d_p/2\lambda)} \right), \quad (14)$$

is the Stokes-Cunningham factor (with parameters set for air) for a particle with diameter  $d_p$ . The mean free path  $\lambda = 67$  nm accounts for the fact that for



very small particles, the surrounding medium can no longer be regarded as a continuum but rather distinct particles. Further, the particle drag coefficient is given by:

$$C_{D,p} = \frac{24}{Re_p} (1 + 0.15Re_p^{0.687}) , \quad (15)$$

for particle Reynolds number  $Re_p = d_p |\mathbf{v}_p - \mathbf{u}| / \nu \lesssim 1000$ . With this, the particle drag force can be re-written as

$$\mathbf{F}_{D,p} = \frac{m_p}{\tau_p} (\mathbf{u} - \mathbf{v}_p) , \quad (16)$$

where

$$\tau_p = \frac{Sd_p^2 C_c}{18\nu(1 + f_c)} \quad (17)$$

is the particle response time, with  $f_c = 0.15Re_p^{0.687}$  and  $S = \rho_p/\rho$ . Note that this equals Stokes drag in the limit  $C_c = 1$  and  $f_c = 0$ . Using the convention of [19], the Stokes number ( $St = \tau_p/\tau_f$ ) is defined with a fluid time scale

$$\tau_f = \frac{D}{2U_0} . \quad (18)$$

The fluid velocity is interpolated from surrounding grid points by bi-linear interpolation on the Cartesian grid and bi-quadratic interpolation on the curvilinear grid. The order of the interpolation is higher on the curvilinear grid as the velocity components (the radial, in particular) are expected to be close to quadratic near the cylinder surface. For three-dimensional simulations, linear interpolation is used for the velocity component along the z-direction (the cylinder's spanwise direction) on all grids.

For particles very close to the cylinder surface, special handling is used to interpolate the radial component of the fluid velocity. By very close to the cylinder we mean in-between a surface grid point and a grid point neighboring the surface, or, alternatively, within the pre-calculated momentum thickness of the boundary layer. The special handling in use for particles at such positions is a quadratic interpolation that guarantees no overshoots in the interpolation. Since all velocities are zero at the surface, this can be achieved by:

$$u_{r,p} = u_{i,g} (\delta r_p / \delta r_g)^2 , \quad (19)$$

where  $u_{r,p}$  and  $u_{r,g}$  are radial velocity components at the position of the particle and at the position of the interception between a surface normal and the first grid line further from the surface than the particle, respectively. The distances  $\delta_p$  and  $\delta_g$  are distances from the surface to the particle and to said grid line, respectively.

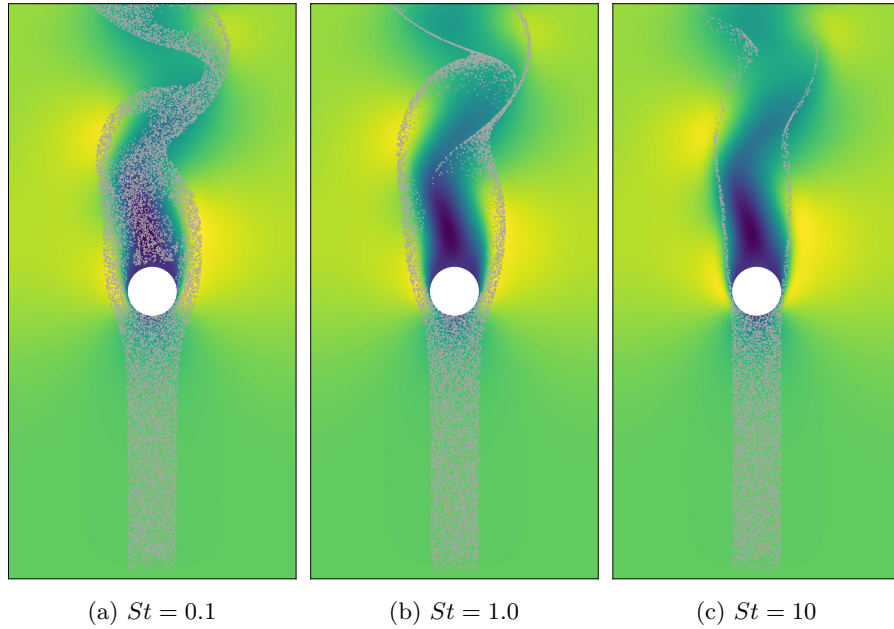


Figure 5: Particle-laden flow interacting with a circular cylinder at  $Re = 100$ . An unhindered particle will cross the flow domain, from the inlet (bottom) to the outlet (top) in approximately two shedding periods at this Reynolds number. Contours of the streamwise velocity component make up the background.

#### 4.2. Particle impaction

After the flow has developed to unsteady periodic vortex shedding, particles are inserted continuously at the inlet. The particles are inserted randomly, as a homogeneous distribution over a rectangle covering the possible particle trajectories that can impact the cylinder. From here they are convected downstream, and removed from the flow either by impacting the cylinder or by reaching the outlet (see Fig. 5). An impaction is registered (and the particle removed) if the distance between the cylinder surface and the particle's center of mass is less than or equal to  $d_p/2$ . Every particle impaction simulation is run until all particles have been removed from the flow. In total  $3.1 \times 10^6$  particles are inserted, distributed over particles with Stokes numbers in the range 0.01–10, with a progressive particle distribution with respect to particle radius (approximately  $2 \times 10^2$  more particles with  $St = 0.01$  than  $St = 10$  inserted).

The resulting impaction efficiency ( $\eta = N_{imp}/N_{ins}$ ) can be split into front ( $\eta_f$ ) and back side impaction ( $\eta_b$ ). At the low Reynolds number flow in this study, backside impaction hardly occurs and we focus on the front side impaction. Figure 6 depicts the particle front side impaction from the present simulations, compared to results from literature. The present results are computed on the grid with grid spacing defined as refinement level four in Tab. 2, for the  $r_{cg} = 3r_c$  case with Lagrangian interpolation. With the  $L_x \times L_y = 6D \times 12D$

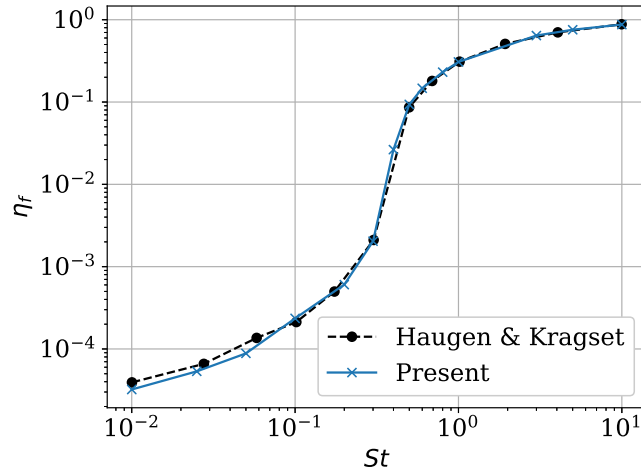


Figure 6: Front side impactation efficiency ( $\eta_f$ ) as a function of Stokes number ( $St$ ) for Reynolds number 100. Present results compared to a previous study by Haugen & Kragset [19]

domain used here, this means we are using a grid  $(N_r \times N_\theta) + (N_x \times N_y) = (48 \times 240) + (144 \times 288)$ . The results from Haugen & Kragset [19] were computed on an equidistant grid with  $512 \times 1024$  grid points, using an immersed boundary method to resolve the cylinder surface.

The particle impactation results from our study agree very well with the results from literature, although the results from the present study are computed on the grid with only 10.1% as many grid points as used by Haugen & Kragset [19]. An additional efficiency improvement was achieved due to the possibility to use a time step of a factor 3.5 larger, due the time steps proportionality to the grid spacing, although some extra work is needed at each time step (computation on two grids, communication of data, filtering on cylinder grid, etc.). Note that for very small particles, the time step can also be restricted by the particle time scale. That is, the time step must be small enough to resolve the time-dependent particle equations. Particles are updated only at the Cartesian time step.

#### 4.3. Investigating the accuracy of the computed impactation efficiencies

The coarseness of the grid used in the computation of particle impactation efficiencies in the previous section allow us to assess, at moderate computational expense, some of the assumptions that must be made in order to regard these impactation results as quantitatively accurate results. These assumptions are, firstly, that blockage effects from the limited domain (with  $L_x \times L_y = 6D \times 12D$ ) have a negligible impact on the particle impactation. Secondly, using the coarsest resolution where grid independency of drag and lift coefficients was reached, means assuming that the transport of the particles is dependent on an accurate flow field only.

A critical assessment of these assumptions leads us to expect a somewhat higher impactation result for particles on a domain where the blockage effect

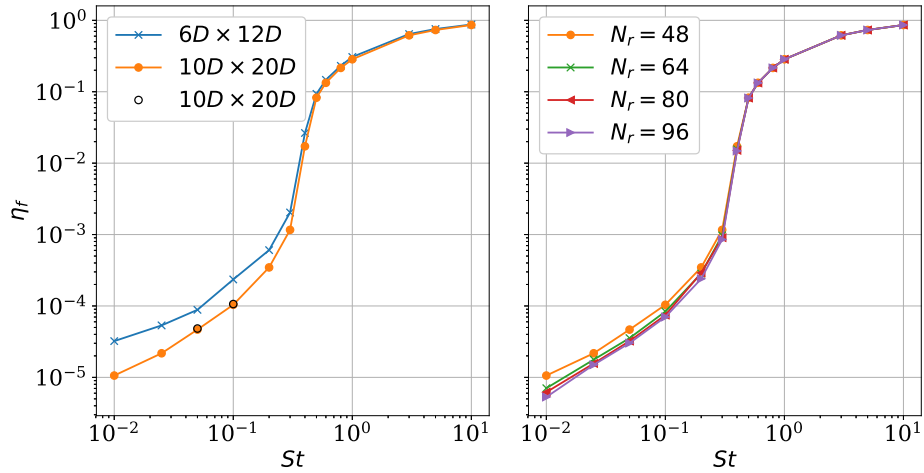


Figure 7: Front side impact efficiency ( $\eta_f$ ) as a function of Stokes number ( $St$ ) for Reynolds number 100 for different domain sizes (left) and grid resolutions (right).

is large, due to a squeezing of the flow field and, consequently, less particles being directed away from the cylinder. In particular, this is expected to affect particle that follow the flow to a large extent, that is, particles with small Stokes numbers. Further, the flow velocities at particle positions are not only dependent on an accurately computed flow field, but also accurate interpolation. The latter aspect can be very sensitive to grid spacing, even if the flow is resolved accurately. Haugen & Kragset [19] used linear interpolation to compute flow velocity at particle positions, except withing the grid point closest to the surface, where an expression similar to that of Eq. 19 was used. Linear interpolation of velocities that are proportional to  $-(\delta r)^2$  (as the upstream flow field at the centerline through the cylinder is) will lead to a systematic over-estimation of these velocities. Hence, an over-prediction in particle impaction can be expected from their results. What is important in this respect, is how large this possible over-prediction is, and for what particle sizes it occurs.

To investigate accuracy of the computed impaction efficiencies we perform particle-laden flow simulations at a larger domain size,  $L_x \times L_y = 10D \times 20D$ , that is, the size used in the grid independence study of Section 3.2. At this larger domain several refined grids are used. These are grids denoted refinement levels 4–7 in Tab. 2, with  $r_{cg} = 3r_c$ . Thus, from 48 (coarsest) to 96 (finest) grid points are used in the radial direction on the cylindrical grid, and the background grid is refined accordingly. The number of inserted particles is  $1.1 \times 10^7$ , whereof  $7 \times 10^6$  are particles with  $St \leq 0.1$ . The results are seen in Fig. 7.

Very few of the smallest particles deposit on the cylinder. To get enough particle impaction at the smallest Stokes numbers to give reliable statistics, we only insert particles with  $St \leq 0.1$  over a region covering one tenth of the cylinder’s projected area, around the centerline of the cylinder, and divide the resulting impaction efficiency by ten. No small Stokes number particles inserted

outside the insertion area are expected to hit the cylinder. To control this, a simulation with  $St = 0.05$  and  $0.1$  inserted over the whole projected cylinder area has been performed, and the results are included as black circles (o) in Fig. 7. There is close to an exact overlap between the impaction efficiencies from the particles inserted in the two different ways.

From Fig. 7 it is clear that the blockage effect from the limited domain size has a significant effect on the particle impaction efficiencies. For  $St \leq 0.5$  this effect is larger than 10%, and it increases as the Stokes number is decreased. The largest difference in impaction efficiencies is seen at  $St = 0.01$ , where 200% more impaction occurs for the smallest domain size. The resolution plays a smaller, but not insignificant, role in the impaction efficiencies. Increasing from the coarsest grid, with  $N_r = 48$ , to  $N_r = 64$ , noticeably reduces the impaction efficiencies. The reduction is more than 10% for  $St \leq 0.3$ . A further refinement of the grid has some effect, but this effect is negligible for  $N_r \geq 80$ . Comparing the results from the larger domain with  $N_r = 80$  to impaction results by Haugen & Kragset [19] suggests that Haugen & Kragset have found a qualitatively correct result, but have somewhat quantitatively over-predicted the particle impaction, in particular in the boundary interception region  $St \lesssim 0.3$ . For the smallest Stokes number ( $St = 0.01$ ) the over-prediction is of approximately a factor 6.3, but at  $St = 0.1$  this factor has decreased to 1.7.

## 5. Concluding remarks

In this work, we have presented a high-order overset grid method, implemented in the open-source code known as the Pencil code. The method uses high-order finite-difference discretization to solve the compressible Navier-Stokes equations on several grids, and communicates necessary flow data between the grids by linear or quadratic interpolation. Unique for the overset grid implementation described here, is the use of local time step restriction and summation-by-parts finite-difference operators. The relaxed time stepping restriction on the coarser grid is very cost efficient for a weakly compressible flow, while the summation-by-parts operators enhance numerical stability together with the use of Padé filtering. The purpose of developing the method is to compute particle impaction on a cylinder in a cross flow, and for this purpose a body-fitted cylindrical grid is an appropriate choice to resolve the boundary layer around the cylinder with high accuracy.

An investigation of the formal order of accuracy of the overset grid implementation revealed that high-order accuracy is indeed reached. Regardless of the choice of bi-linear or bi-quadratic interpolation, the radial velocity component was above third-order (and approximately fifth order at the grid point closest to the surface) and the tangential velocity components was in-between second and third-order in most of the domain covered by the body-fitted cylindrical grid. For unsteady flow the method converges quite rapidly to grid independent solutions for the essential flow variables (drag, lift and Strouhal number) for most of the cases considered. An exception is the smaller cylindrical grid where inaccuracy from spline interpolation was seen in the lift coefficient of the flow.

Using a larger cylindrical grid, with radius five times as large as the cylinder radius, decreased the effect of the interpolation, but increased blockage effect of the restricted size of the flow domain.

When applied to the problem of inertial particles impacting on a cylinder, impaction efficiencies of previously published results were reproduced at a significantly reduced cost. The computational cost was reduced due the coarser background grid required to resolve the flow, which yielded both a much smaller number of grid point (90% reduction in 2D) and the possibility to use a larger time step in a most of the solution domain.

A critical assessment of the particle impaction results revealed that the limited domain size had a significant impact on particle impaction, particularly for the smaller Stokes numbers. Further, although the flow was deemed grid independent, using a finer grid, and thus a more accurate interpolation of flow velocity to particle positions, reduced the number of particles that hit the cylinder. The resulting impaction curves suggest that particle impaction has been over-estimated in previous studies, in particular for very light particles where impaction occurs by boundary interception.

The overset grid method implementation in the Pencil Code is ready for three-dimensional simulations, and extending DNS studies of particle impactions on a cylinder to Reynolds number for real-world application (factor 10-20 larger than the investigation here, for industrial boilers) is within reach. However, even with the highly accurate and efficient method presented here, increasing the Reynolds number and computing three-dimensional flow will be computationally costly. How large Reynolds numbers that can be considered will depend largely on the Stokes numbers of the particles in the study, and on what is deemed acceptable accuracy when particle impaction efficiencies are computed. If the focus is not just qualitative trends, but quantitatively accurate results, we recommend a careful assessment of grid independence (not just of flow variables, but of the particle impaction itself), and care in selection of domain size and set-up.

## 6. Acknowledgements

We would like to acknowledge valuable discussions on numerical methods and code development with our colleagues Prof. Bernhard Müller and Dr. Ehsan Khalili.

The work was supported by the Research Council of Norway (Norges Forskningsråd) under the FRINATEK Grant [grant number 231444]. Partial funding was provide by the GrateCFD project, which is funded by: LOGE AB, Statkraft Varme AS, EGE Oslo, Vattenfall AB, Hitachi Zosen Inova AG and Returkraft AS together with the Research Council of Norway through the ENERGIX program [grant number 267957/E20]. Computational resources were provided by UNINETT Sigma2 AS [project numbers NN9405K and NN2649K].

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