

DATA-DRIVEN SPATIAL DECOMPOSITION ALGORITHM FOR PARTICLE AGGLOMERATION

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TITLE

Data-driven spatial decomposition algorithm for particle agglomeration in hybrid Euler-Lagrange approaches

RESUME

Nous rapportons ici une nouvelle amélioration d'un algorithme de décomposition spatiale d'un domaine physique en fonction de la répartition spatiale des particules. Cet algorithme est utilisé dans les simulations CFD pour le calcul de l'agglomération des particules fondée sur des approches hybrides Euler-Lagrange. Il permet d'éviter les erreurs induites par une répartition non-homogène des particules dans l'espace en calculant une décomposition spatiale optimale (utilisant uniquement les informations sur les positions des particules). L'efficacité et la précision de l'algorithme sont testées dans des configurations simples ainsi que sur un cas représentatif de la dispersion de particules dans une couche limite atmosphérique.

ABSTRACT

We report here new improvement of a recent algorithm for spatial decomposition of a physical domain according to the spatial repartition of particles. This algorithm is used in CFD simulations for the computation of particle agglomeration using hybrid Euler-Lagrange approaches. It allows to avoid errors induced by non-homogeneous particle repartition in space by computing an optimal spatial decomposition using information solely on particle locations. The efficiency and accuracy of the improved algorithm is tested in simple configurations as well as on a case representative of particle dispersion in an atmospheric boundary layer.

MOTS-CLÉS : suspension de particules, agglomération, modélisation, décomposition de domaine /

KEYWORDS: particle suspension, agglomeration, modeling, domain decomposition

1. INTRODUCTION

1.1. General context

CFD simulations of dispersed two-phase flows in practical industrial/environmental cases often involve non-homogeneous concentrations of particles (Schmidt & Rutland, 2004). In hybrid Euler-Lagrange simulations, this can induce the propagation of numerical error when the number of collision/agglomeration events is computed using mean-field approaches (Pischke et al., 2015). In fact, mean-field statistical collision models allow to sample the number of collision events using a priori information on the frequency of collisions (the collision kernel). Yet, since such methods often rely on the mesh used for the Eulerian simulation of the fluid phase, the particle number concentration within a given cell might not be homogeneous, leading to numerical errors.

1.2. Objective

The objective of this study is to minimize the error induced by the spatial decomposition used. For that purpose, we rely on a recently developed spatial decomposition algorithm, called D2SD (Martinez et al., 2021). Its efficiency has been improved to be compatible with standard CFD software and to remain tractable in practical atmospheric cases.

2. METHOD & RESULTS

2.1. Methodology

In this article, we apply the data-driven spatial decomposition (D2SD) algorithm to control such error in simulations of particle agglomeration \cite{bib:ref_3}. Significant improvements are made to design a fast D2SD version, minimizing the additional computational cost by developing re-meshing criteria.

2.2. Results

Through the application to some practical simulation cases, we show the importance of splitting the domain when computing agglomeration events in Euler/Lagrange simulations (Martinez et al., 2022), so that within each elementary cell there is a spatially uniform distribution of particles.

As displayed in Figure 1, the technique can be used to provide an optimal spatial decomposition in the case of particle dispersion over an obstacle (here 100 μm solid particles). This case is representative of typical situations in atmospheric boundary layers (with aerosol dispersion near buildings).

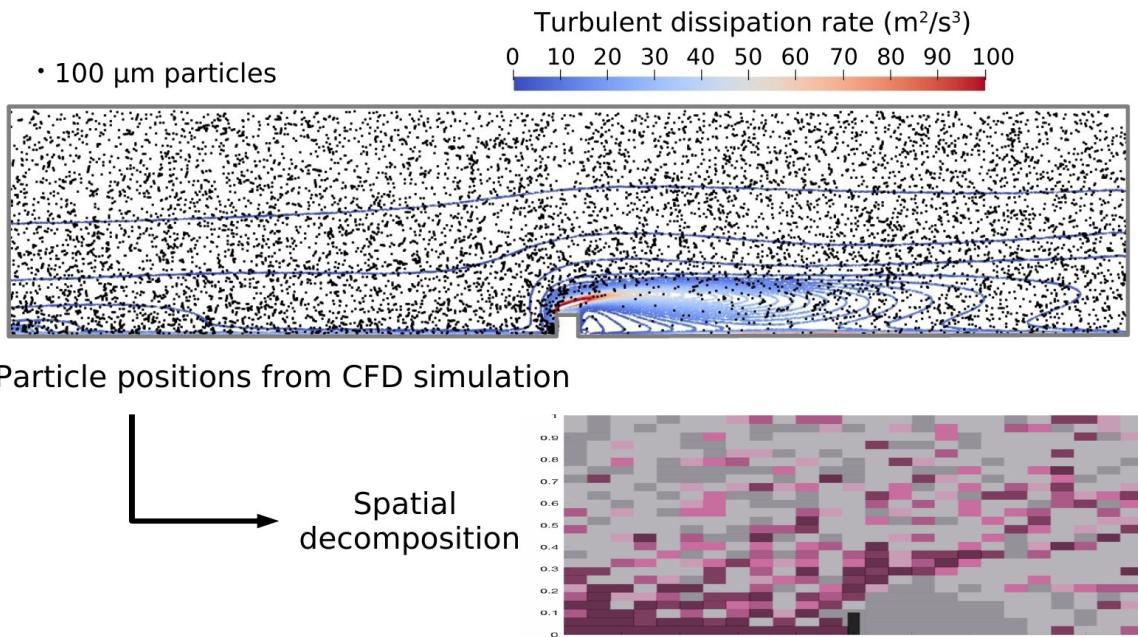


Figure 1. Spatial decomposition (bottom) obtained from the set of particle positions (top), together with the isocontours of the turbulent dissipation rate.

As shown in Table 1, the number of agglomeration events computed with this spatial decomposition is twice smaller than the one that would be obtained using the CFD mesh (used for the computation of the carrier fluid flow). Surprisingly, it can be noted that the results are similar to the ones obtained considering a single cell for the whole domain. However, even when such crude estimations are correct (which might not be the case using other spatial repartitions of particles), they do not provide information on where the aggregates are formed (while the D2SD algorithm does provide this information).

Computational method	D2SD method	PBE on a single-cell	PBE on the CFD mesh
Average number of agglomeration events	29,9	28,5	58,3
CPU / CPU _{CFD}	11,11	0,0029	1

Table 1. Comparison of the average number of agglomeration events computed with the D2SD algorithm, the PBE on a single-cell and the PBE on the CFD mesh (together with the CPU time rescaled by the one obtained for the CFD mesh).

3. CONCLUSION

This shows the importance of using proper spatial decomposition techniques to avoid introducing numerical errors when relying on hybrid Euler-Lagrange approaches for the computation of particle agglomeration in practical cases. Yet, it also highlights the limitations of resorting to such methodologies, especially regarding the numerical costs required to obtain accurate predictions (possible routes for improvements will be discussed).

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