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A COUPLED FLUID-GRANULAR APPROACH TO MODELLING POWDER STREAM IN DIRECTED ENERGY DEPOSITION

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ABSTRACT

Metal-based Directed Energy Deposition as one of the technological variations of additive manufacturing has been recognized as a highly promising technology for the space industry, mostly due to its inherent capacity to perform in microgravity conditions, with no imposed limitations on the size of manufactured objects, and relatively short manufacturing times. The technology however faces a host of problems mostly related to relatively low dimensional accuracy and recurring defects which appear to originate in poor control and understanding of the material deposition. ESA acknowledges the need for consistent, cost-effective, and adaptable software strategies and introducing Virtual Testing for the Process-Structure-Property (PSP) modeling as a complementary alternative to more traditional experimental approaches. A novel numerical approach is thus proposed for simulating the powder stream dynamics by fully coupling a Discrete Element solver to model the powder phase and computational fluid dynamics to model the gas phase.

INTRODUCTION

Metal-based Additive Manufacturing (AM), particularly Directed Energy Deposition (DED), is a potentially disruptive technology for the space market in demand of high-performance and low-weight structures for spacecraft [1], [2]. However, before the advantages of this technology can be fully harvested, the technology itself, as well as our understanding of it must fully mature. Unlocking the full potential of AM and DED would not only boost the European space program but also increase the competitiveness of the European manufacturing industry with respect to global competition.

The inherent stochastic nature of the powder stream has long been associated with poor manufacturing accuracy and recurring defects in DED [3]–[5]. A host of various models have been developed over the course of the last two decades to improve our understanding and predictive capabilities of material deposition in DED.

Conventional approaches to modeling the powder stream in DED are predominantly analytical and aimed at predicting the spatial distribution of powder particles and their interaction with the laser beam. In most cases, it is assumed that particles travel from the nozzle outlet along undisturbed linear trajectories and that particle density distribution along any cross-section of the powder stream is Gaussian [5]–[7]. Modern approaches can account for variable particle velocity [8] but continue to rely on estimated experimental values for variables such as stream divergence [9]. Nevertheless these models are widely used by manufacturers due to their relative simplicity and computational efficiency [10].

Numerical approaches largely apply computational fluid dynamics (CFD) to resolve a two-phase flow problem involving a dispersed second phase with the additional transport equation for the powder phase [11]–[14]. In these approaches one-way coupling is applied, implying that the carrier gas influence on the powder particles is taken into account, while the reactive force of the powder particles on the surrounding gas as well as inter-particle interactions are neglected. Many of the assumptions usually adopted in the numerical approaches are not needed when applying the numerical schemes and it has been shown that some of them, such as linear powder particle trajectories and constant particle speed, may not be warranted [9]. While inter-particle collisions are regularly neglected in the numerical models of powder stream [4], [11]–[13], [15], [16] on account of the powder occupying a relatively small volume fraction in the carrier gas flow [13], recent studies indicate a strong influence of powder particle collisions on the powder stream dynamics [17], [18]. It has been proposed to expand the conventional CFD approach by detecting powder particle collisions and resolving them using the Hertz theory [17] to overcome this deficiency.

The proposed CFD-based approaches to modeling the powder stream in DED face an additional challenge of correctly identifying the boundary conditions for the powder phase at the nozzle outlet. While some approaches simply assume a uniform velocity field for the powder and gas phase at the nozzle outlet [11], other authors chose to model a limited section of the inner walls of the nozzle and the powder particle interactions with the nozzle walls [4], [12], [13], [15], [16]. The powder velocity distribution at the nozzle outlet thus necessarily depends on the chosen powder boundary condition further upstream (usually uniform velocity), powder particle/wall collision restitution coefficient and particle shape (usually assumed spherical), some of which vary considerably in the cited studies. Some of these studies concluded that the powder particle speed at the nozzle outlet depends on the particle size as the larger particles lose momentum during consecutive collisions with the inner nozzle walls, while smaller particles with sufficiently low Stokes numbers follow the carrier gas streamlines and maintain speed [4], [13], [15]. It should however be underlined that these claims stem strictly from the performed numerical simulations and have not been experimentally validated.

We therefore propose a comprehensive approach to overcome the shortcomings and open challenges of the current state of the art regarding the simulative models of DED powder stream. A full coupling of Discrete Element Method (DEM) to handle the powder phase and Computational Fluid Dynamics (CFD) to handle the gas phase is proposed for improved accuracy of the blown powder dynamics. The full coupling implies that the proposed approach accounts for the drag force that the fluid exerts on the powder particles, the reactive force that the powder particles exert on the fluid as well as the inter-particle interaction during powder grain collisions. The boundary conditions for the powder phase at the nozzle outlet are experimentally evaluated to determine the powder particle velocity distribution as a function of powder grain size.

THE POWDER PHASE

Open-source discrete element solver YADE [19] is used to model the powder phase of the stream. Employing DEM allows us to harvest state-of-the-art computational efficiency in granular dynamics and inter-particle interaction, while the open-source platform grants us the necessary freedom to perform the coupling with the CFD solver. Due to high particle sphericity requirements for the DED powders, the powder particles are modelled as completely spherical, while the choice of DEM allows us to later modify the model to account for particle non-sphericity. The powder particles are generated at homogeneously distributed random locations along the nozzle outlet (see Figure 1) with a frequency determined by the mass deposition rate of the powder. The generated powder particles feature randomly chosen radii according to the measured particle size distribution for the simulated powder and randomly chosen initial velocities according to the experimentally determined boundary condition velocity distribution (see section Powder Boundary Conditions). Gravitational force is applied to the powder particles according to the orientation of the simulated DED head and zero Cundall's non-viscous damping is applied. Perfectly elastic inter-granular collisions are considered, accounting for normal and shear contact forces [19]. Since DEM is an explicit numerical method, a critical timestep exists above which the simulation becomes unstable. The timestep for the DEM side of the simulation is thus defined as a fraction of the critical timestep, ensuring that the elastic waves do not propagate further than the minimum distance between the integration points.

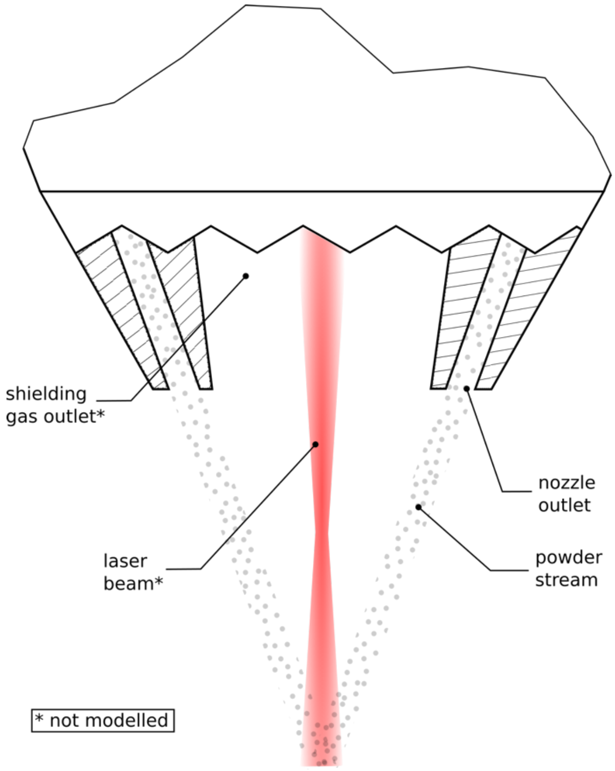

Figure 1: A schematic representation of the modelled Fraunhofer COAX12 V5 discrete coaxial nozzle.

Powder Boundary Conditions

The boundary conditions for the powder are experimentally evaluated at the chosen DED head by implementing an original approach. The state-of-the-art approach of using a combination of a high-speed camera and illuminated light plane to record a series of particle trace images [13], [15], [16] during DED operation is expanded by adding a second high-speed camera as shown in Figure 2. The two cameras are perpendicularly directed and triggered in unison to produce pairs of images that enable the recovery of 3D trajectories of passing particles in post-processing. The trajectories of passing particles on each image are deduced from the illuminated traces on the image that formed during the

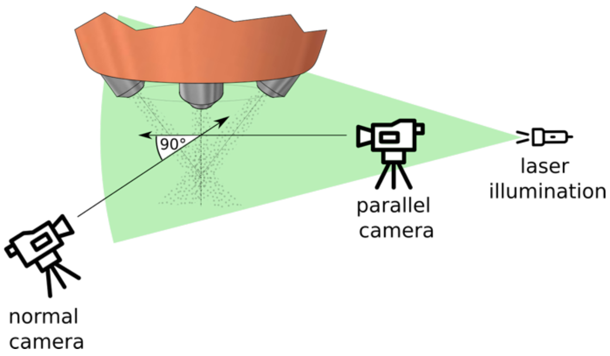

Figure 2: Experimental setup for measuring the powder boundary conditions at the DED nozzle outlet.

exposure time of the camera. Individual traces from two perpendicular images are paired by matching the traces that share a common vertical coordinate of the two extremities of the trace (Figure 3). While most established approaches of this type [13], [15], [16] deduce particle speed from the particle trace length on the recorded image, an error can be introduced due to particles moving in/out of the illuminated plane, and thus the camera only recording a fraction of the actual distance that the particle covered during exposure time. This uncertainty is avoided by introducing frequency modulation to the light source and deducing the particle speed from the wavelength of the dashed particle traces that form due to light source modulation. In order to analyze the potential effect of the powder particle size on its initial speed at the nozzle outlet, the powder is divided into individual size fractions by sieving prior to performing the experiment. Results of this experimental analysis are thus obtained in the form of trajectory angle and speed distributions at the DED nozzle outlet for individual size fractions of powder particles.

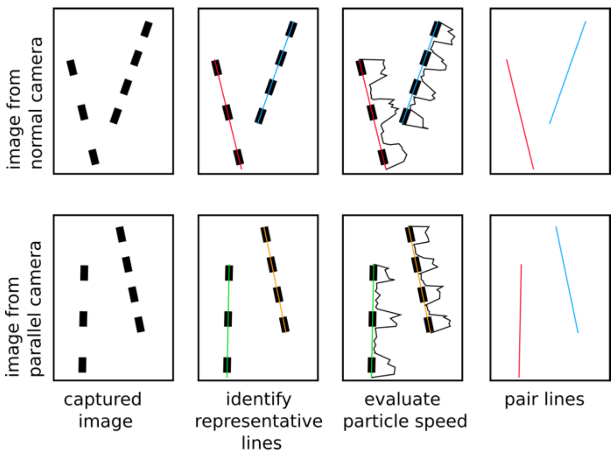

Figure 3: Post-processing of the experimental data to obtain 3D powder particle trajectories.

THE GAS PHASE

Open-source CFD solver openFoam is used to model the gas phase of the powder stream. The Reynolds number for the flow of argon through the channels of the considered DED nozzle at highest recommended carrier gas volumetric flux is $Re \approx 2260 < 2300$ [20], suggesting a laminar flow, while the Reynolds carrier gas flow past the powder particles is difficult to assess due to unknown velocity difference between the powder particles and the carrier gas. Since the flow velocity is below about one-half of the speed of sound, incompressibility can be expected to be a reasonable assumption [21]. An incompressible, laminar flow is thus considered at this point. PISO pressure-velocity coupling is used to solve the pair of continuity and momentum Navier-Stokes equations:

$$\nabla \cdot \boldsymbol{u} = 0 \qquad (1)$$

$$\frac{\partial}{\partial t}(\boldsymbol{u}) + \nabla \cdot (\boldsymbol{u}\boldsymbol{u}) - \nabla \cdot (\nu \nabla \boldsymbol{u}) = -\nabla p + \boldsymbol{f}, \qquad (2)$$

where $\boldsymbol{u}$ is the fluid velocity vector, t is time, p is pressure, ν is kinematic viscosity and $\boldsymbol{f}$ is body force per unit mass.

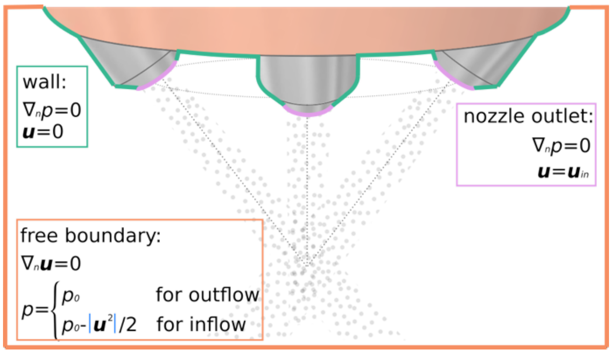

Figure 4: Fluid phase boundary conditions for the modelled system.

Boundary conditions for the gas phase are set as follows (see Figure 4):

- for the nozzle outlet: fixed velocity ($\boldsymbol{u} = \boldsymbol{u}_{in}$) and zero pressure gradient ($\nabla_n p = 0$);
- for the free boundary: zero gradient velocity condition ($\nabla_n \boldsymbol{u} = 0$) and total pressure condition ($p = p_0$ for outflow; $p = p_0 - |\boldsymbol{u}^2|/2$) for inflow);
- for the solid walls: zero velocity ($\boldsymbol{u} = 0$) and zero pressure gradient ($\nabla_n p = 0$).

The coupling between the powder and fluid phase is performed through the body force $\boldsymbol{f}$ by accounting for the reactive force to powder particle drag for each discrete element.

COUPLING OF THE GAS AND POWDER PHASE

The Coupling Regime

The choice of the coupling regime for the developed numerical model is based on the volume fraction of the powder [22]. For the considered DED nozzle (Fraunhofer COAX 12V5), the latter can be derived from the manufacturer-recommended mass deposition rates (10g/

min $< \Phi_m^p <$ 50g/min) and typical range of values for the carrier gas volumetric flux (2L/min $< \Phi_V^f <$ 8L/min) [23], [24]. Depending on the utilized mass deposition rate and carrier gas volumetric rate as well as materiral density (typically in the range of 4000-8000 kg/m^3), the volume fraction of the powder at the outlet of the considered nozzle can be evaluated to $1.5 \cdot 10^{-4} < \alpha < 6 \cdot 10^{-3}$. Depending on the particle diameter within the typical DED powder size range $50\mu m < d_p < 150\mu m$ and fluid velocity $5m/s < |\boldsymbol{u}| < 20m/s$, Stokes number for the considered two-phase flow will result in different values of the magnitude $St \approx 10^4$. These values fall close to the limit between dilute suspension (where the influence of the fluid on the particles and the reactive force of the particles on the fluid are considered relevant) and dense suspension (where inter-particle interaction is also considered relevant) according to [22]. The need for four-way coupling is additionally supported by our recent study evaluating the relevance of inter-particle interactions for the considered nozzle and reporting large potions of grains being involved in inter-granular collisions [18].

The Choice of Coupling Approach

When discussing the dispersed multiphase flows it could be argued that point-particle approach is uniquely suited to handling large particles ($St > 1$). While computationally more efficient Eulerian two-fluid approaches are limited to low Stokes numbers, the fully resolved approaches are not possible for large numbers of suspended particles due to extreme computational costs [25]. While the point-particle approach is on sound theoretical ground only when particle size d_p is smaller than the Kolmogorov length scale η, it remains the only viable approach even for $d_p \gtrsim \eta$.

The Lagrangian point-particle approaches can be divided into the point-force coupling approach and the volumetric-coupling approach (also referred to as the perturbation field scheme) [7]. The point force coupling interpolates the fluid velocity at the particle center from the nearest fluid cell centers to calculate the drag force on the particle and then interpolates the reactive force on the fluid back to the nearest fluid cell centers. The volume-averaged coupling approach on the other hand distributes the reactive drag force from the particle back to a larger volume of the finite volume grid based on a chosen envelope distribution.

Point force coupling successfully captures the effects of particles on the flow when the particles are much smaller than the Kolmogorov scale [26]. At higher Reynolds numbers $Re \approx 100$ and high Stokes numbers, numerical results seem to differ significantly from the experimental measurements [27]. This discrepancy was attributed to the fact that the numerical approach is not able to capture the significant unsteady particle wake and its effect on the turbulence modulation [26], [27]. The volume-averaged coupling on the other hand produces much more accurate results and has been reported to be nearly exact in reproducing turbulence modulation at low Reynolds numbers ($Re \approx 10$) [27]. The volume-coupling approach however comes at a high computational cost due to repeated coordinate transformations required to calculate the force field and apply it onto the Cartesian grid. Eaton [26] reports over 95% of CPU time being used on calculating the particle force term.

While the volume-averaged approach is more accurate, these advantages appear to be mostly limited to modelling turbulence modulation. Since a laminar flow is considered for modelling the DED nozzle powder stream, the point force coupling scheme might prove advantageous due to significantly lower numerical cost and is hence the selected coupling strategy.

The Numerical Coupling Scheme

Adopting the Lagrangian point-force coupling approach, the hydrodynamic force on a particle is represented by a point force. Applying the Stokes drag force ($\boldsymbol{F}_{hyd}$) formulation, the letter can be expressed as:

$$\boldsymbol{F}_{hyd} = 3\pi\mu_f d_p(\boldsymbol{u}_f - \boldsymbol{u}_p), \tag{3}$$

where μ_f is the fluid dynamic viscosity. The reaction force of the particle on the surrounding fluid is formulated as a body force and applied in the cell, where the particle resides. The body force $\boldsymbol{f}$ from Eq. 3 can thus be expressed as:

$$f_{hyd} = \frac{-F_{hyd}}{V_c \rho_f} \tag{4}$$

where V_c is the cell volume and ρ_f is the fluid density.

The coupling methodology involves data exchange between YADE and openFoam solvers, which is performed using the coupling interface developed by Kunhappan et al. [27], [28]. YADE requires the velocity and and velocity gradient tensor at particle positions in 3D space and openFoam requires the body force of particle nodes. The data exchange required to perform the solver coupling is executed by sending and receiving messages using the open MPI library. N_y processes are assigned to YADE where one of them is set up as the master process and is responsible for communication with the worker processes; N_o processes are assigned to openFoam.

The coupling is performed in the manner presented in Figure 5. YADE master process sends the powder particle coordinates to openFoam processes which locate the coordinates in element groups and return the information on velocity and velocity gradients of individual particles to YADE master process. YADE calculates the hydrodynamic force $\boldsymbol{F}_{hyd}$ on individual particles and performs the time stepping. YADE master process then sends the particle hydrodynamic forces and updated coordinates to the openFoam processes, which locate the relevant mesh cells. Applying the body forces, openFoam solves the Navier-Stokes equations and advances the time.

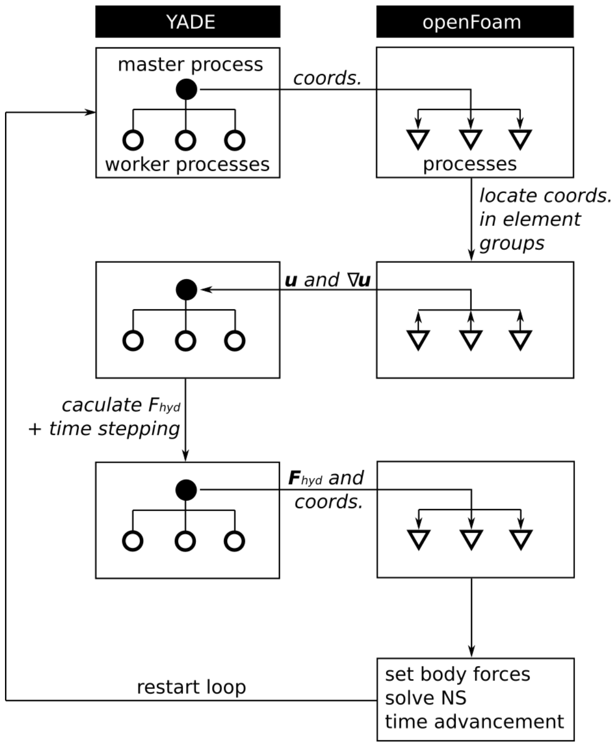

Figure 5: YADE-openFoam coupling flowchart.

CONCLUSIONS

The presented numerical approach demonstrates our strategy to address some of the pressing issues that still hinder the DED technology from achieving its full potential. Assuming that the poor dimensional quality and structural defects in DED manufacturing stem from insufficient control over the powder stream condition, an increased understanding of the powder stream dynamics might be the key to improved control over it. We identify the inter-particle interactions as the missing ingredient in the state-of-the-art powder stream numerical models that could significantly alter the powder dynamics and propose a robust and efficient numerical strategy to overcome this issue.

A fully coupled DEM-CFD approach is utilized to account for the entirety of the relevant interactions in the DED powder stream: the drag of the gas phase on the powder particles, the reactive force of the powder particles on the gas phase, and the inter-particle collisions. State-of-the-art open-source solvers are used for each of the powder stream phases: openFoam CFD solver is used for the gas phase, while YADE DEM solver is used for the powder phase. The computational process is parallelized for both phases and the coupling communication is performed using open MPI library. While the currently proposed numerical model assumes an incompressible, laminar flow of the gas phase and perfectly spherical particles with purely elastic interactions for the powder phase, the choice of the solvers for each of the phases allows us to further develop the model in the future to account for turbulent flows, non-spherical particles, plastic interactions, etc.

The presented model thus marks the next step in the evolution of numerical models of powder stream in DED and is expected to improve the simulational accuracy of the blown powder dynamics.

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