Master Thesis Proposal

Title: Numerical simulation of sub-micron particle coating by smooth hybrid mesoscopic model

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Abstract:

The surfaces of sub-micron particles can be altered by coating them with other materials for improving properties such as adhesion, hydrophobicity, hydrophilicity, printability, corrosion resistance, etc. The specific and broad spectrum of applications of coated particles includes, as examples, removal of metal ions from water; photo-catalyst for water decontamination; reinforcing materials; pharmaceutical dosage; field emission display technology; ferromagnetic iron particles; solid fuel for combustor; etc.

In particular, in the thesis proposal sub-micron particle coating in low-pressure non-equilibrium plasma will be considered. The essential point of this technology is to improve the growth rate of at the particle surface by controlling the main plasma parameters.

Some models exist, based on a detailed chemical kinetics scheme of the reactions occurring in the plasma, namely, electron-neutral, ion-neutral, and neutral-neutral reactions, to predict the species fluxes toward the surface of a sub-micron particle in a low-pressure environment. The usual approach is to apply kinetic theory in the collisionless region within a distance of one mean free path away from the grain, while continuum theory is implemented to solve for species transport in the outer region where reactive-diffusive phenomena occur [1].

From the computational point of view, the matching between the kinetic region and the continuum region is imposed by ensuring the continuity of the fluxes at the interface. However the two descriptions strongly differ, because the collisionless kinetic solution assumes that there are no interactions among the particles, while the continuum description is valid only where a large number of interactions allows one to consider the particles as a fluid. This model, which defines a description somehow in between macroscopic and microscopic phenomena, can be defined a sharp hybrid mesoscopic model.

In this thesis proposal a different approach is investigated. Since for this particular application the electrostatic interactions are weak if compared to thermal energy of ions and electrons and so the interactions mainly happen as collisions, it is possible to describe the rarefied region close the particle to be coated by means of simplified kinetic models. These simplified models prescribe that the time dynamics of the distribution function of the charged particles is driven by the difference between the actual value and the local equilibrium value, according to a given relaxation parameter ruled by the local particle number. Some generalizations of this concept exist for mixtures, i.e. when different particles can interact each other [2-3] (see in particular the Hamel's model). For the present application, three different model equations can be considered by taking into account self-collisions, i.e. collisions among particles of the same type, and cross-collisions, mainly ion-neutrals and electron-neutrals collisions. The local equilibrium conditions can be generalized for taking into account the interaction potential between the charged particles and the grain to be coated.

This kind of models can smoothly describe the behavior of the particles from the collisionless region to the continuum region by properly tuning the relaxation parameter. For this reason, they lead to a smooth hybrid mesoscopic model. The idea is to solve the simplified model equations by

the finite difference method (FDM), in the rarefied region for describing the approach of the distribution function to the local equilibrium. Once the distribution function is no more far away from the local equilibrium, the system of equations can be automatically converted to the continuum based approach. In particular, far from the coated grain the lattice Boltzmann method (LBM) seems the most reasonable candidate for this goal, since it is already formulated in terms of very rough discrete distribution functions for a finite number of microscopic velocities (lattice). In this case, no matching of the fluxes is required and the data from the kinetic approach can be immediately translated in the LBM framework, by performing some integrals depending on the microscopic velocity (quadrature formula).

The main goals of thesis and the innovative contents are:

- to define a very simple kinetic model based on simplified collisional kernels for the main interactions (electron-neutrals and ion-neutrals collisions) in order smoothly take into account both rarefied and continuum regime;
- to define the switching procedure between kinetic model and mesoscopic model based on the LBM framework;
- to solve numerically the previous smooth hybrid model consistently in all the computational domain:
- to compare advantages and drawbacks of both sharp and the sooth hybrid models in dealing with this application.

Please fell free to ask additional information !

[1] A.L. Yarin, B. Rovagnati, F. Mashayek, T. Matsoukas, "Reaction model for plasma coating of nanoparticles by amorphous carbon layers*", Journal of Applied Physics*, vol. 99, n. 6, 15 2006, p 64310-1-12.

[2] P. Asinari, “Viscous coupling based lattice Boltzmann model for binary mixtures”, *Physics of Fluids*, vol. 17, n. 067102, 2005.

[3] P. Asinari, “Semi-implicit-linearized multiple-relaxation-time formulation of lattice Boltzmann schemes for mixture modeling”, *Physical Review E*, vol. 73, n. 056705, 2006.