Flexible High Fidelity Chemistry Model for Kinetic Particle Codes

Sufficiently rarefied gases and plasmas are commonly simulated with so-called kinetic approaches in which the flow is not modelled as a continuum but as a collection of a huge number of particles. To solve technically relevant problems, non-deterministic approaches like Particle-In-Cell (PIC) solvers for plasmas and Direct Simulation Monte Carlo (DSMC) solvers for gases are regularly used and are still subject to continuous improvements.

Gradel sàrl is developing its own software solution since proper tools are unavailable. Within the scope of this project the candidate will develop a flexible data structure for a cross section based plasma chemistry model. The data structure should allow arbitrary plasma compositions and respective particle interactions, automatic/manual neglect of unlike interactions, and automatic calculation of effective interaction probabilities. Implementation of data structure and cross section data initially based on plasma chemical processes will be verified on basis of rate constants. Respective reference values can be derived by mathematical operation on the cross sections assuming equilibrium energy distribution functions.

The perfect candidate has OO/C++ programming experience and a background in a related field (chemistry, engineering, physics, and mathematics). Furthermore, he/she will work in a team of experts with backgrounds in plasma physics, fusion technology, space propulsion, and kinetic particle code development.

Interested students should send their application (including CV) to Dr.-Ing. Dejan Petkow, Gradel sàrl, d.petkow@gradel.lu, Tel: +352 39 00 44 202.