The Research Center Pharmaceutical Engineering GmbH (RCPE) is a global leader in pharmaceutical engineering sciences. We help our partners create and manufacture advanced medicines for patients worldwide through optimizing products and processes.

PAID DIPLOMA / MASTER'S THESIS

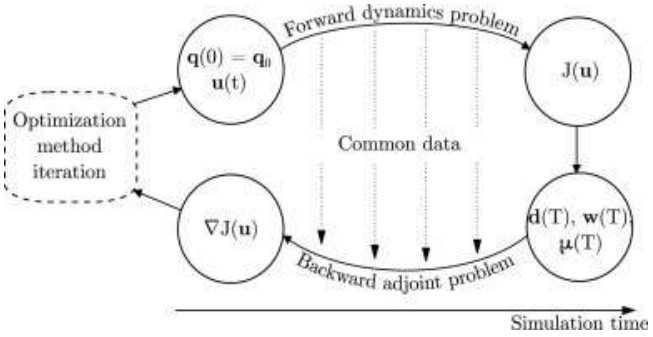
ADJOINT STATE METHOD FOR DEM

Ref. No. DA172

To dedicated students of mathematics, physics, chemical engineering, mechanical engineering and related disciplines we offer an opportunity to write a paid Diploma/Master's thesis.

Objective

Pharmaceutical tablets are made from powders and the pharmaceutical industry is heavily reliant on tools to predict powder flow. One such tool is the Discrete Element Method in which Newton's equations are solved for individual particles. Since the particles have a diameter on the order of 50 µm, DEM simulations typically include a huge number of particles, which makes them time- and energy-consuming.



In order to develop a DEM model of a powder, the parameters of the DEM model (e.g. contact stiffness, friction and restitution coefficients, etc.) have to be calibrated. This calibration is usually done by carrying out small-scale characterization test and simulating those test using different parameter combinations to identify a set of parameters that provides an adequate description of all tests.

In addition to simulating the manufacturing process, it is also desitrable to understand to what extent the simulation is senstive to the DEM parameters. This understanding can be generated in a straightfoward but time-consuming way by varying one parameter at a time and doing as many simulations as there are parameters. An approach that potentially is more efficient uses the adjoint state method. The adjoint state method treats the sensitivity determination as a contrained optimization problem that is solved using Lagrangian multipliers. In the adjoint state approach, one DEM simulation involving N initial value problems is carried out and the sensitivities are then obtained by solving N ODEs for the Lagrangian multipliers (followed by evaluating an integral via quadrature).

In this work, you will develop a proof-of-concept for the adjoint state method for DEM simulations by developing a simple 2- or 3D DEM code for the DEM simulation, a method to solve the ODE for the Lagrangian multipliers, as well as a method to evaluate the integral. The outcome of the project is a prototype DEM code and, more importantly, an outlook on the prospects of implementing the capability to perform sensitivity analysis using the adjoint state method in a commercial DEM code.

Required skills

- Mathematics (numerical solution of ordinary differential equations), programming.

Withing the framework of this diploma / master's thesis we offer the following

- Extensive participation in a top-level and industrially relevant research project in an international environment
- Supervised training in the task
- Assistance of experienced staff with the implementation of innovative ideas
- Access to highly modern infrastructure on campus of Graz University of Technology
- Assistance with the publication of results

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Financing

- Compensation on the basis of a service contract

If you are interested in writing your thesis at the interface between university research and industry/ business and to contribute to the optimization of product and process development in the pharmaceutical industry, please contact us indicating the reference number.

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