Schlussbericht:

Verbundprojekt SimPaTurS
Teilprojekt: Integralterme

Projektleiter:

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21. Dezember 2010

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Teil I

Problem formulation

1 Problem formulation

1.1 Problem formulation

A key point describing a population balance model are the birth and death terms. These are usually integral (linear or non-linear) operators. In particular for aggregation and breakage models birth and death terms are

$$\begin{aligned} Q^+_{brk}(f)(x) &= \int_0^x b(y)\mathbf{B}(x,y)f(t,r,y)dy \\ Q^-_{brk}(f)(x) &= b(x)f(t,r,x) \\ Q^+_{agg}(f)(x) &= \int_0^x \mathbf{A}(x-y,y)f(t,r,x-y)f(t,r,y)dy \\ Q^-_{agg}(f)(x) &= f(t,r,x)\int_0^\infty \mathbf{A}(x,y)f(t,r,y)dy \end{aligned}$$

The aggregation and breakage rates A and B may have different forms, and the numerical approach to compute the integral term depends on the mathematical properties of these kernel functions. The goal of this part of the project was to develop numerical methods for efficient computation of these terms.

1.2 Background

The group of Prof Hackbusch works several years on fast methods and many modern methods for fast evaluations of linear integral operators were at our disposal. However, the Q^+_{agg} is not a linear operator, and for some breakage rates novel methods were required for efficient computation of Q^+_{brk}.

1.3 Planning and elaboration of the project

At the start of the project several examples of breakage and aggregation rates were introduced. The group started with development of mathematical methods and corresponding software for this examples. After about a year and half the model was fixed and the main work was concentrated on aggregation kernels. In particular, a fast method, with *almost linear* complexity was introduced for computing integrals from Q^+_{agg} (*coalescence integrals*).

1.4 Scientific and technical state at the beginning of the project

In the literature there are several various methods for evaluation of coalescence integrals. However, in these works the attention was paid to the accuracy of the method. When handling a 3D / 4D system, a fast method becomes crucial, since the large number of degrees of freedom may lead to weeks or even months of computations. Some fast methods for computing coalescence integrals were known, given that the input and output are defined on certain meshes (e.g. *uniform*, *geometrically refined*). The method proposed here covers much larger class of meshes.

1.5 Co-operation with other groups

During the first half of the project the group was mainly cooperating with Prof Sundmachers group, considering several possible models and discussing their mathematical treatments. When the model was fixed, co-operation with Prof Johns group entered a new phase and several local meetings were organized for combining, improving and making easy-to-use the software from both groups.

Teil II

Results