Value Simulation of the Interacting Pair Number for Solution of the Monodisperse Coagulation Equation

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The pure coagulation Smoluchowski equation with linear coefficients of the form $K_{ij} = a + b(i + j)/2$ is considered for the spatially homogeneous case. These coefficients can be found, for example, in the classical polymer model A—R—B_{f-1}. In this model the molecules with $f - 1$ chemically active units of one kind (B), and one unit of another kind (A), are regarded as monomers. Between A and B units form chemical bonds, which leads to branched molecules if $f \geq 3$. For this model the coagulation (or polymerization) rate $K_{ij}^{(f)}$ is proportional to $(i + j)(f - 2) + 2$.

We construct the value algorithms and analyze their efficiency for estimating two functionals: the total monomer concentration as well as the total monomer and dimer concentration in ensemble at the fixed time T. We suggest using the *value simulation of the interacting pair number* algorithm. It aims at preservation of the monomers (or monomers and dimers) in the simulated ensemble, which is taken into account when multiplicative weight is constructed.

A considerable gain in computational costs is achieved via value simulation of both elementary transitions:

1. simulation of the time between interactions in the ensemble;

2. simulation of the interacting pair number.

Analogous results for the constant ($K_{ij} = 1$) and additive ($K_{ij} = [i+j]/2$) coagulation coefficients were obtained previously by the author and this work presents a generalization of this method for the case of linear coefficients.

Moreover, proposed method not only allows to reduce computational costs of estimating the functionals, but also makes it possible to implement the parametric analysis (with respect to parameters a and b) using the standard weight Monte Carlo technique.