Abstract Submitted
for the APR15 Meeting of
The American Physical Society

Stochastic coalescence in finite systems: an algorithm for the numerical solution of the multivariate master equation.[1] LESTER ALFONSO, Universidad Autonoma de la Ciudad de Mexico, JOSE ZAMORA, PEDRO CRUZ, LUFAC Computacion S.A. de CV — The stochastic approach to coagulation considers the coalescence process going in a system of a finite number of particles enclosed in a finite volume. Within this approach, the full description of the system can be obtained from the solution of the multivariate master equation, which models the evolution of the probability distribution of the state vector for the number of particles of a given mass. Unfortunately, due to its complexity, only limited results were obtained for certain type of kernels and monodisperse initial conditions. In this work, a novel numerical algorithm for the solution of the multivariate master equation for stochastic coalescence that works for any type of kernels and initial conditions is introduced. The performance of the method was checked by comparing the numerically calculated particle mass spectrum with analytical solutions obtained for the constant and sum kernels, with an excellent correspondence between the analytical and numerical solutions. In order to increase the speedup of the algorithm, software parallelization techniques with OpenMP standard were used, along with an implementation in order to take advantage of new accelerator technologies. Simulations results show an important speedup of the parallelized algorithms.

[1]This study was funded by a grant from Consejo Nacional de Ciencia y Tecnologia de Mexico SEP-CONACYT CB-131879. The authors also thanks LUFAC® Computacion SA de CV for CPU time and all the support provided.

Lester Alfonso
Universidad Autonoma de la Ciudad de Mexico

Date submitted: 08 Jan 2015 Electronic form version 1.4