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Analytical and Numerical Approaches in Coagulation of Particles

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***Abstract*—**In this paper we discuss the effect of unbounded particle interaction operator on particle growth and we study how this can address the choice of appropriate time steps of the numerical simulation. We provide also rigorous mathematical proofs showing that large particles become dominating with increasing time while small particles contribute negligibly. Second, we discuss the efficiency of the algorithm by performing numerical simulations tests and by comparing the simulated solutions with some known analytic solutions to the Smoluchowski equation.

***Keywords*—**Stochastic processes; Coagulation of particles; Numerical scheme.

I. Introduction

THE coagulation of particles is observed in various areas ranging from the formation of stars and planets in astrophysics to the behaviour of fuel mixtures in engines. In 1916, M.V. Smoluchowski [1] has proposed an infinite system of differential equations which models the dynamic of such phenomena and describes the evolution of a large number of particles that can coagulate to form clusters which in turn can coalesce in order to form bigger clusters.

In the simplest situation, the space homogeneous discrete Smoluchowski equation reads, for i=1,2,3,…and t >0:

$$\begin{cases} \dfrac{\partial c}{\partial t}(i,t) = \dfrac{1}{2}\sum_{j=1}^{i-1} K(i-j,j)c(i-j,t)c(j,t) - \sum_{j=1}^{\infty} K(i,j)c(i,t)c(j,t) \\ c(i,0) = c_i(0). \end{cases} \quad (1)$$

Where, $c(i,t)$ is the concentration of particles of size i at time t. In fact, this system describes a nonlinear evolution equation of infinite dimension, where the initial conditions $(c_i(0))_{i\geq 1}$ satisfy the equation $\sum_{i\geq 1} c_i(0) = 1$. The rate of merging of particles of size i with those of size j at time t is given by the coagulation kernel $K(i,j)$ that is naturally supposed to be Nonnegative ($K(i,j) > 0$) and symmetric ($K(i,j) = K(j,i)$).

Equation (1) has a transport differential operator on the left hand side and a local quadratic particle interaction operator on the right hand side. The first term on the right hand side shows that the concentration of particles of size i increases as a result of coagulation of particles of sizes (i-j) and j. This is the gain term. The coefficient ½ is due to the fact that K is symmetric. The second term corresponds to the depletion of particles of size i after coalescence with other particles. It represents the loss term. The main numerical tools for solving such equations are Monte Carlo simulations.

Several stochastic algorithms have been proposed [2,4,5] to solve the Smoluchowski system. In particular, H. Babovsky has proposed in [2] a computational method based on a modified Monte Carlo simulation in which the simulated particles represent masses rather than physical particles. We have studied in a previous paper [3], the mathematical convergence of this important numerical algorithm

The objective of the present paper is twofold: First, we extend our study in [3] to analyze the effect of unbounded particle interaction operator on particle growth and how this can address the choice of appropriate time steps of the numerical simulation. In several important applications, particle masses are monotonously increasing with time, and then the operator $K^*(i,j)$ is in fact unbounded and the system of differential equations (1) will contain components related to large particle sizes (i.e., "stiff" components [6]). This implies that there is no possible time step Δt for which the loss term is bounded and at the same time we can no longer guarantee the positivity of the kernel. We provide rigorous mathematical proofs showing that large particles become dominating with increasing time while small particles contribute negligibly. Second, we validate the efficiency of the algorithm by performing numerical simulations tests and by comparing the simulated solutions with some known analytic solutions to the Smoluchowski equation.

II. The Babovsky's Algorithm

We start by some basic notations and concepts. If N_0 is the initial total number of particles, then at time t, $N_0 c(i,t)$ represents the total number of particles of size i and $\sum_{i\geq 1} N_0 c(i,t)$ is the total number of particles. The quantity $ic(i,t)$ represents the fraction at time t of the whole mass produced by the particles of mass i. The whole mass is

$$m(t) = \sum_{i\geq 1} ic(i,t) \cdot$$

Multiplying equation (1) by i and summing over all $i \geq 1$, it can be shown that the whole mass is conserved, i.e.,

$$\frac{d}{dt}\sum_{i\geq 1} ic(i,t) = 0, \quad (2)$$

provided that the relevant summations converge and can be interchanged, which is valid as long as

$$\sum_{i,j\geq 1} K(i,j)c(i,t)c(j,t) < \infty.$$

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Since particles may stick together, the total number of particles is a decreasing quantity and this may display a poor statistics for the simulation. Therefore, to avoid this deficiency it's important to approximate the following mass density function

$$g(i,t) = ic(i,t). \tag{3}$$

If we write $\widetilde{g}_i(t)$ instead of $g(i,t)$, then equation (1) becomes

$$\begin{cases} \dfrac{\partial \widetilde{g}_i}{\partial t}(t) = \displaystyle\sum_{j=1}^{i-1} K^*(i-j,j)\widetilde{g}_{i-j}(t)\widetilde{g}_j(t) - \sum_{j=1}^{\infty} K^*(i,j)\widetilde{g}_i(t)\widetilde{g}_j(t) \\ \widetilde{g}_i(0) = g_{0,i}, \end{cases} \tag{4}$$

with $K^*(i,j) = \dfrac{K(i,j)}{j}$.

Without loss of generality, we assume that at time t=0

$$\sum_{i\geq 1} g_{0,i} = 1. \tag{5}$$

So, the conservation of mass leads to

$$\sum_{i\geq 1} \widetilde{g}_i(t) = 1. \tag{6}$$

We start with an initial N-tuple:

$$Z_0^{(N)} = \left(z_{0,1}^{(N)}, z_{0,2}^{(N)}, ..., z_{0,N}^{(N)}\right) \in IN^N.$$

The entry $z_{0,i}^{(N)}$ represents a particle of mass $1/N$ with 'label' i and such that

$$\forall i \in IN^* \quad \frac{1}{N}\#\{\ell : z_{0,\ell}^{(N)} = i\} \approx \widetilde{g}_i(0), \tag{7}$$

where the symbol $\#$ represents the cardinality of the set.

If we assume the monodisperse initial condition

$$\widetilde{g}_1(0) = 1,\ \widetilde{g}_2(0) = \widetilde{g}_3(0) = \cdots\cdots = 0 \tag{8}$$

we can set

$$z_{0,1}^{(N)} = z_{0,2}^{(N)} = \cdots\cdots = z_{0,N}^{(N)} = 1 \tag{9}$$

Also, we choose a time step Δt such that

$$\Delta t \ \underset{i,j\in IN}{Sup} K^*(i,j) < 1 \tag{10}$$

This means that the time step has to be permanently reduced while particles progress in the domain of increasing mass.

For $n \in IN$, we set $t_n = n\Delta t$. At t=t_n, we consider a point set $Z^{(N)}(n)$ of N particles $z_1^{(N)}(n), ..., z_N^{(N)}(n)$ such that $\forall i \in IN^*$

$$\frac{1}{N}\#\{\ell : z_\ell^{(N)}(n) = i\} \approx \widetilde{g}_i(t_n) \tag{11}$$

For $i \in IN^*$, we define the following independent equally distributed random numbers

$$\chi_{i,\ell}^{(N)}(n) = \begin{cases} 1 & \text{if } z_\ell^{(N)}(n) = i, \\ 0 & \text{otherwise.} \end{cases} \tag{12}$$

such that

$$G_i^{(N)}(n) = \frac{1}{N}\sum_{\ell=1}^{N} \chi_{i,\ell}^{(N)}(n), \tag{13}$$

with

$$\sum_{i=1}^{\infty} G_i^{(N)}(n) = 1. \tag{14}$$

Notice that

$$G_i^{(N)}(n) = \frac{1}{N}\#\{\ell : z_\ell^{(N)}(n) = i\}. \tag{15}$$

Applying the Euler time discretization for $\widetilde{g}_i(t_n)$ will lead to

$$\frac{1}{\Delta t}(\widetilde{g}_i(t_{n+1}) - \widetilde{g}_i(t_n)) = \sum_{j=1}^{i-1} K^*(i-j,j)\widetilde{g}_{i-j}(t_n)\widetilde{g}_j(t_n) - \sum_{j=1}^{\infty} K^*(i,j)\widetilde{g}_i(t_n)\widetilde{g}_j(t_n), \quad i \in IN^*, n \in IN.$$

Using now the fact that $\sum_{j\geq 1} \widetilde{g}_j(t_n) = 1$, we conclude that $\widetilde{g}_i(t_{n+1})$ is defined by

$$\widetilde{g}_i(t_{n+1}) = \sum_{j=1}^{i-1} \Delta t K^*(i-j,j)\widetilde{g}_{i-j}(t_n)\widetilde{g}_j(t_n) + \sum_{j=1}^{\infty}(1 - \Delta t K^*(i,j))\widetilde{g}_j(t_n)\widetilde{g}_i(t_n) \tag{16}$$

Then the Babovsky's scheme proposed in [2] can now be described as follows:

- For $1 \leq i \leq N$, choose at time $t = 0$, $z_i^{(N)}(0) \in \{1,2,3....\}$ such that $\forall i \in IN^*,\ G_i^{(N)}(0) \approx g_{0,i}$.
- For $1 \leq \ell \leq N$, the transition from $z_\ell^{(N)}(n)$ to $z_\ell^{(N)}(n+1)$ is given by the following random game:

1. For i=1,…,N choose equidistributed random numbers $\pi_i^{(N)} \in \{1,2,...,N\}$ and $r_i^{(N)} \in [0,1]$.
2. Choose a time step Δt such that:
$$\Delta t \ \underset{i,j\in IN}{Sup} K^*(i,j) < 1$$
3. Let $p(i,j) = \Delta t K^*(i,j)$ and define for $1 \leq \ell \leq N$

$$z_\ell^{(N)}(n+1) := \begin{cases} z_\ell^{(N)}(n) + z_{\pi_\ell^{(N)}(n)}^{(N)}(n) & \text{if } r_\ell^{(N)}(n) \leq p(z_\ell^{(N)}(n), z_{\pi_\ell^{(N)}(n)}^{(N)}(n)), \\ z_\ell^{(N)}(n) & \text{otherwise.} \end{cases} \tag{17}$$

III. Growth of Particle Size

The convergence of the numerical scheme has been concluded for the case where the operator $K^*(i,j)$ is nonnegative and bounded, and so according to (17), we should have $\forall \ell, m \in \{1...N\},\ p(z_\ell, z_m) < 1$. But in several important applications, particle masses are monotonously increasing with time, and then the operator $K^*(i,j)$ is in fact unbounded and the system of differential equations (4) will contain components related to large particle sizes (i.e., "stiff" components [10]). This implies that there is no possible time step Δt for which the loss term $\sum_{j=1}^{\infty} K^*(i,j)\widetilde{g}_i(t)\widetilde{g}_j(t)$ is less than $\kappa.\widetilde{g}_i(t)$ with $|\kappa| < 1$, and at the same time we can no longer guarantee the positivity of the kernel. In this section, we provide rigorous mathematical proofs showing that large particles become dominating with increasing time while small particles contribute negligibly. In this respect, Babovsky

suggested in [2] a modification of the scheme by choosing a limit value N_L and allowing the particles whose mass has crossed this level from below to contribute to the clusters by merging only with other small particles. This modification leads to the calculation of subsolutions with fixed lower bounds for the time step, and the solution of the original problem is obtained when N_L approaches infinity.

Lemma 3. Suppose that the coagulation kernel is positive [i.e., $K(i,j)>0$] and assume that there exists a positive solution of the equation (1) on an interval [0,t_0] such that all the applications

$$t \to \sum_{j=1}^{\infty} K(i,j)c(j,t)$$

are integrable and $c(i_0,0)>0$ *for some* $i_0 \in N^*$. *Then, for all* $t \in]0,t_0]$ *the support of* $c(t)$ *defined by* $\text{supp}(c(t)) := \{i \in IN^* : c(i,t) \neq 0\}$ *is unbounded* [*i.e.,* $c(ni_0,t)>0 \ \ \forall n$].

Proof: For $i \in IN^*$, let

$$\phi(i,t) := \int_0^t \sum_{j=1}^{\infty} K(i,j)c(j,s)ds$$

Multiplying equation (1) by $e^{\phi(i,t)}$ we obtain

$$\frac{\partial}{\partial t}c(i,t)e^{\phi(i,t)} = \frac{1}{2}\sum_{j=1}^{i-1} K(i-j,j)c(i-j,t)c(j,t)e^{\phi(i,t)} - \sum_{j=1}^{\infty} K(i,j)\,c(j,t)\,c(i,t)e^{\phi(i,t)}. \quad (18)$$

Now using the following two relations

$$\frac{\partial}{\partial t}(c(i,t)e^{\phi(i,t)}) = e^{\phi(i,t)}\frac{\partial}{\partial t}c(i,t) + c(i,t)e^{\phi(i,t)}\frac{\partial}{\partial t}c(i,t)$$

and

$$\frac{\partial}{\partial t}\phi(i,t) = \sum_{j=1}^{\infty} K(i,j)c(j,t),$$

equation (18) can be rewritten as

$$\frac{\partial}{\partial t}\left(c(i,t)e^{\phi(i,t)}\right) = \frac{1}{2}\sum_{j=1}^{i-1} K(i-j,j)c(i-j,t)c(j,t)e^{\phi(i,t)}. \quad (19)$$

Integrating (19) between 0 to t, we obtain

$$c(i,t)e^{\phi(i,t)} = c(i,0) + \frac{1}{2}\int_0^t \sum_{j=1}^{i-1} K(i-j,j)c(i-j,s)c(j,s)e^{\phi(i,s)}ds$$

or

$$c(i,t) = c(i,0)e^{-\phi(i,t)} + \frac{1}{2}\int_0^t \sum_{j=1}^{i-1} K(i-j,j)c(i-j,s)c(j,s)e^{\phi(i,s)-\phi(i,t)}ds. \quad (20)$$

The relation (20) shows that $c(i,t)$ is the sum of two positive terms from which we can deduce that

$$c(i_0,t) \geq c(i_0,0)e^{-\phi(i_0,t)} > 0. \quad (21)$$

But since

$$c((n+1)i_0,t) = c((n+1)i_0,0)e^{-\phi((n+1)i_0,t)} + \frac{1}{2}\int_0^t \sum_{j=1}^{(n+1)i_0-1} K((n+1)i_0-j,j)c((n+1)i_0-j,s)c(j,s)e^{\phi((n+1)i_0,s)-\phi((n+1)i_0,t)}ds,$$

we have

$$c((n+1)i_0,t) \geq \frac{1}{2}\int_0^t K(ni_0,i_0)c(ni_0,s)c(i_0,s)e^{-\phi((n+1)i_0,t)}ds. \quad (22)$$

By induction, we conclude that

$$\forall n \ \ c(ni_0,t) > 0. \quad (23)$$

Lemma 4. Let $\tilde{g}_i(t)$ *be a solution of (4) such that*

$$\forall i \in IN^*, \forall t > 0 \ \ \tilde{g}_i(t) \geq 0,$$

and for $J \in IN^*$, *let* $\gamma_J(t) := \sum_{i=1}^{J} \tilde{g}_i(t), \quad t > 0.$

If $\forall i,j \in IN^*, K^*(i,j) \geq \tilde{K}^*$ *then*

$$\gamma_J(t) \leq \frac{\gamma_J(0)e^{-\tilde{K}^*t}}{1-\gamma_J(0)(1-e^{-\tilde{K}^*t})}.$$

Proof. By summing equation (4) from i=1 to J, we have

$$\sum_{j=1}^{J}\frac{\partial}{\partial t}\tilde{g}_i(t) = \sum_{i=2}^{J}\sum_{j=1}^{i-1} K^*(i-j,j)\tilde{g}_{i-j}(t)\tilde{g}_j(t)\tilde{g}_i(t) - \sum_{i=1}^{J}\sum_{j=1}^{\infty} K^*(i,j)\tilde{g}_i(t)\tilde{g}_j(t) \quad (24)$$

$$\frac{d}{dt}\sum_{j=1}^{J}\tilde{g}_i(t) = \sum_{i=2}^{J}\sum_{j=1}^{i-1} K^*(i-j,j)\tilde{g}_{i-j}(t)\tilde{g}_j(t)\tilde{g}_i(t) - \sum_{i=1}^{J}\sum_{j=1}^{\infty} K^*(i,j)\tilde{g}_i(t)\tilde{g}_j(t). \quad (25)$$

Now letting h=i-j, one can notice that

$$\left.\begin{matrix} 2 \leq i \leq J \\ 1 \leq j \leq i-1 \end{matrix}\right\} \Leftrightarrow \begin{cases} 1 \leq h \leq J-1 \\ 1 \leq j \leq J-1 \\ 2 \leq h+j \leq J \end{cases} \quad (26)$$

so,

$$\frac{d\gamma_J}{dt}(t) = \sum_{\substack{1\leq h<J, 1\leq j<J \\ h+j\leq J}} K^*(h,j)\tilde{g}_h(t)\tilde{g}_i(t) - \sum_{i=1}^{J}\sum_{j=1}^{\infty} K^*(i,j)\tilde{g}_i(t)\tilde{g}_j(t)$$
$$= \sum_{\substack{1\leq i<J, 1\leq j<J \\ i+j\leq J}} K^*(i,j)\tilde{g}_i(t)\tilde{g}_j(t) - \sum_{i=1}^{J}\sum_{j=1}^{\infty} K^*(i,j)\tilde{g}_i(t)\tilde{g}_j(t)$$
$$= \sum_{\substack{1\leq i\leq J, 1\leq j \\ i+j>J}} K^*(i,j)\tilde{g}_i(t)\tilde{g}_j(t). \quad (27)$$

Let's define the set

$$\Omega := \{(i,j) : 1 \leq i \leq J, 1 \leq j\}, \text{ then}$$

$$\Omega = \Omega_1 \cup \Omega_2,$$

where

$$\Omega_1 := \{(i,j) : 1 \leq i < J, 1 \leq j < J \text{ and } i+j \leq J\}$$

and

$$\Omega_2 := \{(i,j) : 1 \leq i < J, 1 \leq j \text{ and } i+j > J\}.$$

Using now the fact that

$$\forall i, j \in IN^*, K^*(i,j) \geq \widetilde{K}^*,$$

one obtains

$$\frac{d\gamma_J}{dt}(t) \leq -\widetilde{K}^* \sum_{\substack{1\leq i\leq J, 1\leq j \\ i+j>J}} \widetilde{g}_i(t)\widetilde{g}_j(t) \leq -\widetilde{K}^* \sum_{i=1}^{J}\sum_{j=N+1}^{\infty} \widetilde{g}_i(t)\widetilde{g}_j(t),$$

and so

$$\frac{d\gamma_J}{dt}(t) \leq -\widetilde{K}^* \sum_{i=1}^{J} \widetilde{g}_i(t)\left(1-\sum_{j=1}^{N}\widetilde{g}_i(t)\right) \tag{28}$$

with

$$\sum_{j=1}^{\infty}\widetilde{g}_i(t) = 1.$$

For $t > 0$, the function $\gamma_J(t)$ satisfies the following differential inequality

$$\frac{d\gamma_J}{dt}(t) \leq -\widetilde{K}^*\gamma_J(t)(1-\gamma_J(t)) \tag{29}$$

By Gronwell's Lemma [10,11], one can find an upper limit for the function $\gamma_J(t)$ as follows. Let $u(t)$ be the solution of the corresponding Cauchy problem, that is,

$$\begin{cases} \dfrac{du}{dt}(t) = -\widetilde{K}^* u(t)(1-u(t)) \\ u(0) = \gamma_J(0). \end{cases} \tag{30}$$

This is a nonlinear differential equation with an initial condition. The change of variable $\vartheta = u^{-1}$ will reduce it to the linear equation

$$\begin{cases} \dfrac{d\vartheta}{dt}(t) + \widetilde{K}^*\vartheta(t) = \widetilde{K}^* \\ \vartheta(0) = \dfrac{1}{\gamma_J(0)}. \end{cases} \tag{31}$$

The solution of (31) is $\vartheta(t) = 1 + Ae^{-\widetilde{K}^* t}$, where A is a constant. Applying now the initial condition, we get

$$\vartheta(t) = 1 + \left(\frac{1-\gamma_J(0)}{\gamma_J(0)}\right)e^{-\widetilde{K}^* t}. \tag{32}$$

Then, from (32) we deduce that the upper solution $u(t)$ is

$$u(t) = \frac{\gamma_J(0)e^{-\widetilde{K}^* t}}{1-\gamma_J(0)(1-e^{-\widetilde{K}^* t})}. \tag{33}$$

Therefore,

$$\forall t > 0 \quad \gamma_J(t) \leq u(t), \tag{34}$$

which ends the proof of Lemma 4.

IV. Numerical Simulations

In this section, we aim to numerically validate the convergence of the algorithm described above. It is well known that for three particular kernels $K(i,j)$ and in the case of the monodisperse initial configuration, i.e.

$$c(1,0) = 1 \text{ and } \forall i > 1,\ c(i,0) = 0, \tag{35}$$

explicit solutions of Smoluchowski's coagulation equation are available [12]. Here we consider the *unbounded linear kernel* $K(i,j)=i+j$, we compute the simulated solutions and compare them to their corresponding exact solutions.

A. Approximation of the moments

According to our notations, if $c(i,t)$ is the solution of equation (1) at time t, the moment of order k of $c(i,t)$ is

$$m_k(t) = \sum_{i=1}^{\infty} i^k c(i,t) \quad \text{or} \quad m_k(t) = \sum_{i=1}^{\infty} i^{k-1} g(i,t).$$

In particular, the moment of order zero is

$$m_0(t) = \sum_{i=1}^{\infty} \frac{g(i,t)}{i},$$

and $N_0 m_0(t)$ is the total number of clusters at time t. At time t_n, $m_0(t_n)$ is approximated, according to (13) and (15), by

$$m_0(t_n) = \frac{1}{N}\sum_{\ell=1}^{N}\frac{1}{z_\ell^{(N)}(n)}.$$

B. Numerical results

The numerical algorithm derived in section 2 is readily transformed into a computer program. The computations are performed using "Mathematica" but our computer program can be easily implemented with other calculators. We consider N particles, a time interval $[0,t_f]$, and P time steps where $P = 1/\Delta t$ and $0 < \Delta t < t_f$. The quantity $E_{N,P}=m_0(t)- m_0(t_n)$ represents the error between the exact and the approximated solutions for N particles and P time steps.

For the kernel $K(i,j)= i + j$, the exact solution of (1) is

$$c(i,t) = e^{-t}B(i,1-e^{-t}), \text{ where}$$

$$B(i,u) = \frac{(iu)^{i-1}}{i!}e^{-iu}.$$

Then,

$$g(i,t) = ic(i,t) = ie^{-t}B(i,1-e^{-t})$$

and the exact solution is

$$m_0(t) = e^{-t}.$$

Since the linear kernel is not bounded, it's important to determine an appropriate time step Δt before running the numerical simulation. Next we choose a time step small enough so that time discretization error is negligible relative to the Monte Carlo error. Figs 1 (a), 2 (a) and 3 (a) (in the left) represent the exact and the computed solutions for N=1000, 10000 and 100000 with P=400and t_f=2.5. In the right, Figs. 1 (b), 2 (b) and 3 (b) represent the corresponding errors.

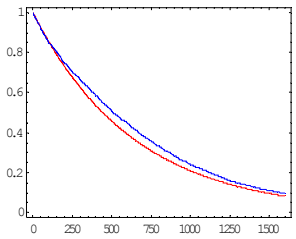

Fig.1 (a) Computed & Exact solutions: N=1000, P=400 t_f=2.5.

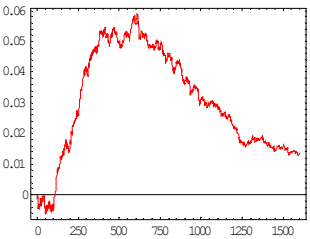

Fig.1 (b) The error $E_{N,P}$.

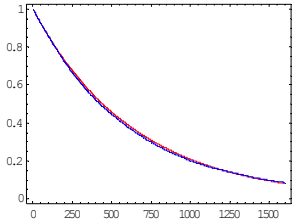

Fig. 2 (a) Computed & Exact solutions: N=10000, P=400 t_f=2.5.

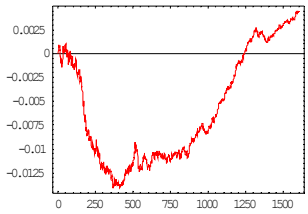

Fig. 2 (b) The error $E_{N,P}$

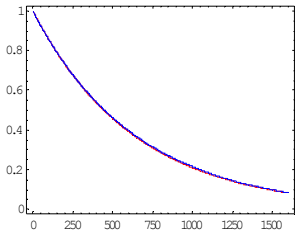

Fig.3 (a) Computed & Exact solutions: N=100000, P=400, t_f=2.5.

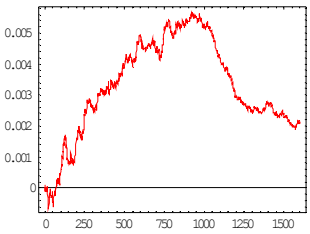

Fig.3 (b) The error $E_{N,P}$

C. Comments on the Results

The analysis of the results shows a good agreement between numerical and exact values for the kernel used in this test. The scheme provides tangible results even for modest particle numbers like 1000 particles or even less. This confirms the efficiency of the scheme. However, the scheme is affected with fluctuations which are hard to be controlled quantitatively. The main source of errors in the computations for a system consisting of mass-one particles only comes from the use of repeated random selections. A forthcoming paper will present numerical simulations that measure the fluctuations which are inherent to the scheme. Despite the flexibility of the scheme, It's important to notice that in some cases the scheme can be quite slow, because its convergence rate is only $\mathcal{O}(1/N^{1/2})$. An approach based on the use of quasi-random numbers can accelerate the convergence and achieve better convergence in certain cases [9], but we lose the randomness in the selection of the particles.

V. Conclusion

In this paper a procedure for solving Smoluchowski's coagulation equation is analyzed. The important case of unbounded interaction operator has been considered and we presented some insights on the mathematical proofs showing that large particles become dominating with increasing time while small particles contribute negligibly. Numerical simulations have also been performed and they show good agreement with analytic solutions of the Smoluchowsi equation. Also convergence of the simulation as the number of particles N increases has been verified. An important addition to this work is to investigate other stochastic schemes for the resolution of the Smoluchowski's system and to modify them in order to increase their numerical efficiency.

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