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A Finite Difference Method for Piecewise Deterministic Processes with Memory. II

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Abstract. We deal with the numerical scheme for the Liouville Master Equation (LME) of a kind of Piecewise Deterministic Processes (PDP) with memory, analysed in [2]. The LME is a linear system of hyperbolic PDEs, written in non-conservative form, with non-local boundary conditions. The solutions of that equation are time dependent marginal distribution functions whose sum satisfies the total probability conservation law. In [2] the convergence of the numerical scheme, based on the Courant-Isaacson-Rees jointly with a direct quadrature, has been proved under a Courant-Friedrichs-Lewy like (CFL) condition. Here we show that the numerical solution is monotonic under a similar CFL condition. Moreover, we evaluate the conservativity of the total probability for the calculated solution. Finally, an implementation of a parallel algorithm by using the MPI library is described and the results of some performance tests are presented.

Key words: Monotonicity, upwind, non-local boundary conditions,memory, semi-Markov,piecewise deterministic.

1 Introduction

Due to the success of stochastic differential equations (SDEs) in modelling many non-deterministic systems, interest is growing in numerical methods for solving them. Usually, stochastic equations include the Wiener process, named also Gaussian white noise, as a source of randomness. This process is a mathematical abstraction provoking some changes in the ordinary differentiation rules, as it was formalized by Itô and Stratonovich [14]. So that, when solving these stochastic equations in the strict sense (or path-wise), numerical methods and concepts for ordinary differential equations, have to be changed, for example, according to the Itô rules (e.g. see [5, 22]). On the other hand, the solution of SDEs can be expressed in statistical sense, by drawing the probability density function (PDF) from a Fokker-Planck (and its generalizations) equation, so that the standard methods for the numerical solution of PDEs can be applied. By following these remarks, in this paper we deal with piecewise

deterministic processes (PDPs) [11, 26], as an alternative framework for modelling non-determinism, and continue the analysis of paper [2] on the numerical solution of a Liouville-Master Equation[1] for the distribution function.

Let us give a brief summary of the PDPs under consideration.

DEFINITION 1. We name $X(t)$, $X : [t_0, \infty[\rightarrow \Omega$, $\Omega := [\Omega_a, \Omega_b] \subset \mathbb{R}$, be a continuous PDP if:

(a) $X(t)$ satisfies the equation:

$$\dot{X}(t) = A_{\mathcal{S}(t)}(X), \tag{1.1}$$

where $\mathcal{S}(t)$ is a discrete stochastic process [2] with *state space* $\{1, \ldots, S\}$. Correspondingly, given $s = \mathcal{S}(t)$, $s \in \{1, \ldots, S\}$, we say that the dynamics is in the (deterministic) state s, driven by function $A_s : \Omega \rightarrow \mathbb{R}$ of the set $\{A_1, \ldots, A_S\}$ of the known functions (or controllers). We require that $A_s(x)$ be Lipschitz continuous, so that, for fixed s, $X(t)$ exists, is unique and non-explosive solution.

(b) The initial condition for the problem is defined by the Cauchy problem to Eq. (1.1), i.e. $X(t_0) = X_0$, and by the initial state $s = s_0$ of the same equation.

(c) Each state s is characterized by a probability density function (PDF) $\psi_s : \mathbb{R}^+ \rightarrow \mathbb{R}^+$, of *transition events* with

$$\int_0^\infty \psi_s(t)\, dt = 1. \tag{1.2}$$

(d) If the dynamics is in the state j, when a transition event occurs, it switches instantaneously from the state j (A_j) to a new state i (A_i), given randomly according to the transition probability matrix (or transition measure) q_{ij}:

$$0 \leq q_{ij} \leq 1, \quad \sum_{i=1}^{S} q_{ij} = 1 \quad \forall i, j = 1, \ldots, S. \tag{1.3}$$

The position $X(t)$ of the process is not affected when the state switches.

Assumptions (1.1), (1.2) and (1.3) define the three *local characteristics* of the PDP. Equation (1.1) can be integrated as an ordinary differential equation until a transition event happens. At this point of time the integration starts to be driven by another controller, and so on. We note that the noise is introduced as a point event, differently from Wiener approach that affects every infinitesimal time scale inducing the changes of differentiation rules. Indeed, $X(t)$ is the result of the action of a semi-Markov process [21, 36], defined by (1.2), (1.3) and the discrete states $1, \ldots, S$, on the differential equation (1.1).

[1] That is the analogue of the Fokker-Plank equation for this kind of processes.
[2] In Ref. [2] the notation has no explicit time dependency.

The mathematical definition of PDP is well-known by researchers working in probability calculus, operation research (e.g. see [10]) and stochastic hybrid systems (SHS), but it is not very popular between those working in applied sciences, nevertheless they use it, at least in a simplified form. This kind of modelling can be used for phenomenas where a deterministic motion is interrupted by a fast interaction that tends to randomize the motion for a small amount of time. We refer to models including the 'dichotomic noise', 'random telegraph process', 'binary noise', and so on, as driving terms for deterministic equations. As examples of such models, we quote: reacting-diffusing systems [17], biological dispersal [16], scattering of radiation [19], non-Maxwellian equilibriums [1, 4, 6, 12, 35], filtered telegraph signals [20, 32], ecological systems [24], harmonic oscillators [25].

From its definition we can understand that PDP, i.e. $X(t)$, is mostly locally deterministic, but the whole trajectory is not: it represents a random path and the meaningful informations can be represented by statistical functions. Formally we write:

$$F_s(x,y,t) := \mathbb{P}(X(t) \le x,\ y \le Y < y+dy,\ \text{ state} = s) \tag{1.4}$$

as the probability to find at time t the process $X(t)$ being in the state s, in a position less than x, and being past the time $Y \in [y, y+dy]$ for an infinitesimal time dy, since the last switching event.

The unknown functions $F_s(x,y,t),\ s = 1,\dots,S$ can be determined by a system of the Liouville-Master equations [2]:

$$\partial_t F_s(x,y,t) + A_s(x)\,\partial_x F_s(x,y,t) + \partial_y F_s(x,y,t) = -\lambda_s(y)\,F_s(x,y,t), \tag{1.5}$$

subject to the non-local boundary conditions:

$$F_s(x,0,t) = \sum_{j=1}^{S} q_{sj} \int_0^t F_j(x,y,t)\,\lambda_j(y)\,dy, \tag{1.6}$$

for $F_s : \mathcal{D} \to \mathbb{R}^+$ and $(x,y,t) \in \mathcal{D} := (\Omega \times [0,T] \times [0,T]) \subset \mathbb{R}^3$. At the initial time moment $t_0 = 0$ the Cauchy initial conditions are settled by:

$$F_s(x,y,0) = F_{0,s}(x)\delta(y), \tag{1.7}$$

where $\delta(y)$ is the δ-Dirac function, and functions $F_{0,s}(x)$ are the known initial marginal distribution functions of the processes subject to the conditions:

$$F_{0,s}(\Omega_a) = 0 \qquad \forall s = 1,\dots,S, \tag{1.8}$$

$$\sum_{s=1}^{S} F_{0,s}(\Omega_b) = 1. \tag{1.9}$$

Here, $\delta(y)$ has only a symbolic validity, with the aim to point out that the process starts without memory. Moreover, we assume that functions $F_s(x,y,t)$ are enough regular, and do not specify exactly the spaces of functions to which they belong, even if they are defined via (1.4).

The assumption $X(t) \in \Omega$ corresponds to

$$\partial_x F_s(x, y, t)|_{x=\partial\Omega} = 0, \tag{1.10}$$

since we are requiring that the probability for the process to be outside the interval Ω is zero. The main difficulty of this formulation deals with the non-local boundary condition (1.6), i.e. the value of the unknown function at the boundary $y = 0$ depends on the integral of this function over the interior of the definition domain.

The functions $\lambda_s(y) \geq 0$ are the *hazard rates*[3] [14, 29] defined as the ratio between the probability function $\psi(\tau)$ and its *survival function*:

$$\lambda_s(y) := \frac{\psi_s(y)}{\int_y^\infty \psi_s(t)\, dt}, \quad y \geq 0.$$

It relates the statistics of the PDF switching times (1.2) to the probability per unit of time that a transition event will occur, i.e. a transition rate, after the process has spent the time y since the last event. Therefore, y plays the role of *memory* because it represents the time from the last switch (see [3] for memoryless processes). The explicit dependence of λ on y makes both the statistics of the switching events and $X(t)$ be non-Markovian.

Eq. (1.5) represents the amount of probability change under the deterministic motion: if no transition event occurs in a small interval Δt, then we get $F_s(x, y, t + \Delta t) \simeq (1 - \lambda(y - \Delta t)\Delta t)\, F_s(x - \Delta x, y - \Delta t, t)$, with $\Delta x \approx A_s(x)\Delta t$. Eq. (1.6) evaluates the amount of process incoming into a new state just after a switching event, that is at $y = 0$, as a sum of the time spent in the previous states, weighted by the stochastic transition matrix $\{q_{ij}\}$.

The system of Eq. (1.5) consists of non-conservative hyperbolic PDEs, nevertheless, the solutions are subject to the total probability conservation law. We first define the distribution function regardless the memory state y as:

$$\mathcal{F}_s(x, t) := \int_0^t F_s(x, y, t)\, dy, \tag{1.11}$$

then the following total probability (norm) conservations are valid for $t \in \mathbb{R}^+$:

$$\lim_{x \to \Omega_b} \sum_{s=1}^{S} \mathcal{F}_s(x, t) = 1, \quad \lim_{x \to \Omega_a} \sum_{s=1}^{S} \mathcal{F}_s(x, t) = 0. \tag{1.12}$$

We verify these equations by integrating Eq. (1.5) over y, as follows:

$$\int_0^t (\partial_t F_s + A_s(x)\partial_x F_s + \partial_y F_s)\, dy = -\int_0^t \lambda_s(y) F_s\, dy$$

that is:

$$\partial_t \mathcal{F}_s - F_s(x, t, t) + A_s(x)\partial_x \mathcal{F}_s + F_s(x, t, t) - F_s(x, 0, t) = -\int_0^t \lambda_s(y) F_s\, dy$$

[3] Also named as hazard function, failure rate, force of mortality.

and inserting Eq. (1.6), we get:

$$\partial_t \mathcal{F}_s(x,t) + A_s(x)\partial_x \mathcal{F}_s(x,t) = \sum_{j=1}^{S}(q_{sj} - \delta_{sj}) \int_0^t \lambda_j(y) F_j(x,y,t)\, dy,$$

where δ_{sj} is the Kronecker symbol. By summing over all states and using the property of stochastic matrix of Eq. (1.3) we get

$$\sum_{s=1}^{S} (\partial_t \mathcal{F}_s(x,t) + A_s(x)\partial_x \mathcal{F}_s(x,t)) = 0.$$

If we suppose that $\lim_{x\to\partial\Omega} A_s(x)\partial_x \mathcal{F}_s(x,t) = 0$ then $\lim_{x\to\partial\Omega} \partial_t \sum_{s=1}^{S} \mathcal{F}_s = 0$. From Eqs. (1.8) and (1.9) we get (1.12).

These conditions make the problem well-posed, and, according to the definition of Eq. (1.4), the solutions are positive:

$$F_s(x,y,t) \geq 0, \tag{1.13}$$

and monotonic in x:

$$F_s(x + \Delta x, y, t) \geq F_s(x,y,t), \quad \text{for } \Delta x > 0. \tag{1.14}$$

In Sect. 3 we will give an explanation of these properties.

In Ref. [2] we have analysed convergence and error bounds of the numerical solution obtained with a first order difference method composed of the Courant-Isaacson-Rees scheme for the PDEs and quadrature for the non-local condition. Here, we investigate the conditions which guarantee that the numerical solution satisfies monotonicity and conservativity properties, in the sense of Eq. (1.12). This is a typical task of analysis for numerical methods of hyperbolic systems of conservation laws [18]

$$u_t + f(u)_x = 0.$$

For example, upwind, Godunov, TVD and WENO are well known schemes that preserve monotonicity and conservativity [9, 18, 23], although the discretization of the transport operator is still an open subject of research [34]. We note, that some research have been performed for non-conservative systems of the form

$$u_t + a(x,t)u_x = 0, \quad u_t + f(u)u_x = 0,$$

see, e.g. [28], and for coupled systems [7], but our equation has both of these two characteristics. Moreover, the coupling is non-local with respect to the memory, so it is interesting to see its influence on the features of the numerical solution.

In the next section we give a review of the numerical scheme defined in [2]. In Sect. 3 we prove a condition for convergence, similar to Ref. [2], that guarantees the monotonicity (non-decreasing) property of the numerical solution. The conservativity of the solution is investigated in Sect. 4. Sect. 5 is devoted to a brief description of a basic parallel algorithm and its scalability analysis. Finally, in Sect. 6 we show some performance results of the MPI implementation of the algorithm for a test problem.

2 The Numerical Scheme

It is convenient to perform the numerical integration along the characteristic lines $\xi = t - y$ (see [2]). With this new variable, we define the unknowns $\phi_s(x, y, \xi) = \phi_s(x, y, t - y) := F_s(x, y, t)$, so that Eq. (1.5) turns into

$$A_s(x)\,\partial_x \phi_s(x, y, \xi) + \partial_y \phi_s(x, y, \xi) = -\lambda_s(y)\phi_s(x, y, \xi), \tag{2.1}$$

for $0 < \xi < t$ and $0 < y < t$. In the same way Eq. (1.6) becomes

$$\phi_s(x, 0, t) = \sum_{l=1}^{S} q_{sl} \int_0^t \phi_l(x, y, \xi)|_{\xi=t-y} \lambda_l(y)\, dy. \tag{2.2}$$

The initial condition reads as

$$\phi_s(x, y, \xi)|_{\xi=-y} = F_{0,s}(x)\delta(y). \tag{2.3}$$

We will assume that similar conditions to Eqs. (1.10), and (1.12) are satisfied for $\phi_s(x, y, \xi)$, i.e.:

$$\partial_x \phi_s(x, y, \xi)|_{\xi=t-y} = 0, \quad x \in \partial\Omega, \tag{2.4}$$

$$\lim_{x\to\Omega_b} \sum_{s=1}^{S} \int_0^t \phi_s(x, y, \xi)|_{\xi=t-y}\, dy = 1, \tag{2.5}$$

$$\lim_{x\to\Omega_a} \sum_{s=1}^{S} \int_0^t \phi_s(x, y, \xi)|_{\xi=t-y}\, dy = 0, \quad \forall t \in [0, T].$$

These conditions state that the probability density function of the given process vanishes outside the interval $[\Omega_a, \Omega_b]$, and the normalizing condition (the second equation) is satisfied. We restrict the analysis to processes having a finite support, in order not only to simplify the numerical treatment, but also to get a non vanishing equilibrium solution on a finite interval, that is useful for the validation of the numerical scheme.

On the domain $\mathcal{D}$, we introduce a uniform mesh

$$\mathsf{M} := \{x_k, y_j, t_n\}, \quad \begin{cases} k = 0, \ldots, K, \\ j, n = 0, \ldots, N, \qquad N = T/\tau, \end{cases}$$

with step size h for the grid on x, and τ for y and t, so that we define the discrete known functions as ${}^lA_k := A_l(x_k)$ and ${}^l\lambda_j := \lambda_l(y_j)$, and the discrete solution

$${}^lF^n_{kj}, \qquad n = 0, \ldots, N, \quad j \le n$$

as an approximation to $F_l(x_k, y_j, t_n)$ at the mesh points. The change of variables $\xi = t - y$ corresponds to the discrete mapping on the mesh:

$$\bar{\mathsf{M}} := (k, j, i)|_{i=n-j} = (k, j, n), \tag{2.6}$$

where the index i identifies the set of mesh points lying on the characteristics lines. Therefore we get the following relation between the discrete solutions

$$F_l(x_k, y_j, t_n) = \phi_l(x_k, y_j, t_n - y_j) = \phi_l(x_k, y_j, \xi_i) \Rightarrow {}^lF^n_{kj} = {}^l\phi^{n-j}_{kj} = {}^l\phi^i_{kj}.$$

The numerical scheme is based on the discrete version of Eq. (2.1) obtained with a first order upwind scheme of the operator ∂_x [27]:

$$ {}^l\phi^i_{k,j+1} = {}^l\phi^i_{kj} - {}^lA_k \frac{\tau}{h} \left({}^l\phi^i_{k+\nu,j} - {}^l\phi^i_{k+\nu-1,j} \right) - \tau \, {}^l\lambda_j \, {}^l\phi^i_{kj}, \; i = 0, \ldots, N, \quad (2.7) $$

where $\nu = 1$ if ${}^lA_k < 0$, $\nu = 0$ if ${}^lA_k > 0$. For the Eq. (2.2), we substitute the integral with a quadrature scheme:

$$ {}^s\phi^i_{k,0} = \tau \sum_{l=1}^{S} q_{sl} \sum_{j=0}^{i} w_j^{(i)} \; {}^l\phi^{i-j}_{k\,j} \; {}^l\lambda_j, \qquad i > 0, \quad (2.8) $$

where $w_j^{(i)} \geq 0$ is a sequence of weights. The boundary condition (1.10) is included by requiring that ${}^l\phi^i_{0j} = {}^l\phi^i_{1j}$ and ${}^l\phi^i_{K-1,j} = {}^l\phi^i_{K,j}$.

The integration proceeds as follows (see [2] for details). Given the initial condition ${}^l\phi^0_{k,0} = \phi_l(x_k, 0, 0) = F_l(x_k, 0, 0)$, we calculate all the ${}^l\phi^i_{kj}$ from $j = 1$ to N with Eq. (2.7), along the characteristic line $i = 0$. In general for a given solution on the boundary ${}^l\phi^i_{k,0}$, we can find all ${}^l\phi^i_{kj}$ starting from $j = 1$ up to $N - i$ for a fixed characteristic line i (see curved arrows of Fig. 1).

But the starting values ${}^l\phi^i_{k,0}$ for upwind are unknown and have to be estimated by using the boundary integration (2.8) (see vertical dot-dashed arrows of Fig. 1). This is a system of equations for the unknowns ${}^l\phi^i_{k,0}$. When all ${}^l\phi^i_{kj}$ are known, the discrete distribution function can be retrieved by ${}^lF^n_{k,j} = {}^l\phi^i_{kj}|_{i=n-j}$. A quadrature formula for Eq. (1.11) gives us the memoryless distribution. The convergence of the numerical solution is ensured by the CFL-like condition studied in [2]:

$$ \tau \Big(\frac{\max_l \|A_l(x)\|_\infty}{h} + \max_l \|\lambda_l(y)\|_\infty \Big) < 1. \quad (2.9) $$

3 Monotonicity (Positivity) Analysis

Each function $F_s(x, y, t)$ represents a marginal probability density for y and distribution for x, this means that it is positive and monotone, as mentioned in (1.13) and (1.14). The validity of such properties can be shown from the following Theorem 1, jointly to the convergence theorem of [2], given for the numerical solution. In fact, by assuming that the analytical solution exists and is unique, from the cited theorems and for the vanishing limit of the step mesh size h, we prove that the solution is positive and monotone.

An alternative argument is given directly by the LME. Eq. (1.14) is equivalent to requirement that densities are positive, i.e. $\partial_x F_s(x, y, t) \geq 0$. If we derive Eq. (1.5) with respect to x, we obtain a totally hyperbolic [13] system for densities. This means that the characteristic curves of the system exist for all points of the domain. Therefore, if the initial condition is non-negative, the characteristic curves propagate non-negative functions into the solution domain. Also, the solution on the boundary $y = 0$, defined by the partial derivative with respect to x of Eq. (1.6), is positive being the integral of non-negative functions.

We wish that the same properties should be valid for the discrete solutions ${}^{l}F^{n}_{k,j}$ or ${}^{l}\phi^{i}_{k,j}$, otherwise the numerical solution could not be meaningful. It is known that [18, 23] for hyperbolic partial differential equations, the first order upwind scheme preserves the solution from oscillations, i.e. the positivity. Here we show that a similar result holds for the numerical scheme (2.7) – (2.8), i.e. that there exists a CFL-like condition that ensures the discrete solution are non-decreasing (monotone) in k (i.e. in x).

Theorem 1. *Let* ${}^{l}\phi^{i}_{k,j}$ *be the solution of* (2.7) – (2.8) *on the mesh* $\bar{\mathsf{M}}$*, for the Cauchy problem* ${}^{l}\phi^{0}_{k,0}$ *with* ${}^{l}\phi^{0}_{k+1,0} \geq {}^{l}\phi^{0}_{k,0} \geq 0$*, furthermore let* $A_s(x)$ *and* $\lambda_s(x)$ *be regular enough functions* $\forall s$*. If conditions*

$$\tau(2 \max_{l} \|A_l(x)\|_\infty / h + \max_{l} \|\lambda_l(y)\|_\infty) < 1, \tag{3.1}$$

$$(\max_{i} w_0^{(i)} \max_{l} {}^{l}\lambda_0)\tau < 1, \tag{3.2}$$

are satisfied, then ${}^{l}\phi^{i}_{k+1,j} \geq {}^{l}\phi^{i}_{k,j} \geq 0,\ \forall i,j \geq 0, k, l.$

Proof. Let $\alpha = \tau/h$ and define ${}^{l}p^{i}_{k,j} := ({}^{l}\phi^{i}_{k+1,j} - {}^{l}\phi^{i}_{k,j})/h$, by subtracting Eq. (2.7) evaluated at k and $k+1$, we get:

$${}^{l}p^{i}_{k,j+1} = (1 - \tau\lambda_j)\, {}^{l}p^{i}_{k,j} + \alpha(-A_{k+1}\, {}^{l}p^{i}_{k+\bar{\nu},j} + A_k\, {}^{l}p^{i}_{k+\nu-1,j}), \tag{3.3}$$

where $\nu = 0$ if $A_k > 0$, $\nu = 1$ if $A_k < 0$, $\bar{\nu} = 0$ if $A_{k+1} > 0$ and $\bar{\nu} = 1$ if $A_{k+1} < 0$. The aim is to find inequalities of the form ${}^{l}p^{i}_{k,j+1} \geq \beta\, {}^{l}p^{i}_{k,j}$ with $0 < \beta < 1$. We suppose that ${}^{l}p^{i}_{k,j} \geq 0$ for all k, then from Eq. (3.3) four cases have to be considered.

Case (i), A_{k+1} and $A_k \geq 0$:

$${}^{l}p^{i}_{k,j+1} = (1 - \tau\lambda_j)\, {}^{l}p^{i}_{k,j} + \alpha(A_k\, {}^{l}p^{i}_{k-1,j} - A_{k+1}\, {}^{l}p^{i}_{k,j}).$$

Then since $A_k \geq 0$ we get:

$${}^{l}p^{i}_{k,j+1} \geq (1 - \tau(A_{k+1}/h + \lambda_j))\, {}^{l}p^{i}_{k,j}.$$

The condition (3.1) ensures that there exists $\beta \in]0,1[$ such that: ${}^{l}p^{i}_{k,j+1} \geq \beta\, {}^{l}p^{i}_{k,j}$.

Case (ii), A_{k+1} and $A_k \leq 0$:

$${}^{l}p^{i}_{k,j+1} = (1 - \tau\lambda_j)\, {}^{l}p^{i}_{k,j} + \alpha(|A_{k+1}|\, {}^{l}p^{i}_{k+1,j} - |A_k|\, {}^{l}p^{i}_{k,j}),$$

so that

$${}^{l}p^{i}_{k,j+1} \geq (1 - \tau(|A_k|/h + \lambda_j))\, {}^{l}p^{i}_{k,j}$$

and as above ${}^{l}p^{i}_{k,j+1} \geq \beta\, {}^{l}p^{i}_{k,j}$.

Case (iii), $A_{k+1} \leq 0, A_k \geq 0$, $\bar{\nu} = 1, \nu = 0$:

$${}^{l}p^{i}_{k,j+1} = (1 - \tau\lambda_j)\, {}^{l}p^{i}_{k,j} + \alpha(|A_{k+1}|\, {}^{l}p^{i}_{k+1,j} + A_k\, {}^{l}p^{i}_{k-1,j}),$$

so we get that ${}^{l}p^{i}_{k,j+1} \geq (1 - \tau\, {}^{l}\lambda_j)\, {}^{l}p^{i}_{k,j}$ and therefore ${}^{l}p^{i}_{k,j+1} \geq \beta\, {}^{l}p^{i}_{k,j}$, for $\beta \in]0,1[$.

Case (iv), $A_{k+1} > 0, A_k < 0$, $\bar{\nu} = 0, \nu = 1$:

$$ {}^{l}p^{i}_{k,j+1} = (1 - \tau((A_{k+1} + |A_k|)/h + \lambda_j))\ {}^{l}p^{i}_{k,j} $$

and ${}^{l}p^{i}_{k,j+1} \geq \beta\ {}^{l}p^{i}_{k,j}$ is valid from (3.1).

We conclude that there exists such a $\beta \in]0,1[$ that ${}^{l}p^{i}_{k,j+1} \geq \beta\ {}^{l}p^{i}_{k,j}$, so that ${}^{l}p^{i}_{k,0} \geq 0$ implies ${}^{l}p^{i}_{k,j} \geq 0,\ \ j > 0$, that is:

$$ {}^{l}\phi^{i}_{k+1,0} \geq {}^{l}\phi^{i}_{k,0}, \text{ then } {}^{l}\phi^{i}_{k+1,j} \geq {}^{l}\phi^{i}_{k,j}, \text{ for all } i \geq 0, j > 0. \tag{3.4} $$

Now we show that if

$$ {}^{l}\phi^{i-j}_{k+1,j} \geq {}^{l}\phi^{i-j}_{k,j} \text{ for } j > 0, i \geq j, \text{ then } {}^{l}\phi^{i}_{k+1,0} \geq {}^{l}\phi^{i}_{k,0}. \tag{3.5} $$

We subtract side by side Eq. (2.8) for $k+1$ and k:

$$ {}^{s}p^{i}_{k,0} = \tau \sum_{l=1}^{S} q_{sl} \sum_{j=0}^{i} w^{(i)}_{j}\ {}^{l}p^{i-j}_{kj}\ {}^{l}\lambda_j, \quad \text{for } i > 0. $$

By moving the term with $j = 0$ to the left hand side, we get

$$ \sum_{l=1}^{S} \left(\delta_{sl} - q_{sl} w^{(i)}_{0}\ {}^{l}\lambda_0 \tau \right)\ {}^{l}p^{i}_{k0} = \tau \sum_{l=1}^{S} q_{sl} \sum_{j=1}^{i} w^{(i)}_{j}\ {}^{l}p^{i-j}_{kj}\ {}^{l}\lambda_j, \tag{3.6} $$

this is a system of equations for $l = 1, \cdots S$ unknowns ${}^{l}p^{i}_{k0}$, for fixed i and k. Let us write it as

$$ Q\mathbf{p} = b, $$

where $\mathbf{p}$ is ${}^{l}p^{i}_{k0}$. We are searching for a condition on Q, that is a Z-matrix, such that all components of $\mathbf{p}$ would be non-negative. Solutions can be found by the Jacobi method, i.e. we split $Q = D - G$ so that for the r-th iteration step:

$$ \mathbf{p}^{(r+1)} = (D^{-1}G)\mathbf{p}^{(r)} + D^{-1}b, $$

where $D = \mathrm{diag}(Q)$ and $G \geq 0$. The hypothesis (3.2) has two consequences. First $D > 0$, so that, b being non-negative, if $\mathbf{p}^{(r)} \geq 0$ for some r, all following $\mathbf{p}^{(r+\bar{r})}, \bar{r} > 0$ will be non-negative. Second the matrix Q is strictly diagonal dominant by column, in fact by summing over s, for the coefficients of (3.6) we get $(1 - \tau \max_i w^{(i)}_0 \max_l {}^{l}\lambda_0) > 0$. Therefore the sequence of non-negative $\mathbf{p}^{(r+\bar{r})}$ converges to the solution ${}^{l}p^{i}_{k0}$, which exists by hypothesis.

Finally, starting from the Cauchy initial condition ${}^{l}\phi^{0}_{k,0} \geq 0$, and applying (3.4) and (3.5) alternately, according to the scheme Fig. 1, the non-decreasing property for ${}^{l}\phi^{i}_{kj}$ holds for the whole definition domain. □

Remark 1. If in Theorem 1 $\max_i w^{(i)}_0 \leq 1$ then $(\max_i w^{(i)}_0 \max_l {}^{l}\lambda_0)\tau < 1$ and only the CFL-like condition (3.1) implies monotonicity.

Remark 2. If $A'_l(\bar{x}) \leq 0$, where $A_l(\bar{x}) = 0$ for $\bar{x} \in \Omega$ and $l = 1, \ldots S$, i.e. there are no repulsive fixed points, then the case (iv) never happens and the condition (2.9), rather than (3.1), is enough for ensuring the statement of the theorem.

4 Conservation Law for the Discrete Scheme

The evolution solution $\phi_s(x, y, \xi)$ is a subject to the total conservation law stated by (2.5). In terms of discrete solution, it is mimicked by the following discrete conservation law:

$$\tau \sum_l \sum_{j=0}^{i} v_j^{(i)} \, {}^l\phi_{K,j}^{i-j} = \tau \sum_l \sum_{j=0}^{i+1} v_j^{(i+1)} \, {}^l\phi_{K,j}^{i+1-j} + E_c^{(i)}. \tag{4.1}$$

Here $v_j^{(i)}$ and $v_j^{(i+1)}$ are the weights of the quadrature formulas at time t_i and t_{i+1} of (2.5), and $E_c^{(i)}$ is the conservation error committed by the numerical scheme between two time steps. For conservative numerical scheme $E_c^{(i)} = 0$, and the discrete total probability is equal to 1 for all i. For hyperbolic PDE's there is a lot of literature [18] on conservative numerical schemes. If we would have to solve the PDE equation (2.1), then we could apply one of the well known conservative schemes. But our mathematical model has two non-standard equations: the non-local boundary condition (2.2) and conservation equation (2.5). We will see that the proposed numerical scheme does not satisfy (4.1) exactly, in general, but under certain conditions we get a satisfactory approximation order of the conservation law. For the sake of simplicity, in what follows we assume that the same scheme is used for quadrature of (1.6) and (1.11), i.e. the equalities $v_j^{(i)} = w_j^{(i)}$ hold.

Theorem 2. *Assume $\phi_l(x, y, \xi)$ is a sufficiently regular solution of* (2.1) *on $\mathcal{D}$, under the boundary conditions* (2.2), (2.4) *and initial condition* (2.3), *and $\lambda_l(y) \in C^1([0, T])$. Assume that the hypothesis of Thm. 1 are satisfied. Let ${}^l\phi_{k,j}^i$ denote the numerical solution of Eqs.* (2.7) *and* (2.8) *on the mesh $\bar{M}$ at the time moment t_i, and assume the same sequence of weights for quadrature of* (1.6) *and* (1.11)*:*

$$\begin{cases} w_0^{(i+1)}, \quad w_1^{(i+1)} = w_0^{(i)} + d_1, \\ w_j^{(i+1)} = w_{j-1}^{(i)}, \quad j \geq 2. \end{cases} \tag{4.2}$$

Then there exist constants C_i, $a_i > 0$, such that the conservation error $E_c^{(i)}$ of (4.1) *is given by*

$$\begin{aligned} E_c^{(i)} &= \tau(1 - w_0^{(i+1)} a_i^{-1} - d_1) \sum_l {}^l\phi_{K,0}^i \\ &\quad + d_1 \tau^2 (1 - w_0^{(i+1)} a_i^{-1}) \sum_l {}^l\lambda_0 \, {}^l\phi_{K,0}^i - w_0^{(i+1)} (\tau^2 a_i^{-1} C_i + o(\tau^2)). \end{aligned} \tag{4.3}$$

Proof. The hypothesis of Theorem 1 ensures that functions ${}^l\phi_{k,j}^i$ own monotonicity and positivity, so that the probabilistic meaning is preserved and the calculation of the total probability (4.1) is meaningful. The CFL-like condition (3.1) ensures that the numerical solution approximates the analytical solution, so the discrete version of (2.4) can be applied.

We start from the left hand side of (4.1) and obtain an equivalence with the right hand side. By using the discrete Eq. (2.7) with $i \to i-j$ we write:

$$\sum_{j=0}^{i} w_j^{(i)}\ {}^l\phi_{k,j}^{i-j} = \sum_{j=0}^{i} w_j^{(i)}\ {}^l\phi_{k,j+1}^{i-j} + \tau \sum_{j=0}^{i} w_j^{(i)}\ {}^l\lambda_j\ {}^l\phi_{k,j}^{i-j} + \sum_{j=0}^{i} w_j^{(i)}\ {}^lA_k\{...\}, \quad (4.4)$$

where ${}^lA_k\{...\}$ is the convective upwind derivative that vanishes when $k = K$, due to the above mentioned boundary condition. The first sum in the r.h.s. can be rewritten to include the point $j = 0$, $t = t_{i+1}$:

$$\sum_{j=1}^{i+1} w_{j-1}^{(i)}\ {}^l\phi_{k,j}^{i+1-j} + d_1\ {}^l\phi_{k,1}^{i} - d_1\ {}^l\phi_{k,1}^{i} + w_0^{(i+1)}\ {}^l\phi_{k,0}^{i+1} - w_0^{(i+1)}\ {}^l\phi_{k,0}^{i+1}$$
$$= \sum_{j=0}^{i+1} w_j^{(i+1)}\ {}^l\phi_{k,j}^{i+1-j} - d_1\ {}^l\phi_{k,1}^{i} - w_0^{(i+1)}\ {}^l\phi_{k,0}^{i+1},$$

here we have used (4.2). From (4.1) and (4.4) we get:

$$E_c^{(i)} = - d_1\tau \sum_l\ {}^l\phi_{K,1}^{i} - w_0^{(i+1)}\tau \sum_l\ {}^l\phi_{K,0}^{i+1}$$
$$+ \tau \sum_l\ {}^lA_K \sum_{j=0}^{i} w_j^{(i)}\{...\} + \tau^2 \sum_l \sum_{j=0}^{i} w_j^{(i)}\ {}^l\lambda_j\ {}^l\phi_{K,j}^{i-j}. \quad (4.5)$$

Now we evaluate the first two summations of the r.h.s. at the point $k = K$. From (2.7), in the first sum we can use the equality

$${}^l\phi_{K,1}^{i} = {}^l\phi_{K,0}^{i} - {}^l\lambda_0\ {}^l\phi_{K,0}^{i}\tau.$$

From (2.8) and using relation $\sum_l q_{ls} = 1$, the second sum of (4.5) can be written as

$$\sum_l\ {}^l\phi_{k,0}^{i+1} = \tau \sum_l \sum_s q_{ls} \sum_{j=0}^{i+1} w_j^{(i+1)}\ {}^s\phi_{kj}^{i+1-j}\ {}^s\lambda_j$$
$$= \tau \sum_l \left(w_0^{(i+1)}\ {}^l\phi_{k0}^{i+1}\ {}^l\lambda_0 + \sum_{j=1}^{i+1} w_j^{(i+1)}\ {}^l\phi_{k,j}^{i+1-j}\ {}^l\lambda_j \right), \quad i > 0.$$

That is:

$$\sum_l\ {}^l\phi_{k0}^{i+1}(1 - w_0^{(i+1)}\ {}^l\lambda_0\tau) = \tau \sum_l \sum_{j=1}^{i+1} w_j^{(i+1)}\ {}^l\phi_{k,j}^{i+1-j}\ {}^l\lambda_j.$$

Since the hypothesis (3.2) of Thm. 1, the terms in parenthesis of the l.h.s. are positive, so that, by applying the average theorem, there exist $a_i > 0$ such that:

$$a_i \sum_l\ {}^l\phi_{K,0}^{i+1} = \tau \sum_l \sum_{j=1}^{i+1} w_j^{(i+1)}\ {}^l\phi_{K,j}^{i+1-j}\ {}^l\lambda_j.$$

Therefore Eq. (4.5) becomes:

$$E_c^{(i)} = - d_1\tau \sum_l {}^l\phi^i_{K0} + d_1\tau^2 \sum_l {}^l\lambda_0\, {}^l\phi^i_{K0} + \tau^2 \sum_l \sum_{j=0}^{i} w_j^{(i)}\, {}^l\phi^{i-j}_{k,j}\, {}^l\lambda_j$$
$$- \tau^2 w_0^{(i+1)} a_i^{-1} \sum_l \sum_{j=0}^{i} w_{j+1}^{(i+1)}\, {}^l\phi^{i-j}_{K,j+1}\, {}^l\lambda_{j+1}.$$

Since $\lambda_l(y)$ is continuous and differentiable, the last term can be evaluated by using equality ${}^l\lambda_{j+1} = {}^l\lambda_j + {}^l\lambda'_j\tau + o(\tau)$, where ${}^l\lambda'_j = \lambda'_l(y_j)$ and $o(\tau)$ means $\lim_{t\to 0} o(\tau)/\tau = 0$. Moreover, it follows from from Eq. (2.7) that ${}^l\phi^{i-j}_{K,j+1} = (1 - {}^l\lambda_j\tau)\, {}^l\phi^{i-j}_{K,j}$. After some algebra, by summarizing this result, we get:

$$-d_1\tau \sum_l {}^l\phi^i_{K0} + \tau^2(1 - w_0^{(i+1)} a_i^{-1}) \sum_l \sum_{j=0}^{i} w_j^{(i)}\, {}^l\phi^{i-j}_{K,j}\, {}^l\lambda_j - d_1\tau^2 w_0^{(i+1)} a_i^{-1}$$
$$\times \sum_l {}^l\phi^i_{K,0}\, {}^l\lambda_0 + d_1\tau^2 \sum_l {}^l\lambda_0\, {}^l\phi^i_{K,0} - w_0^{(i+1)}\tau^2 a_i^{-1} C_i + w_0^{(i+1)} o(\tau^2),$$

where $C_i = \tau \sum_l \sum_{j=0}^{i} w_j^{(i)}\, {}^l\phi^{i-j}_{K,j}({}^l\lambda'_j - {}^l\lambda_j^2)$. By using Eq. (2.8), summed over the states s, for the double summation, we get the proof. □

Remark 3. For quadrature of (2.8), we adopt the rectangle scheme [2]:

$$w_j^{(i)} = \begin{cases} 0 \ \text{ for } j = 0 \\ 1 \ \text{ for } j > 0 \end{cases} \qquad i > 0. \tag{4.6}$$

This scheme has the first order of approximation for the integration of the boundary condition (2.2), the same as the upwind approximation, so the overall numerical scheme has the first approximation order.

We note that for $w_0^{(i)} = 0$ the system of equations (2.8) becomes explicit. If the term ${}^l\phi^i_{k,0}$ is bounded, the error committed by suppressing it from the quadrature vanishes as $\tau \to 0$. We see that in Eq. (4.3) the first term is equal to zero, because $d_1 = 1$ and $w_0^{(i+1)} = 0$, and it remains only $E_c^{(i)} = \tau^2 \sum_l {}^l\lambda_0\, {}^l\phi^i_{K,0} \geq 0$, this means also that the conservation error has constant sign that tends to drain the total probability. Further, if ${}^l\lambda_0 = \lambda_l(0) = 0$, then $E_c^{(i)} = 0$, and the scheme becomes conservative, despite of the rough precision of quadrature.

Remark 4. The conservation error committed after the time step $N = T/\tau$ is the sum of the errors $E_c^{(i)}$, for $i = 0, \ldots N$, that is $T\mathcal{O}(\tau)$. For the discrete total probability conservation, we have

$$\tau \sum_l \sum_{j=0}^{N} w_j^{(N)}\, {}^l\phi^{N-j}_{K,j} = 1 - T\mathcal{O}(\tau), \quad \mathcal{O}(\tau) \geq 0.$$

Remark 5. The CFL condition (3.1) jointly with quadrature (4.6) is sufficient to get a reasonable the first order approximated numerical solution. By the way, when investigating a long time transient to the equilibrium solution, a small time step τ can be required to reduce the conservation error. Such a choice can alter the correctness of the approximation due to round-off errors.

5 The Parallel Algorithm

The parallel algorithm has been implemented as described in Sect. 2 and represented in Fig. 1. A matrix for iteration is not assembled, such as in [3]: the numerical solution is calculated step-by-step, according to (2.7) and (2.8). The main novelty, with respect to numerical solution of PDE's, is the presence of a quadrature due to the non local boundary condition (2.8). However, the variable change (2.6) does not affect the possibility to distribute the computational load between processors.

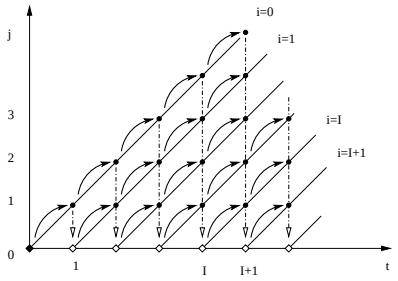

Figure 1. Representation of the integration scheme for the regular mesh on (t, y) plane. Full curved arrows: upwind step of (2.7). Dot-dashed vertical arrows: quadrature of (2.8).

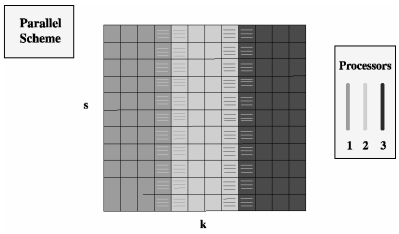

Figure 2. Schematic representation of the splitting of the computational load into three stripes.

5.1 Domain decomposition and scalability analysis

A basic way consists in splitting the products on the spatial index k for each temporal step, i.e. we use a domain decomposition with *striped partitioning* (see Fig. 2). Due to upwind that involves indexes $k-1$ or $k+1$ for computing the step k, each process associated to a stripe requires communication with the two neighbouring stripes (see dashed cells of Fig. 2).

In order to analyse the scalability of the partitioning scheme [15] we define the following terms: p is the number of processors, t_w is the time for transferring bytes between two processors, t_c is the unit computation time, $M = SKN$ is the mesh size, $K_{loc} = K/p$ is the portion of the mesh that is distributed to each processor (we assume K_{loc} to be integer for a sake of load balance). $T_p(i)$ and $T_e(i)$ are correspondingly the parallel and serial execution time needed to calculate the solution ${}^{l}\phi_{kj}^{i+1}$ at the time step i, and $T_p = \sum_{i=0}^{N} T_p(i)$, $T_e = \sum_{i=0}^{N} T_e(i)$ the total times. T_0 is the total overhead due to the time spent in

communications between processors, $S_p = T_e/T_p$ is the speed-up and $E_p = S_p/p$ is the efficiency.

For striping, the amount of communication required by a partition is $T_0 = t_s + 2t_w SN$, where t_s is the start up time, the calculation time for upwind is $t_c K_{loc} S i$ and quadrature $t_c K_{loc} S^2 i$, having assumed the same time t_c for both numerical steps. The parallel run time at time i is given by:

$$T_p(i) = K_{loc} t_c S(S+1)i + t_s + 2t_w SN + C_2 \log(p),$$

where the last term results from overhead due to synchronization. The serial time is

$$T_e(i) = K t_c S(S+1)i.$$

We are interested in the total parallel computation time

$$T_p = \sum_{i=1}^{N} T_p(i) = K_{loc} t_c S(S+1)\frac{N^2}{2} + t_s N + 2t_w SN^2 + C_2 \log(p)N,$$

and the total serial time:

$$T_e = \sum_{i=1}^{N} T_e(i) = K t_c S(S+1)\frac{N^2}{2},$$

valid for large N. We note that terms $C_2 \log(p)N$ and $t_s N$ can be neglected in an asymptotic analysis. So we have the speed-up:

$$S_p \approx \frac{p}{1 + 4pt_w/Kt_c(S+1)} \tag{5.1}$$

and the efficiency:

$$E_p \approx \frac{1}{1 + 4pt_w/Kt_c(S+1)}. \tag{5.2}$$

From this equations we see that the efficiency remains constant (isoefficiency) if the number of processors p scales as the size of the space mesh K.

Here we give a sketch of the algorithm implemented by using the MPI libraries [30].

```
// Finite difference method for Liouville-Master Equation

MPI_Init();

IF (Process == 0)
BEGIN
        Parameters reading.
        NEW phi.   // allocates memory for the initial condition
END

   // All processes:
   MPI_Bcast( common parameters )
```

```
   NEW local_phi.   // allocates memory for the solution of
                       the local process

   // Breaks matrix phi into local matrixes for all processes
   MPI_Scatter(init. cond. phi, local init. cond. loc_phi)


   // main time cycle:

WHILE ( n < N )
BEGIN
        // Communicate spatial boundaries between submatrixes:
        COMM_BOUND( proc,loc_phi[end] -> proc+1,loc_phi[-1]  )
        COMM_BOUND( proc+1,loc_phi[0] -> proc,loc_phi[end+1] )

        IF (Process == 0)  // save data on the main process.
        BEGIN
            SAVE_DATAS
        END

        FOR s:=1 TO S   // states cycle
        BEGIN
            FOR j:=0 TO jMAX // memory cycle:
            BEGIN
                FOR k:=0 TO kMAX // spatial cycle:
                BEGIN
                   // Updates loc_phi to new time step
                   UPWIND(loc_phi)
                END
            END
        END

        // Calculates boundary for j=0
        BOUNDARY_INTEGRATION(loc_phi)

     n=n+1
END
MPI_Finalize();
```

First, process 0 reads the parameters and prepares the initial condition, then common parameters are broadcasted to all processes. Each process allocates memory for the matrix that will contain the solution, an `MPI_Scatter` distribute the initial condition to all processes.

Then the main temporal cycle starts. The function COMM_BOUND implements the exchange of the boundary of the matrix, by using a task with a pair of `MPI_Send` and `MPI_Recv` functions. SAVE_DATAS takes care of saving partial computation on permanent memory. UPWIND and BOUNDARY_INTEGRATION, implementing Eqs. (2.7) and (2.8), are executed until

the end of the integration (see Fig. 3).

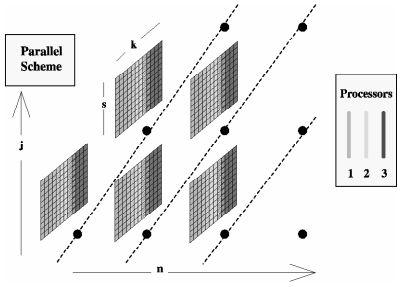

Figure 3. Schematic representation of the computing load of the numerical algorithm.

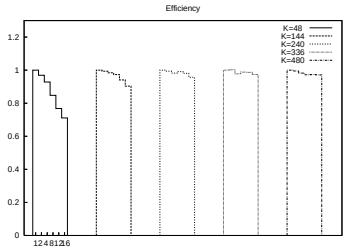

Figure 4. Results of the efficiency test for the McFadden problem. Data are grouped in five histograms. Each one represents the efficiency vs. the number of processes involved in the computation, for a fixed K.

6 Performance Tests

Tests for the parallel algorithm have been executed on the IBM BCX/5120 Cluster located at CINECA Supercomputing Centre in Italy. BCX is an IBM BladeCenter LS21 Cluster, made 1280 4-way nodes (blades). Each computing node contains 2 Opteron dual-core processors, with a clock of 2.4 GHz. All the nodes are interconnected to each other through a Infiniband network, capable of a maximum bandwidth of 10 Gbit/s between each pair of nodes. The global peak performance of BCX is of 26.6 TFlops. The code has been compiled with the Intel `icc` compiler, with optimization option `-O3`, and by including the OpenMPI-1.2.5 libraries.

As above described, the finite difference scheme (2.7) – (2.8) has been applied, with quadrature weights (4.6), to solve the problem of filtering of dichotomous noise with McFadden [31] interval PDF treated in [2]. The Cauchy problem for starting the numerical integration has been set according to (1.7):

$$ {}^sF^0_{k0} = \begin{cases} 0, & k < 0, \\ 0.5/(2\tau), & k = 0, \\ 1/(2\tau), & k > 0, \end{cases} \qquad {}^sF^0_{kj} = 0, \quad j > 0 $$

for all $s = 1, 2$. This choice approximates (1.7) with $F_{0,s}(x) = H(x)$, where $H(x)$ is the Heaviside function: $H(x) = 0$ if $x < 0$, $H(x) = 0.5$ if $x = 0$ and $H(x) = 1$ if $x > 0$. Such Cauchy condition for the Liouville-Master Equation, also named the Riemann problem, corresponds to having placed the process $X(t)$ at the initial position $X_0 = 0$, to an equiprobable random initial state, $s = 1$ or $s = 2$, and having spent a vanishing time in it (i.e. $\delta(y)$ in (1.7)). The other parameters are:

$$ q_{11} = q_{22} = 0, \;\; q_{12} = q_{21} = 1, \;\; \gamma_1 = \gamma_2 = 1, \;\; W_1 = -W_2 = 1. $$

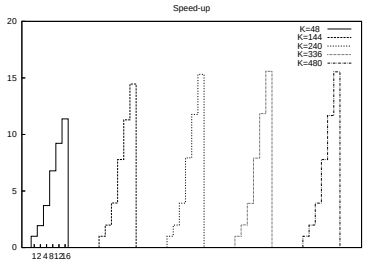

Figure 5. Results of the speed-up test for the McFadden problem. Data are grouped in five histograms. Each one represents the speed-up vs. the number of processes involved in the computation, for a fixed K.

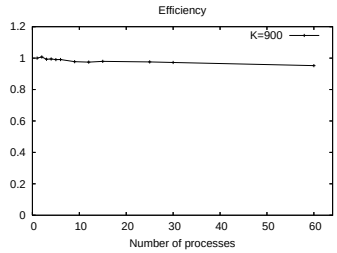

Figure 6. Results of the efficiency test for the McFadden problem with 900 spatial mesh points.

Then the numerical integration proceeds as discussed at the end of Sect. 2 until T.

The CPU time for solving the McFadden problem till $T = 3.249$ with a fixed temporal step $\tau = 0.0015$ has been measured. In order to reduce fluctuations in computation time, caused by other concurrent processes running on the cluster, each test was repeated eight times, then averaged. We note that averaged results were affected by $2 \div 5\%$ standard deviation error. Moreover, in order to do tests on an uniform communication network, only one process on a node was used. Up to four processes could run on a node, causing a mismatch with the theoretical analysis due to the wider intra-node (and intra-core) than node-node communication bandwidth, and, due to the concurrency in using global memory on multi-core nodes (the well-known botle-neck of such type architeture) efficiency of the parallel can degrade if 2-4 processes are run on one node [8, 33].

Speed-up, S_p and Efficiency, E_p, have been calculated by different combinations of K and p.

Fig. 4 shows the efficiency versus the number of processors $p = \{1, 2, 4, 8, 12, 16\}$, for five groups of spatial mesh size: $K = \{48, 144, 240, 336, 480\}$. The same scheme is used for the representation of the speed-up of Fig. 5. In Figs. 6, 7 and 8 we show similar tests for $K = 900$, $T = 3.25$, $\tau = 0.001$. All plots follow the expected behaviour of Eqs. (5.1) and (5.2), i.e. the efficiency decreases when the number of processes increases and the speed-up decrease is less enhanced for small size problems. Also, the efficiency degrades faster for small size problems (see Fig. 4 with $K = 48$). Isoefficiency result test ($\tau = 0.0015$, $T = 3.249$) is reported in Fig. 9 as the efficiency versus the number of processes, when $K_{loc} = K/p$ is kept fixed. The three lines, related to $K_{loc} = \{9, 12, 15\}$, confirm that the efficiency improves when K/p increases according to Eq. (5.2), with a slight decrement for increasing p.

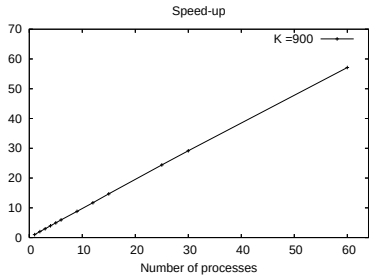

Figure 7. Results for the speed-up test for the McFadden problem with 900 spatial mesh points.

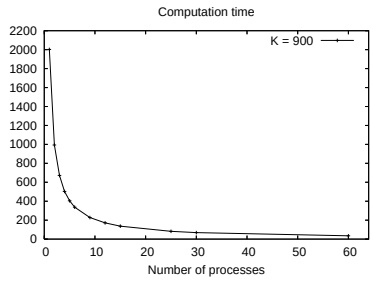

Figure 8. Computation time, in seconds, vs. the number of processes, for the McFadden problem with 900 spatial mesh points.

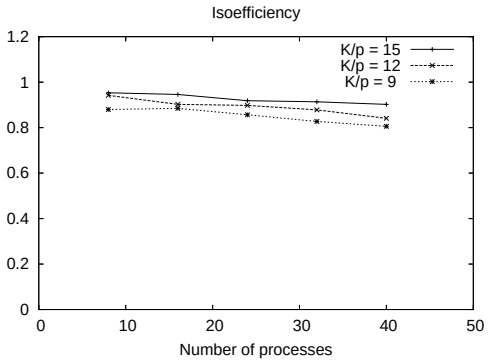

Figure 9. Efficiency vs. number of processes, when the fixed ratio of K/p equals to $9, 12, 15$.

7 Summary and Conclusions

In this paper we have completed the basic analysis, started in [2], on the properties of the numerical solution of the Liouville Master Equation for a class piecewise deterministic process. We have found that the CFL-like condition (3.1) and the sequence of weights (4.6), plus some other conditions, are able to guarantee the monotonicity and the total conservativity of the solution of the first order numerical scheme, which is derived by using the Courant-Isaacson-Rees scheme and a direct quadrature. We note that the system of equations under consideration is non-standard due to the non-locality of the boundary condition. By using the proposed numerical scheme we can get one of the first algorithms for the calculation of the statistical properties of this kind of stochastic processes, directly from a LME. Moreover, this scheme has given us a possibility to study the effects on the numerical solution of the well-known discretization schemes in the case of this not so well-known problem. Future work will be done to get high order numerical approximations, better conservation discrete properties, and extension to higher dimensional space problems. Finally, we have shown some tests on a parallel implementation of the associated

numerical algorithm.

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