PARTICLE APPROXIMATION OF FIRST ORDER SYSTEMS*

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Introduction

By particle methods of approximation of time-dependent problems in partial differential equations, we mean numerical methods where, for each time t, the exact solution is approximated by a linear combination of Dirac measures in the space variables x. Although these methods have not yet a very large range of applications as that of classical methods (finite difference methods, finite element methods or even spectral methods), they provide an effective way of solving convection-dominated problems. In fact, particle methods are commonly used in some problems of Physics and Fluid Mechanics.

In Physics, these methods have been considered very early for the numerical solution of kinetic equations such as Boltzmann, Vlasov or Fokker-Planck equations and have been mainly based on a Monte Carlo methodology. More recently, particle methods have received a great deal of attention in Plasma Physics and are now currently used in a number of physical problems. In that direction, see the book of Hockney and Eastwood[9].

In Fluid Mechanics, vortex simulations of incompressible fluid flows at high Reynolds numbers have been first introduced by Rosenhead and subsequently developed by Chorin, Leonard and Rehbach among other contributors (see the survey of Leonard[10]). On the other hand, particle in cell (P.I.C.) methods have been introduced by Harlow[8] for the numerical computation of compressible multifluid flows. Recently Gingold and Monaghan[7] have proposed a new particle method which may be viewed as an improvement of the P.I.C. method.

The purpose of this paper is to review some recent results recently obtained by the author in joint works with S. Gallic and J. Ovadia concerning the particle approximation of hyperbolic and parabolic systems and which are related to the approach of Gingold and Monaghan. In Section 1, we describe a particle method of approximation of first-order linear symmetric systems. Convergence results are stated in Section 2: they generalize previous results of the author on the particle approximation of hyperbolic equations[12,13]. We show in Section 3 how to adapt the method to the nonlinear hyperbolic system of gas dynamics, hence generalizing the ideas of [7]. Finally, Section 4 is devoted to the extension of the method to the numerical treatment of convection-diffusion equations.

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For a mathematical study of the vortex method, we refer to Beale and Majda[1,2] and the thesis of Cottet[3]; see also [12]. For a proof of convergence of the particle method for the Vlasov–Poisson equations arising in Plasma Physics, see [4].

§ 1. Description of the Particle Method

Let us consider the Cauchy problem for first-order systems written in conservation form

$$\begin{cases} \frac{\partial u}{\partial t}+\sum_{i=1}^{n}\frac{\partial}{\partial x_i}(A^i u)+A^0 u=f, & x\in \mathbb{R}^n,\ t>0, \\ u(x,0)=u_0(x). \end{cases} \tag{1.1}$$

Here $u=u(x,t)$, $f=f(x,t)$ are column vectors with p components and $A^i=A^i(x,t)$, $0\leqslant i\leqslant n$, are $p\times p$ matrices. Setting $Q_T=\mathbb{R}^n\times]0,T[$, $T>0$, we assume that

$$\begin{cases} A^i\in L^\infty(Q_T;\,\mathfrak{L}(\mathbb{R}^p)), & 0\leqslant i\leqslant n, \\ \frac{\partial A^i}{\partial x_j}\in L^\infty(Q_T;\,\mathfrak{L}(\mathbb{R}^p)), & 1\leqslant i,\ j\leqslant n \end{cases} \tag{1.2}$$

and

$$A^i(x,t)=A^i(x,t)^T,\quad 1\leqslant i\leqslant n. \tag{1.3}$$

Then, given $u_0\in L^2(\mathbb{R}^n)^p$ and $f\in L^1(0,T;\,L^2(\mathbb{R}^n)^p)$, it is a classical result that Problem (1.1) has indeed a unique weak solution $u\in C^0(0,T;\,L^2(\mathbb{R}^n)^p)$.

Assume next that the data A^i, $0\leqslant i\leqslant n$, u_0 and f are continuous functions. In order to approximate the solution u of Problem (1.1) by a particle method, we begin by introducing a system of moving coordinates. We write

$$A^i=a^iI+B^i,\quad 1\leqslant i\leqslant n, \tag{1.4}$$

where I is the $p\times p$ identity matrix and the functions a^i are continuous and satisfy

$$a^i,\ \frac{\partial a^i}{\partial x_j}\in L^\infty(Q_T),\quad 1\leqslant i,\ j\leqslant n. \tag{1.5}$$

Then, we consider the differential system

$$\frac{dx}{dt}=a(x,t),\quad a=(a_1,\cdots,a_n), \tag{1.6}$$

whose solutions are the characteristic curves associated with the first order differential operator

$$\frac{\partial}{\partial t}+\sum_{i=1}^{n}a_i\frac{\partial}{\partial x_i}.$$

We denote by $t\to x(\xi,t)$ the unique solution of (1.6) which satisfies the initial condition

$$x(0)=\xi,\quad \xi\in\mathbb{R}^n \tag{1.7}$$

and we set

$$J(\xi,t)=\det\left(\frac{\partial x_i}{\partial \xi_j}(\xi,t)\right). \tag{1.8}$$

Then it is a simple and classical matter to check that

$$\frac{\partial J}{\partial t}(\xi,t)=J(\xi,t)(\operatorname{div} a)(x(\xi,t),t),\quad \operatorname{div} a=\sum_{i=1}^{n}\frac{\partial a^i}{\partial x_i}. \tag{1.9}$$

Note that (ξ, t) may be viewed as a system of Lagrangian coordinates associated with the "velocity" vector field $a=(a_1, \cdots, a_n)$.

The next step consists in deriving a general approximation of a continuous function by a linear combination of Dirac measures. Let $g\in C^0(\mathbb{R}^n)$ and let $\varphi\in C_0^0(\mathbb{R}^n)$, i.e., φ is a continuous function with compact support. By using the change of variables $x=x(\xi, t)$, we have

$$\int_{\mathbb{R}^n} g\varphi\, dx=\int_{\mathbb{R}^n} g(x(\xi, t))\varphi(x(\xi, t))J(\xi, t)d\xi.$$

Now, if we approximate the integral

$$\int_{\mathbb{R}^n} \psi\, d\xi \quad \text{by} \quad \sum_{k\in K} \omega_k \psi(\xi_k)$$

for some set $(\xi_k, \omega_k)_{k\in K}$ of points $\xi_k\in\mathbb{R}^n$ and weights $\omega_k\in\mathbb{R}$, we obtain

$$\int_{\mathbb{R}^n} g\varphi\, dx \simeq \sum_{k\in K} w_k(t) g(x_k(t))\varphi(x_k(t)),$$

where

$$x_k(t)=x(\xi_k, t), \quad w_k(t)=\omega_k J(\xi_k, t), \quad k\in K. \tag{1.10}$$

This amounts to approximate the function g by the measure

$$\sum_{k\in K} w_k(t) g(x_k(t))\delta(x-x_k(t)),$$

where $\delta(x-x_0)$ means the Dirac measure located at the point $x_0\in\mathbb{R}^n$ and h refers to a discretization parameter to be specified later on.

We are now looking for a *particle approximation* u_h of the solution u of Problem (1.1) of the form

$$u_h(x, t)=\sum_{k\in K} w_k(t) u_k(t)\delta(x-x_k(t)), \tag{1.11}$$

where $u_k(t)$ stands for an approximation of $u(x_k(t), t)$. In fact, we need to associate with the measure $u_h(\cdot, t)$ a continuous function $u_h^\varepsilon(\cdot, t)$ which will approximate the exact solution $u(\cdot, t)$ in a more classical sense. Therefore, we introduce a cut-off function $\zeta\in C_0^1(\mathbb{R}^n)$, i.e., a C^1 function with compact support, such that

$$\int_{\mathbb{R}^n} \zeta\, dx=1.$$

We set for all $\varepsilon>0$

$$\zeta_\varepsilon(x)=\frac{1}{\varepsilon^n}\zeta\left(\frac{x}{\varepsilon}\right) \tag{1.12}$$

and

$$u_h^\varepsilon(\cdot, t)=u_h(\cdot, t)*\zeta_\varepsilon$$

or equivalently

$$u_h^\varepsilon(x, t)=\sum_{k\in K} w_k(t) u_k(t)\zeta_\varepsilon(x-x_k(t)). \tag{1.13}$$

It remains to derive a discretized form of Problem (1.1) in order to define the unknown functions $t\to u_k(t)$, $k\in K$, and therefore the approximate solutions u_h and u_h^ε. Using (1.4), the first equation (1.1) becomes

$$\frac{\partial u}{\partial t}+\sum_{i=1}^n \frac{\partial}{\partial x_i}(a^i u)+\sum_{i=1}^n \frac{\partial}{\partial x_i}(B^i u)+A^0 u=f \quad \text{in } Q_T.$$

We first notice that we have in the sense of distributions on Q_T

$$\frac{\partial u_h}{\partial t}+\sum_{i=1}^{n}\frac{\partial}{\partial x_i}(a^i u_h)=\sum_{k\in K}\frac{d}{dt}(w_k(t)u_k(t))\delta(x-x_k(t)). \tag{1.14}$$

Indeed, let φ be in $C_0^\infty(Q_T)$; we have by (1.6)

$$\frac{d}{dt}\varphi(x(\xi,t),t)=\Big(\frac{\partial\varphi}{\partial t}+\sum_{i=1}^{n}a^i\frac{\partial\varphi}{\partial x_i}\Big)(x(\xi,t),t).$$

Hence

$$\Big\langle\frac{\partial u_h}{\partial t}+\sum_{i=1}^{n}\frac{\partial}{\partial x_i}(a^i u_h),\ \varphi\Big\rangle=-\int_0^T\sum_{k\in K}w_k u_k(t)\Big(\frac{\partial\varphi}{\partial t}+\sum_{i=1}^{n}a^i\frac{\partial\varphi}{\partial x^i}\Big)(x_k(t),t)dt$$

$$=-\int_0^T\sum_{k\in K}w_k u_k(t)\frac{d}{dt}\varphi(x_k(t),t)dt$$

and (1.14) follows.

Next, for deriving a particle approximation of $\dfrac{\partial}{\partial x_i}(B^i u_h)$, we write

$$\frac{\partial}{\partial x_i}(B^i u_h)=\frac{\partial B^i}{\partial x_i}u_h+B^i\frac{\partial u_h}{\partial x_i}\simeq\frac{\partial B^i}{\partial x_i}u_h+B^i\frac{\partial u_h^\varepsilon}{\partial x_i}$$

and we use the following approximations for B^i and $\dfrac{\partial B^i}{\partial x_i}$:

$$B^i\simeq\sum_{k\in K}w_k(t)B_k^i(t)\delta(x-x_k(t)),$$

$$\frac{\partial B^i}{\partial x_i}\simeq\sum_{k\in K}w_k(t)B_k^i(t)\frac{\partial\zeta_\varepsilon}{\partial x_i}(x-x_k(t)),$$

where $B_k^i(t)=B^i(x_k(t),t)$. This gives

$$\frac{\partial}{\partial x_i}B^i u_h\simeq\sum_{k,l\in K}w_k(t)w_l(t)(B_k^i(t)u_l(t)$$

$$+B_l^i(t)u_k(t)\frac{\partial\zeta_\varepsilon}{\partial x_i}(x_k(t)-x_l(t))\delta(x-x_k(t)). \tag{1.15}$$

Finally, we have

$$A^0u_h=\sum_{k\in K}w_k(t)A_k^0(t)u_k(t)\delta(x-x_k(t)) \tag{1.16}$$

and we consider the following approximation of f

$$f\simeq\sum_{k\in K}w_k(t)f_k(t)\delta(x-x_k(t)), \tag{1.17}$$

where $A_k^0(t)=A^0(x_k(t),t)$ and $f_k(t)=f(x_k(t),t)$.

Now, using (1.14), (1.15), (1.16) and (1.17), we find that a (semi-) discretized form of Problem (1.1) consists in finding functions $t\in[0,T]\to u_k(t)\in\mathbf{R}^p$, $k\in K$, solutions of the differential system

$$\frac{d}{dt}(w_k u_k)+w_k\Big\{\sum_{i=1}^{n}\sum_{l\in K}w_l(B_k^i u_l+B_l^i u_k)\frac{\partial\zeta_\varepsilon}{\partial x_i}(x_k-x_l)+A_k^0u_k\Big\}=w_k f_k, \tag{1.18}$$

$$u_k(0)=u_0(\xi_k),\quad k\in K. \tag{1.19}$$

On the other hand, using (1.6), (1.7), (1.9) and (1.10), we note that the functions $t\to x_k(t)$ and $t\to w_k(t)$, $k\in K$, can be characterized as the solutions of the differential equations

$$\begin{cases} \dfrac{dx_k}{dt} = a(x_k, t), \\ x_k(0) = \xi_k \end{cases} \tag{1.20}$$

and

$$\begin{cases} \dfrac{dw_k}{dt} = w_k(\operatorname{div} a)(x_k, t), \\ w_k(0) = \omega_k. \end{cases} \tag{1.21}$$

The numerical method is thus defined by the equations (1.18), (1.19), (1.20) and (1.21). It remains however to perform a suitable time-discretization in order to obtain a practically implementable numerical scheme.

If problem (1.1) is a purely convective problem, i.e., if $B^i=0$, $1\leqslant i\leqslant n$, $A^0=0$, $f=0$, (1.18) reduces to

$$\frac{d}{dt}(w_k u_k)=0.$$

Hence, in that case, the problem is solved by moving the particles k along the characteristic curves $t\to x_k(t)$ without changing their weights $w_k u_k$. On the other hand, when there is no convection, i.e., when $a^i=0$, $1\leqslant i\leqslant n$, the positions of the particles remain fixed but their weights are modified through (1.18). In fact, the scheme (1.18) can be viewed as a *generalized finite-difference scheme* using an arbitrary moving grid defined by the positions of the particles.

It is often required in practice that the analogue of the conservation property

$$\frac{d}{dt}\int_{R^n} u(x, t)dx+\int_{R^n} A^0(x, t)u(x, t)dx=\int_{R^n} f(x, t)dx$$

holds for any numerical approximation of the solution of Problem (1.1). Hence, we require that

$$\frac{d}{dt}\Big(\sum_{k\in K} w_k(t)u_k(t)\Big)+\sum_{k\in K} w_k(t)A_k^0(t)u_k(t) = \sum_{k\in K} w_k(t)f_k(t). \tag{1.21$'$}$$

Note that this is indeed the case if the cut-off function ζ satisfies the condition

$$\zeta(-x)=\zeta(x) \quad \forall x\in\mathbb{R}^n. \tag{1.22}$$

In fact, using (1.22), we have

$$\frac{\partial\zeta_\varepsilon}{\partial x_i}(-x)=-\frac{\partial\zeta_\varepsilon}{\partial x_i}(x),$$

so that (interchange k and l)

$$\sum_{k,l\in K} w_k w_l(B_k^i u_l+B_l^i u_k)\frac{\partial\zeta_\varepsilon}{\partial x_i}(x_k-x_l)=0$$

and (1.21) follows at once.

§ 2. Convergence of the Particle Method

For simplicity, we shall restrict ourselves in this section to the model situation where

$$K=\mathbb{Z}^n,\ \xi_k=(k_i h)_{1\leqslant i\leqslant n},\ \omega_k=h^n \quad \forall k=(k_1, \cdots, k_n)\in\mathbb{Z}^n. \tag{2.1}$$

In this case, we are able to prove a precise convergence result for the particle method. Before stating the theorem, we need to introduce for any integer $m\geqslant1$ and any $q\in[1,\infty]$ the classical Sobolev spaces

$$W^{m,q}(\mathbb{R}^n)=\{v\in L^q(\mathbb{R}^n);\ \partial^\alpha v\in L^q(\mathbb{R}^n)\leqslant|\alpha|\leqslant m\}$$

provided with the norms

$$\|v\|_{m,q,\mathbb{R}^n}=\Big(\sum_{|\alpha|\leqslant m}\|\partial^\alpha v\|^q_{L^q(\mathbb{R}^n)}\Big)^{1/q}$$

and semi norms

$$|v|_{m,q,\mathbb{R}^n}=\Big(\sum_{|\alpha|=m}\|\partial^\alpha v\|^q_{L^q(\mathbb{R}^n)}\Big)^{1/q}$$

for $q<+\infty$ and their usual modifications for $q=+\infty$.

We begin by considering the case

$$B^i=0,\quad 1\leqslant i\leqslant n, \tag{2.2}$$

so that equation (1.18) reduces to

$$\frac{d}{dt}(w_k u_k)+w_k A_k^0 u_k=w_k f_k.$$

Assuming that the solution u of Problem (1.1) is smooth enough, we set

$$e_k(t)=u(x_k(t),\ t)-u_k(t).$$

Since we have by (1.6), (1.9) and (1.10)

$$\frac{d}{dt}(w_k(t)u(x_k(t),\ t))=w_k(t)\Big(\frac{\partial u}{\partial t}+\sum_{i=1}^n\frac{\partial}{\partial x_i}(a_i u)\Big)(x_k(t),\ t)$$

we obtain

$$\begin{cases}\dfrac{d}{dt}(w_k e_k)+w_k A_k^0 e_k=0,\\ e_k(0)=0\end{cases}$$

and therefore $e_k(t)=0$, $k\in\mathbb{Z}^n$.

Hence, setting for any $v\in C^0(\mathbb{R}^n)$

$$\pi_h(t)v=h^n\sum_{k\in\mathbb{Z}^n}J(\xi_k,\ t)v(x_k(t))\delta(x-x_k(t))$$

and

$$\pi_h^\varepsilon(t)v=\pi_h(t)v*\zeta_\varepsilon, \tag{2.3}$$

we see that, in the case (2.2), we have

$$u_h^\varepsilon(\cdot,\ t)=\pi_h^\varepsilon(t)u(\cdot,\ t).$$

Therefore, finding a bound for the error $u(\cdot,\ t)-u_h^\varepsilon(\cdot,\ t)$ exactly reduces in the case (2.2) in estimating the approximation error:

$$u(\cdot,\ t)-\pi_h^\varepsilon(t)u(\cdot,\ t).$$

Let us then state an approximation theorem.

Theorem 1. *Let $m>n$ be an integer. We assume that*

$$a^i\in L^\infty(0,\ T;\ W^{m+1,\infty}(\mathbb{R}^n)),\quad 1\leqslant i\leqslant n. \tag{2.4}$$

We assume in addition that the cut-off function ζ has a compact support and satisfies the following conditions:

(i) *there exists an integer $r\geqslant1$ such that*

$$\begin{cases} \int_{\mathbb{R}^n} \zeta\, dx = 1, \\ \int_{\mathbb{R}^n} x^\alpha \zeta\, dx = 0 \quad \forall \alpha \in \mathbb{N}^n \text{ with } 1 \leqslant |\alpha| \leqslant r-1 \text{ [1)]}; \end{cases} \tag{2.5}$$

(ii) *the function* ζ *belongs to the space* $W^{m+s,1}(\mathbb{R}^n)$ *for some other integer* $s \geqslant 0$.
Then, there exists a constant $C = C(T) > 0$ *independent of* h *and* ε *such that, we have for all function* $v \in W^{\mu,q}(\mathbb{R}^n)$, $\mu = \max(r+s, m)$, $1 \leqslant q \leqslant +\infty$

$$|v - \pi_h^\varepsilon(t) v|_{s,q,\mathbb{R}^n} \leqslant C\Big(\varepsilon^r |v|_{r+s,q,\mathbb{R}^n} + \frac{h^m}{\varepsilon^{m+s}} \|v\|_{m,q,\mathbb{R}^n} \Big), \quad 0 \leqslant t \leqslant T. \tag{2.6}$$

For the proof of this result, we refer to [5]; cf. also [12].

In the case (2.2), we may apply Theorem 1 in order to get a bound for the error. Assuming that the hypotheses of Theorem 1 hold with $s=0$, we obtain if the solution u of Problem (1.1) is smooth enough:

$$\|u(\cdot, t) - u_h^\varepsilon(\cdot, t)\|_{L^r(\mathbb{R}^n)} \leqslant C\Big(\varepsilon^r + \frac{h^m}{\varepsilon^m} \Big), \quad 0 \leqslant t \leqslant T.$$

In the general case however, the situation appears to be more complex. On the one hand, we are only able to derive a L^2 error bound. On the other hand, this bound is not optimal compared with the approximation error (2.6) for $s=0$, $q=2$. In fact, we have

Theorem 2. *Assume that the hypotheses of Theorem* 1 *hold with* $s=1$. *Assume in addition that the condition* (1.22) *is satisfied and that there exists a constant* $c_1 > 0$ *independent of* h *and* ε *such that*

$$\frac{h^m}{\varepsilon^{m+1}} \leqslant c_1. \tag{2.7}$$

Suppose finally that the solution u *of Problem* (1.1) *belongs to the space* $C^0(0, T; W^{\mu,\infty}(\mathbb{R}^n)^p)$ *where* $\mu = \max(r+1, m)$ *and satisfies for some* $\gamma < \frac{n}{2}$ *and for all* $\beta \in \mathbb{N}^n$ *with* $|\beta| \leqslant \mu$

$$|\partial^\beta u(x, t)| \leqslant c_2 (1 + |x|)^{-\gamma}, \quad x \in \mathbb{R}^n, \ t \in [0, T]. \tag{2.8}$$

Then, there exists a constant $C = C(u, T) > 0$ *independent of* h *and* ε *such that*

$$\|u(\cdot, t) - u_h^\varepsilon(\cdot, t)\|_{L^2(\mathbb{R}^n)} \leqslant C\Big(\varepsilon^r + \frac{h^m}{\varepsilon^{m+1}} \Big), \quad 0 \leqslant t \leqslant T. \tag{2.9}$$

Again, we refer to [5] for the proof of this theorem. Note that the error bound (2.9) depends on:

(i) the moment properties (2.5) of the cut-off function ζ,

(ii) the smoothness of this function ζ.

In fact, (2.5) implies that ζ_ε is in some sense an approximation of order $O(\varepsilon^r)$ of the Dirac measure δ. Moreover, we are able to prove the convergence of the particle method only if

$$\frac{h^m}{\varepsilon^{m+1}} \text{ tends to zero as } h \text{ and } \varepsilon \text{ tend to zero.}$$

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1) $x^\alpha = x_1^{\alpha_1} \cdots x_n^{\alpha_n}$ if $x = (x_1, \cdots, x_n) \in \mathbb{R}^n$, $\alpha = (\alpha_1, \cdots, \alpha_n) \in \mathbb{N}^n$.

This means that the support of the function $y \to \zeta_\epsilon(x-y)$ must contain sufficiently many particles in order to obtain a reasonable approximation $u_h^\epsilon(x, t)$ of $u(x, t)$.

Remark 1. Theorem 2 can be easily generalized to first-order symmetrizable systems. Instead of (1.3), we require that there exists a $p\times p$ symmetric matrix $P=P(x, t)$ which depends smoothly of x and t and is uniformly positive definite in Q_T such that the matrices $PA^i(x, t)$, $1\leqslant i\leqslant n$, are symmetric.

Such symmetrizable first order systems occur when linearizing a nonlinear system of conservation laws for which an entropy function exists. We shall discuss the particle approximation of such a nonlinear first order system in the next section.

§ 3. Application: A Free Lagrangian Method for the Euler Equations of Gas Dynamics

The numerical approximation of the Euler equations for a compressible perfect fluid is a practically important and challenging problem which is extensively studied. Finite-difference Eulerian methods (using a fixed mesh) have been considerably developed recently but are still not well suited for the numerical simulation of *complex multifluid* flows. In fact, for such flows, the use of a fixed finite-difference mesh appears to be inappropriate. On the other hand, classical Lagrangian finite-difference methods (using a mesh attached to the fluid) become ineffective in presence of great distortions of the fluid.

In order to overcome the above difficulties, one could think to use a Lagrangian particle method, i.e., where the particles have the fluid velocity. This was first done by Harlow[8] when he derived the particle in cell (P.I.C.) method: in the original method of Harlow, the convective terms are discretized via a particle method while the pressure terms are discretized via a finite-difference technique using a fixed Eulerian mesh. Recently, a new particle method has been proposed by Gingold and Monaghan[7]: the smoothed particle hydrodynamics (S.P.H.) method which improves the P.I.C. method in several respects, in particular by avoiding the use of a fixed finite-difference mesh.

Now, by taking into account the considerations of Section 1, we are able to extend the S.P.H. method of Gingold and Monaghan method. For simplicity, we shall restrict ourselves to the one-dimensional case but the analysis can be easily extended to multi-dimensional problems. Therefore, we consider the one-dimensional gas dynamics equations in slab symmetry:

$$\begin{cases} \dfrac{\partial\rho}{\partial t}+\dfrac{\partial}{\partial x}(\rho u)=0, \\ \dfrac{\partial}{\partial t}(\rho u)+\dfrac{\partial}{\partial x}(\rho u^2+p)=0, \\ \dfrac{\partial}{\partial t}(\rho E)+\dfrac{\partial}{\partial x}(\rho E+p)u=0. \end{cases} \tag{3.1}$$

In (3.1), ρ is the density of the fluid, u is its velocity, p is its pressure and E is its total energy per unit mass. In order to close the system of equations (3.1), we need to add an equation of state

$$p=p(\rho, e), \tag{3.2}$$

where $e=E-\frac{1}{2}u^2$ is the internal energy of the fluid per unit mass. Hence, setting

$$\phi=\begin{pmatrix}\rho\\ \rho u\\ \rho E\end{pmatrix},\quad A(\phi)=\begin{pmatrix}u & 0 & 0\\ p/\rho & u & 0\\ 0 & p/\rho & u\end{pmatrix}, \tag{3.3}$$

the system of equations (3.1) can be equivalently written in the form

$$\frac{\partial\phi}{\partial t}+\frac{\partial}{\partial x}(A(\phi)\phi)=0. \tag{3.4}$$

Next, we decompose the matrix $A(\phi)$ in the following way

$$A(\phi)=uI+B(\phi),\quad B(\phi)=\begin{pmatrix}0 & 0 & 0\\ p/\rho & 0 & 0\\ 0 & p/\rho & 0\end{pmatrix}, \tag{3.5}$$

hence separating the convective terms from the pressure terms. Thus (3.4) becomes

$$\frac{\partial\phi}{\partial t}+\frac{\partial}{\partial x}(u\phi)+\frac{\partial}{\partial x}(B(\phi)\phi)=0. \tag{3.6}$$

Now, we apply the particle method of Section 1 to the first-order system (3.6). We are looking for a particle approximation ϕ_h of ϕ

$$\phi_h(x, t)=\sum_{k\in K}w_k(t)\phi_k(t)\delta(x-x_k(t)),$$

where

$$\phi_k=\begin{pmatrix}\rho_k\\ \rho_k u_k\\ \rho_k E_k\end{pmatrix}$$

and $t\to x_k(t)$, $k\in K$, is the solution of the differential equation

$$\begin{cases}\dfrac{dx_k}{dt}(t)=u_k(t),\\ x_k(0)=\xi_k.\end{cases} \tag{3.7}$$

The functions $t\to w_k(t)$ will be specified in the sequel.

The method of discretization (1.18) gives here:

$$\frac{d}{dt}(w_k\phi_k)+w_k\sum_{l\in K}w_l(B(\phi_k)\phi_l+B(\phi_l)\phi_k)\zeta'_s(x_k-x_l)=0,\quad k\in K.$$

By using the form (3.5) of the matrix $B(\phi)$, we obtain

$$\begin{cases}\dfrac{d}{dt}(w_k\rho_k)=0,\\ \dfrac{d}{dt}(w_k\rho_k u_k)+w_k\sum\limits_{l\in K}w_l\Big(\dfrac{p_k}{\rho_k}\rho_l+\dfrac{p_l}{\rho_l}\rho_k\Big)\zeta'_s(x_k-x_l)=0,\\ \dfrac{d}{dt}(w_k\rho_k E_k)+w_k\sum\limits_{l\in K}w_l\Big(\dfrac{p_k}{\rho_k}\rho_l u_l+\dfrac{p_l}{\rho_l}\rho_k u_k\Big)\zeta'_s(x_k-x_l)=0.\end{cases} \tag{3.8}$$

The first equation (3.8) gives

$$w_k \rho_k = m_k = \text{constant mass of the particle } k. \tag{3.9}$$

This expresses the conservation of mass. Next, using (3.9), the second and third equations (3.8) of conservation of momentum and conservation of energy become respectively

$$\frac{du_k}{dt} + \sum_{l \in K} m_l \left(\frac{p_l}{\rho_l^2} + \frac{p_k}{\rho_k^2} \right) \zeta_\varepsilon'(x_k - x_l) = 0 \tag{3.10}$$

and

$$\frac{dE_k}{dt} + \sum_{l \in K} m_l \left(\frac{p_l}{\rho_l^2} u_k + \frac{p_k}{\rho_k^2} u_l \right) \zeta_\varepsilon'(x_k - x_l) = 0. \tag{3.11}$$

By setting

$$e_k = E_k - \frac{1}{2} u_k^2$$

and using (3.10), we note that (3.11) may be also written in the form

$$\frac{de_k}{dt} + \frac{p_k}{\rho_k^2} \sum_{l \in K} m_l (u_k - u_l) \zeta_\varepsilon'(x_k - x_l) = 0. \tag{3.12}$$

Finally, it remains to specify w_k or equivalently $\rho_k = \frac{m_k}{w_k}$. We take

$$\rho_k = \sum_{l \in K} m_l \zeta_\varepsilon(x_k - x_l). \tag{3.13}$$

Therefore, the particle method of approximation of the gas dynamic equations (3.1) is defined by (3.7), (3.10), (3.12) and (3.13).

It remains to introduce a time-discretization in order to obtain a practical numerical method. This is done by using a leap-frog time-stepping exactly as in Richtmyer and Morton [14, p. 295]. Moreover, in order to prevent the resulting scheme from the development of nonlinear instabilities, we have to add to the pressure p and "ad hoc" pseudo-viscosity term q of Von Neumann-Richtmyer type

$$q = \begin{cases} -\alpha \varepsilon \rho c \dfrac{\partial u}{\partial x}, & \dfrac{\partial u}{\partial x} \leqslant 0, \\ 0, & \dfrac{\partial u}{\partial x} \geqslant 0, \end{cases}$$

where c is the local sound speed and α is a numerical parameter. For details, we refer to [7] and [11]; see also Section 4.

In fact, one-dimensional numerical experiments show that this Lagrangian particle method is simple and robust and produces very satisfactory results. Again, we refer to [7] and [11] for more details in that direction. The application of the method to the numerical approximation of two-dimensional problems is in progress. On the other hand, the study of the convergence of the method is an open mathematical question.

§ 4. Extension of the Particle Method: Convection-Diffusion Problems

The particle method can be easily extended to the numerical approximation of convection-diffusion problems. Let us consider the Cauchy problem for a convection diffusion equation

$$\begin{cases} \dfrac{\partial u}{\partial t}+\sum_{i=1}^{n}\dfrac{\partial}{\partial x_i}(a^i u)-\sum_{i=1}^{n}\dfrac{\partial}{\partial x_i}\left(b\dfrac{\partial u}{\partial x_i}\right)=f, \quad x\in\mathbb{R}^n,\ t>0, \\ u(x,0)=u_0(x). \end{cases} \tag{4.1}$$

In (4.1), $u=u(x,t)$ and $f=f(x,t)$ are scalar functions and the coefficients a^i satisfy the conditions (1.5). Moreover, we assume that

$$b\in L^\infty(Q_T), \quad b(x,t)\geqslant\beta>0. \tag{4.2}$$

Again, we look for a particle approximation u_h of the solution u of (4.1) defined by (1.11). A first approach consists in putting (4.1) in the form of a first order system.

Setting $p^i=-b\dfrac{\partial u}{\partial x_i}$, the first equation (4.1) becomes

$$\begin{cases} \dfrac{\partial u}{\partial t}+\sum_{i=1}^{n}\dfrac{\partial}{\partial x_i}(a^i u+p^i)=f, \\ p^i+b\dfrac{\partial u}{\partial x_i}=0, \quad 1\leqslant i\leqslant n. \end{cases}$$

Now, assuming that the functions a^i, b and f are continuous and applying the ideas of Section 1, we want to find the scalar functions $t\to u_k(t)$ and $t\to p_k^i(t)$, $1\leqslant i\leqslant n$, $k\in K$, solutions of the differential system:

$$\begin{cases} \dfrac{d}{dt}(w_k u_k)+w_k\sum_{i=1}^{n}\sum_{l\in K}w_l(p_l^i+p_k^i)\dfrac{\partial\zeta_\varepsilon}{\partial x_i}(x_k-x_l)=w_k f_k, \\ p_k^i+b_k\sum_{l\in K}w_l(u_l-u_k)\dfrac{\partial\zeta_\varepsilon}{\partial x_i}(x_k-x_l)=0, \quad 1\leqslant i\leqslant n, \\ u_k(0)=u_0(\xi_k). \end{cases} \tag{4.3}$$

For the convergence of this method, we refer again to [5].

Let us now describe another way of approximating Problem (4.1) which appears to be more effective in some practical problems. Starting from (1.14), we have only to derive a particle approximation of $\dfrac{\partial}{\partial x_i}\left(b\dfrac{\partial u_h}{\partial x_i}\right)$. This is based on the following result concerning the approximation of differential operators by *generalized finite-differences*.

Theorem 3. *Assume that the coefficients a^i and b are smooth enough. Assume in addition that the cut-off function ζ is radially symmetric, i.e., there exists a function $\bar\zeta$: $\mathbb{R}^+\to\mathbb{R}$ such that*

$$\zeta(x)=\bar\zeta(|x|). \tag{4.4}$$

Moreover, we suppose that the function ζ belongs to the space $W^{m+1,1}(\mathbb{R}^n)$ and satisfies the conditions (2.5). Then, if the function v belongs to the space $W^{s,\infty}(\mathbb{R}^n)$, $s=\max(r+2, m+1)$, we have:

$$\sum_{l\in K}w_l(b(x_k)+b(x_l))(v(x_l)-v(x_k))\frac{D\zeta_\varepsilon(x_k-x_l)\cdot(x_l-x_k)}{|x_l-x_k|^2}$$
$$=\sum_{i=1}^{n}\frac{\partial}{\partial x_i}\left(b\frac{\partial v}{\partial x_i}\right)(x_k)+O\left(\varepsilon^r+\frac{h^m}{\varepsilon^{m+1}}\right). \tag{4.5}$$

In (4.5), $D\zeta_\varepsilon(x)$ is the total derivative of the function ζ_ε at the point x so that

$$D\zeta_\varepsilon(x)\cdot y=\sum_{i=1}^{n}\frac{\partial\zeta_\varepsilon}{\partial x_i}(x)y_i.$$

Hence, assuming that (4.4) holds, a natural particle approximation of Problem (4.1) consists in finding the functions $t\to u_k(t)$, $k\in K$, solutions of

$$\begin{cases}\dfrac{d}{dt}(w_k u_k)+w_k\displaystyle\sum_{l\in K}w_l(b_l+b_k)(u_l-u_k)\frac{D\zeta_\varepsilon(x_k-x_l)\cdot(x_l-x_k)}{|x_l-x_k|^2}=w_k f_k,\\ u_k(0)=u_0(\xi_k).\end{cases}\tag{4.6}$$

For a mathematical study of this numerical method of approximation of convection-diffusion problems, see [6].

Let us point out that the previous method is well adapted to the particle discretization of the pseudo-viscosity term introduced in Section 3. In this direction, the method may be viewed as a generalization of a method considered by Gingold and Monaghan[7].

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