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High Order Computation of the History Term in the Equation of Motion for a Spherical Particle in a Fluid

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The historical evolution of the equation of motion for a spherical particle in a fluid and the search for its general solution are recalled. The presence of an integral term that is nonzero under unsteady motion and viscous conditions allowed simple analytical or numerical solutions for the particle dynamics to be found only in a few particular cases. A general solution to the equation of motion seems to require the use of computational methods. Numerical schemes to handle the integral term of the equation of motion have already been developed. We present here adaptations of a first order method for the implementation at high order, which may employ either fixed or variable computation time steps. Some examples are shown to establish comparisons between diverse numerical methods.

KEY WORDS: High order method; equation of motion; history term.

1. THE EQUATION OF MOTION FOR A SPHERICAL PARTICLE IN A FLUID

The description of the dynamics of particles in fluids is of fundamental importance in many scientific and engineering fields. In order to predict the corresponding behaviour, an adequate equation of motion is required. Boussinesq [6], Basset [5], and Oseen [24] have been respectively credited with the original derivation of the equation governing the transient motion

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of a spherical particle at small Reynolds number ($\mathrm{Re} = 2a\,|\vec{v}|\,\rho/\mu$) immersed in an otherwise stationary fluid

$$\frac{4}{3}\,\pi a^3 \delta\,\frac{d\vec{v}}{dt} + \frac{2}{3}\,\pi a^3 \rho\,\frac{d\vec{v}}{dt} = -6\pi a \mu \vec{v} - \frac{4}{3}\,\pi a^3\,\vec{\nabla} p + \frac{4}{3}\,\pi a^3\,\delta \vec{g} - 6a^2\sqrt{\pi\rho\mu}\int_0^t \frac{d\vec{v}/dt'}{\sqrt{t-t'}}\,dt' \tag{1}$$

for a particle of velocity $\vec{v}$, density δ, radius a, and at rest when $t = 0$, moving in a fluid with viscosity μ, density ρ, pressure gradient $\vec{\nabla} p$ and in the presence of gravity $\vec{g}$. The first and second term on the left-hand side are respectively due to the net force on the particle and the added mass (one half of the fluid mass displaced by its volume), also called inertial drag. On the other side of the equation we respectively find the forces related to the steady state aerodynamic drag, pressure gradient (usually replaced by the hydrostatic condition $\vec{\nabla} p = \rho \vec{g}$) and weight, whereas the last part is called the history term (it is applicable under Stokes flow regime, roughly $\mathrm{Re} < 1$). This component increases the drag and represents the resistance to the unsteady motion of the particle due to fluid viscosity and it is associated with the diffusion of vorticity away from it (a kind of feedback of the surrounding flow field, which contains information of the particle velocity at previous times, as the momentum that was transferred from one to the other cannot disappear). The effect on particle velocity may be integrable even if the integrand tends to infinity.

The above expression has been successively extended. The equation of motion in an unsteady and nonuniform ambient flow at small particle Reynolds number ($\mathrm{Re} = 2\,a\,|\,\vec{v} - \vec{u}\,|\,\rho/\mu$), as used for example by [4], is as given by Maxey and Riley in 1983 [18], except for the added mass term, whose more appropriate form was first derived in 1928 [28], but was just recalled in 1988 [3]

$$\delta\,\frac{d\vec{v}}{dt} + \frac{1}{2}\,\rho\,\frac{d\vec{v}}{dt} = \frac{1}{2}\,\rho\,\frac{D\vec{u}}{Dt} - \frac{9\mu}{2a^2}\,(\vec{v} - \vec{u}) + \rho\,\frac{D\vec{u}}{Dt} + (\delta - \rho)\,\vec{g} - \frac{9}{2a}\sqrt{\frac{\rho\mu}{\pi}}\int_0^t \frac{d(\vec{v} - \vec{u})/dt'}{\sqrt{t-t'}}\,dt' \tag{2}$$

where $\vec{u}$ represents the fluid velocity at the current position of the particle and the flow is assumed to be incompressible and characterized by a small shear. The terms on the right-hand side respectively correspond to a new part of the added mass (due to fluid acceleration), steady state drag, local fluid element dynamics (also called dynamic buoyancy), body (weight and buoyancy) and history forces. Notice that D/Dt and d/dt are respectively the total derivatives following a fluid element and the particle. The initial velocities of the particle and the fluid in that position are assumed to be equal, so a few modifications must be introduced if that is not the case [16, 17]. Some authors (see below) have also investigated or suggested modifications to the expression for the history integral, but a term of this kind is always present. All these additional points will not alter the nature of our problem and the proposed solutions to be discussed below. The equation of motion may be applied to any sphere which is small compared to the scale of the ambient fluid flow. Semiempirical or more complex analytical versions in order to extend the validity have also been presented. One common approach for large Reynolds numbers has been the use of an expression for the steady state drag force valid in that range, but neglecting the added mass and history forces. Michaelides [23] presented a thorough review of the study of the problem. Henceforth, unless otherwise stated we will refer always to the equation of motion (2).

The history force expression as written above and originally derived has well known limitations because it ignores the advective term in the Navier–Stokes equation, leading to an overestimation of the behaviour at long times. Some extensions for finite Reynolds number have been summarized by [23]. Diverse works [10, 14, 19–21] for example allude to a different decay of the history integral, that varies as the classical expression for short times and faster later. However, the description by [20, 21] was obtained by extrapolating results in the frequency domain for small amplitude perturbations of a steady flow and it has been questioned by other authors, who presented alternatives (see, e.g., [15]). In another approach the classical history term is multiplied by an empirical coefficient that depends on fluid and particle velocities (see, e.g., [23]) to account for finite Reynolds number. This method became very popular in engineering calculations of the drag force due to its agreement with experimentally observed quantities. More appropriate expressions of the history integral than the presently well-known ones may be extremely complex or they may emerge in the near future. However, when using the classical expression some works [9] have found small relative differences with full simulations of the flow configuration or with experimental data. Results are not conclusive and are still open to discussion, so the uncertainty about appropriate options keeps different approaches. In brief, the history term must be taken into account and here it is assumed to have the form of the classical expression. This may not capture the physical process in the most faithful manner, but it could be representative in a simple form of the difficulties to be found in the search for numerical solutions in a variety of present or future extensions of the integral expression. In addition, the corresponding simulation results should be valuable for the description of the system involved. Our goal is to obtain a minimal scheme with the classical expression with which we may search numerical solutions. If there appear differences against other methods in this approach, with the inclusion of a more complex kernel we expect the advantages to remain or be even enhanced. However, there is no warranty that any positive aspects observed for the numerical method described below will also apply for other versions of the history integral.

2. NUMERICAL METHODS TO SOLVE THE EQUATION OF MOTION

The history integral yields a term that is clearly different from the form of all the other ones and it poses a particular problem, as an integro-differential equation implicit in $\vec{v}$ results. Tatom [27] noted that in the field of fractional calculus, analytical solutions may be obtained in closed form for certain special cases. Numerical solutions will require a priori an iterative method, but they may then become very much time consuming. Different approaches have been followed in order to overcome this difficulty. There is an additional drawback for computations at first sight: the integral term needs to recall the past of the particle and fluid and it therefore increasingly devours memory.

The search for a general solution of the particle velocity from the equation of motion has remained a difficult task. An analytical solution to Eq. (2) in the presence of an uniform background flow field has been obtained by the use of fractional calculus [11]. However, for more complex cases this has not been possible. On the other hand, while there are efficient numerical algorithms for differential equations, methods for the above type of integrodifferential equations have not been developed to the same degree. From the whole equation of motion only the history term represents an inconvenient for numerical solutions. Different ways have been attempted in order to overcome this complication. An obvious procedure would imply the search for an implicit technique that involves iterations, but this often proved to be cumbersome. One common approach to avoid this inconvenient has been the restriction to cases where the history term might be considered negligible (basically when the particle is much denser than the fluid). This reduces the order of the equation of motion and makes it explicit in the velocity, which diminishes the memory requirements and increases the speed of the computations (there is no need to retain information on the past motion of the particle and no iterations are required). However, under certain conditions the assumption is not physically appropriate and may therefore lead to erroneous results if groundlessly applied [13, 29]. Appropriate solutions when $\mathrm{Re} < 1$ may require the inclusion of the history term in the equation of motion [2]. By the way, the wide and ever increasing availability of computational power makes it now possible to perform simulations which were considered very expensive in terms of memory and speed some years ago, only feasible at large institutional computers, but pose no challenge to a PC at the present time. Anyway, our schemes below will always be guided towards a minimum computational cost.

By using an integrodifferential transformation, Michaelides [22] has changed the equation of motion of the particle into a differential equation explicit in the particle velocity, as the latter is not present in his history integral. Therefore, solutions may be found with any numerical technique appropriate for differential equations. The history of the fluid must still be stored, the differential equation becomes second order and it includes a larger number of terms, but a significant computer memory demand reduction occurs as it becomes no longer necessary to keep the past information of the particle.

Another alternative in order to attack the problem without iterations is to use a discretisation of the history integral, as considered in [1, 26]. Both works employ first order techniques with respect to the time step of the numerical integration. We adopt here both options and pursue to increase their order. To achieve this aim some handling will become necessary. We will present here as a guide for other cases the implementation of Runge–Kutta methods of order four and five. However, it should be kept in mind that higher order does often but certainly not always mean higher accuracy. Notwithstanding, a first order calculation of the history term places a priori a constraint on the potential accuracy of a numerical solution to Eqs. (1) or (2).

We may now roughly classify the possible solution alternatives to the integrodifferential equation and outline their advantages and drawbacks:

- Implicit methods by iterations: the particle velocity, which is the dependent variable, appears in the integral, computations may become time consuming and cumbersome and there are memory requirements in order to store the particle and fluid acceleration history for recall at each step

- Integral discretisation with first order scheme: the particle velocity appears explicitly in the integral discretisation and the equation therefore becomes easier and faster to solve, but low accuracy is expected and there are memory requirements for the particle and fluid acceleration history

- Integrodifferential transformation: the particle velocity appears explicitly in a way (not part of a history integral) that memory requirements for the particle past do not exist, but they still do for the fluid (there is a history integral for the second time derivative of the fluid velocity), the differential equation has now become second order and it has many more terms
- Integral discretisation with high order scheme: the particle velocity appears explicitly, it remains a first order differential equation with a few terms, but there are memory requirements in order to store the particle and fluid acceleration history

In the last three methods the operation count at step k is $O(k)$, as the largest amount of arithmetics stems in both cases from the calculation of the corresponding history integrals, which are obtained by addends over all the previous solution points. Then, for the whole computation they would be $O(K*(K-1)/2) \sim O(K^2)$ if K is the total number of steps. It is not clear a priori whether if any of the last two alternatives may represent a better trade-off between desired accuracy and computer time, so it will become advisable after the implementation of the present method in the next chapter to perform some numerical tests.

3. HIGH ORDER COMPUTATION OF THE HISTORY TERM

We consider a problem where t is time, $\vec{x}$ are the spatial coordinates, $\vec{u}(t, \vec{x})$ the fluid velocity field, $\vec{X}(t)$, $\vec{v}(t)$ the particle position and velocity. The following formulations will be applied to Runge–Kutta schemes, but they can also be simply extended to other methods and these examples should serve as a guide in those cases.

3.1. Implementation for One Type of Discretisation

The discretisation by Reeks and McKee [26] of the history integral at time t, reached after M fixed computational steps Δt, is given by

$$\int_0^t \frac{d(\vec{v}-\vec{u})/dt'}{\sqrt{t-t'}}\,dt' = \frac{1}{\sqrt{\Delta t}} \sum_{n=0}^{M-1} (\vec{v}^{n+1} - \vec{v}^{n})\, \lambda(M-n)$$

$$- \sqrt{\Delta t} \sum_{n=0}^{M-1} \frac{d\vec{u}^{n+1}}{dt}\, \lambda(M-n) \tag{3}$$

where the superscripts 0,..., M refer to the successive solution points in $[0, t]$,

$$\lambda(k) = 2(\sqrt{k} - \sqrt{k-1})$$

and

$$\frac{d\vec{u}}{dt} = \left(\frac{\partial}{\partial t} + \vec{v}.\vec{\nabla}\right)\vec{u}(t, \vec{x} = \vec{X}(t))$$

Notice that there are some typos in the expressions of the original article.

With the above discretisation, the $d\vec{v}/dt$ integral can be replaced by an expression explicit in $\vec{v}(t)$ (given by $\vec{v}^M$), so Eqs. (1) or (2) now resemble a set of three coupled first order differential equations for the functions v_j ($j = 1, 2, 3$), having the general form

$$\frac{dv_j(t)}{dt} = f_j(t, v_1, v_2, v_3) \tag{4}$$

where the expressions of the functions $f_j(t, v_1, v_2, v_3)$ are known. In order to advance a solution from t_n to t_{n+1} with a fourth order Runge–Kutta method we need to make the following calculations:

$$\begin{aligned} a_j &= f_j(t_n, v_1^n, v_2^n, v_3^n) \\ b_j &= f_j(t_n + 0.5\,\Delta t, v_1^n + 0.5\,\Delta t\, a_1, v_2^n + 0.5\,\Delta t\, a_2, v_3^n + 0.5\,\Delta t\, a_3) \\ c_j &= f_j(t_n + 0.5\,\Delta t, v_1^n + 0.5\,\Delta t\, b_1, v_2^n + 0.5\,\Delta t\, b_2, v_3^n + 0.5\,\Delta t\, b_3) \\ d_j &= f_j(t_n + \Delta t, v_1^n + \Delta t\, c_1, v_2^n + \Delta t\, c_2, v_3^n + \Delta t\, c_3) \end{aligned} \tag{5}$$

In the above formulas there is at first glance an inconvenient: the rule of fixed steps has been broken, as b_j, c_j make a 0.5 Δt jump, which is half as large as all the previous ones. However, that does not pose an unavoidable obstacle to the discretized history expression given by Eq. (3), which can be calculated when time t equals M full steps plus the additional 0.5 Δt according to

$$\begin{aligned} \int_0^t \frac{d(\vec{v}-\vec{u})/dt'}{\sqrt{t-t'}}\,dt' = {} & \frac{1}{\sqrt{\Delta t}} \sum_{n=0}^{M-1} (\vec{v}^{n+1} - \vec{v}^n)\,\lambda(M + 0.5 - n) + 2\,\frac{\vec{v}^{M+0.5} - \vec{v}^M}{\sqrt{0.5\,\Delta t}} \\ & - \sqrt{\Delta t} \sum_{n=0}^{M-1} \frac{d\vec{u}^{n+1}}{dt}\,\lambda(M + 0.5 - n) \\ & - 2\,\frac{d\vec{u}^{M+0.5}}{dt}\sqrt{0.5\,\Delta t} \end{aligned} \tag{6}$$

where $\vec{v}^{M+0.5}$ and $\vec{u}^{M+0.5}$ are the velocities at time t. The above formula may be considered an extension to the derivation of the discretisation for equal steps by [26].

A fourth order Runge–Kutta now yields

$$v_j^{n+1} = v_j^n + \frac{\Delta t}{6}(a_j + 2b_j + 2c_j + d_j)$$

whereas for a simpler second order

$$v_j^{n+1} = v_j^n + \Delta t\, b_j$$

A Runge–Kutta scheme of fourth-order is usually found to be superior to higher-order ones, which includes the fact that the amount of function evaluations (i.e., overload) increases with order. It is the most often used formula due to its balance between computational efficiency and expected accuracy [7, 8, 25].

Some numerical methods require variable steps and in that case the above discretisation will become inapplicable. We must generalize Eq. (3). Some additional manipulations to the derivation by [26] yield

$$\int_0^t \frac{d(\vec{v}-\vec{u})/dt'}{\sqrt{t-t'}}\,dt' = \sum_{n=0}^{M-1} \frac{\vec{v}^{n+1}-\vec{v}^n}{\Delta t_n}\, 2\left(\sqrt{t-t_n}-\sqrt{t-t_{n+1}}\right)$$
$$-\sum_{n=0}^{M-1} \frac{d\vec{u}^{n+1}}{dt}\, 2\left(\sqrt{t-t_n}-\sqrt{t-t_{n+1}}\right) \tag{7}$$

By exerting an adaptive stepsize control over its action, an integrator may aim some predetermined accuracy in the solution with the least computational effort. Many small steps should advance through intricate parts while a few long jumps should speed through gentle sectors. When applying this idea to the fourth order Runge–Kutta method it is even possible to transform it into fifth order [25]. The discretisation in Eq. (7) may be applied straightforward.

3.2. Implementation for a Second Type of Discretisation

In order to show another option to manage the history term we will also present below a different discretisation, worked out by AEA [1]. Some clarifications, which have not been stated in the original documentation should be made for an appropriate application of the technique: t_n and

$(d\vec{v}/dt - d\vec{u}/dt)^n$ respectively correspond to the midpoint and endpoint of step n. At time t after M computational steps Δt_n

$$\int_0^t \frac{d(\vec{v}-\vec{u})/dt'}{\sqrt{t-t'}}\, dt' = \sum_{n=1}^{M-1} \frac{\left(\frac{d\vec{v}}{dt}-\frac{d\vec{u}}{dt}\right)^n}{\sqrt{t-t_n}}\, \Delta t_n + \frac{\left(\frac{d\vec{v}}{dt}-\frac{d\vec{u}}{dt}\right)^M}{\sqrt{\Delta t_M/2}}\, \Delta t_M \tag{8}$$

where the superscripts 1,..., M refer to the steps. The first term on the right-hand side gives the history force for all previous times and it can be explicitly calculated. The second part represents the current time step, which must be separated into two components: the unknown particle acceleration $d\vec{v}/dt^M(\approx d\vec{v}/dt)$ is moved to the left-hand side whereas the fluid acceleration, which is a given function, does not change place. The significant difference in this type of discretisation is that it does use $d\vec{v}/dt$ instead of $\vec{v}$. However, its unknown value at the new point has been moved to the left-hand side and causes no problem because it appears in a linear way. Moreover, in equation set (5) there is no inconvenient in making the necessary evaluations at the trial positions 0.5 Δt and Δt ahead of t_n (b_j, c_j, d_j), as Eqs. (1) and (2) have again the format for numerical solution given by Eq. (4).

The particular case of constant steps yields

$$\int_0^t \frac{d(\vec{v}-\vec{u})/dt'}{\sqrt{t-t'}}\, dt' = \Delta t \left(\sum_{n=1}^{M-1} \frac{\left(\frac{d\vec{v}}{dt}-\frac{d\vec{u}}{dt}\right)^n}{\sqrt{t-(n-1/2)\,\Delta t}} + \frac{\left(\frac{d\vec{v}}{dt}-\frac{d\vec{u}}{dt}\right)^M}{\sqrt{\Delta t/2}} \right) \tag{9}$$

When time t equals M full steps plus an additional 0.5 Δt

$$\int_0^t \frac{d(\vec{v}-\vec{u})/dt'}{\sqrt{t-t'}}\, dt' = \Delta t \left(\sum_{n=1}^{M} \frac{\left(\frac{d\vec{v}}{dt}-\frac{d\vec{u}}{dt}\right)^n}{\sqrt{t-(n-1/2)\,\Delta t}} + \frac{\left(\frac{d\vec{v}}{dt}-\frac{d\vec{u}}{dt}\right)^{M+0.5}}{\sqrt{\Delta t/4}} \right) \tag{10}$$

By arguments similar to those of the previous section we see that fixed or variable step methods may be implemented without trouble for this discretisation.

4. NUMERICAL EXAMPLES

A few simulations are now exhibited as examples and in order to establish some comparisons along the different solution alternatives. We followed [22] in defining a characteristic time for the spherical particle

$$t* = \frac{2\,\delta a^2}{9\mu}$$

to express dimensionless times and frequencies. The maximum fluid velocity in each case has been taken to be 1 cm/s. The initial particle velocity was set equal to the fluid velocity in that location for simplicity. The values used for the computations were: $\delta = 2.7$ g/cm^3, $\rho = 1.0$ g/cm^3, $\mu = 0.01$ g/cm·s, and $a = 0.01$ cm. Figures 1a and 1b depict the particle response obtained from the integral discretisation with a fourth order Runge–Kutta described in Sec. 3.1, where a sinusoidal flow field $u = \sin(\omega t)$ in cm/s has been considered, with $\omega/\omega*$ the dimensionless frequency being respectively 1 and 10. At very low frequencies (not shown) the particle follows the flow rather well, whereas at the highest frequencies both phase lag and amplitude reduction with respect to the fluid increase. We also found solutions with an integral discretisation under a first order method and the fourth order solution without the history integral in the equation of motion has been in addition computed to evaluate the effects and importance of that term. Both features have been included in the figure. We have also found the behaviour of the particle in a step and a more randomlike flow, which may be seen in Figs. 1c and 1d. The field in the latter was given by fluctuations within positive values and accompanied by an increasing trend. Notice that Re < 1 in all cases. The computational time step in the calculations for Figs. 1a and 1c was 0.02 $t*$ and 0.002 $t*$ for Figs. 1b and 1d. Solutions by an implicit iterative method (the required accuracy was set similar to the one expected for a fourth order method) and by the integrodifferential transformation [22] implemented with a fourth order Runge–Kutta were also found, but they are not exhibited because they cannot be discerned from the plot for the integral discretisation under the fourth order Runge–Kutta. In each of the four flow fields the solutions of the diverse methods coalesce for sufficiently small stepsizes, which leads to a kind of reference curve that has also been included. We obtained it by using our method with time steps of 0.01 $t*$ for Figs. 1a and 1c and 0.001 $t*$ for Figs. 1b and 1d. As stated above, we used the same grid for the fourth and first order methods in each case and it may be clearly seen that the former produces a curve much closer to the reference numerical solution in the four panels.

We had previously repeated the computations for the integrodifferential transformation scheme and for our method on a series of successively halved steps and found that the solutions converged to a stepsize independent behaviour. We then checked the order p by replacing the results for three consecutive halved stepsizes into the formula [12]

$$p = \frac{\log((\phi_{2\,\delta t} - \phi_{4\,\delta t})/(\phi_{\delta t} - \phi_{2\,\delta t}))}{\log 2}$$

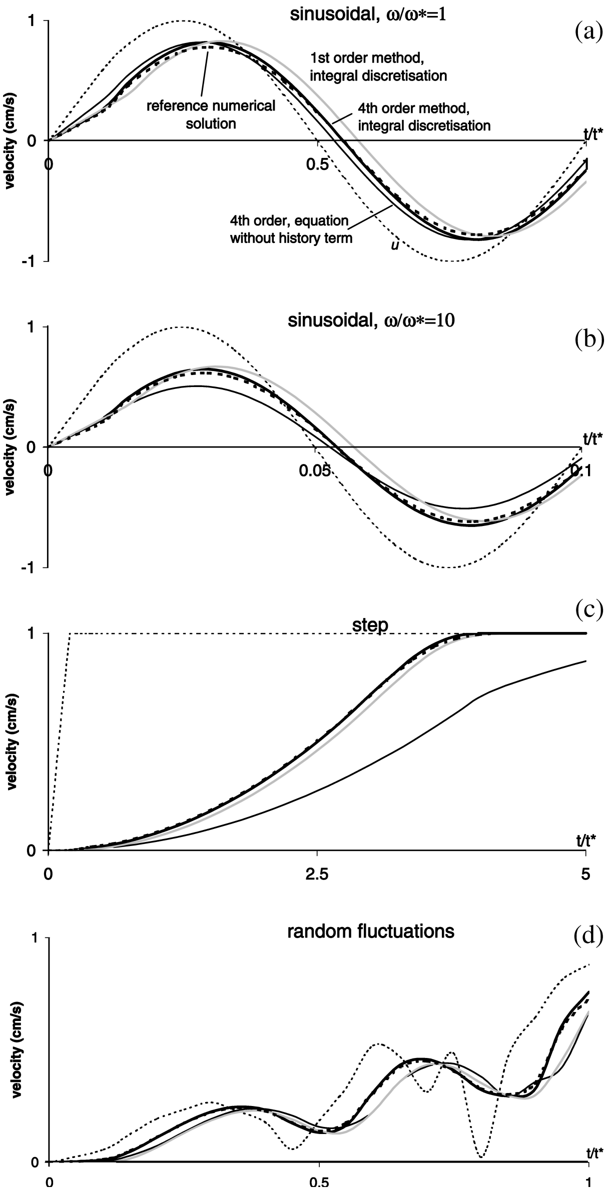

Fig. 1. Numerical solutions for particle velocity in diverse flow fields (parameter values are given in the text). The results correspond to integral discretisation with first and fourth order methods. The solution from the equation of motion without history term (integral discretisation with fourth order Runge–Kutta), the reference numerical curve and the fluid velocity are exhibited for convenience.

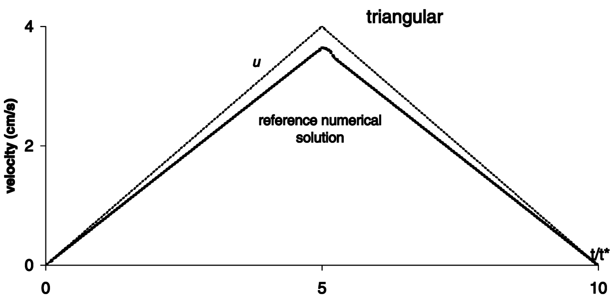

Fig. 2. The reference numerical solution for particle velocity in a triangular flow field.

where $\phi_{\delta t}$ denotes the solution with stepsize δt. In all cases the result for our method was around 4 and in average 5% larger than for the other alternative. Both were found to be one order of magnitude faster than the implicit iterative method, but ours was in average 10% faster.

For further analysis we include an additional one-dimensional case with a triangular flow field. It is shown in Fig. 2 with the reference numerical solution obtained when using our method for $\delta t = 0.01t*$. The initial particle and fluid velocity were set equal. A summary of relevant characteristics of runs with first and fourth order methods using integral discretisation are presented in Table I. The advantage regarding CPU time of using the latter becomes clear. It should be noted that time consumption may become extremely significant whenever repeated calculations are made, as in the computation of particle transport and diffusion coefficients.

Table I. Relevant Run Characteristics of Methods with Integral Discretisation on a Triangular Flow Field

Parameter	First order method	Fourth order method
$\lvert(\phi_{2\,\delta t} - \phi_{4\,\delta t})/\phi_{\delta t}\rvert_{\mathrm{rms}}$ for $\delta t = 0.0005t*$	1.8×10^{-2}	1.9×10^{-9}
$\lvert(\phi_{\delta t} - \phi_{2\,\delta t})/\phi_{\delta t}\rvert_{\mathrm{rms}}$ for $\delta t = 0.0005t*$	9×10^{-3}	1.4×10^{-10}
p for $\delta t = 0.0005t*$	1.0	3.8
δt for $\lvert(\phi_{\delta t} - \phi_{2\,\delta t})/\phi_{\delta t}\rvert_{\mathrm{rms}} < 0.01$[a]	$0.0005t*$ (20000 steps)	$0.1t*$ (100 steps)
Run time for $\delta t = 0.002t*$ (5000 steps)[b]	90 s	90 s
Run time for $\delta t = 0.001t*$ (10000 steps)[b]	3 min	3 min
Run time for $\delta t = 0.0005t*$ (20000 steps)[b]	13 min	13 min

[a] Largest stepsize that suited the specified error target.
[b] We used a 1.2 GHz PC with 256 MB of memory.

5. DISCUSSION

It has been shown that the first order procedures for the numerical solution of the motion equation of a spherical particle in a fluid that have been described can be generalized to a Runge–Kutta or to other methods of any order. The main concern refers to the history term of that equation. Constant or variable step discretisations of that complicate part may be implemented.

Fixed step methods may be applied even though some trial evaluations of the higher order methods must be performed at positions which are shifted with respect to the equally spaced solution points, as shown in Eqs. (6) and (10).

When using variable steps the memory needs will be higher, because all past calculation times must be kept. This would imply a 50% larger average storage requirement in a one dimensional problem (this percentage represents an increase of 40 KB every additional 10000 steps), because in the fixed discretisation only the particle velocity and position must be kept in each step (the last one in order to be always able to recalculate the fluid acceleration at past times in the appropriate place). When using a variable discretisation it is more efficient to store the fluid and particle acceleration in each step.

The scheme here developed and an alternative one were implemented with a fourth order Runge–Kutta method and they exhibited significant time saving and accuracy improvement as compared to respectively an iterative and a first order method when applied in a few representative numerical examples. However, the present development exhibited a slightly better performance. In summary, it has been shown that a high order Runge–Kutta method may be formulated to treat the history term efficiently. The importance of this relies on the fact that particularly computer time may become very significant whenever repeated calculations of particle trajectories are essential.

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