

Innovative Algorithm for Particles Transport in a Fluid

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Abstract-Particles transport in a fluid simulations have plenty of applications in the medicine or different fields of the engineering; from drug delivery simulation in the respiratory system to the friction of a car's break with its wheels or the icing of water droplets on a wing. But its implementation has also very different possible approaches: depending on the fluid, the size of the particle and the number of particles, literature proposes different solutions. In this paper, we want to show a generalized solution and compare it with proposed algorithms in the literature.

I. INTRODUCTION

Particles in a fluid are transported because of the action of different forces. Depending on the case, gravity, buoyancy, Coriolis, Brownian motion or other forces may become necessary. Although involved forces may vary in every problem, drag force [1] and lift force [2] become essential when transported by a fluid.

Let F_p , a_p and m_p be the force, acceleration and mass of particle p . Applying the Newton's second law, the total acceleration applied on each particle is given by the summatory of all the forces involved

$$\Sigma F_p = m_p a_p \quad (1)$$

The calculation of a_p every step from initial time t_i to final time t_f requires an integration scheme. The time interval Δt of every step will be

$$\Delta t = t_f - t_i.$$

II. INTEGRATION SCHEME

The proposed integration scheme is a semi-implicit Newmark- β [3]. In this scheme, the actualization of the velocity u_{n+1} and position x_{n+1} of the next time step is given by two equations:

$$u_{n+1} = u_n + [(1-\gamma)a_n + \gamma a_{n+1}]\Delta t \quad (2)$$

$$x_{n+1} = x_n + u_n \Delta t + [(1-2\beta)a_n + 2\beta a_{n+1}]\Delta t^2/2 \quad (3)$$

Where β and γ are constants. If $\beta=1/4$ and $\gamma=1/2$ the method is implicit unconditionally stable and acceleration

within the time interval Δt is presumed to be constant. If, otherwise, a linear variation of the acceleration during the time interval is assumed, then the values will be $\beta=1/6$ and $\gamma=1/2$. As far as these values are the most commonly used in our simulations, becoming in both cases in an implicit method, a Newton-Raphson is needed in order to solve the dependence on u_{n+1} .

Let u_{n+1} be the function whose root is desired. The Newton-Raphson is described in this case by:

$$u_{n+1} = u_n - w(u_n) \quad (4)$$

Where,

$$w(u_n) = f(u_n)/f'(u_n) \quad (5)$$

And

$$f(u_n) = u_{n+1} + [(1-\gamma)a_n + \gamma a_{n+1}]\Delta t - u_n \quad (6)$$

$$f'(u_n) = -1 + \Delta t \gamma da/du|_{n+1} \quad (7)$$

To ensure the convergence

$$\|w(u_n)\| / \|u_n\| < \epsilon_c \quad (8)$$

is imposed. ϵ_c means the desired precision in the convergence.

The Newton-Raphson will be compared to an explicit Runge-Kutta 4, which is one of the most widely integration schemes used when particles transport, e.g. [4],[5] or [6]. The behavior of both cases will be discussed in terms of mathematics and High Performance Computing (HPC).

III. ADAPTIVE TIME STEP

When particles transport is solved, firstly, the fluid is solved in the chosen interval Δt_{fluid} . The particles must be solved during the same time interval, but using adaptive intervals Δt_p for each particle in figure 1. A constant variation of the velocity of the fluid is supposed during Δt_p .

Figure 1: Scheme of adaptive time step. Particles can adopt a smaller time step than the fluid.

The time step may vary because of three reasons:

A. One element per time step

Particles cannot cross more than one element from one time step to another. Otherwise, time step is automatically decreased. This is why, if particles change subdomain, only

the first neighborhoods list is looped. These elements are called halo elements. In *figure 2* an example is shown.

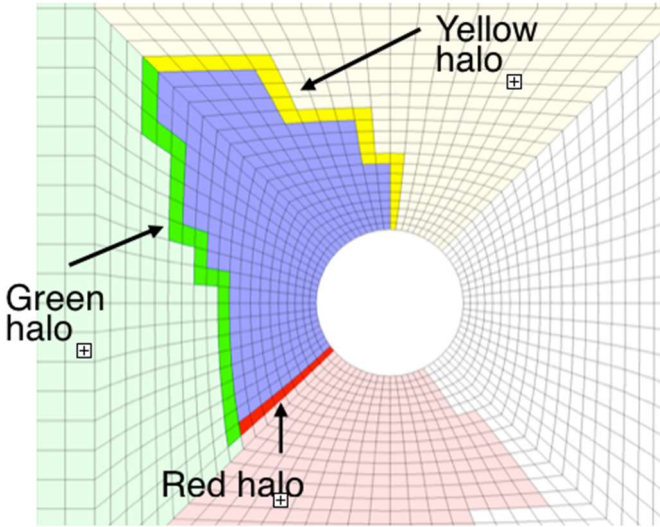


Figure 2: Blue subdomain is bordering red, green and yellow subdomains. In the case, a particle in blue subdomain changes subdomain, time step will be decreased if necessary, until it belongs to a halo element.

B. Reaching convergence of the integration scheme

Time step is decreased when convergence in Newmark- β is not reached. The convergence factor can be controlled by the user before the simulation starts, choosing the value ε_c defined by (8).

C. Control the error due to discretization of the time

As in the point B, before the simulation starts, the user must define the maximum acceptable error of the discretization ε_{err} . This error is normalized using a characteristic length L .

Some of the proposed characteristic lengths are the diameter of the particle, the length of the element or the instant velocity of the particle multiplied by a characteristic time τ . The discussion about which is the right characteristic length is not always straightforward and may vary depending on the properties of the problem.

In order to estimate the new Δt_{err} , let x_{n+1}^{exa} be the exact solution applying Taylor series.

$$x_{n+1}^{exa} = x_n + u_n \Delta t + 1/2 a_n \Delta t^2 + 1/6 (da_n/dt) \Delta t^3 \quad (9)$$

It is necessary to subtract the equation (9) and (3), obtaining as result

$$x_{n+1}^{exa} - x_{n+1} = \beta(a_{n+1} - a_n) \Delta t^2 - 1/6 (da_n/dt) \Delta t^3 \quad (10)$$

Now, applying the approximation

$$da_n/dt = (a_{n+1} - a_n) / \Delta t \quad (11)$$

Dividing by characteristic length L , and finally isolating Δt , it is obtained

$$\Delta t_{err} = \{ \varepsilon_{err} L / [(\beta - 1/6)(a_{n+1} - a_n)] \}^{1/2} \quad (12)$$

Let define ε_{trn} as the truncation error. According to equation (3), we also require the second order term (dependent on the velocity u_n) to be ε_{trn} times smaller than the first order term (dependent on the accelerations a_n, a_{n+1}). This means:

$$[(1-2\beta)a_n + 2\beta a_{n+1}] \Delta t^2 / 2 = \varepsilon_{trn} u_n \Delta t \quad (13)$$

Therefore, the truncation time step Δt_{trn} which satisfies this criteria is

$$\Delta t_{trn} = 2 \varepsilon_{trn} |u_n / [(1-2\beta)a_n + 2\beta a_{n+1}]| \quad (14)$$

Both time steps will be used to estimate a new time step. To obtain that, we define the accuracy α as

$$\alpha = \min(\Delta t_{trn}, \Delta t_{err}) / \Delta t \quad (15)$$

The new time interval is only accepted if $\alpha > 0.9$. Otherwise, the process is repeated using $\Delta t_{new} = \Delta t$.

When showing results we will compare the error accuracy with the adaptive time step and without. Inasmuch as its impact on the performance of the code.

REFERENCES

- [1] G.H. Ganser (1993) A rational approach to drag prediction of spherical and nonspherical particles. Powder Technol.
- [2] A. Li, G. Ahmadi (1992) Dispersion and deposition of spherical particles from point sources in a turbulent channel flow. Aerosol Science and Technology.
- [3] N.M. Newmark (1959) A method of Computation for Structural Dynamics. Journal of the Engineering Mechanics Division, ASCE, pp. 67-94.
- [4] B.Asharian, S.Anjivel (1994) Inertial and Gravitational Deposition of Particles in a Square Cross Section Bifurcating Airway. Aerosol Science and Technology.
- [5] ST Jayaraju, M Brouns, S Verbanck, C Lacor (2007) Fluid flow and particle deposition analysis in a realistic extrathoracic airway model using unstructured grids. Journal of Aerosol Science

- [6] J.M. Dias, J.F. Lopesa, I. Dekeyserb (2001) Lagrangian transport of particles in Ria de Aveiro lagoon, Portugal. *Physics and Chemistry of the Earth, Part B: Hydrology, Oceans and Atmosphere*