Equations of motion for hybrid Molecular Dynamics/Continuum Hydrodynamics particles

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Introduction

The main idea of this project is combine the two types of Equations. The first equation describes continuous fluid dynamics in a conceptually different way which was shown by Pep Espanol. The second equation is basic equation from molecular dynamics. We use the fractional derivative operatores to solve this problem.

The goal

The goal of this project is to choose the right defenition of the fractional derivative and to programme this and get some numerical results.

Discrete fluid particles formulation of hydrodynamics by Pep Espanol

Pep Espanol has shown that the Navier-Stokes equations, when rewritten in Lagrangian form (go with the flow), can be reformulated to describe continuous fluid dynamics in a conceptually different way. Here, fluid particles of mass $\boldsymbol{M_i}$ and volume $\boldsymbol{V_i}$ with coordinates $\boldsymbol{R_i}$ move with the velocity $\boldsymbol{U_i}$, their momentum is $\boldsymbol{P_i = M_i U_i}$

$$\frac{dM_i}{dt} = 0 \tag{1}$$
$$\frac{dR_i}{dt} = U_i$$
$$\frac{dP_i}{dt} = \sum_j \frac{\partial V_j}{\partial R_i} P_j + \sum_j \frac{\partial V_j}{\partial R_i} \sigma_i$$

Transition to atomistic Newtonian dynamics

To convert (1) into Newtonial equation of motion we need to (i) convert the first term (reversible part) into the gradient of interatomic potential

$$P_i' = \sum_j f_{ij} = \sum_j \phi_{ij}'(|R_i - R_j|)\frac{R_i - R_j}{|R_i - R_j|} \tag{2}$$

where $\boldsymbol{\phi_{ij}}$ is the interatomic potential, and nullify the second term (irreversible or dissipative part). For both we will use the apparatus of fractional derivatives.

Fractional derivative

By a fractional derivative we will mean an operator $\boldsymbol{D^\alpha f}$ satisfying the following properties $\boldsymbol{D^\alpha f = D^n I^{n-\alpha} f}$ where $\boldsymbol{n - 1 < \alpha <= n}$, $\boldsymbol{D^n f = \frac{\partial^n f}{\partial x^n}}$ and $\boldsymbol{I^\alpha}$ is the fractional integral defined by the Cauchy formula for repeated integration:

$$(I^\alpha f)(x) = \frac{1}{\Gamma(\alpha)} \int_0^x (x-t)^{\alpha-1} f(t) dt \tag{3}$$

There are several different definitions of fractional derivative, with different results. Here we used the Riman-Liuville derivative:

$$f_\delta^{(\alpha)}(x) = \frac{1}{\Gamma(1-\alpha)} D_x^1 \int_\delta^x (x-\xi)^{-\alpha} f(\xi) d\xi \tag{4}$$

Reversible part of the dynamics

The discrete $\boldsymbol{(gradP)_i}$ operator for pressure, can be generalised by introducing the discrete $\boldsymbol{(grad^\alpha P)_i}$, and $\boldsymbol{(V^\alpha_\nabla P)_i}$ operators as follows:

$$(grad^\alpha P)_i = -V_i^{-1} \sum_j \frac{\partial V_j}{\partial R_i^\alpha} P_j^\alpha \tag{5}$$
$$(V^\alpha_\nabla P)_i = -V_i^{-1} \sum_j [V_j^{\alpha-1} \frac{\partial V_j}{\partial R_i^\alpha} P_j^\alpha]$$

Therefore, a continuous transition of the reversible part between the hydrodynamic and atomistic representation of fluid particles can be achieved by multiplying $\boldsymbol{(grad^\alpha P)_i}$ by another operator of the order $\boldsymbol{1 - \alpha}$ acting on $\boldsymbol{\phi_{ij}}$

$$P_i' = \sum_j V_j^{\alpha-1} \frac{\partial^\alpha V_j}{\partial R_i^\alpha} P_j^\alpha \frac{\partial^{1-\alpha} \phi_{ij}}{\partial R_i^{1-\alpha}} \phi_{ij}^{-\alpha} \tag{6}$$

Irreversible part of the dynamics

For nullifying the second term of (2) with reducing the spatial scale we need to introduce an operator that satisfies $\boldsymbol{\lim_{\alpha\to 0} Q^\alpha[\sigma] = 0}$ and $\boldsymbol{\lim_{\alpha\to 1} Q^\alpha[\sigma] = \sigma}$ We use the following operator that has suitable limits

$$V_0^\alpha f = f^{-1} \frac{\partial^{1-\alpha} f}{\partial x^{1-\alpha}} [\frac{\partial^\alpha f}{\partial x^\alpha} - (1-\alpha) f x^{-\alpha}] \tag{7}$$

Thus, the final equation for the momentum of the particle is

$$\begin{aligned} P_i' = \sum_j V_j^{\alpha-1} \frac{\partial^\alpha V_j}{\partial R_i^\alpha} P_j^\alpha \frac{\partial^{1-\alpha}\phi_{ij}}{\partial R_i^{1-\alpha}} \phi_{ij}^{-\alpha} + \\ +\zeta \sum_j [\frac{\partial^\alpha V_i}{\partial R_j^\alpha} - (1-\alpha) R_j^{-\alpha} V_i] V_i^{-1} \frac{\partial^{1-\alpha} V_i}{\partial R_j^{1-\alpha}} U_j + \\ +2\eta \sum_j [\frac{\partial^\alpha V_i}{\partial R_j^\alpha} - (1-\alpha) R_j^{-\alpha} V_i] V_i^{-1} \frac{\partial^{1-\alpha} V_i}{\partial R_j^{1-\alpha}} U_j \end{aligned} \tag{8}$$

Conclusions

We have already choosen the defenition of fractional derivative and we are trying to use it for functions where it is necessary. Also we have programmed some expressions and we continue to develop programme code.

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