Hybrid molecular hydrodynamics simulation

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Intro

Pep Espanol has shown that Navier-Stokes equations, in Lagrangian form ('go with the flow'), can be reformulated to describe continuous fluid dynamics in a conceptually different way using 'discrete versions' of differential operators:

$$\dot{\mathbf{P}}_i = -\mathcal{V}_i\,(\mathrm{grad}\,P)_i - \mathcal{V}_i\,(\mathrm{Div}\,\boldsymbol{\sigma})_i\,,$$

To convert it into Newtonian equation of motion we need to

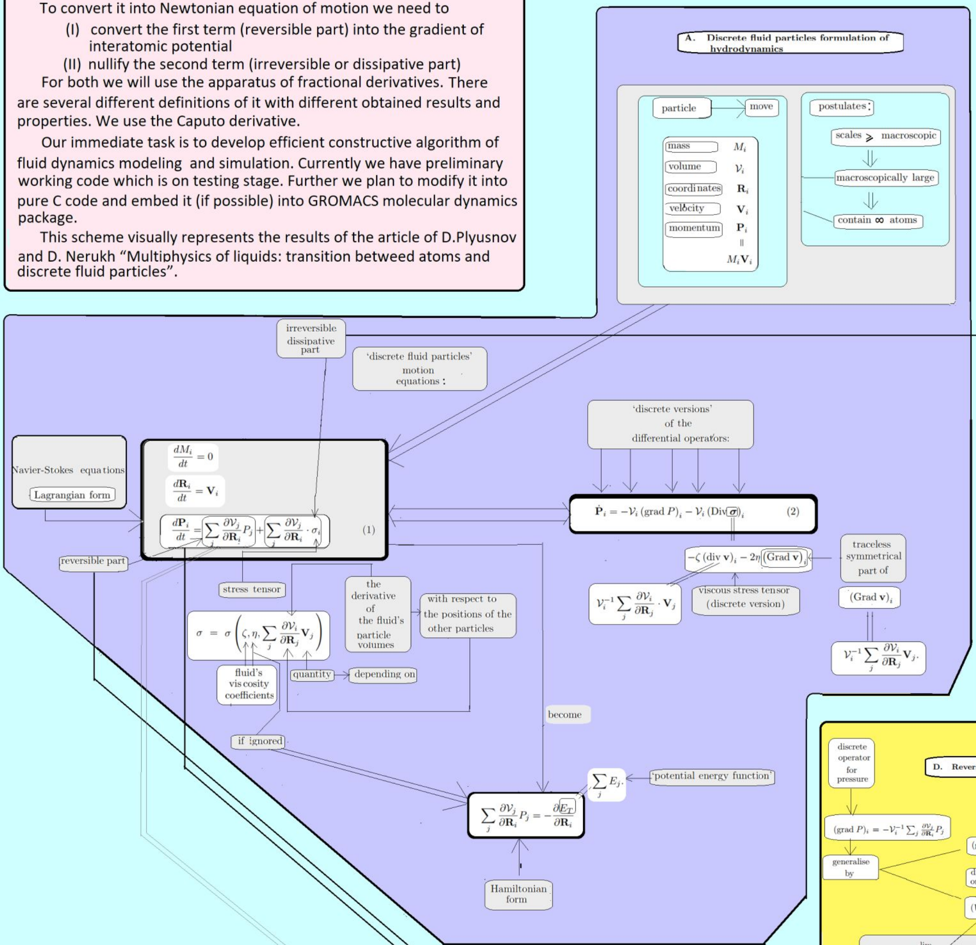
(I) convert the first term (reversible part) into the gradient of interatomic potential

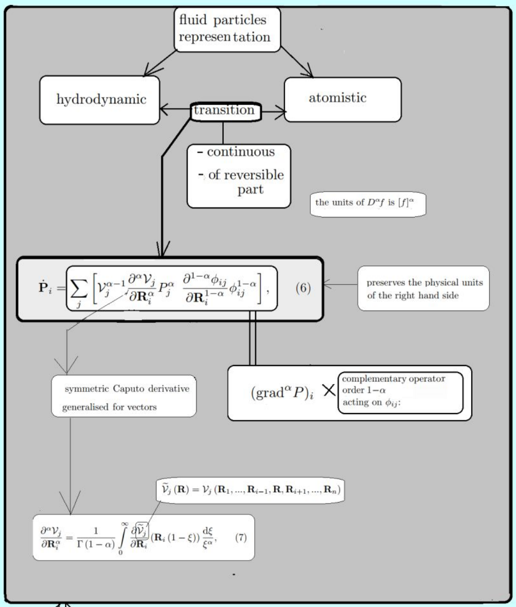
(II) nullify the second term (irreversible or dissipative part)

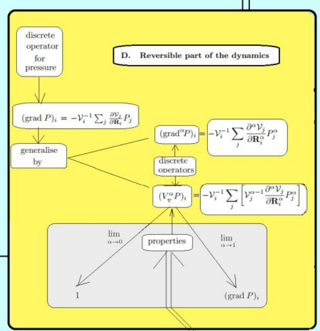
For both we will use the apparatus of fractional derivatives. There are several different definitions of it with different obtained results and properties. We use the Caputo derivative.

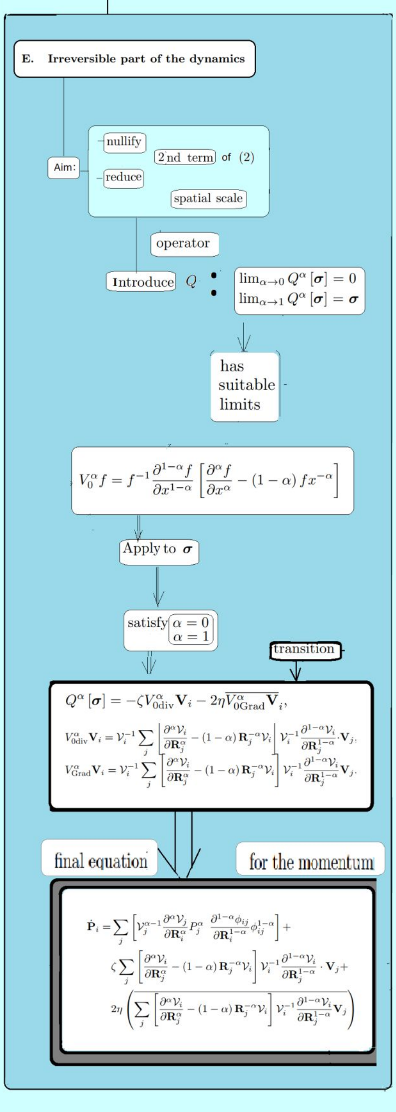
Our immediate task is to develop efficient constructive algorithm of fluid dynamics modeling and simulation. Currently we have preliminary working code which is on testing stage. Further we plan to modify it into pure C code and embed it (if possible) into GROMACS molecular dynamics package.

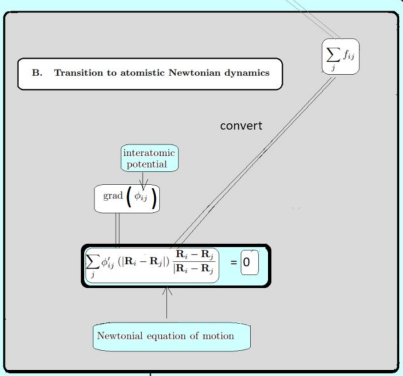
This scheme visually represents the results of the article of D.Plyusnov and D. Nerukh "Multiphysics of liquids: transition betweed atoms and discrete fluid particles".

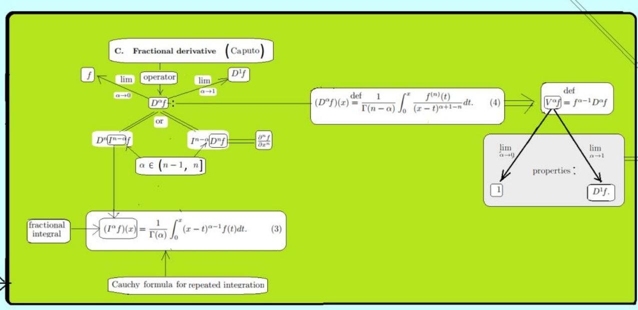


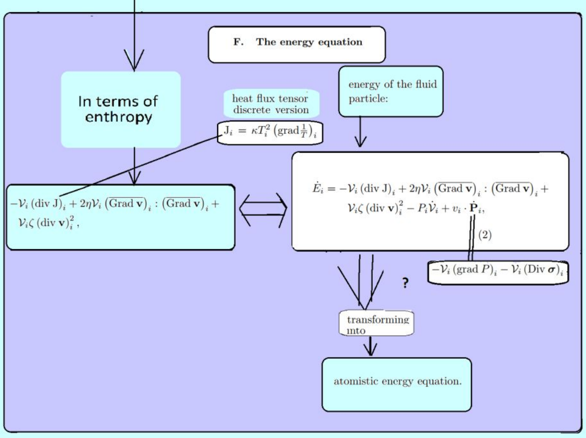












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