## **Hybrid molecular hydrodynamics simulation Ihor Rusnak** 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: $\dot{\mathbf{P}}_{i} = -\mathcal{V}_{i} \left( \operatorname{grad} P \right)_{i} - \mathcal{V}_{i} \left( \operatorname{Div} \boldsymbol{\sigma} \right)_{i},$ To convert it into Newtonian equation of motion we need to (I) convert the first term (reversible part) into the gradient of A. Discrete fluid particles formulation of hydrodynamics interatomic potential (II) nullify the second term (irreversible or dissipative part) fluid particles representation 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 hydrodynamic fluid dynamics modeling and simulation. Currently we have preliminary volume macroscopically large working code which is on testing stage. Further we plan to modify it into coordinates $\mathbf{R}_i$ pure C code and embed it (if possible) into GROMACS molecular dynamics package. velocity V contain ∞ atoms of reversible 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". $M_i V_i$ $\dot{\mathbf{P}}_{i} = \sum_{i} \left[ \mathcal{V}_{j}^{\alpha-1} \frac{\partial^{\alpha} \mathcal{V}_{j}}{\partial \mathbf{R}_{i}^{\alpha}} P_{j}^{\alpha} \frac{\partial^{1-\alpha} \phi_{ij}}{\partial \mathbf{R}_{i}^{1-\alpha}} \phi_{ij}^{1-\alpha} \right]$ preserves the physical units of the right hand side symmetric Caputo deriv generalised for vectors $\frac{d\mathbf{R}_i}{dt} = \mathbf{V}_i$ $\frac{d\mathbf{P}_{i}}{dt} = \sum_{j} \frac{\partial V_{j}}{\partial \mathbf{R}_{i}} P_{j} + \left[ \sum_{j} \frac{\partial V_{j}}{\partial \mathbf{R}_{i}} \cdot \sigma_{i} \right]$ $\widetilde{V}_{i}(\mathbf{R}) = V_{i}(\mathbf{R}_{1}, ..., \mathbf{R}_{i-1}, \mathbf{R}, \mathbf{R}_{i+1}, ..., \mathbf{R}_{n})$ $-\zeta \left(\operatorname{div} \mathbf{v}\right)_{i} - 2\eta \left(\operatorname{Grad} \mathbf{v}\right)_{i} + \zeta \left(\operatorname{Grad} \mathbf{v}\right)$ $\frac{\partial^{\alpha} V_{j}}{\partial \mathbf{R}_{i}^{\alpha}} = \frac{1}{\Gamma(1 - \alpha)} \int_{0}^{\infty} \frac{\partial \widetilde{V_{j}}}{\partial \mathbf{R}_{i}} (\mathbf{R}_{i} (1 - \xi)) \frac{d\xi}{\xi^{\alpha}},$ (Grad v) of the fluid's $= \sigma \left( \zeta, \eta, \sum_{i} \frac{\partial V_{i}}{\partial \mathbf{R}_{i}} \mathbf{V}_{j} \right)$ $V_i^{-1} \sum_j \frac{\partial V_i}{\partial \mathbf{R}_i} \mathbf{V}_j$ . D. Reversible part of the dynamics $\sum E_j$ . [potential energy function] E. Irreversible part of the dynamics $\sum_{i} \frac{\partial V_{j}}{\partial \mathbf{R}_{i}} P_{j} = - \frac{\partial E_{T}}{\partial \mathbf{R}_{i}}$ $(\mathrm{grad}\; P)_i = -\mathcal{V}_i^{-1} \sum_j \frac{\partial \mathcal{V}_j}{\partial \mathbf{R}_i} P_j$ $(\operatorname{grad}^{\alpha}P)_{i} = -V_{i}^{-1}\sum_{i}\frac{\partial^{\alpha}V_{j}}{\partial \mathbf{R}_{i}^{\alpha}}P_{j}^{\alpha}$ nullify Hamiltonian form 2nd term of (2) $(V_v^{\alpha}P)_i$ = $-V_i^{-1}\sum_i \left[V_j^{\alpha-1}\frac{\partial^{\alpha}V_j}{\partial \mathbf{R}_i^{\alpha}}P_j^{\alpha}\right]$ Aim: spatial scale operator $\sum f_{ij}$ B. Transition to atomistic Newtonian dynamics Introduce Q $\lim_{\alpha \to 0} Q^{\alpha} [\boldsymbol{\sigma}] = 0$ $\lim_{\alpha \to 1} Q^{\alpha} [\boldsymbol{\sigma}] = \boldsymbol{\sigma}$ has f lim operator lim D<sup>1</sup>f suitable limits $D^{\alpha}f)(x) \stackrel{\text{def}}{=} \frac{1}{\Gamma(n-\alpha)} \int_{0}^{x} \frac{f^{(n)}(t)}{(x-t)^{\alpha+1-n}} dt.$ $I^{n}$ $\xrightarrow{g}$ $D^{n}f$ $\xrightarrow{g^{n}f}$ $V_0^{\alpha}f = f^{-1}\frac{\partial^{1-\alpha}f}{\partial x^{1-\alpha}}\left[\frac{\partial^{\alpha}f}{\partial x^{\alpha}} - (1-\alpha)\,fx^{-\alpha}\right]$ fractional integral $I(I^{\alpha}f)(x) = \frac{1}{\Gamma(\alpha)} \int_{0}^{x} (x-t)^{\alpha-1}f(t)dt.$ Apply to $\sigma$ use satisfy $\alpha = 0$ $\alpha = 1$ F. The energy equation $Q^{\alpha}\left[\boldsymbol{\sigma}\right] = -\zeta V_{0\mathrm{div}}^{\alpha} \mathbf{V}_{i} - 2\eta \overline{V_{0\mathrm{Grad}}^{\alpha}}$ energy of the fluid particle: $V_{0\text{div}}^{\alpha} \mathbf{V}_{i} = V_{i}^{-1} \sum_{i} \left| \frac{\partial^{\alpha} V_{i}}{\partial \mathbf{R}_{i}^{\alpha}} - (1 - \alpha) \mathbf{R}_{j}^{-\alpha} V_{i} \right| V_{i}^{-1} \frac{\partial^{1-\alpha} V_{i}}{\partial \mathbf{R}_{i}^{1-\alpha}} \cdot \mathbf{V}_{j}$ In terms of enthropy heat flux tensor discrete version Acknowledgements $V_{Grad}^{\alpha} \mathbf{V}_{i} = V_{i}^{-1} \sum_{i} \left[ \frac{\partial^{\alpha} V_{i}}{\partial \mathbf{R}_{j}^{\alpha}} - (1 - \alpha) \mathbf{R}_{j}^{-\alpha} V_{i} \right] V_{i}^{-1} \frac{\partial^{1-\alpha} V_{i}}{\partial \mathbf{R}_{j}^{1-\alpha}} \mathbf{V}_{j}.$ $J_i = \kappa T_i^2 \left( \operatorname{grad} \frac{1}{T} \right)_i$ I would like to thank: $\dot{E}_{i} = -V_{i} \left( \text{div J} \right)_{i} + 2\eta V_{i} \left( \overline{\text{Grad } \mathbf{v}} \right)_{i} : \left( \overline{\text{Grad } \mathbf{v}} \right)_{i} +$ $-V_i \left(\text{div J}\right)_i + 2\eta V_i \left(\overline{\text{Grad }\mathbf{v}}\right)_i : \left(\overline{\text{Grad }\mathbf{v}}\right)_i +$ $V_i \zeta \left( \text{div } \mathbf{v} \right)_i^2 - P_i \dot{V}_i + v_i \cdot \dot{\mathbf{P}}_i$ final equation for the momentum Aston University, for his expert advices and encouragemenet; • Jessica Neumann, International Partnerships $-V_i (\operatorname{grad} P)_i - V_i (\operatorname{Div} \sigma)_i$ $\dot{\mathbf{P}}_{i} = \sum_{i} \left[ \mathcal{V}_{j}^{\alpha-1} \frac{\partial^{\alpha} \mathcal{V}_{j}}{\partial \mathbf{R}_{i}^{\alpha}} P_{j}^{\alpha} \right. \left. \frac{\partial^{1-\alpha} \phi_{ij}}{\partial \mathbf{R}_{i}^{1-\alpha}} \phi_{ij}^{1-\alpha} \right] +$ Development Officer, for her help with obtaining of Erasmus+ Grant; $\zeta \sum_{i} \left[ \frac{\partial^{\alpha} V_{i}}{\partial \mathbf{R}_{j}^{\alpha}} - (1 - \alpha) \mathbf{R}_{j}^{-\alpha} V_{i} \right] V_{i}^{-1} \frac{\partial^{1-\alpha} V_{i}}{\partial \mathbf{R}_{j}^{1-\alpha}} \cdot \mathbf{V}_{j} +$ • Mr Stephen Baker, Postgraduate Research $2\eta \left( \sum_{j} \left[ \frac{\partial^{\alpha} \mathcal{V}_{i}}{\partial \mathbf{R}_{j}^{\alpha}} - (1 - \alpha) \mathbf{R}_{j}^{-\alpha} \mathcal{V}_{i} \right] \mathcal{V}_{i}^{-1} \frac{\partial^{1 - \alpha} \mathcal{V}_{i}}{\partial \mathbf{R}_{j}^{1 - \alpha}} \mathbf{V}_{j} \right) \right.$ Admissions Officer, for dealing with PhD application and help with enrollment; atomistic energy equation • Dr Vitaliy Yu. Bardik , Senior Research Associate, responsible person at Taras Shevchenko National University of Kyiv for his help with preparing for this program.