MULTISCALE HYBRID MODEL OF LIQUIDS: CONSERVATION OF THE TOTAL ENERGY OF THE SYSTEM

Yelyzaveta Berezovska, Erasmus+ exchange student from
Taras Shevchenko National University of Kyiv, Ukraine in Aston University, UK

SUMMARY

Fluctuations of liquids at the scales where the hydrodynamic and atomistic descriptions overlap are considered. For a smooth transition between the atomistic and continuum representations, an analogy with two-phase hydrodynamics is used that leads to a strict preservation of macroscopic mass and momentum conservation laws [1]. To get a more realistic theory of liquids energy conservation law is added in the multiscale model.

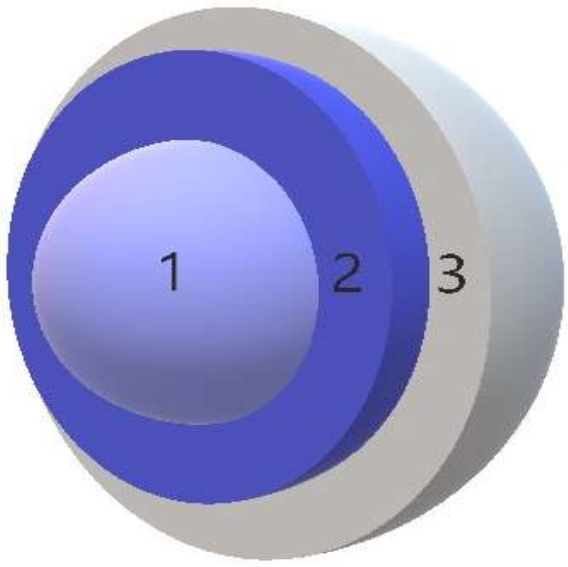
Hybrid system

Total internal energy of the mixture is a combination of the total energy of the molecular dynamics (MD) part and the internal energy of the hydrodynamics (HD) part. For the first approximation:

$$E = xE_{HD} + (1-x)H_0,$$

where x is the mole fraction of the HD phase.
Systems in macroscopic equilibrium are considered. Therefore, it is assumed that the changes of the total energy in control volumes are only due to thermal fluctuations. Since $\dot{H}_0 = 0$,

$$\dot{E} = \dot{E}_{HD}$$



Model

On the image basic model is illustrated. In the centre is pure molecular dynamics zone (1). Then comes hybrid molecular dynamics (2) and pure hydrodynamics region (3).

General idea

System of N atoms interacting via potential forces is described using dynamics that obeys the Gauss principle of least constraint [2]:

$$\dot{\mathbf{q}}_i = \mathbf{p}_i/m + \mathbf{C}_i \cdot \mathbf{F}(t)$$
$$\dot{\mathbf{p}}_i = \mathbf{F}_i - \mathbf{D}_i \cdot \mathbf{F}(t) - \lambda(t)\mathbf{p}_i$$

where $F(t)$ is some external vector field and the term $\lambda(t)pi$ is the force of constrain derived on the basis of Gauss principle to maintain a constant energy $\dot{H}_0 = 0$.
Considering fundamental assumption of HD – local equilibrium hypothesis – from MD phase point of view the energy of the system (each control volume) remains constant.
Using modified equations of motion for the MD phase [1] an equation for multiplier $\lambda(t)$ and afterwards for parameter β was found.
Future computer simulations in GROMACS will show if total energy of the system is constrained under this conditions.

Main results

An equation for multiplier $\lambda(t)$:

$$\lambda(t) = -\frac{\rho_p}{\sum_{k=1}^{N}\rho_k}\left[s_p(1-s_p)\alpha\left[\Delta\left\{ \tilde{\rho} - \sum_{k=1}^{N}\rho_k \right\}\right]_p \Big/ \sum_{k=1}^{N}\rho_k \right]_p$$

An equation for parameter β:

$$\beta(p,\mathbf{r}) = \left(\frac{\sum_p \frac{\mathbf{p}_p^2}{m_p}}{\sum_{p,i}\mathbf{p}_p \bullet \left[\frac{\partial}{\partial x_i}\left(s(1-s)\frac{\partial}{\partial x_i}\left\{ \tilde{u}_j\tilde{\rho} - \sum_{j,k=1}^{N} u_{jk}\rho_k \right\}\right)\right]_p \Big/ \sum_{k=1}^{N}\rho_k} \right) \frac{1}{\sum_{k=1}^{N}\rho_k} \frac{\alpha s_p(1-s_p)\rho_p\left[\Delta\left\{\tilde{\rho} - \sum_{k=1}^{N}\rho_k\right\}\right]_p}{\sum_{k=1}^{N}\rho_k} - \frac{1}{\sum_p \frac{\mathbf{p}_p^2}{m_p}} \sum_p \left[\mathbf{F}_\mathbf{p}^{\mathbf{MD}} \bullet \left(s_p(\tilde{\mathbf{u}} - \mathbf{u}_p) + \alpha s_p(1-s_p) grad\left\{ \tilde{\rho} - \sum_{k=1}^{N}\rho_k \right\} \Big/ \sum_{k=1}^{N}\rho_k \right)\right] -$$

$$- \frac{1}{\sum_p \frac{\mathbf{p}_p^2}{m_p}} \sum_p \frac{\mathbf{p}_p}{m_p} \bullet \left\{ s_p\mathbf{F}_\mathbf{p}^{\mathbf{MD}} - s_p\mathbf{F}_\mathbf{p} - \frac{m_p}{\sum_{p=1}^{N}\rho_p} \left(\frac{\sum_{k=1,k\neq p}^{N}\left[\alpha s_k(1-s_k)\mathbf{u}_\mathbf{k}\rho_k\left[\Delta\left\{\tilde{\rho} - \sum_{k=1}^{N}\rho_k\right\}\right]_k\right]}{\sum_{p=1}^{N}\rho_p} \right) - \frac{m_p}{\sum_{p=1}^{N}\rho_p} \frac{\sum_p^N\left[\alpha s_p(1-s_p)\rho_p\left[grad\left\{ \tilde{\rho} - \sum_{p=1}^{N}\rho_p \right\}\right]_p \sum_i \frac{\partial u_{jp}}{\partial x_i}\right]}{\sum_{p=1}^{N}\rho_p} \right\}$$

REFERENCES

1. Markesteijn A, Karabasov S, Scukins A, Nerukh D, Glotov V, Goloviznin V. 2014 Concurrent multiscale modelling of atomistic and hydrodynamic processes in liquids. Phil. Trans. R. Soc. A 372: 20130379. http://dx.doi.org/10.1098/rsta.2013.0379
2. Denis J. Evans, G. P. Morriss 1984 Non-Newtonian molecular dynamics. North-Holland Physics Publishing – Amsterdam

Acknowledgements

I'm thankful to Erasmus+ programme, Aston University, Dr. Dmitry Nerukh, Ivan Korotkin, Maryna Bakumenko and Physics Department of Taras Shevchenko National University of Kyiv for all the support and help with this work