Hybrid modelling based on two-phase flow analogy: advances and challenges

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Acknowledgement

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Queen Mary University of London,
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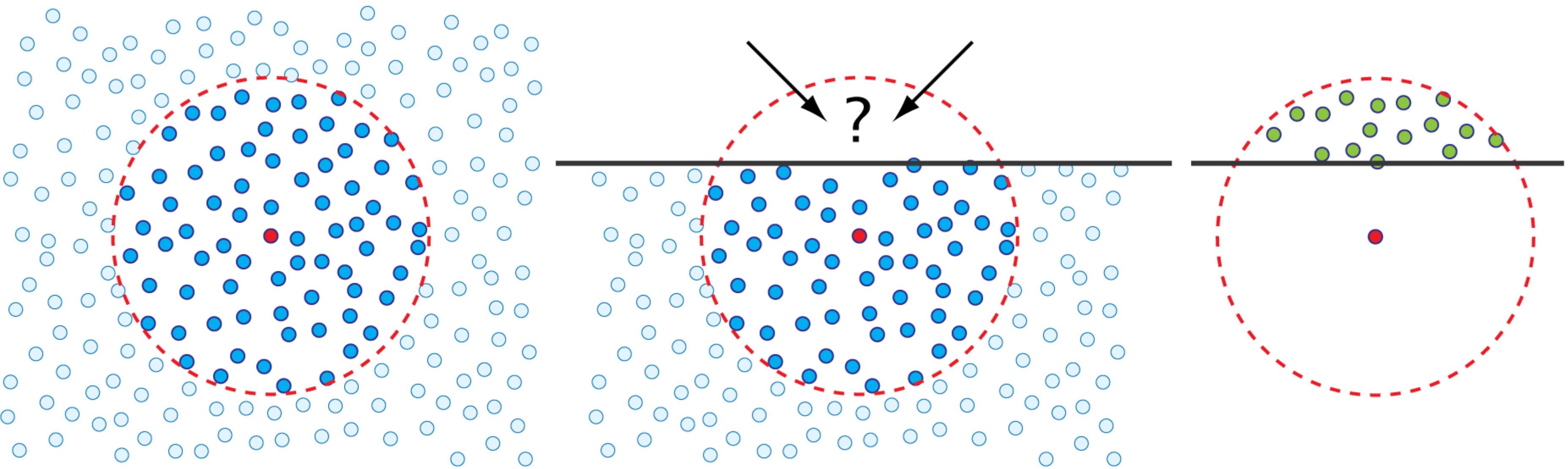
Cambridge University,
Immanuel Kant Baltic Federal University,
Kharkov National University

Continuum ⇔ Atoms ??

- **Problem**: Missing interactions near "wall"
  - Results in unnatural "wiggles"

- **Possible** solutions to mimic the missing force:
  - Average force normally "felt" by particle
  - Value of force function of distance to wall

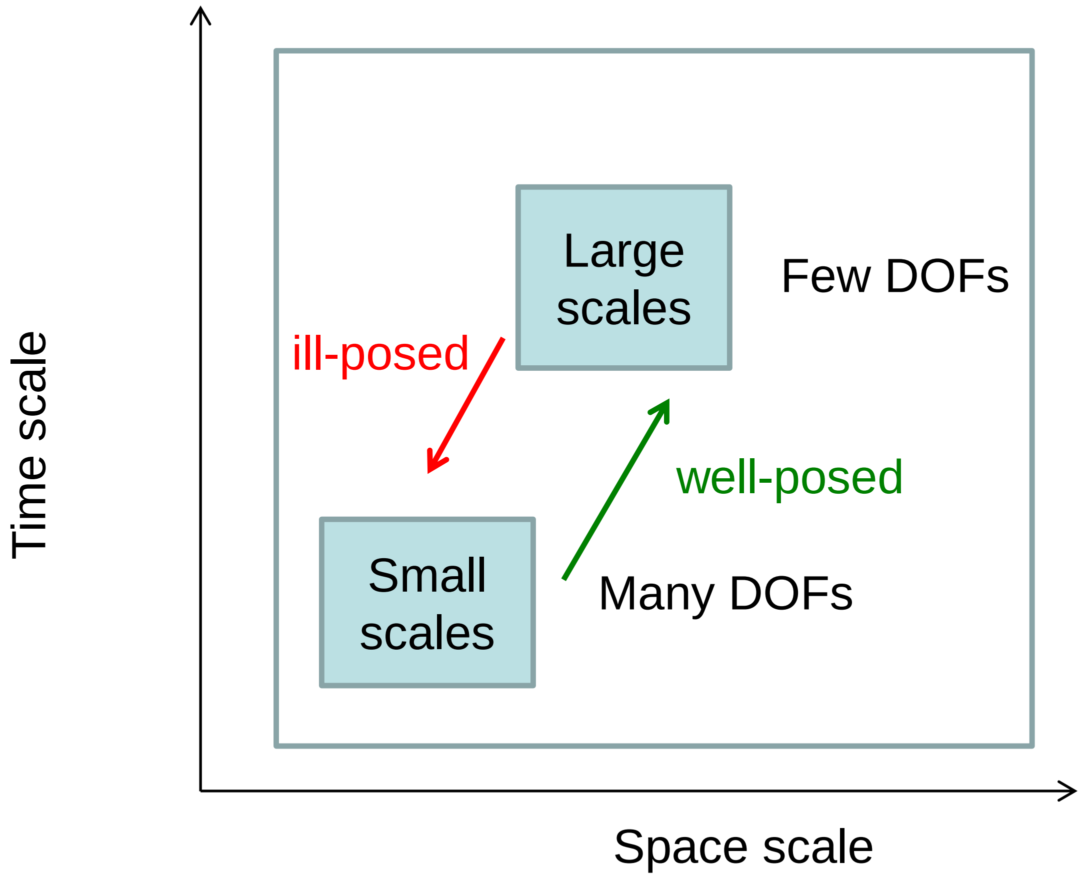


Particle in bulk
all force interactions OK

Particle near specular wall
missing force interactions due to wall

Missing part
try to mimic this force

Multiscale modelling: cyclic (fully coupled) approach



Physical analogies as a multiscale modelling method

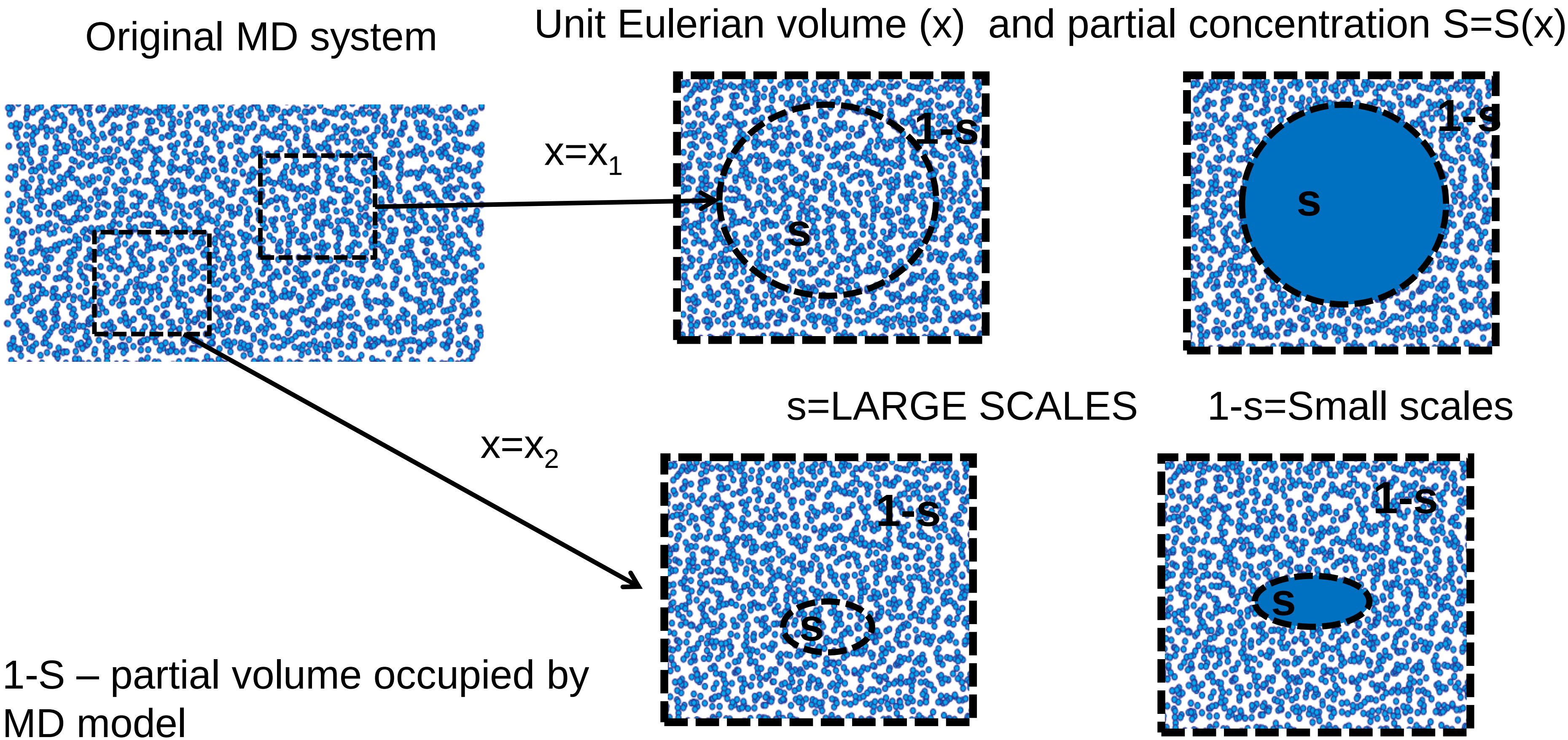
Examples from physics: electrical circuits, acoustics…

pros: may allow efficient solutions for very complex systems, may be “physically insightful” (depending on the question asked)

cons: the solution is not unique, not from the “first principles”, “too engineering”, etc..

MD/FH coupling based on the two-phase analogy

S.E. Buckley and M.C. Leverett (1942). "Mechanism of fluid displacements in sands"



1-S – partial volume occupied by MD model

S – partial volume occupied by continuum model

The two ‘phases’ occupy the same elementary volume of the same liquid, no interface forces are relevant

Two-phase hydrodynamic analogy: mass conservation

S.E. Buckley and M.C. Leverett (1942). "Mechanism of fluid displacements in sands"

Continuum phase

$$\delta_t(sm) + \sum_{\gamma=1,6} \left(s\rho\bar{\mathbf{u}}\right) d\mathbf{n}^{\gamma} dt = \delta_t J^{(\rho)}$$

Particle phase

$$\delta_t\left((1-s) \sum_{p=1,N(t)} m_p \right) + \sum_{\gamma=1,6} \left((1-s) \sum_{p=1,N_\gamma(t)} \rho_p \mathbf{u}_p \right) d\mathbf{n}^{\gamma} dt = -\delta_t J^{(\rho)}$$

Conservation law is satisfied for the mixture density

$$\overline{\rho} = s\rho + (1-s) \sum_{p=1,N(t)} \rho_p$$

J is the model birth/death function that depends on S for the solution to satisfy compatibility conditions: for S-> 1 all phases -> continuum phase, for S-> 0 all phases -> atomistic phase

Two-phase hydrodynamic analogy : momentum conservation

S.E. Buckley and M.C. Leverett (1942). "Mechanism of fluid displacements in sands"

Continuum phase

Landau-Lifshitz' deterministic + stochastic stresses

$$\delta_t(smu_i) + \sum_{\gamma=1,6}\left(s\rho u_i \bar{\mathbf{u}}\right) d\mathbf{n}^\gamma dt = s\sum_{j=1,3}\sum_{\gamma=1,6}\left(\Pi_{ij} + \tilde{\Pi}_{ij}\right) dn_j^\gamma dt + \delta_t J_i^{(\mathbf{u})} dt, i = 1,3$$

Particle phase

$$\delta_t\left((1-s)\sum_{p=1,N(t)} m_p u_{ip}\right) + \sum_{\lambda=1,6}\left((1-s)\sum_{p=1,N_\gamma(t)} \rho_p u_{ip} \mathbf{u}_p\right) d\mathbf{n}^\gamma dt = (1-s)\sum_{p=1,N(t)} F_{ip} dt - \delta_t J_i^{(\mathbf{u})} dt, i = 1,3$$

2nd Newton's law is satisfied: the change of the mixture momentum

$$\bar{\rho}\cdot\bar{u}_i \text{, where } \bar{u}_i = \left[s\rho u_i + (1-s)\sum_{p=1,N(t)} \rho_p u_{ip}\right]$$

= force

Closing the hybrid model

Specify the source birth/death terms in the 'buffer zone' 0< s < 1 the continuum solution is **forced (softly diffused or exponentially forced)** towards the 'target' MD solution;

$$D_t\left(\overline{m} - \sum_{p=1,N(t)} m_p\right) = L^{(\rho)} \bullet \left(\overline{m} - \sum_{p=1,N(t)} m_p\right),$$

$$D_t\left(\overline{u}_i\overline{m} - \sum_{p=1,N(t)} u_{ip} m_p\right) = L^{(u)} \bullet \left(\overline{u}_i\overline{m} - \sum_{p=1,N(t)} u_{ip} m_p\right) + s\sum_{j=1,3}\sum_{\gamma=1,6}\left(\Pi_{ij} + \tilde{\Pi}_{ij}\right) dn_j^{\gamma}\, dt,$$

for s=1 and s=0 allow the model to become pure continuum (fluctuating hydrodynamics) and pure MD, respectively.

Consistent modification of the MD equations

- Add forcing terms to the molecular dynamics kinematic and dynamic equations to satisfy the macroscopic equations of the hybrid model

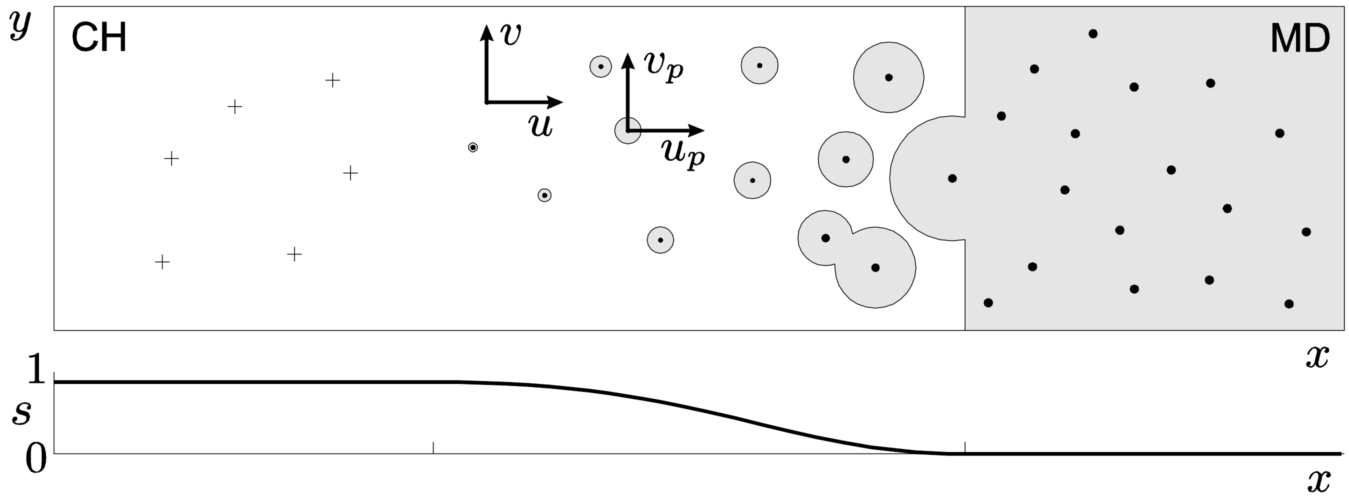
$$\frac{dx_{ip}}{dt^{MD}} = u_{ip}{}^{Newton} + ?..$$

$$\frac{d}{dt} u_{ip}{}^{Newton} = -\frac{d}{dx_i} V_p{}^{MD} + ?..$$

Can work out the expressions for the "?" terms from the corresponding discrete conservation laws for MD particles

Note that $dx_p/dt \neq u_p$ for the "two phase flow" model

2D examples of two-way coupled hybrid models



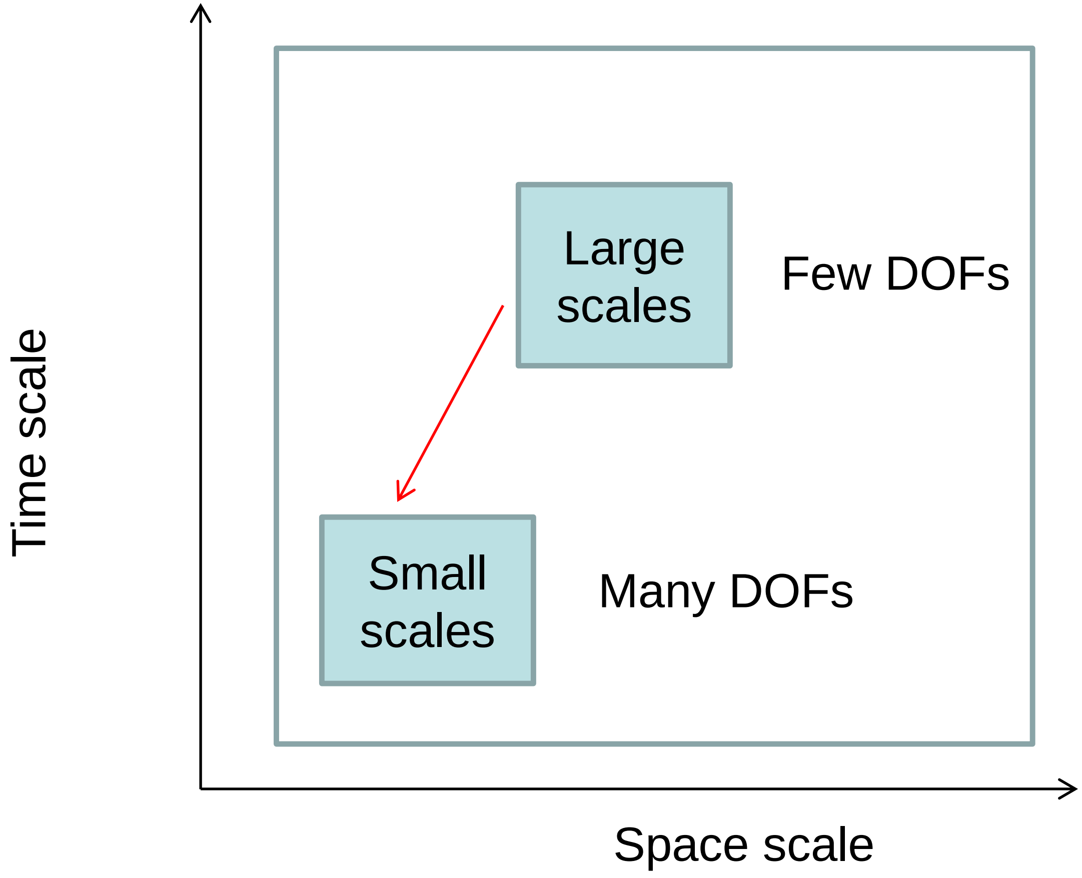
PHILOSOPHICAL TRANSACTIONS OF THE ROYAL SOCIETY A | MATHEMATICAL, PHYSICAL & ENGINEERING SCIENCES

Concurrent multiscale modelling of atomistic and hydrodynamic processes in liquids

Anton Markesteijn, Sergey Karabasov, Arturs Scukins, Dmitry Nerukh, Vyacheslav Glotov and Vasily Goloviznin

Phil. Trans. R. Soc. A 2014 **372**, 20130379, published 30 June 2014

(Current) Multiscale modelling in 3D: acyclic "top-bottom"/ "boundary-condition" approach



Effectively works like an 'open-domain' boundary condition in CFD

Large scales: Fluctuating Hydrodynamics

- Fluctuating Hydrodynamics
  - Dissipative fluxes treated as stochastic variables
    - Random variables, mimicking molecular motion
- Fluctuation-Dissipation theorem
- Equations of Fluctuating Hydrodynamics
  - Conservation of Mass / Conservation of Momentum
    - Added fluctuating stress tensor

$$\langle \delta\Pi_{ij}(\mathbf{r},t)\cdot\delta\Pi_{kl}(\mathbf{r}',t')\rangle = 2k_{\mathrm{B}}T\left[\eta\left(\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk}\right)+\left(\eta_{\mathrm{v}}-\frac{2}{3}\eta\right)\delta_{ij}\delta_{kl}\right] \times \delta(\mathbf{r}-\mathbf{r}')\ \delta(t-t').$$

Landau-Lifshitz Fluctuating Hydrodynamics Equations

One dimensional case

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} = 0$$

Stochastic fluxes

$$\frac{\partial \rho u}{\partial t} + \frac{\partial\left(\rho u^2 + P\right)}{\partial x} - \frac{4}{3}\cdot\eta\cdot\frac{\partial^2 u}{\partial x^2} - \frac{\partial s}{\partial x} = 0$$

$$\frac{\partial \rho E}{\partial t} + \frac{\partial\left(\rho E + P\right)u}{\partial x} - \frac{\partial}{\partial x}\cdot\left(\frac{4}{3}\cdot\eta u\frac{\partial u}{\partial x} + \kappa\cdot\frac{\partial T}{\partial x}\right) - \frac{\partial\left(q + u\cdot s\right)}{\partial x} = 0$$

$$\left\langle s(x,t)s(x',t')\right\rangle = \frac{8\cdot k\cdot\eta\cdot T}{3\cdot\sigma}\cdot\delta(x-x')\cdot\delta(t-t');$$

$$\left\langle q(x,t)q(x',t')\right\rangle = \frac{2\cdot k\cdot\kappa\cdot T^2}{\sigma}\cdot\delta(x-x')\cdot\delta(t-t');$$

$$\rho E = c_v\rho T + \frac{\rho u^2}{2};$$

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Comput. Methods Appl. Mech. Engrg. 281 (2014) 29–53

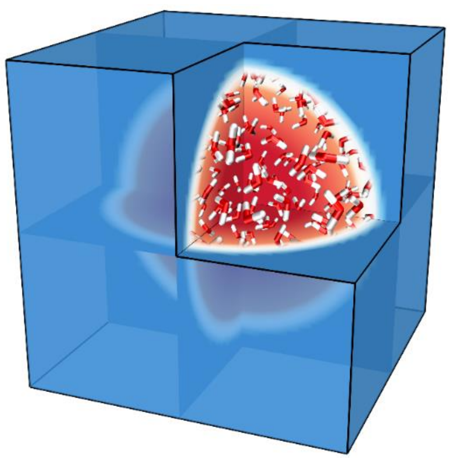
Computer methods in applied mechanics and engineering

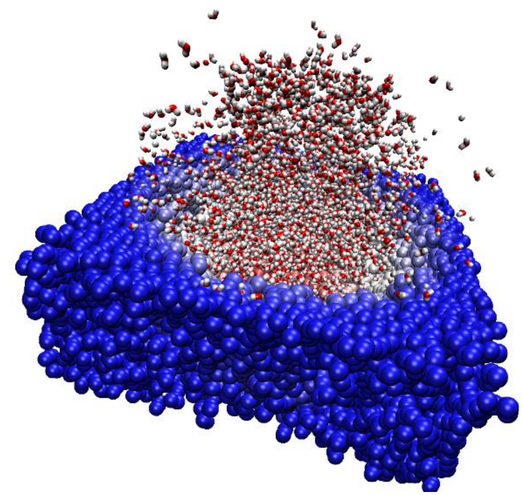
www.elsevier.com/locate/cma

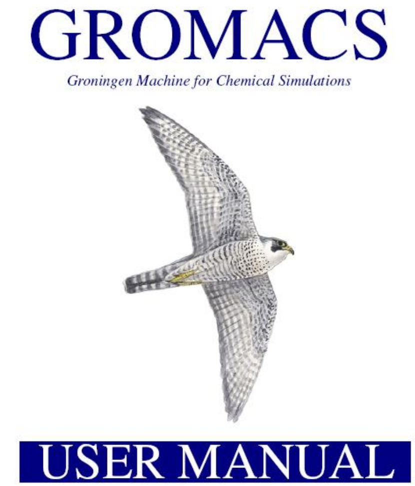
A new non-linear two-time-level Central Leapfrog scheme in staggered conservation–flux variables for fluctuating hydrodynamics equations with GPU implementation

A.P. Markesteijn[a,*], S.A. Karabasov[a], V.Yu. Glotov[b], V.M. Goloviznin[b]

From fluctuating hydrodynamics to all-atom resolution







AIP | The Journal of Chemical Physics

A hybrid molecular dynamics/fluctuating hydrodynamics method for modelling liquids at multiple scales in space and time

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Ivan Korotkin[1,a)], Sergey Karabasov[1], Dmitry Nerukh[2], Anton Markesteijn[1], Arturs Scukins[2], Vladimir Farafonov[3] and Evgen Pavlov[2,4]

+ VIEW AFFILIATIONS

[a)] Author to whom correspondence should be addressed. Electronic mail: i.korotkin@qmul.ac.uk

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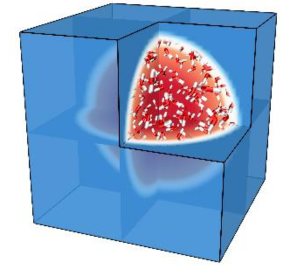
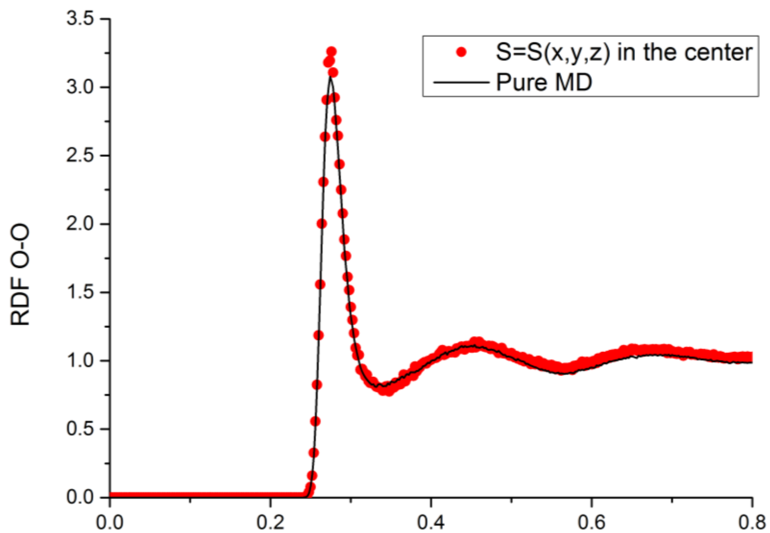
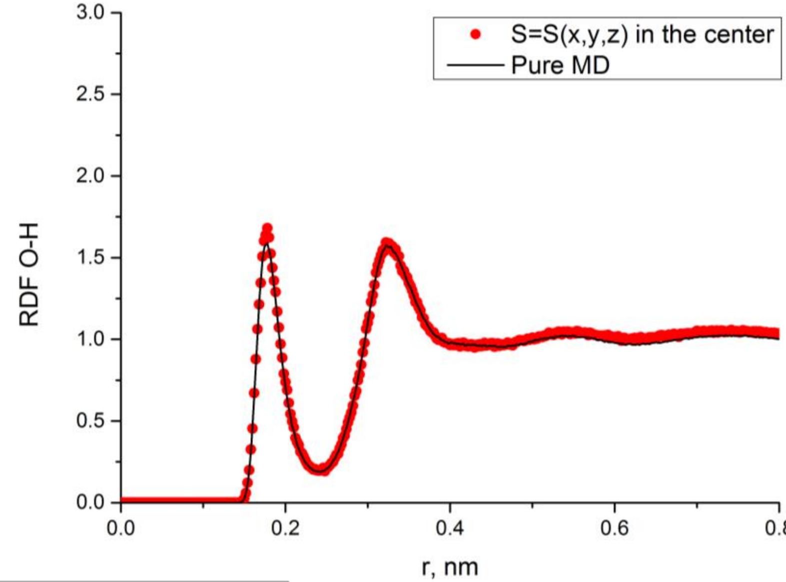
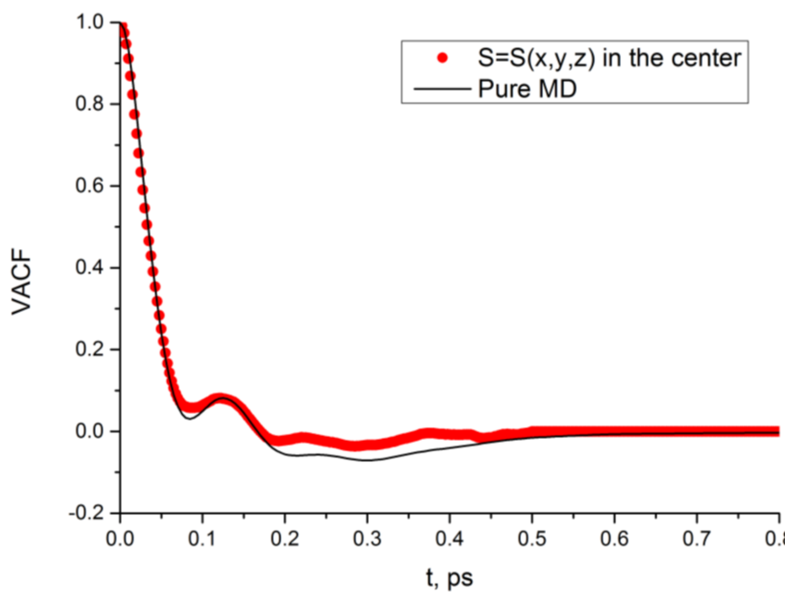
J. Chem. Phys. **143**, 014110 (2015); http://dx.doi.org/10.1063/1.4923011

‘Simple water’: radial distributions and velocity correlations

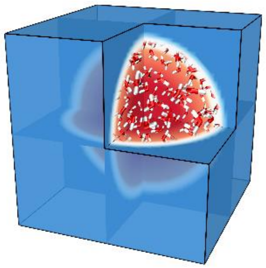


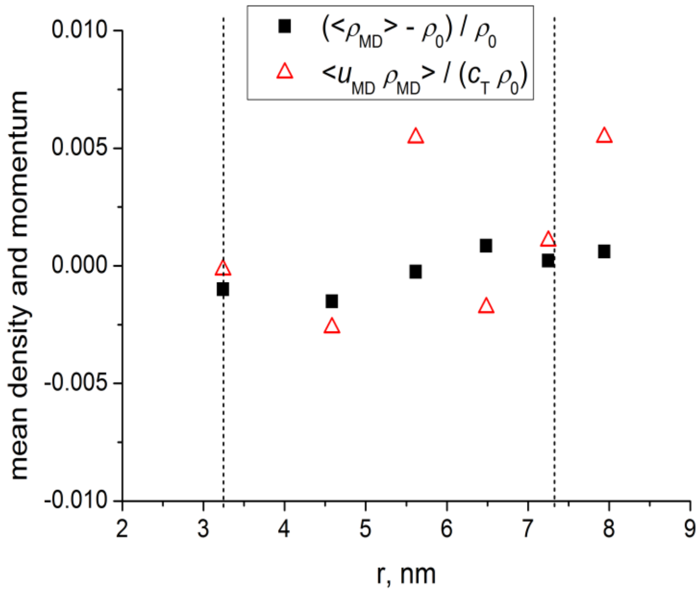




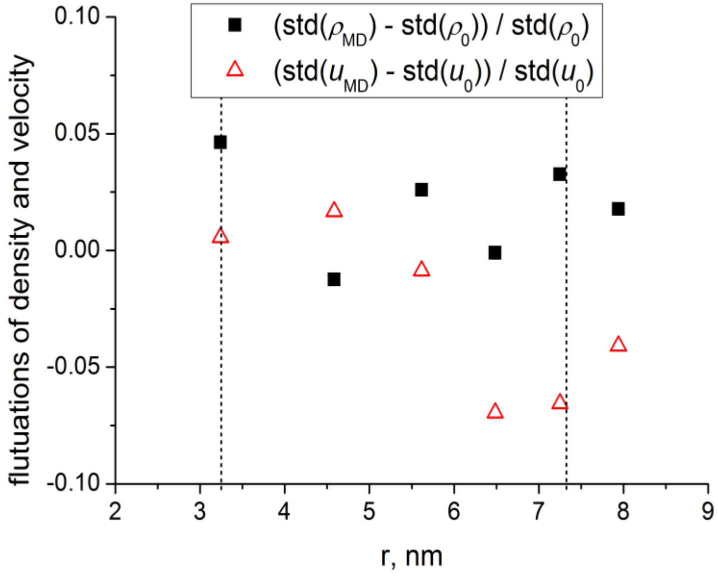


Preservation of mass, momentum, and correct fluctuation amplitudes across the hybrid zone



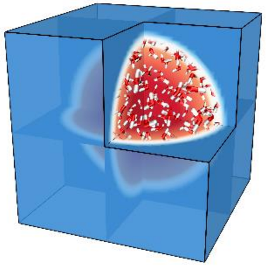


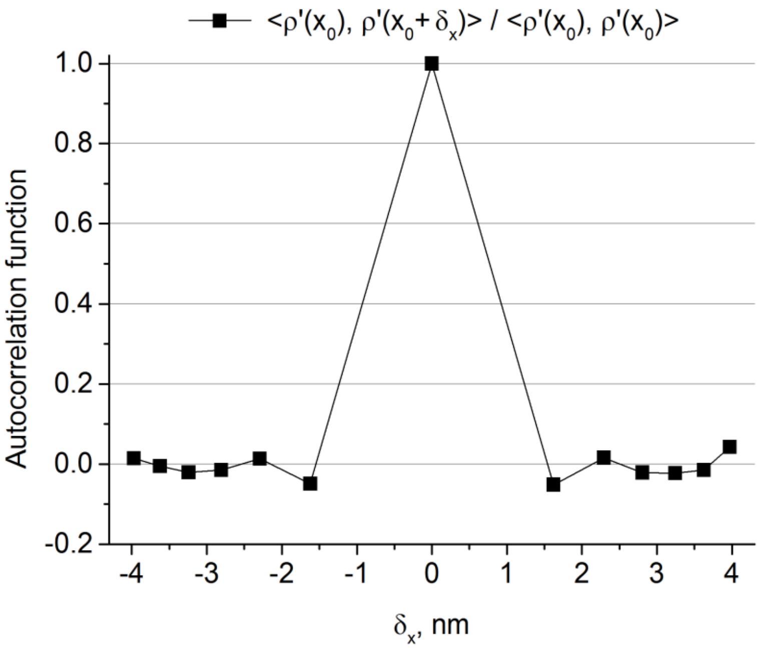
means



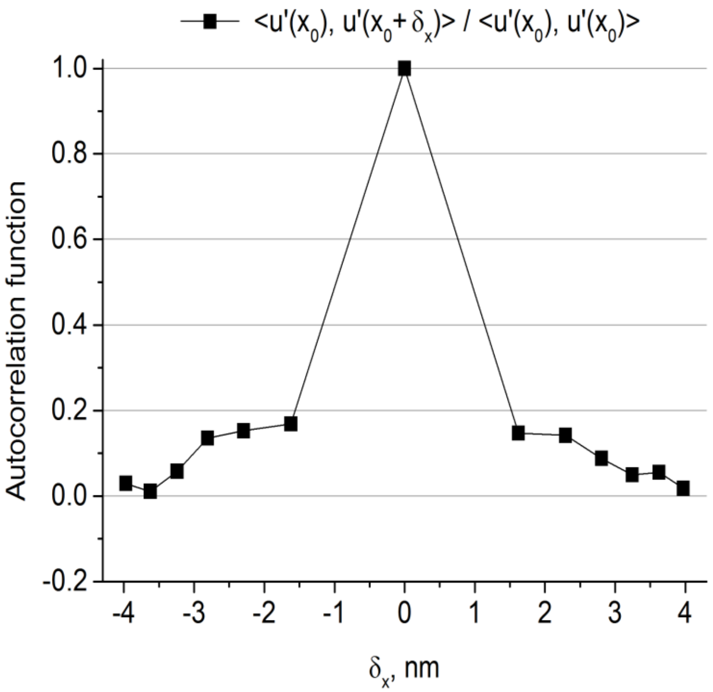
fluctuations

Preservation of random fluctuations across the hybrid zone



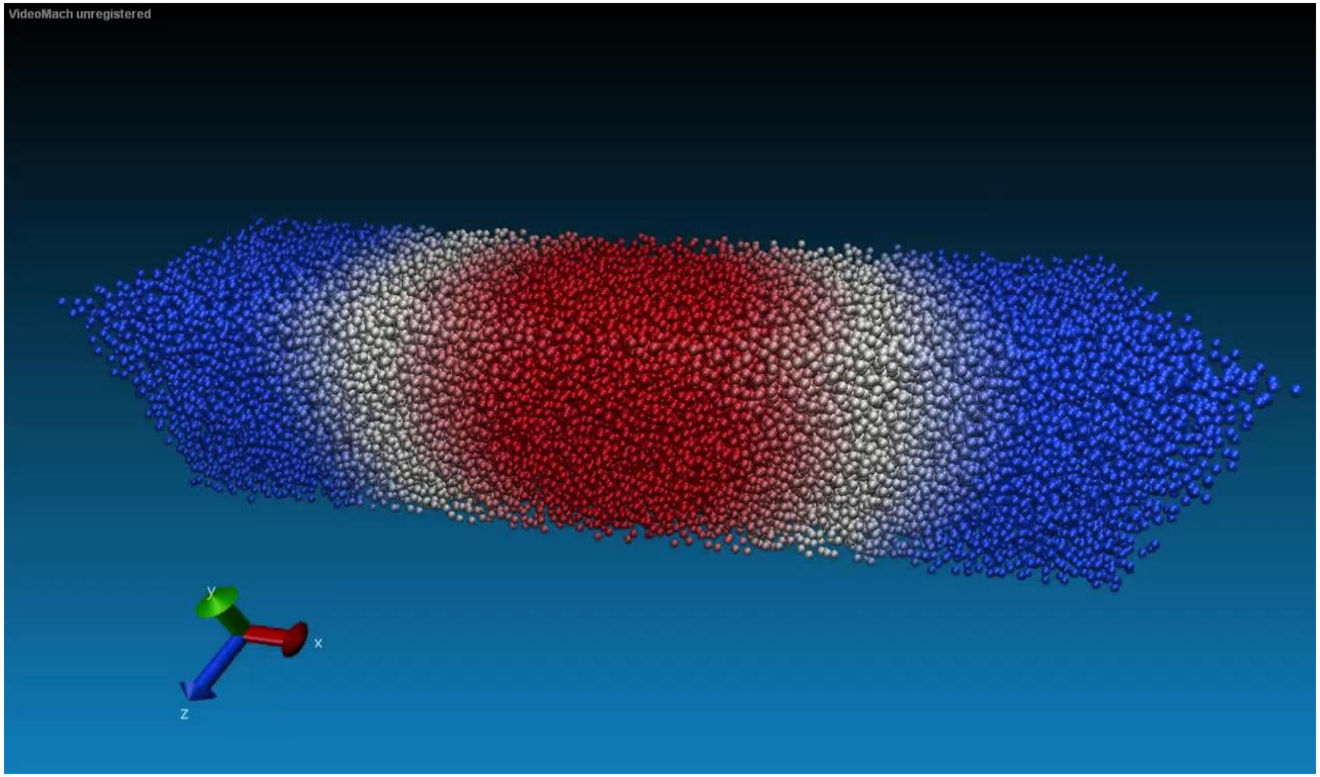


density

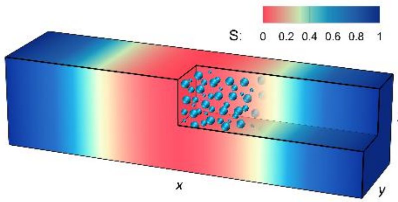


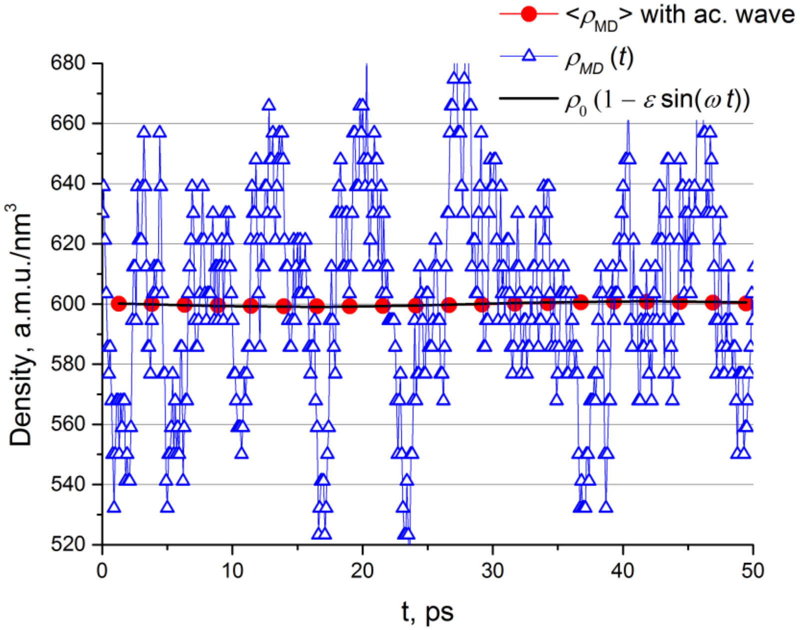
velocity

Test problem: hydrodynamic waves travelling through the hybrid MD/FH zone (20x5x5 FH cells)

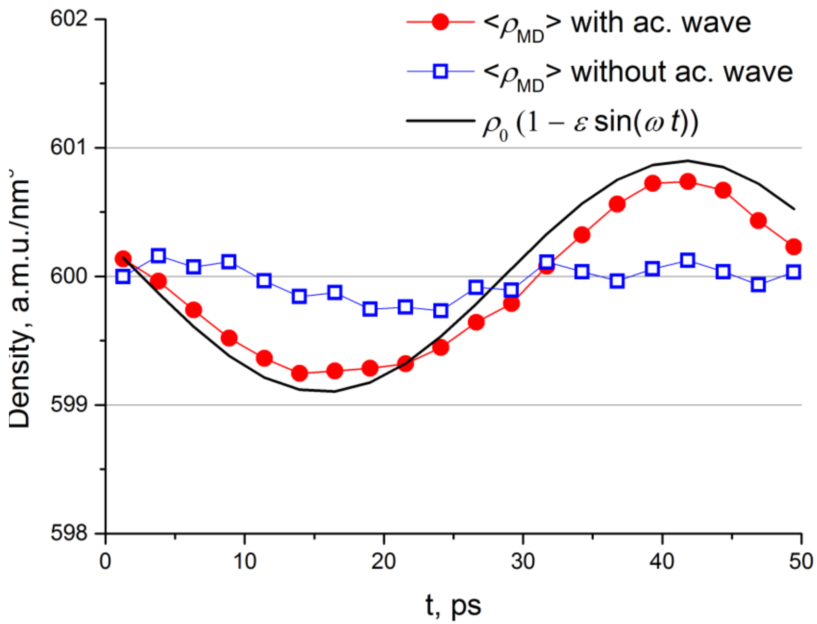


Case 1: acoustic wave





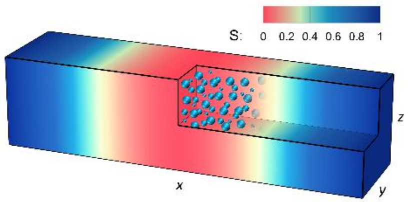
Original signal

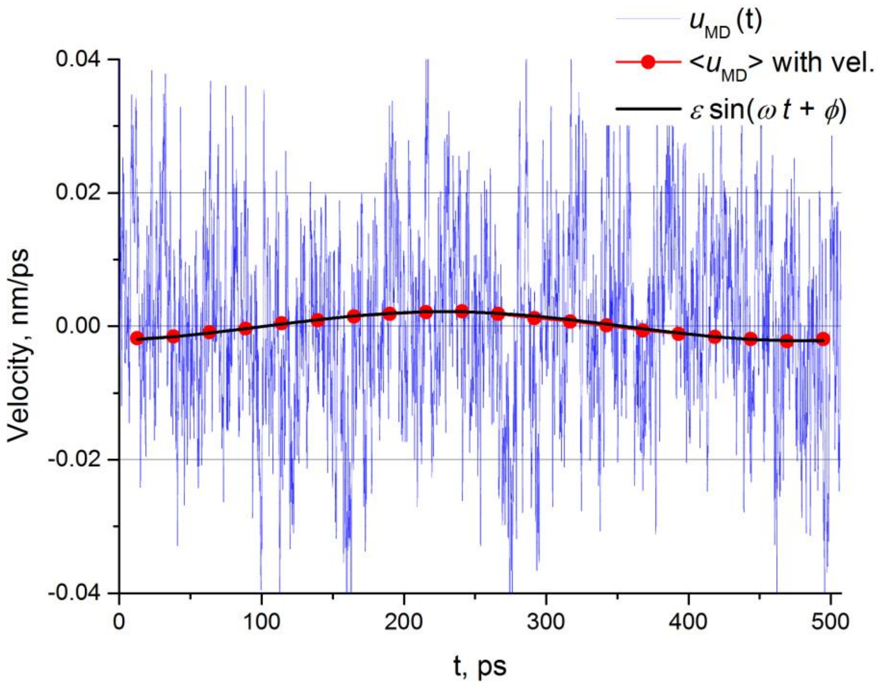


Phase and y&z averaged signal

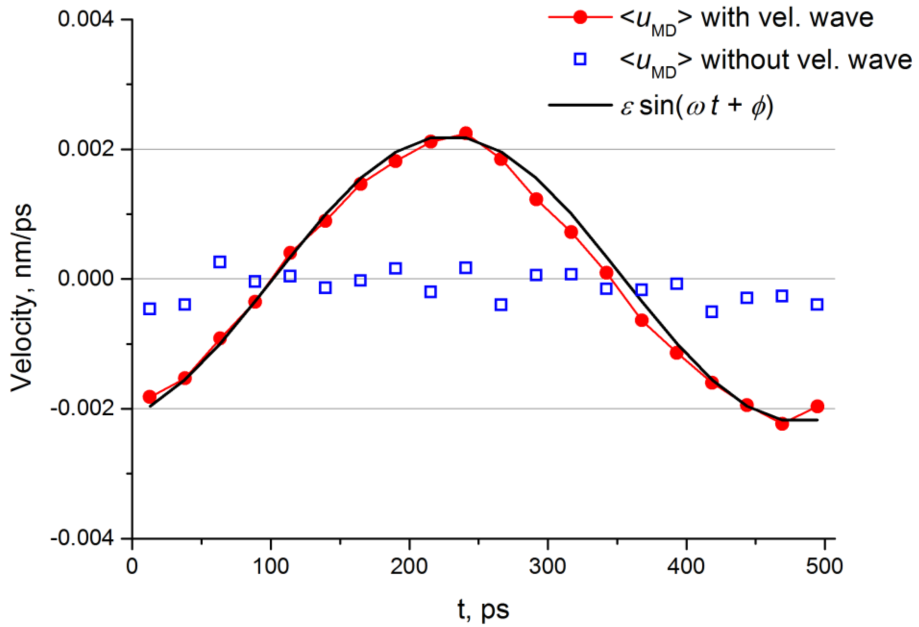
Signal/noise ~0.01

Case 2: shear wave





Original signal



Phase and y&z averaged signal

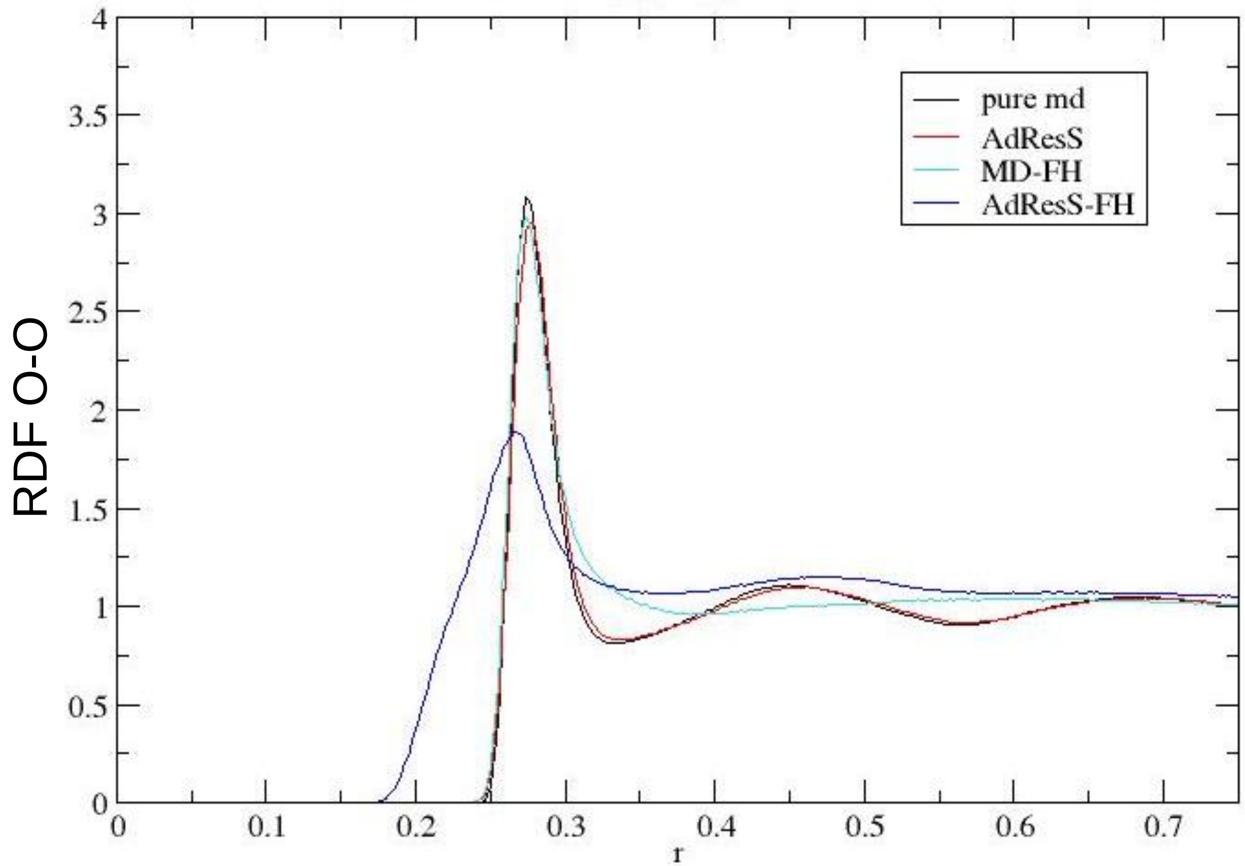
Signal/noise ~0.05

Unsolved issue: sensitivity to the hybrid model parameters

Keep away the redundant MD particles from the FH zone using the space-time expansion ?

Introduce MD (+CG) +FH?

Effect of the macroscopic equation of state?

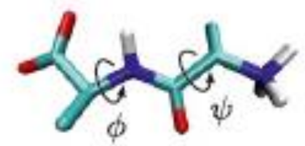


Application: dialanine molecule in water

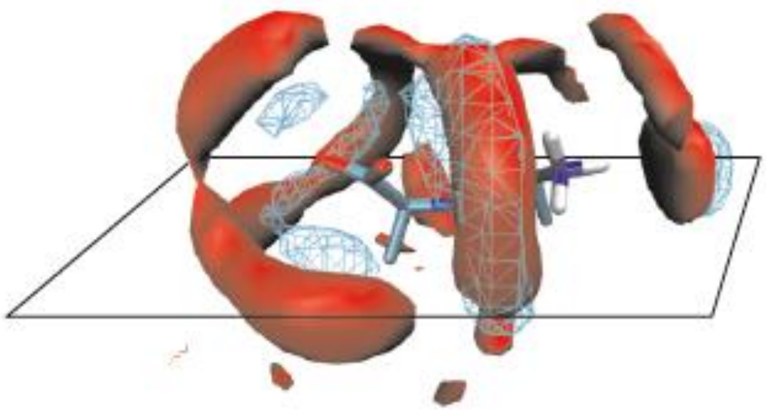
The Journal of Physical Chemistry Letters
Letter
pubs.acs.org/JPCL

Water–Peptide Dynamics during Conformational Transitions

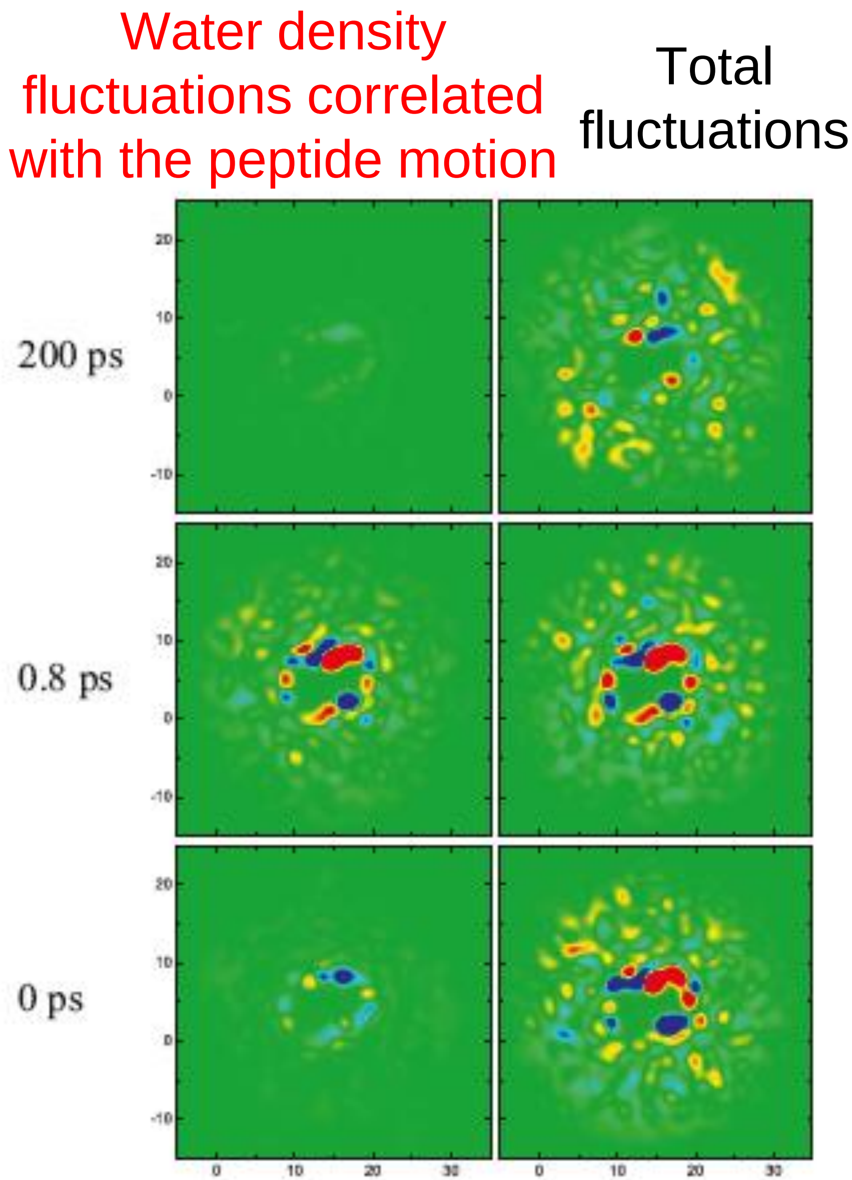
Dmitry Nerukh*,† and Sergey Karabasov‡



Surrounding water density changes as the dialanine molecule changes its conformation

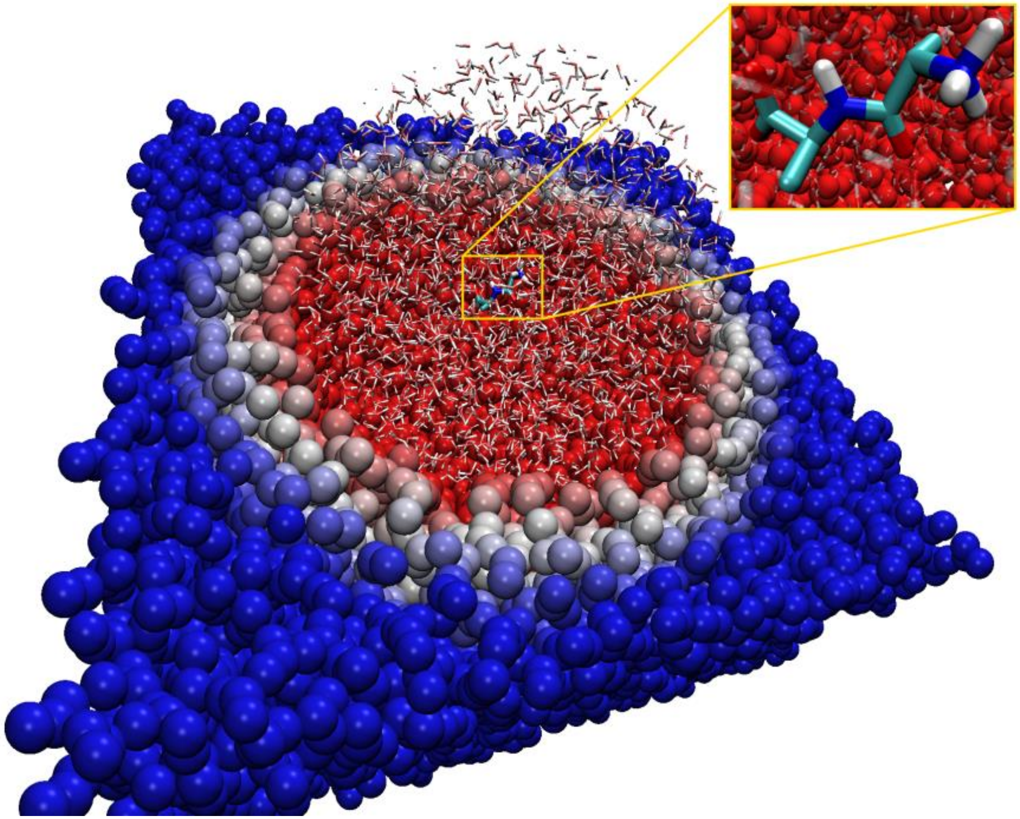


Question: to what extend the dynamics of water density (fluctuations) is connected with the dynamics of the peptide (quantified by its dihedral angles ϕ and ψ)?



Answer: strongly correlated but *only* at very specific periods, when the conformational transitions occur

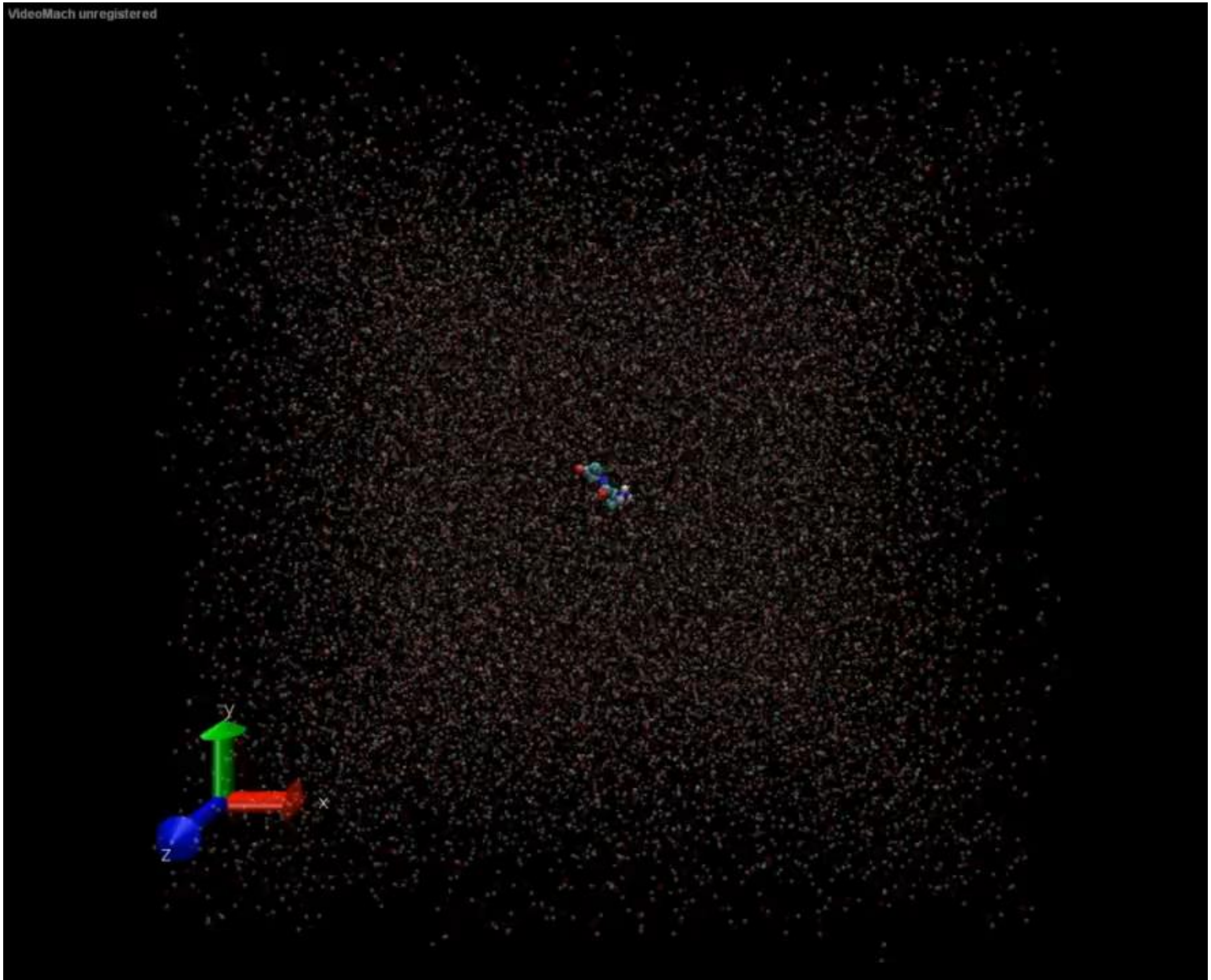
Dialanine in water: a multiscale model



“Static sphere” MD/FH algorithm

- Define S-function, which specifies the (stationary) space decomposition between the MD and the hydrodynamics driven parts of the computational domain,
- For each particle location, find the corresponding control volume it belongs to, interpolate the hydrodynamic fields obtained, compute S-function value at the particle location, and integrate MD equations over one time step,
- Update positions of all particles and repeat.

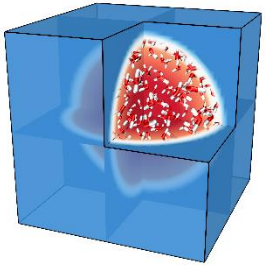
Dialanine diffusion in water, s=s(**x**)

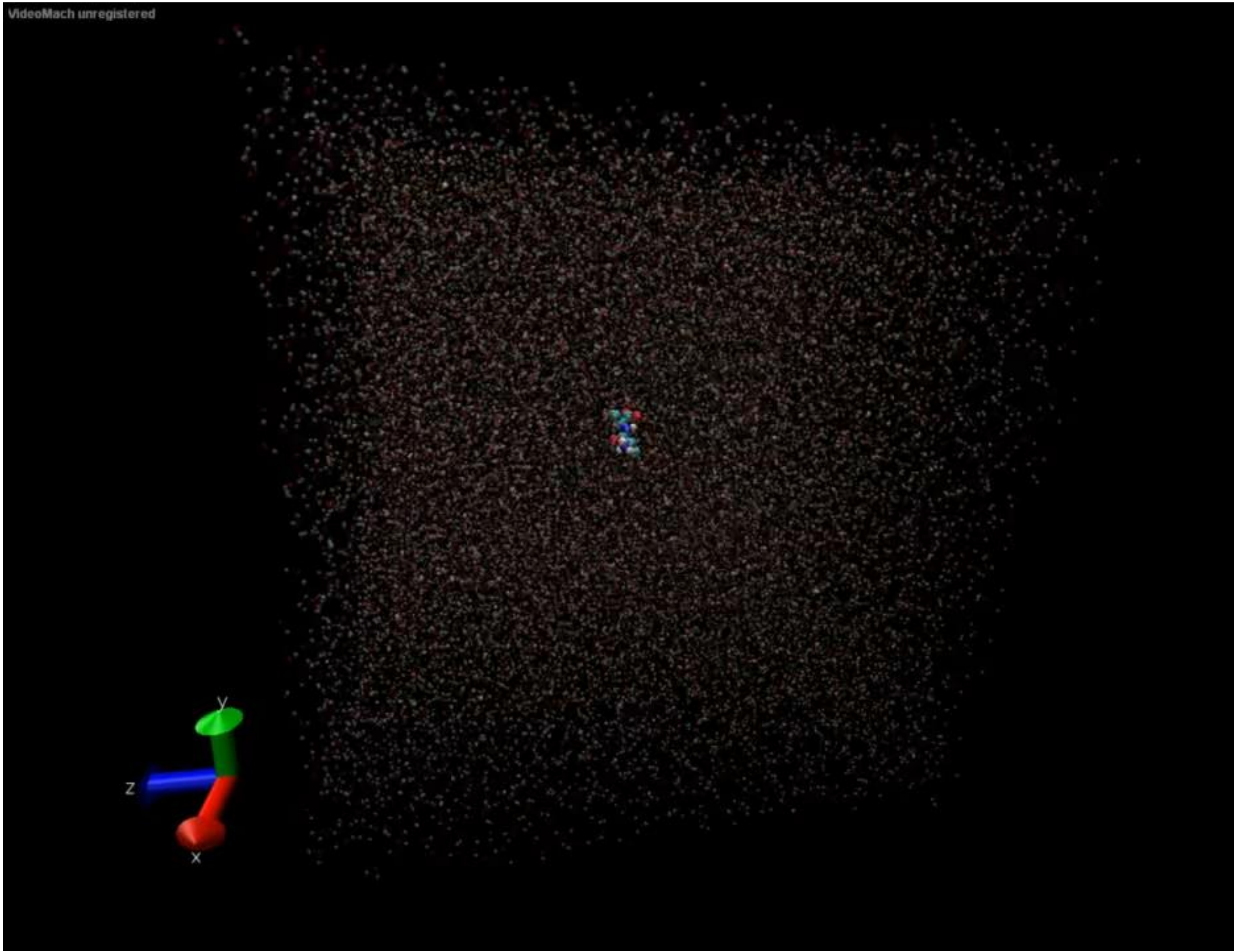


“Dynamic sphere” MD/FH algorithm

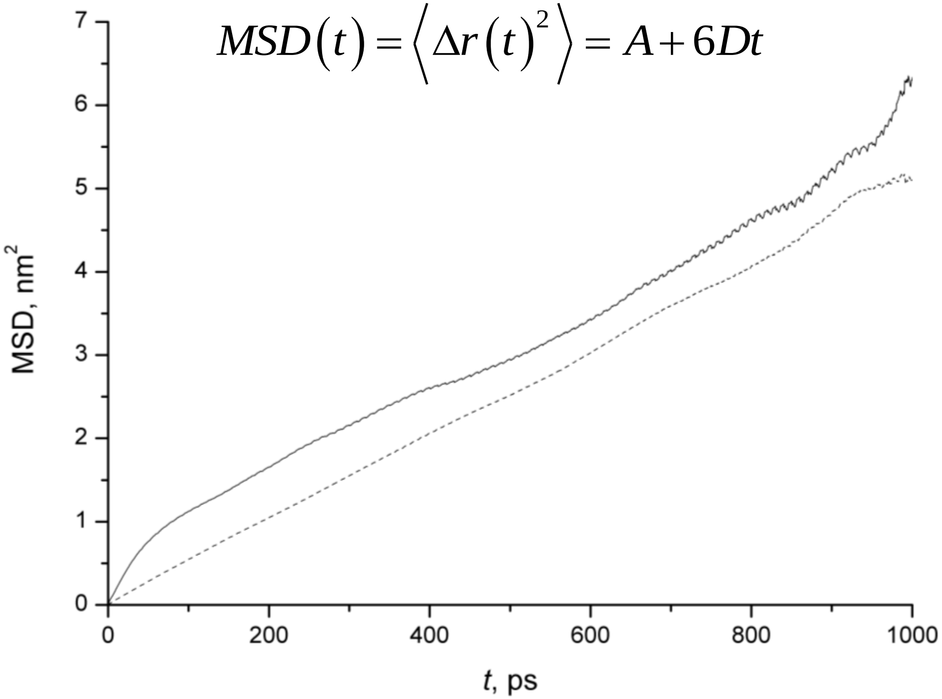
- Specify the feature of interest, e.g. the centre of mass of a complex molecule that needs to be treated at all-atom resolution.
- Lock the centre of S-function to this feature so that the coordinates of the origin are updated at each time step.
- For each particle location corresponding to a certain time moment, find the control volume it belongs to, interpolate the hydrodynamic fields to its location, calculate the space-time variable S-function at that location, and integrate MD equations over one time step, then update positions of all particles, move the origin of S-function in accordance with the kinematics of the feature of interest, and repeat.

Dialanine diffusion in water, s=s(**x**,t)

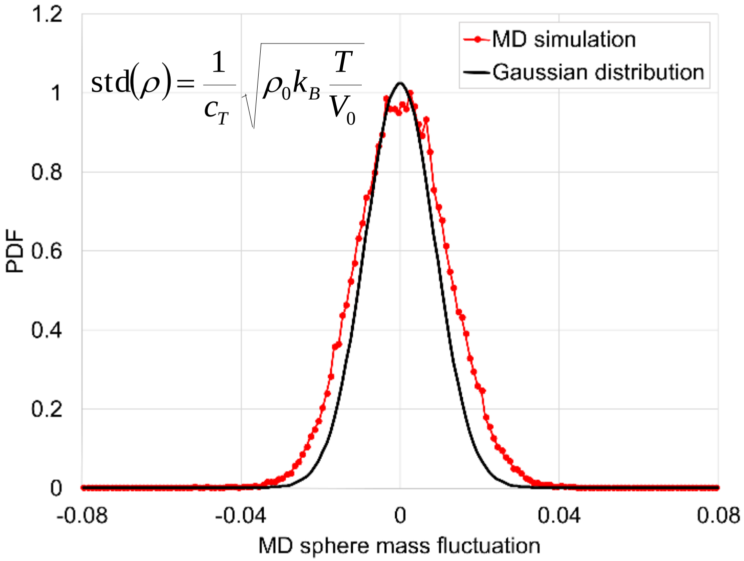


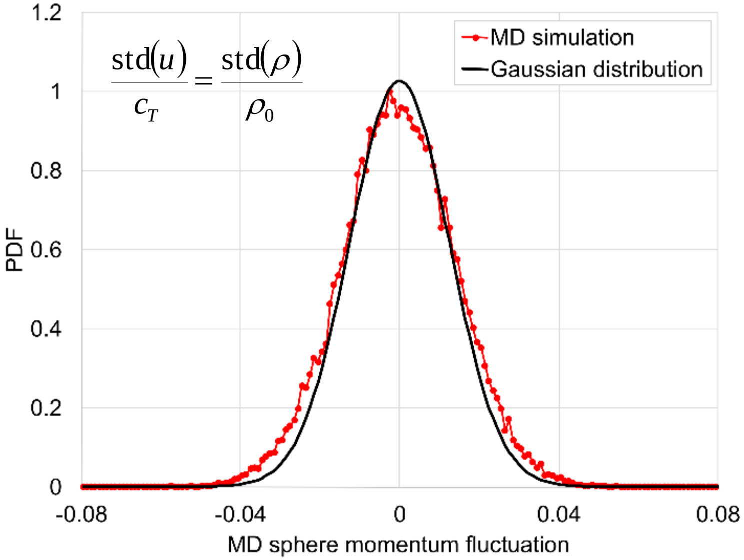


Dialanine in water: mass and momentum fluctuations and diffusion coefficient



D=(**0.83**±0.08)·10^{-5} cm²/s
(D_{ref}= **0.86**·10^{-5} cm²/s)





Application for “Micro/ Nano Fluidics for Health and Diagnostics”?

<u>Dr. Ajay Agarwal</u>

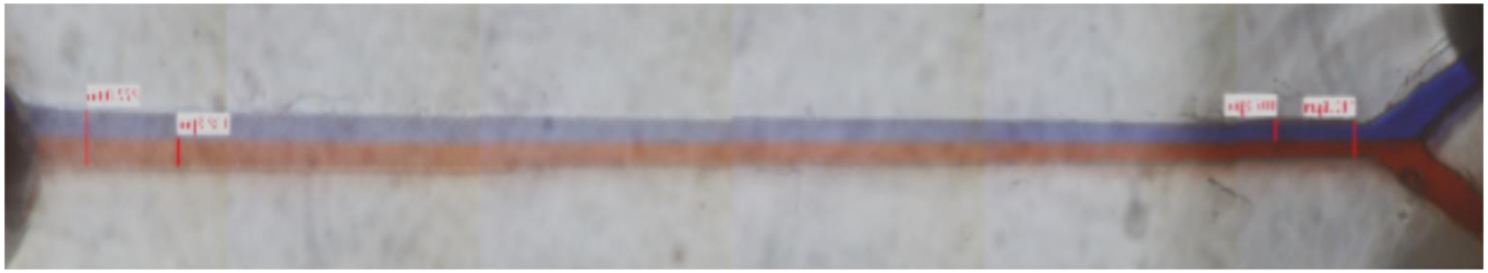
- ***Principal Scientist, CSIR-CEERI, Pilani, INDIA***
- ***Associate Professor, AcSIR, New Delhi, INDIA***

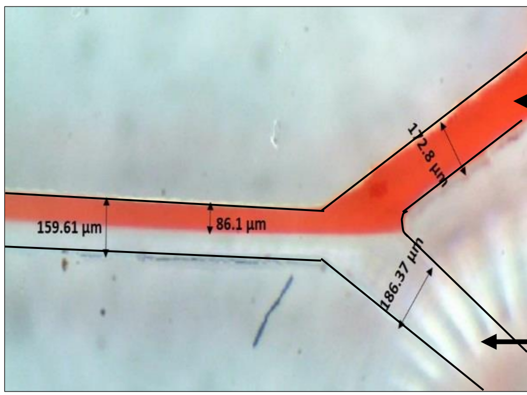
<u>Prof. Pankaj Vadgama</u>

- ***Director, IRC in Biomedical Materials,***
- ***Queen Mary Univ. of London, UK***

- **Versatile microfluidic platforms for medical diagnostics**
- **Controlled flow for kinetically and diffusion controlled assays**
- **Dual flow regimens for liquid-liquid interfacing of sample and reagent streams**
- **Integration of sensor arrays into micro flow devices for practical assay and reaction modeling.**
- **Development of pump-less fluid flow using porous absorbent phases**

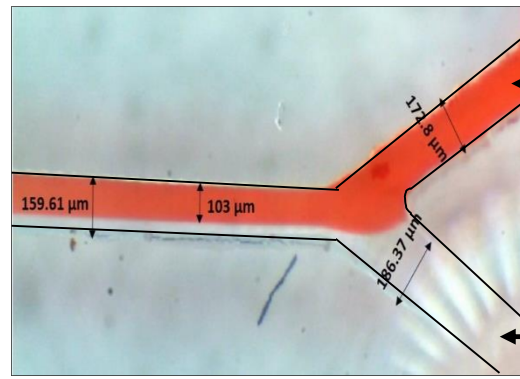
Effect of flow rates on laminar flow width





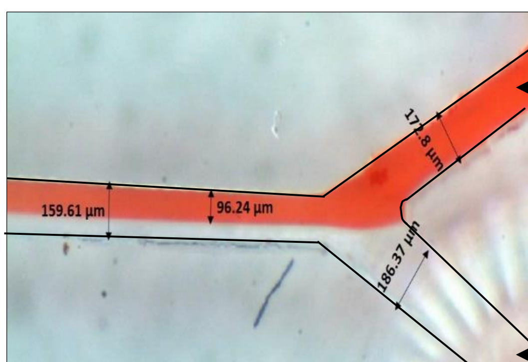
Water with Red ink at flow rate = 1ml/hr

Water at fixed flow rate = 1ml/hr



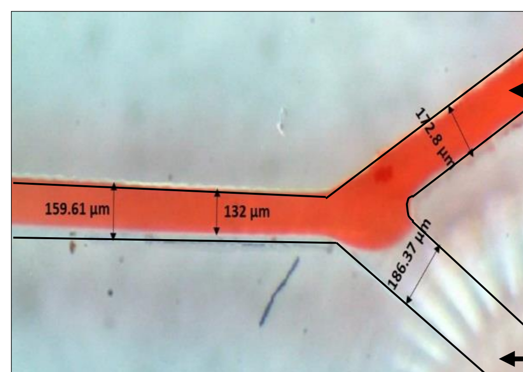
Water with Red ink at flow rate = 5ml/hr

Water at flow rate = 1ml/hr



Water with Red ink at flow rate = 2ml/hr

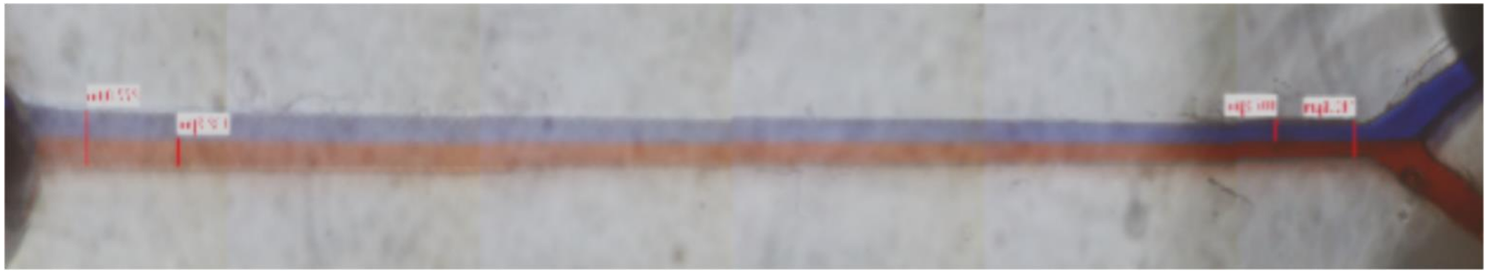
Water at flow rate = 1ml/hr

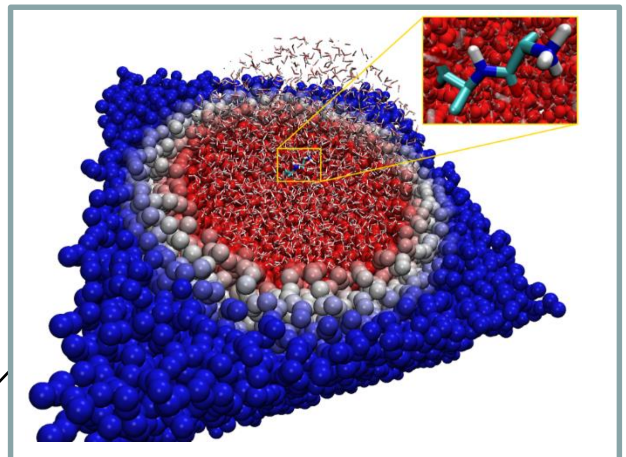


Water with Red ink at flow rate = 10 ml/hr

Water at flow rate = 1ml/hr

Effect of flow rates on protein diffusion and conformational changes

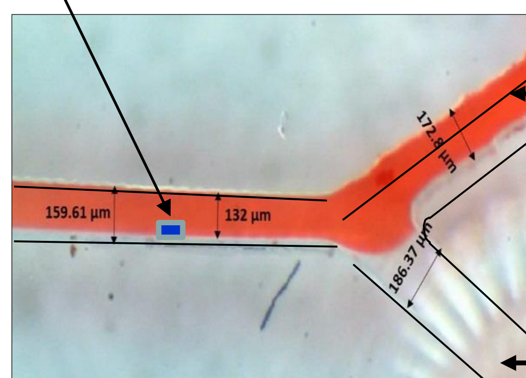




Challenge:
bridging of the time scales?

Water with Red ink at flow rate = 1ml/hr

Water at fixed flow rate = 1ml/hr



Water with Red ink at flow rate = 10 ml/hr

Water at flow rate = 1ml/hr

Multiscale Computing, e.g. TARDIS=Time Asynchronous Relative Dimension In Space

"Time And Relative Dimensions In Space"
Doctor Who

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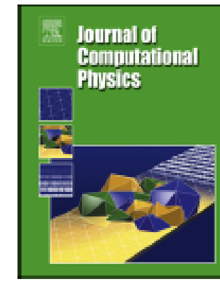


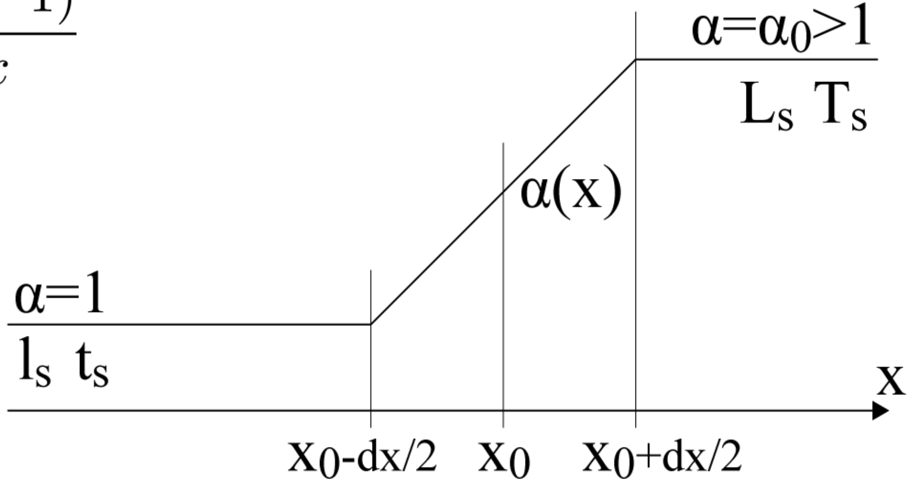
Time asynchronous relative dimension in space method for multi-scale problems in fluid dynamics

CrossMark

A.P. Markesteijn, S.A. Karabasov *

Time Asynchronous Relative Dimension in Space (TARDIS)

- Simple advection equation: $$\frac{\partial \rho}{\partial t} + c\frac{\partial \rho}{\partial x} = 0$$
- Transformation: $$\bar{x} - x_0 = \alpha\left(x - x_0\right) \qquad \bar{t} - t_0\left(t\right) = \alpha t$$ $$\alpha = \left(\frac{L_s}{l_s}\right) = \left(\frac{T_s}{t_s}\right)$$
- Introduce time-delay: $$\frac{d}{dt}t_0\left(t\right) = \left(x - x_0\right)\frac{d}{dx}\alpha\left(x\right)$$
  - Where: $$\frac{d}{dx}\alpha\left(x\right) = \frac{\left(\alpha_0 - 1\right)}{dx}$$



- Final transformations:

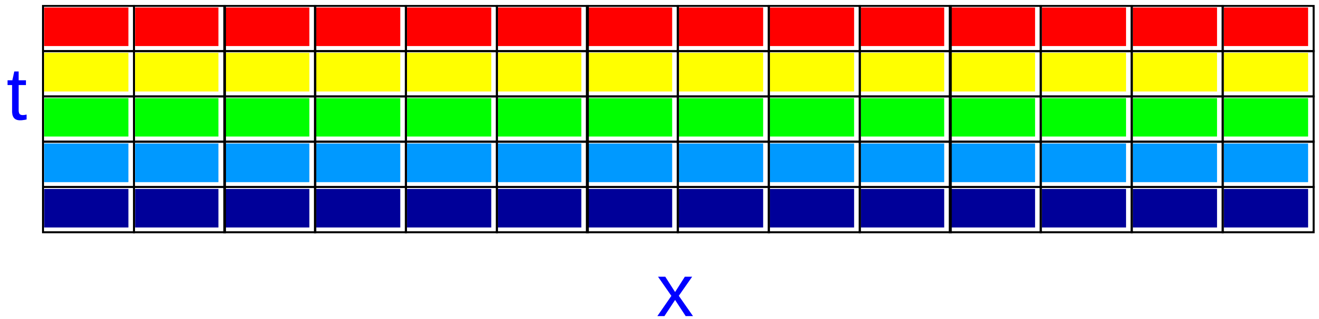
$$\frac{\partial}{\partial x} = \frac{\partial}{\partial \bar{x}}\left(\alpha + \left(x - x_0\right)\frac{d}{dx}\alpha\right)$$

$$\frac{\partial}{\partial t} = \frac{\partial}{\partial \bar{t}}\left(\alpha + \left(x - x_0\right)\frac{d}{dx}\alpha\right)$$

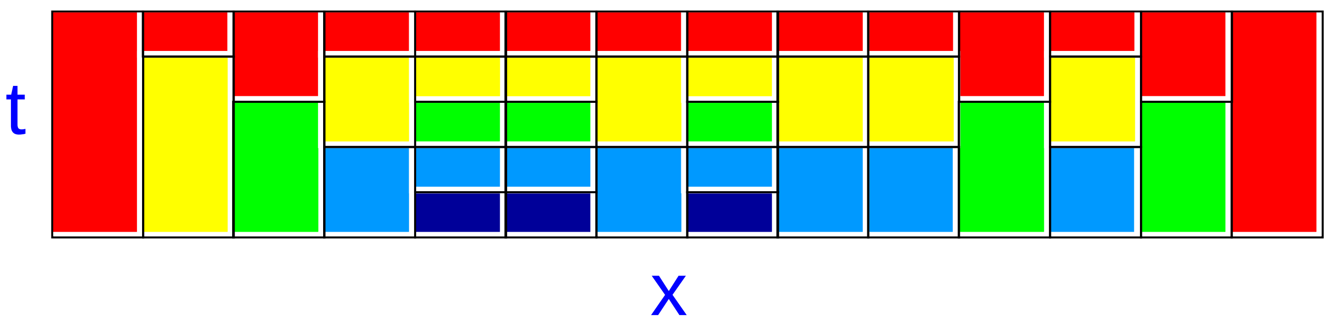
- With compatibility condition:

$$dx \to 0 : \rho\left(x, t\right) \sim \rho\left(x_0, \bar{t}\left(x_0\right) - \left(\alpha_0 - 1\right)t\right) = \rho\left(x_0, \bar{t}\left(x_0\right)\right)$$

Homogeneous time-stepping



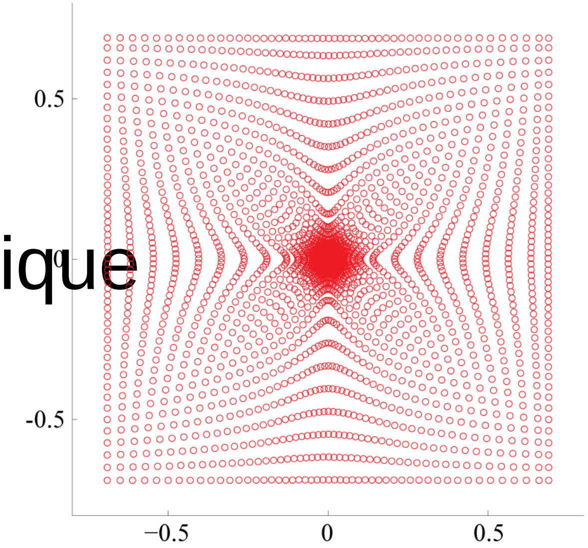
Asynchronous time-stepping

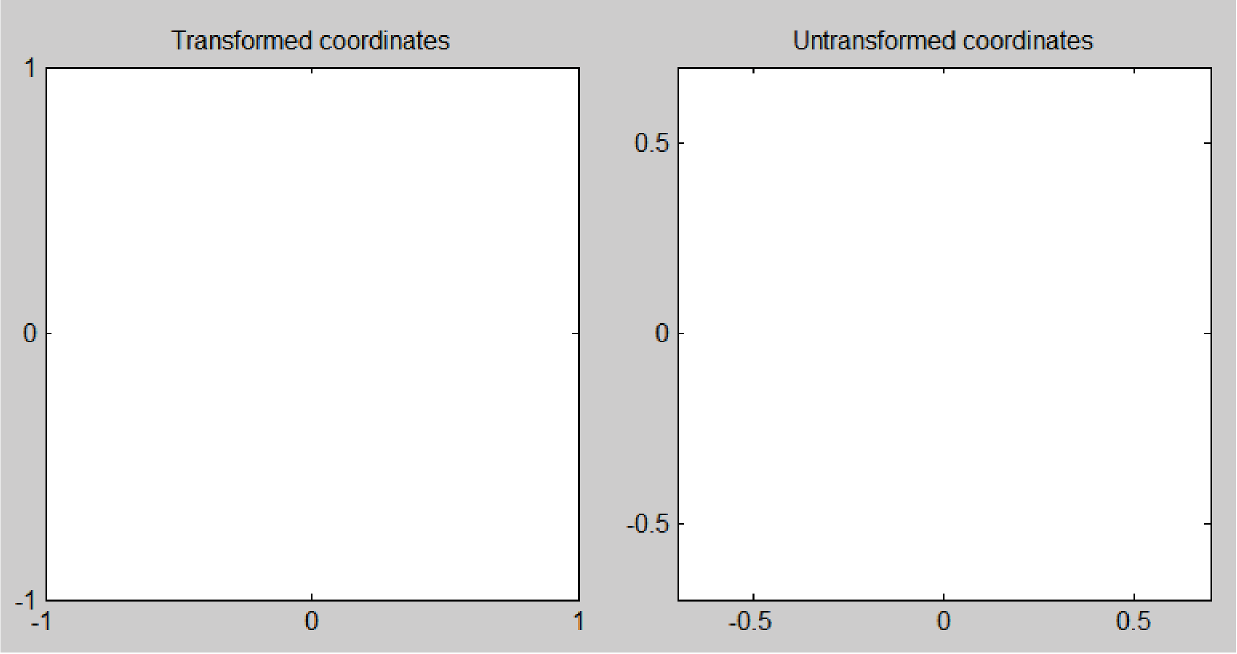


1st 2nd 3rd 4th step

Example: 2D space-time zoom for advection

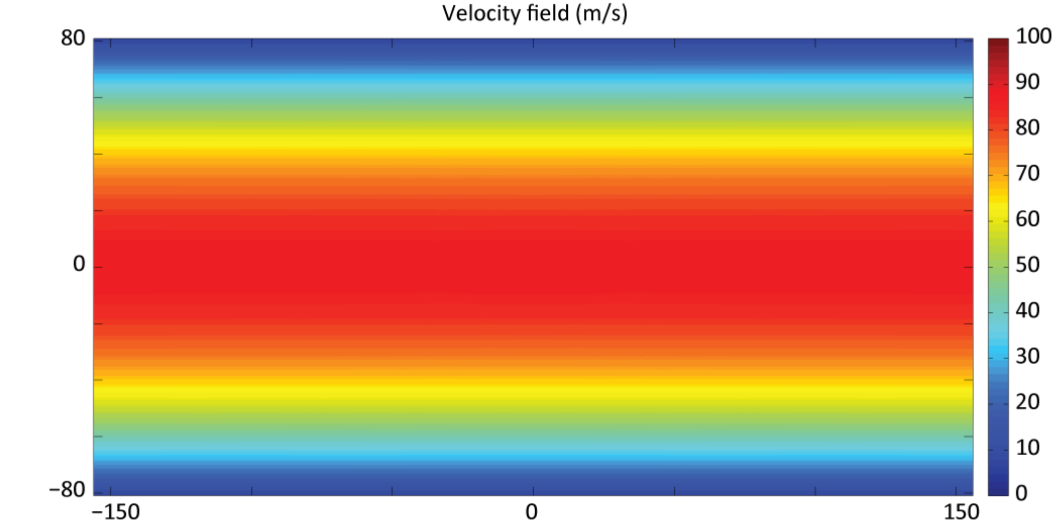
- Flat boundary equivalent
  - Adjusting aspect ratios of cells
  - Accomplished in ray-tracing technique

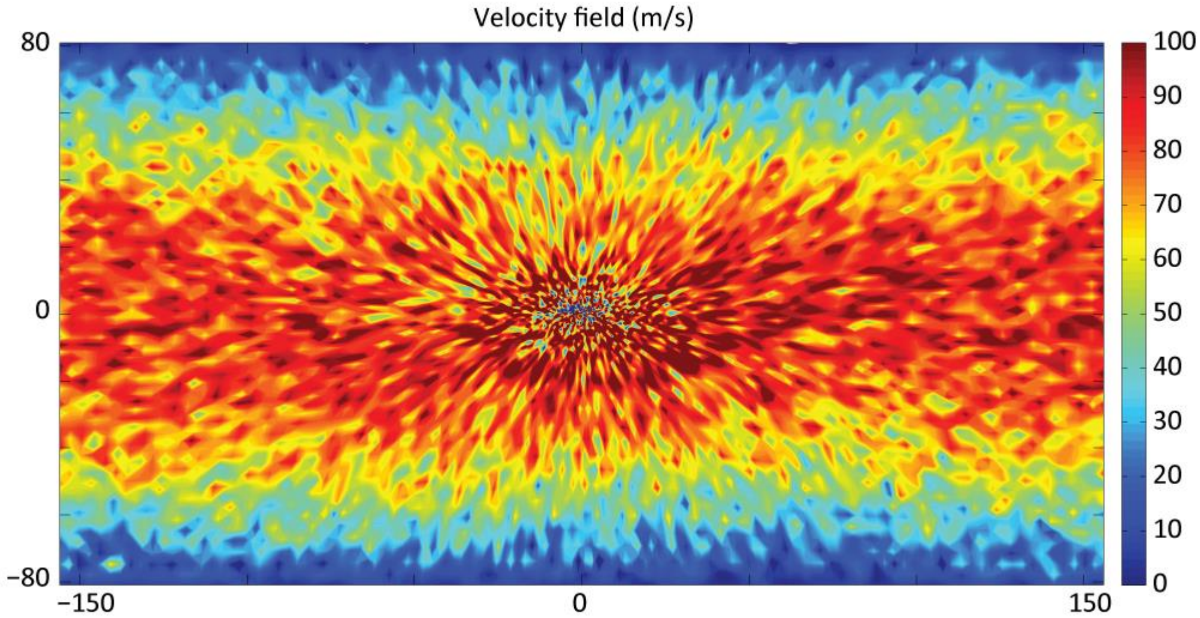


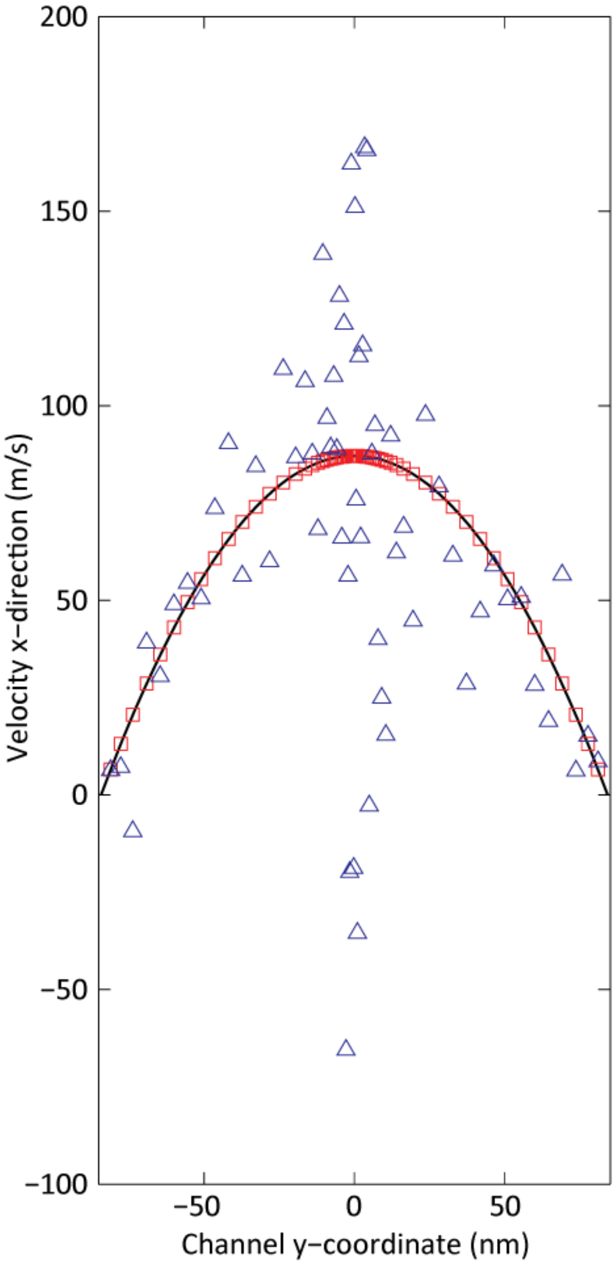


2D channel flow with Fluctuating Hydrodynamics

- Velocity profile and fluctuations

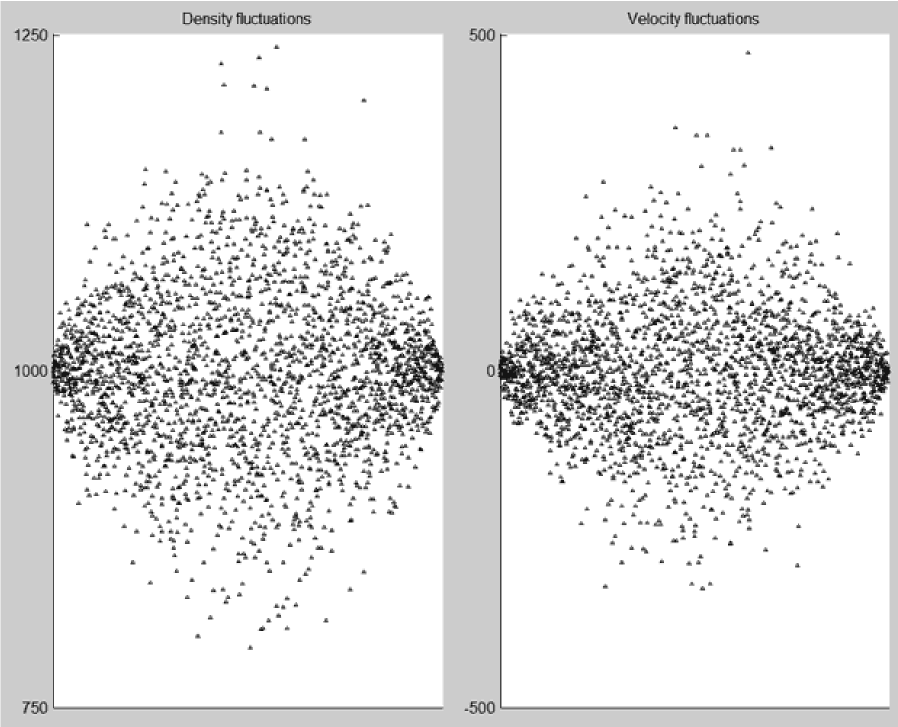




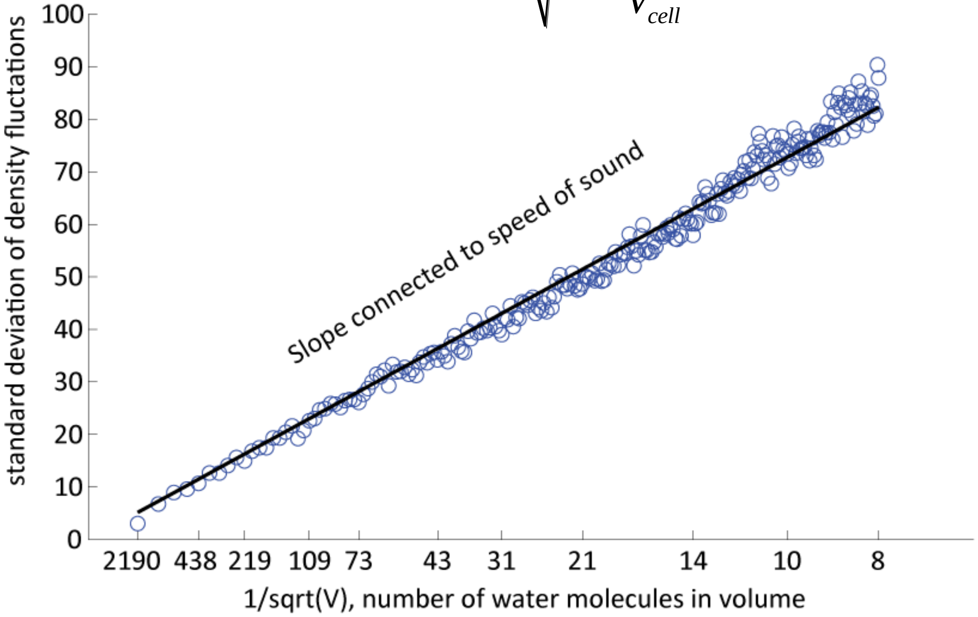


Effect of the scale change on Fluctuating Hydrodynamics

- Density fluctuations and the speed of sound
  - Domain 2560x10, Scale: 1 to 256 to 1 in plateaus
  - Volumes: 2190 → 8 water molecules
  - Speed of sound, relation density, momentum, volume
    - Determined from linear fit: ~1510 m/s (equal to MD results)

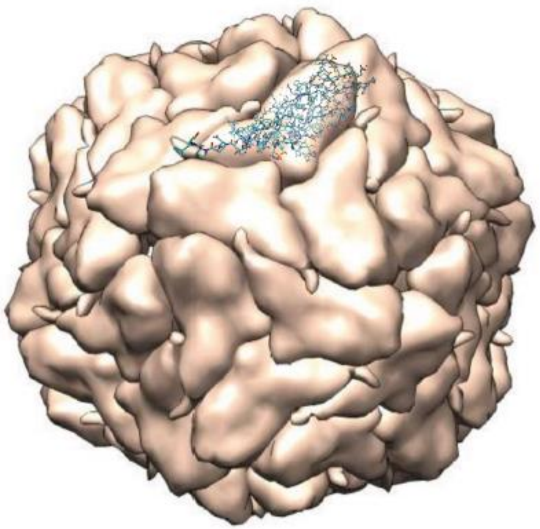


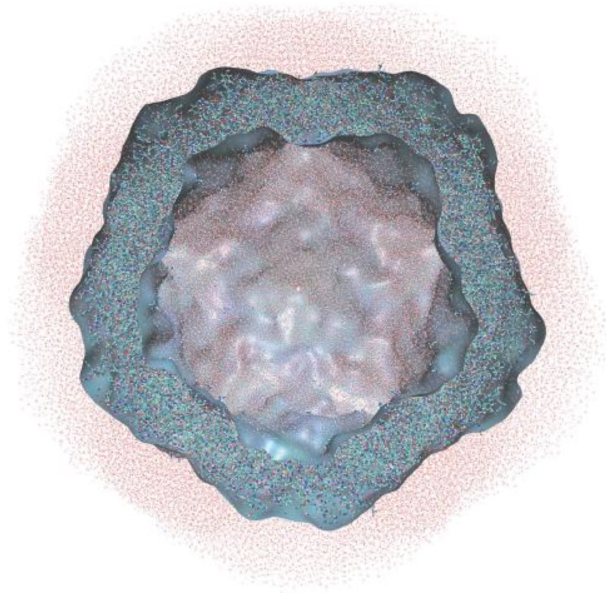
$$STD(\rho') = c_T^{-1}\sqrt{\rho k_B \frac{T}{V_{cell}}},$$



Application: simulation of porcine circovirus (PCV2) capsid in water at normal conditions

Capsid diameter of
~18-20 nm (126 180 atoms)
Total box domain size
~ 26.68 nm (~1 180 000 atoms)





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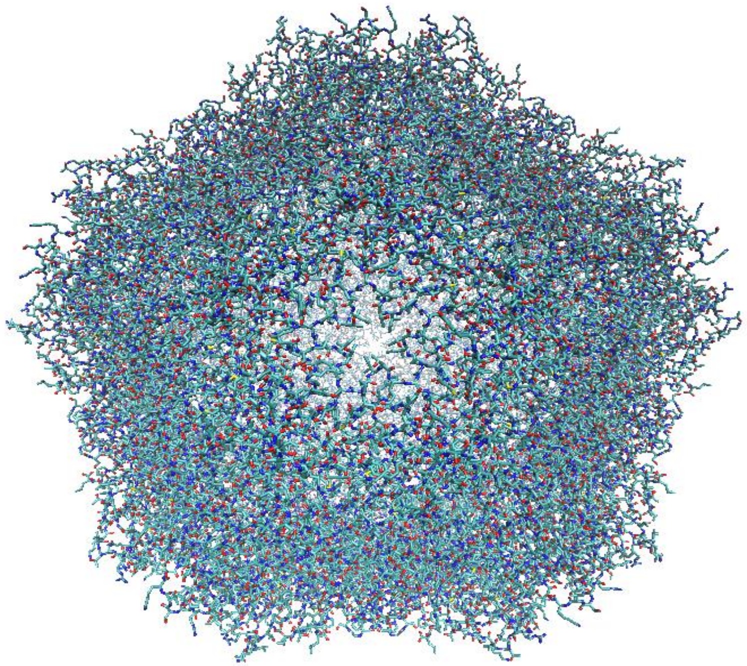
In Press, Corrected Proof — Note to users

Two-phase flow analogy as an effective boundary condition for modelling liquids at atomistic resolution

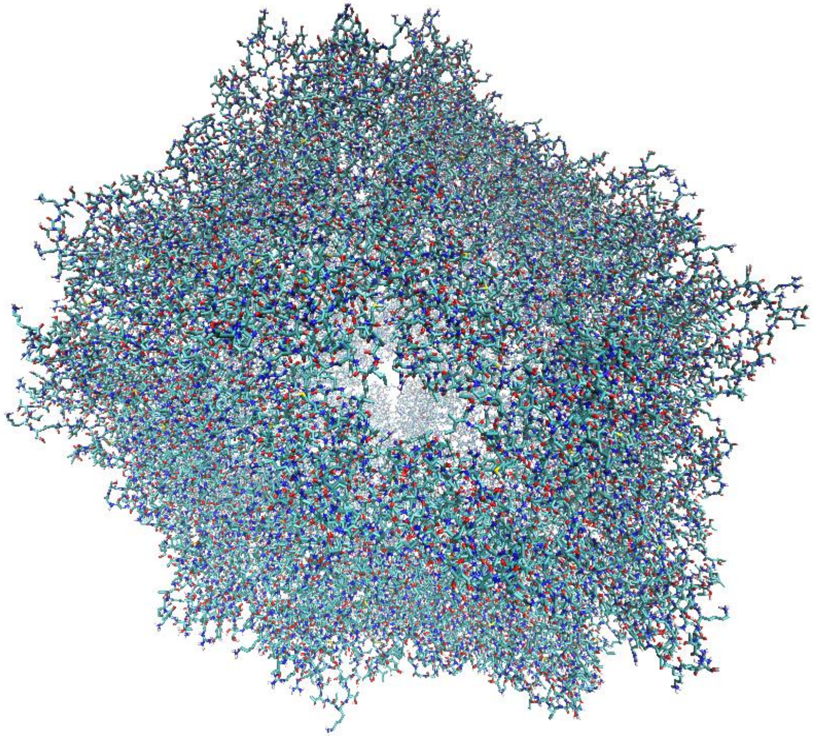
Ivan Korotkin[a, e], Dmitry Nerukh[b], Elvira Tarasova[c], Vladimir Farafonov[d], Sergey Karabasov[e]

Show more

Pure MD simulation in a periodic water cube

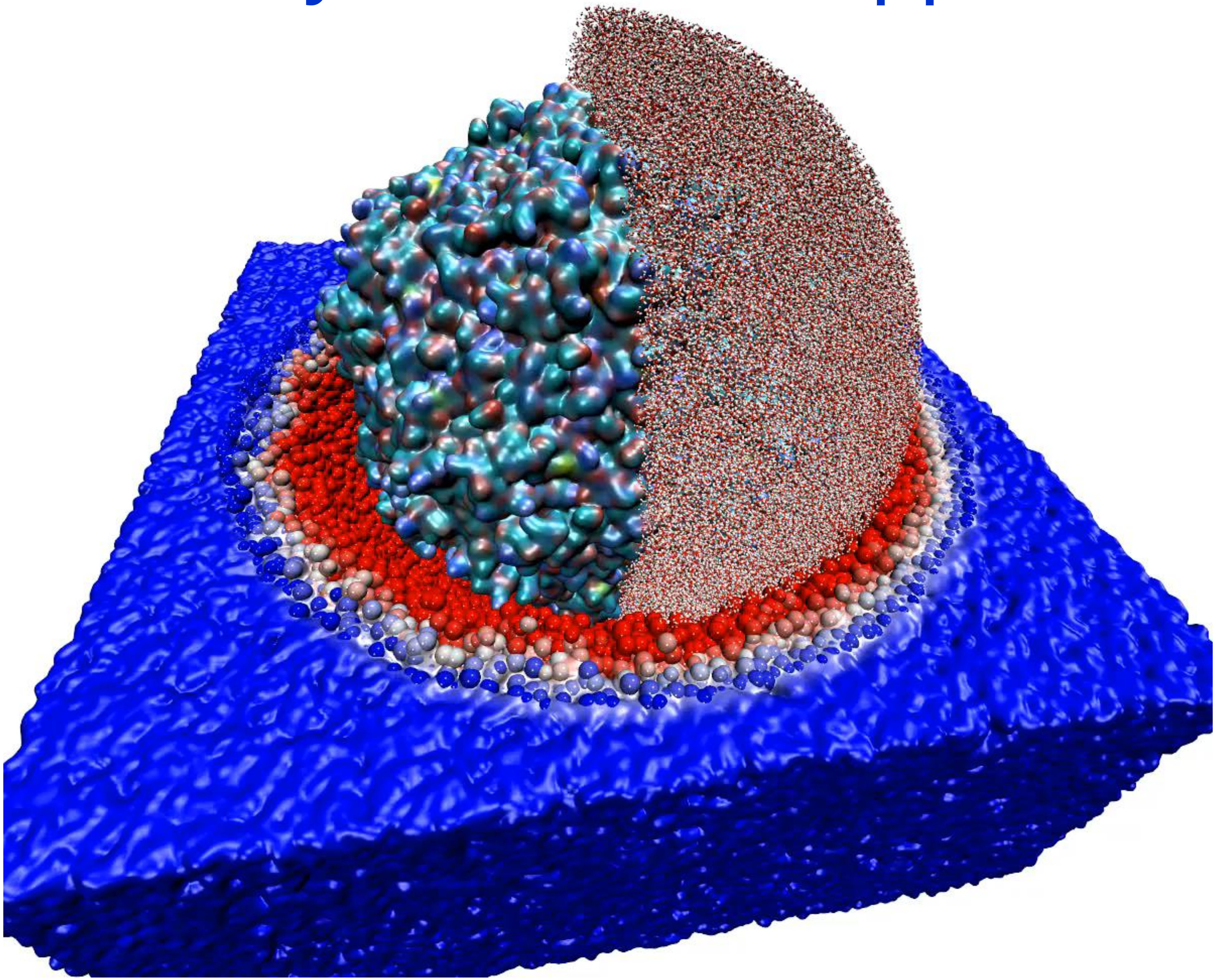


PCV2 capsid initial configuration from the experimental X-ray data



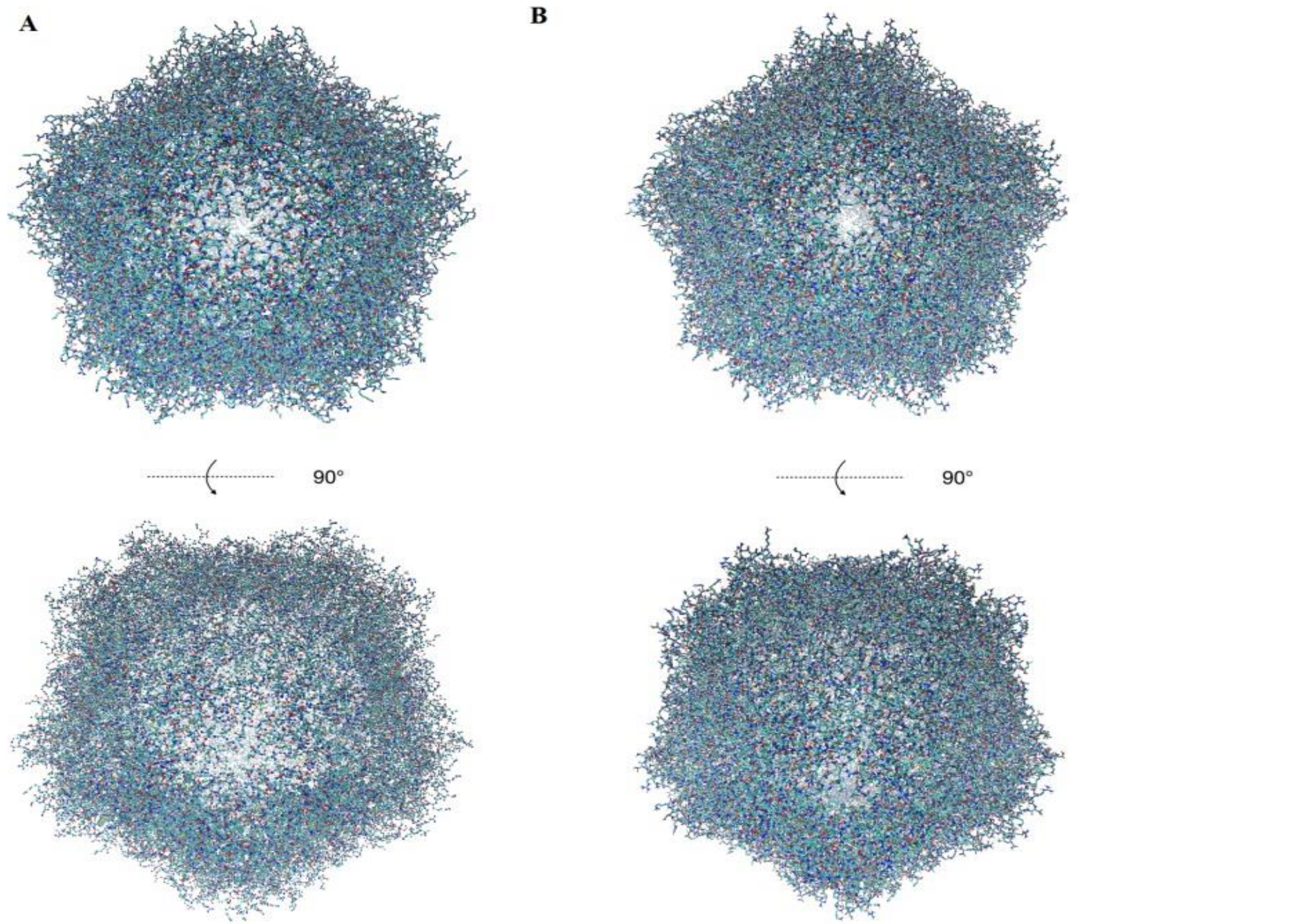
PCV2 capsid becomes unstable in pure MD

Hybrid MD/FH approach

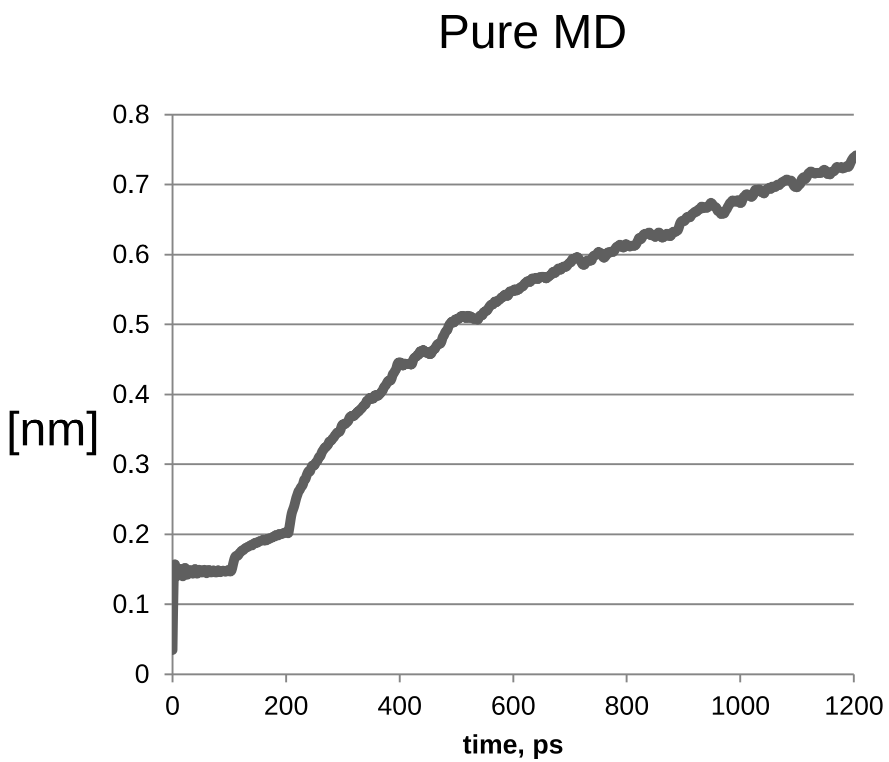


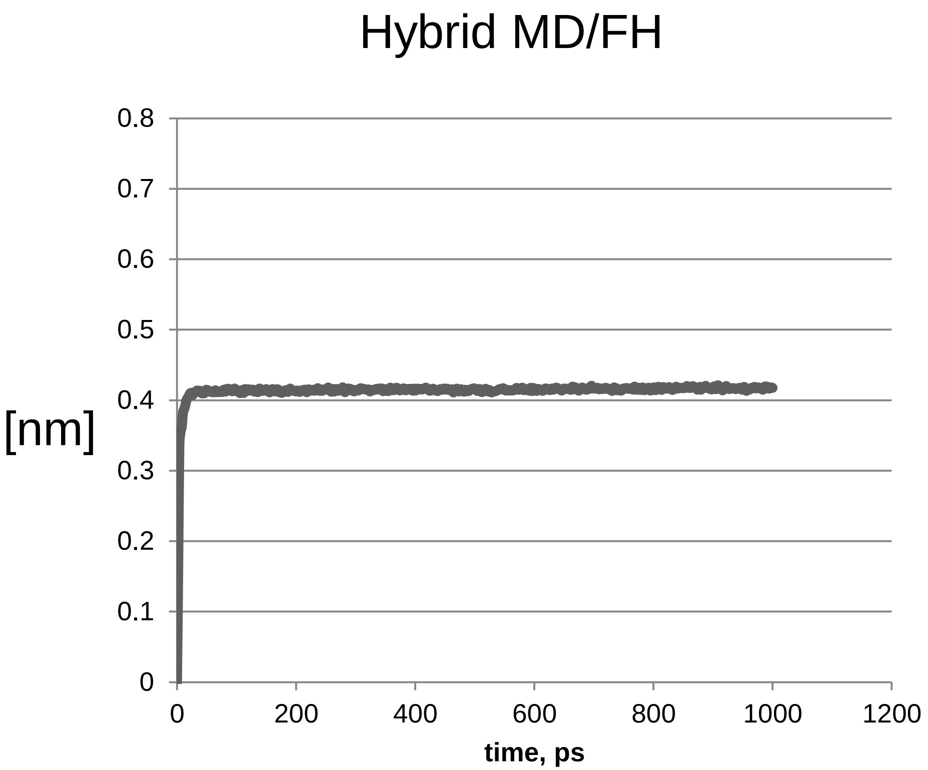
Hybrid MD/FH simulation in a periodic water cube

Initial configuration   simulated structure from hybrid MD/FH



Root-mean-square displacement (RMSD) of the backbone atoms





Reference value of RMSD of large molecular systems for stability ~ 0.3nm

Open questions

- A fully coupled MD/FH approach in 3D
- Simulation of large biochemical systems (e.g. more than 1 virus or virus peptide interaction, long simulation times)
- Incorporation of 2d objects (e.g. membranes)
- Adding electrostatic charges to the macroscopic part of the hybrid model
- Generalisations for liquid/solid systems