An Eulerian -Lagrangian framework for multi-scale/multi-physics (continuum-atomistic) modelling of liquids based on a hydrodynamic analogy

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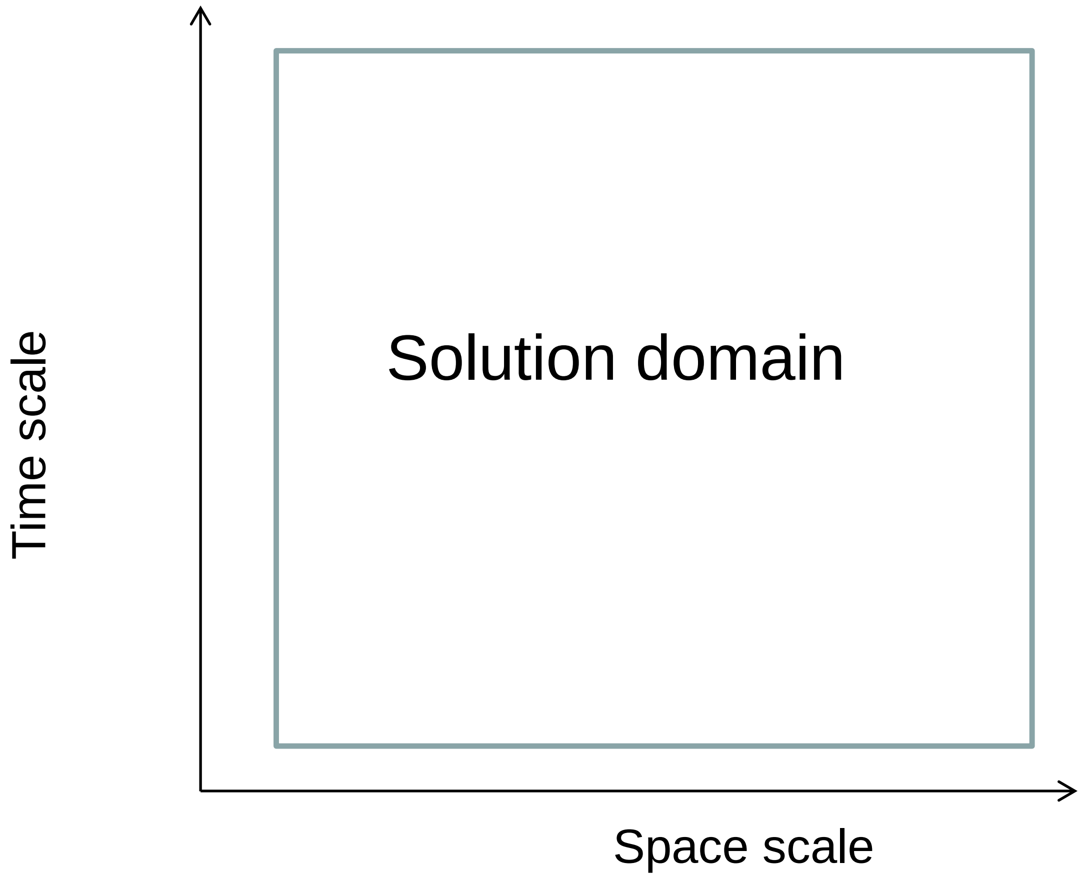
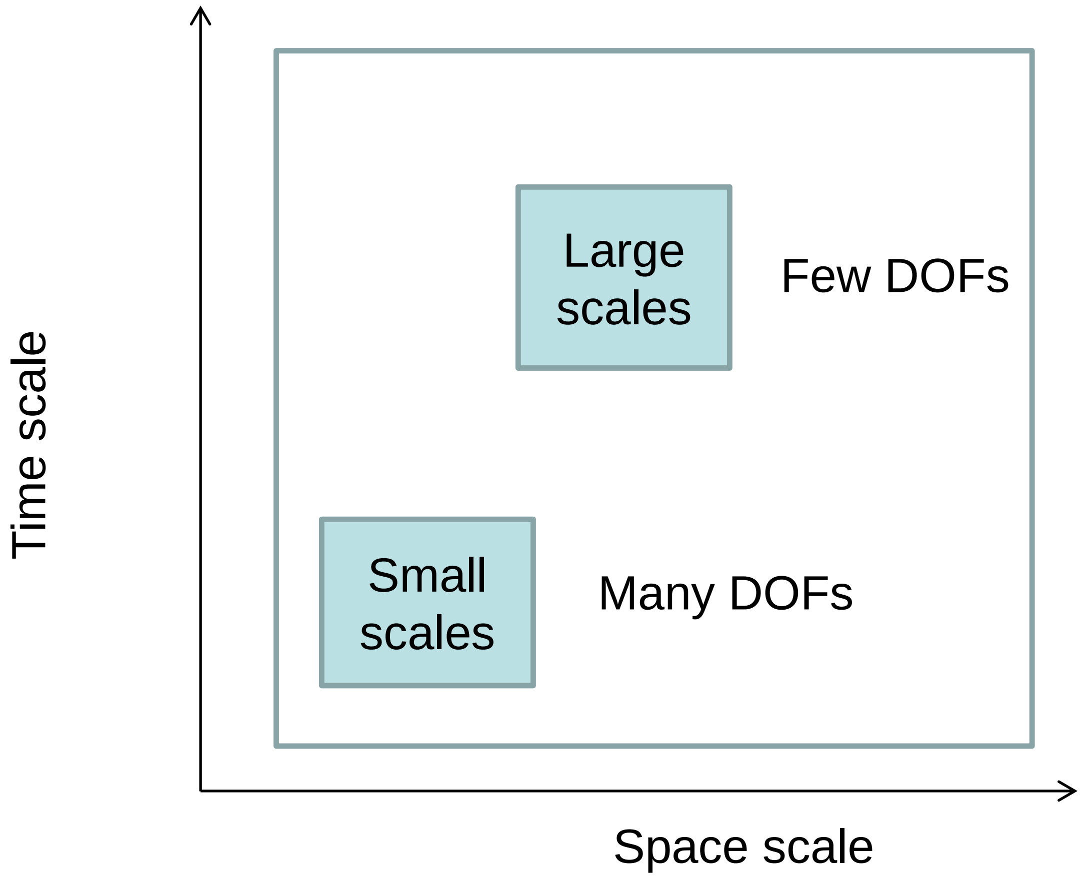
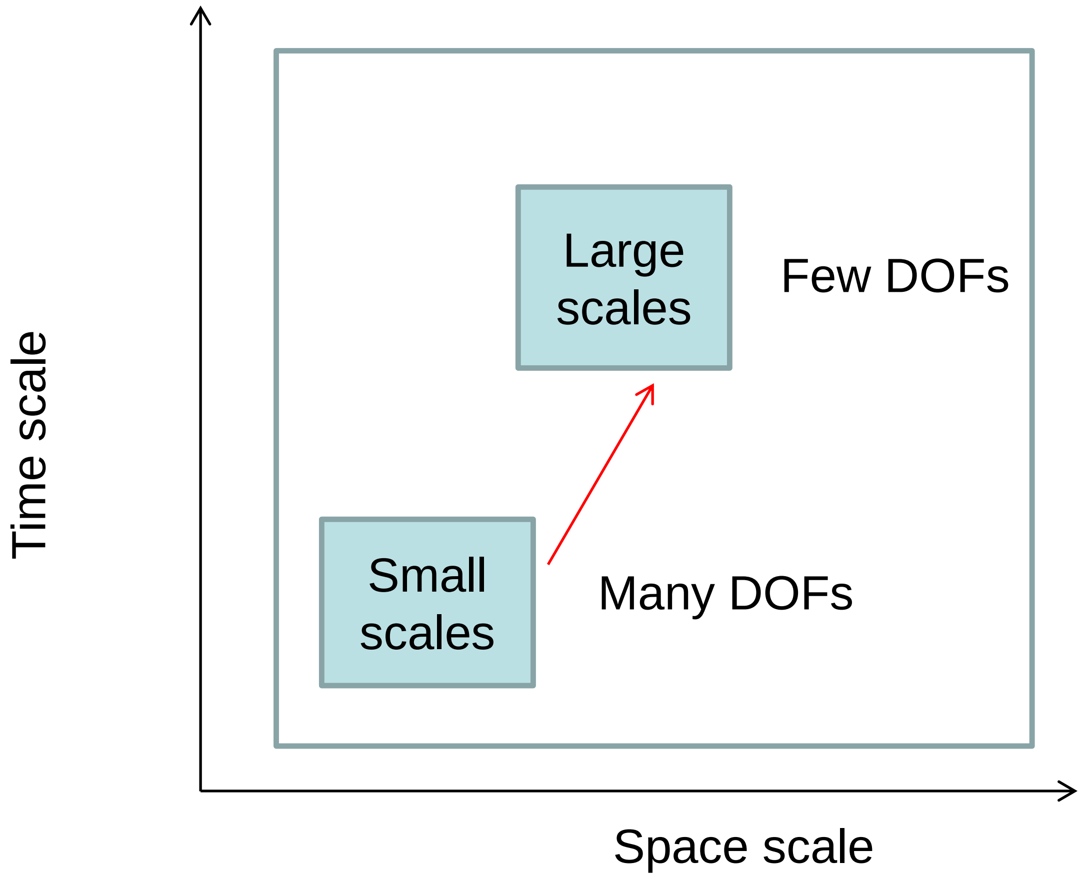
Multiscale modelling



Multiscale modelling: areas of interest

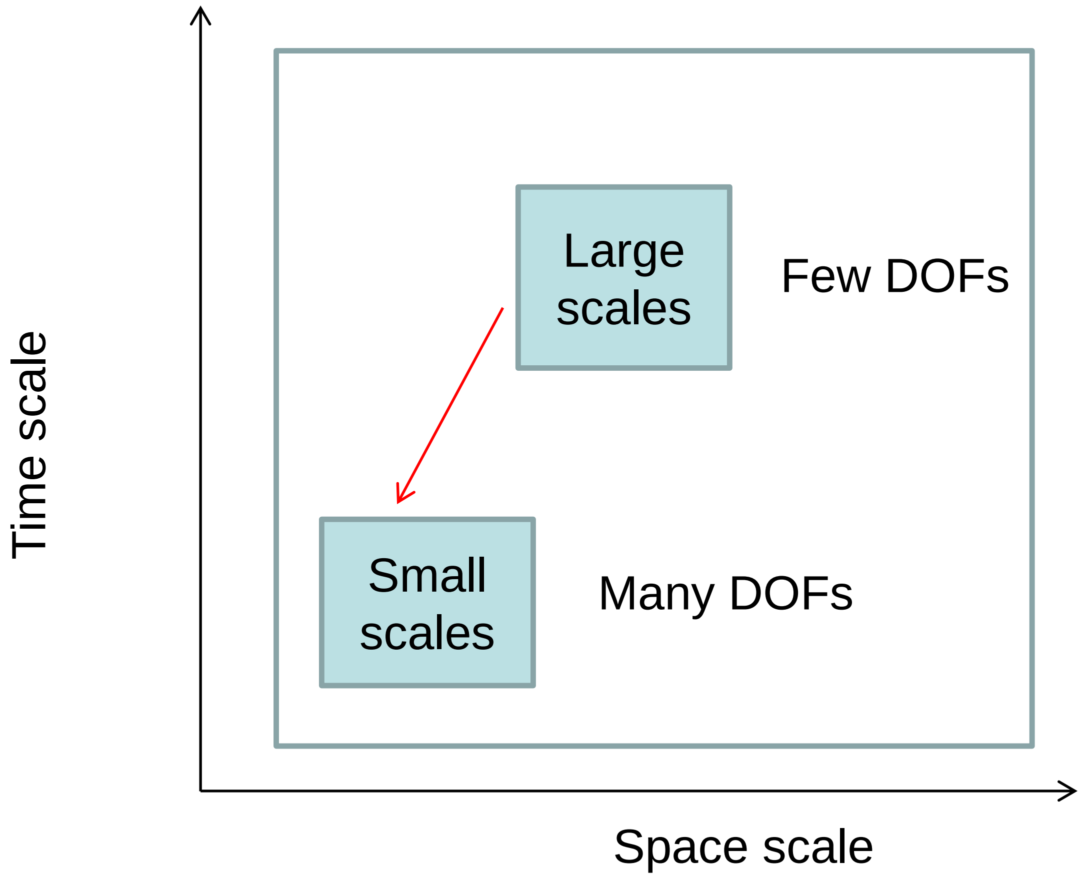


Multiscale modelling: acyclic “bottom-top” approach



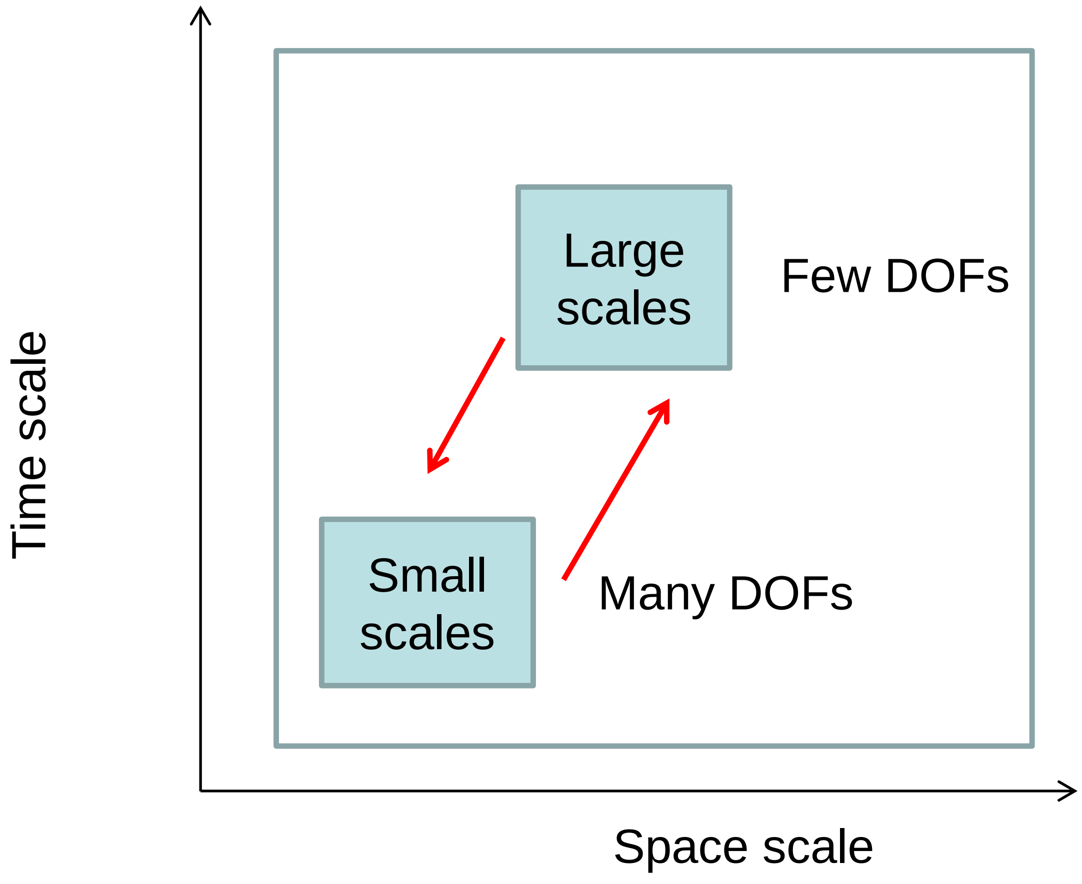
Integration, interpolation,…

Multiscale modelling: acyclic “top-bottom” approach



Typically, ill-posed/ none-unique

Multiscale modelling: cyclic (fully coupled) approach



General strategy for hybrid schemes

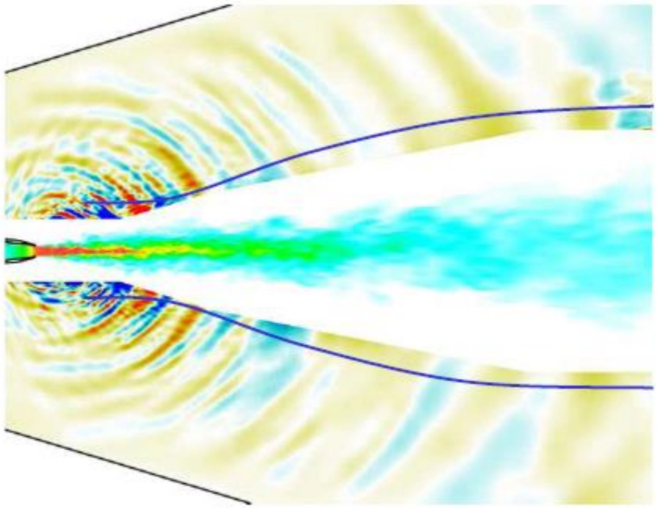
- Define the large scale and the small scale
- Specify their interaction (‘hand shaking’) (arrows on the multiscale schematic)
- Develop efficient computational framework for multiscale simulations

Physical analogies as a multiscale modelling method

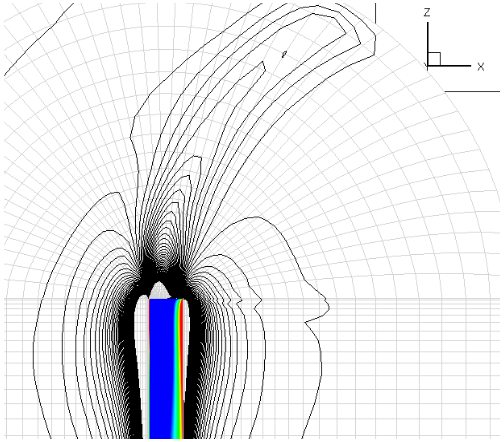
pros: may be physically insightful (depending on the construction) … tractable solutions for complex systems!

cons: the solution method not unique, not from the first principles, “not elegant”, etc..

Aerospace applications: sound generated by engineering flows



Vorticity and acoustic dilatation field of a turbulent jet



Acoustic pressure contours of a high-speed helicopter blade

For jets: Acoustic energy ~ 10^{-5} Mechanical energy

Aerodynamic scales << Acoustic scales

δ b.layer/D~ 0.01-0.001 L/D~100-1000

Aerodynamic fluctuations >> Acoustic fluctuations

Acoustic analogy

$$\frac{\partial}{\partial t}\rho + \frac{\partial}{\partial x_i}\rho v_i = 0 \qquad \frac{\partial}{\partial t}\rho v_i + \frac{\partial}{\partial x_j}\rho v_j v_i + \frac{\partial}{\partial x_i} p = \frac{\partial}{\partial x_j}\sigma_{ij}$$

d/dt

d/dx

$$\frac{\partial^2}{\partial t^2}\rho = \frac{\partial^2}{\partial x_i \partial x_j}\rho v_j v_i + \frac{\partial^2}{\partial x_i \partial x_i} p - \frac{\partial^2}{\partial x_i \partial x_j}\sigma_{ij}$$

James Lighthill

Lighthill, M. J. (1952). "On sound generated aerodynamically. I. General theory". Proceedings of the Royal Society A 211 (1107): 564–587

Acoustic analogy

$$\frac{\partial}{\partial t}\rho + \frac{\partial}{\partial x_i}\rho v_i = 0 \qquad \frac{\partial}{\partial t}\rho v_i + \frac{\partial}{\partial x_j}\rho v_j v_i + \frac{\partial}{\partial x_i} p = \frac{\partial}{\partial x_j}\sigma_{ij}$$

$$\frac{\partial^2}{\partial t^2}\rho = \frac{\partial^2}{\partial x_i \partial x_j}\rho v_j v_i + \frac{\partial^2}{\partial x_i \partial x_i} p - \frac{\partial^2}{\partial x_i \partial x_j}\sigma_{ij}$$

$$\frac{\partial^2}{\partial t^2}\rho' - \frac{\partial^2}{\partial x_i \partial x_i}\rho' c_0{}^2 = \frac{\partial^2}{\partial x_i \partial x_j} T_{ij}$$

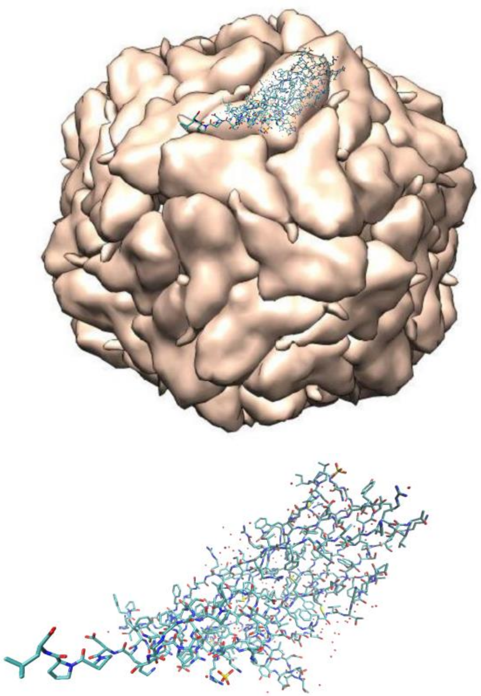
Model: T_{ij} doesn't include ρ' variable

$$p(\mathbf{x},t) = \frac{1}{4\pi}\frac{\partial^2}{\partial x_i \partial x_j}\int \frac{1}{|\mathbf{x}-\mathbf{y}|} T_{ij}\left(\mathbf{y}, t-\tau-\frac{|\mathbf{x}-\mathbf{y}|}{c_0}\right) d^3\mathbf{y}, \qquad T_{ij} = \rho v_i v_j + (p' - c_0{}^2\rho')\delta_{ij} - \sigma_{ij}$$

Application to microscopic flow modelling

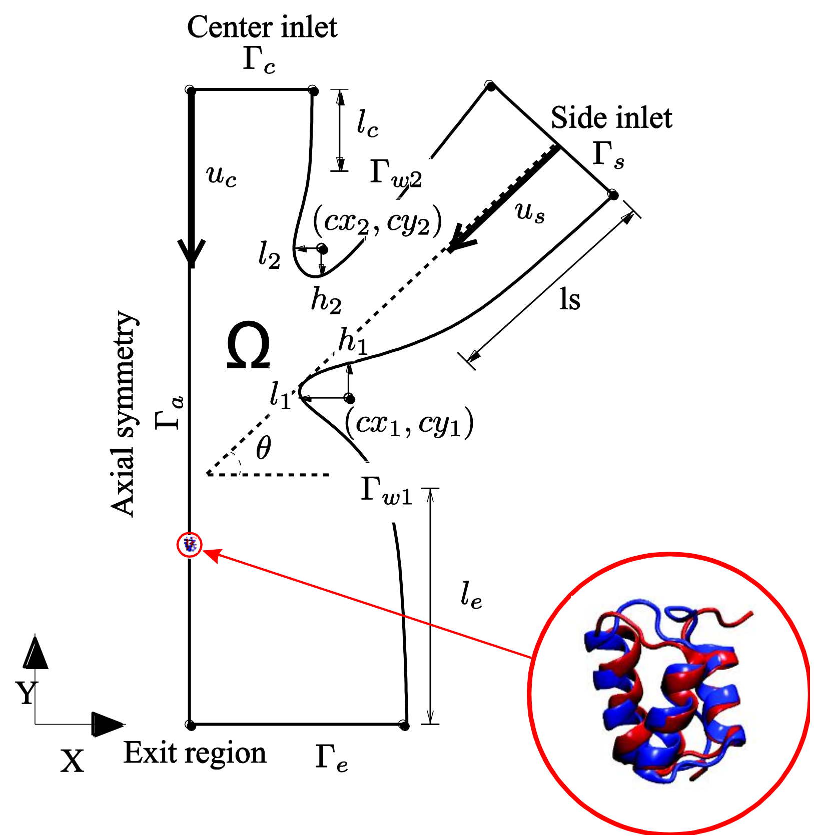
Grand challenges

Resolution adaptive all-atom simulation of a nano-scale living organism (virus) in water

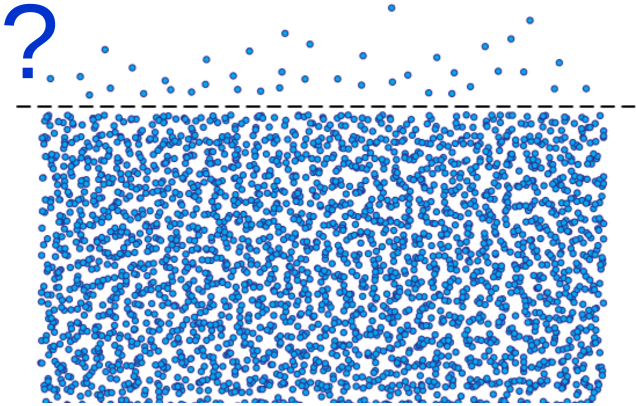


porcine circovirus in water

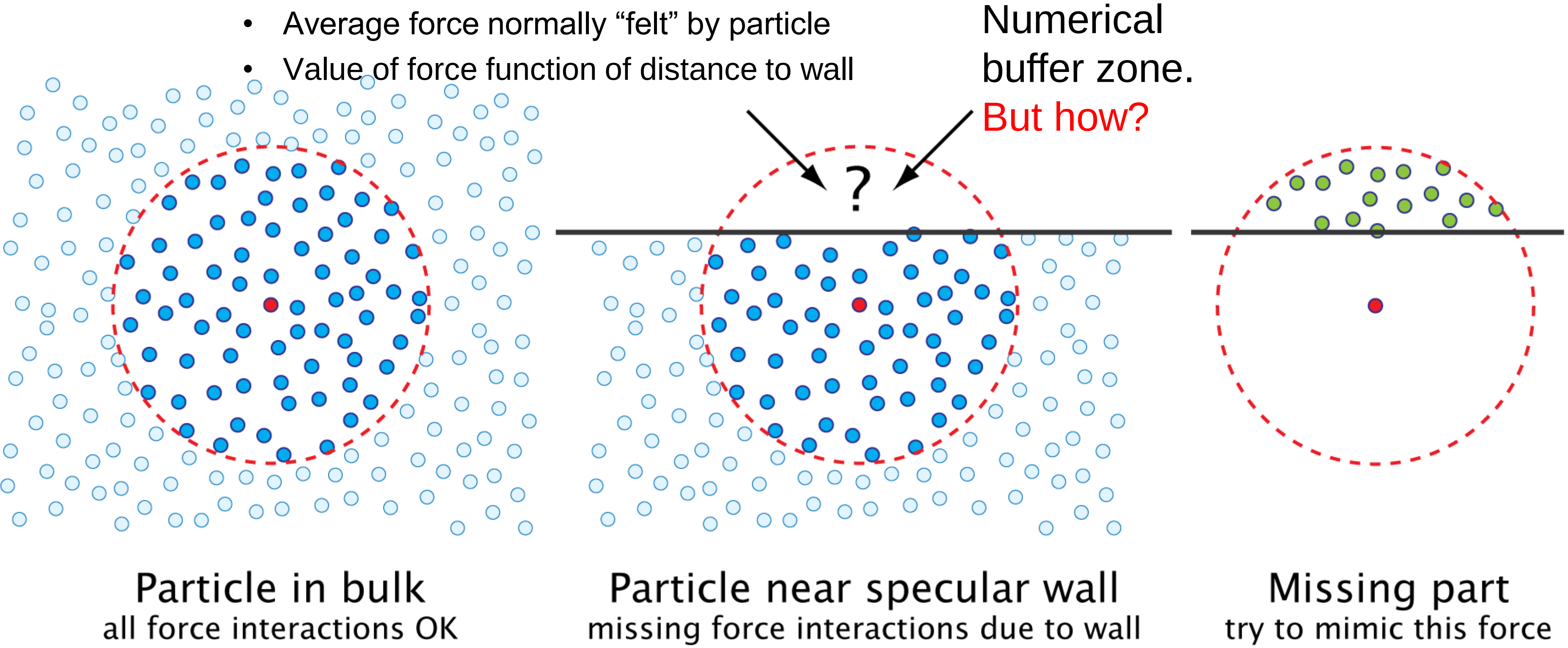
Conformational changes of macromolecules under the effect of hydrodynamics



Continuum-> MD ??



- Prevent particles from drifting away
  - **Problem**: Missing interactions near wall
    - Results in unnatural “wiggles”
  - **Partial** Solution: Mimic missing force
    - Average force normally “felt” by particle
    - Value of force function of distance to wall



Small scales = Molecular dynamics (MD)

Large scales = ?

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 Hyrodynamics Equations

One dimensional case

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

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

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

Stochastic fluxes

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

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

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

Characteristic form of LL-NS equations

$$\left(\frac{\partial u}{\partial t}+\frac{1}{\sqrt{c^2\cdot\rho^2-\rho\left(\gamma-1\right)s}}\cdot\frac{\partial P}{\partial t}\right)+\left\{u+\sqrt{c^2-\frac{\left(\gamma-1\right)s}{\rho}}\right\}\cdot\left(\frac{\partial u}{\partial x}+\frac{1}{\sqrt{c^2\cdot\rho^2-\rho\left(\gamma-1\right)s}}\cdot\frac{\partial P}{\partial x}\right)=G_1;$$

$$\left(\frac{\partial u}{\partial t}-\frac{1}{\sqrt{c^2\cdot\rho^2-\rho\left(\gamma-1\right)s}}\cdot\frac{\partial P}{\partial t}\right)+\left\{u-\sqrt{c^2-\frac{\left(\gamma-1\right)s}{\rho}}\right\}\cdot\left(\frac{\partial u}{\partial x}-\frac{1}{\sqrt{c^2\cdot\rho^2-\rho\left(\gamma-1\right)s}}\cdot\frac{\partial P}{\partial x}\right)=G_2;$$

$$\left[\frac{\partial}{\partial t}\left(\ln\frac{P}{\rho^\gamma}\right)-\frac{s}{c_v T}\cdot\frac{\partial}{\partial t}\left(\frac{1}{\rho}\right)\right]+u\cdot\left[\frac{\partial}{\partial x}\left(\ln\frac{P}{\rho^\gamma}\right)-\frac{s}{c_v T}\cdot\frac{\partial}{\partial x}\left(\frac{1}{\rho}\right)\right]=G_3;$$

Condition for hyperbolicity $|s|<\dfrac{\rho\cdot c^2}{(\gamma-1)}$

Stochastic fluxes

Stochastic fluxes approximation

$$\left.\begin{aligned}\langle s(x,t)s(x',t')\rangle &= \frac{8\cdot k\cdot\eta\cdot T}{3\cdot\sigma}\cdot\delta(x-x')\cdot\delta(t-t');\\ \langle q(x,t)q(x',t')\rangle &= \frac{2\cdot k\cdot\kappa\cdot T^2}{\sigma}\cdot\delta(x-x')\cdot\delta(t-t');\end{aligned}\right\}\Rightarrow$$

$$s_h(x,t)=\sqrt{\frac{8\cdot k\cdot\eta\cdot T}{3\cdot\sigma\cdot\Delta x\cdot\Delta t}}\cdot Gauss(0,1);$$

$$q_h(x,t)=\sqrt{\frac{2\cdot k\cdot\kappa\cdot T^2}{\sigma\cdot\Delta x\cdot\Delta t}}\cdot Gauss(0,1);$$

System size

- For high value of stochastic forcing (large s and q fluxes) the solution of the LL Navier-Stokes equations is challenging (but possible with the use of high-resolution schemes)

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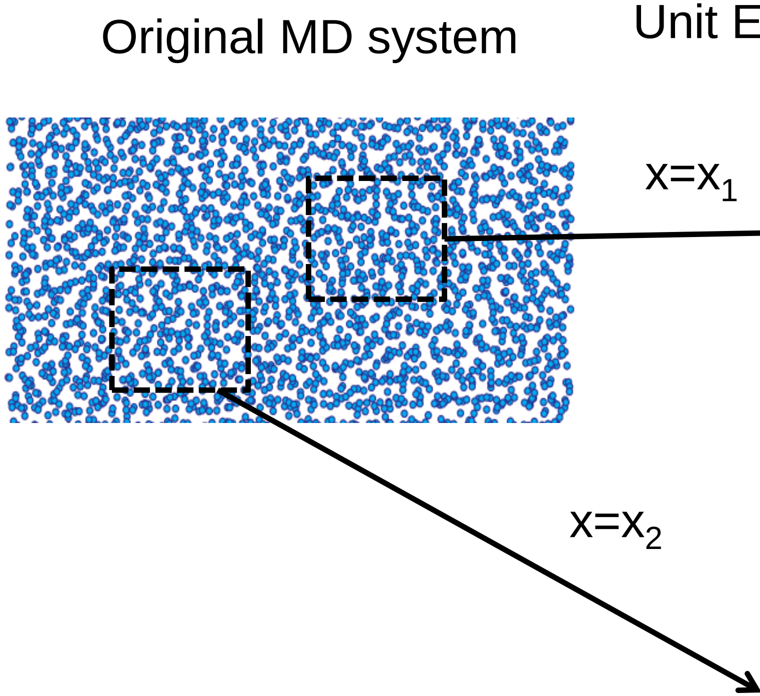
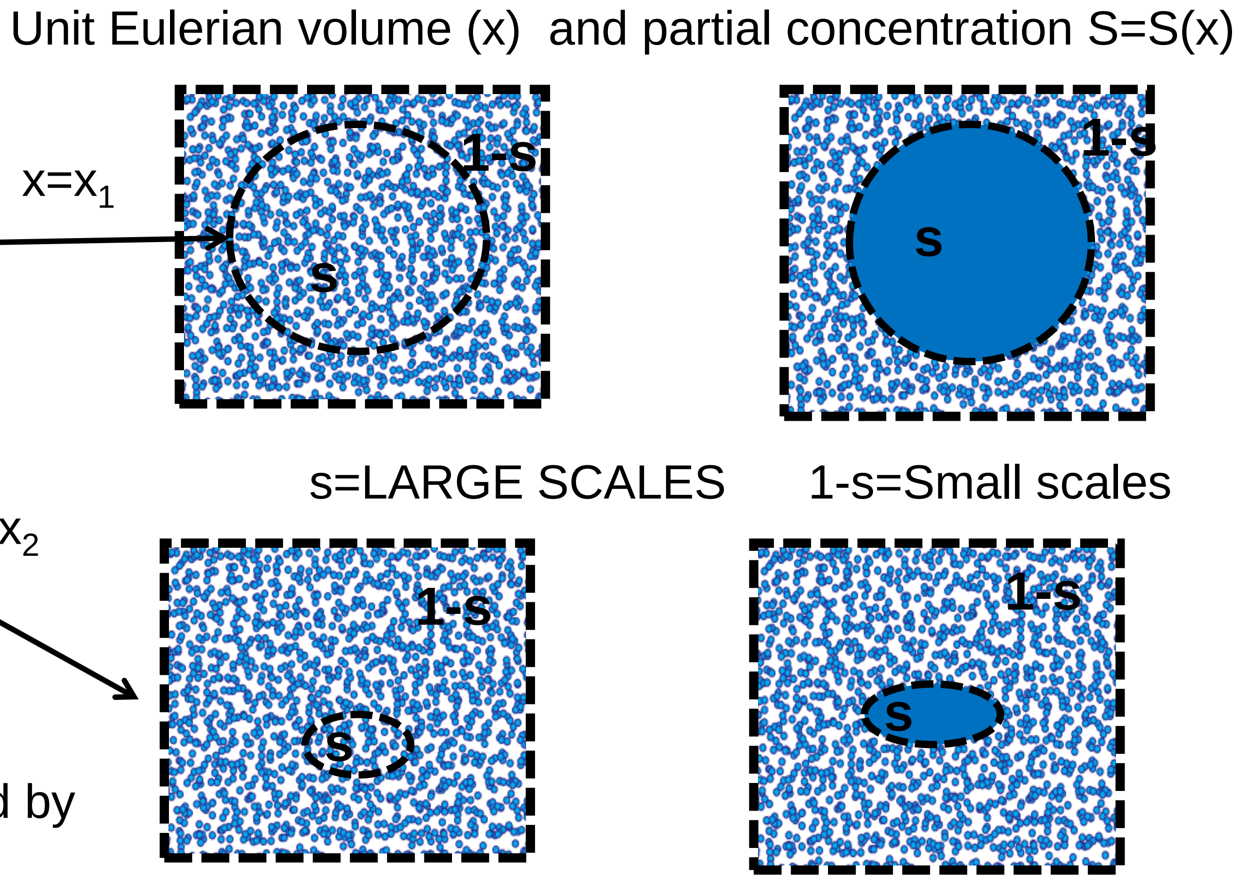
A new non-linear two-time-level Central Leapfrog scheme in staggered conservation–flux variables for fluctuating hydrodynamics equations with GPU implementation

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

FH - MD coupling: the idea

Two-phase hydrodynamics analogy

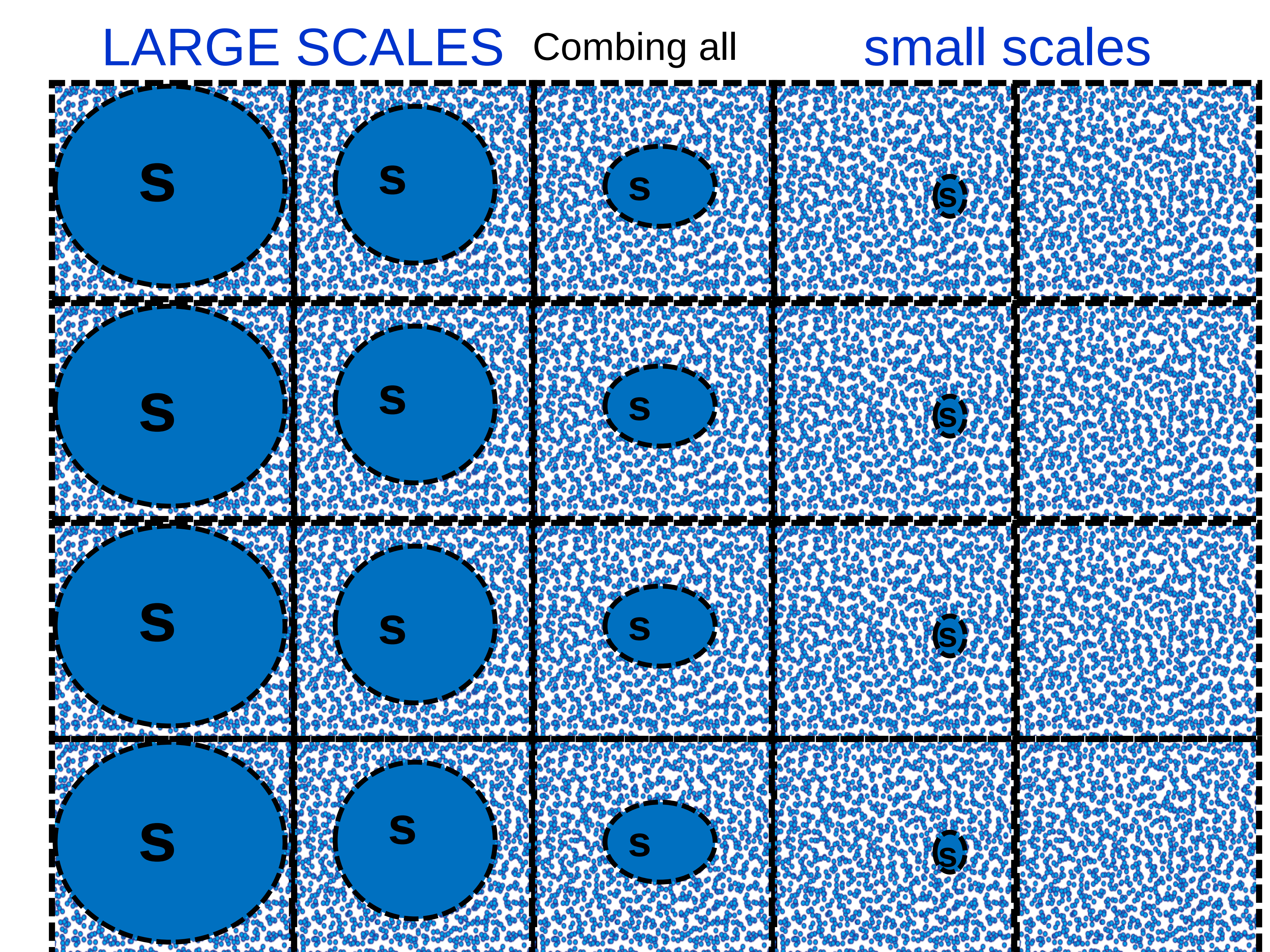




1-S – partial volume occupied by MD model

S – partial volume occupied by continuum model

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


LARGE SCALES
Combing all
small scales
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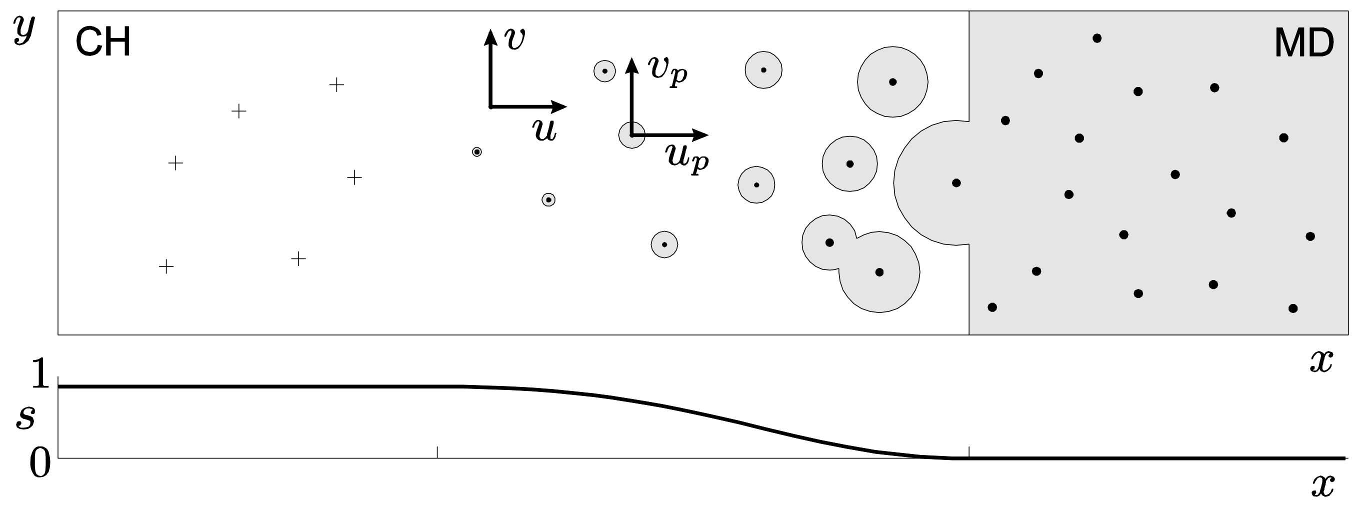
1D Schematic



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

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Two-phase hydrodynamic analogy: mass conservation

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 automatically 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

Continuum phase

Landau-Lifshitz'
deterministic + stochastic stresses

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

Particle phase

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

Conservation law is automatically satisfied for the mixture momentum

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

Modified macroscopic equations

Specify the source birth/death terms so that the density equation becomes a material balance equation for perturbation with respect to the averaged MD values where the right hand side is some linear (algebraic or diffusion) operator, same for the momentum equations (+continuum force)

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

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

So that in the ‘buffer zone’ 0< s < 1 the continuum solution is **exponentially sponged (hard)**, or **diffused (soft)**, towards the ‘target’ MD solution

Integral form of the convection derivative

$$\frac{D}{Dt_0}\bullet = \frac{\partial}{\partial t}\bullet + div(\overline{\mathbf{u}}\bullet)$$

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

$$D_t\left(\overline{u}_i\overline{m} - \sum_{p=1,N(t)} u_{ip} m_p\right) = \delta_t\left(\overline{u}_i\overline{m} - \sum_{p=1,N(t)} u_{ip} m_p\right) + \sum_{\gamma=1,6}\left(\overline{u}_i\overline{\rho} - \sum_{p=1,N_\gamma(t)} u_{ip}\rho_p\right)\mathbf{u}d\mathbf{n}^\gamma dt,$$

Integral form of the diffusive forcing

~∂ (α ∂/∂x ρ') /∂x

$$L^{(\rho)} \bullet \left(\overline{m} - \sum_{p=1,N(t)} m_p \right) = \sum_{k=1,3} \sum_{\gamma=1,6} \left(s(1-s) \cdot \alpha \cdot \frac{1}{V} \left(\sum_{\lambda=1,6} \left(\overline{\rho} - \sum_{p=1,N_\lambda(t)} \rho_p \right) dn_k^\lambda \right) \right) dn_k^\gamma dt,$$

$$L^{(u)} \bullet \left(\overline{u}_i \overline{m} - \sum_{p=1,N(t)} u_{ip} m_p \right) = \sum_{k=1,3} \sum_{\gamma=1,6} \left(s(1-s) \cdot \beta \cdot \frac{1}{V} \left(\sum_{\lambda=1,6} \left(\overline{u}_i \overline{\rho} - \sum_{p=1,N_\lambda(t)} u_{ip} \rho_p \right) dn_k^\lambda \right) \right) dn_k^\gamma dt,$$

~∂ (β ∂/∂x (ρu)') /∂x

Consistent modification of the MD equations

- Add forcing terms to the molecular dynamics kinematic and dynamic equation so that the macroscopic conservations for two “phases” hold:

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

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

Can work out the expressions for these terms from the corresponding conservation laws for MD particles

$$\delta_t \sum_{p=1,N(t)} m_p + \sum_{\gamma=1,6} \left(\sum_{p=1,N_\gamma(t)} \frac{d\mathbf{x}_p}{dt} \rho_p \right) d\mathbf{n}^\gamma \cdot dt = 0$$

$$\delta_t \sum_{p=1,N(t)} m_p u_{ip} + \sum_{\gamma=1,6} \left(\sum_{p=1,N_\gamma(t)} \frac{d\mathbf{x}_p}{dt} \rho_p u_{ip} \right) d\mathbf{n}^\gamma \cdot dt = \sum_{p=1,N(t)} m_p a_{ip} dt, \qquad a_{ip} = \frac{du_{ip}}{dt}$$

Result for the modified MD equations:

~ α ∂/∂x ρ'

$$\frac{d\mathbf{x}_p}{dt} = \mathbf{u}_p + s(\bar{\mathbf{u}} - \mathbf{u}_p) + s(1-s)\cdot\alpha\cdot\frac{\sum\limits_{\gamma=1,6}\left(\bar{\rho} - \sum\limits_{q=1,N_\gamma(t)}\rho_q\right)d\mathbf{n}^\gamma}{\sum\limits_{q=1,N(t)} m_q},$$

$$\frac{du_{ip}}{dt} = (1-s)F_{ip} / m_{ip} +$$

~∂ (α ∂/∂x ρ') /∂x

$$+\sum_{k=1,3}\sum_{\gamma=1,6}\left(s(1-s)\cdot\alpha\cdot\sum_{q=1,N_\gamma(t)}\rho_q u_{iq}\cdot\left(\frac{\sum\limits_{\lambda=1,6}\left(\bar{\rho} - \sum\limits_{q=1,N_\lambda(t)}\rho_q\right)dn_k^\lambda}{\sum\limits_{q=1,N(t)} m_q}\right)\right)dn_k^\gamma \Big/ \sum_{q=1,N(t)} m_q$$

$$+\sum_{k=1,3}\sum_{\gamma=1,6}\left(s(1-s)\cdot\beta\cdot\frac{1}{V}\left(\sum_{\lambda=1,6}\left(\bar{\rho}\cdot\bar{u}_i - \sum_{q=1,N_\lambda(t)}\rho_q u_{iq}\right)dn_k^\lambda\right)\right)dn_k^\gamma \Big/ \sum_{q=1,N(t)} m_q, \qquad i = 1,3,$$

~∂ (β ∂/∂x (ρu)') /∂x

Features of the hybrid model

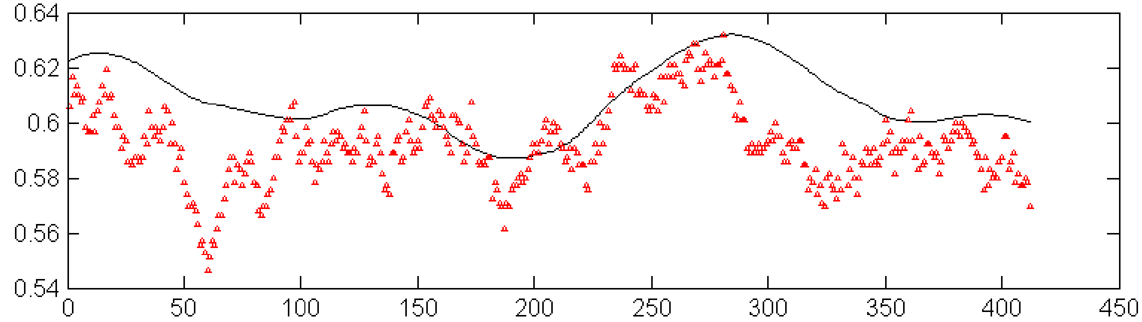
- Strict preservation of mass and momentum macroscopic conservation laws
- Convergence to the classical Fluctuating Hydrodynamics model for s->1 and no particles with capturing both the mean and the fluctuations
- Automatic satisfaction of the fluctuation-dissipation theorem for S=0 and S=1 and, for equilibrium, in between too

Example 1
Fluctuations of liquid argon at equilibrium conditions, s=const

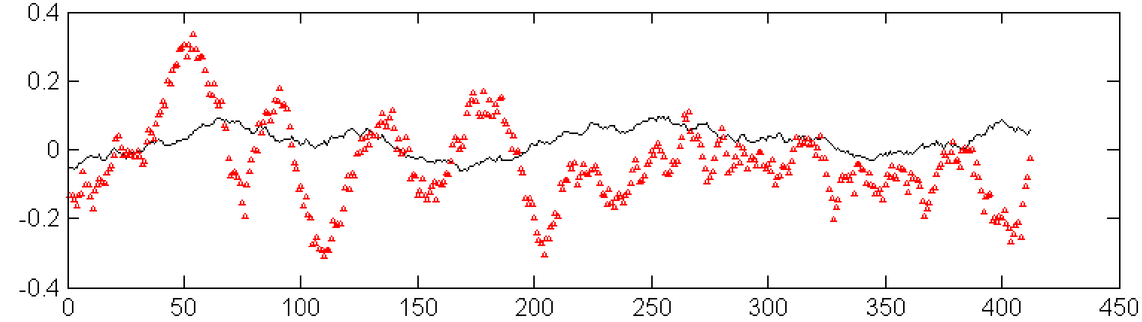
Toy model:
15x15 cell domain, each cell contains 400 atoms with Leonard-Jones potential

Consistency of MD-FH coupling for s=0.01 (~pure MD)

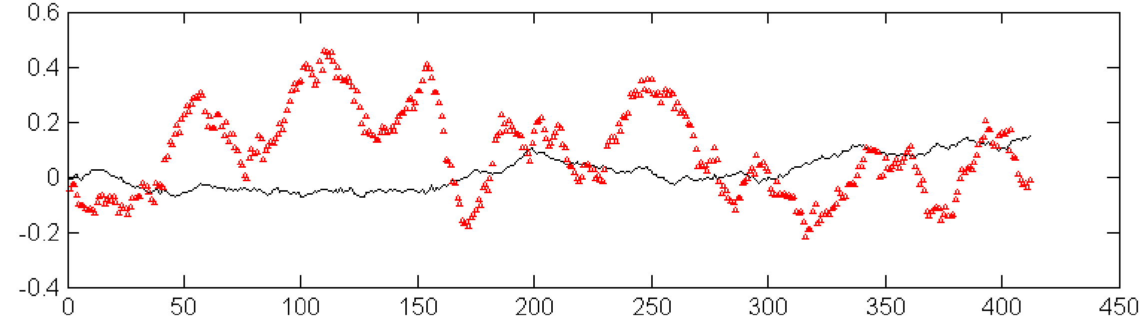
density



x-vel



y-vel

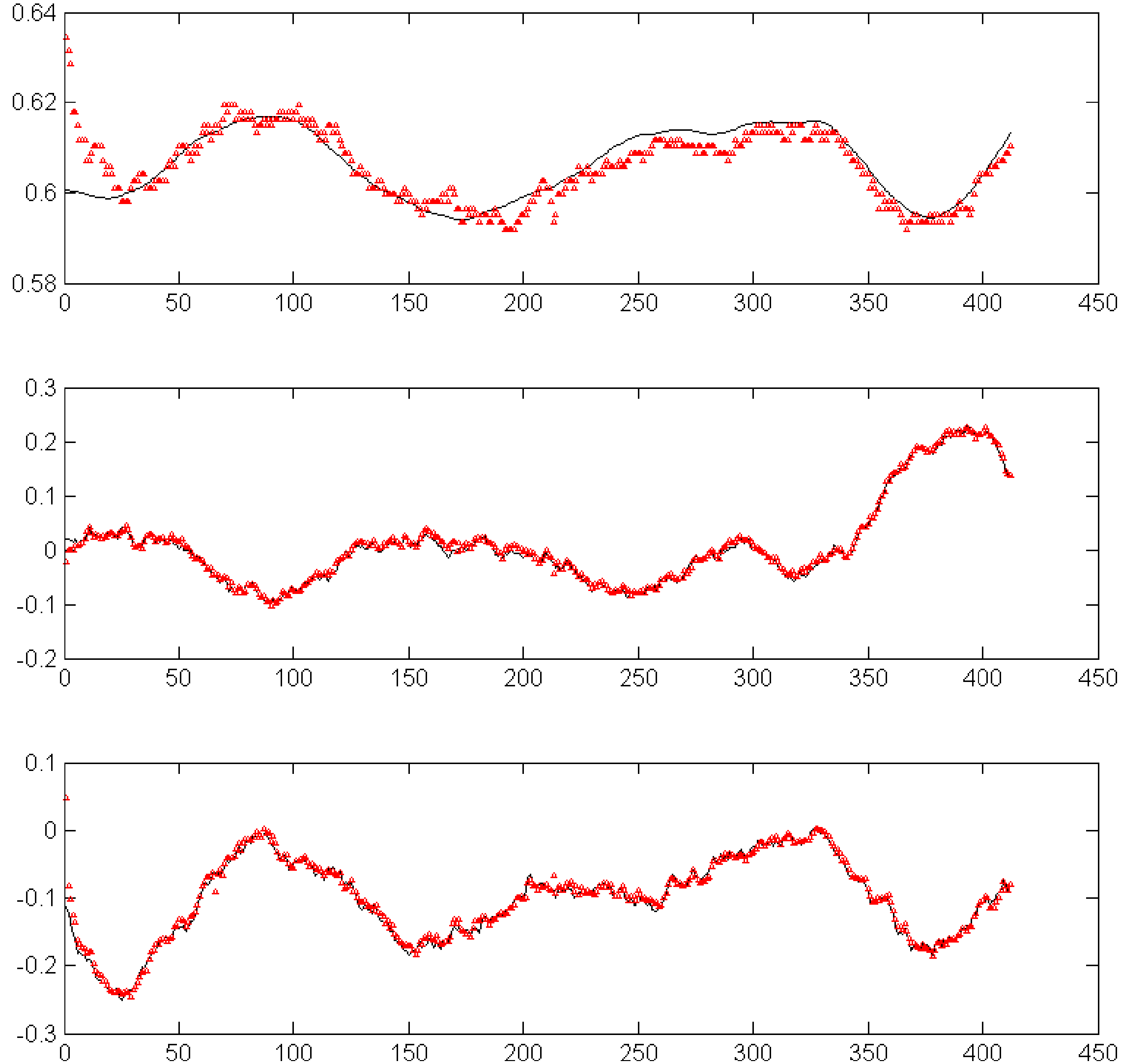


Consistency of MD-FH coupling for s=0.99 (~pure FH)

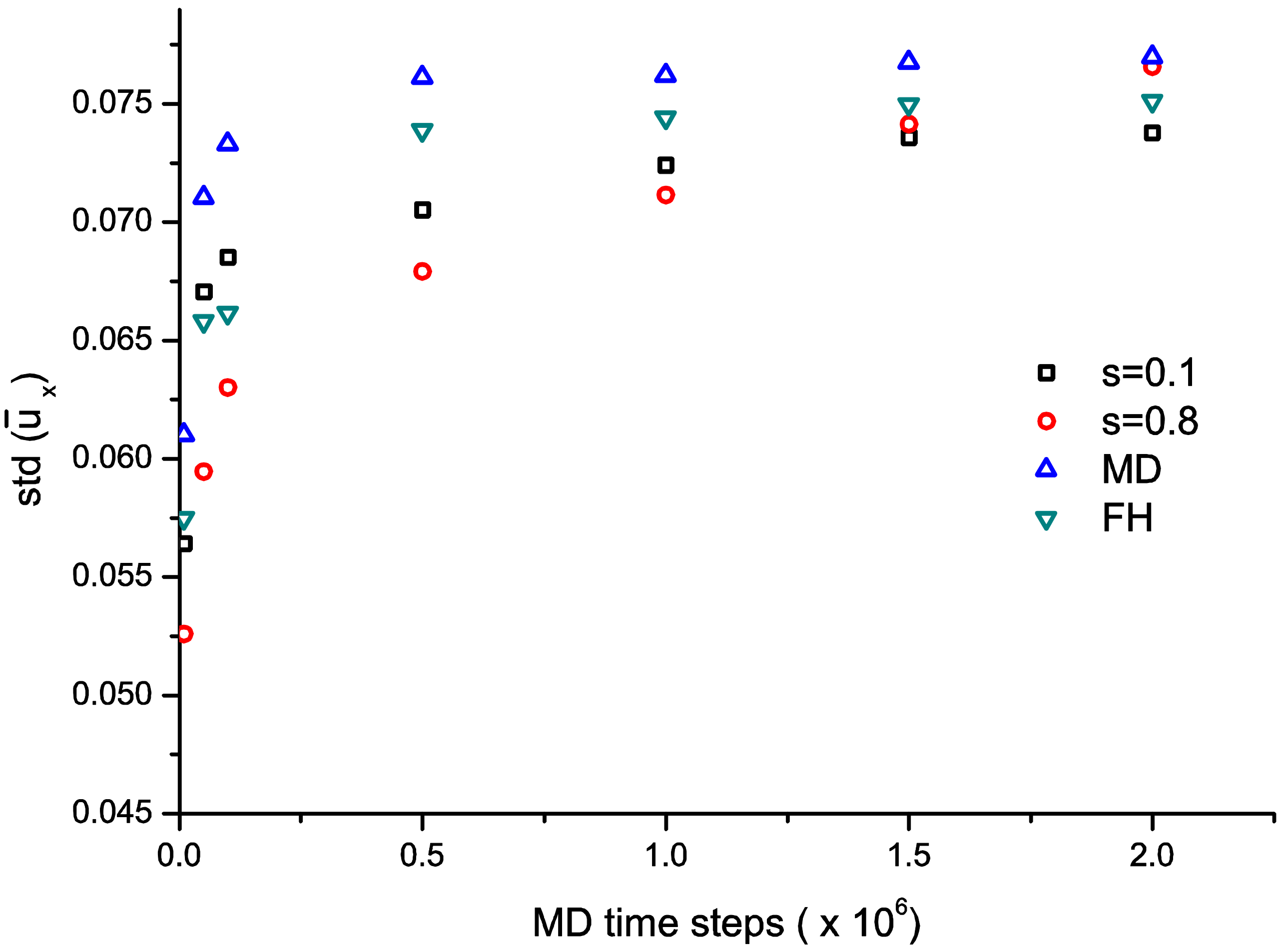
density

x-vel

y-vel



Second order statistics



3D Open Source MD Code: Groningen Machine for Chemical Simulations

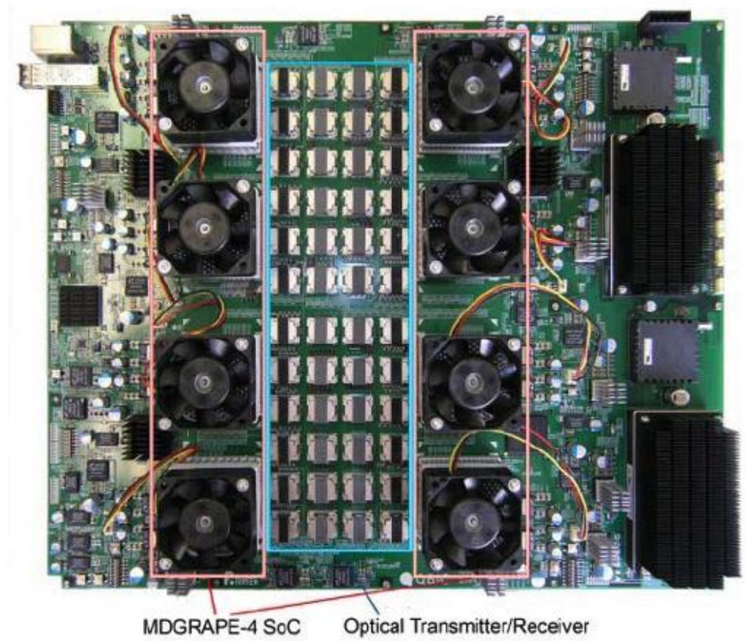
GROMACS

Groningen Machine for Chemical Simulations

USER MANUAL

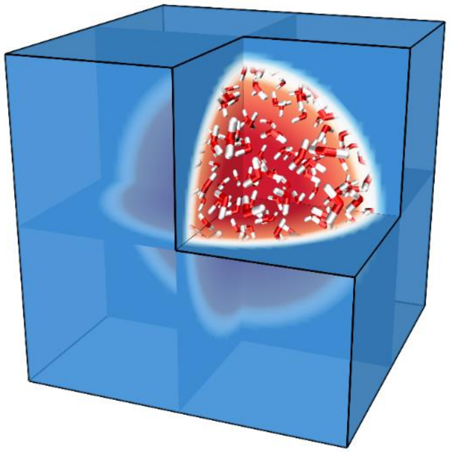
Specialised hardware

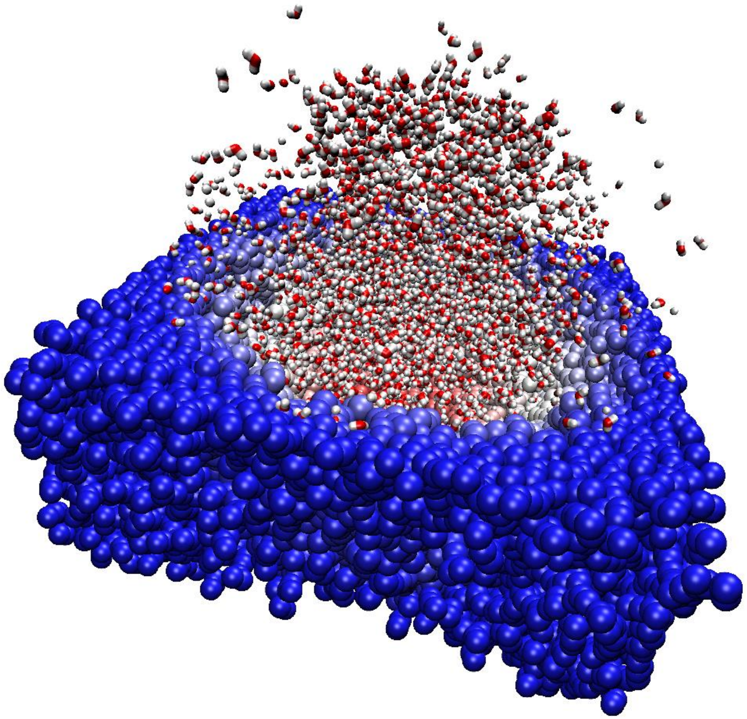
MDGRAPE-4: 100 ps per day for a 100K atoms system



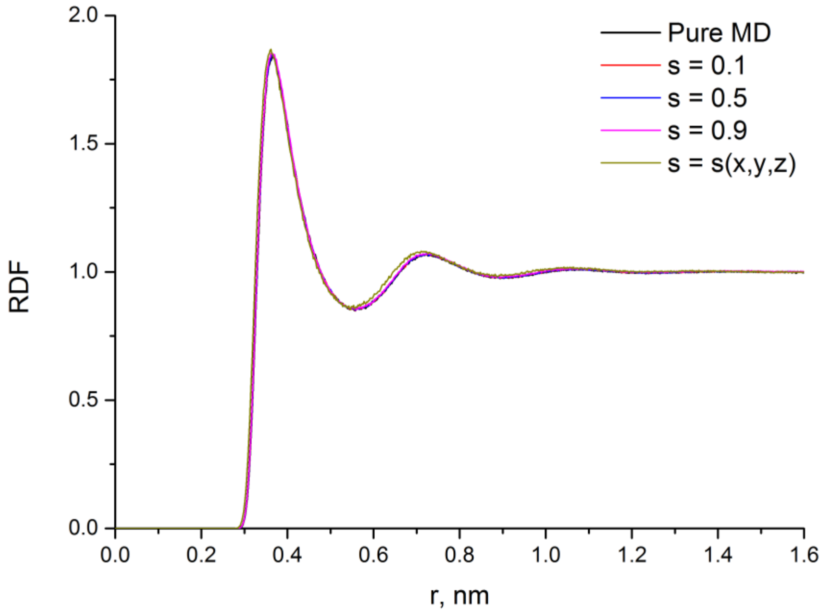
Can do up to ~ 0.001 s
for relatively small MD systems ~ 100,000 atoms

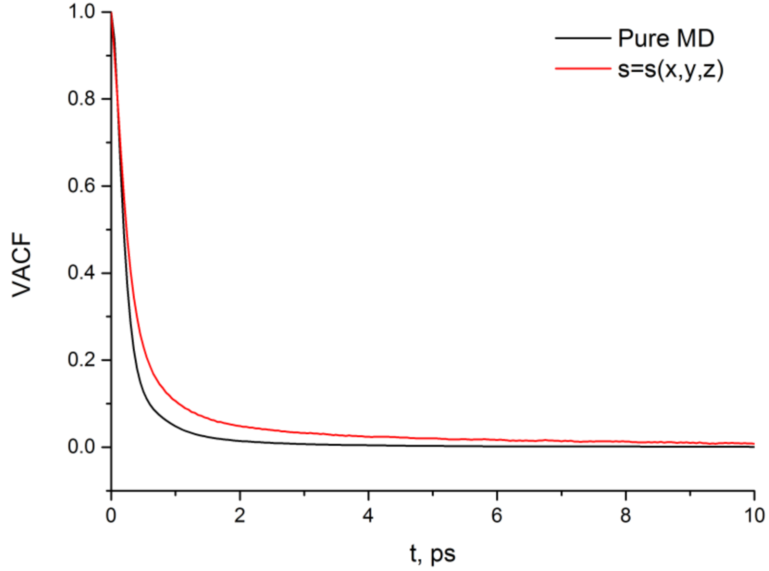
Example 2: 3D liquid argon and water at equilibrium (domain: 5x5x5 FH cells)



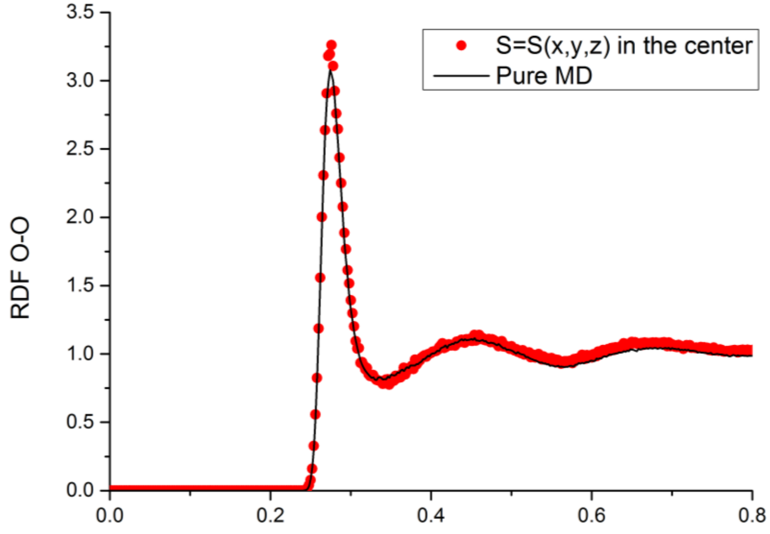


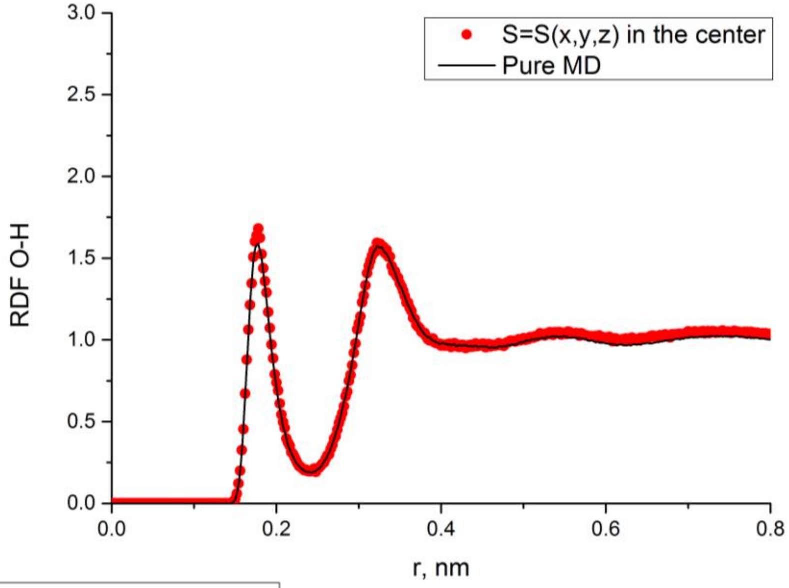
RDF and VACF for liquid argon

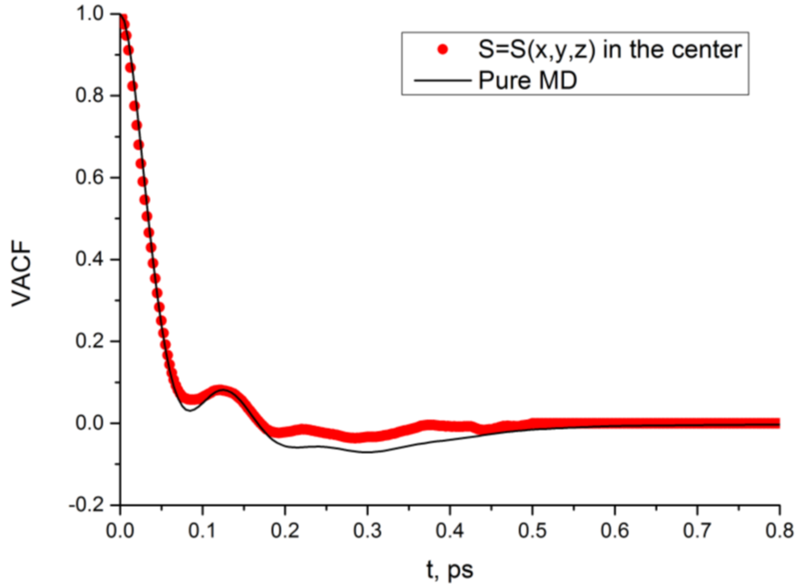




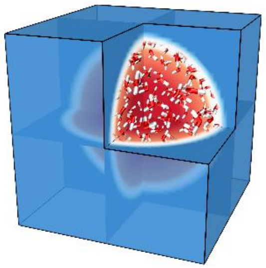
RDF and VACF for water

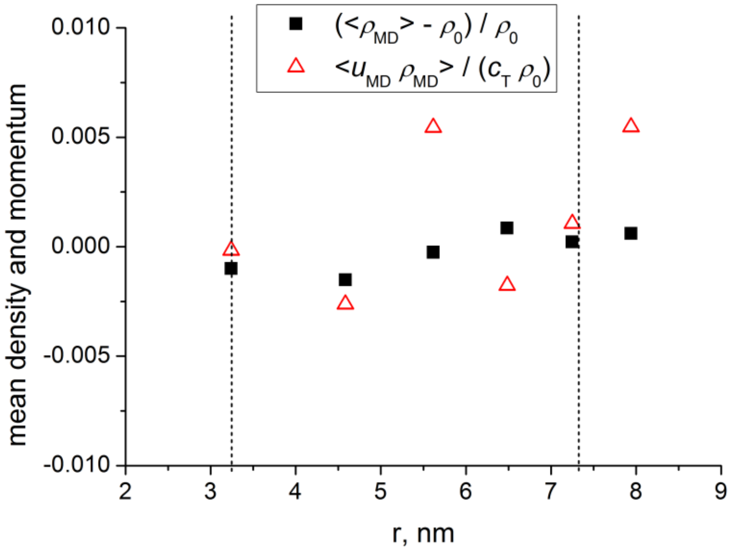


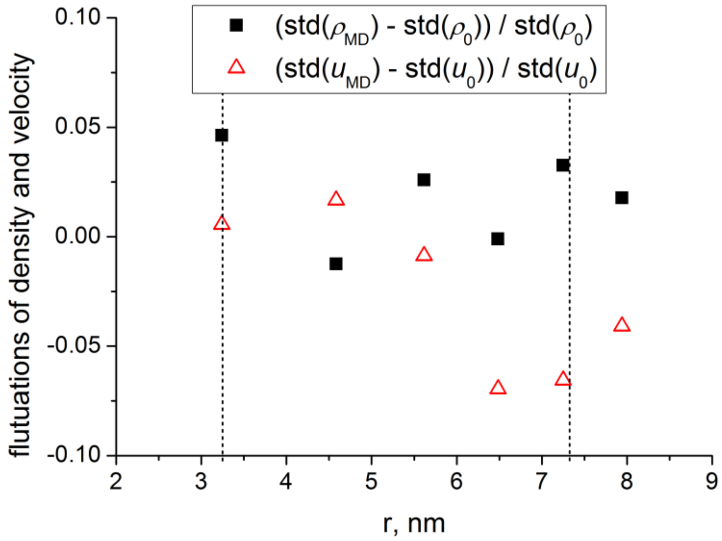




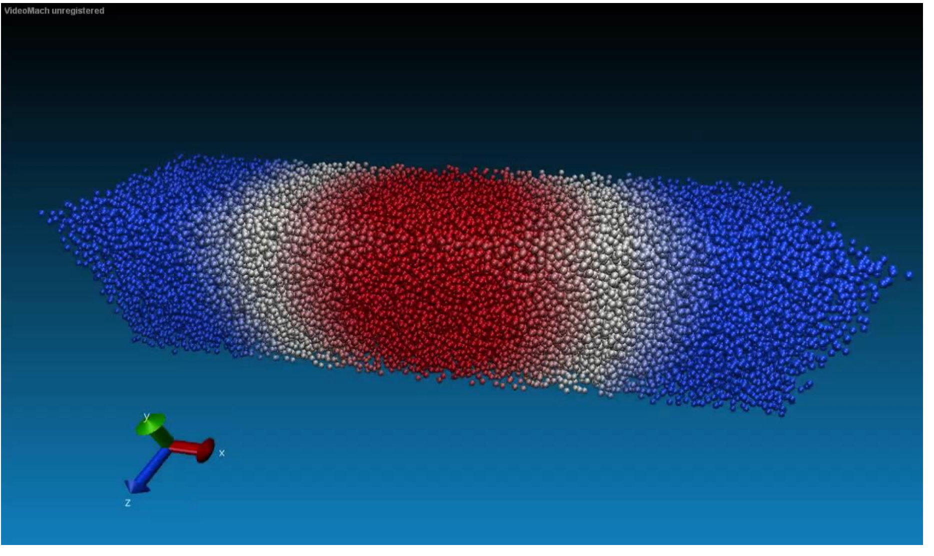
Preservation of mass, momentum, and correct fluctuations across the hybrid zone



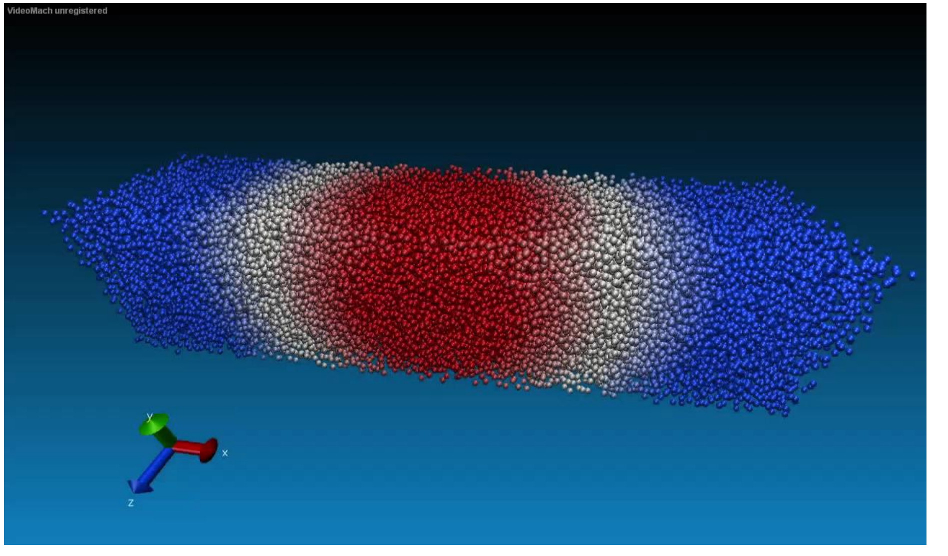




Example 3: Acoustic wave passing through the hybrid MD/FH zone (20x5x5 FH cells)

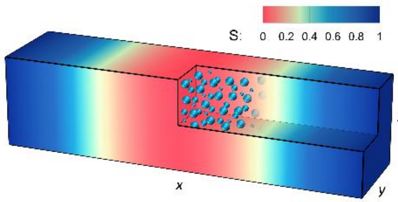


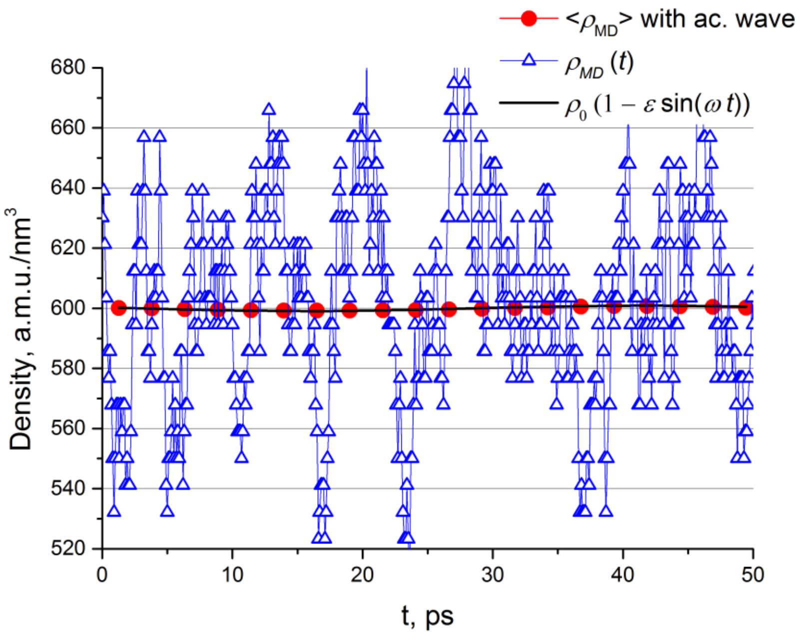
With acoustic wave



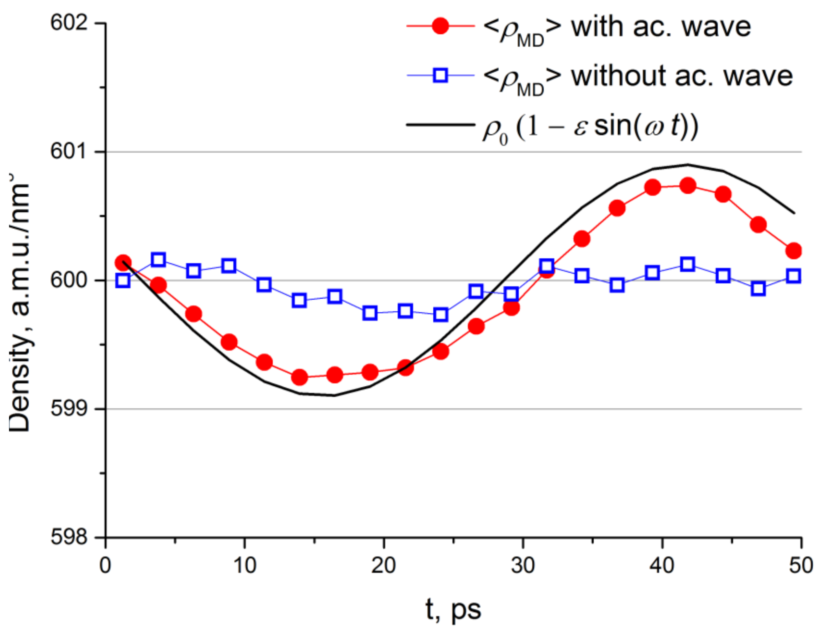
Without acoustic wave

Acoustic wave passing through the hybrid MD/FH zone





Original signal

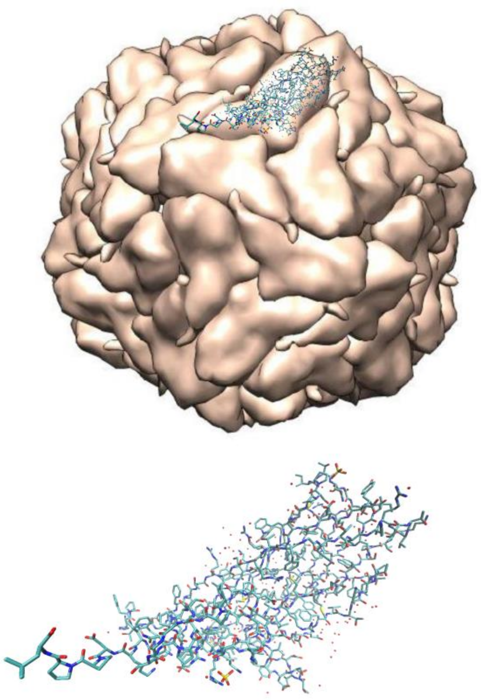


Phase and y&z averaged signal

Signal/noise ~0.01

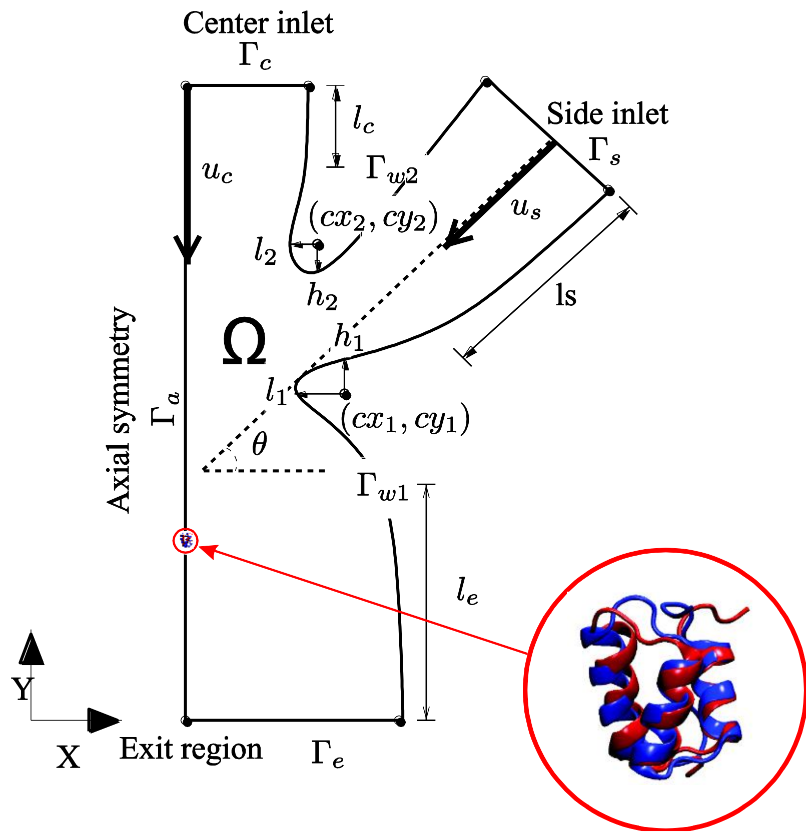
Grand challenges – bridging the space/time scales?

Resolution adaptive all-atom simulation of a nano-scale living organism (virus) in water



porcine circovirus

Conformational changes of macromolecules under the effect of hydrodynamics



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

"Time And Relative Dimensions In Space"
Doctor Who

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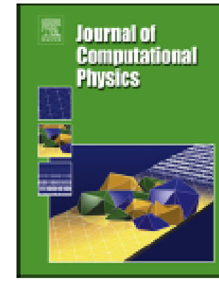


ELSEVIER

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

CrossMark

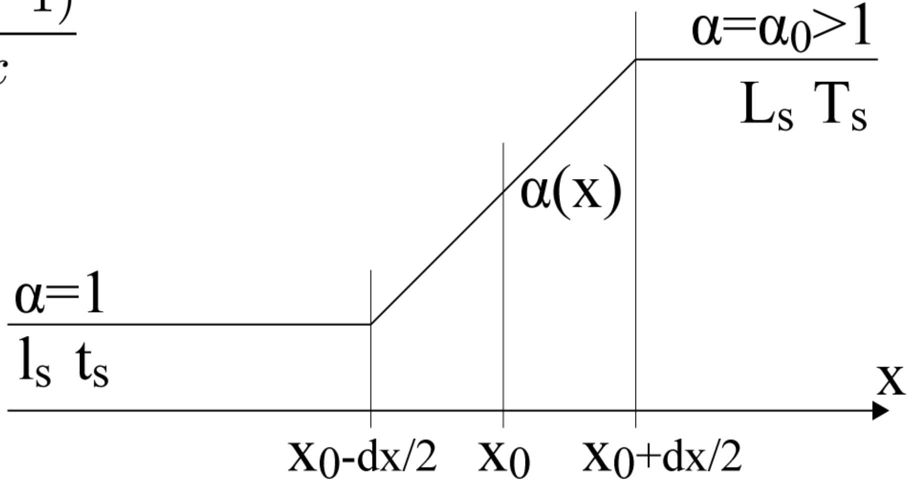
A.P. Markesteijn, S.A. Karabasov *

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:

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

Time Asynchronous Relative Dimension in Space (TARDIS)

- Result of transformations:
  - Advection equation in transformed space-time coordinates has the same form as original equation

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

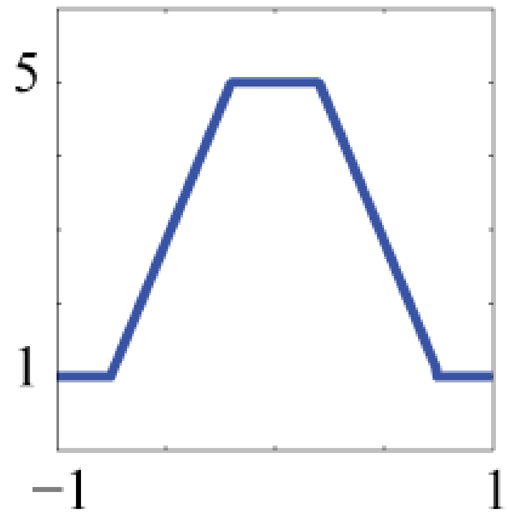
  - The compatibility condition amounts to a time-delay boundary condition between the large scale/small scale solution domains

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

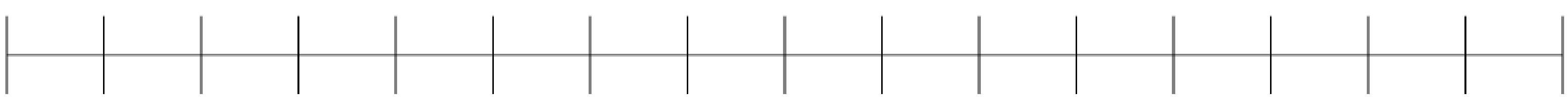
  - Frequency of a wave propagating from the large scales to the small scales will reduce its frequency α_0 times
  - Due to time delay, wavelength will broaden α_0 times

Example: 1D Plane Wave

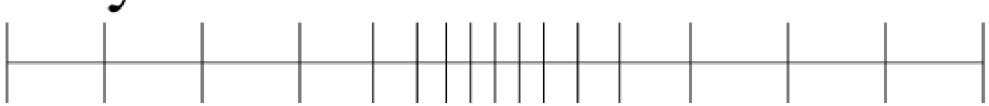
- Incoming acoustics wave
  - Scale difference of 5
  - Both mesh size and local time scal
- Results:
  - Wave length should increase 5x
  - Frequency should decrease 5x
  - Physical domain: normal wave



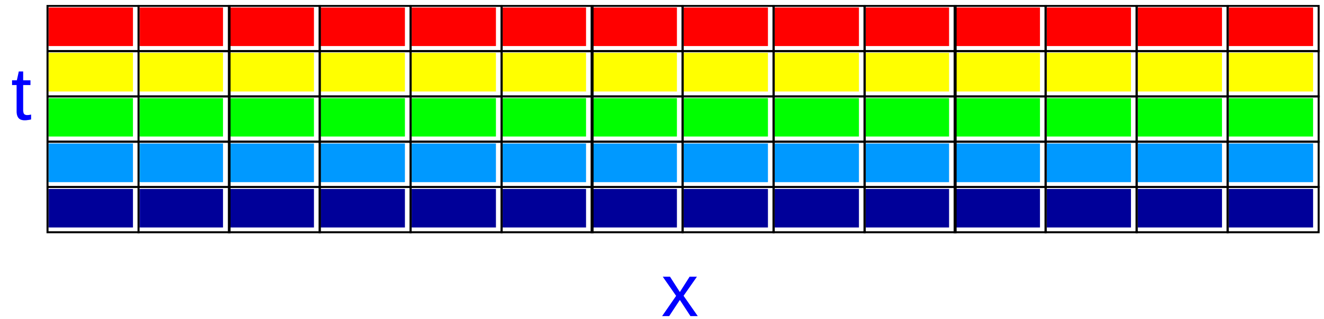
Computational Domain - Transformed Coordinates



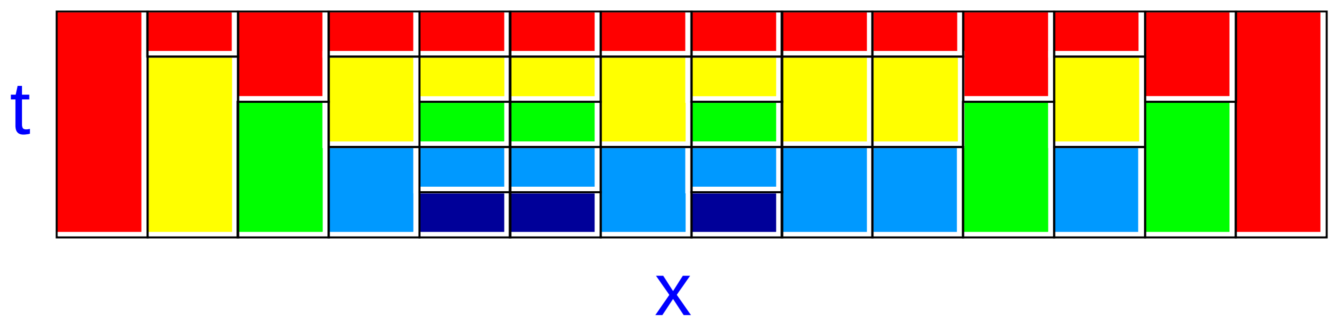
Physical Domain - Untransformed Coordinates



Homogeneous time-stepping

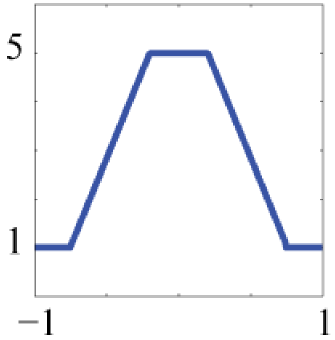


Asynchronous time-stepping

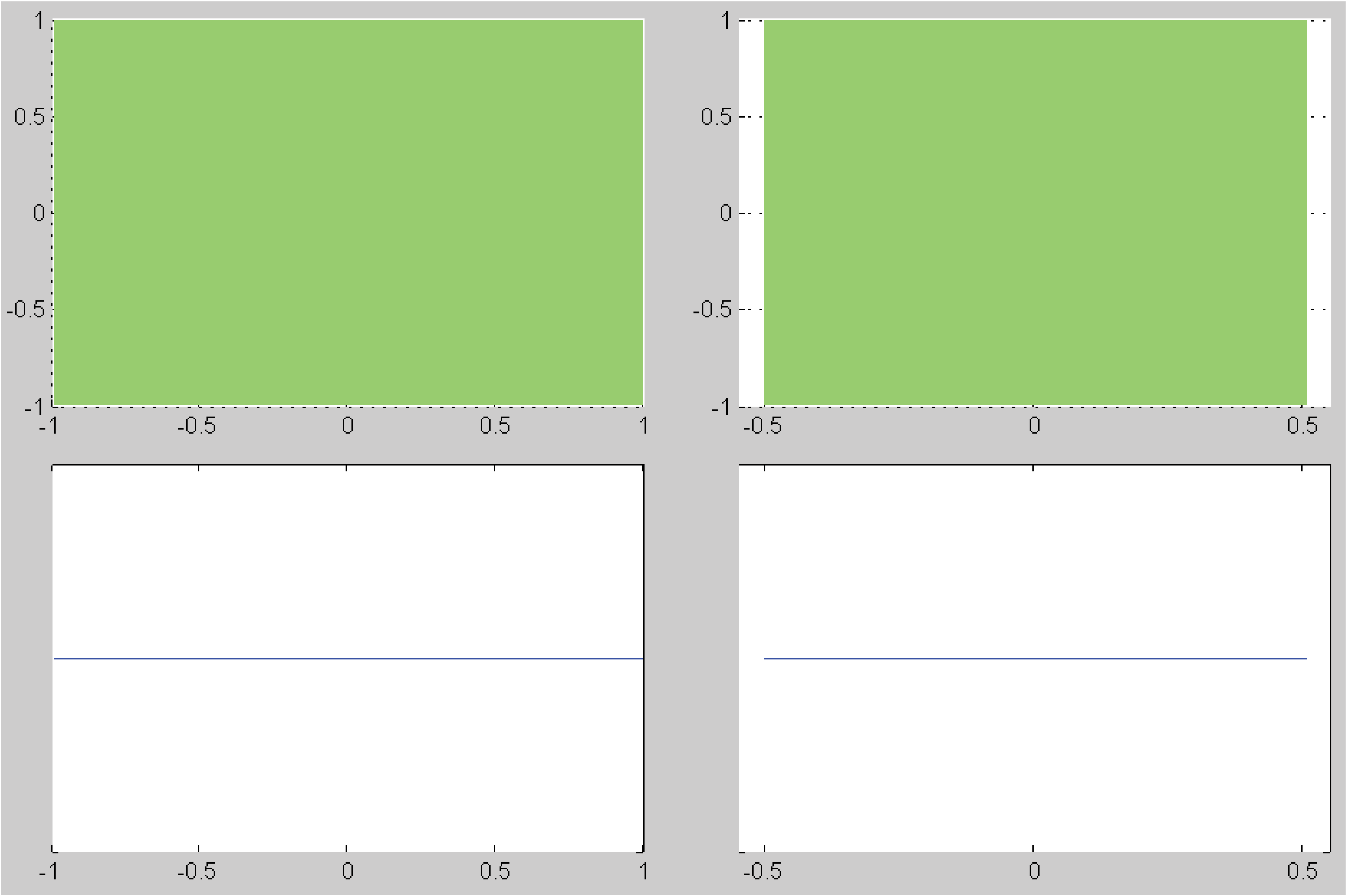


step

Example: 1D Plane Wave

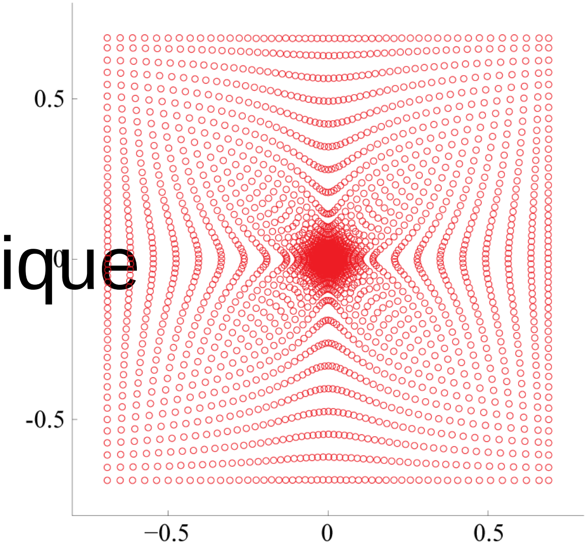


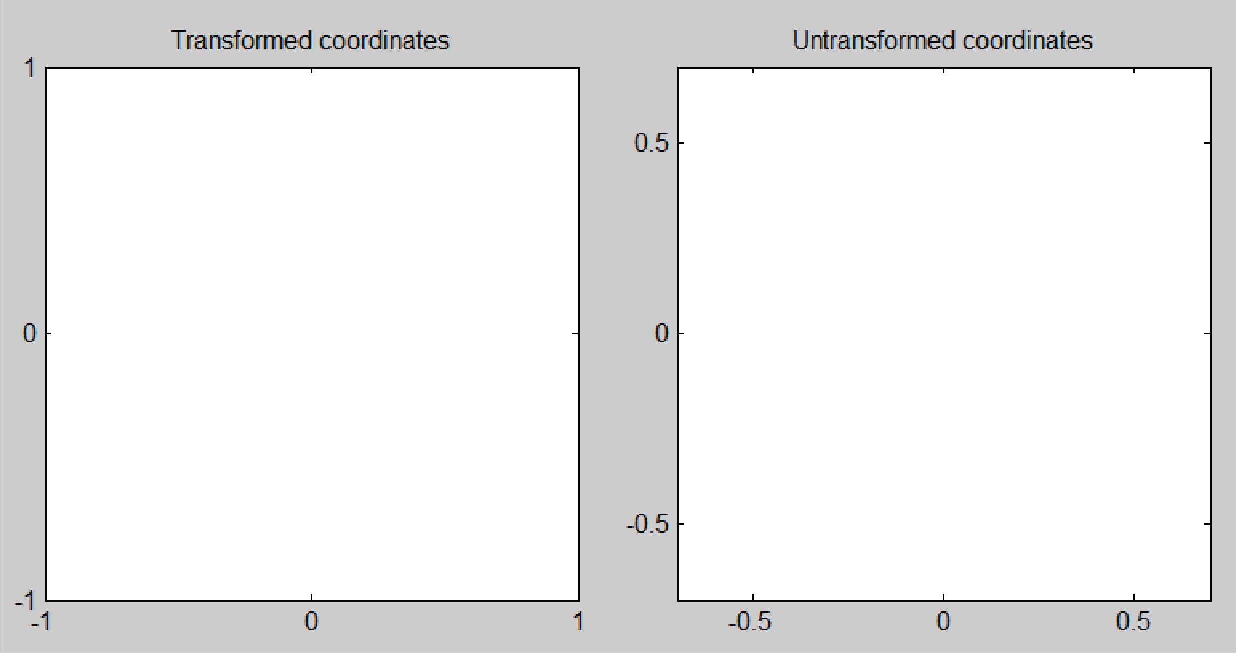
- Scale function: 1 to 5 to 1 linearly
  - Incoming acoustic wave: 20 PPW



Example: 2D Radial Zoom-In Grid Generation

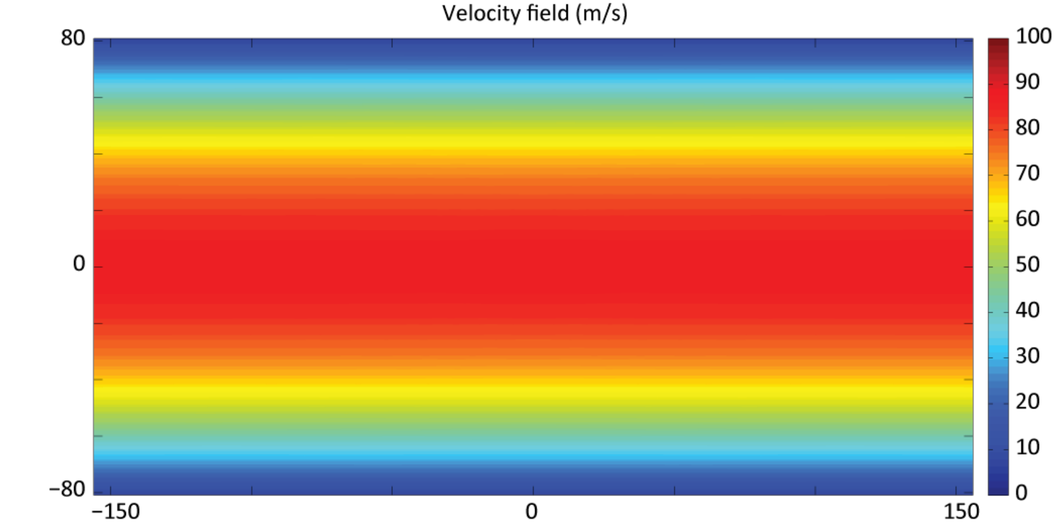
- Flat boundary equivalent
  - Adjusting aspect ratios of cells
  - Accomplished in ray-tracing technique

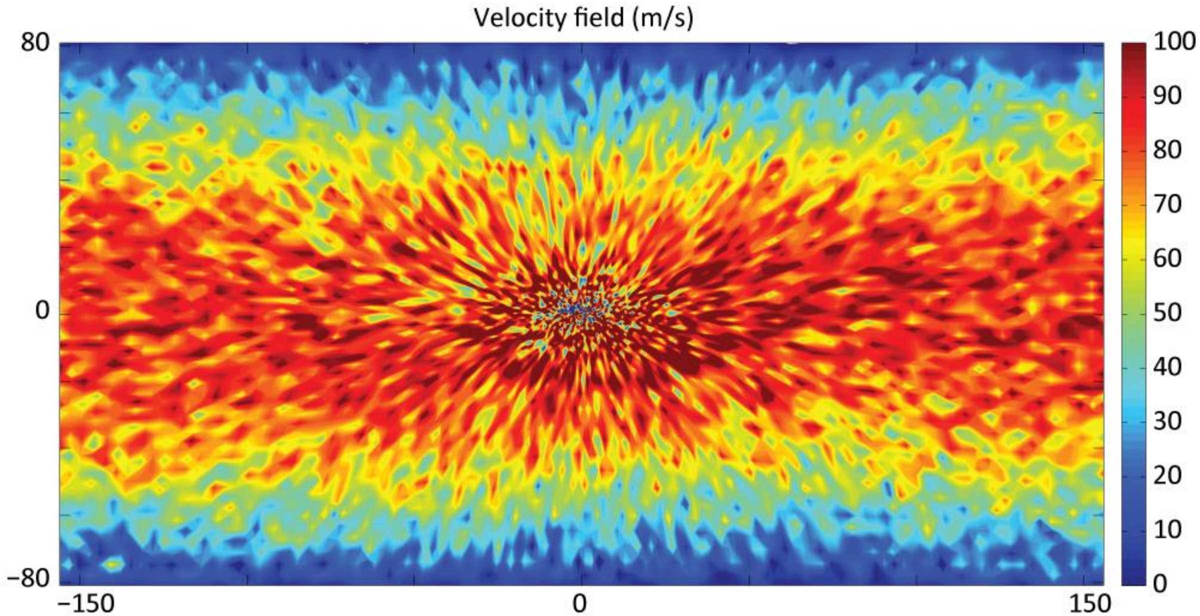


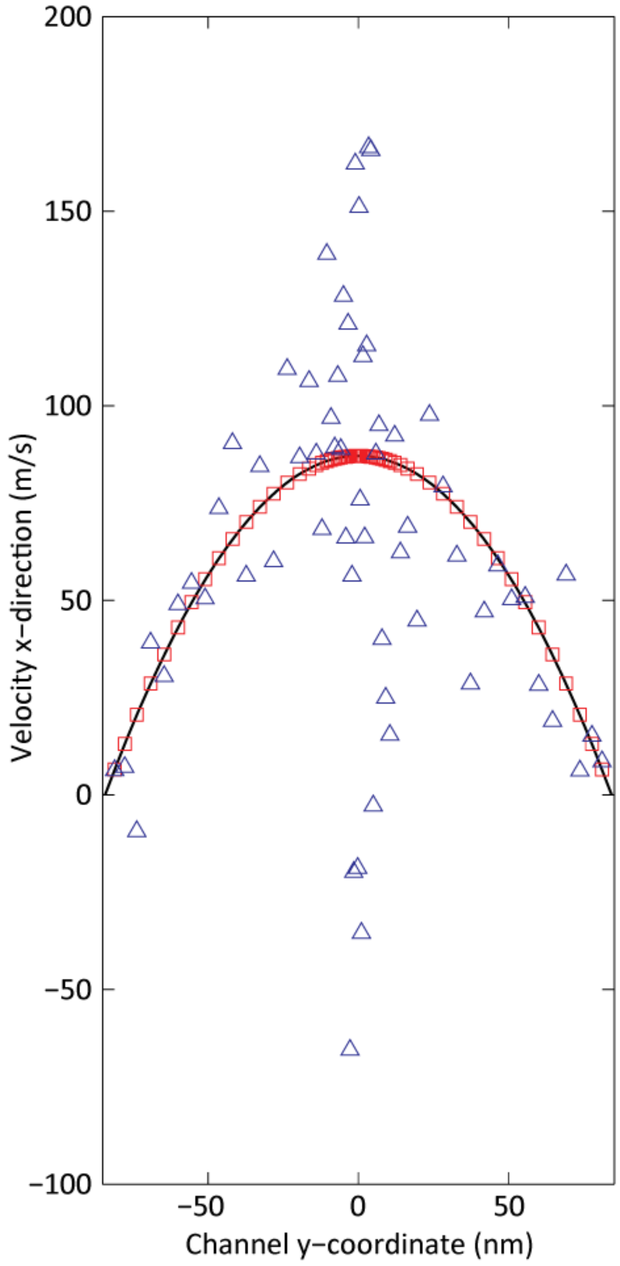


2D Example: Fluctuating Hydrodynamics

- Velocity profile and fluctuation

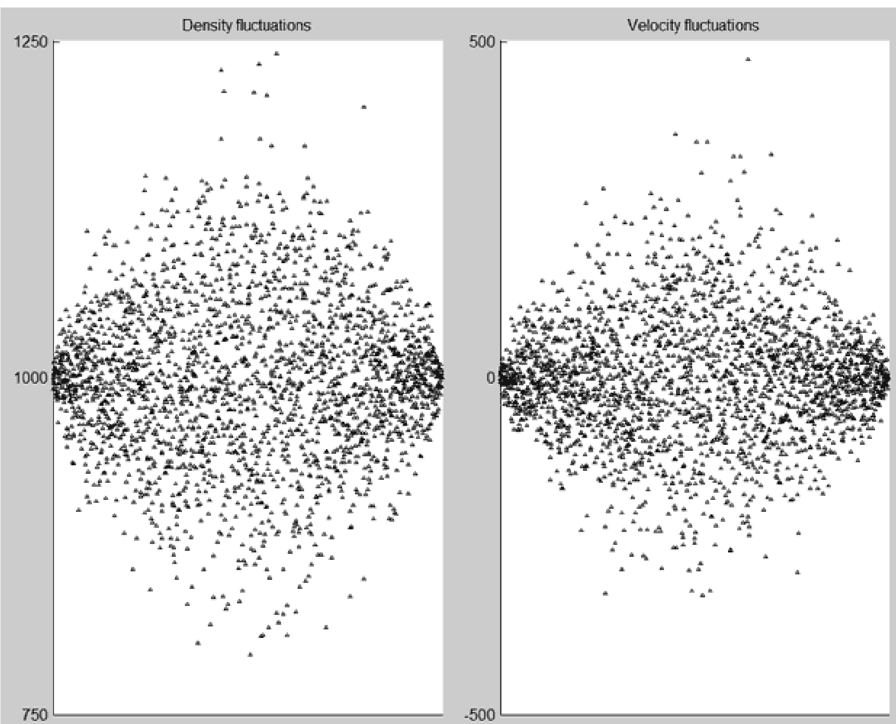


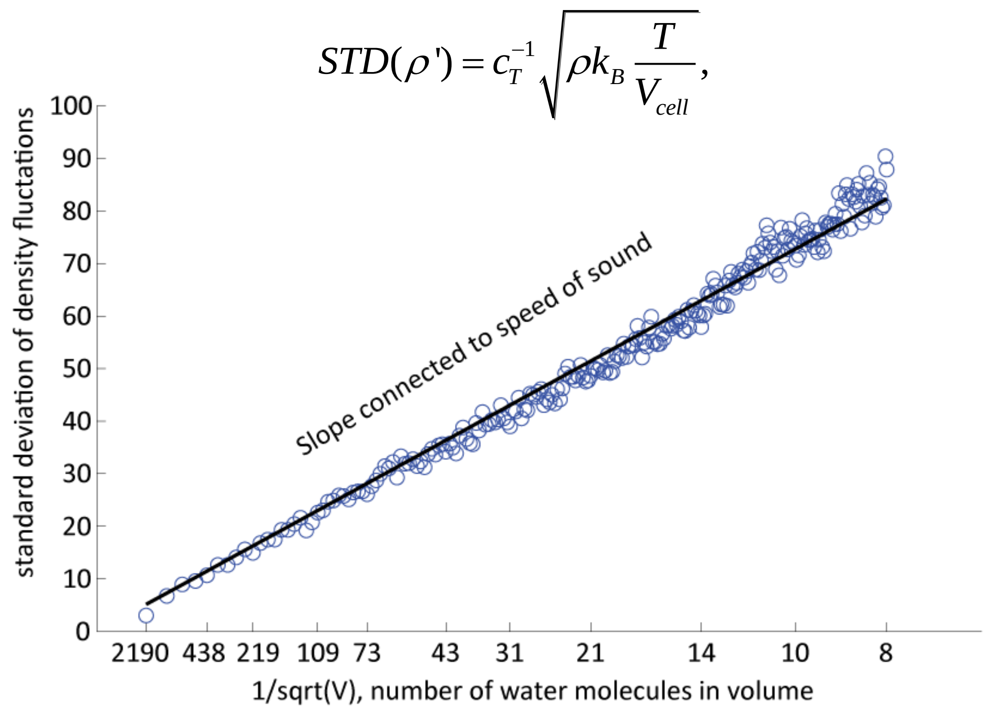




2D Example: Fluctuating Hydrodynamics

- 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)





Conclusions

- Physical analogy approach for MD/FH simulations is discussed for liquid argon and water
  - Pros: conservation laws, physical interpretation of "interpolation parameter" s (including s(t)) and the hybrid MD/FH region, potentially can bridge MD with very large HD scales/ be computationally efficient for engineering applications
  - Cons: the current fully-atomistic MD/FH zone needs calibration, extensions of TARDIS to fully atomistic MD?
- Possible solution: fully atomistic MD/FH -> MD/CG/FH

MD

FH

AdResS?