Non-reflecting boundaries for ultrasound in fluctuating hydrodynamics of open systems

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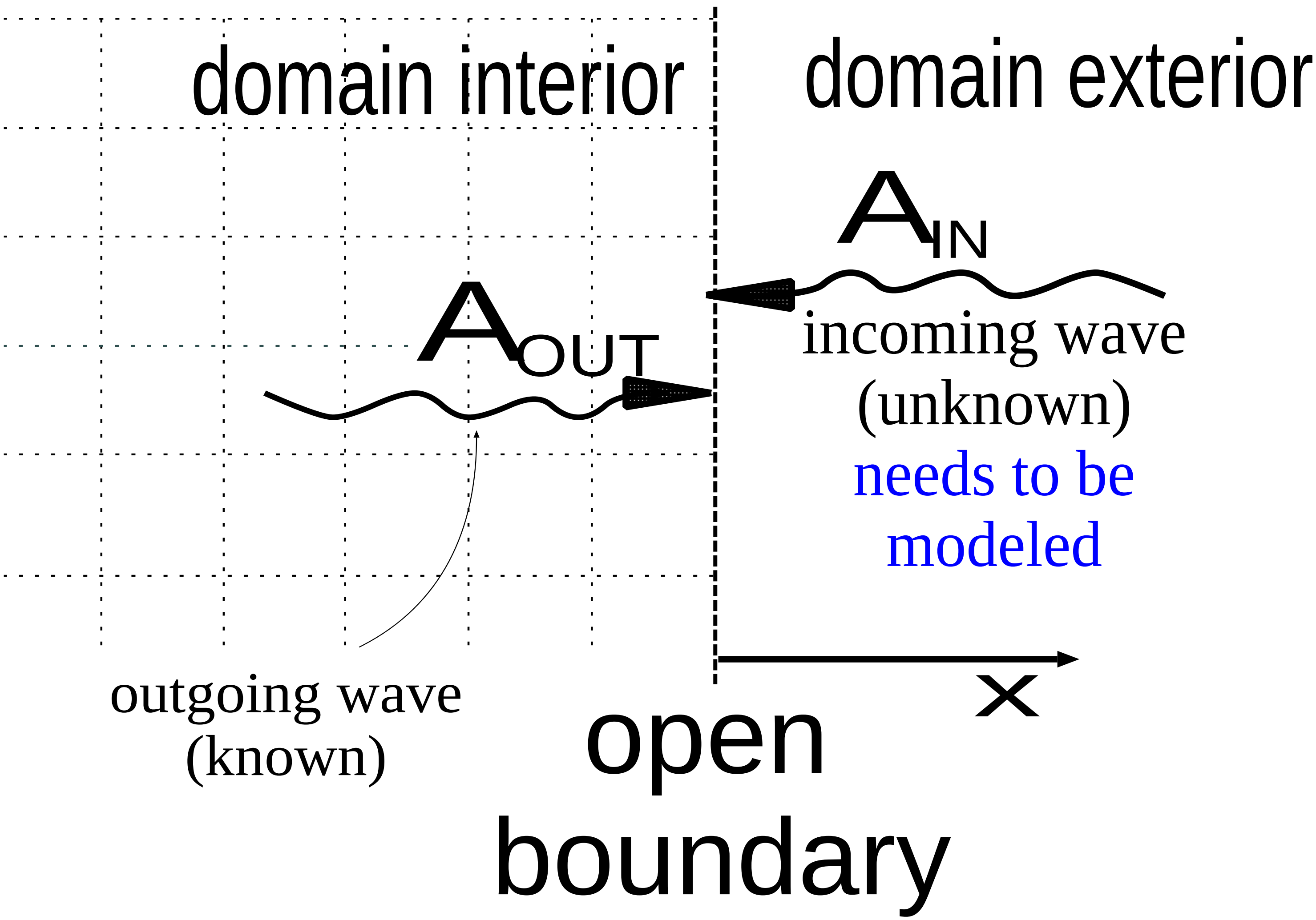
Open boundaries: applications

- Open boundaries are needed in most CFD applications: turbulence, combustion, simulation of sound devices...
- Evacuate **sound**, shear or heat waves out of the simulation domain.
- Open boundaries have been derived for standard CFD.
- This work generalizes them to **fluctuating hydrodynamics**
- ULTRASOUND $f \sim GHz$ scales ranging from **microns to nanometers**.
- Ultrasound applications are wide-spread,
  - Transport and manipulation of nanoparticles [ETH, Zurich]
  - Complex rheological behaviour of viscoelastic fluids.
  - Microflows, Nanoflows.
  - Macromolecules-sound interaction (proteins) [*Science*, 309:1096, 2005.]
  - The present NRBC can be combined with hydrid molecular-continuum simulations involving sound [PRL, 97, 134501 (2006)].

Non-reflecting boundary conditions for CFD: set-up



Non-reflecting boundary conditions in terms of sound modes.

- Amplitude of **sound waves**

$$A_{IN} = \frac{1}{2}\left(\frac{\delta p}{\rho_e c} - \delta u\right) \quad \text{moving} \leftarrow \tag{1}$$

$$A_{OUT} = \frac{1}{2}\left(\frac{\delta p}{\rho_e c} + \delta u\right) \quad \text{moving} \rightarrow \tag{2}$$

with $\delta p = p - p_e$, $\delta u = u - u_e$, pressure and velocity fluctuations.

- **NRBC formulation:** At the boundary solve linear Navier-Stokes Eqs. in the normal-to-boundary direction:

$$\frac{\partial A_i}{\partial t} + \frac{L_i}{\rho_e c} = \pm \frac{1}{\rho_e} \frac{\partial \Pi_{xx}}{\partial x},$$

with $i = IN \rightarrow +$ and $i = OUT \rightarrow -$

- Amplitude variations:

$$\frac{L_i}{\rho_e c} = (u \mp c)\frac{\partial A_i}{\partial x}$$

Non-reflecting boundary conditions: implementation for primitive variables.

- **NRBC:** Solve for pressure and velocity at the boundary:

$$\frac{\partial p}{\partial t} + \frac{1}{2}\left(L_{OUT} + L_{IN}\right) = 0$$

$$\frac{\partial u}{\partial t} + \frac{1}{2\rho_e c}(L_{OUT} - L_{IN}) = -\frac{1}{\rho_e}\frac{\partial}{\partial x}\left(\Pi_{xx}\right).$$

we work with density $\delta\rho = \delta p/c^2$, where c is the sound velocity.

Closure models for the incoming waves

$L_{OUT} = \lambda_{OUT}\left(\frac{\partial P}{\partial x} + \rho c \frac{\partial u}{\partial x}\right)$	Evaluated at the interior domain
$L_{IN} = 0$	`cons:` ill posed, overall pressure drift
$L_{IN} = K(p - p_{eq}) \quad K = \frac{\sigma c}{L}$	`cons:` reflection of low freqs.
$L_{IN} = K(p - p_{eq} - \rho c A_{OUT})$	`pros:` no drift, no reflection at low freq.("wave masking")
$L_{IN} = K(\rho c A_{IN})$	`pros:` enables fluctuation-dissipation balance, based on wave masking.

NRBC for FH: Fluctuation-dissipation balance for incoming waves

- Stochastic eq. for incoming wave amplitude:

$$\frac{dA_{IN}(x_b)}{dt} + KA_{IN}(x_b) = F(t)$$

- Fluctuating stress: $F(t) \equiv \frac{1}{\Delta x \rho_e}\left[\tilde{\Pi}_{xx}(x_b + \frac{\Delta x}{2}) - \tilde{\Pi}_{xx}(x_b - \frac{\Delta x}{2})\right]$

$$\langle F(t)F(0)\rangle = 2\Phi\delta(t) = \frac{4k_BT\eta_L}{\Delta x^2 \rho_e^2 V_c}\delta(t)$$

- Stochastic boundary **dynamics**: $\langle A_{IN}(t)A_{IN}(0)\rangle = \frac{\Phi}{K}\exp(-Kt)$.

  $\langle A_{IN}\rangle = 0$ and $\boxed{\langle A_{IN}^2\rangle = \frac{\Phi}{K}}$.

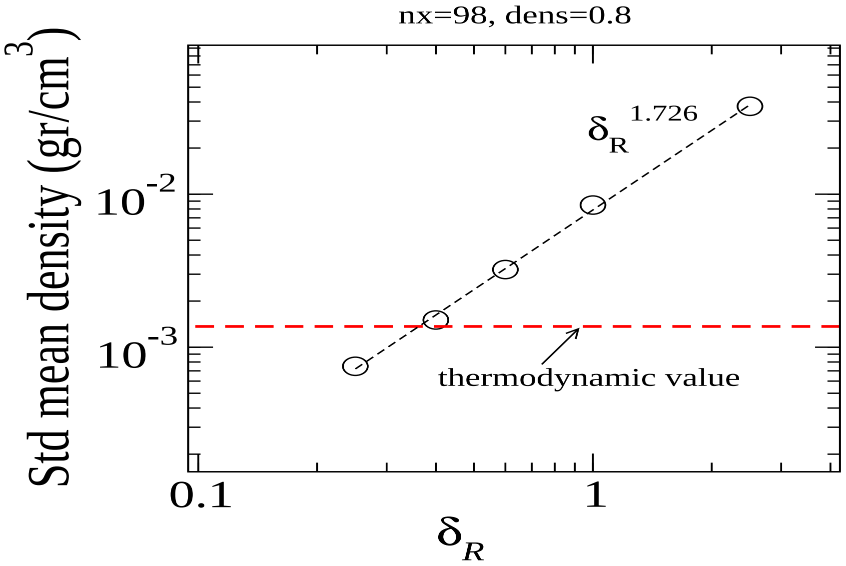
- Sound amplitude variance, **thermodynamics,** $A_{IN} = (1/2)(c\delta\rho/\rho_e - \delta u)$.

  $\boxed{\langle A_{IN}^2\rangle = \frac{1}{2}\frac{k_BT}{\rho_e V_c}}$

- **Relaxation rate**: $\boxed{K = \frac{\nu_L}{(\delta_R \Delta x)^2}}$ with $\delta_R^{(theor)} = 0.5$

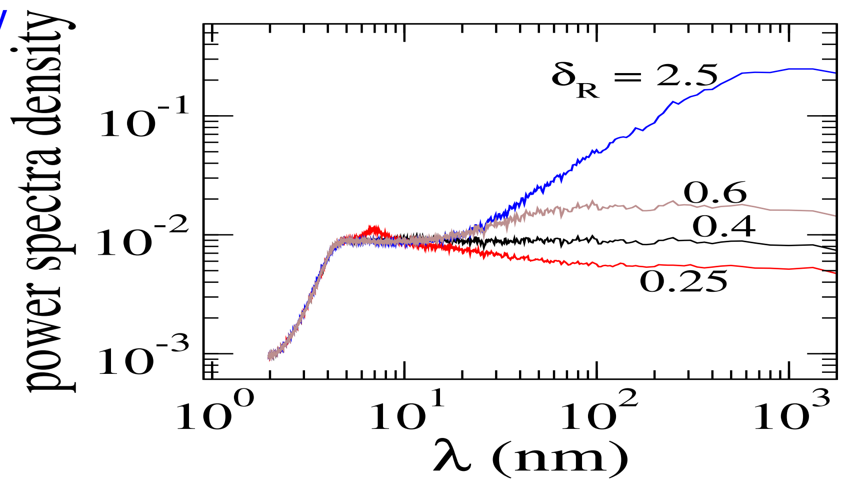
Mean density fluctuation at equilibrium: grand canonical ensemble,

$$\langle(\delta\bar{\rho})^2\rangle = \frac{k_B T}{c^2 V}$$



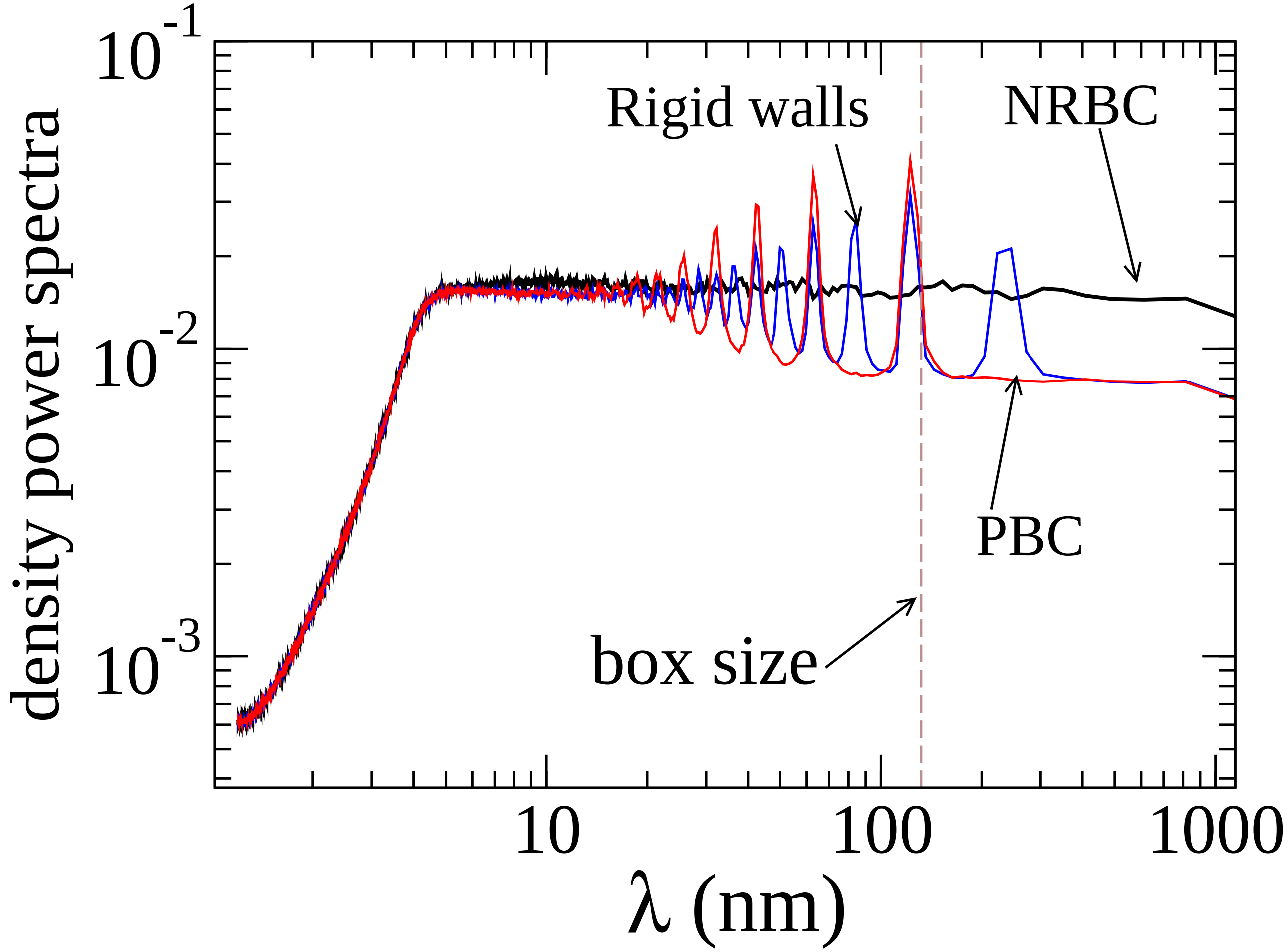
$$\delta_R^{(num)} = 0.4$$

Sound power spectral density within the system interior

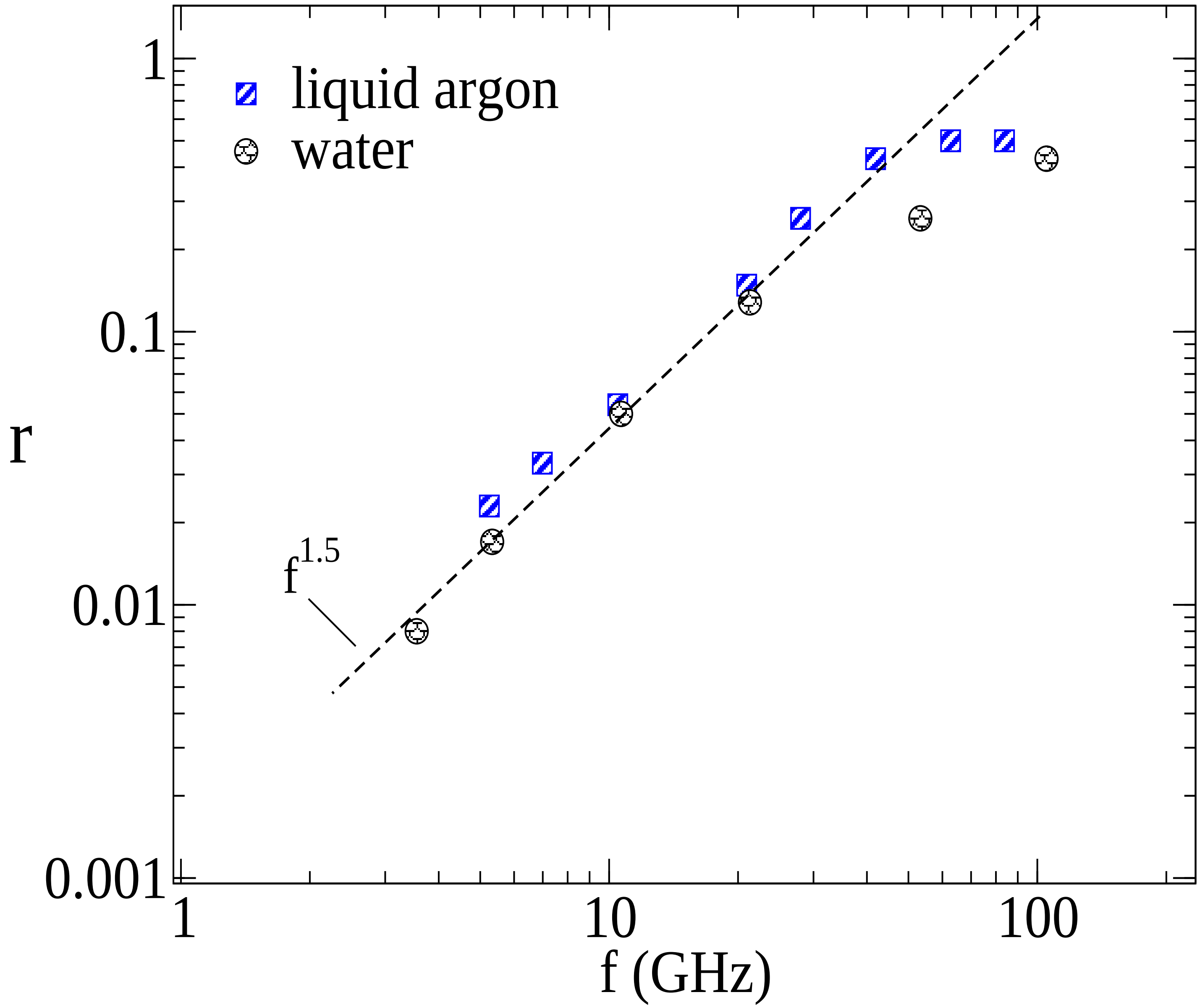


Comparison with PBC and Rigid walls:

PSD of waves within the system



Reflection coefficient



Conclusions

- Simulation of ultrasound in microenviroments, via fluctuating hydrodynamics
- Open boundaries for sound, low reflection.
- Respect hydrodynamics and thermodynamics fluctuations (grand-canonical)
- **Applied to**
  - Sound-macromolecule interactions
  - Micro-devices (e.g. collimators, microring ultrasound detectors, ...)