CATCH-U-DNA
UAM group
Theory and simulations

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CATCH-U-DNA Kick-off Meeting

Outline

- Objetives
- Methods and models
  - Continuum level
  - Mesoscopic level
  - Atomistic level
- Questions

Modelling of Quartz Micro Balance

1. **Reproduce experiments** (results/trends)
   - Frequency decay rate shifts, ΔF, ΔD
   - Relation between acoustic ratio (dissipation/frequency) and molecule intrinsice viscosity.
2. **Insights**
   - How the mechanic energy dissipates into the fluid-macromolecule system?
   - Role of the protein linker in dissipation.
   - Origin of the intercept “a” in $\Delta D/\Delta F = a + m\,[\eta]$ (related with the linker stiffness).
   - Plateau regime in the relation $\Delta D/\Delta F$ versus $[\eta]$ (viscous limit?)

Modelling of Quartz Micro Balance

Figure 2 shows the relation between experimental $\Delta D/\Delta F$ values and the corresponding intrinsic viscosities for linear

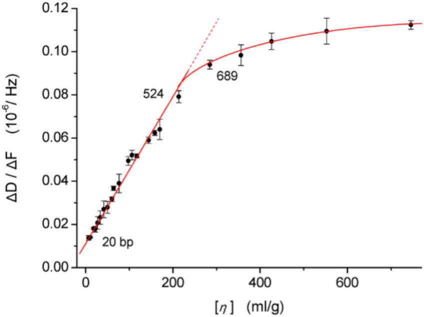
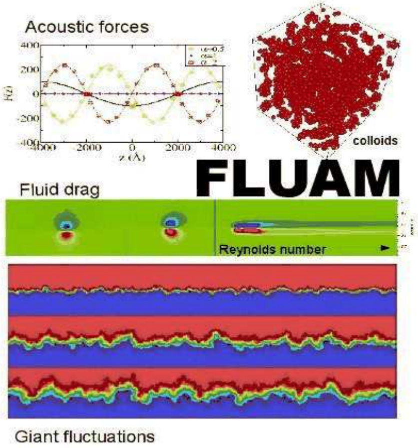


Figure 2. Acoustic ratio/intrinsic viscosity relationship for linear dsDNA for the 35 MHz frequency of the QCM device. The $[\eta]$ values are from the experimentally obtained eq 5. The numbers adjacent to the line indicate the number of base pairs giving an approximate value of 600 bp at the "break" point.

1. Continous description (partial differential eqs.)
2. Mesoscopic level
   FLUAM: *FLuid And Matter*. GPU code
   Fluid phase is solved via fluctuating Navier-Stokes.
   - Lenght resolution: 2 nm. DNA: Worm like chain, beads.
   - Lenght resolution: 0.5 nm. DNA: Elastic network model.
3. Atomistic level
   UAMMD: *Universally Adaptable Multiscale Molecular Dynamics*.
   GPU code
   Fluid solved at discrete molecular level.

FLUid And Matter
GPU code (CUDA)

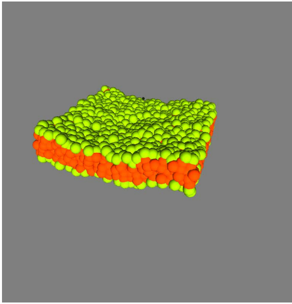
Complex Fluids Group
Dept. Theoretical Physics
For Condensed Matter
UAM



https://github.com/fbusabiaga/fluam

Eulerian-Lagrange, Immersed Boundary Method (Peskin)

- **Objetive**: Fluid-structure interaction
- **Accurate**: Fluid based on finite volume (Eulerian), including thermal fluctuations
- **Flexible**: Surfaces are mesh-free (Lagrangian)
- **Adaptable**: Surfaces resolved by a mesh of "Lagrangian markers"
- **Fast**: Regular fluid mesh, pseudospectral, Fast-Fourier.
- **Versatile**: *Inertia*, no-Inertia (Stokes), particle compressibility, chemical reactions, sound-matter interaction, etc.



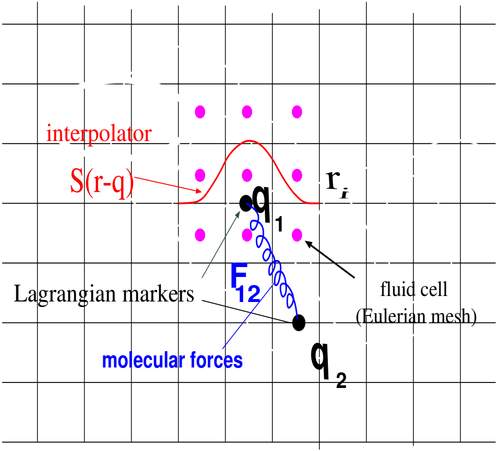
Fluid average around each Lagrangian marker J

- Compact support interpolator $\mathrm{S}(\mathbf{r}-\mathbf{q})$

$$\mathrm{J}_{\mathbf{q}}[\mathbf{v}] \equiv \sum_{i \in \mathrm{mesh}} \mathrm{S}(\mathbf{r}_i - \mathbf{q})\mathbf{v}(\mathbf{r}_i)$$

- Instantaneous fluid-particle coupling (no-slip)

$$\mathbf{u} = \frac{\mathrm{d}\mathbf{q}}{\mathrm{d}t} = \mathrm{J}_{\mathbf{q}}[\mathbf{v}(\mathbf{r})]$$



Equations of motion

$$\text{Fluid} \quad : \quad \rho\left[\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v}\cdot\nabla\mathbf{v}\right] = -\nabla\mathbf{P} - \sum_i \boldsymbol{\lambda}_i\,\mathrm{S}(\mathbf{q}_i - \mathbf{r})$$

$$\text{Particle} \quad : \quad m_e^{(i)}\frac{\mathrm{d}\mathbf{u}_i}{\mathrm{d}t} = \boldsymbol{\lambda}_i + \mathbf{F}_i$$

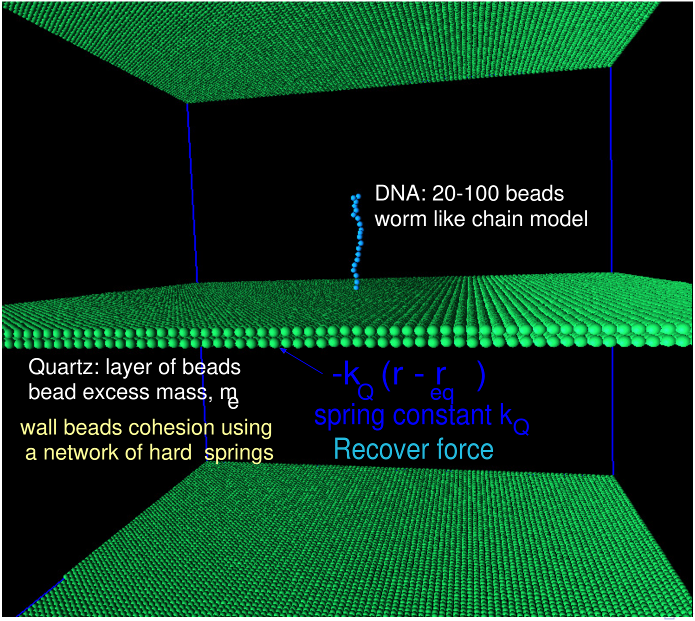
$$\text{Coupling} \quad : \quad \mathrm{J}_{\mathbf{q}_i}[\mathbf{v}] = \frac{d\mathbf{q}}{dt} = \mathbf{u}_i \text{ (no slip)}$$

Pressure tensor

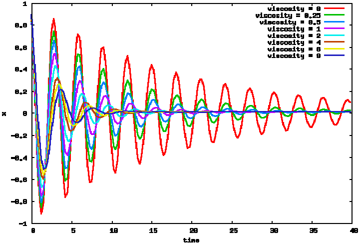
$$\mathbf{P} = \nabla p\boldsymbol{I} - \eta\nabla^{\mathrm{sym}}\mathbf{v} + \sqrt{2k_BT\eta}\,\boldsymbol{\mathcal{W}}$$

- Particle mass: $m_p = m_e + \rho\mathbb{V}$
- Particle volume $\mathbb{V} = 8h^3$ (fluid mesh-size h)
- Fluid-particle force $\boldsymbol{\lambda}_i$ (obtained from the no-slip condition, instantaneous)

Mesoscopic model
Low resolution: 2 nm


DNA: 20-100 beads
worm like chain model
Quartz: layer of beads
bead excess mass, m_e
wall beads cohesion using
a network of hard springs
$-k_Q (r - r_{eq})$
spring constant k_Q
Recover force

Relaxation upon perturbation
from equilibrium position



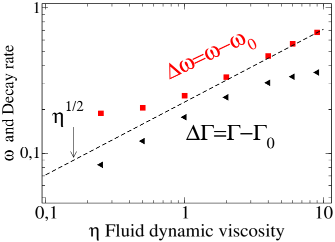
Pure fluid change in
frequency and decay
(theory)

$$x(t) = x(0)\exp(-\Gamma t)\cos(\omega t + \phi)$$

$$\omega_0 = \sqrt{k_Q/(2\,m_e)}$$

$$\Delta\omega = \omega - \omega_0 \sim \eta^{1/2}$$

Change in frequency and Decay rate



$$(u = 20,\ \phi = 3 \times 10^{-3})$$

A short movie

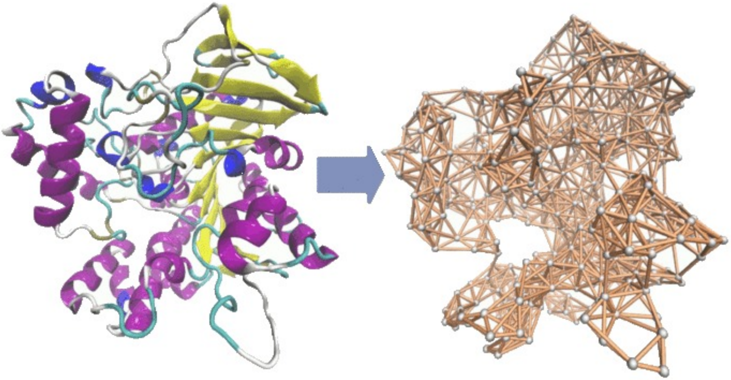
$$(u = 20,\ \phi = 3 \times 10^{-3})$$

Larger chain coverage (from another problem)

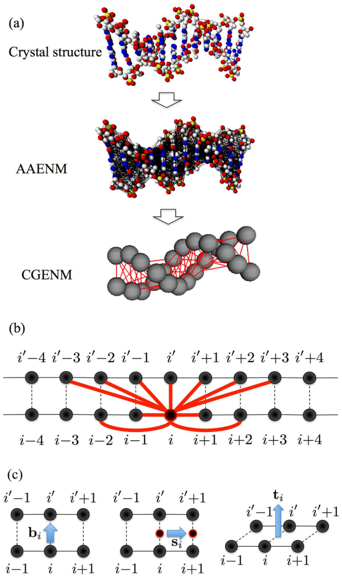
$$(u = 20,\ \phi = 3 \times 10^{-3})$$

Mesoscopic model
High resolution: 0.5 nm

Elastic Network Model for linker protein



Elastic Network Model for DNA strands



Some questions to discuss

- Coverage (decrease witht the DNA-strand lenght?)
- Boundary conditions: **No-slip or partial slip**
- Other molecules aside from DNA: vesicles ?
- Adding salts: Debye interactions with the wall

- Marc Meléndez Schofield (post-doc expert in mesoscale modeling)
- Raul Pérez Peláez (pHD, UAMMD coder)
- Another postdoc? expertise (CGMD of proteins?, Fluid dynamics?)

Scientific advisor: Pedro Tarazona Lafarga

External groups

- Pep Español: Theoretical description on energy dissipation for mesoscale descriptions
- Aleks Donev: Fluctuating hydrodynamics with constraints

Thanks !