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Bridging atomistic and continuum scales with a view to solving tribological problems

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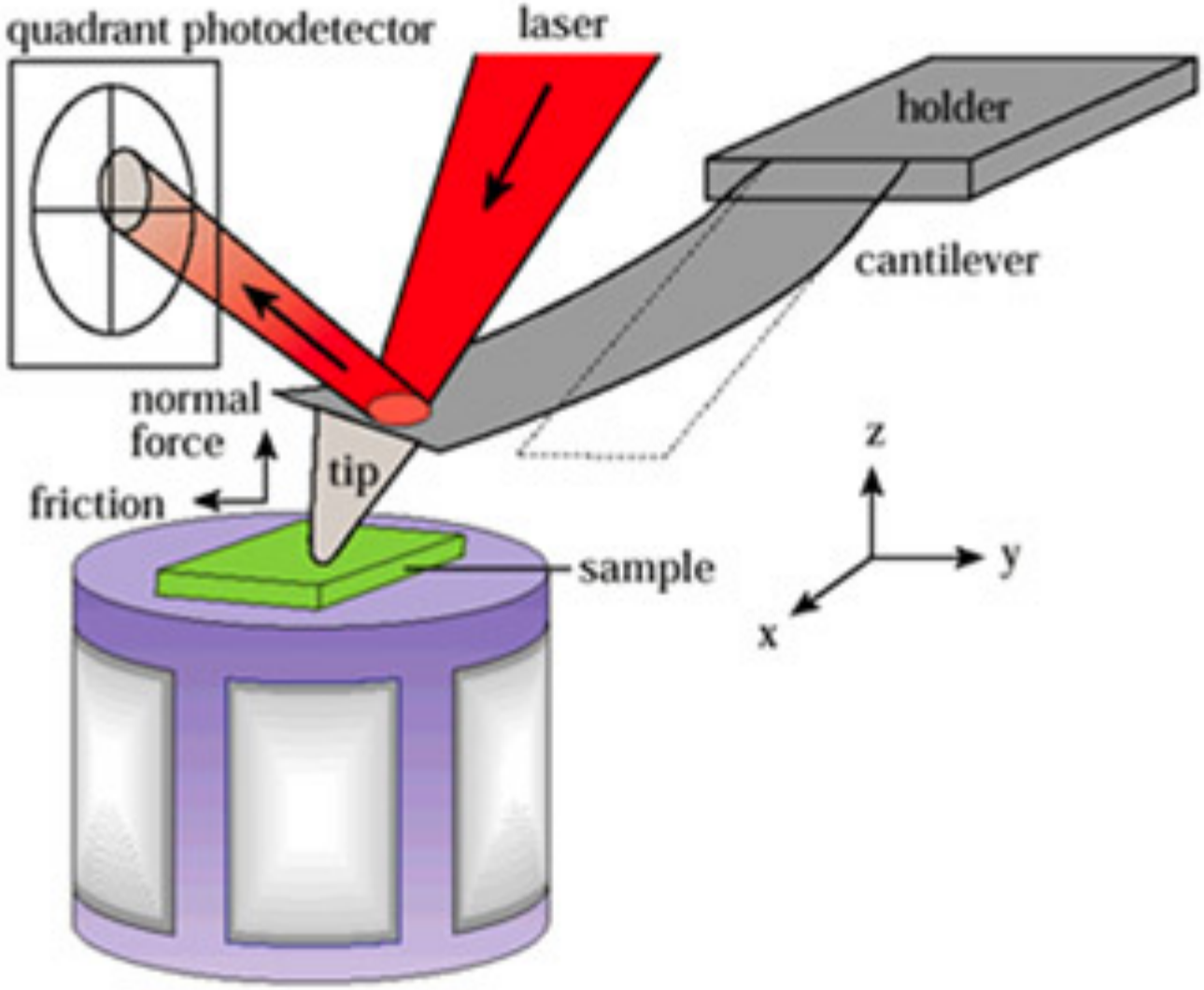
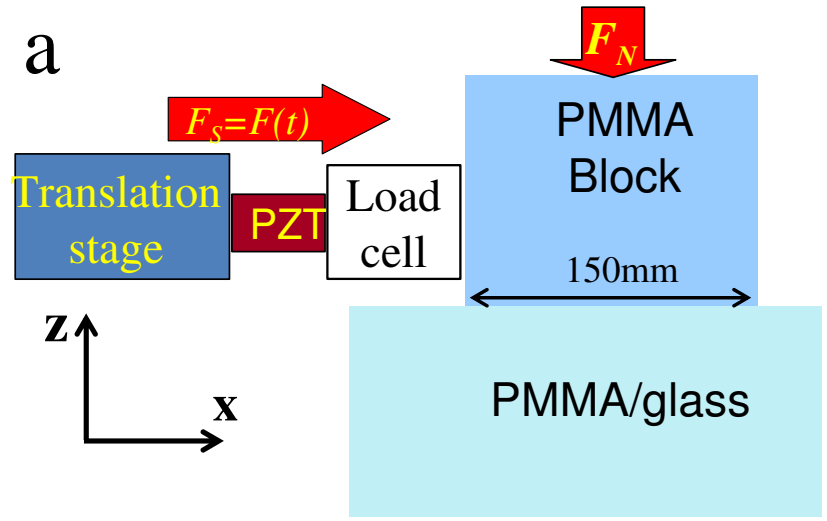
Nanotribological motivation

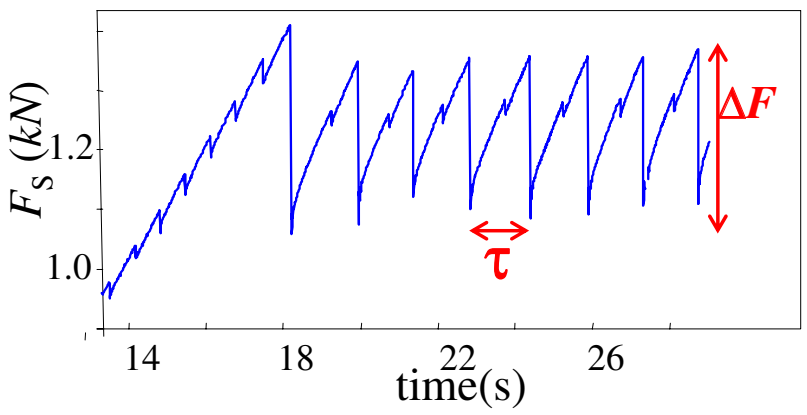
A cartoon diagram of the AFM

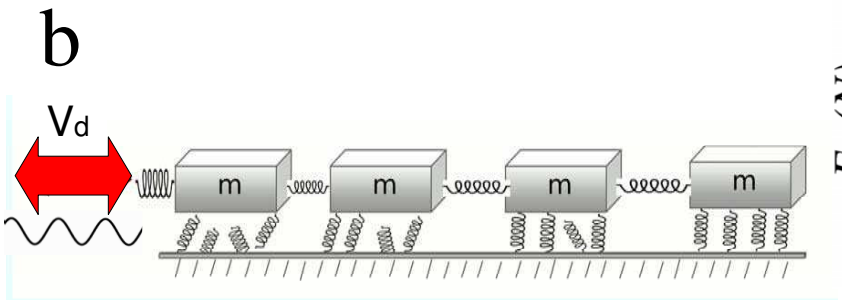


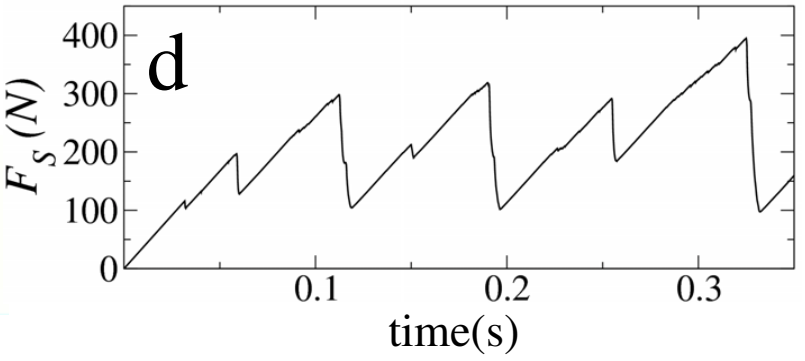
Nanotribological motivation

A large test piece (from Capozza et al. 2011)



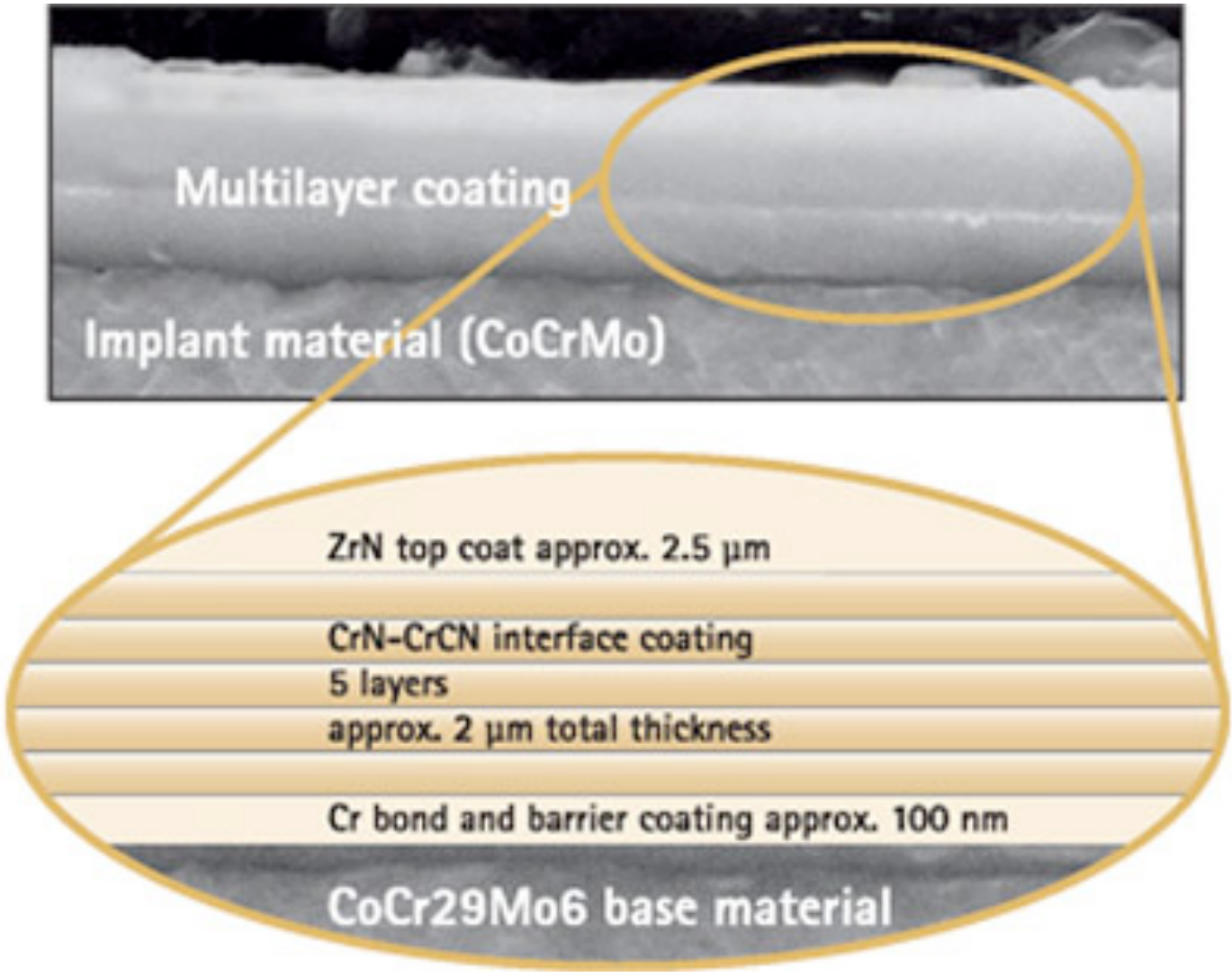






Nanotribological motivation

A typical surface coating



Straightforward Newtonian MD

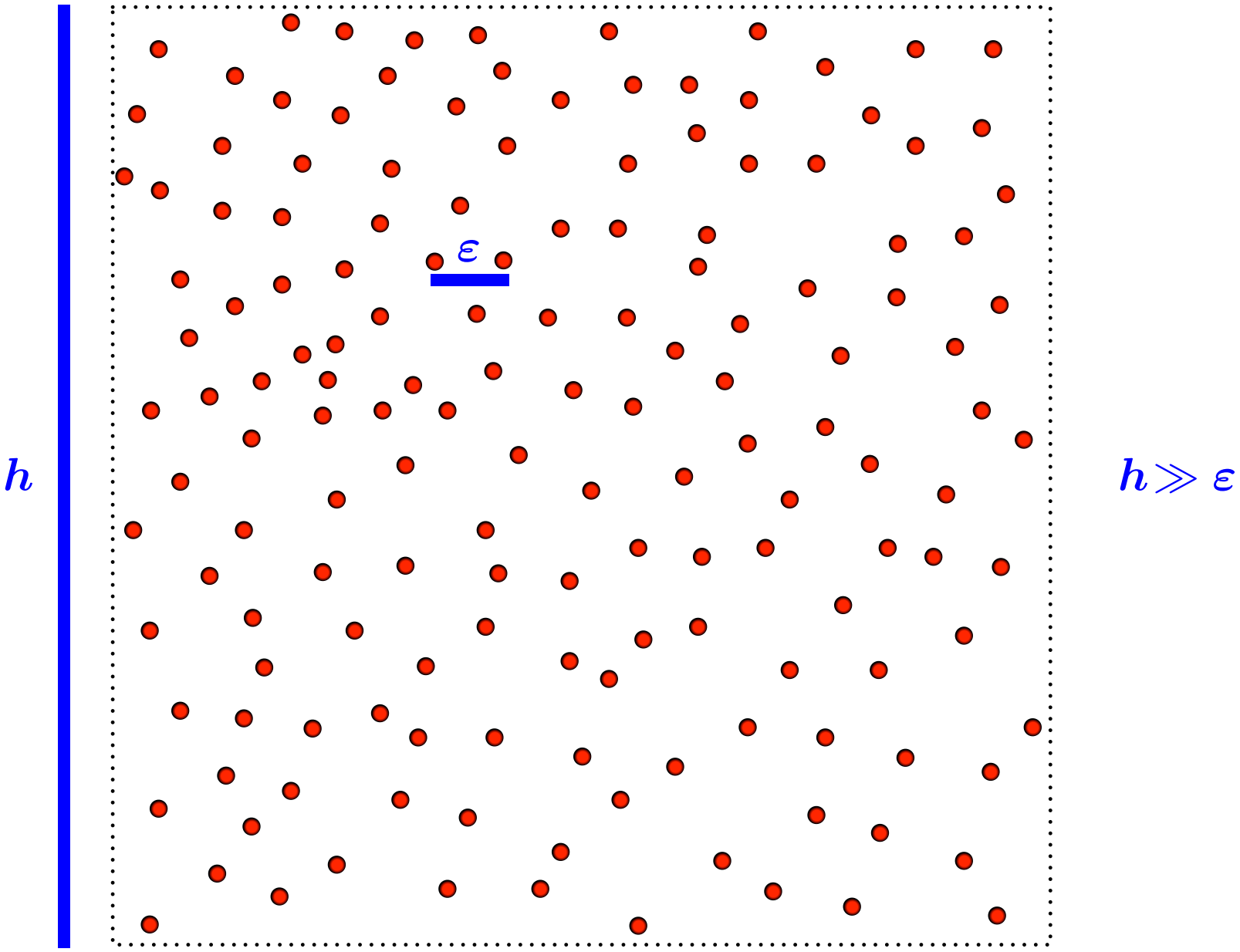
$$\mathscr{L} : (\mathfrak{x}, \dot{\mathfrak{x}}) \mapsto \tfrac{1}{2} \sum_{i=1}^{N} m_i |\dot{\boldsymbol{x}}_i|^2 - \mathscr{V}(\mathfrak{x})$$

$$\mathfrak{x} := (\boldsymbol{x}_1, \ldots, \boldsymbol{x}_i, \ldots, \boldsymbol{x}_N)$$

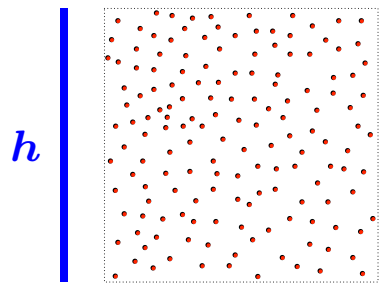
$$\mathscr{V}(\mathfrak{x}) = \sum_{i=1}^{N} \mathscr{V}_1{}^{i}(\boldsymbol{x}_i) + \mathscr{V}_>(\mathfrak{x})$$

$$\mathscr{V}_>(\mathfrak{x}^{\circlearrowleft}) = \mathscr{V}_>(\mathfrak{x})$$

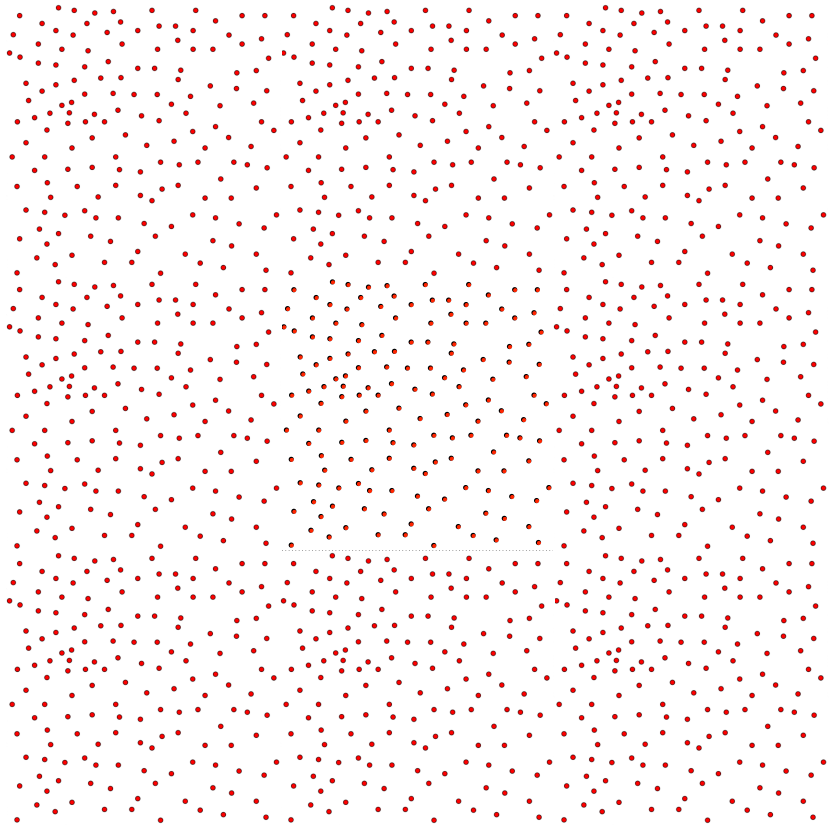
MD cell: a cartoon

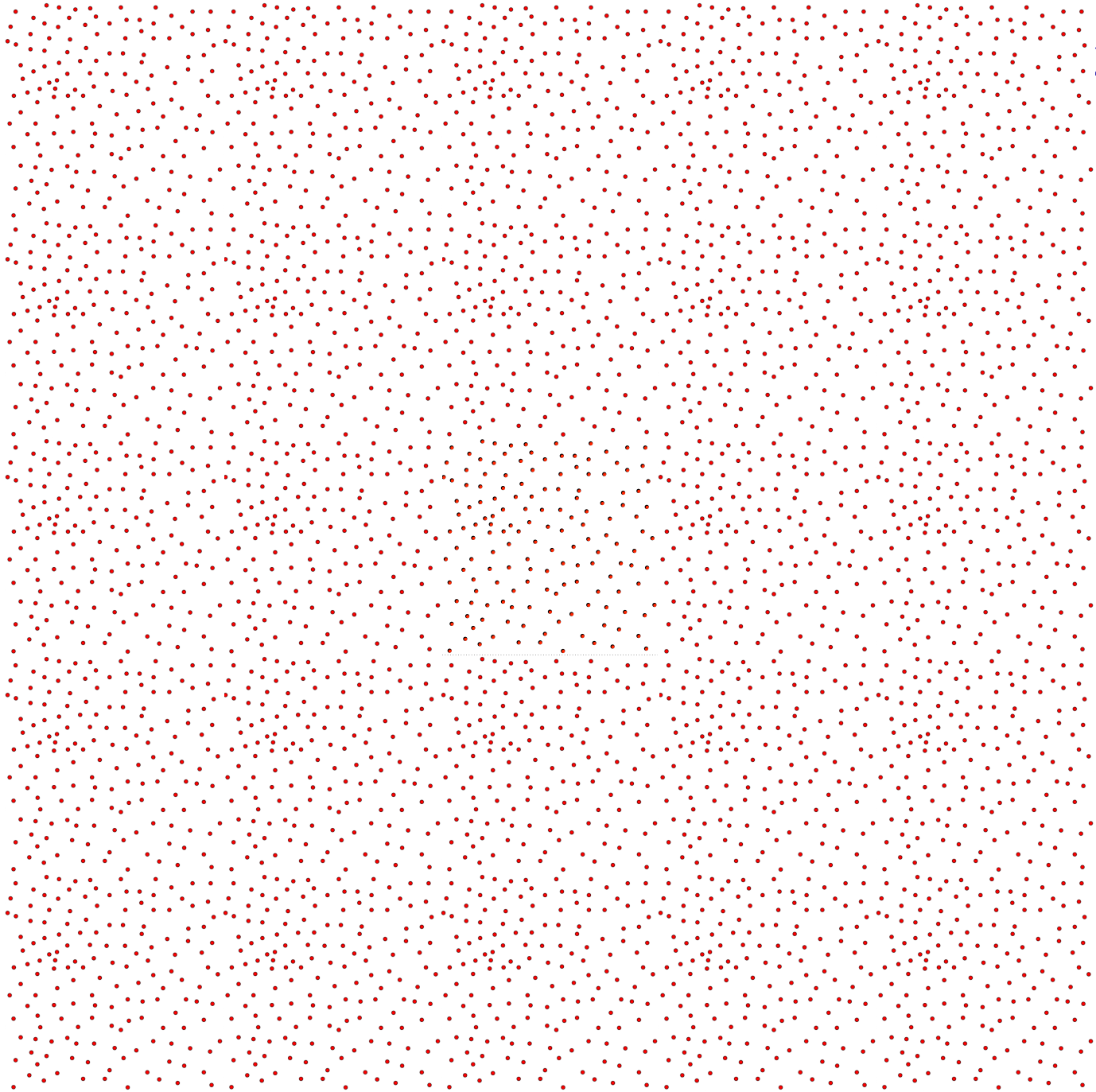


The periodicity trick



The periodicity trick





Drawbacks of straightforward MD

- Number of particles, total energy, and volume (N, E, V) stay constant over time ($\Longrightarrow$ *microcanonical ensemble*) —as remarked in 1980 by H.C. Andersen.
- Also the shape of the MD cell does not change —as pointed out by M. Parrinello & A. Rahman.
- Collective degrees of freedom enabling coarse-graining are lacking—my own focus today.

APR seminal papers

- H.C. Andersen, Molecular dynamics simulations at constant pressure and/or temperature. *Journal of Chemical Physics*, **72**(4):2384–2393, 1980.
- M. Parrinello and A. Rahman, Crystal structure and pair potentials: A molecular-dynamics study. *Physical Review Letters*, **45**(14):1196–1199, 1980.
- M. Parrinello and A. Rahman, Polymorphic transitions in single crystals: A new molecular dynamics method. *Journal of Applied Physics*, **52**(12):7182–7190, 1981.

APR cure

(rephrased and slightly extended)

$$\tau \mapsto (\mathbf{h}_1(\tau), \ldots, \mathbf{h}_\ell(\tau), \ldots, \mathbf{h}_n(\tau))$$

$$\mathbf{h}_\ell(\tau) = \mathbf{F}(\tau)\, \mathbf{e}_\ell \quad (1 \leq \ell \leq n)$$

$$\boldsymbol{x}_i(\tau) = \boldsymbol{p}(\tau) + \mathbf{r}_i(\tau) = \boldsymbol{p}(\tau) + \mathbf{F}(\tau)\, \mathbf{s}_i(\tau)$$

- $\boldsymbol{p}$ ... cell mass centre
- $\mathfrak{r} := (\mathbf{r}_1, \ldots, \mathbf{r}_i, \ldots, \mathbf{r}_N)$ ... radius vectors (w.r.t. $\boldsymbol{p}$)
- $\mathbf{F}$ ... cell deformation
- $\mathfrak{s} := (\mathbf{s}_1, \ldots, \mathbf{s}_i, \ldots, \mathbf{s}_N)$ ... scaled radius vectors

APR cure

(discussion)

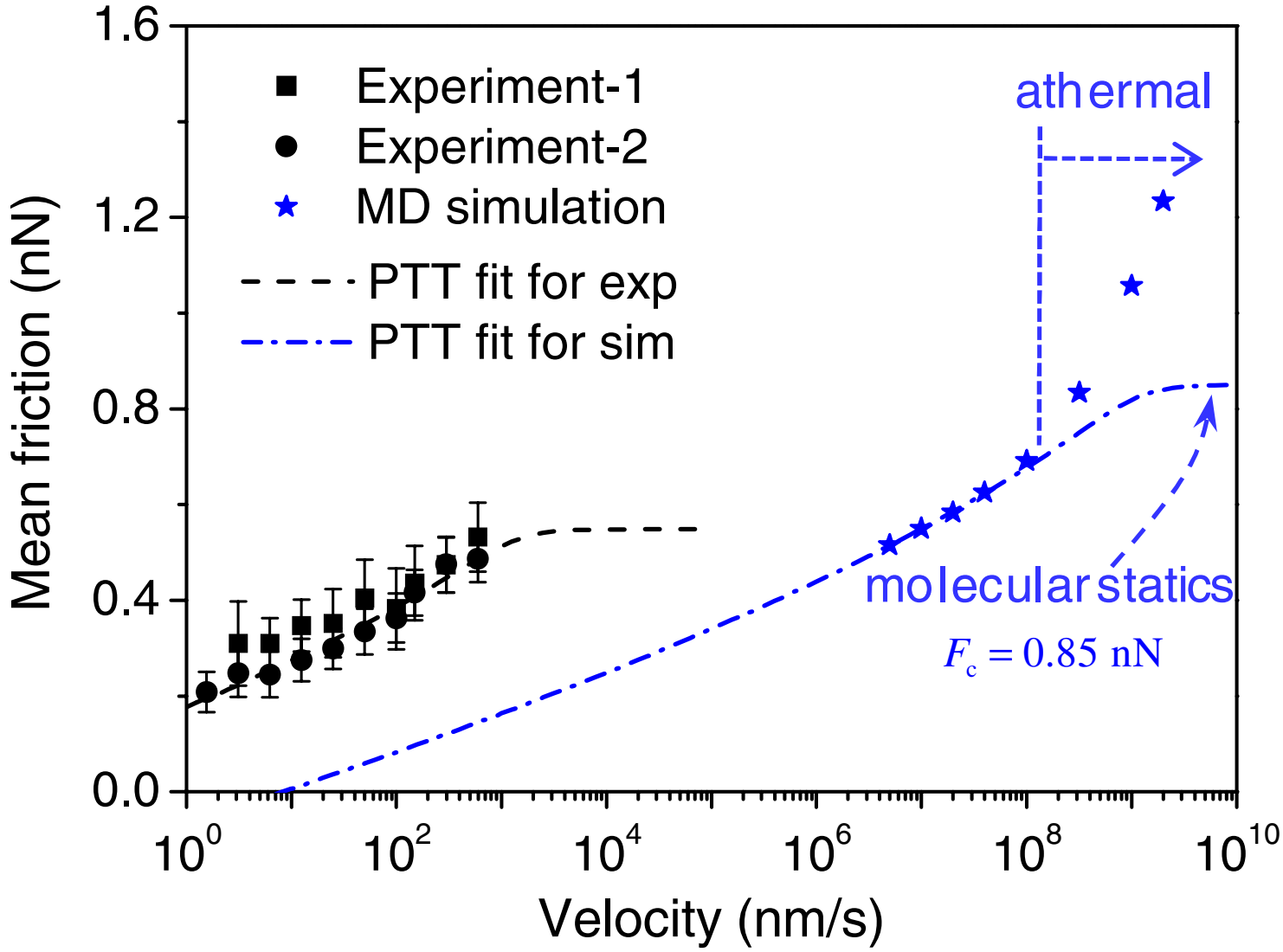
(a) $\mathbf{F}(\tau) = \mathbf{F}(\tau_0)$ ... pre-Andersen MD

(b) $\mathfrak{s}(\tau) = \mathfrak{s}(\tau_0)$ ... Cauchy-Born rule

(c) $\mathfrak{s}(\tau) = \mathrm{Relax}\big(\mathbf{F}(\tau); \mathfrak{s}(\tau_0)\big)$ ... Molecular Statics

Molecular Statics vs. Molecular Dynamics

(from Li et al. 2011)



APR recipe:

ad hoc extended Lagrangian

$$\mathscr{L}_{APR} : (\mathfrak{s}, \dot{\mathfrak{s}}; \mathbf{F}, \dot{\mathbf{F}}) \mapsto$$

$$\frac{1}{2} \sum_{i=1}^{N} m_i \, \dot{\mathbf{s}}_i \cdot (\mathbf{C} \, \dot{\mathbf{s}}_i) + \frac{1}{2} \, \mathbf{M} \cdot (\dot{\mathbf{F}}^\top \dot{\mathbf{F}}) - \mathscr{V}_{\text{near}}(\mathbf{F}\mathfrak{s}) + V_0 \mathbf{S} \cdot \mathbf{F}$$

- $\mathbf{C} := \mathbf{F}^\top \mathbf{F}$ ... cell metric distortion
- $\mathbf{M} \, (= W \, \mathbf{I})$ ... scaled cell inertia tensor (given)
- $V_0 \mathbf{S}$ ... prototype volume $\times$ applied stress (given)

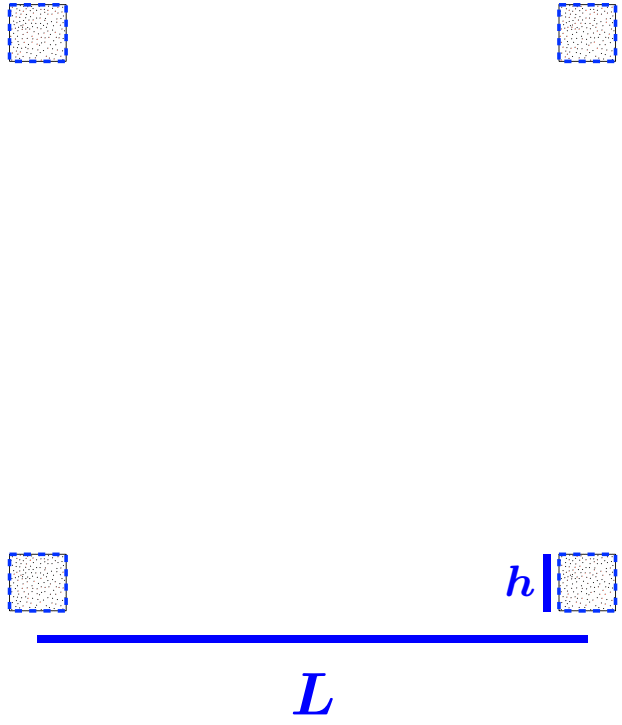
APR recipe:

equations of motion

$$m_i\big(\ddot{\mathbf{s}}_i + \mathbf{C}^{-1}\dot{\mathbf{C}}\,\dot{\mathbf{s}}_i\big) = -\mathbf{F}^{-1}\,D_i\mathscr{V}_{\text{near}}\big|_{\mathbf{F}\mathfrak{s}}$$

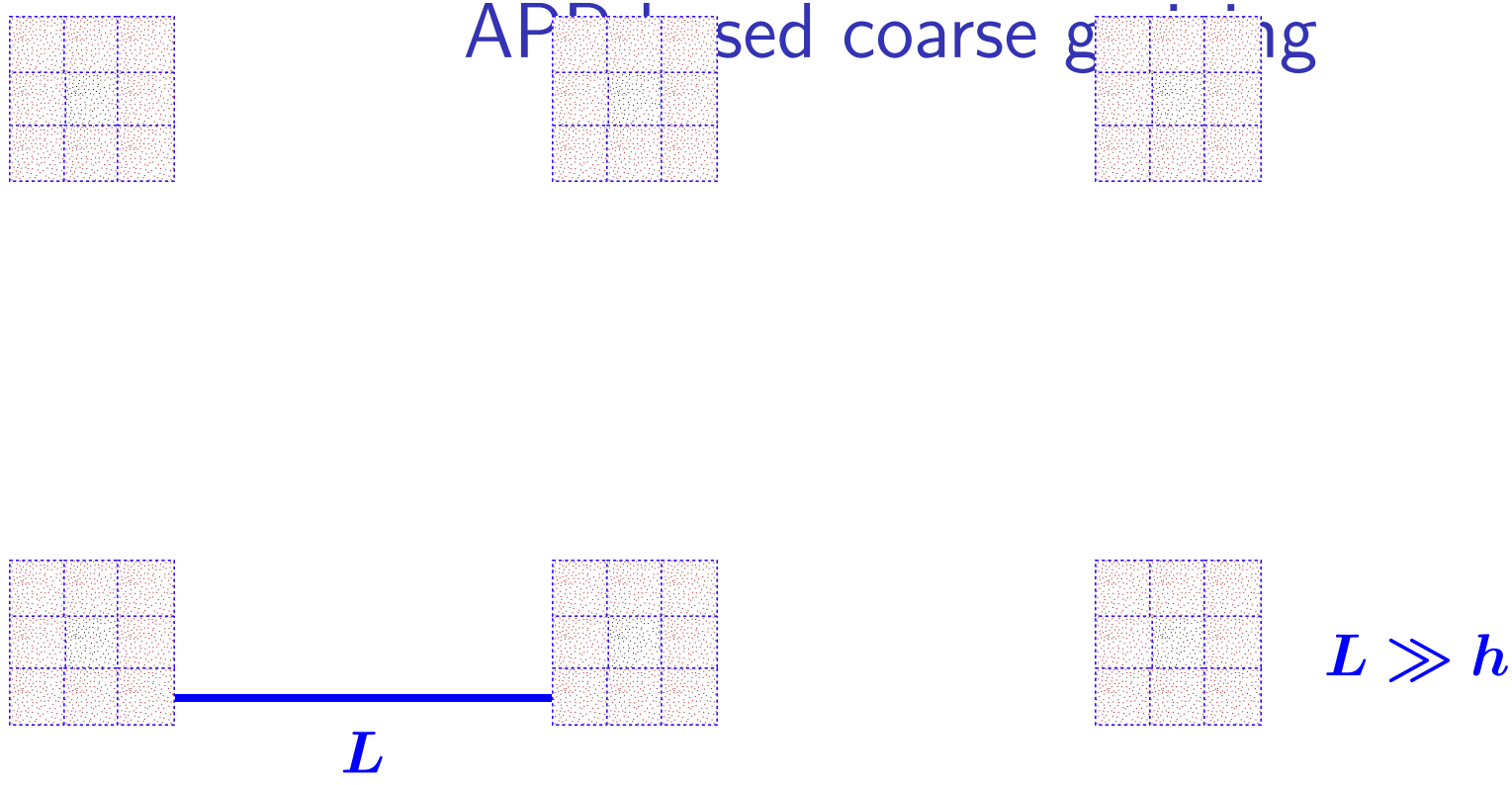
$$\mathbf{M}\,\ddot{\mathbf{F}} = V_0\mathbf{S} - \sum_{i=1}^{N}\big(\mathbf{s}_i \otimes D_i\mathscr{V}_{\text{near}}\big|_{\mathbf{F}\mathfrak{s}} - \mathbf{F}\big(m_i\,\dot{\mathbf{s}}_i \otimes \dot{\mathbf{s}}_i\big)\big)$$

APR-based coarse graining



$L \gg h$

APD-based coarse graining



Interacting APR-like cells I:

the surrounding medium as a *hard* loading device

- Associate an APR-like cell with each body element $\mathsf{T}_b\mathscr{B}$.
- ▷ Fix a prototype field $\mathbf{P}_0$, and assume the gross motion $\boldsymbol{p}$ to be known over body-time $\mathscr{B} \times \mathscr{T}$.
- Compute the gross deformation $\mathbf{F} = (\nabla \boldsymbol{p})\mathbf{P}_0^{-1}$.
- For each b-cell, compute the reactive Piola stress $\mathbf{S}^b$ over time, taking $\mathbf{F}^b = \mathbf{F}(b, \cdot\,)$ as the enforced cell deformation.
- Construct a slowly varying stress field $\widetilde{\mathbf{S}}$ over the medium via $\mathbf{S}(b, \cdot\,) = \mathbf{S}^b$ and $\widetilde{\mathbf{S}} := \mathrm{slw}\,\mathbf{S}$.
- Enforce balance: $\mathrm{Div}\,\widetilde{\mathbf{S}} = \varrho_0\,\ddot{\boldsymbol{p}}$.
- ◁ Balance pinpoints the gross motion $\boldsymbol{p}$ (to within a rigid motion).

Interacting APR-like cells II:

the surrounding medium as a *soft* loading device

- Associate an APR-like cell with each body element $\mathsf{T}_b\mathscr{B}$.
- ▷ Assume the stress field $\mathbf{T} \in \mathrm{Slw}$ to be known over $\mathscr{B} \times \mathscr{T}$.
- For each $b \in \mathscr{B}$, compute the b-cell deformation $\mathbf{F}^b$ over time, taking $\mathbf{T}^b := \mathbf{T}(b, \cdot\,)$ as the applied Cauchy stress.
- Construct a slowly varying deformation field $\widetilde{\mathbf{F}}$ over the medium via $\mathbf{F}(b, \cdot\,) = \mathbf{F}^b$ and $\widetilde{\mathbf{F}} := \mathrm{slw}\,\mathbf{F}$.
- Compute the corresponding metric: $\widetilde{\mathbf{C}} := \widetilde{\mathbf{F}}^{\top}\widetilde{\mathbf{F}}$.
- ○ Enforce compatibility over $\mathscr{B}$: $\mathrm{Riem}(\widetilde{\mathbf{C}}) = \mathbf{0}$.
- Compute the rotation field $\mathbf{R}^{\times}$ and the gross motion $\boldsymbol{p}$ such that $\nabla\boldsymbol{p} = \mathbf{R}^{\times}\widetilde{\mathbf{F}}\,\mathbf{P}_0$ (existence ensured by ○).
- Enforce balance: $\mathrm{Div}\,\mathbf{S} = \varrho_0\,\ddot{\boldsymbol{p}}$.
- ◁ Compatibility & balance pinpoint the stress field $\mathbf{T}$.

A quote from Parrinello & Rahman 1981

Whether such a Lagrangian is derivable from first principles is a question for further study.

The APR functional revisited

- Basic Lagrangian ... $\mathscr{L}(\boldsymbol{x}, \dot{\boldsymbol{x}}) = \mathscr{K}(\dot{\boldsymbol{x}}) - \mathscr{V}(\boldsymbol{x})$
- APR-like assumption ... $\boldsymbol{x} = \boldsymbol{p} + \mathbf{r} = \boldsymbol{p} + \mathbf{F}\,\mathbf{s}$

  Leibniz rule $\Rightarrow$ $\dot{\boldsymbol{x}} = \dot{\boldsymbol{p}} + (\dot{\mathbf{F}}\,\mathbf{s} + \mathbf{F}\,\dot{\mathbf{s}}) = (\dot{\boldsymbol{p}} + \mathbf{L}\,\mathbf{r}) + \mathbf{F}\,\dot{\mathbf{s}}$
- $\mathbf{L} := \dot{\mathbf{F}}\,\mathbf{F}^{-1}$ ... cell velocity gradient: $\mathbf{W} := \mathrm{skw}\,\mathbf{L}, \mathbf{D} := \mathrm{sym}\,\mathbf{L}$
- $\dot{\boldsymbol{p}} + \mathbf{L}\,\mathbf{r}$ ... entrainment velocity; $\mathbf{F}\,\dot{\mathbf{s}}$ ... streaming velocity

$\Rightarrow$ $\dot{\boldsymbol{x}} = \big(\dot{\boldsymbol{p}} + \mathbf{W}\,\mathbf{r}\big) + \big(\mathbf{D}\,\mathbf{r} + \mathbf{F}\,\dot{\mathbf{s}}\big)$

The APR functional revisited

$$\mathscr{L}_{\square} : (\mathbf{s}, \dot{\mathbf{s}}; \boldsymbol{p}, \dot{\boldsymbol{p}}; \mathbf{F}, \dot{\mathbf{F}}) \mapsto$$

$$\tfrac{1}{2} \sum_{i \in \mathfrak{S}} m_i \, \dot{\mathbf{s}}_i \cdot (\mathbf{C} \, \dot{\mathbf{s}}_i) + \tfrac{1}{2} \left(\sum_{i \in \mathfrak{S}} m_i \, \mathbf{s}_i \otimes \mathbf{s}_i \right) \cdot (\dot{\mathbf{F}}^{\top} \dot{\mathbf{F}})$$

$$+ \tfrac{1}{2} \left(\sum_{i \in \mathfrak{S}} m_i \right) |\dot{\boldsymbol{p}}|^2 + \left(\sum_{i \in \mathfrak{S}} m_i \, \dot{\mathbf{s}}_i \otimes \mathbf{s}_i \right) \cdot (\dot{\mathbf{F}}^{\top} \mathbf{F})$$

$$+ \tfrac{1}{2} \left(\sum_{i \in \mathfrak{S}} m_i (\mathbf{F} \, \mathbf{s}_i)^{\cdot} \right) \cdot \dot{\boldsymbol{p}} - \mathscr{V}_{\text{near}}(\mathbf{F}\mathbf{s}) + V_0\big(\mathbf{S} \cdot \mathbf{F} + \mathbf{b} \cdot (\boldsymbol{p} - \boldsymbol{o})\big)$$

Time-scale separation requirements

- $\mathbf{M} := \sum_{i \in \mathfrak{S}} m_i \, \mathbf{s}_i \otimes \mathbf{s}_i$ ... scaled cell inertia tensor
- $\dot{\mathbf{M}} = \mathbf{0} \quad \Rightarrow \quad \sum_{i \in \mathfrak{S}} m_i \, \dot{\mathbf{s}}_i \otimes \mathbf{s}_i \in \mathrm{Skw}$
- $\mathrm{skw}(\dot{\mathbf{F}}^{\top}\mathbf{F}) = \mathbf{0} \quad \Leftrightarrow \quad \mathrm{skw}(\dot{\mathbf{F}}\mathbf{F}^{-1}) = \mathrm{skw}\,\mathbf{L} = \mathbf{W} = \mathbf{0}$
- $\dot{\boldsymbol{p}} = \mathbf{0}$

Time-scale separation requirements

- The APR-like Lagrangian reproduces the Newtonian dynamics of the *tensostatted* particle system iff:
- The applied Cauchy stress is slowly varying: $\dot{\mathbf{T}} \simeq \mathbf{0}$.
- The scaled inertia tensor is slowly varying: $\dot{\mathbf{M}} \simeq \mathbf{0}$.
- The rigid component of the cell motion is slow, i.e.,
  - the cell mass centre moves slowly: $\dot{\boldsymbol{p}} \simeq \mathbf{0}$;
  - the cell spin is small: $\mathbf{W} = \mathrm{skw}(\dot{\mathbf{F}}\mathbf{F}^{-1}) \simeq \mathbf{0}$.