Accelerating a multiscale continuum-particle fluid dynamics model with on-the-fly machine learning

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Micro and Nano Flows for Engineering

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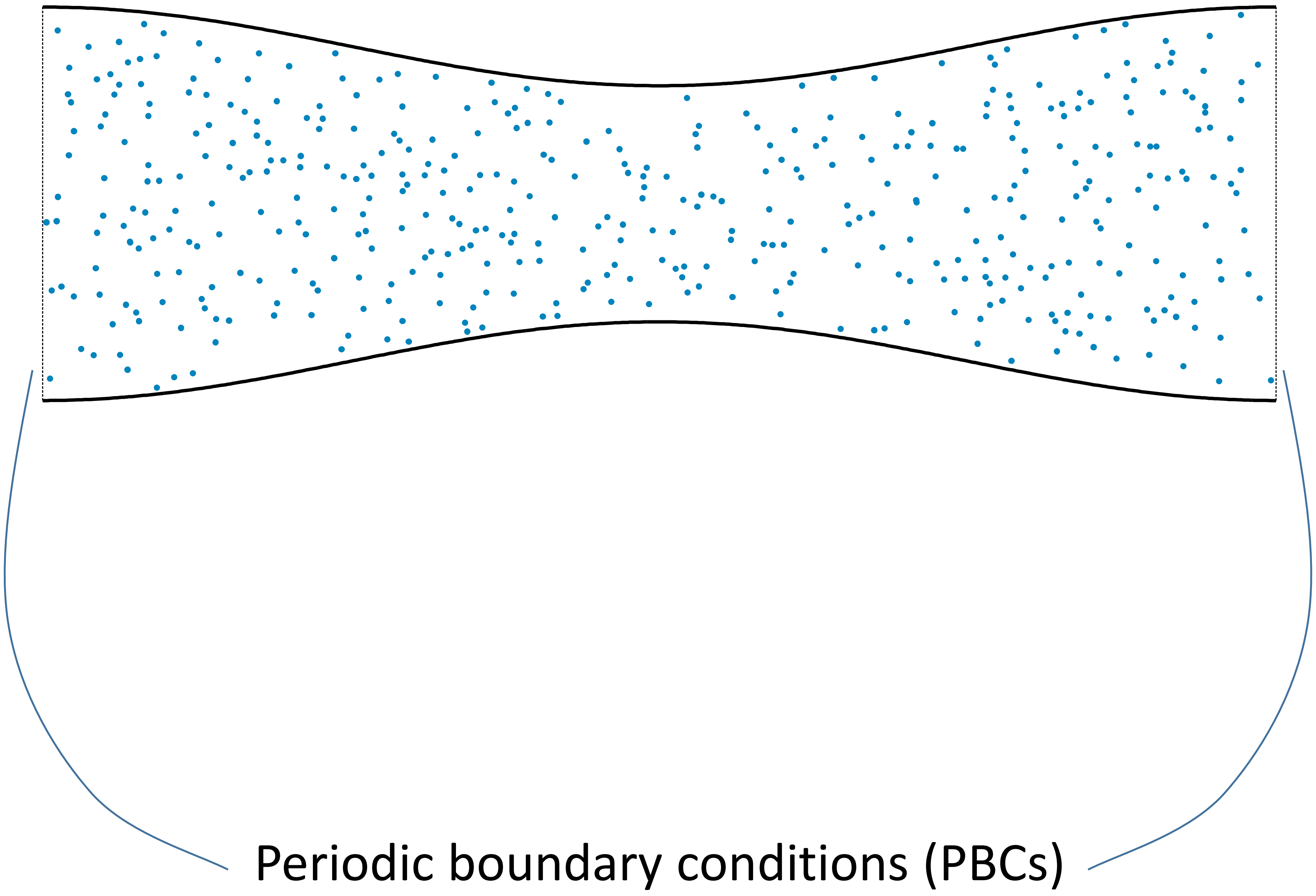
The problem with hybrid methods…

…too many similar and repetitious simulations.

Consider a converging-diverging nanochannel:



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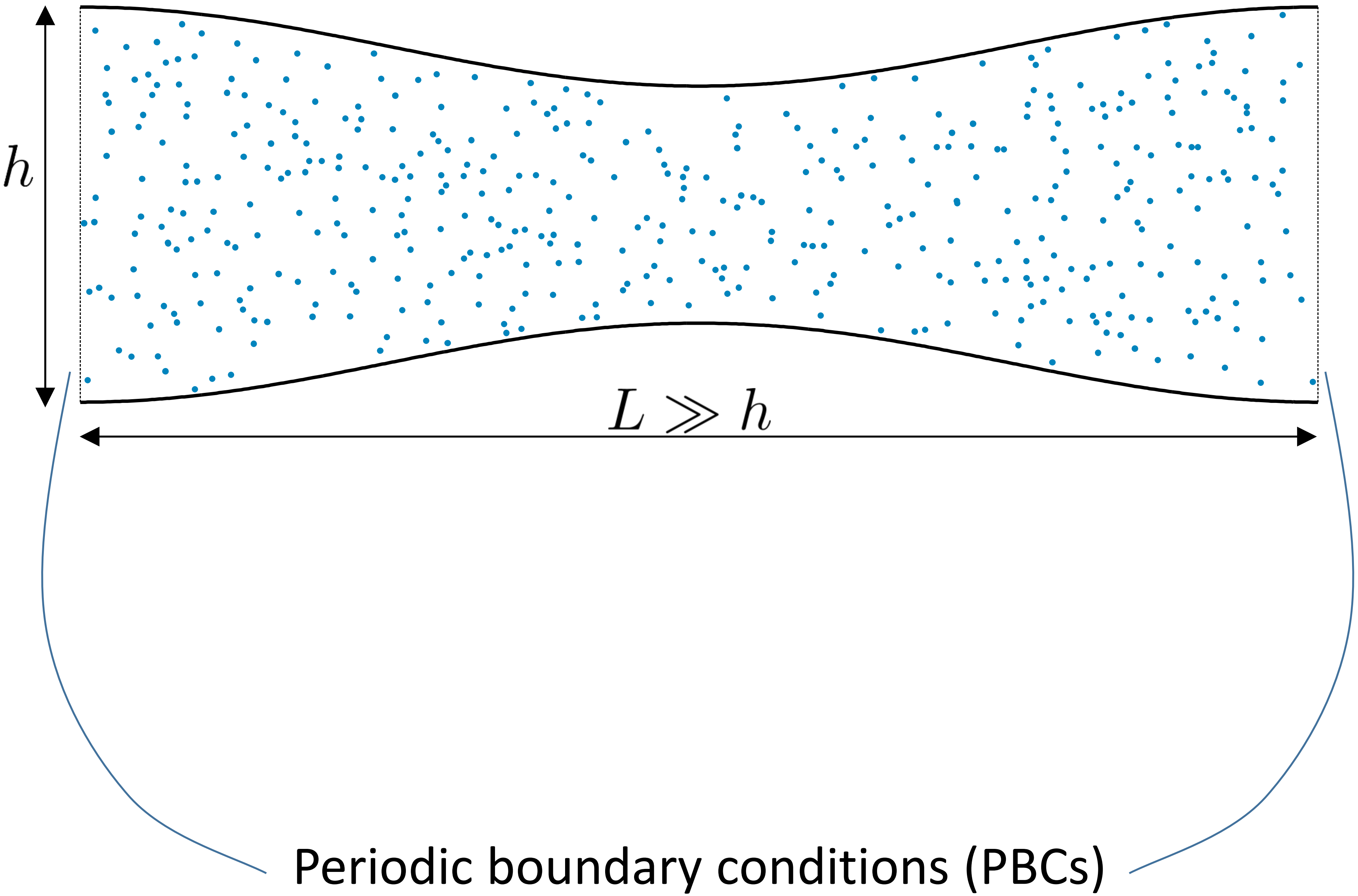
- Channel height



The problem with hybrid methods…

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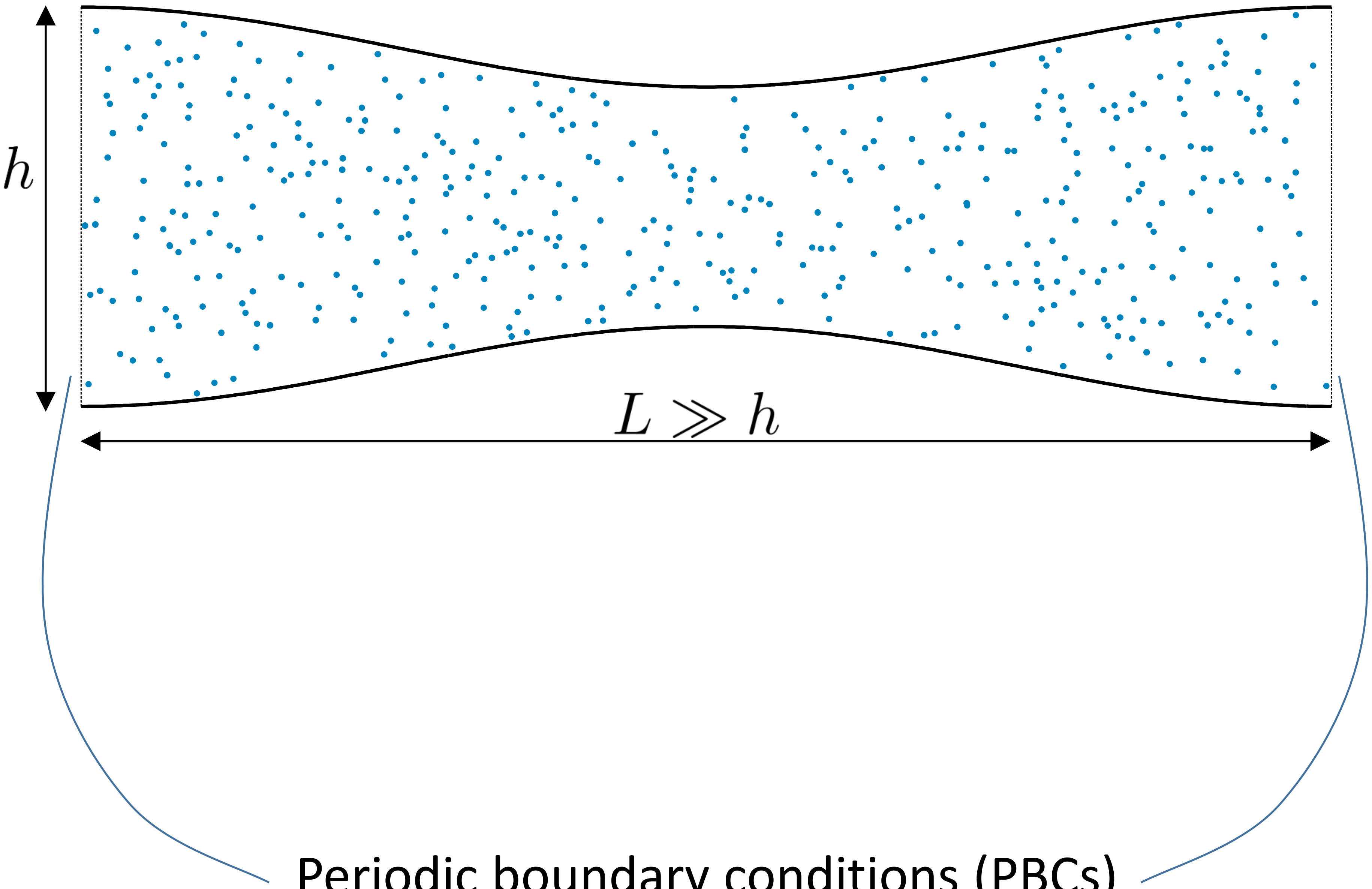
Consider a converging-diverging nanochannel:

- Channel height
- Density



The problem with hybrid methods...

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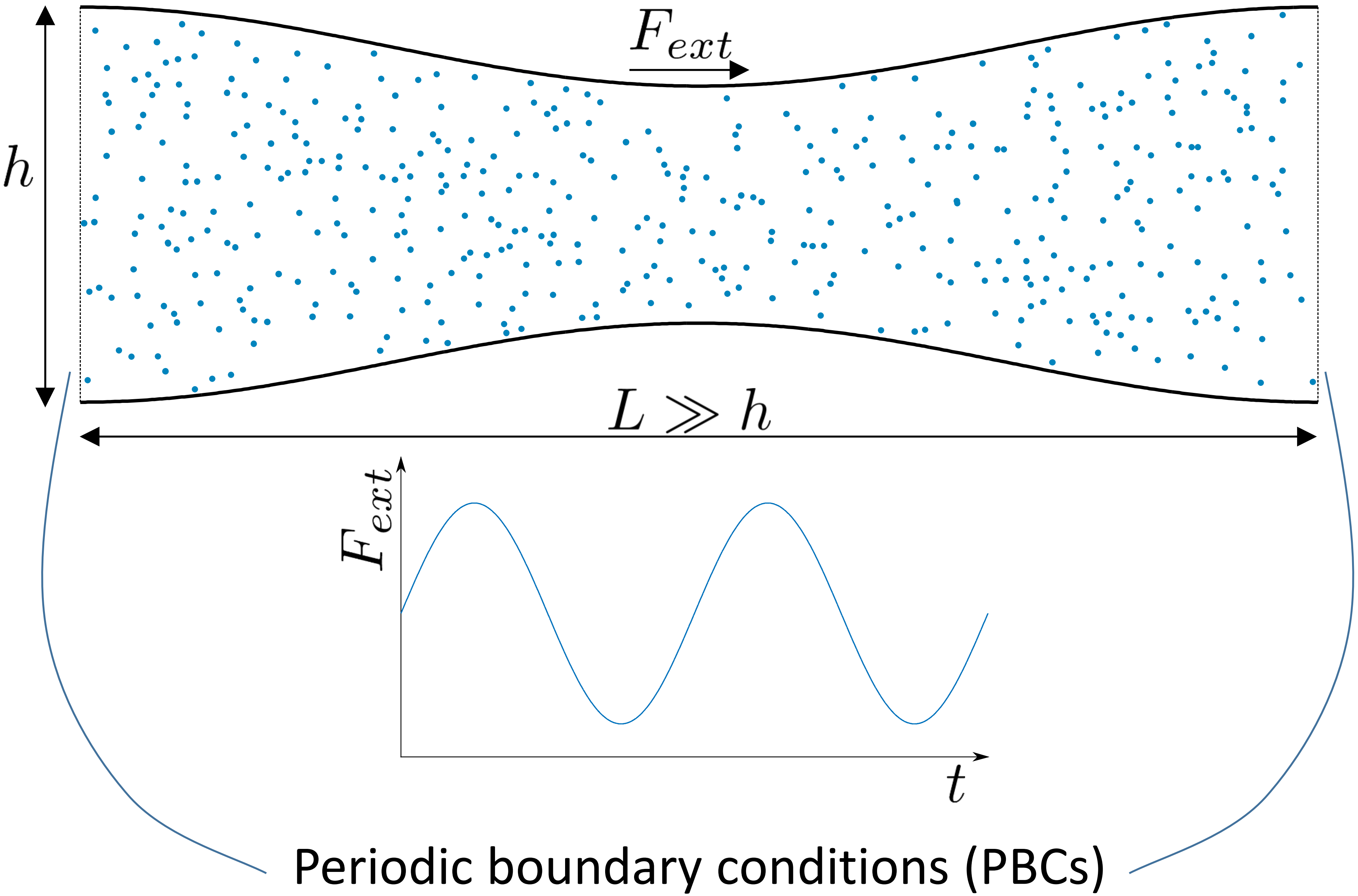
Consider a converging-diverging nanochannel:

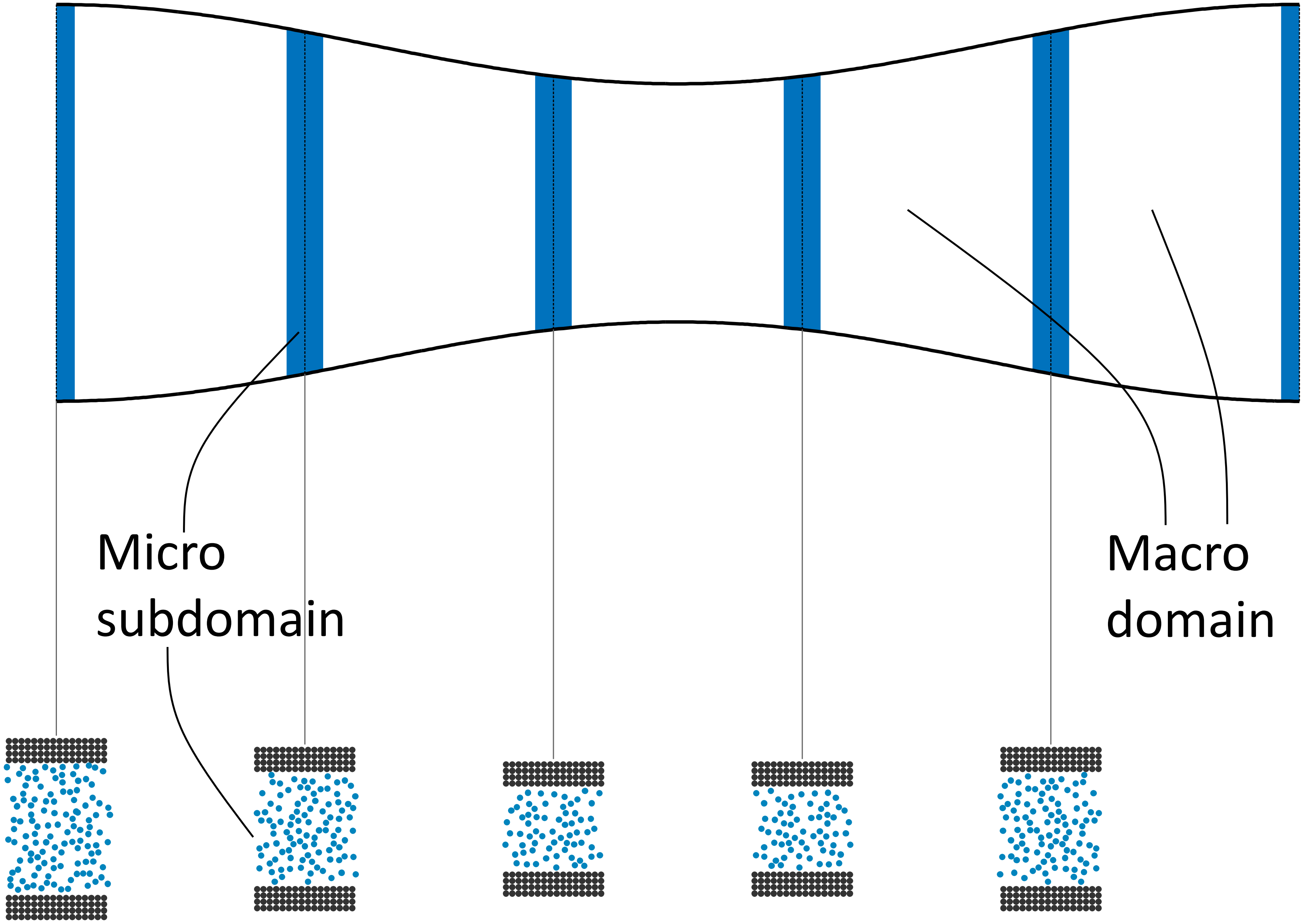
- Channel height
- Density
- Forcing



Hybrid method

We split the macro domain into micro subdomains.

These individual periodic subdomains are simulated using molecular dynamics (MD).



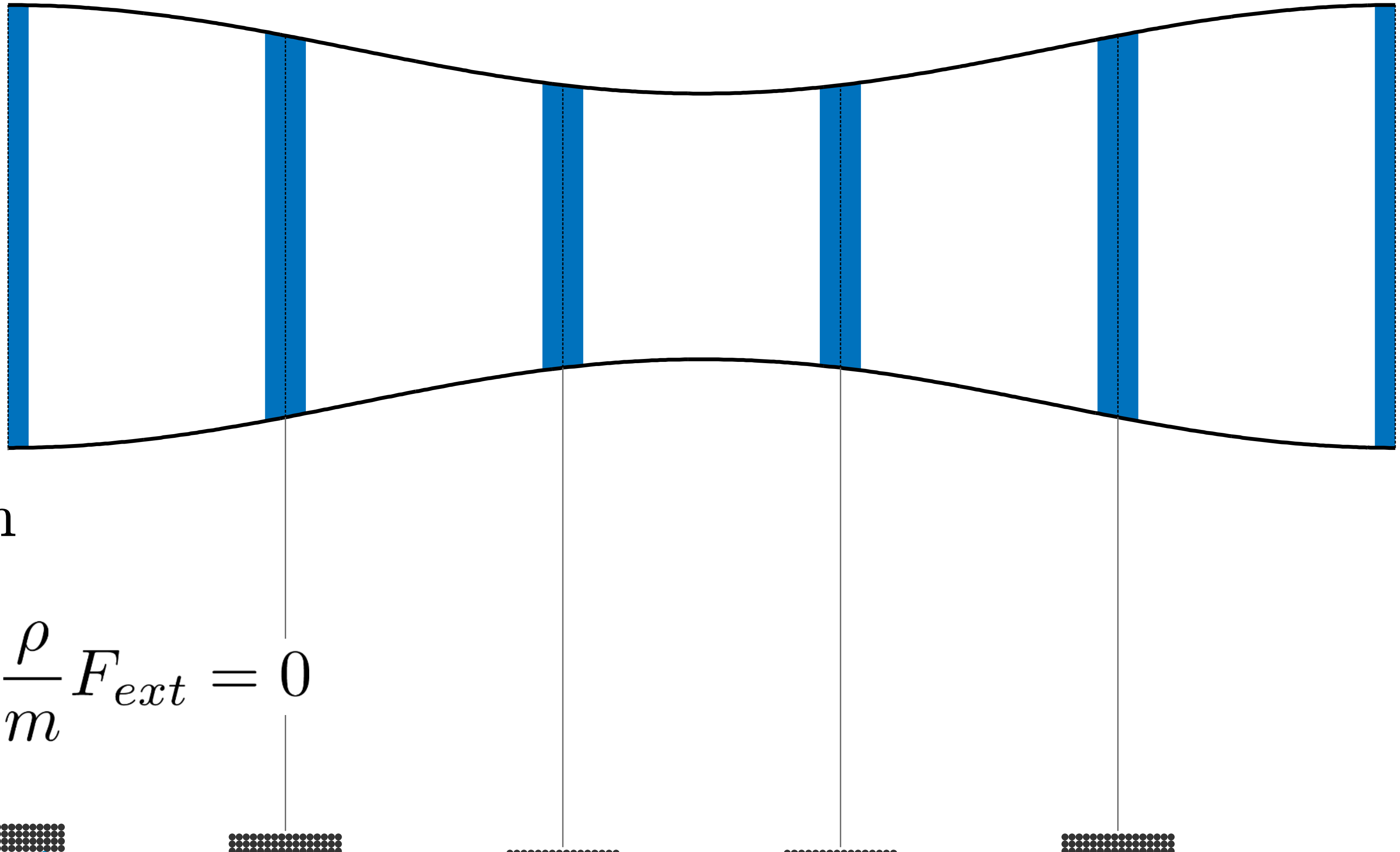
Hybrid method – macro model

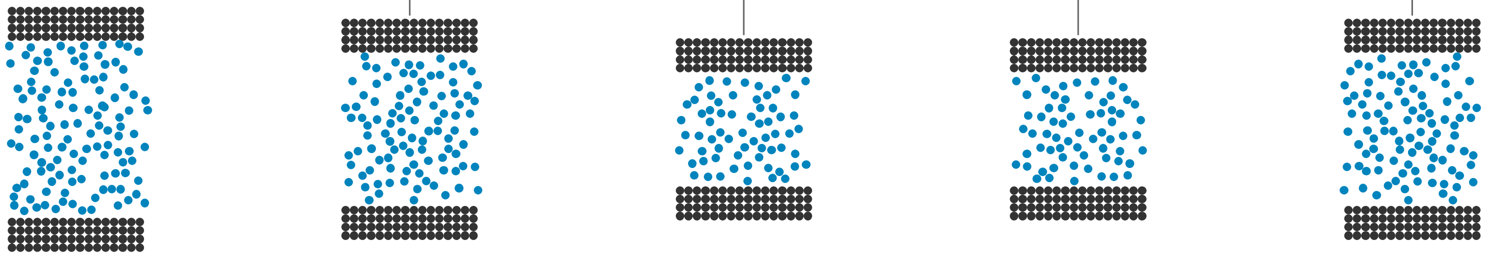
Mass conservation

$$\frac{\partial \rho}{\partial t} + \frac{1}{A}\frac{\partial q}{\partial s} = 0$$

Momentum conservation

$$-\frac{\partial p}{\partial s} + \frac{\partial \tau_{sy}}{\partial y} + \frac{\partial \tau_{sz}}{\partial z} + \frac{\rho}{m}F_{ext} = 0$$



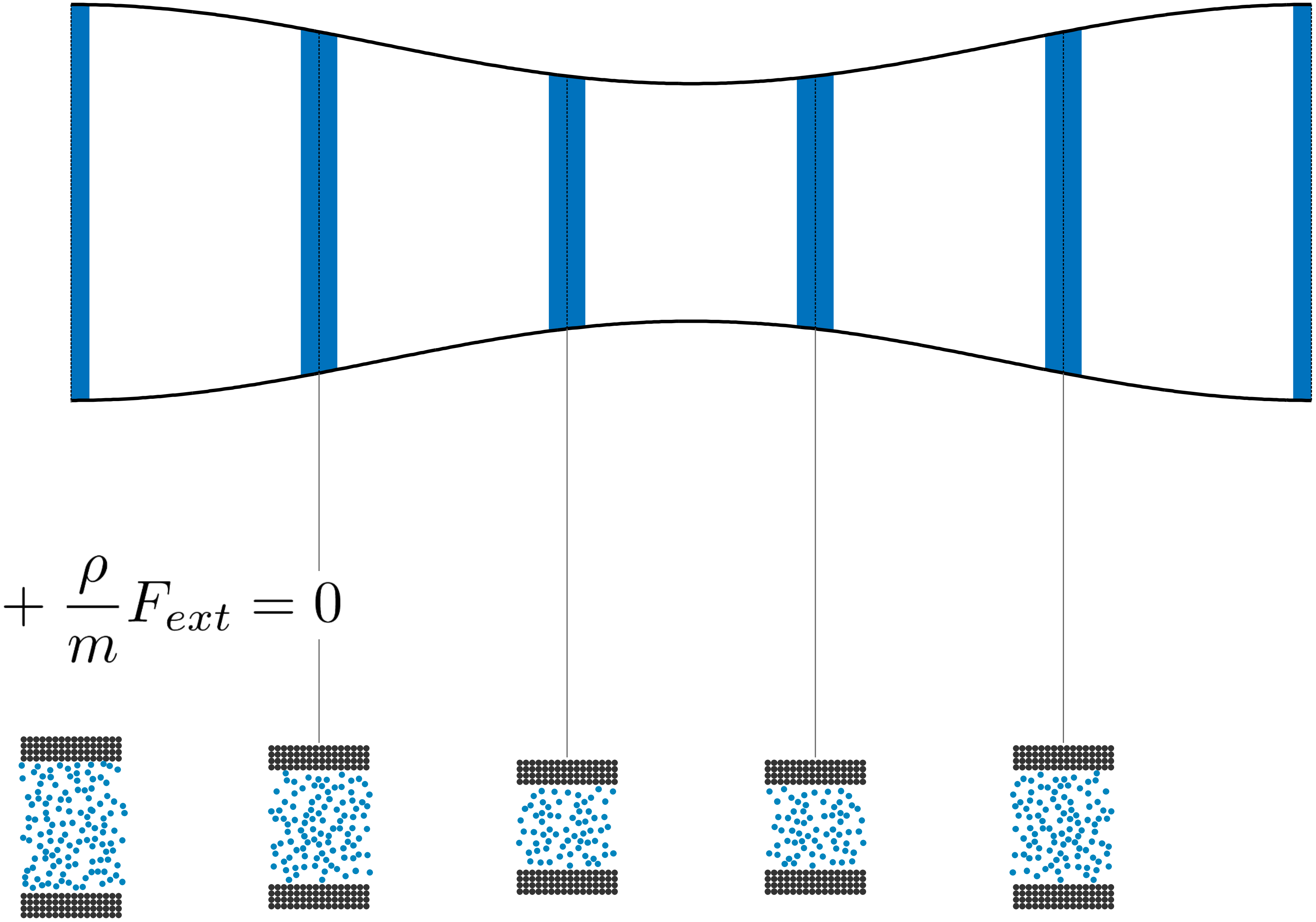


Hybrid method – micro model

MD subdomain simulations conserve mass.

MD cannot support a pressure gradient.

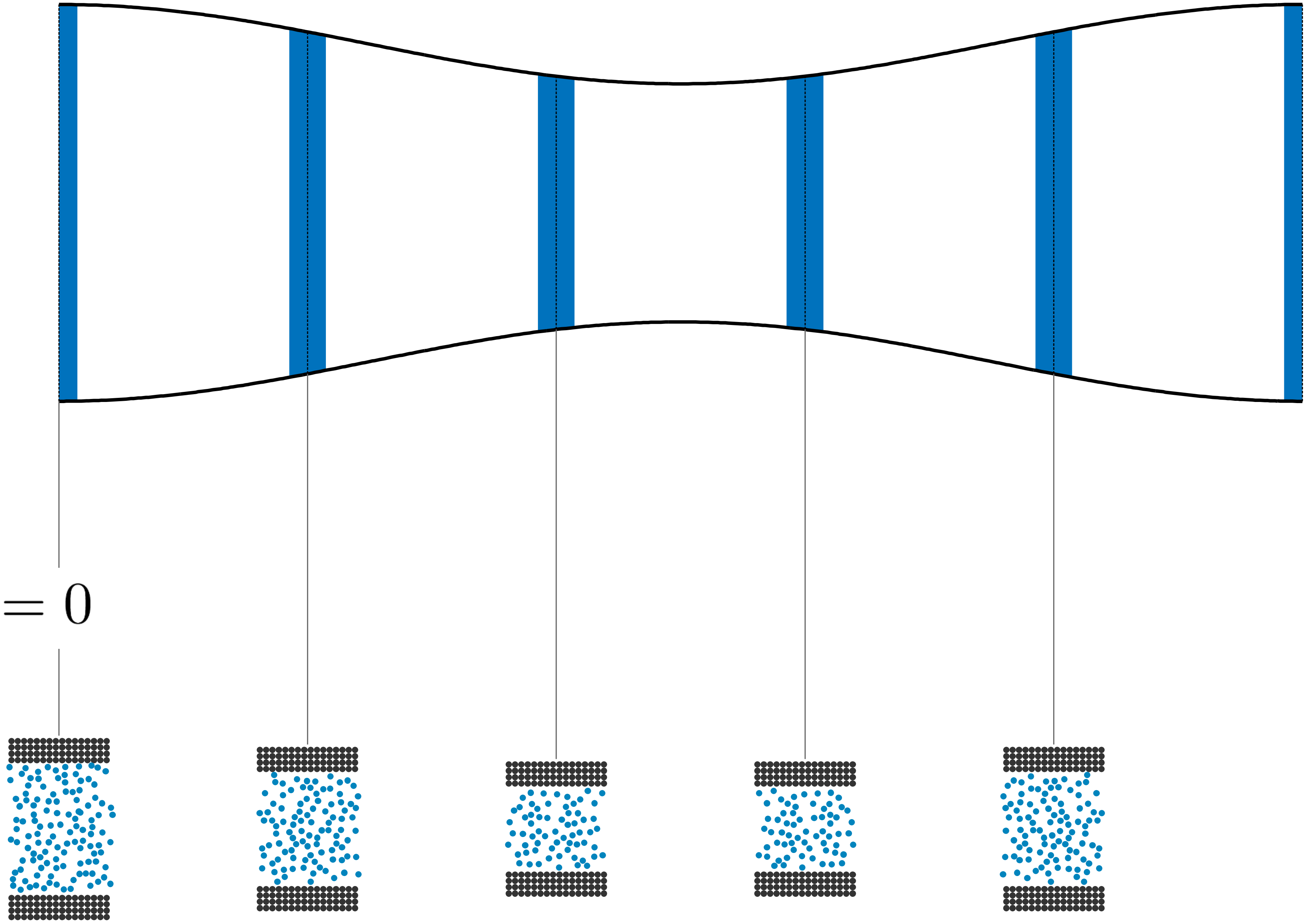
$$-\frac{\partial p}{\partial s} + \frac{\partial \tau_{sy}}{\partial y} + \frac{\partial \tau_{sz}}{\partial z} + \frac{\rho}{m} F_{ext} = 0$$



Hybrid method – micro model

MD subdomain simulations conserve mass.

Instead, we apply a larger body force.



$$\frac{\partial \tau_{sy}}{\partial y} + \frac{\partial \tau_{sz}}{\partial z} + \frac{\rho}{m} F_\mu = 0$$

$$F_\mu = F_{ext} - \frac{m}{\rho}\frac{\partial p}{\partial s}$$

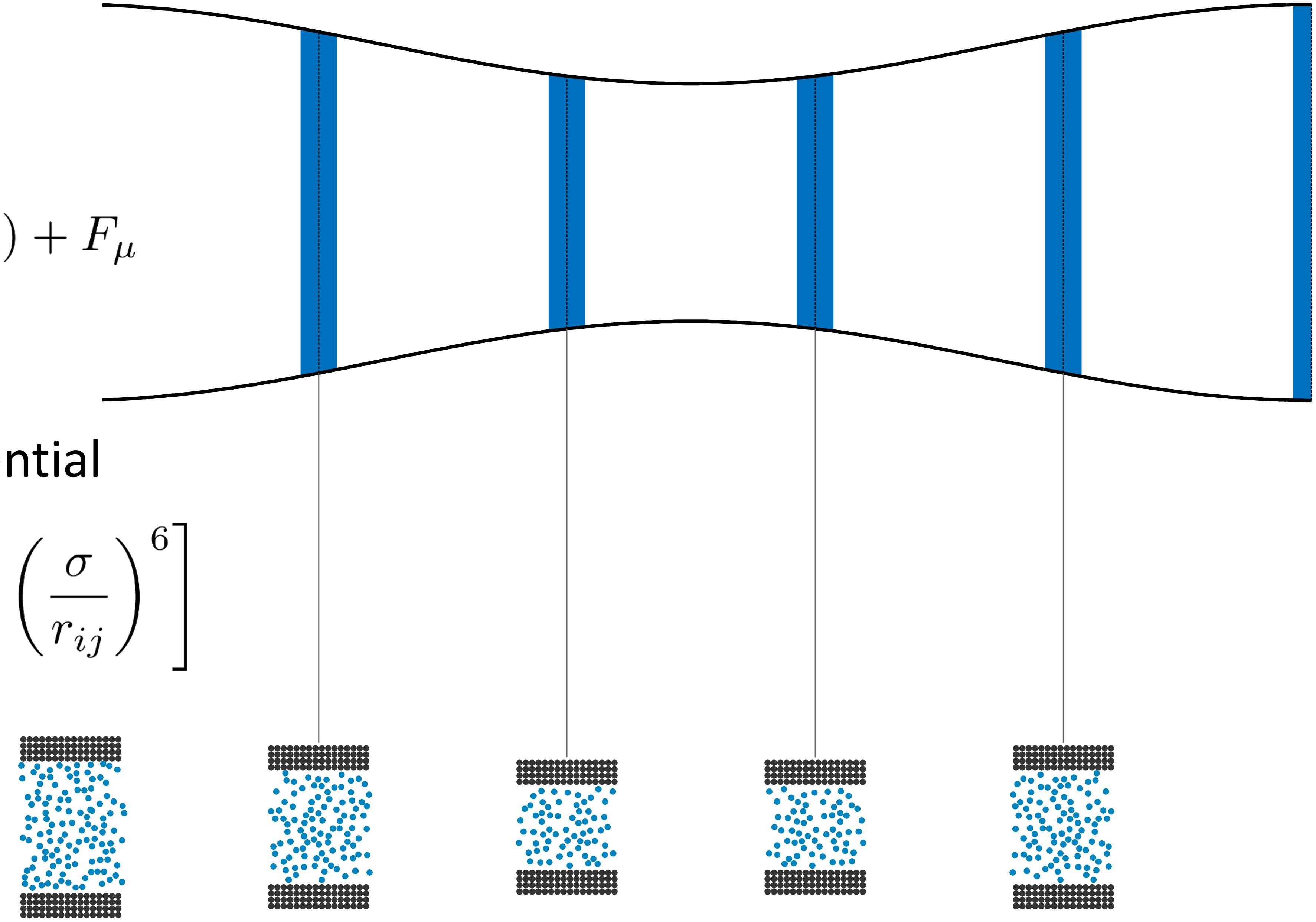
Hybrid method – micro model

Newton's 2nd law

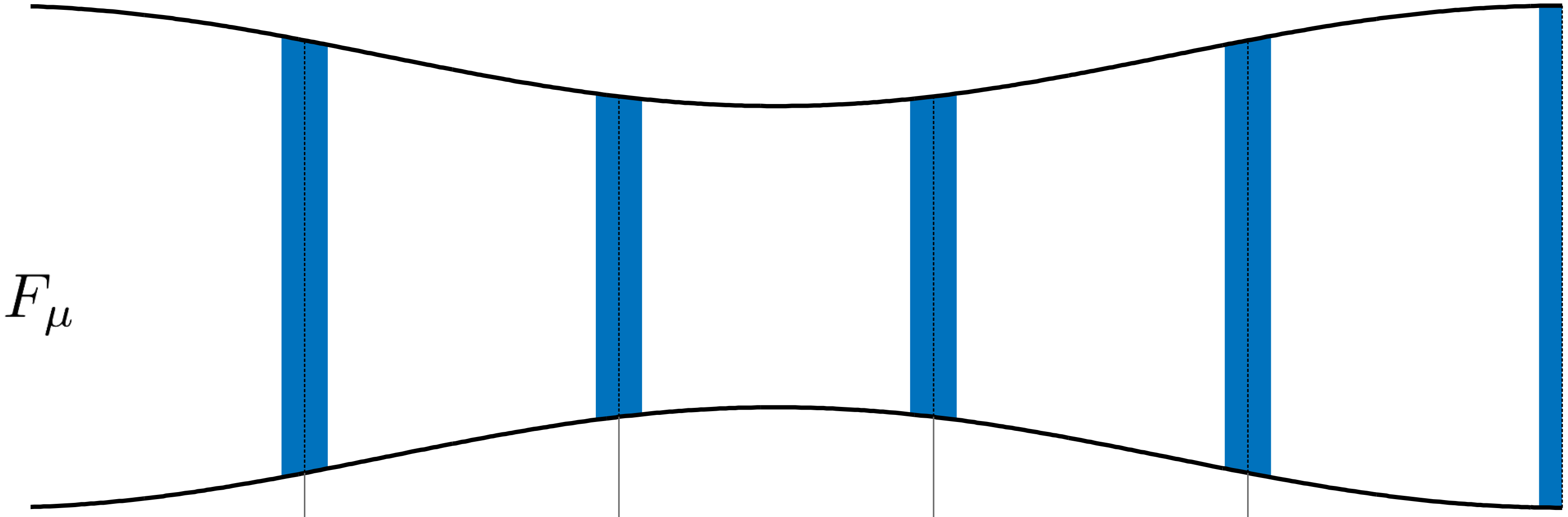
$$m_i \ddot{\mathbf{r}}_i = \sum_{j=1(\neq i)}^{N_m} -\nabla U(r_{ij}) + F_\mu$$

Lennard Jones potential

$$U(r_{ij}) = 4\epsilon \left[\left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^{6} \right]$$



Hybrid method – micro model



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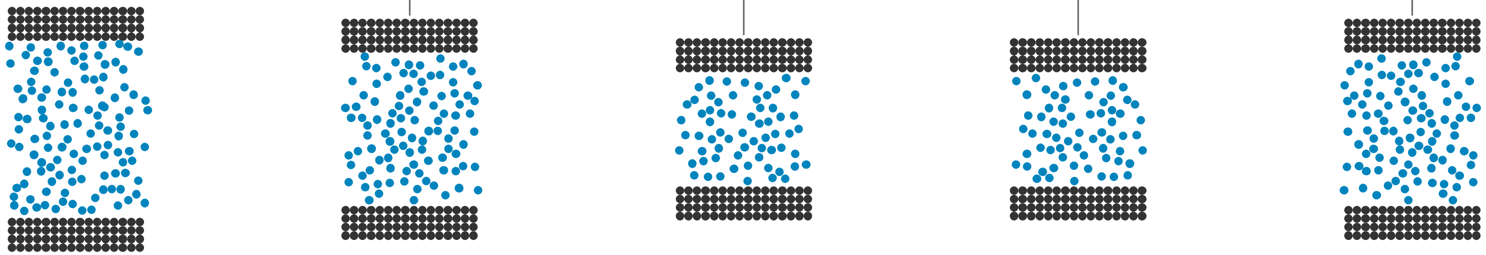
Distance to zero potential

Potential well depth



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Potential well depth

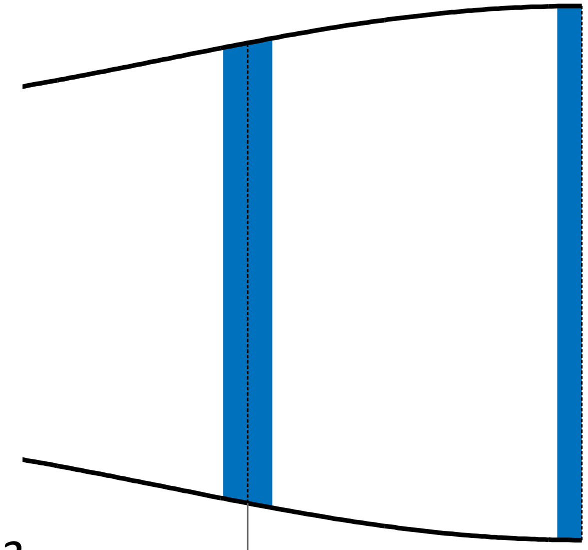
Distance to zero potential

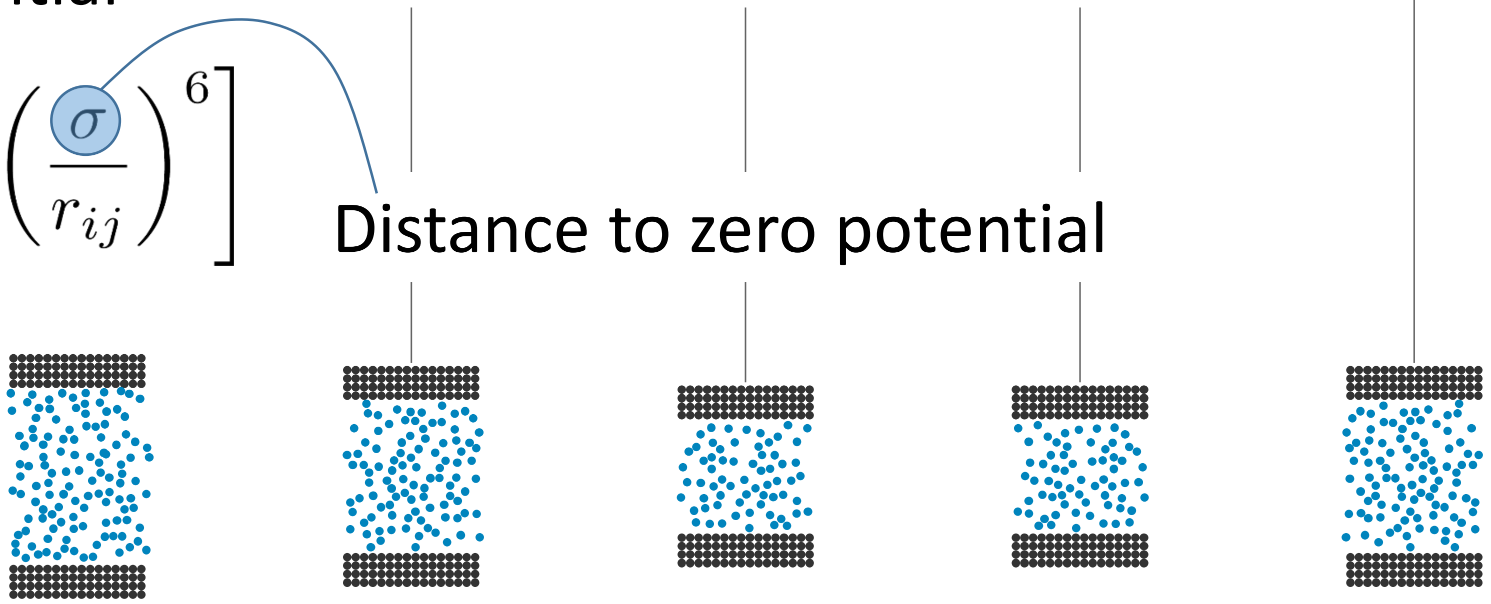
For argon:

$$\sigma_{w-f} = 2.55 \times 10^{-10}\ m$$
$$\epsilon_{w-f} = 0.33 \times 10^{-21}\ J$$

$$\sigma_{f-f} = 3.4 \times 10^{-10}\ m$$
$$\epsilon_{f-f} = 1.65 \times 10^{-21}\ J$$

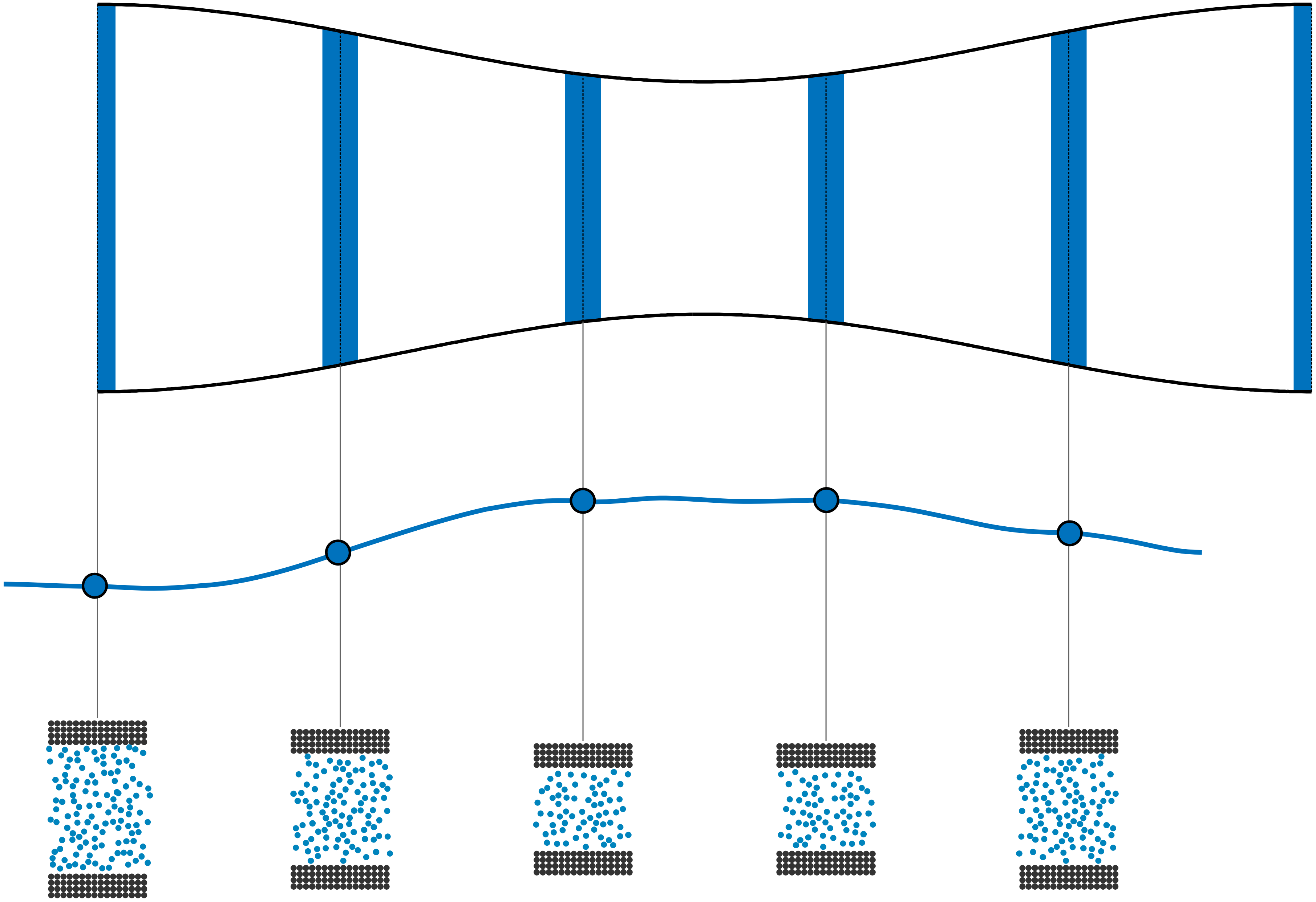
Thompson and Troian (1997), Nature, 389:360:362





Hybrid methods – machine learning

We'd like to use the existing information to make predictions.

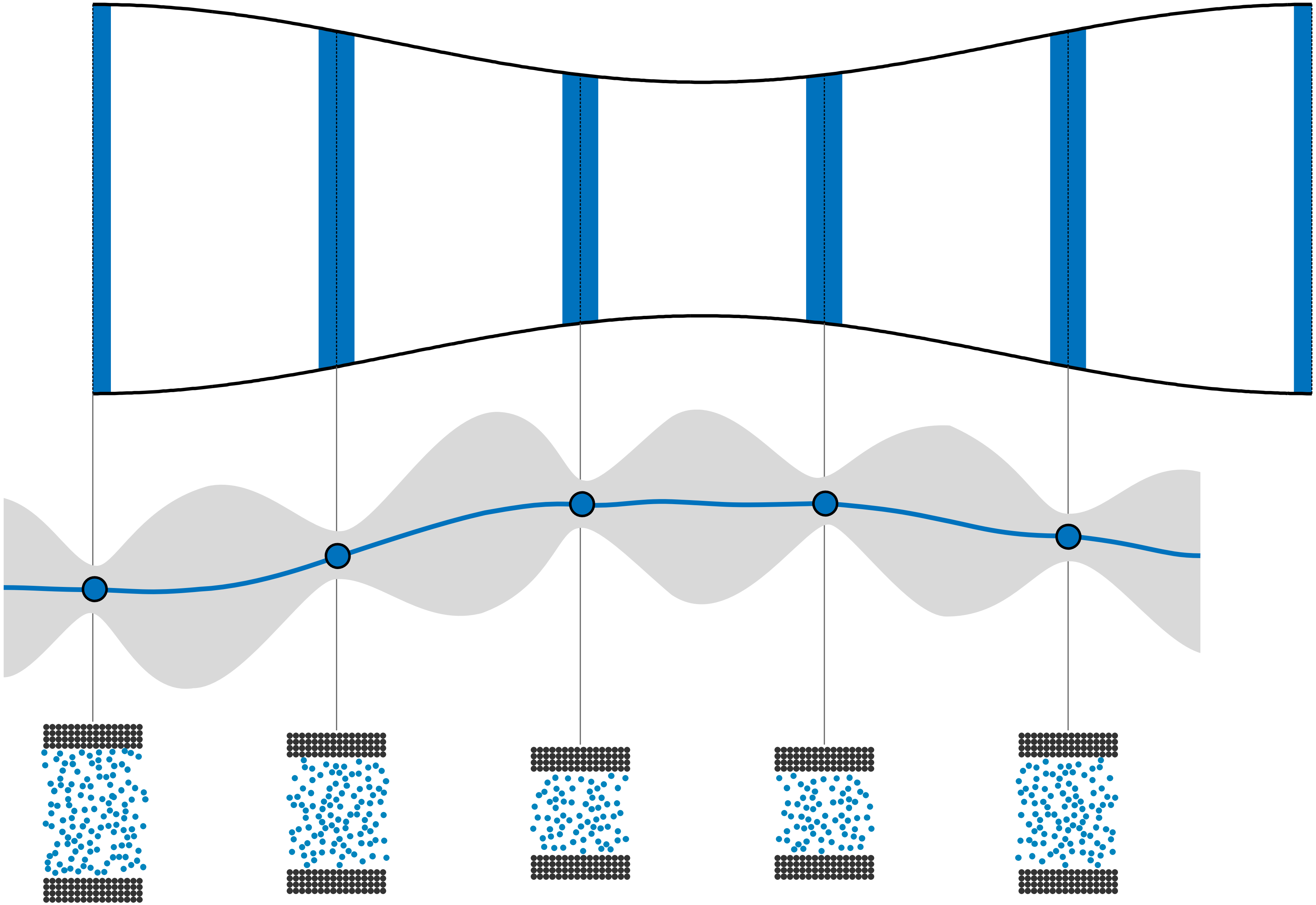


Hybrid methods – machine learning

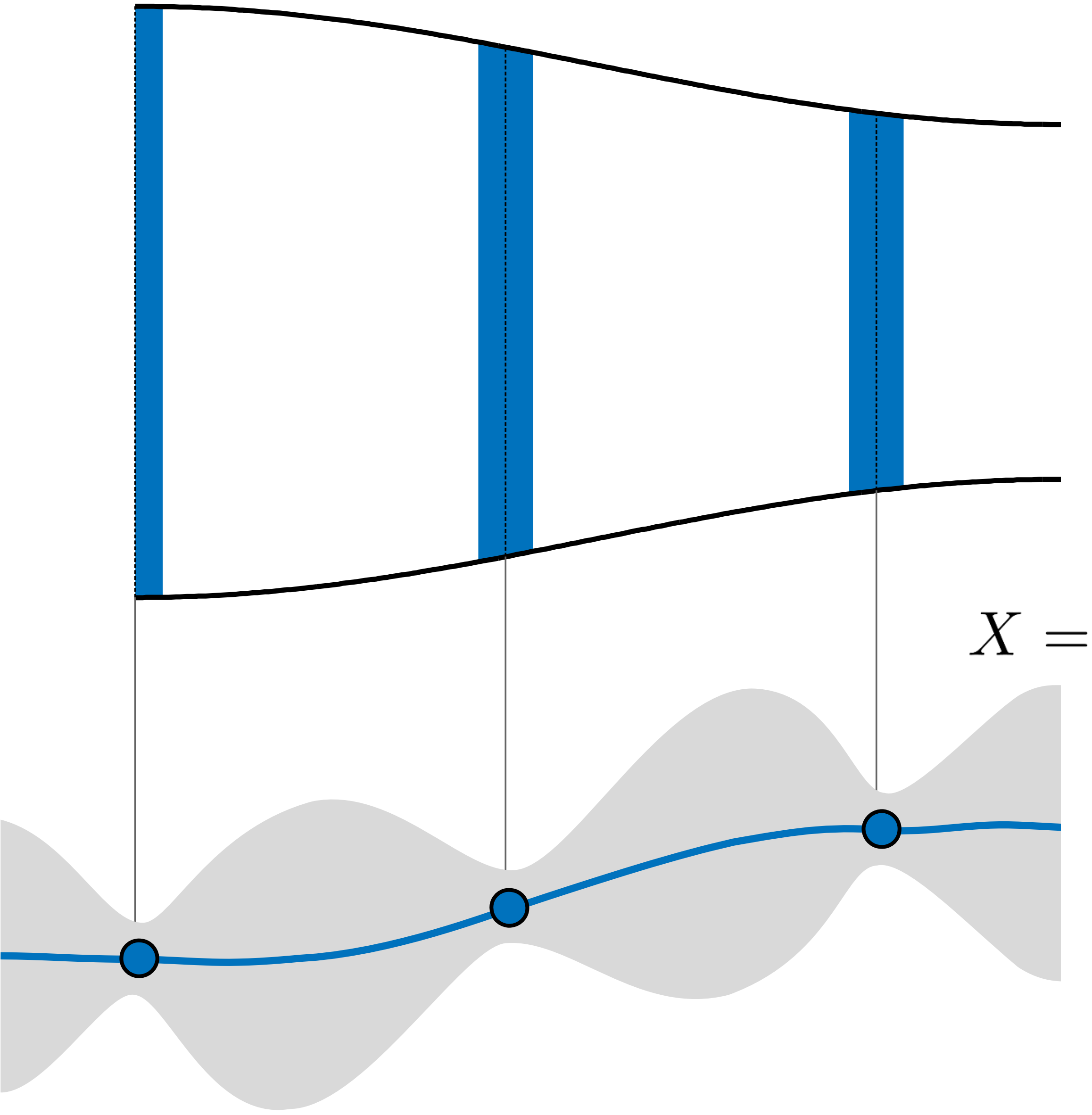
We'd like to use the existing information to make predictions.

We want to judge on-the-fly if a new simulation is required.

For this, we use a Gaussian process (GP).



GP regression for our multiscale system



input

$$\boldsymbol{x}_i = \{h_i,\ \rho_i,\ F_i\}$$

output

$$y_i = q_i \text{ or } p_i$$

Gaussian process

$$f(\mathbf{x}_i) \sim \mathcal{GP}\big(\mu(\mathbf{x}_i), K(\mathbf{x}_i, \mathbf{x}_j)\big)$$

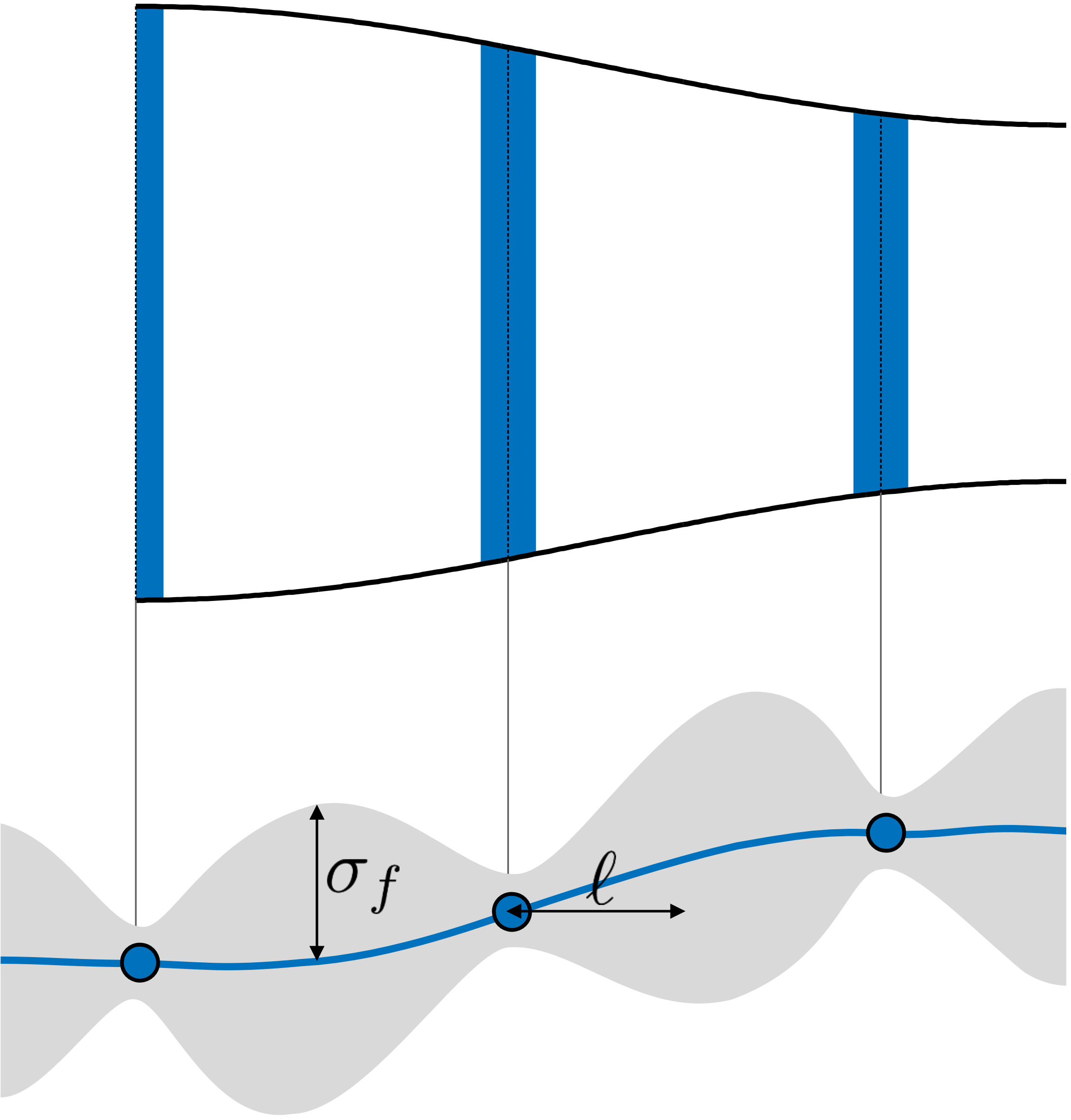
training points

$$X = \begin{bmatrix} h_1 & h_2 & \dots & h_M \\ \rho_1 & \rho_2 & \dots & \rho_M \\ F_1 & F_2 & \dots & F_M \end{bmatrix} \quad \langle \boldsymbol{y} \rangle = [\langle y_1 \rangle\ \langle y_2 \rangle\ \dots\ \langle y_M \rangle]$$

posterior distribution – Bayes' theorem

$$P(f|\langle \mathbf{y} \rangle, X) = \frac{P(\langle \mathbf{y} \rangle | X, f) P(f)}{P(\langle \mathbf{y} \rangle | X)}$$

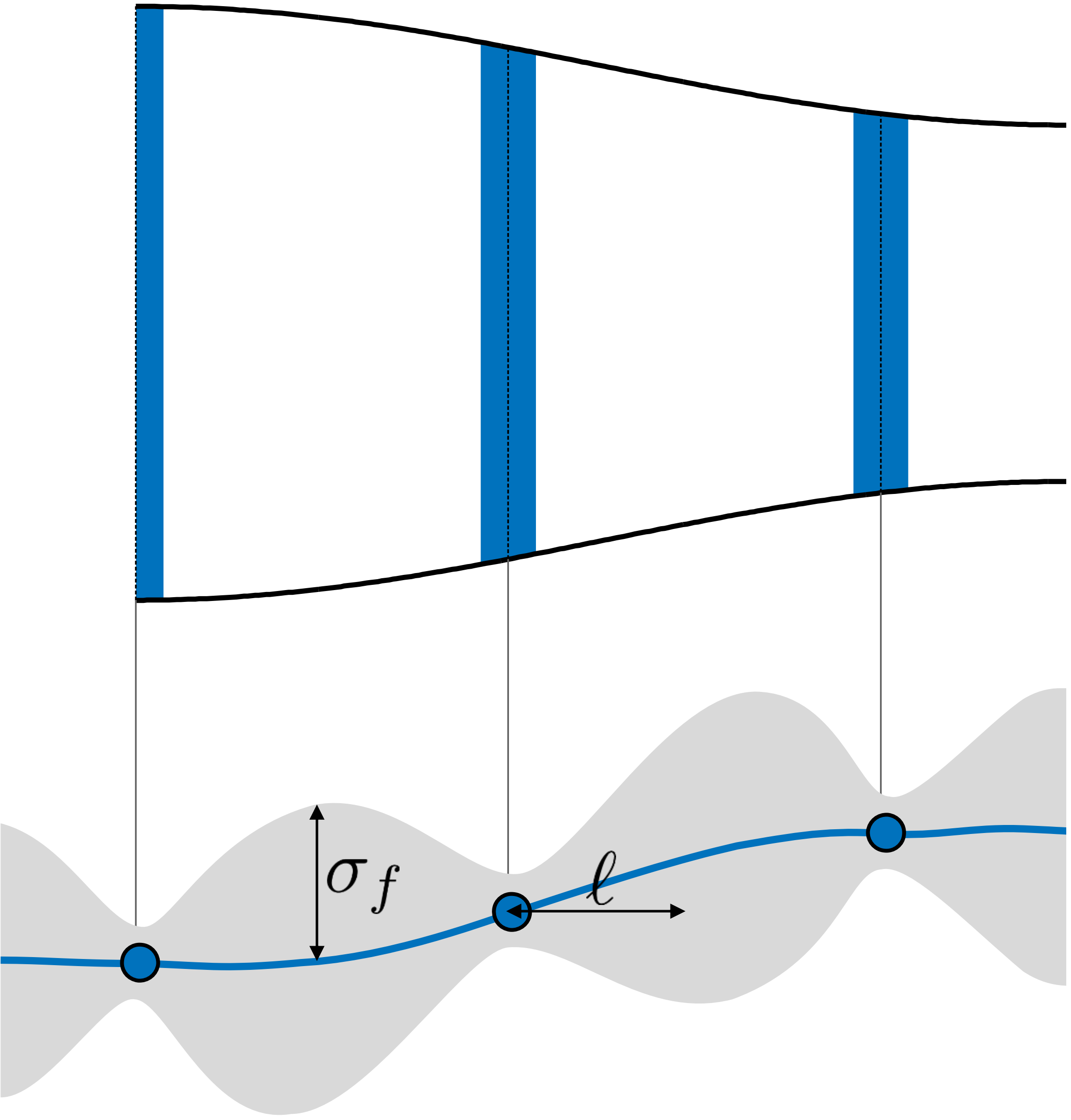
GP regression for our multiscale system



function covariance –
squared exponential kernel

$$K(\mathbf{x}_i, \mathbf{x}_j) = \sigma_f^2 \exp\left(-\frac{d_{ij}^2}{2\ell^2}\right)$$

GP regression for our multiscale system



function covariance –
squared exponential kernel

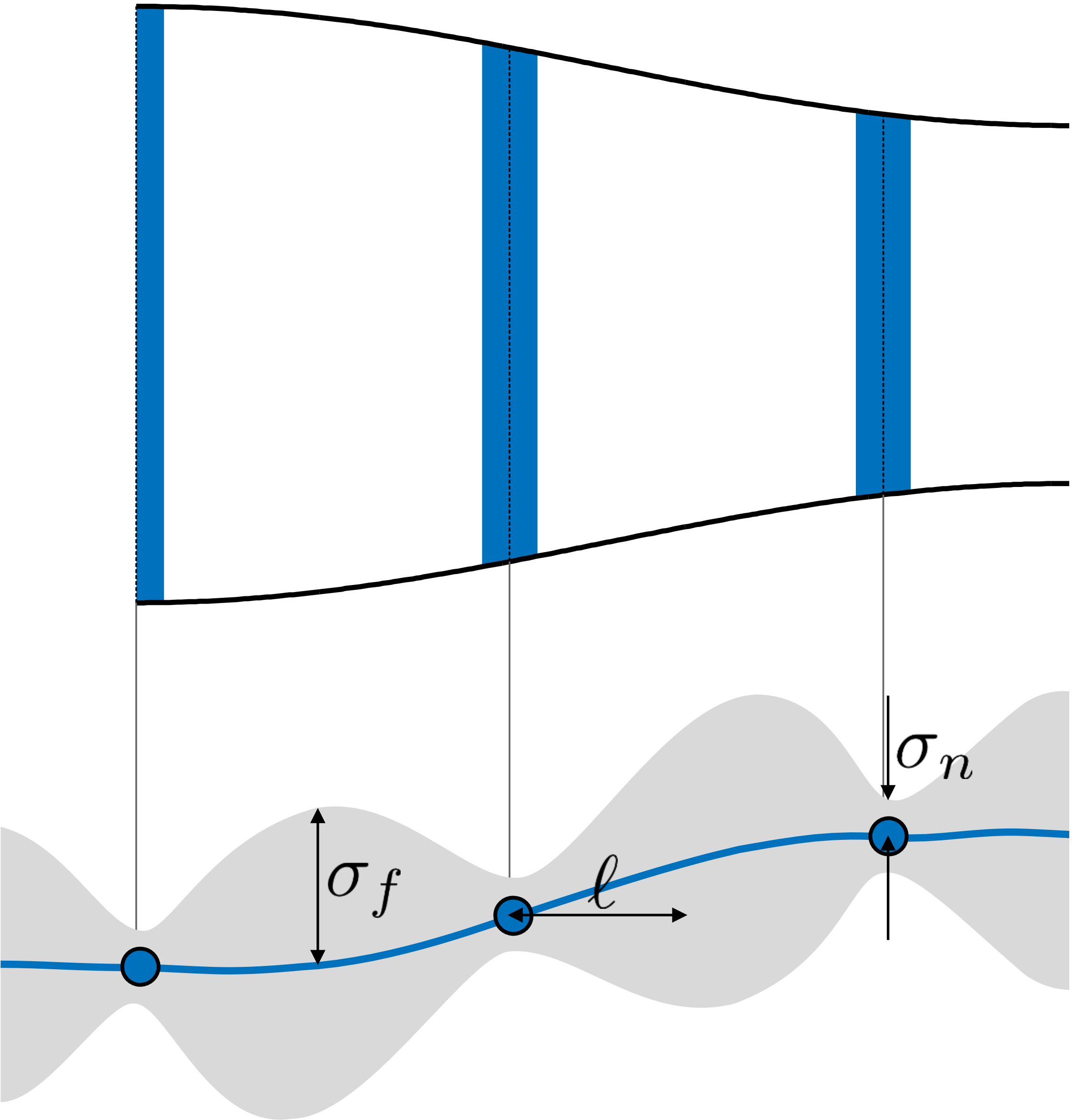
$$K(\mathbf{x}_i, \mathbf{x}_j) = \sigma_f^2 \exp\left(-\frac{d_{ij}^2}{2\ell^2}\right)$$

input difference

$$d_{ij}^2 = \left(\frac{h_i - h_j}{\overline{\Delta h}}\right)^2 + \left(\frac{\rho_i - \rho_j}{\overline{\Delta \rho}}\right)^2 + \left(\frac{F_i - F_j}{\overline{\Delta F}}\right)^2$$

$$\overline{\Delta h} = \mathbb{E}\begin{bmatrix} \Delta h_{11} & \Delta h_{12} & \dots & \Delta h_{1M} \\ \Delta h_{21} & \Delta h_{22} & \dots & \Delta h_{2M} \\ \vdots & \vdots & \ddots & \vdots \\ \Delta h_{M1} & \Delta h_{M2} & \dots & \Delta h_{MM} \end{bmatrix}$$

GP regression for our multiscale system



function covariance

$$K(\mathbf{x}_i, \mathbf{x}_j) = \sigma_f^2 \exp\left(-\frac{d_{ij}^2}{2\ell^2}\right)$$

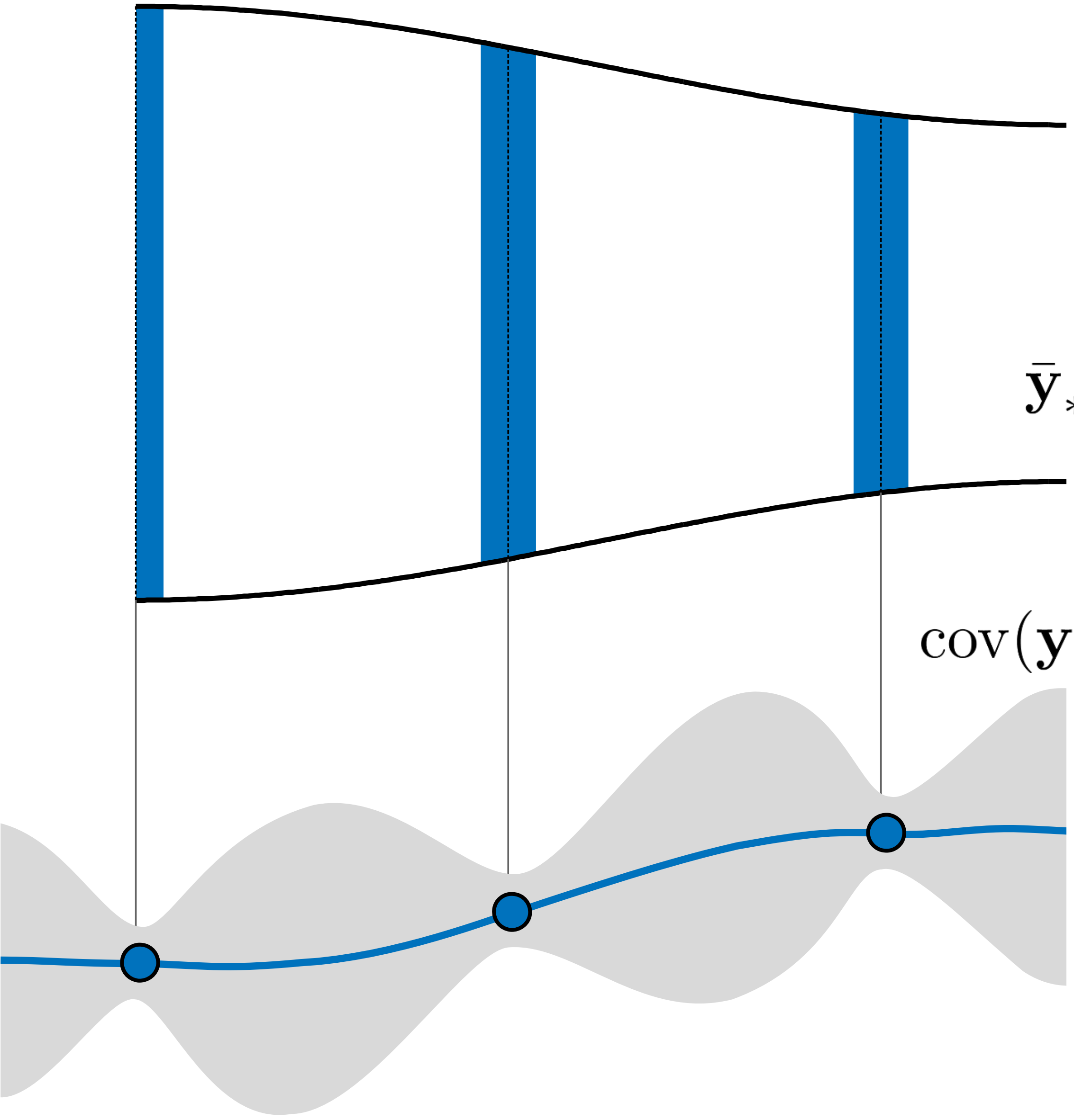
output covariance

$$C(X, X) = K(X, X) + \sigma_n^2 I$$

hyperparameters

	q (ng/s)	p (MPa)
σ_n	0.05	0.003
σ_f	1	1
ℓ	1	1

GP regression for our multiscale system



posterior distribution at test points

$$\mathbf{y}_*|X, \mathbf{y}, X_* \sim \mathcal{N}\left(\bar{\mathbf{y}}_*, \mathrm{cov}(\mathbf{y}_*)\right)$$

posterior mean

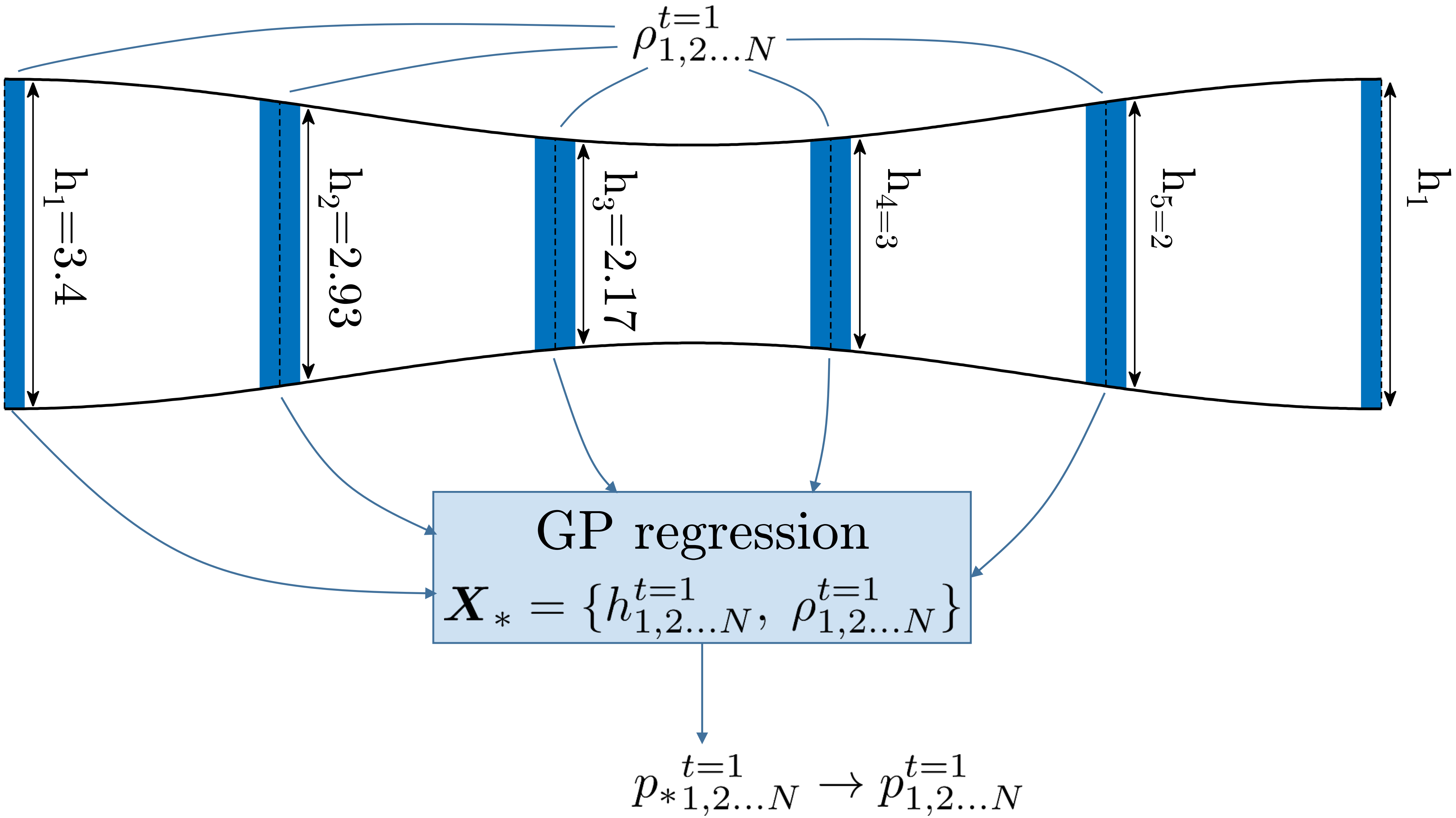
$$\bar{\mathbf{y}}_* = \mu(X_*) + K(X_*, X)C(X, X)^{-1}\left(\langle\mathbf{y}\rangle - \mu(X)\right)$$

posterior covariance

$$\mathrm{cov}(\mathbf{y}_*) = K(X_*, X_*) - K(X_*, X)C(X, X)^{-1}K(X, X_*)$$

$$\text{if } \mathrm{cov}(\mathbf{y}_*) < \sigma_t \text{ then } = y = y_*$$

Implementation procedure



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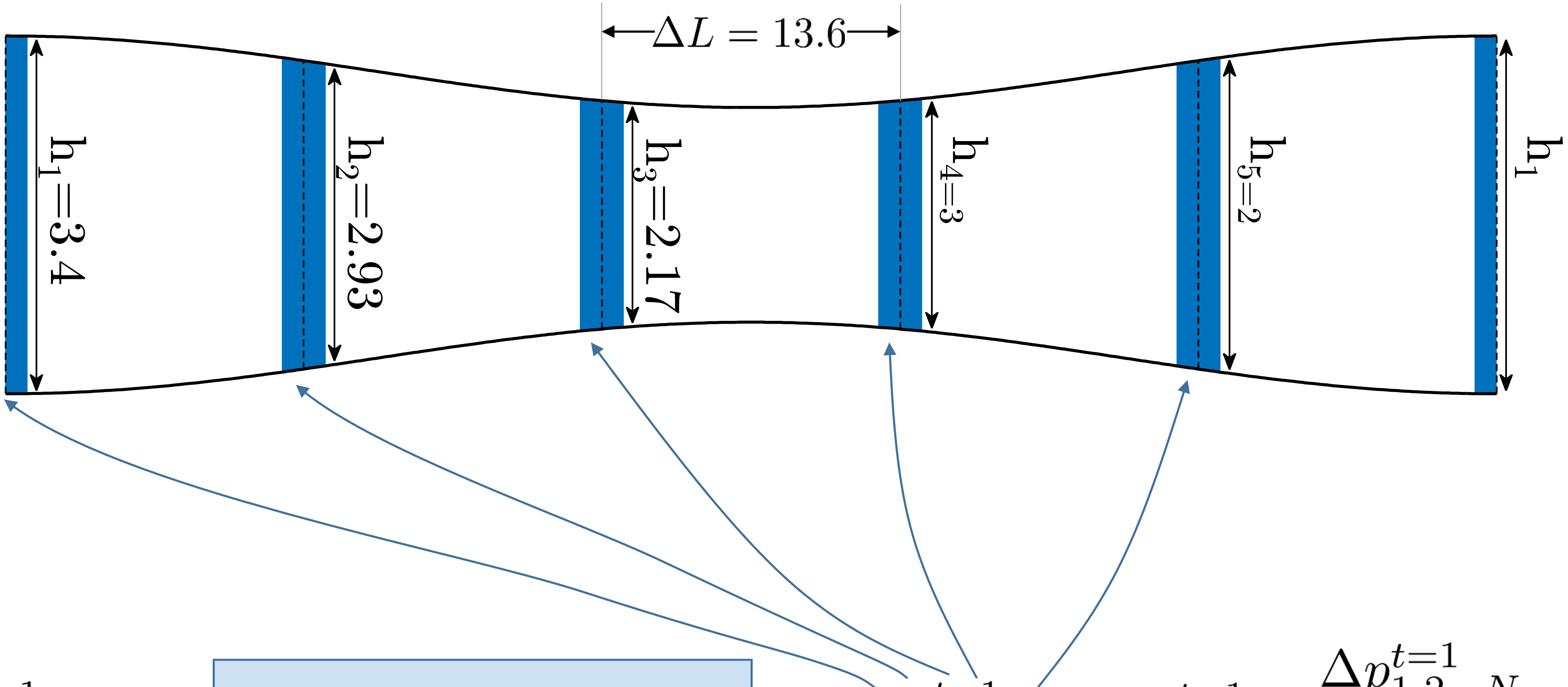
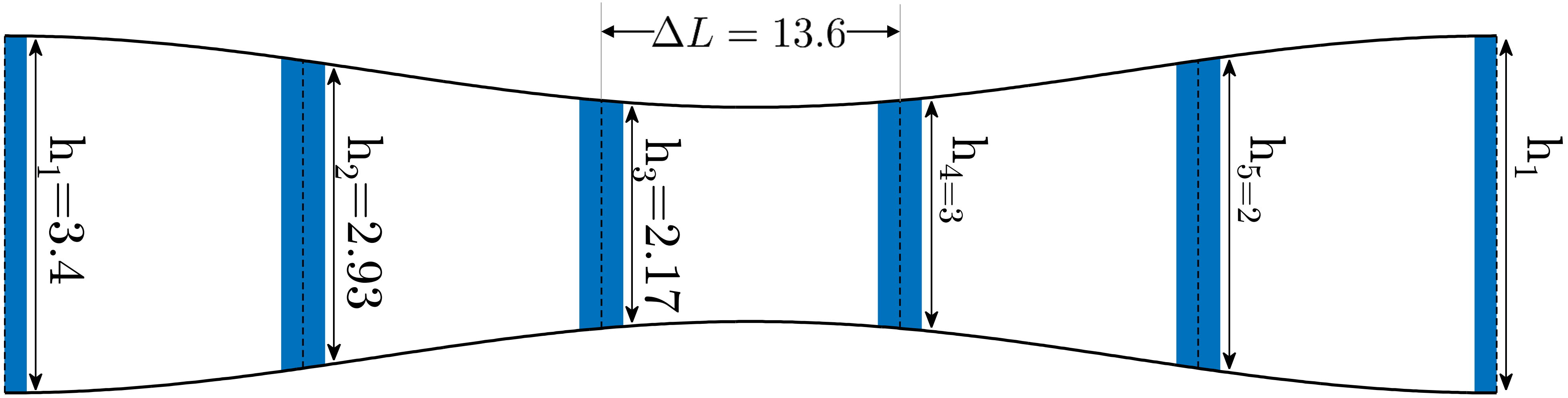


$p^{t=1}_{1,2\ldots N}$ → momentum balance → $F_{\mu}{}^{t=1}_{1,2\ldots N} = F^{t=1}_{ext} - \frac{\Delta p^{t=1}_{1,2\ldots N}}{2\Delta L}$

Implementation procedure



$$F_{ext} = 0.487 \sin\left(\frac{2\pi t}{10.8}\right) \ \text{pN}$$

$p^{t=1}_{1,2\ldots N}$ → **momentum balance** → $F_{\mu}{}^{t=1}_{1,2\ldots N} = F^{t=1}_{ext} - \dfrac{\Delta p^{t=1}_{1,2\ldots N}}{2\Delta L}$

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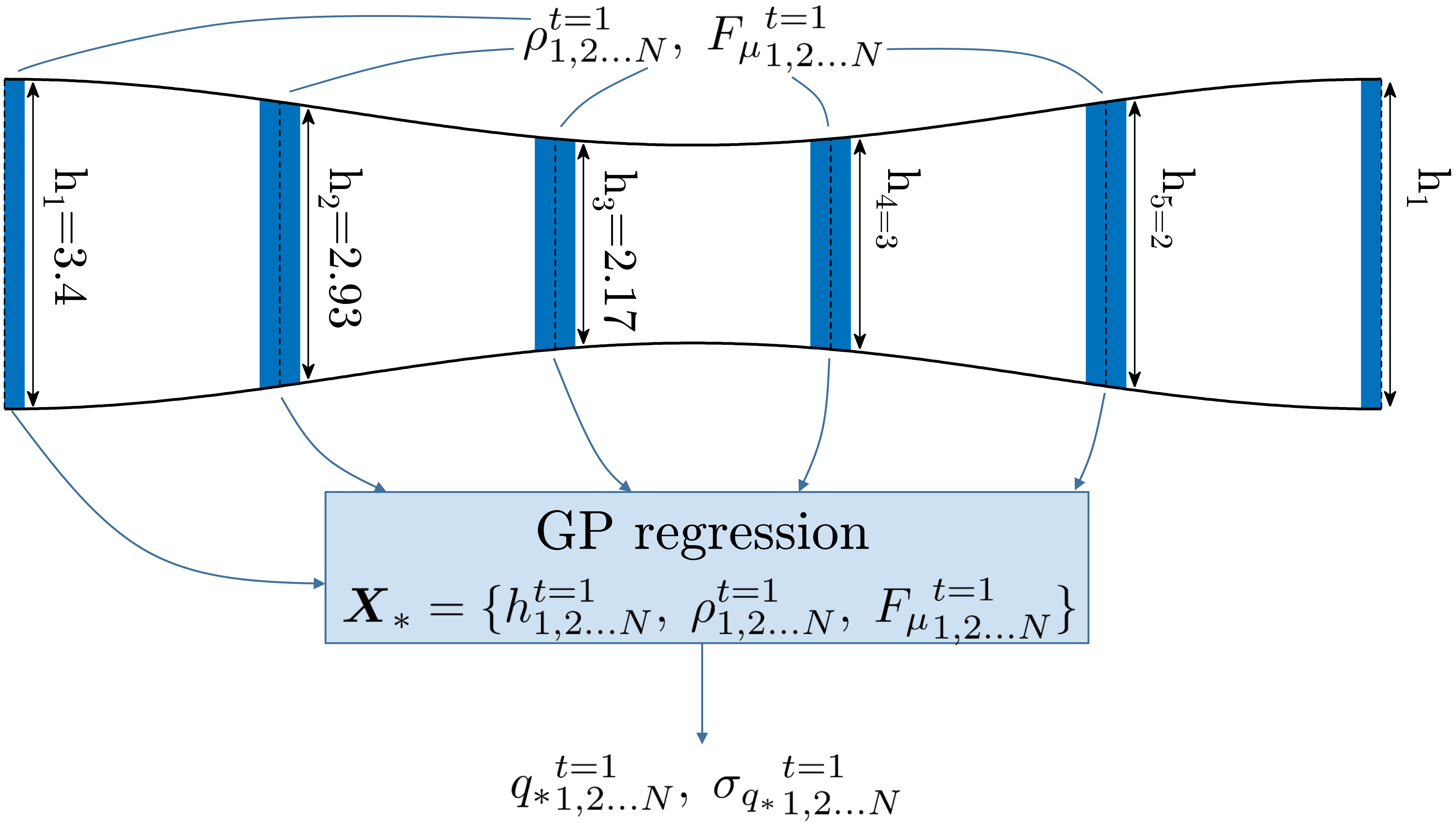

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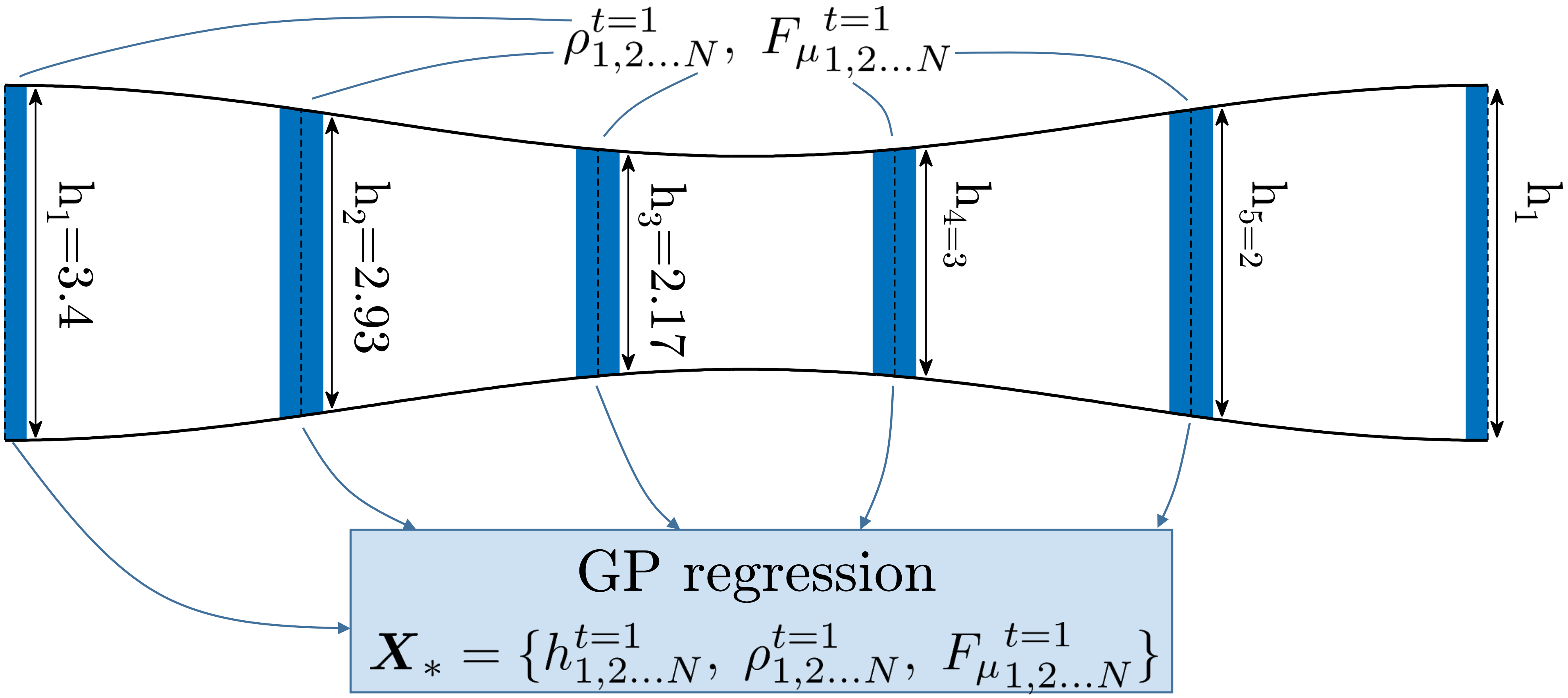
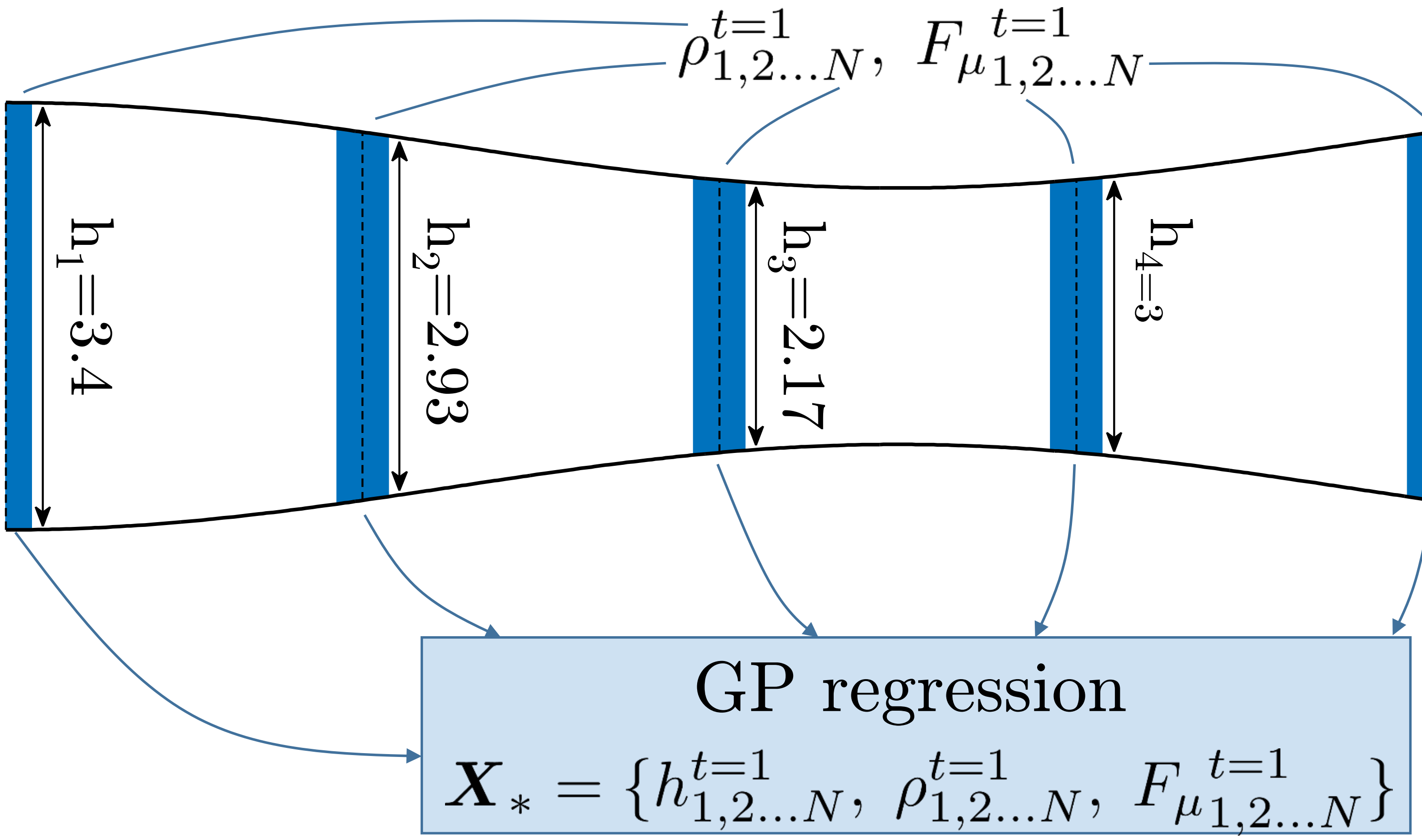


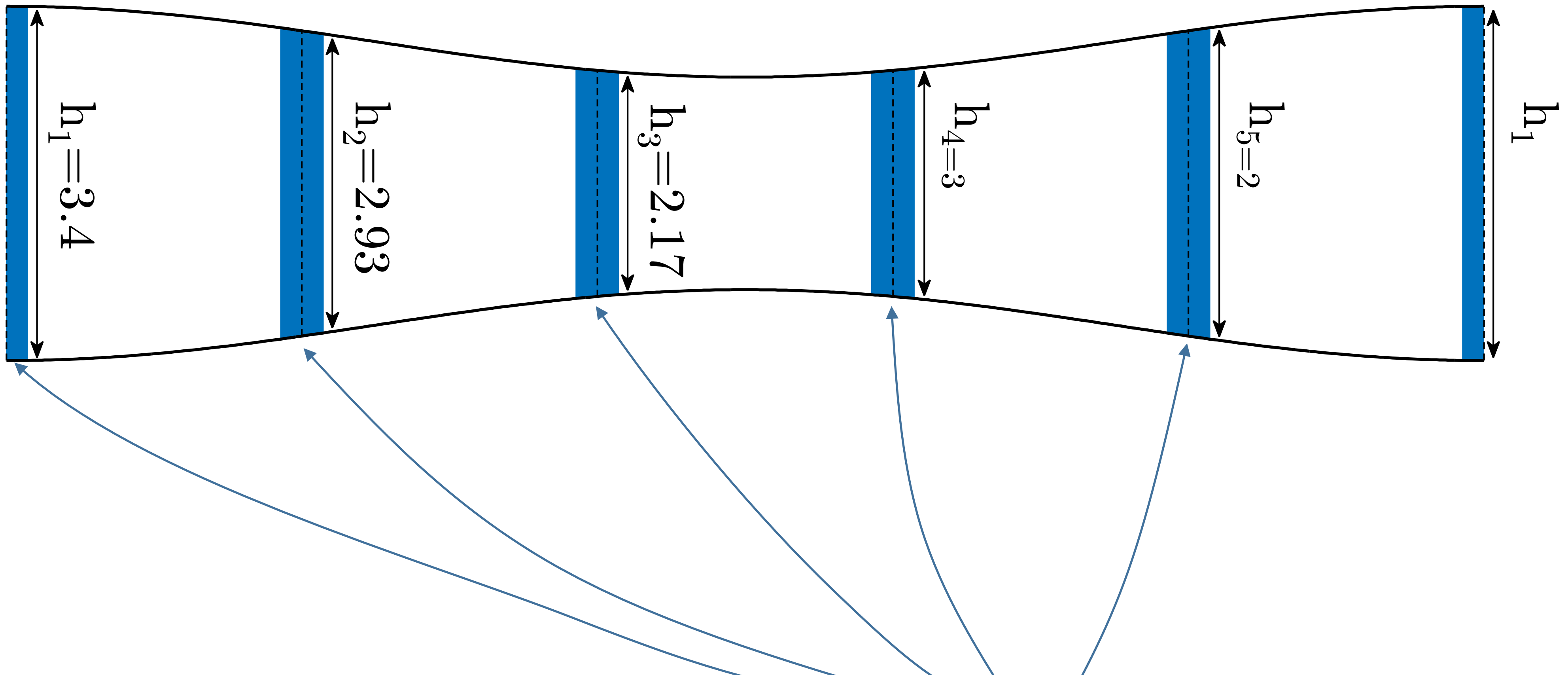
$$\text{if } \sigma_{q_*}{}^{t=1}_{i} < \sigma_t; \quad \text{then } q_*{}^{t=1}_{i} \rightarrow q^{t=1}_{i}$$

Implementation procedure



if $\sigma_{q_*\,i}^{\ t=1} > \sigma_t$ → MD simulation → $q_i^{t=1} = \langle q_i^{t=1} \rangle$ → update database

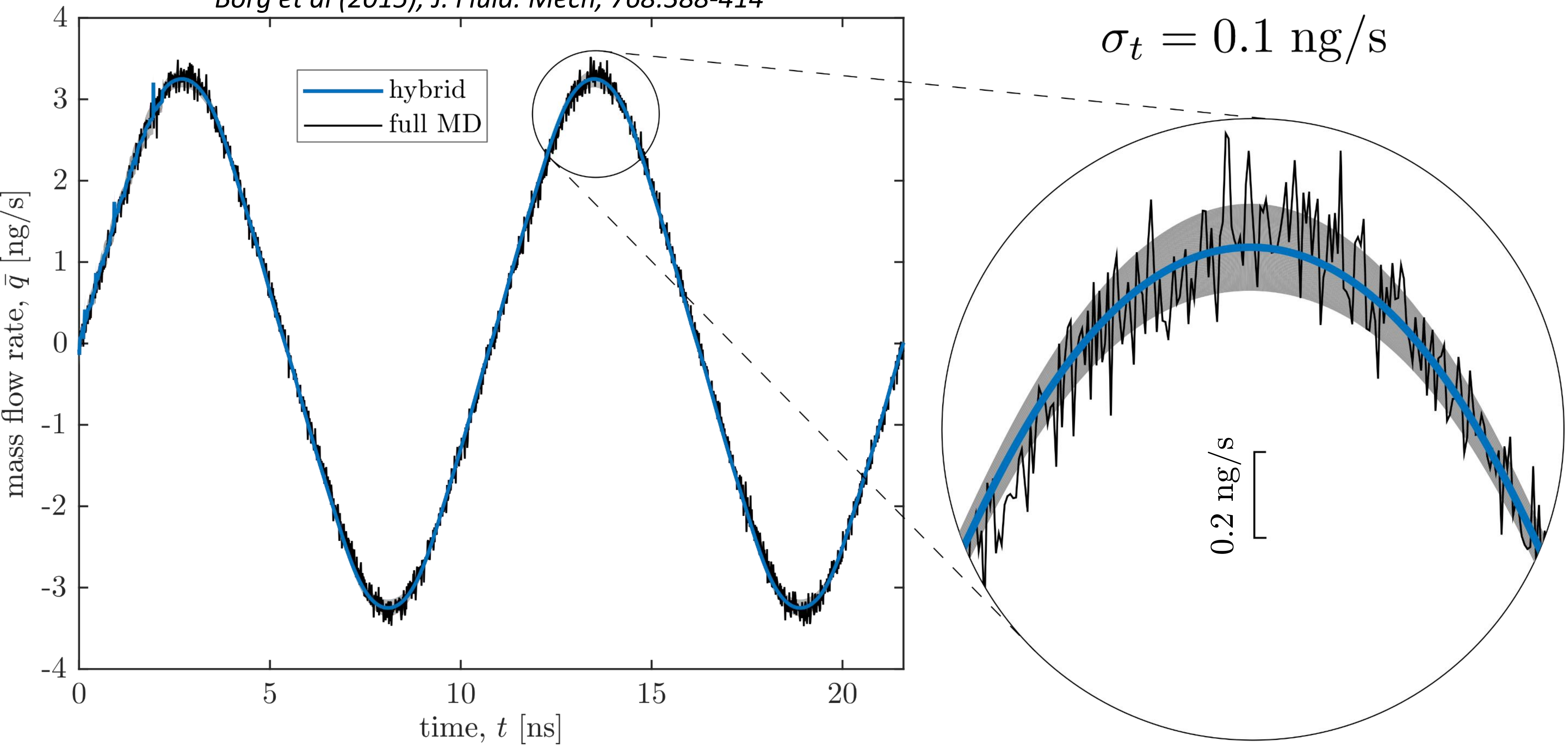
Implementation procedure



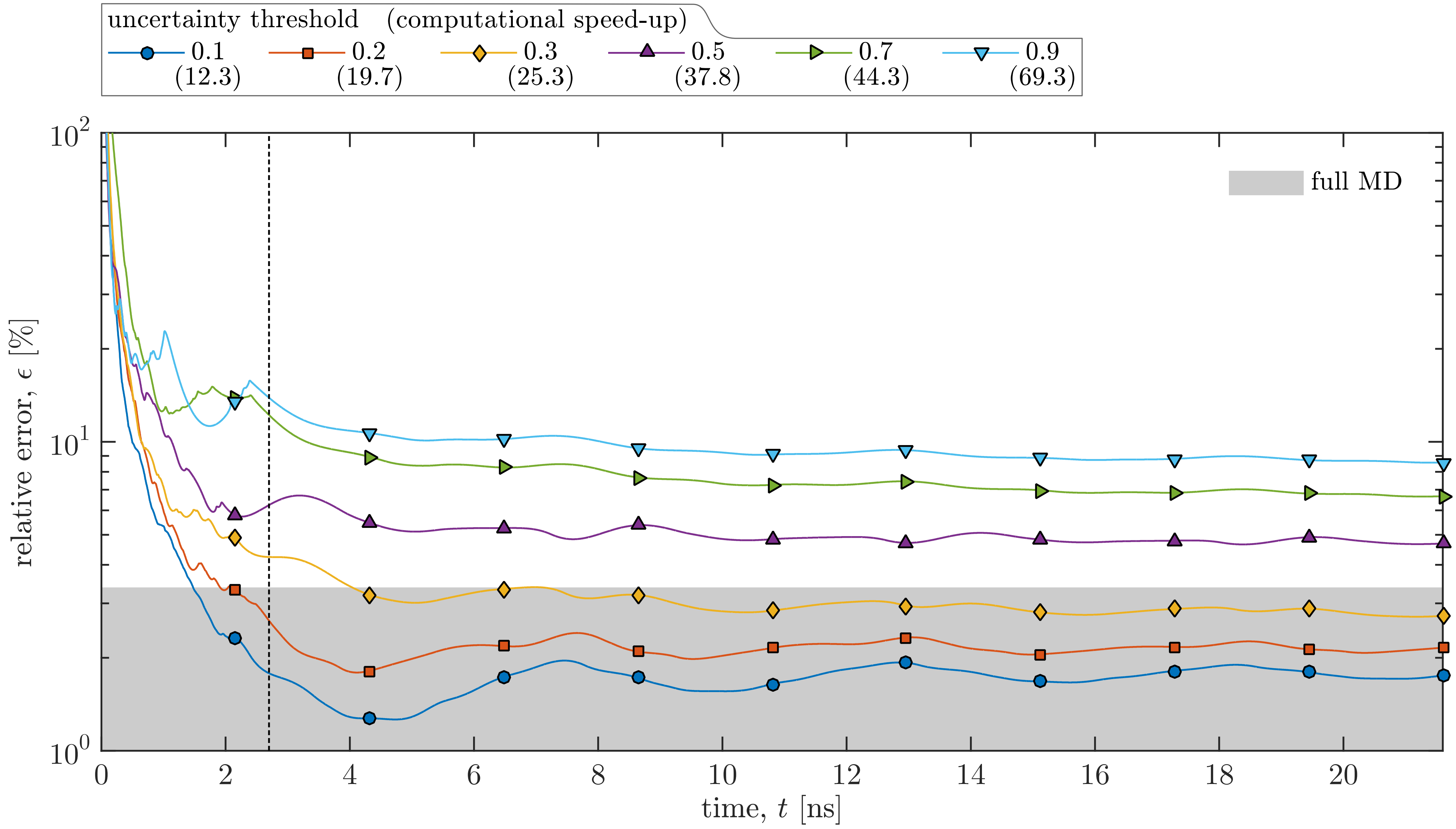
$q^{t=1}_{1,2\ldots N}$ → mass conservation → $\rho^{t=2}_{1,2\ldots N} = -\frac{\Delta t}{A}\frac{\Delta q^{t=1}_{1,2\ldots N}}{2\Delta L}$

Results – empty database, low uncertainty threshold

Borg et al (2015), J. Fluid. Mech, 768:388-414



Results – empty database, varying uncertainty threshold



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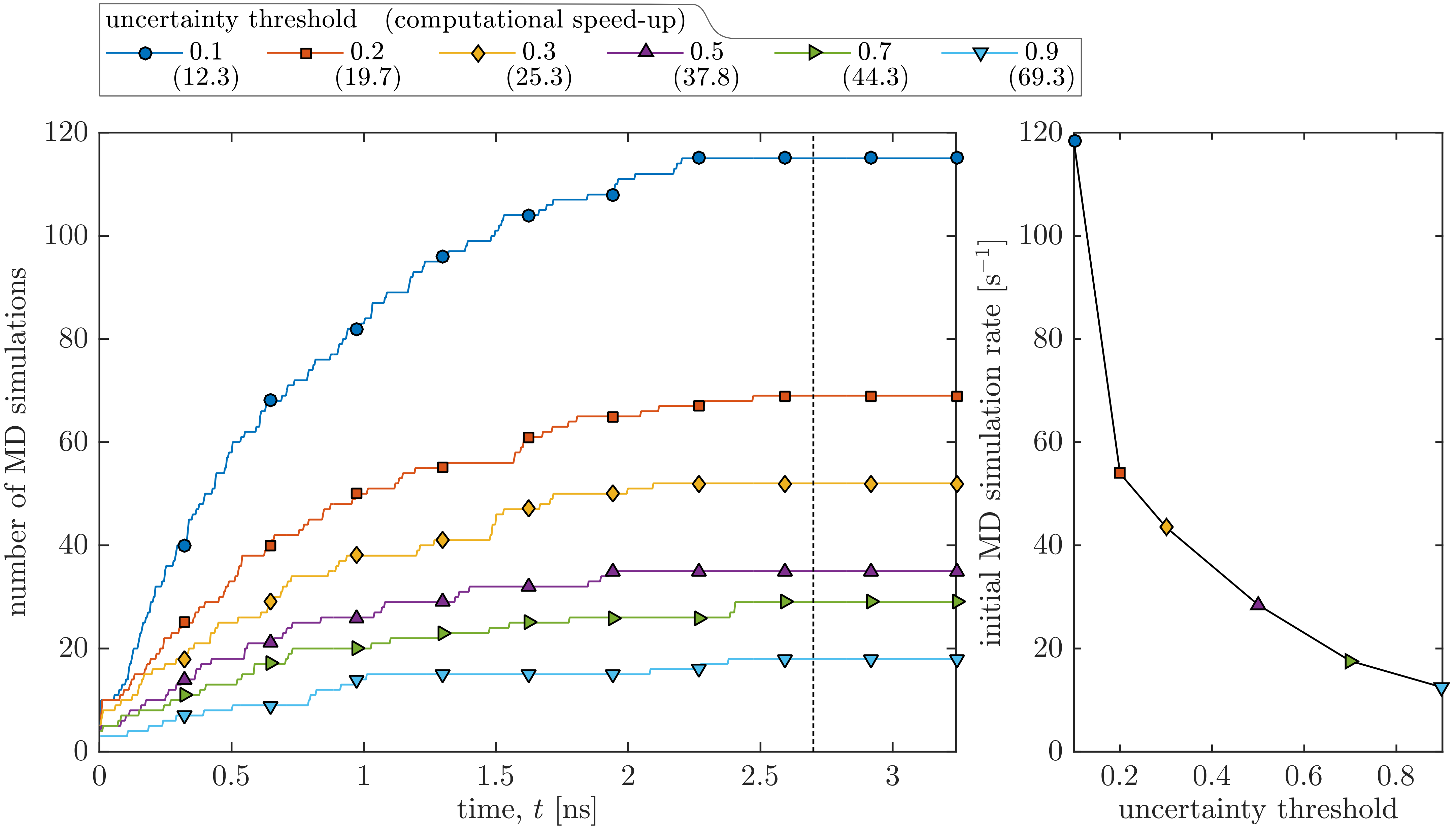

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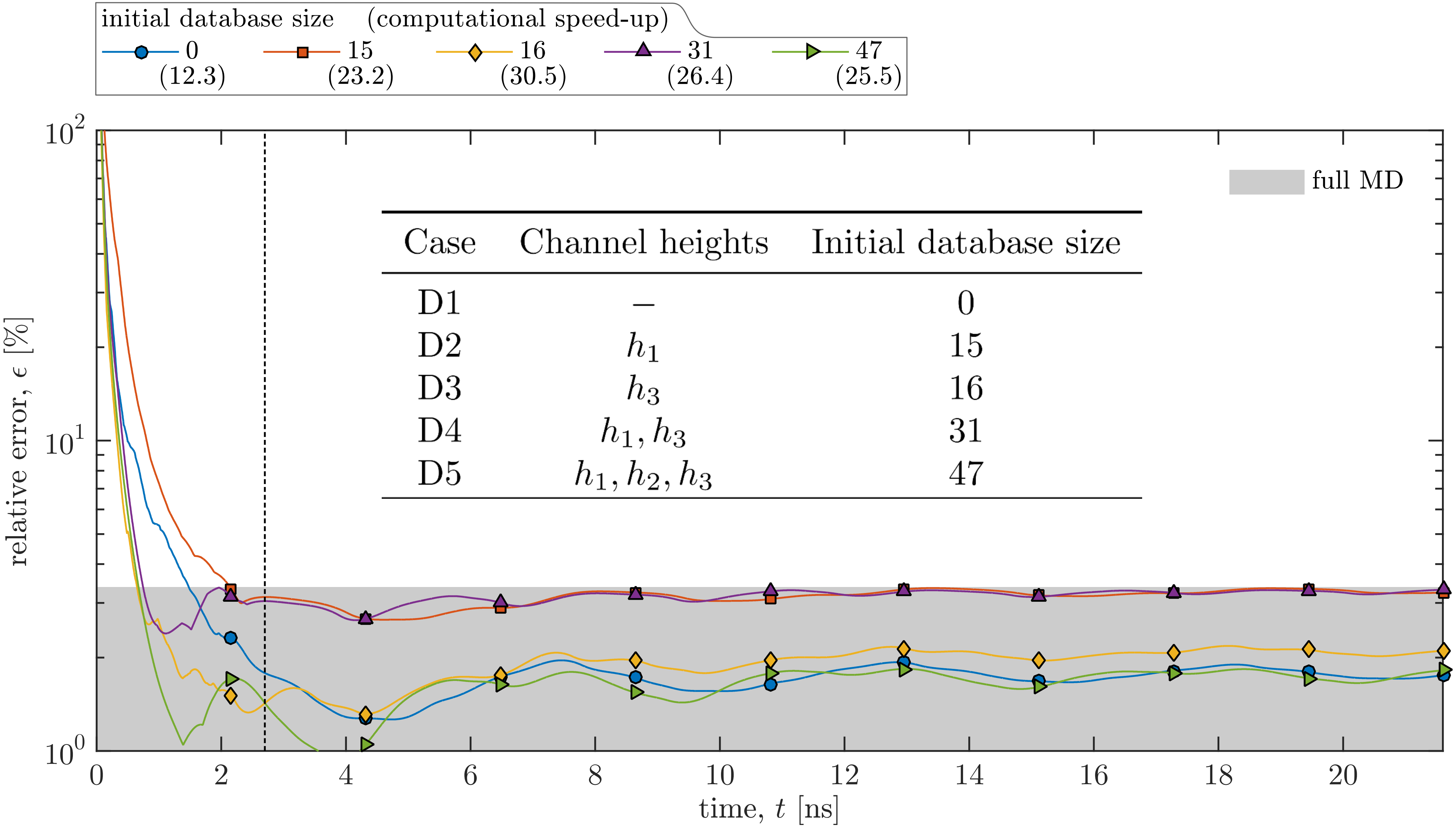
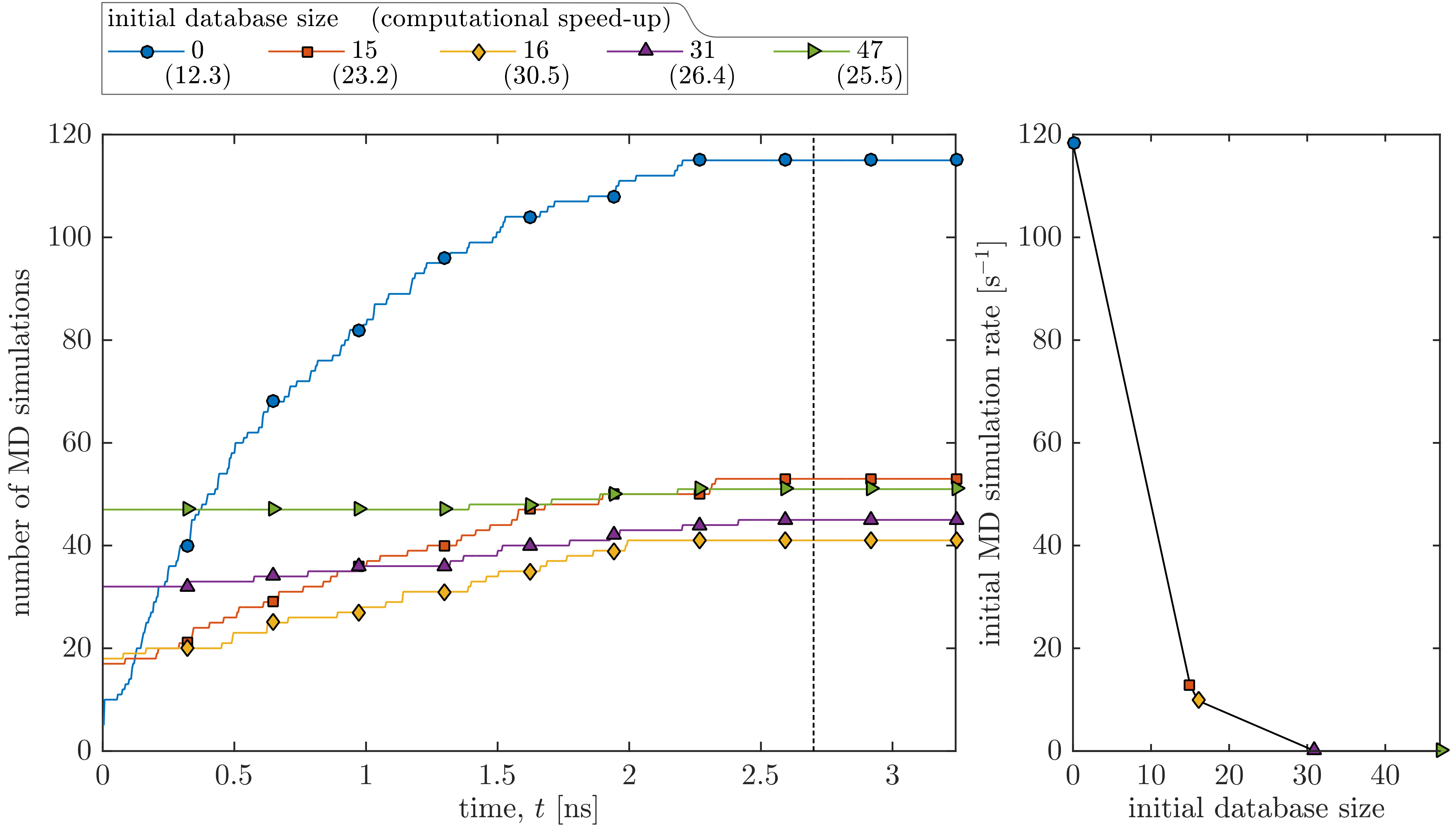
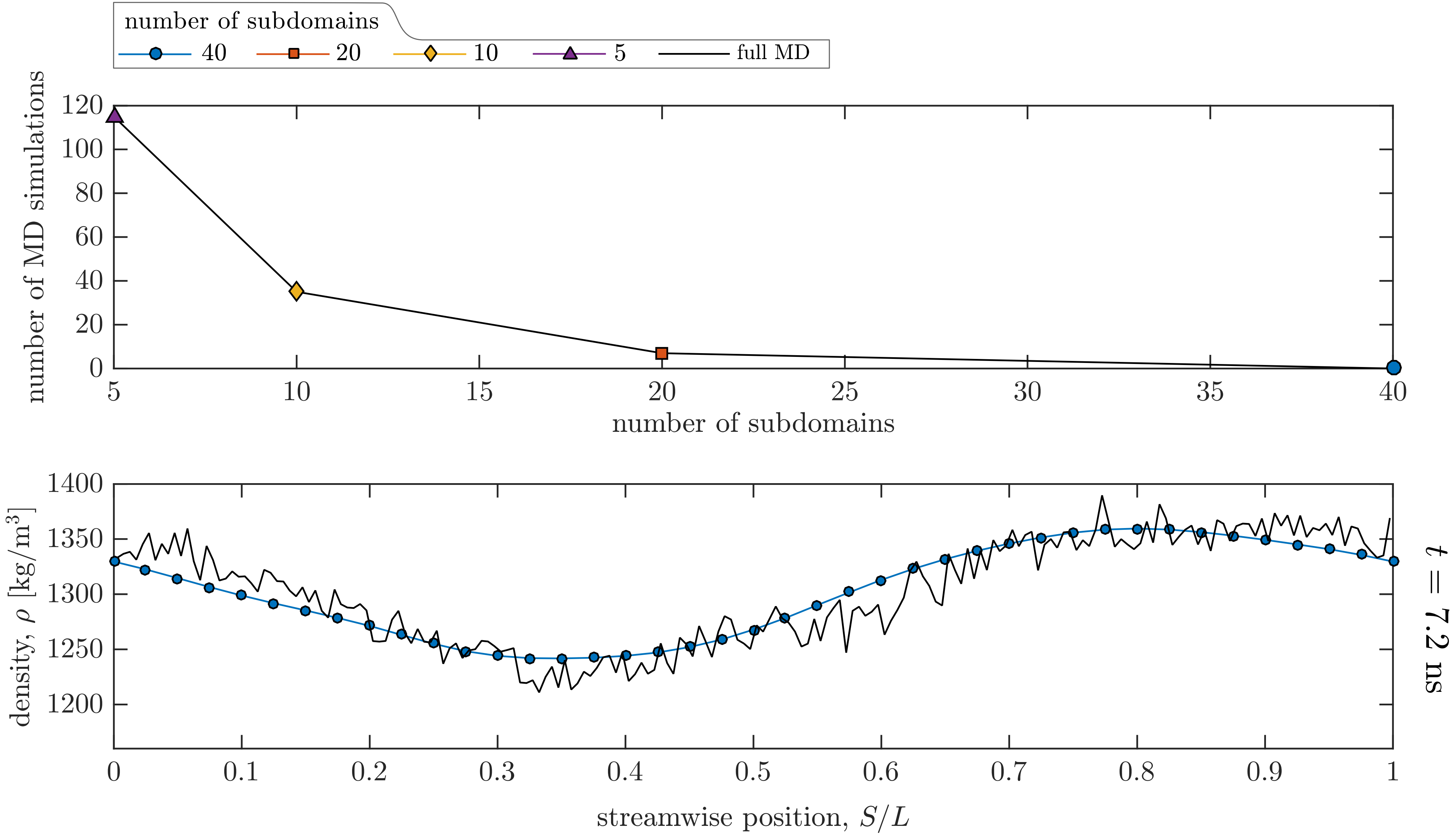


Case	Channel heights	Initial database size
D1	–	0
D2	h_1	15
D3	h_3	16
D4	h_1, h_3	31
D5	h_1, h_2, h_3	47

Results – varying database, low uncertainty threshold



Results – expanding a database: subdomains



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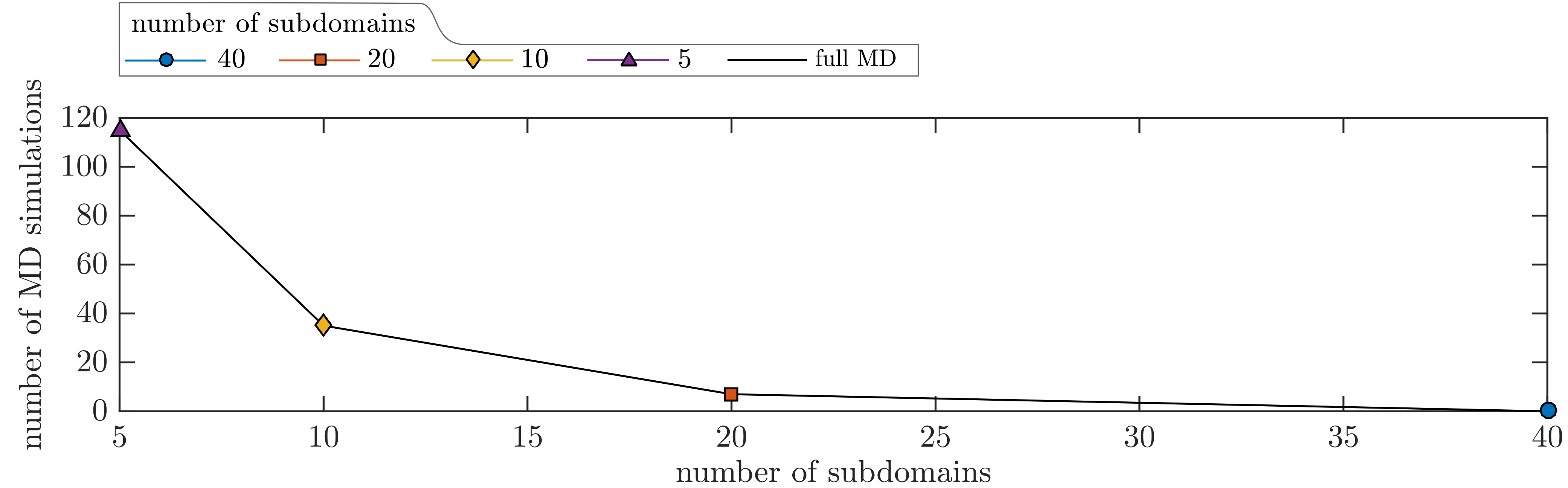

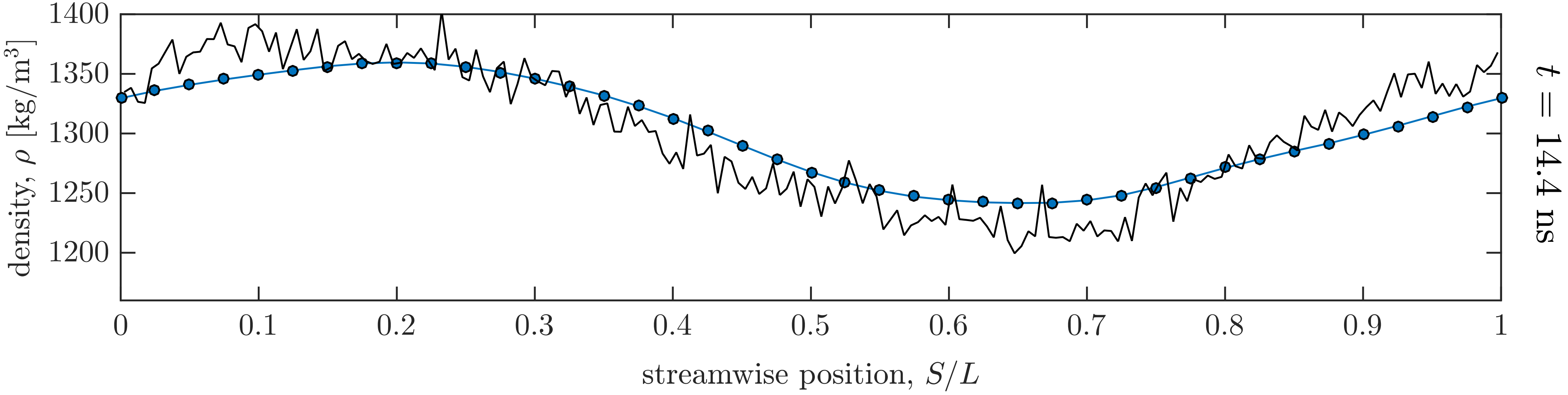

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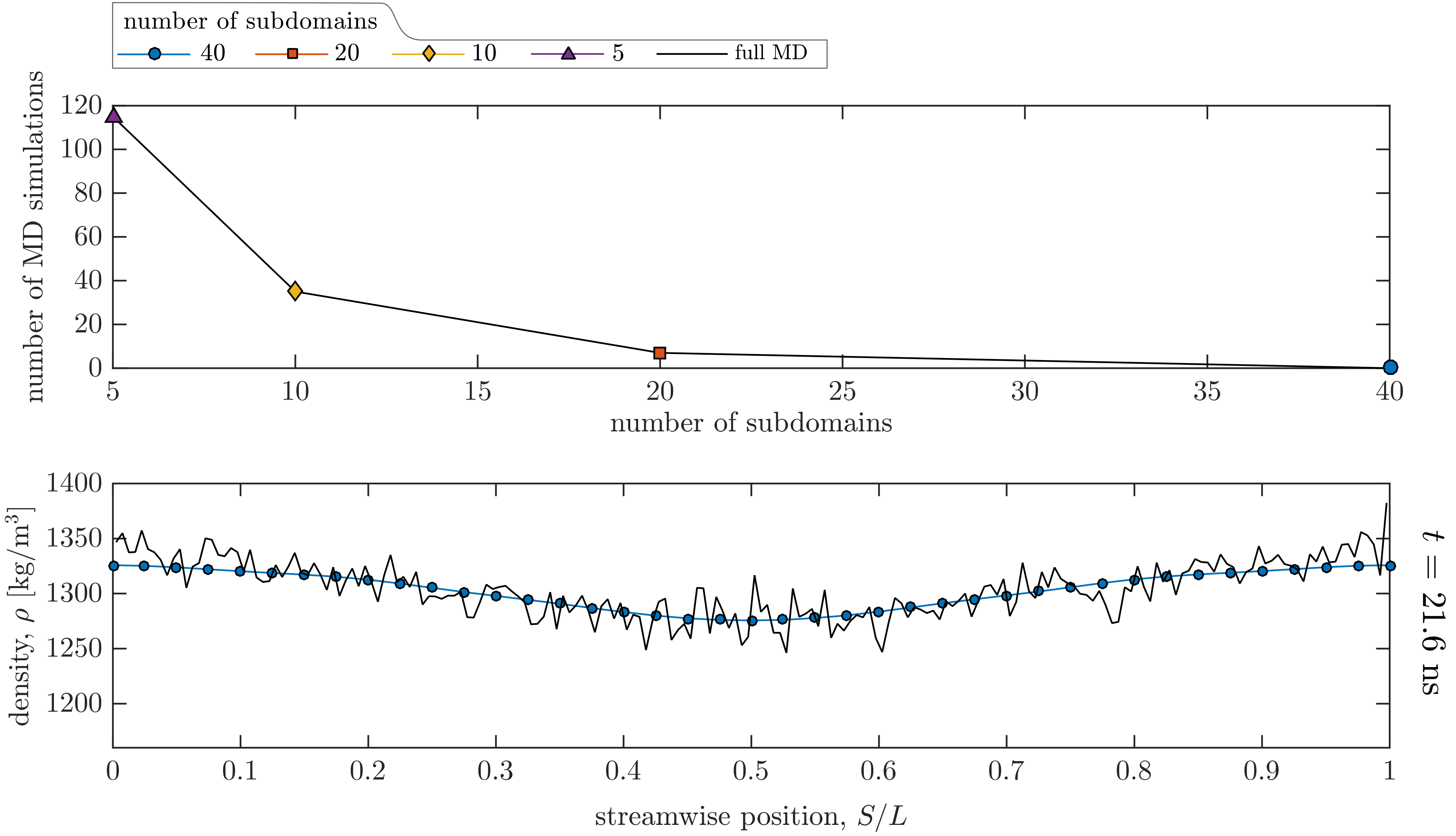
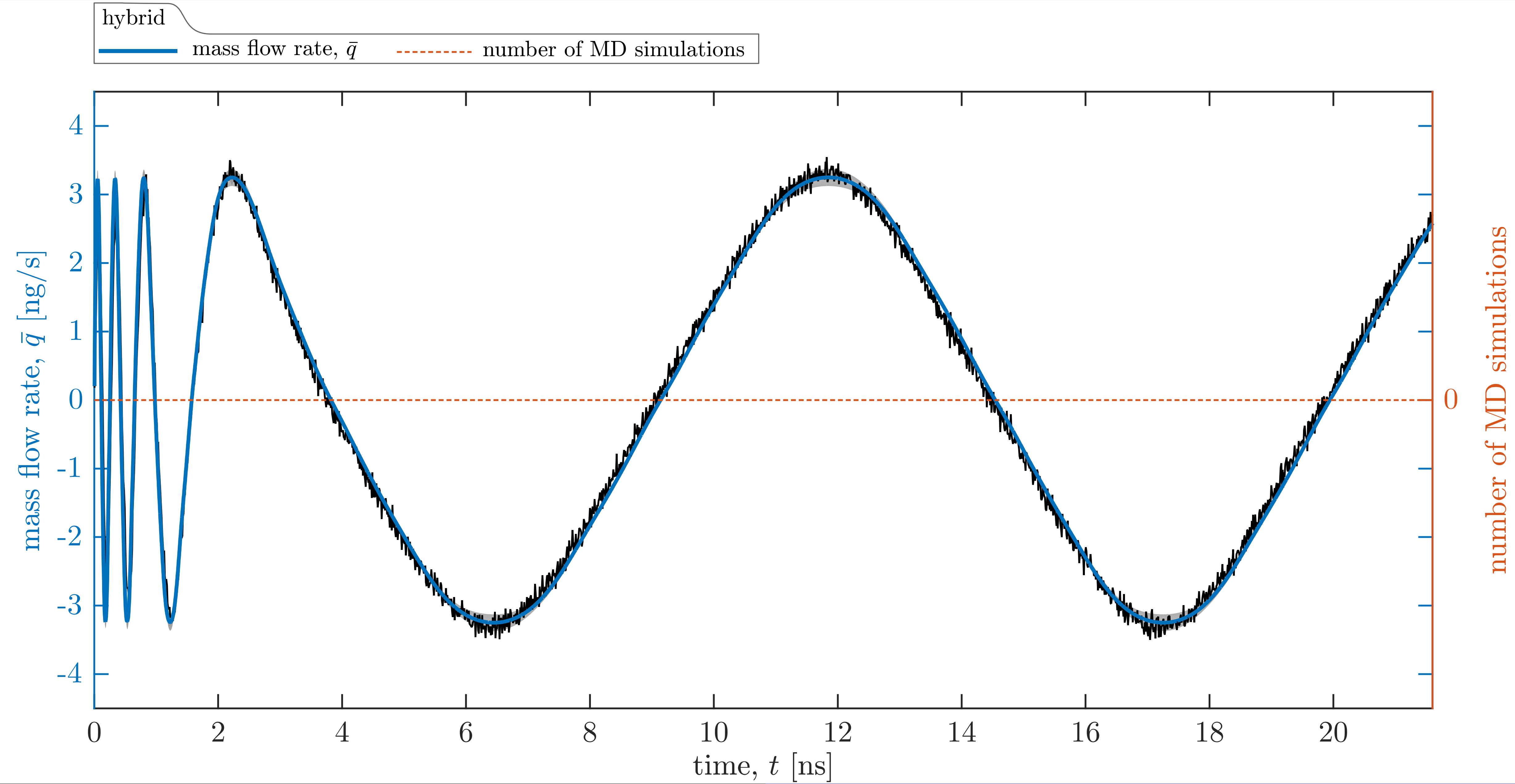


Results – expanding a database: forcing functions



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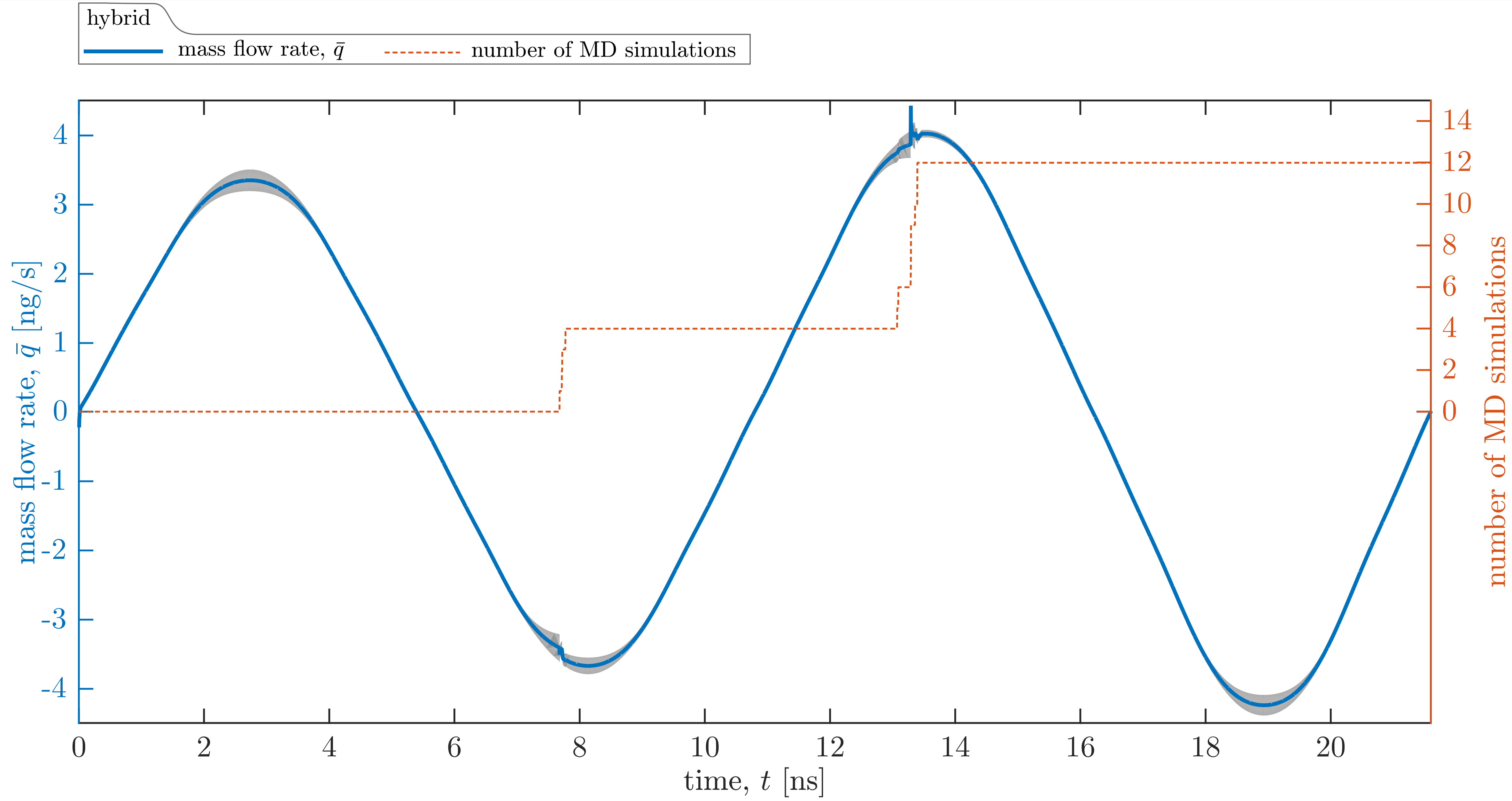

Conclusions

- Near-optimal information efficiency.
- Potential for uncertainty quantification.
- Strong agreement with full MD solutions.
- Dramatically enhanced computational speed (when database is extensive).
- Uncertainty threshold is a trade-off between accuracy and efficiency.
- Constructing an initial database is likely beneficial.
- Future work includes making the subdomain selection “smarter” and applying our algorithm to more complex engineering problems.

Thanks for listening