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Stochastic Atomistic-to-Continuum Coupling using Bayesian Inference

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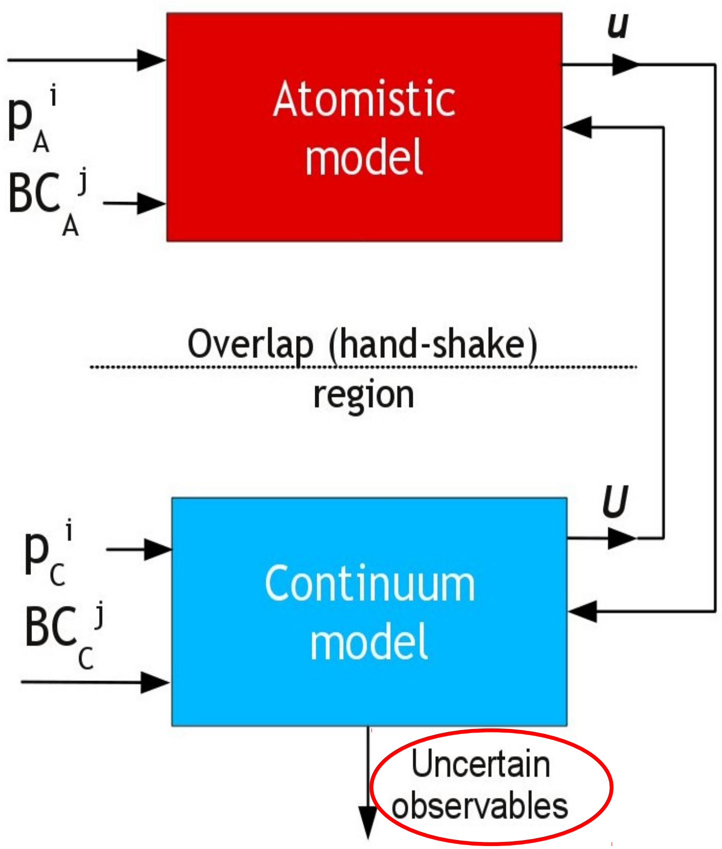
Overview

- Introduction and Motivation
  - Motivation
  - Main Objectives
  - Approach
- Quantifying Uncertainty in the Atomistic Simulation Output
  - Drawing samples from the atomistic simulation
  - Inference of the Output variable
- Application and Results
- Conclusions

Motivation

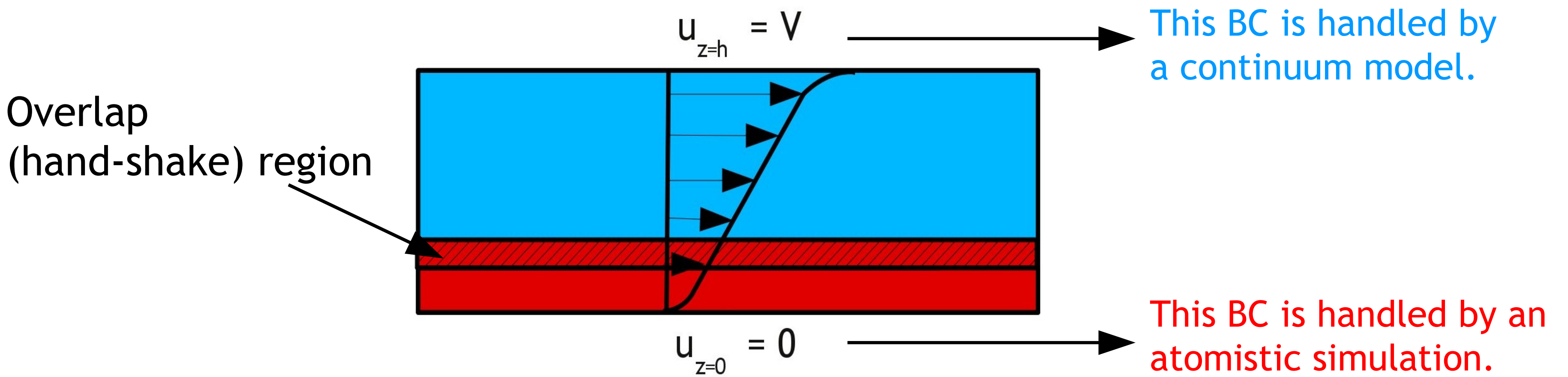
- Physical systems often require multiscale simulations to capture phenomena occurring at both bulk and interface.
- Modeling such systems requires exchange of information between the different scales.
- Uncertainty quantification is needed in order to get a predictive fidelity of the multiscale simulation.



Based on all inputs into the simulation, what is the resulting uncertainty in the predicted value of the coupling variables?

The main objective is to quantify uncertainty of an atomistic simulation output in a stochastic coupled multiscale setting.

We develop and validate a theoretical framework for stochastic multi-scale coupling based on a simple plane Couette flow.

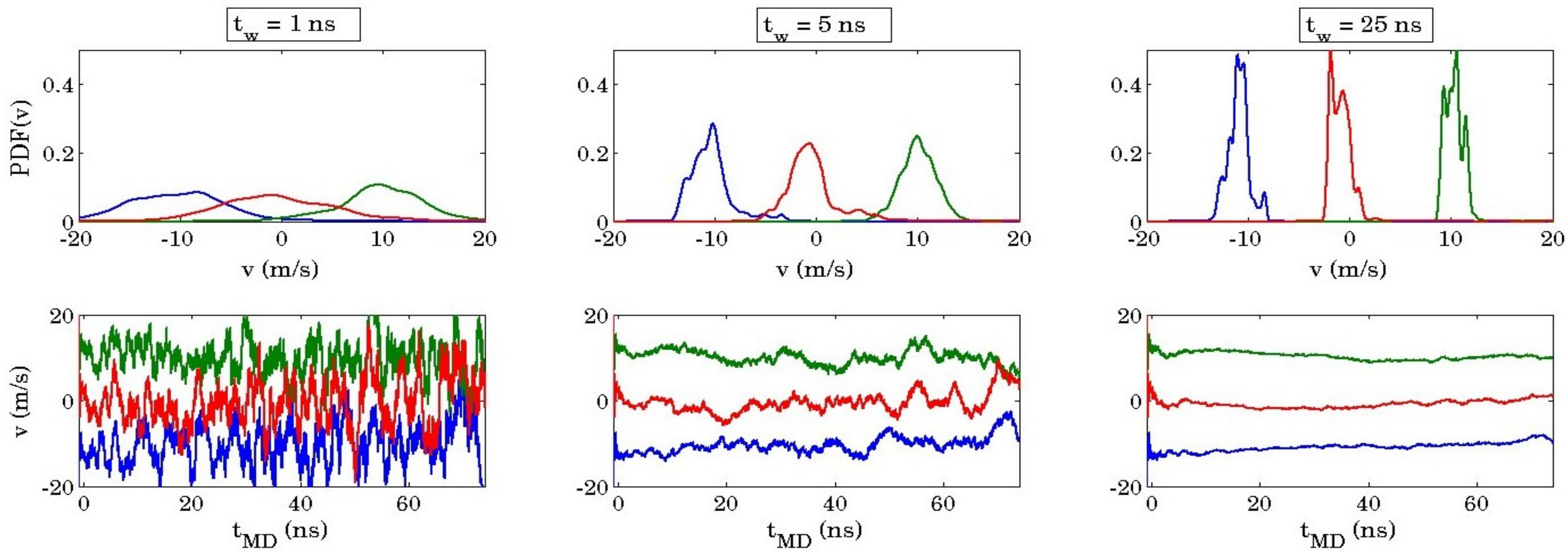


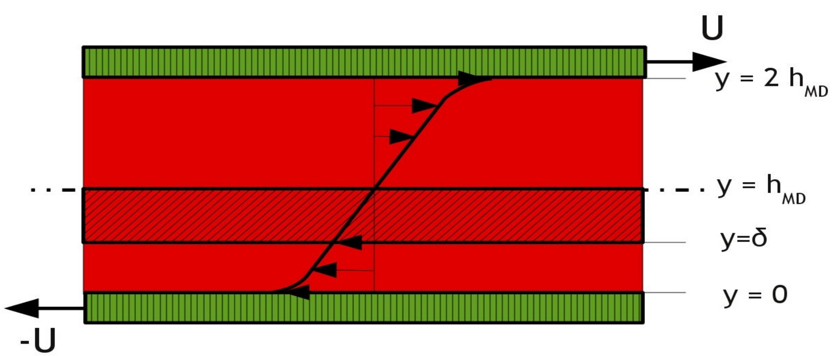
A simple plane Couette flow

Benefits of studying a simple Couette flow:

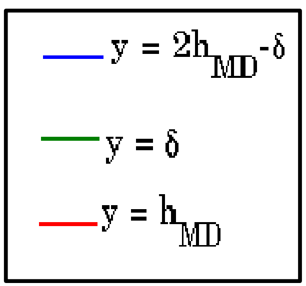
- Analytical solution available on the continuum level
- Sufficiently simple for methods development and validation
- Sufficiently complex to address all hurdles towards the final solution

Atomistic simulations output is uncertain due to Molecular Dynamics (MD) finite sampling.





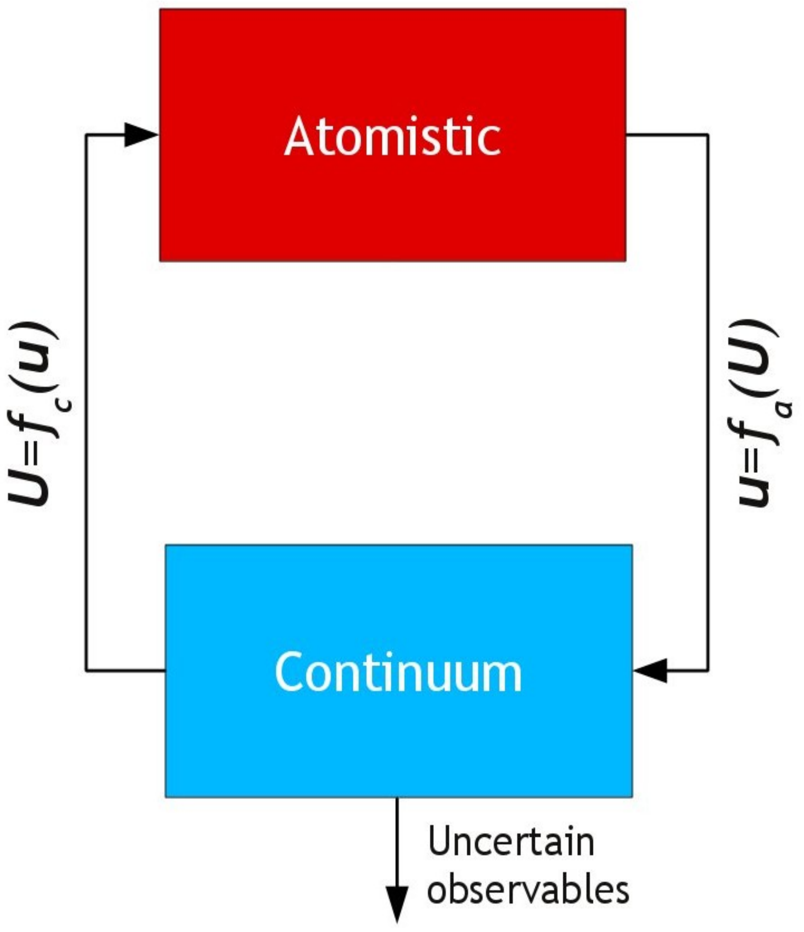
t_w = time averaging window width
U = 20 m/s



Stochastic coupling is needed in order to feed uncertainty back to continuum.

In order to evaluate any uncertain observable, we first evaluate the exchanged variables and their uncertainty between the atomistic and continuum models.

- To this end, we focus on the uncertainty due to MD noise and finite sampling.
- We use Polynomial Chaos Expansions (PCE) to express the uncertain variables ***u*** and ***U***.
- We use Bayesian inference to propagate uncertainty in an atomistic simulation and to compute the PCE model of $\boldsymbol{u}=f_a(\boldsymbol{U})$.
- We then iterate between the atomistic and continuum simulations until convergence.



Polynomial Chaos Expansions (PCE) are used in uncertainty quantification for an efficient representation of a random variable

Let X be a random variable with finite variance.

$$X : \Omega \rightarrow \mathbb{R}$$

$$X(\omega) = \sum_{k=0}^{\infty} X_k \Psi_k(\xi_1, \xi_2 \ldots \xi_{N_d})$$

$\{\xi_i\}_{i=1}^{N_d}$ are *i.i.d.* random variables (e.g., Gaussian)

$\{\Psi_k\}_{k=0}^{\infty}$ are multivariate orthogonal polynomials (e.g., Hermite)

We truncate the expansion at order N_o and dimension N_d such that:

$$X = \sum_{k=0}^{P} X_k \Psi_k(\boldsymbol{\xi}) \qquad P+1 = \frac{(N_d + N_o)!}{N_o! \, N_d!}$$

Bayesian Inference

Let *m* be a hypothesis and *D* observed data.

Posterior Likelihood Prior

$$\mathcal{P}(m|D) = \frac{\mathcal{P}(D|m)\mathcal{P}(m)}{\int \mathcal{P}(D|m)\mathcal{P}(m)dm}$$

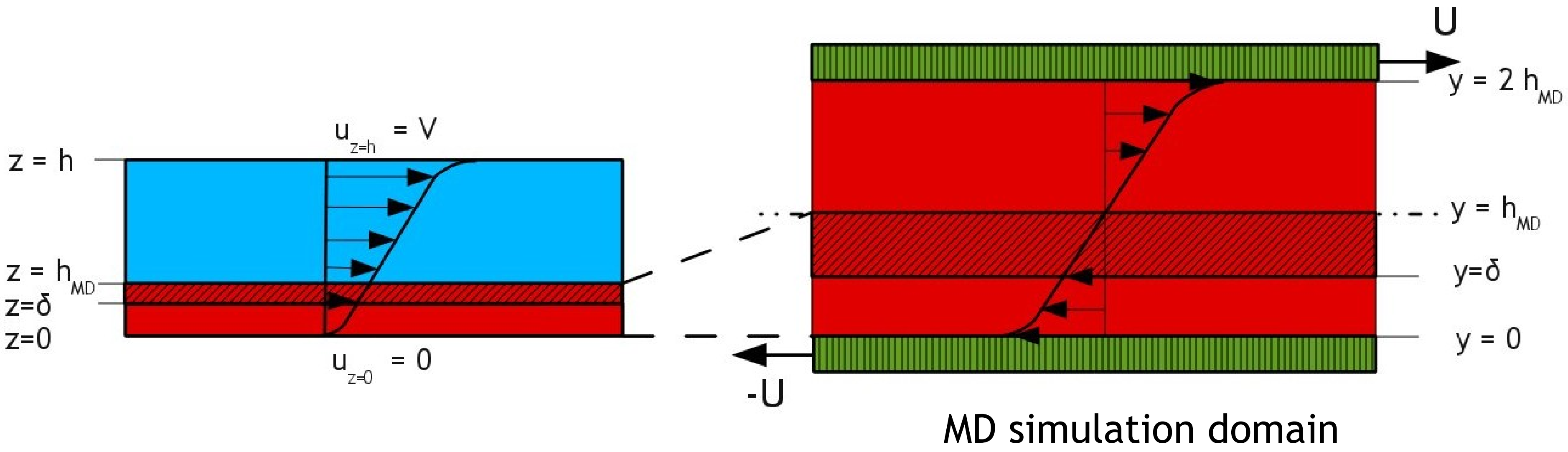
• The prior expresses the initial knowledge about the hypothesis *m* (*e.g.* uniform distribution, expert's knowledge...)

• The likelihood is the probability of observing the data *D* given the hypothesis *m*. It encompasses the forward model of *m*.

• The denominator is a normalization constant.

• The posterior is the probability of the hypothesis *m* given the data *D* : offers an enhanced knowledge of *m*.

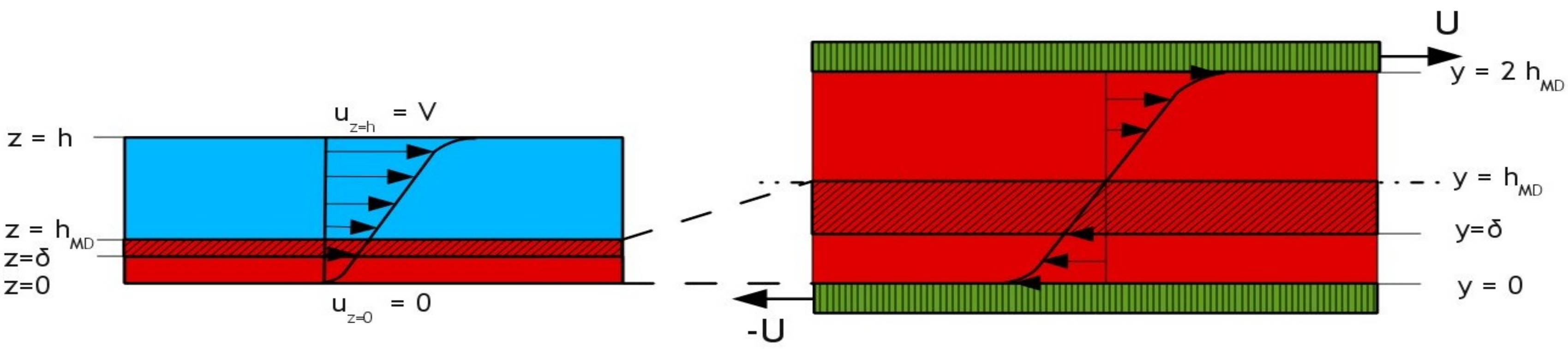
Variables exchange between continuum and atomistic models within the overlap region



• A velocity *u* is extracted from the atomistic simulation at y=δ and imposed on continuum at z=δ.

• A velocity *U* is evaluated by the continuum model at $z=h_{MD}$ and it is imposed on the atomistic simulation at y=0 and $y=2h_{MD}$ (in opposite directions)

Propagating of uncertainty in a MD simulation

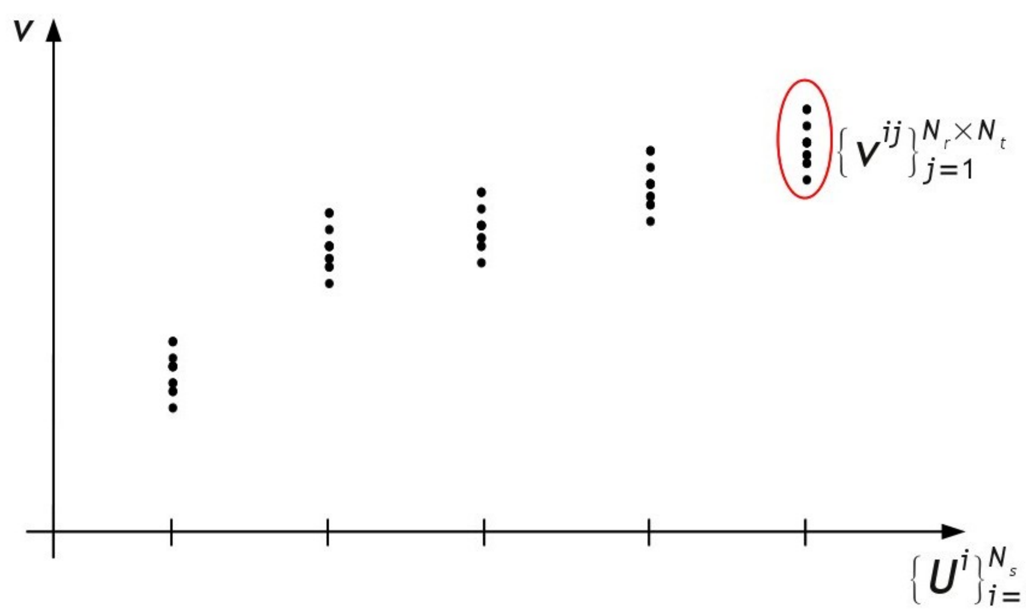


1) We draw N_s samples U_i from the PCE of ***U*** based on quadrature points.

2) For each sample U_i, we perform N_r replica MD simulations.

3) From each replica MD simulation, we draw N_t samples v^{ij}.

4) **We use all these $N_s \times N_r \times N_t$ values of v as data D_v to infer the PCE of u.**

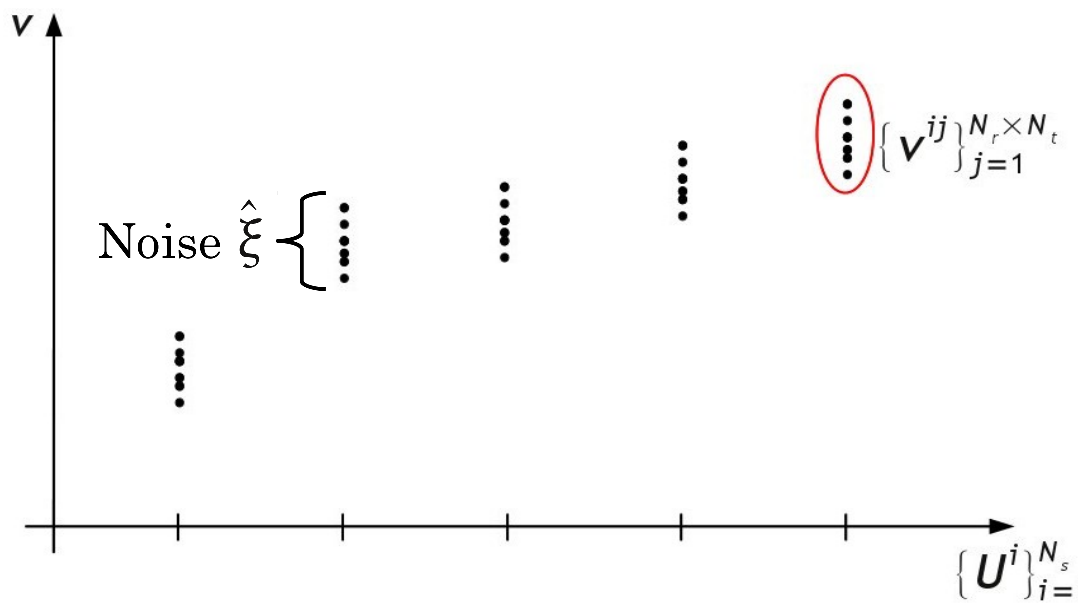


Inferring the Output Variable

$$\mathcal{P}(\tilde{\boldsymbol{u}}, \sigma^2 | D_v) \propto \mathcal{P}(D_v | \tilde{\boldsymbol{u}}, \sigma^2)\mathcal{P}(\tilde{\boldsymbol{u}}, \sigma^2)$$

$$v = \sum_{k=0}^{P} \tilde{u}_k \Psi_k(\xi) + \underbrace{\sigma\hat{\xi}}_{\text{Noise term}}$$

We draw samples from the posterior using Markov Chain Monte Carlo (MCMC) sampling.



ξ relates to the spread in U^i

Folding the input uncertainty and the sampling noise into one uncertain output

After marginalizing over σ^2, we obtain a joint posterior on the $\{\tilde{u}_k\}_{k=0}^{P}$:

$$\tilde{u} = \sum_{k=0}^{P} \tilde{u}_k \Psi_k(\xi)$$

We approximate $\{\tilde{u}_k\}_{k=0}^{P}$ as a Multivariate Normal Distribution (MVN) as follows:

$$\{\tilde{u}_k\}_{k=0}^{P} \sim \mathcal{MVN}(\boldsymbol{\mu}, \Sigma) = \boldsymbol{\mu} + L\boldsymbol{\zeta} \quad \text{where} \quad L^T L = \Sigma$$

We obtain:

$$\tilde{u} = \boldsymbol{\Psi}(\xi)^T \cdot \boldsymbol{\mu} + \zeta \sqrt{\boldsymbol{\Psi}(\xi)^T \cdot \Sigma \cdot \boldsymbol{\Psi}(\xi)}$$

Folding the input uncertainty and the sampling noise into one uncertain output

$$\tilde{u} = \mathbf{\Psi}(\xi)^T \cdot \boldsymbol{\mu} + \zeta \sqrt{\mathbf{\Psi}(\xi)^T \cdot \Sigma \cdot \mathbf{\Psi}(\xi)}$$

This expression of $\tilde{u}$ is "cheap" for sampling in ζ and ξ !

Inverse Cumulative Distribution Function (CDF) transform

- $F(.)$ is the CDF of $\tilde{u}$

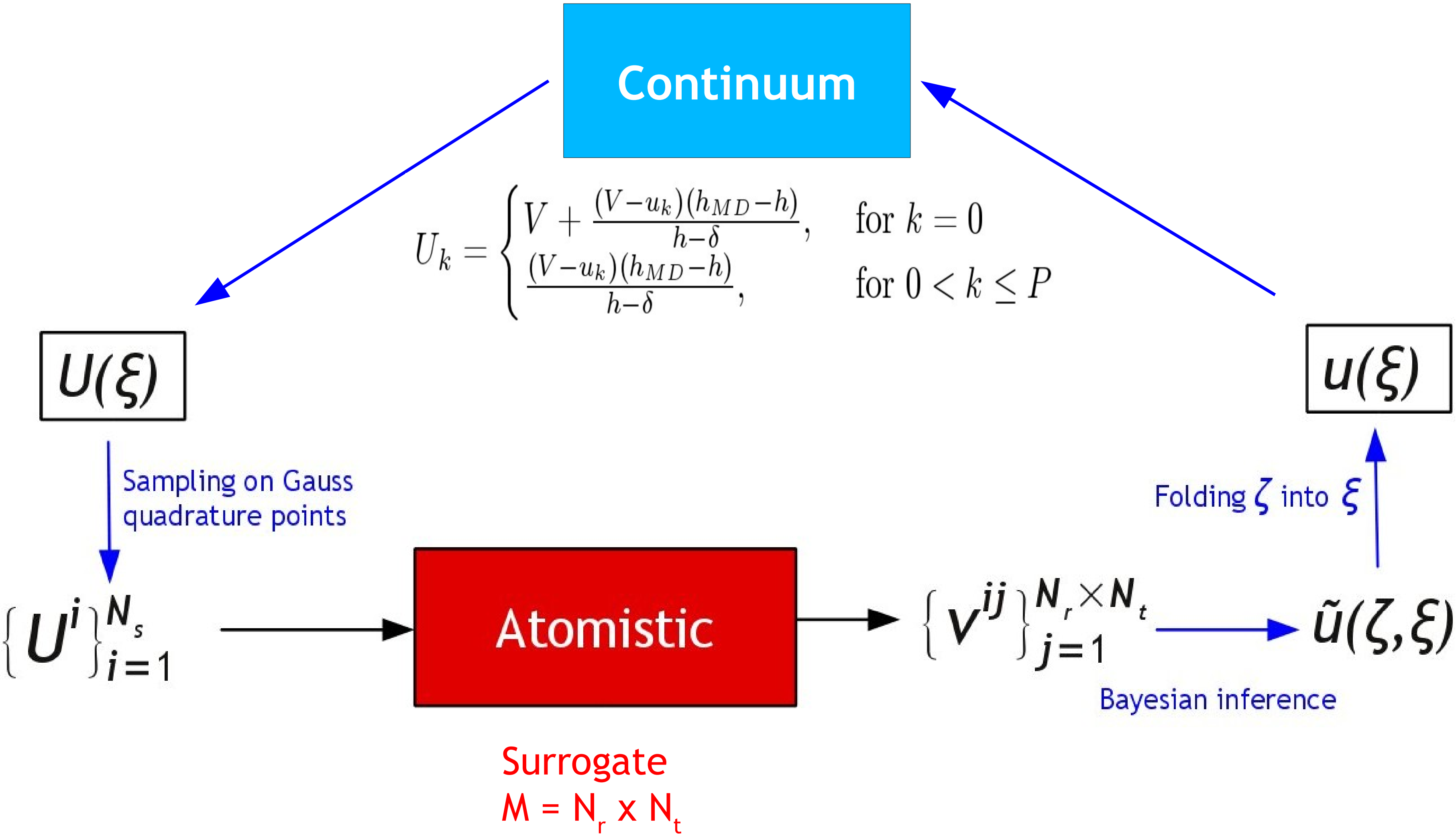
$$u_k = \frac{\langle F^{-1}(\Phi(\xi))\Psi_k(\xi)\rangle}{\langle \Psi_k(\xi)^2 \rangle}$$

$$u = \sum_{k=0}^{P} u_k \Psi_k(\xi)$$

ξ is the degree of freedom associated with the sampling noise

Summary of the Different Steps for Coupling

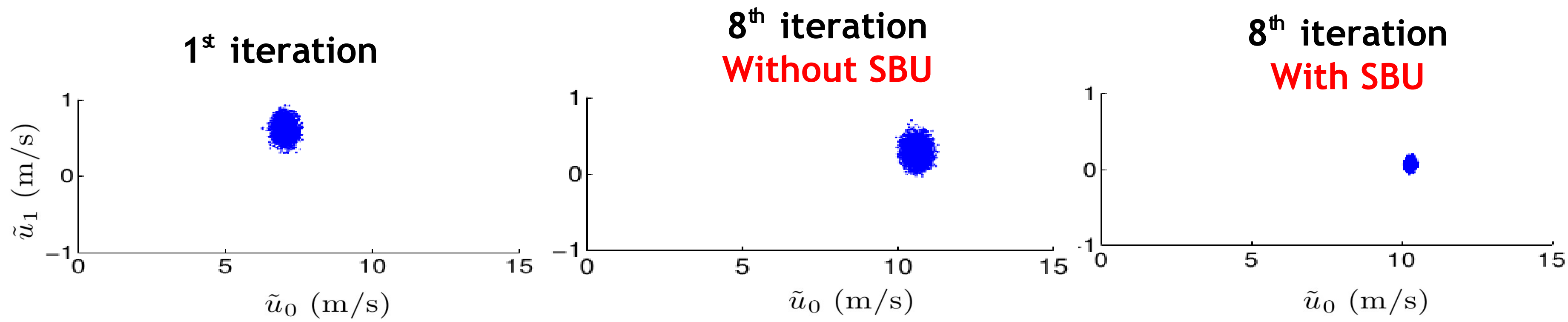
Laminar Newtonian Couette flow
The analytical solution is available

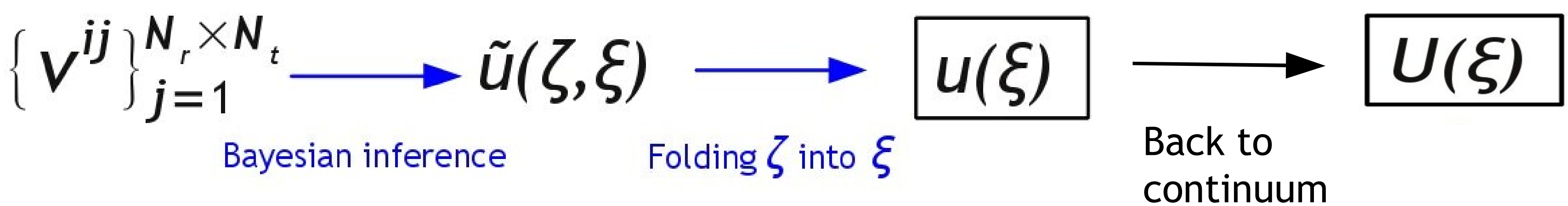


$$U_k = \begin{cases} V + \frac{(V-u_k)(h_{MD}-h)}{h-\delta}, & \text{for } k = 0 \\ \frac{(V-u_k)(h_{MD}-h)}{h-\delta}, & \text{for } 0 < k \leq P \end{cases}$$

$$\{U^i\}_{i=1}^{N_s} \qquad \{V^{ij}\}_{j=1}^{N_r \times N_t} \qquad \tilde{u}(\zeta,\xi)$$

Joint Posterior of $\{\tilde{u}_0, \tilde{u}_1\}$

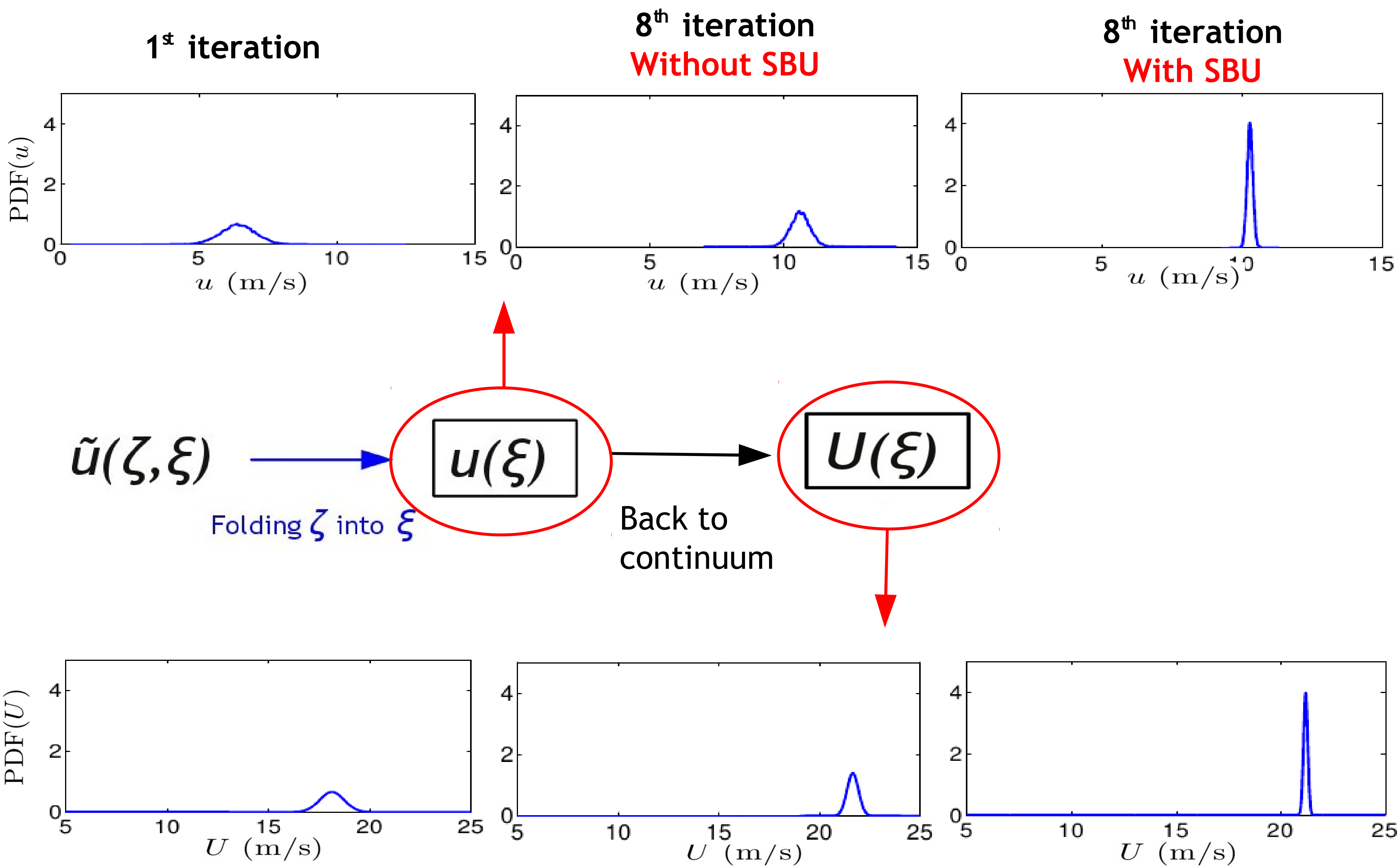




Sequential Bayesian Updating (SBU)

The posterior of the previous iteration is used as the prior in the current iteration.

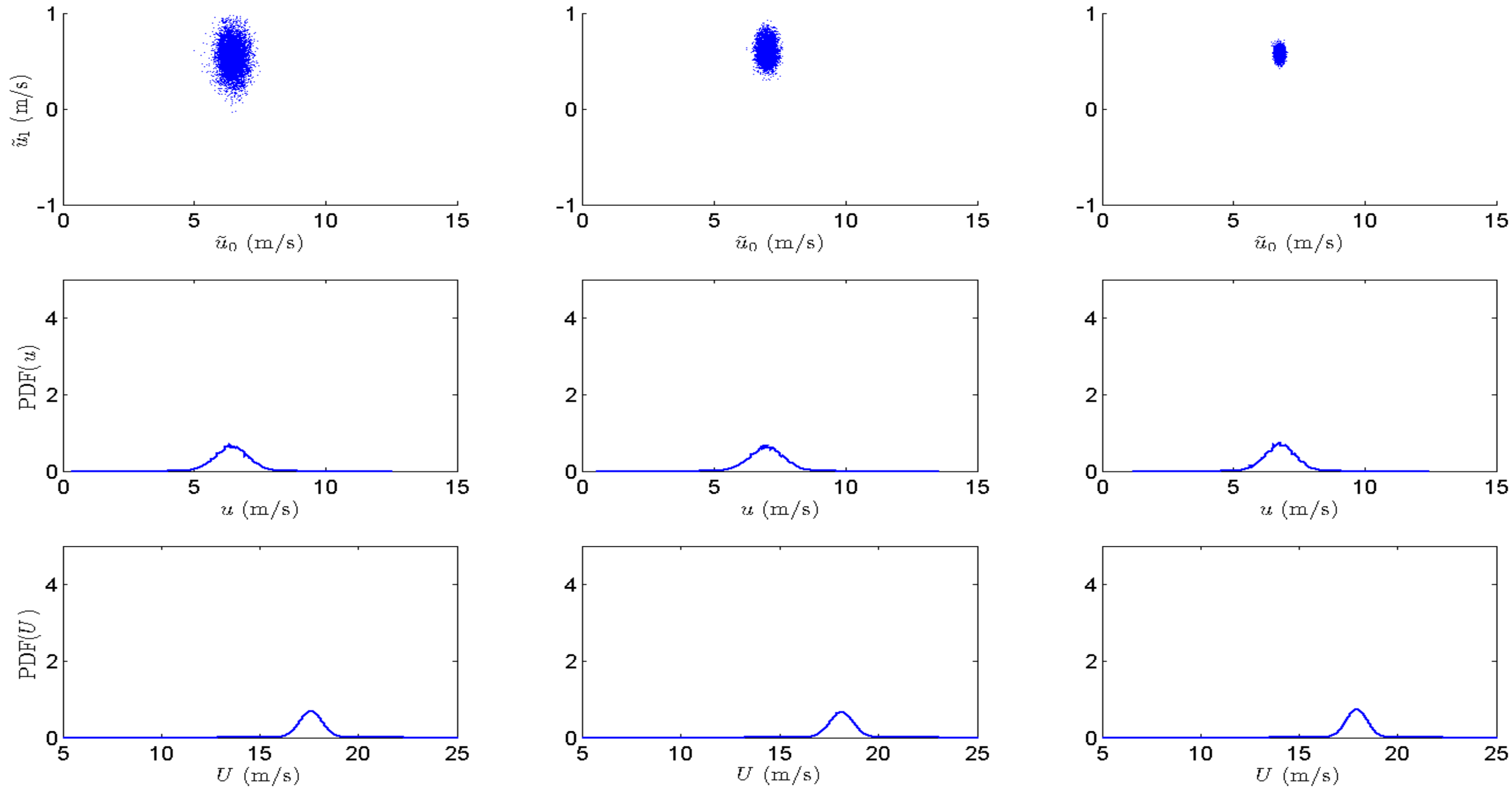
PDFs of *u* and *U*



Stochastic Coupling Algorithm Convergence *Without* SBU

t_w = Time averaging window width

t_w=1 ns　　t_w=5 ns　　t_w=25 ns



Stochastic Coupling Algorithm Convergence *With* SBU

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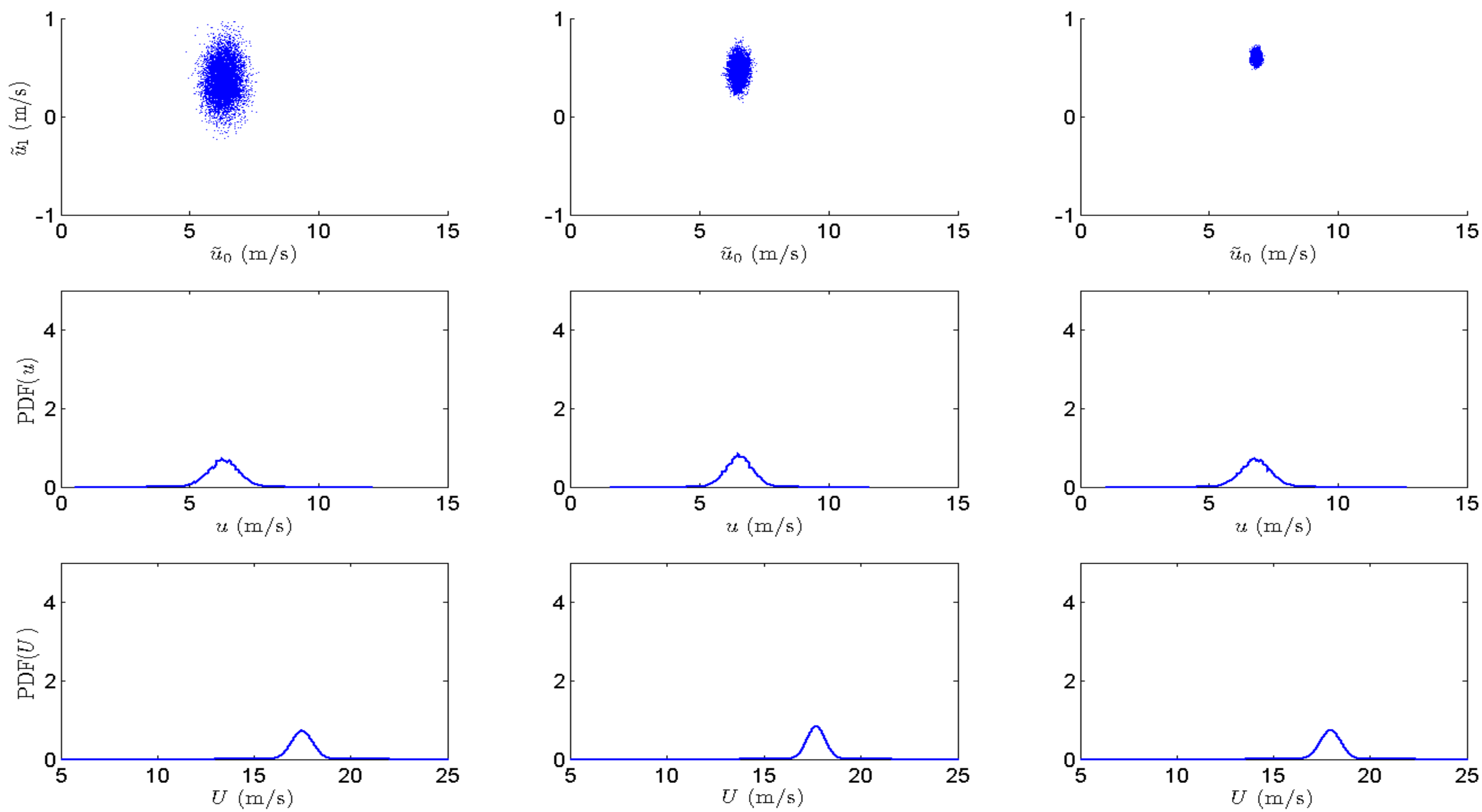
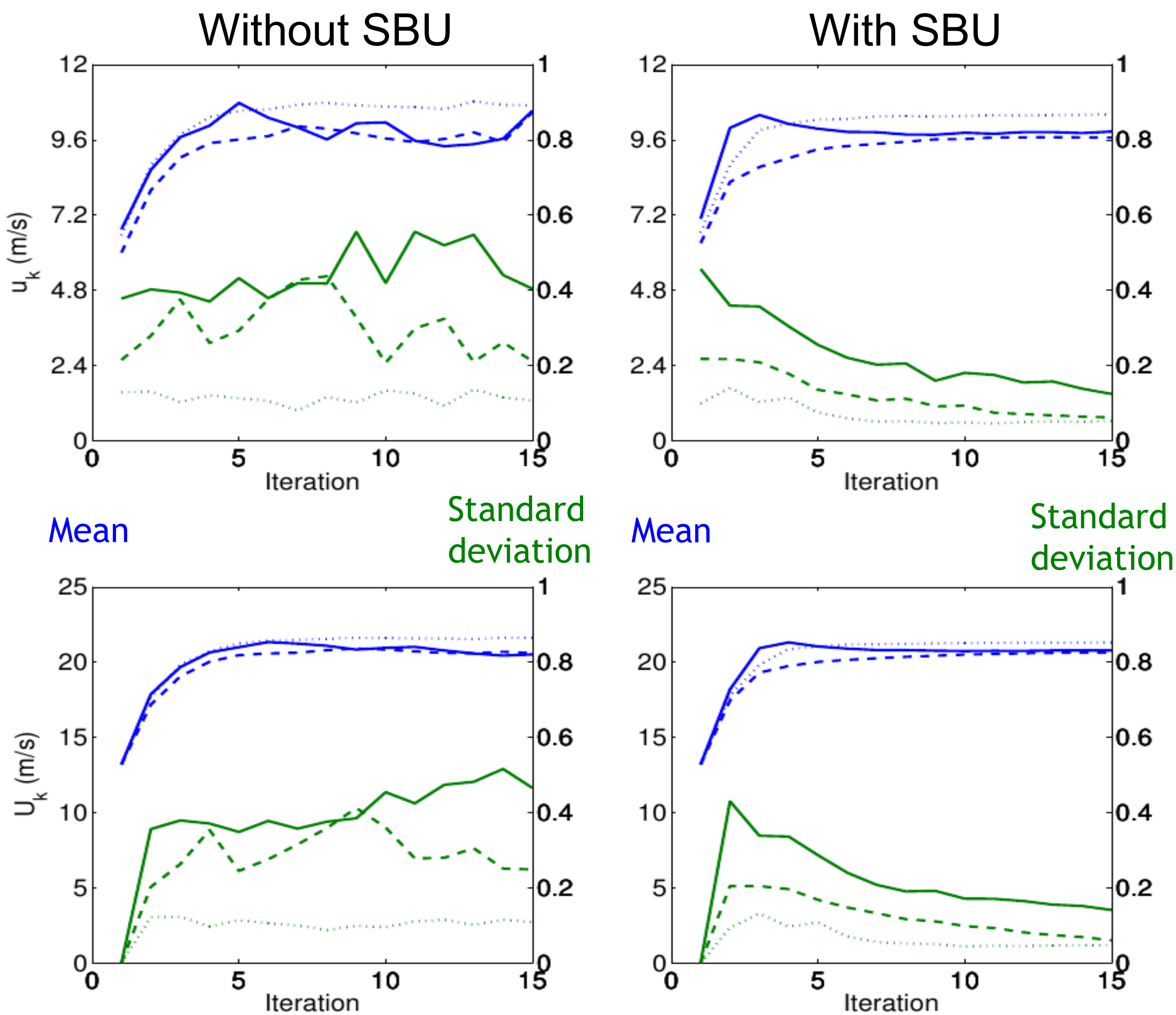


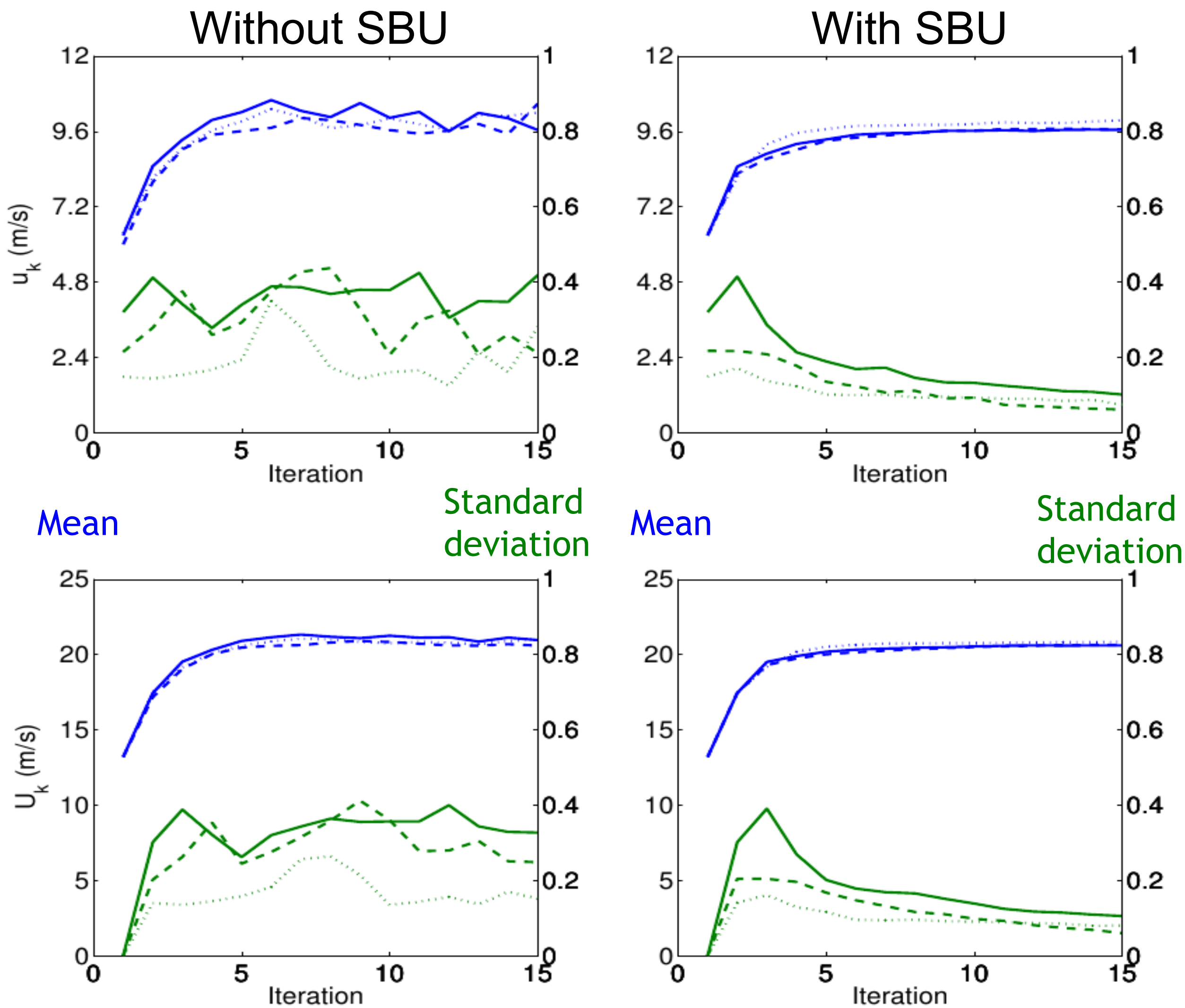
Effect of the time averaging window t_w on the convergence of the mean and standard deviation

Solid: t_w=1 ns Dashed: t_w=5 ns Dotted: t_w=25 ns



Effect of the number of samples *M* on the convergence of the mean and standard deviation

Solid: M=10 Dashed: M=20 Dotted: M=40



Conclusions

- Uncertainty quantification enables predictive modeling of multi-scale systems.
- We showed a method to derive the PCE of a variable extracted from MD simulations.
- We developed an algorithm that couples atomistic and continuum simulation models through variable exchange in terms of PCEs.
- The coupling iterative algorithm converges in a reasonable number of iterations.
- Sequential Bayesian Updating enhances the accuracy of the converged variables by including additional data at each iteration.

Acknowledgments

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- Omar Knio (JHU)
- Kevin Long (TTU)
- Youssef Marzouk (MIT)

THANK YOU FOR YOUR ATTENTION

Questions???

Uncertainty Propagation in the Atomistic Simulation

Inferring the Output Variable

$$\mathcal{P}(\tilde{\boldsymbol{u}}, \sigma^2_{\hat{\xi}} | D_v) \propto \mathcal{P}(D_v | \tilde{\boldsymbol{u}}, \sigma^2_{\hat{\xi}}) \mathcal{P}(\tilde{\boldsymbol{u}}) \mathcal{P}(\sigma^2_{\hat{\xi}})$$

Log-likelihood function:

$$\log\left(\mathcal{P}(D_v | \tilde{\boldsymbol{u}}, \sigma^2_{\hat{\xi}})\right) = -0.5 N_s N_r N_t \left(\log(2\pi) + \log(\sigma^2_{\hat{\xi}})\right) - 0.5 \frac{\boldsymbol{d}^T \boldsymbol{d}}{\sigma^2_{\hat{\xi}}}$$

$$d_{j+(i-1)N_r N_t} = v^{ij} - \sum_{k=0}^{P} \tilde{u}_k \Psi_k(\xi_i)$$

Priors:

For the PC coefficients:

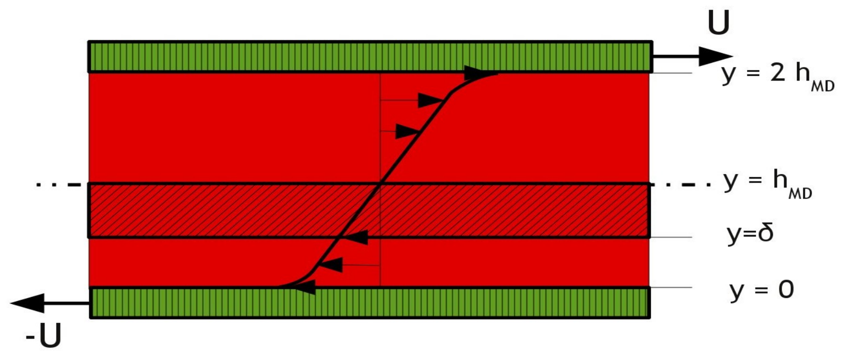
$$\mathcal{P}(\tilde{\boldsymbol{u}}) = \begin{cases} \prod_{k=0}^{P} \frac{1}{\alpha_k - \beta_k} & \text{for } \beta_k \leq \tilde{u}_k \leq \alpha_k \\ 0 & \text{otherwise} \end{cases}$$

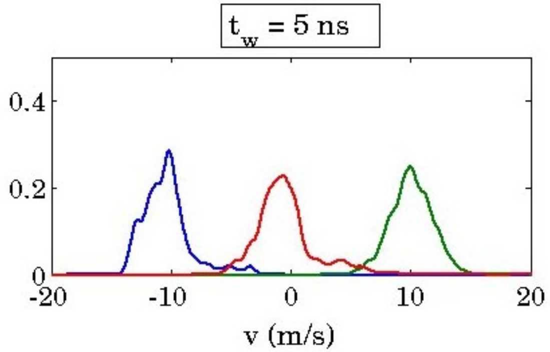
For $\sigma^2_{\hat{\xi}}$*:*

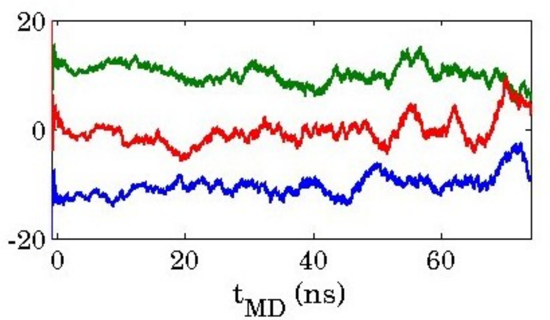
$$\mathcal{P}(\sigma^2_{\hat{\xi}}) = \begin{cases} \frac{1}{\sigma^2_{\hat{\xi}}} & \text{for } \sigma^2_{\hat{\xi}} > 0 \\ 0 & \text{otherwise} \end{cases}$$

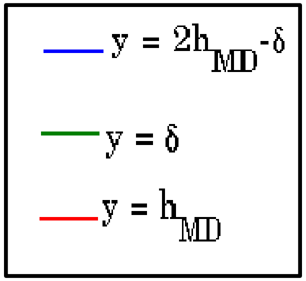
Results

Molecular Dynamics Simulations









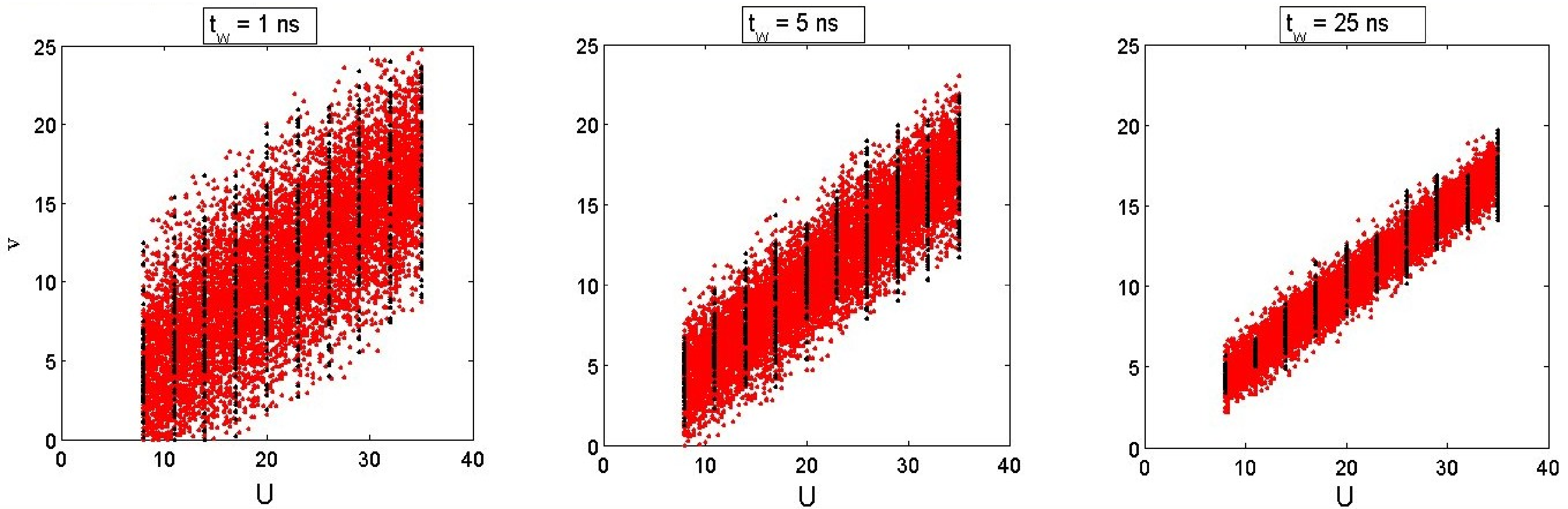
t_w = time averaging window width
U = 20 m/s

- MD simulations are a lot more expensive than continuum simulations.

- Hence, we infer a surrogate of these MD simulations and use in the coupling algorithm.

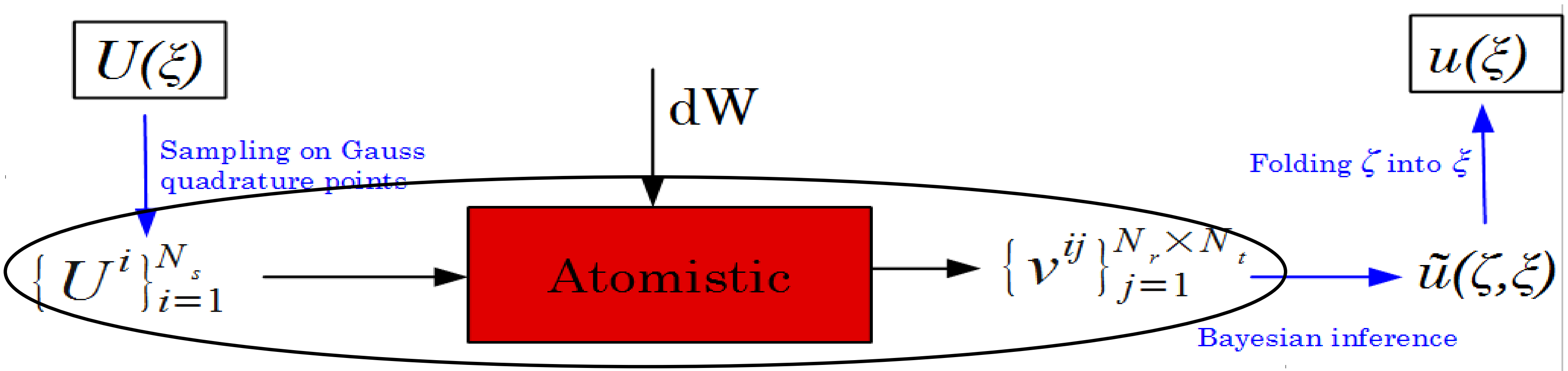
Results

MD Simulations Surrogate



t_w = Time averaging window width

For each sample of U, we now draw *M* data points from the surrogate equal to $N_r \times N_t$ data points drawn from MD simulations.



Using the MD simulations surrogate

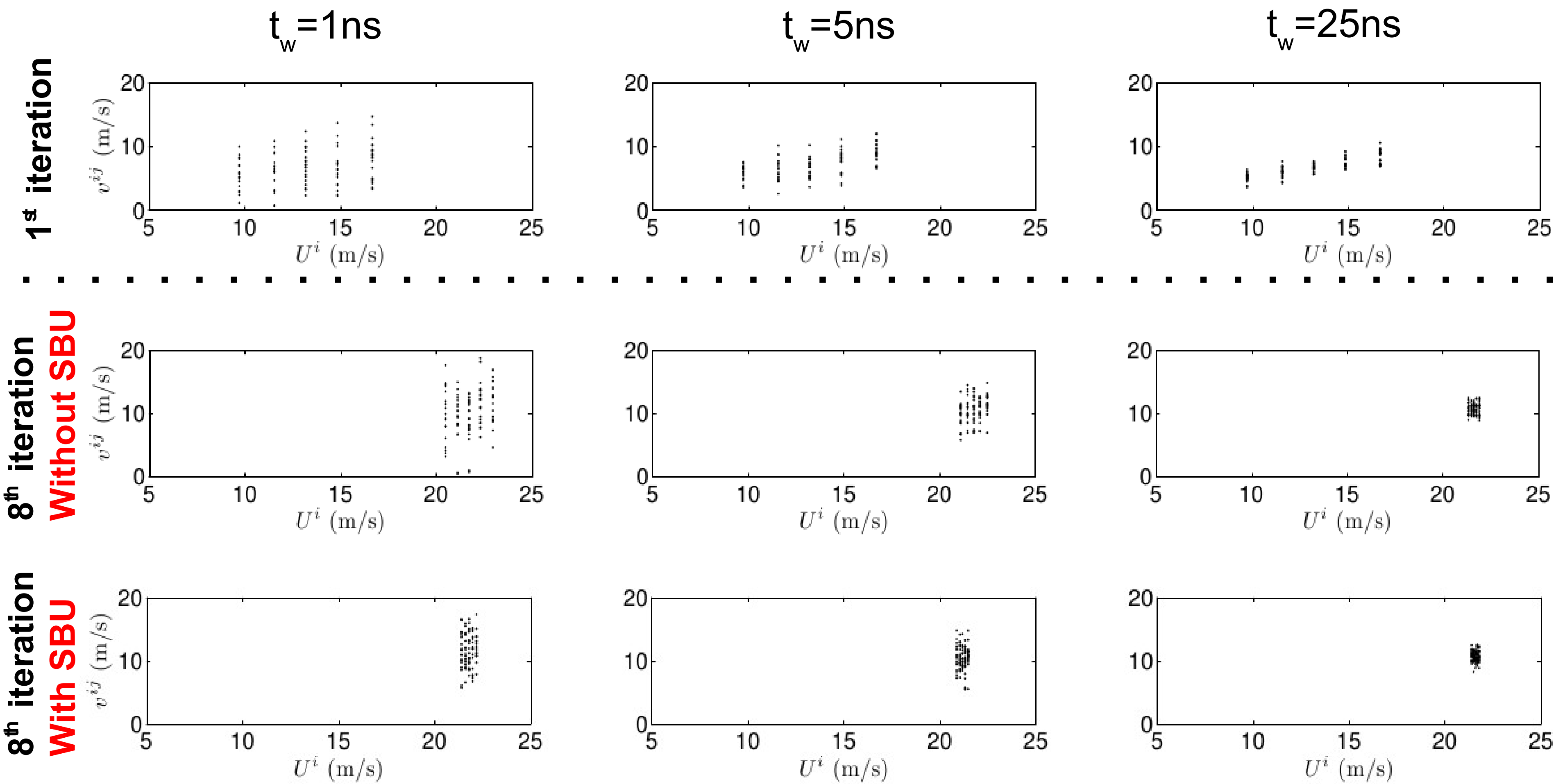
Sequential Bayesian Updating (SBU)

The posterior of the previous iteration is used as prior in the current iteration

Results

Uncertainty Propagation in the Atomistic Simulation

Inference data

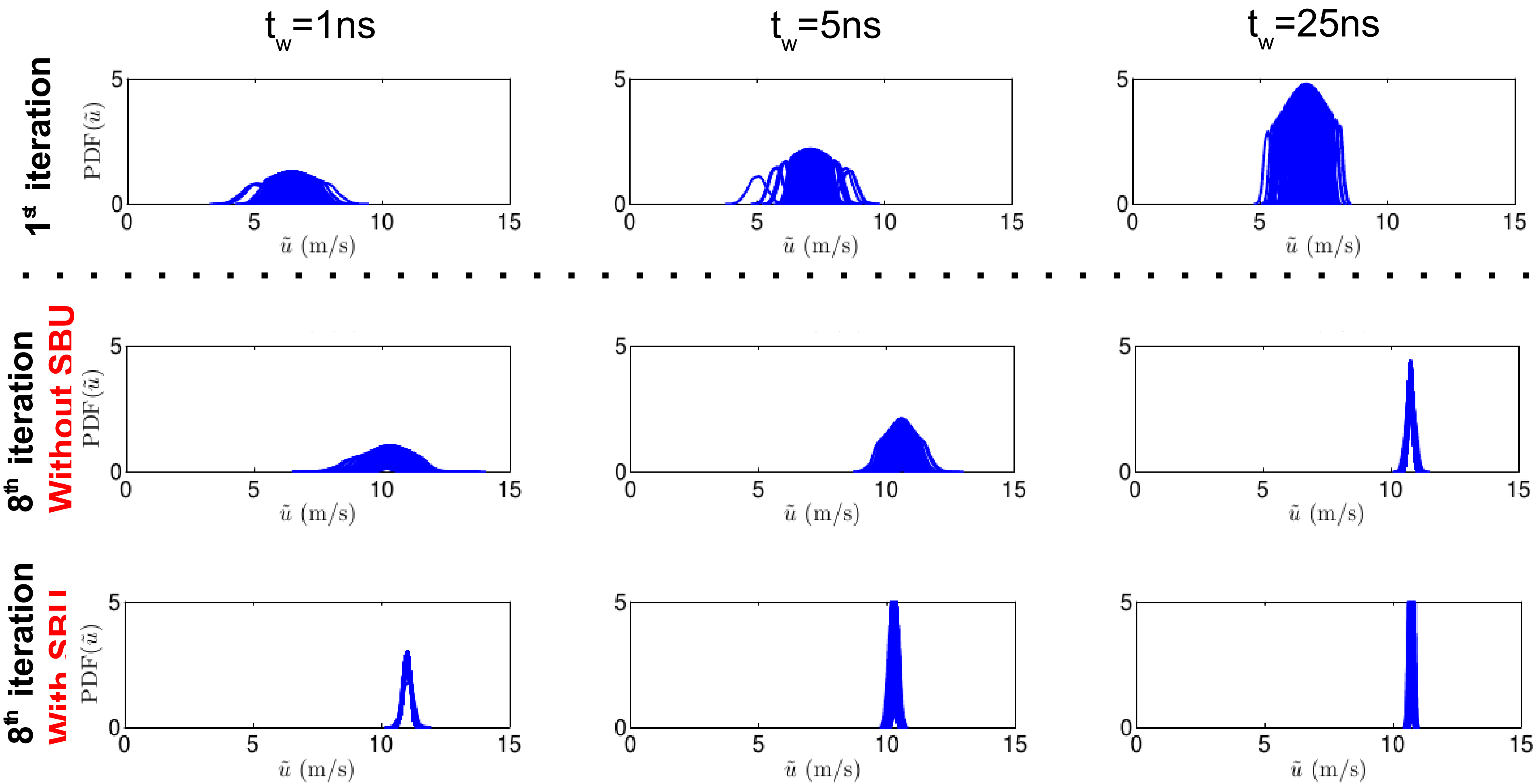


- N_s = 5
- M=20

Results

Uncertainty Propagation in the Atomistic Simulation

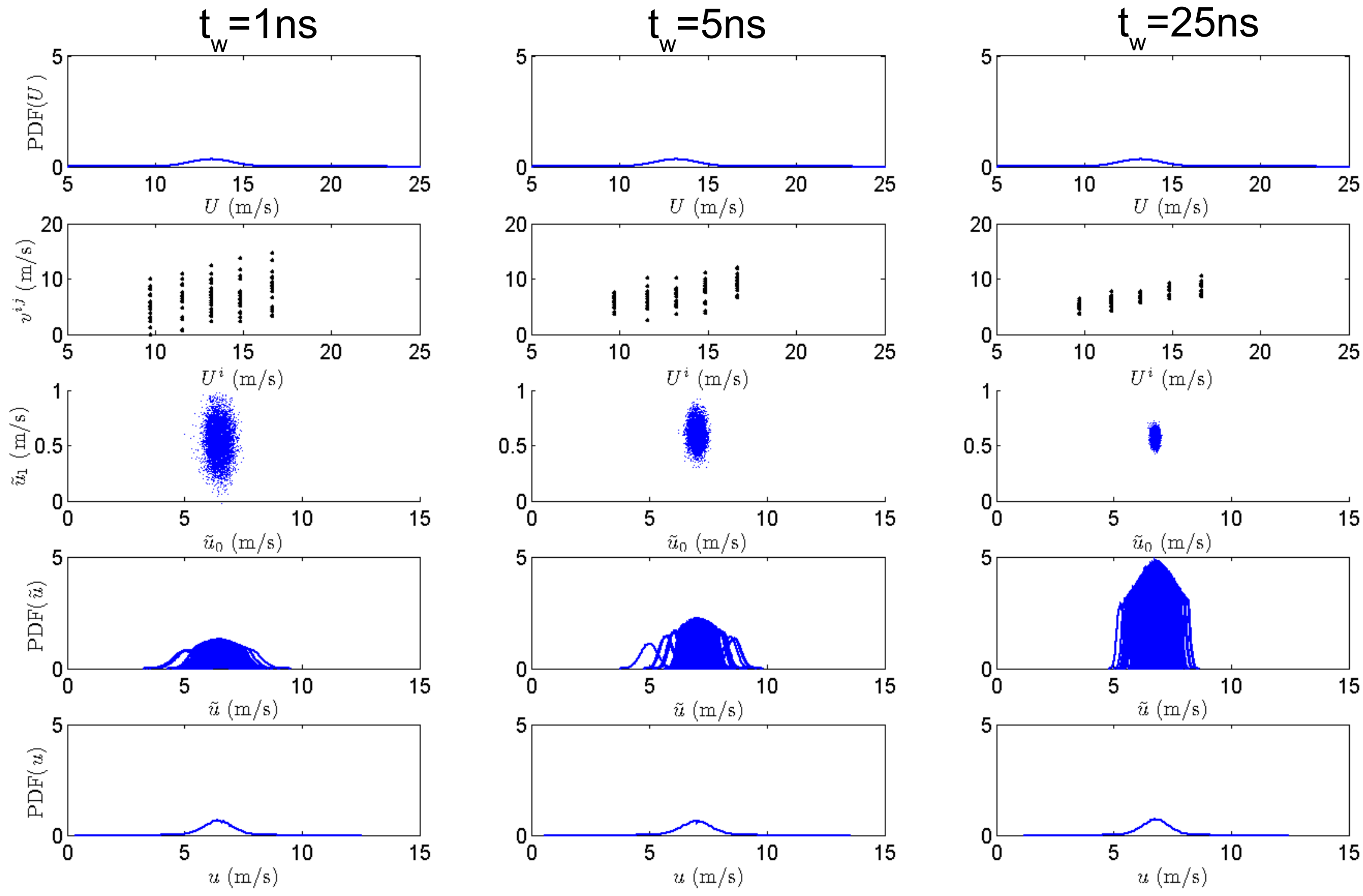
PDFs of ũ



Results

Uncertainty Propagation in the Atomistic Simulation

Without SBU (M=20)



Results

Uncertainty Propagation in the Atomistic Simulation

With SBU (M=20)