Spatial Model Aggregation (X-MA) of stochastic Explicit Algebraic Reynolds Stress models

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1. Introduction
   - Context
   - Our contribution
2. Learning of stochastic SBL-EARSM closures
   - Reynolds stress representation
   - Sparse Bayesian Learning (SBL)
   - Spatial Model Aggregation (X-MA)
3. Results
   - Training flow cases
   - Collaborative Testing Challenge

- RANS (Reynolds-Averaged Navier-Stokes) simulations for engineering, design and optimisation
  + Simplicity, low cost, robustness
  – Low fidelity
- Mostly Linear Eddy Viscosity Models (LEVM): "Boussinesq" analogy
- Non-linear corrections in the baseline LEVM:
  1. Work well for a limited set of flow cases
  2. Based on local equilibrium assumptions + some empiricism
  3. Complex coefficient expressions, numerical stiffness
  4. No information about uncertainties
- Choice of a 'best' turbulence model often based on 'expert judgement'
- Recent trends:
  - Increasing availability of high-Fidelity databases
  - Development of ML-augmented turbulence models [1][2] [3]

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GOAL:

→ Learn customized non linear eddy viscosity models for selected flow classes:

- Stochastic (equipped with measure of uncertainty)
- Physically interpretable
- Sparse (less complex, more robust, less likely to overfit)

→ Automatically combine these customized models to yield predictions better than LEVM throughout the flows of the Collaborative Testing Challenge

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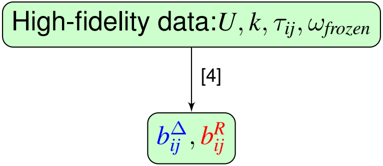
Algorithm overview

High-fidelity data: $U, k, \tau_{ij}, \omega_{frozen}$

Algorithm overview



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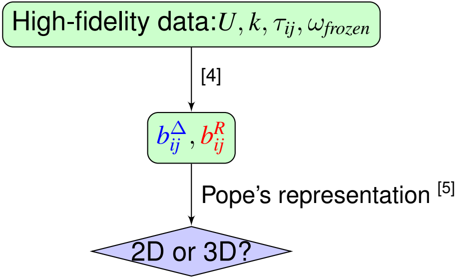

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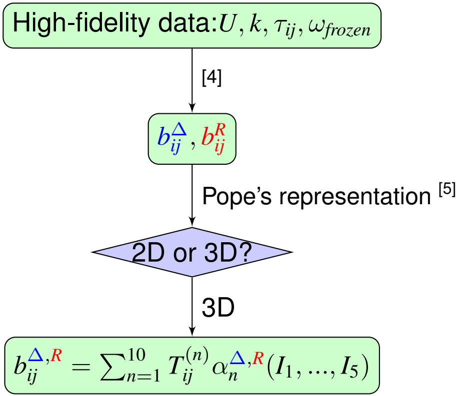

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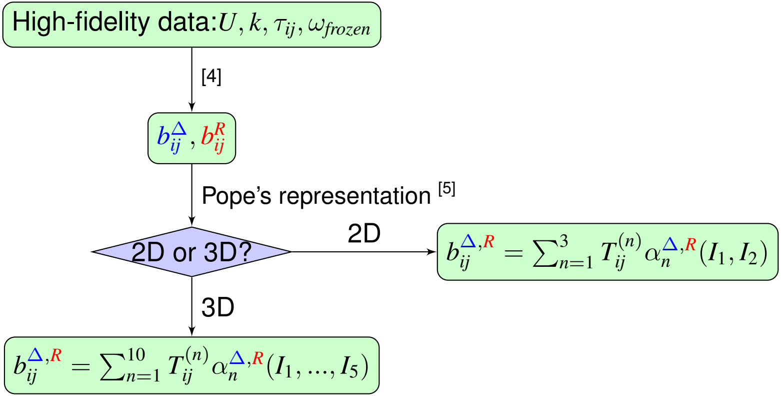

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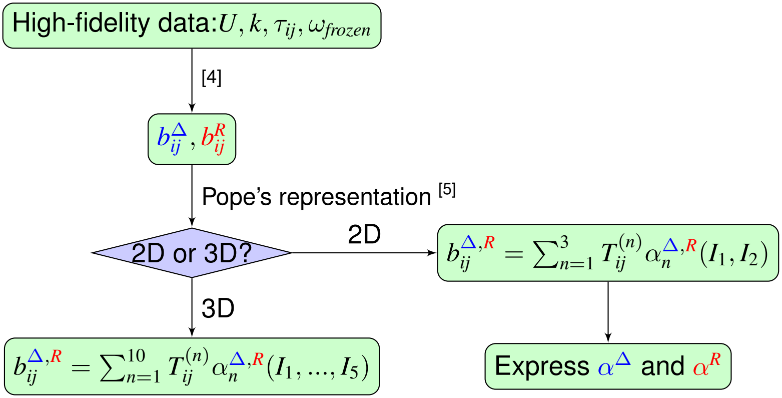

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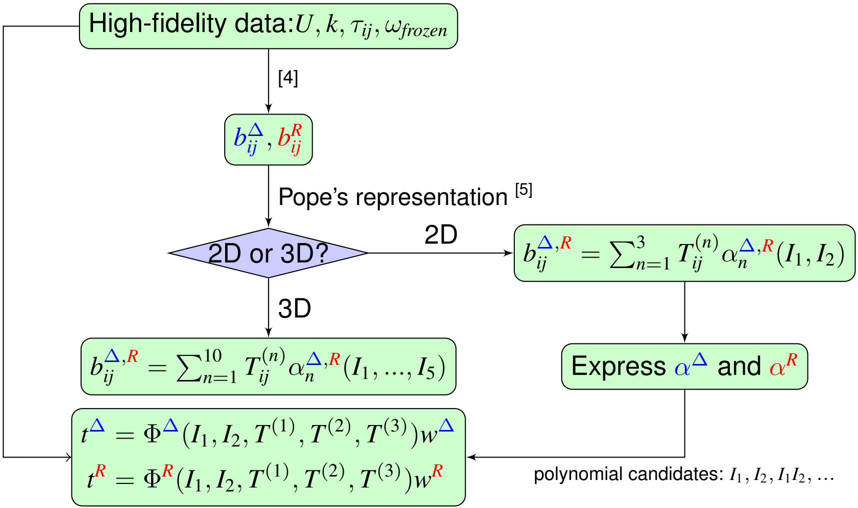

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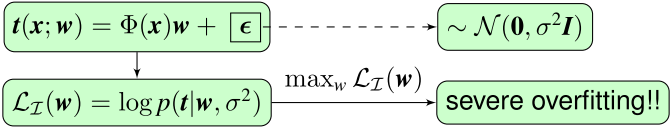

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Bayes rule

$$p(\boldsymbol{w}|\boldsymbol{t}, \boldsymbol{\alpha}, \boldsymbol{\sigma^2}) \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$$

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$$\max_{\alpha,\sigma^2}(\mathcal{L}_{\mathcal{II}}(\boldsymbol{\alpha}, \boldsymbol{\sigma^2}))$$

$$\boldsymbol{\alpha}_{MP}, \sigma^2_{MP}$$

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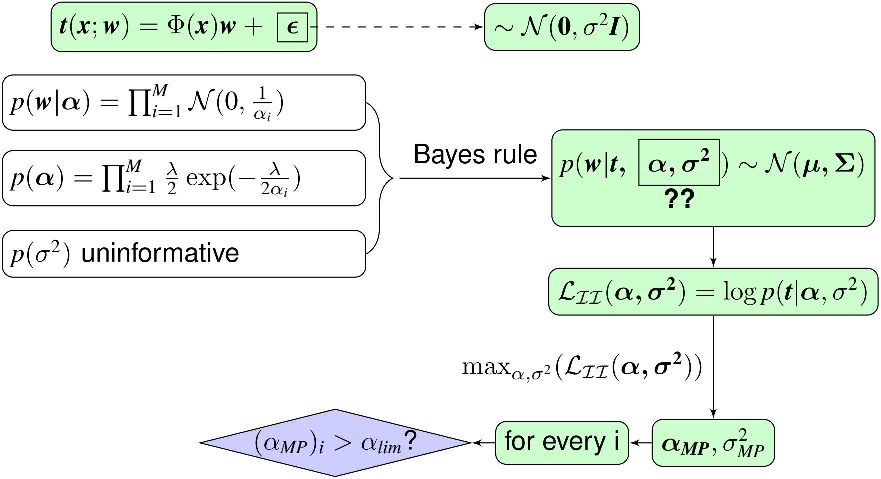

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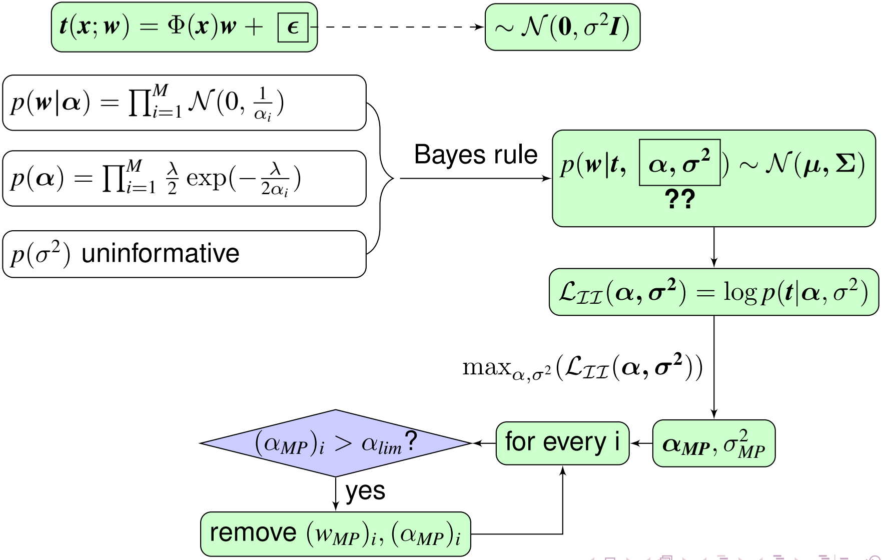

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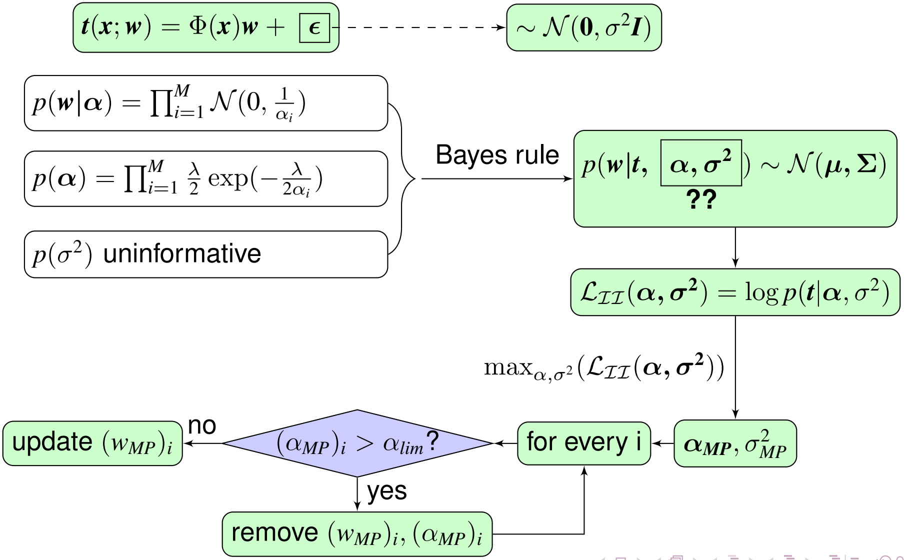

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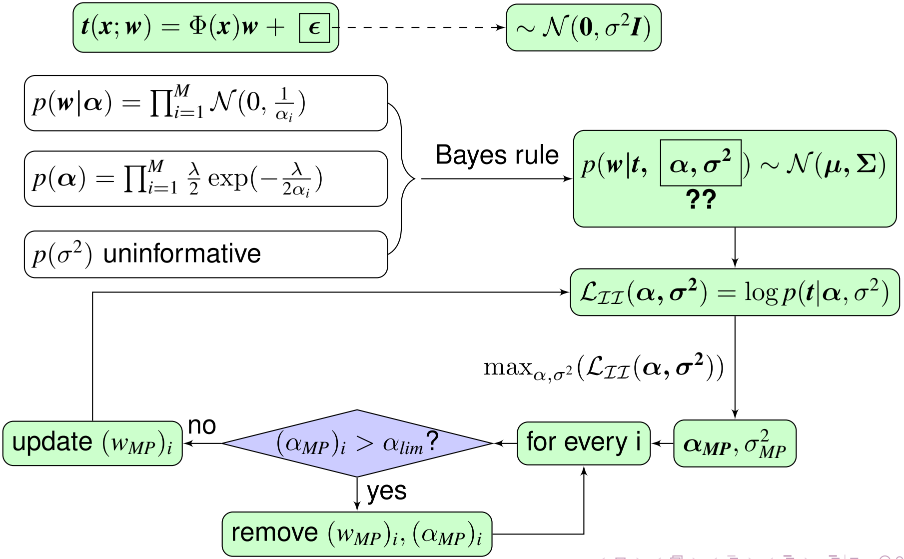
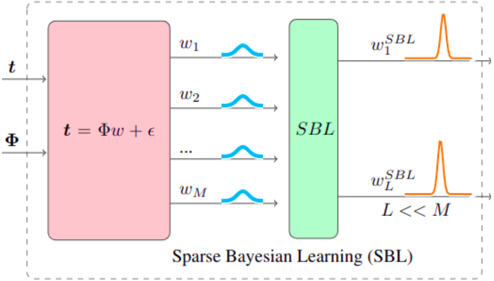
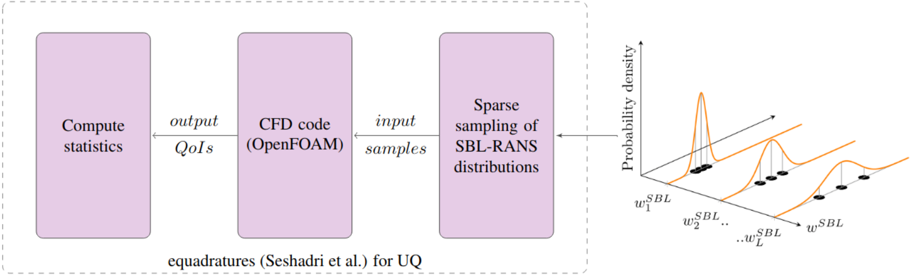


SBL - Uncertainty Quantification





Model Aggregation (MA)

Let us consider K SBL-EARSM models, learned in different environments. We **aggregate** their individual solutions d_k to produce robust predictions of new flows

- **Mixture of Experts**: Exponentially Weighted Average (EWA) of models

$$w_k(\delta^k;\bar{\delta};\sigma_w) = \frac{g_k(\delta^k;\bar{\delta};\sigma_w)}{\sum_{l=1}^{K} g_l(\delta^l;\bar{\delta};\sigma_w)} \quad (1)$$

  where:
  - $\bar{\delta}$ is a vector of high-fidelity data
  - δ^k is a vector of the k^{th} individual model predictions for $\bar{\delta}$ (Nota: $\delta^k \neq d_k$!)
  - σ_w is a hyperparameter
  - g_m is a cost function of the form

$$g_k(\delta^k;\bar{\delta};\sigma_w) = \exp\left(-\frac{1}{2}\frac{(\delta^k-\bar{\delta})^T.(\delta^k-\bar{\delta})}{\sigma_w^2}\right) \quad (2)$$

- The aggregated prediction of quantity d writes:

$$d_{MA} = \sum_{k=1}^{K} w_k d_k \quad (3)$$

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X-MA

MA: constant weights do not account for "regional" model behavior
X-MA: '**local**' and '**physics-aware**' aggregation:

$$\underbrace{\boldsymbol{\eta}(\vec{\boldsymbol{x}}) = (\eta_1(x), \ldots, \eta_{10}(x))}_{\text{local flow features}} \xrightarrow[W]{CART} \underbrace{(w_1(\delta^1(x); \bar{\delta}(x); \sigma_w), \ldots, w_K(\delta^K(x); \bar{\delta}(x); \sigma_w))}_{\text{local models weights}} \quad (4)$$

$$d_{X-MA}(x) = \sum_{k=1}^{K} W_k(\boldsymbol{\eta}(\vec{\boldsymbol{x}}); \sigma_w) d_k(x) \quad (5)$$

Feature	Description	Formula	Feature	Description	Formula
η_1	Normalized Q criterion	$\frac{\|\|\mathbf{\Omega}\|\|^2 - \|\|\mathbf{S}\|\|^2}{\|\|\mathbf{\Omega}\|\|^2 + \|\|\mathbf{S}\|\|^2}$	η_6	Viscosity ratio	$\frac{\nu_T}{100\nu + \nu_T}$
η_2	Turbulence intensity	$\frac{k}{0.5 U_i U_i + k}$	η_7	Ratio of pressure normal stresses to normal shear stresses	$\frac{\sqrt{\frac{\partial P}{\partial x_i}\frac{\partial P}{\partial x_i}}}{\sqrt{\frac{\partial P}{\partial x_j}\frac{\partial P}{\partial x_j}} + 0.5\rho\frac{\partial U_k^2}{\partial x_k}}$
η_3	Turbulent Reynolds number	$\min\left(\frac{\sqrt{k}\lambda}{50\nu}, 2\right)$	η_8	Non-orthogonality marker between velocity and its gradient [28]	$\frac{\left\|U_k U_l \frac{\partial U_k}{\partial x_l}\right\|}{\sqrt{U_n U_n U_i \frac{\partial U_i}{\partial x_j} U_m \frac{\partial U_m}{\partial x_j}} + \left\|U_i U_j \frac{\partial U_i}{\partial x_j}\right\|}$
η_4	Pressure gradient along streamline	$\frac{U_k \frac{\partial P}{\partial x_k}}{\sqrt{\frac{\partial P}{\partial x_j}\frac{\partial P}{\partial x_j} U_i U_i} + \left\|U_l \frac{\partial P}{\partial x_l}\right\|}$	η_9	Ratio of convection to production of k	$\frac{U_i \frac{\partial k}{\partial x_i}}{\|\overline{u'_j u'_l} S_{jl}\| + U_l \frac{\partial k}{\partial x_l}}$
η_5	Ratio of turbulent time scale to mean strain time scale	$\frac{\|\|\mathbf{S}\|\| k}{\|\|\mathbf{S}\|\| k + \varepsilon}$	η_{10}	Ratio of total Reynolds stresses to normal Reynolds stresses	$\frac{\|\|\overline{u'_i u'_j}\|\|}{k + \|\|\overline{u'_i u'_j}\|\|}$

Training Data

Ref	case	Data
D_1	ZPG-TBL	DNS of turbulent boundary layer, $670 \leq Re_\theta \leq 4060$[7]
D_2	FDC	DNS of turbulent channel flow, $180 \leq Re_\tau \leq 590$[8]
D_3	ANSJ	PIV of near sonic axisymmetric jet [9]
D_4	APG	LES of adverse pressure-gradient TBL [10] $Re_\theta \leq 4000$, $\beta = 4$, 5 different pressure gradients
D_5	SEP	LES of Periodic Hills at Re=10595 [11] DNS of converging-diverging channel at Re=13600 [12] LES of curved backward facing step at Re = 13700 [13]
D_6	N4412	LES of NACA4412 at $\alpha = 5$, $Re_c = 10^5, 2.10^5, 4.10^5, 10^6$ [14]

- SBL-EARSM models are infered using Reynolds stress data
- The aggregation of models is using streamwise velocity data

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[12] Laval, J.-P. and Marquillie, M. (2011). In *Progress in wall turbulence: understanding and modeling*, pages 203–209. Springer

[13] Bentaleb, Y., Lardeau, S., and Leschziner, M. A. (2012). *Journal of Turbulence*, (13):N4

[14] Vinuesa, R., Negi, P. S., Atzori, M., Hanifi, A., Henningson, D. S., and Schlatter, P. (2018). *International Journal of Heat and Fluid Flow*, 72:86–99

Case 2DZP: zero pressure boundary layer

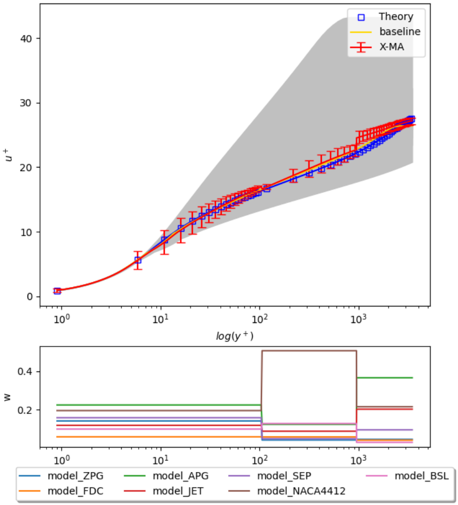

Figure 2: u^+ vs. $log(y^+)$

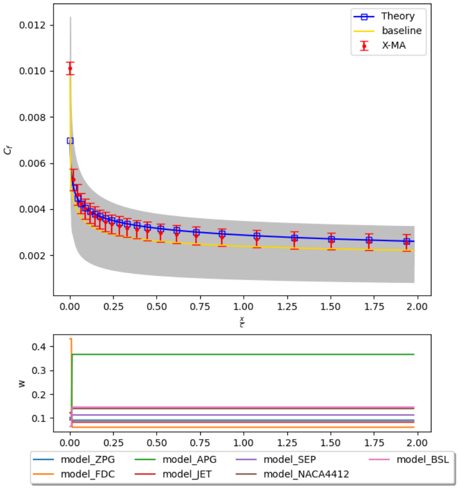

Figure 3: C_f vs. x

Case 2DFDC: Fully-developed channel flow

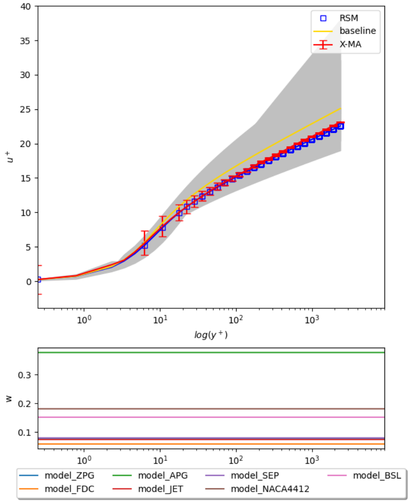

Figure 4: u^+ vs. $log(y^+)$

Case 2DWMH: Wall-Mounted Hump

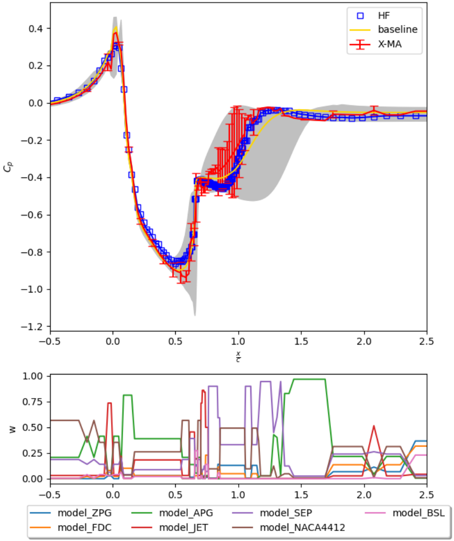

Figure 5: C_p vs. x

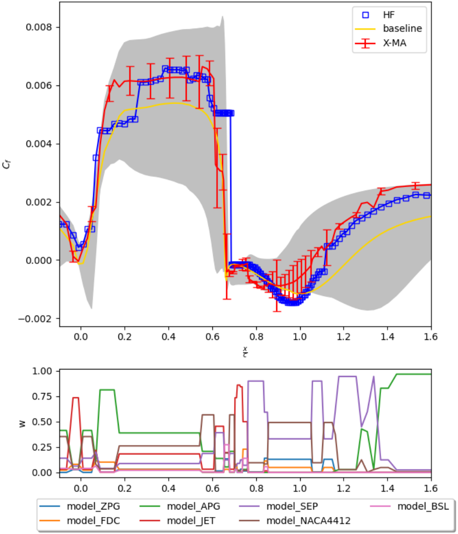

Figure 6: C_f vs. x

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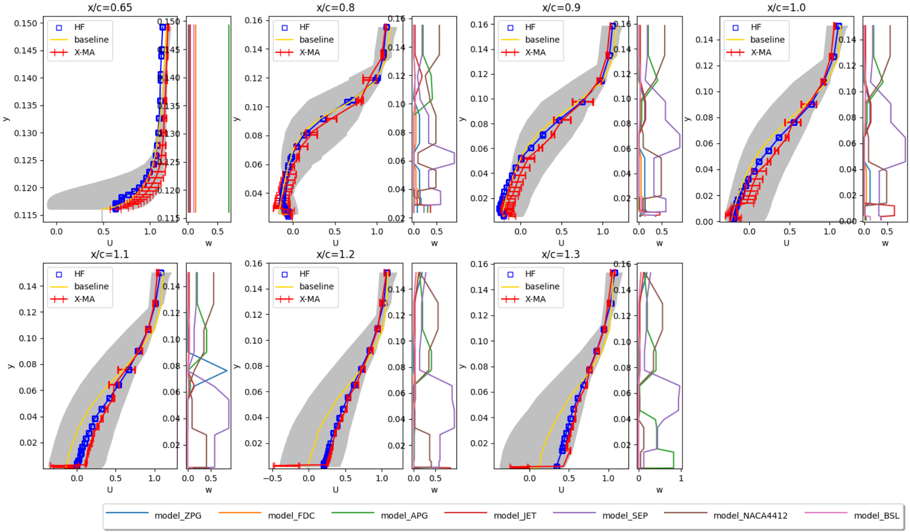

Figure 7: Streamwise velocity U at different streamwise stations

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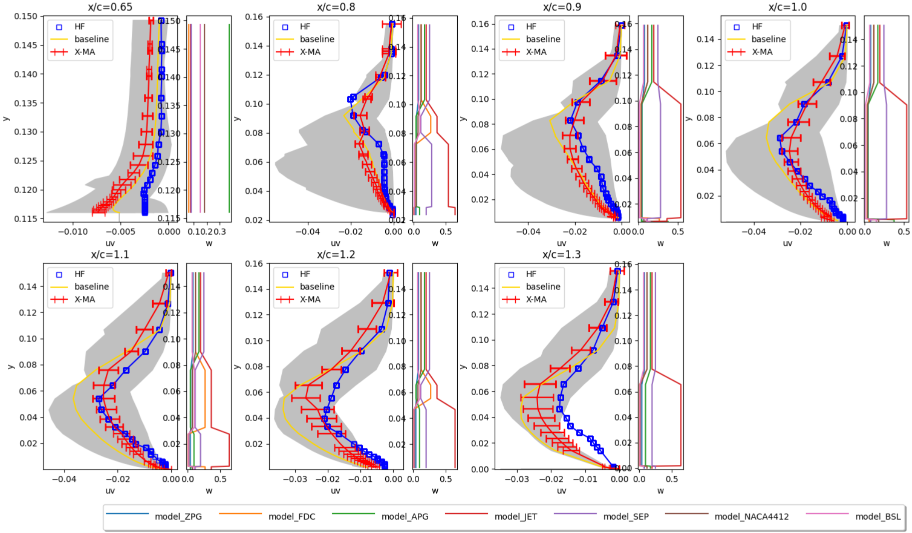

Figure 8: Reynolds shear stress τ_{xy} at different streamwise stations

Case ASJ: Axisymmetric Subsonic Jet

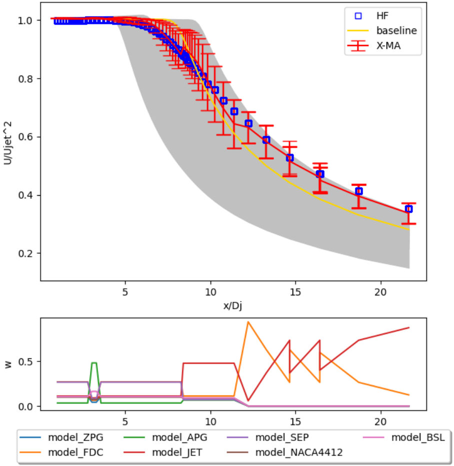

Figure 9: Streamwise velocity along symmetry axis

Case ASJ: Axisymmetric Subsonic Jet

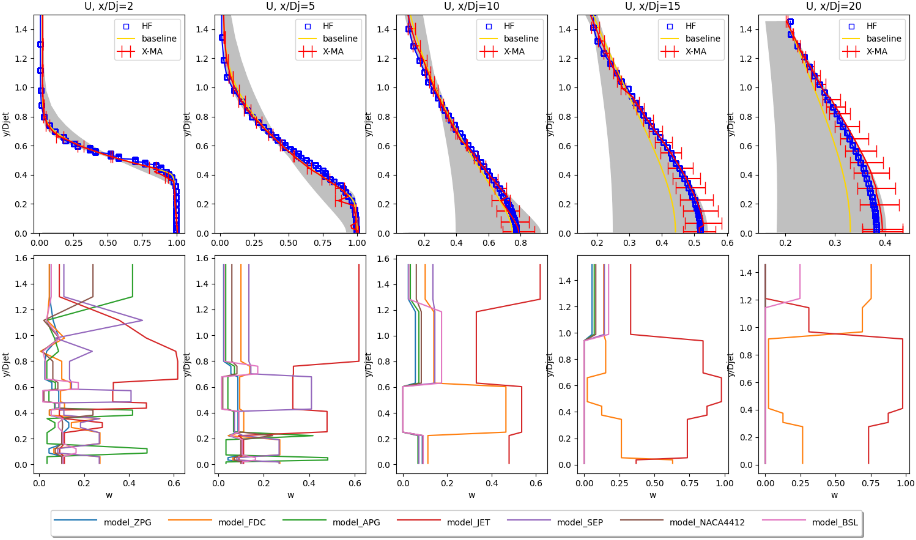

Figure 10: Streamwise velocity U along symmetry axis

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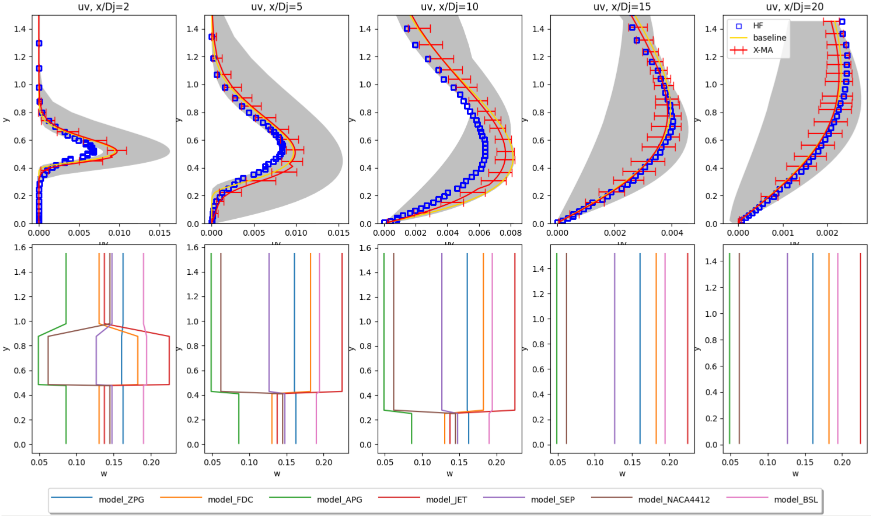

Figure 11: Reynolds shear stress τ_{xy} at different stations along x

Case 2DN00: NACA 0012 Airfoil

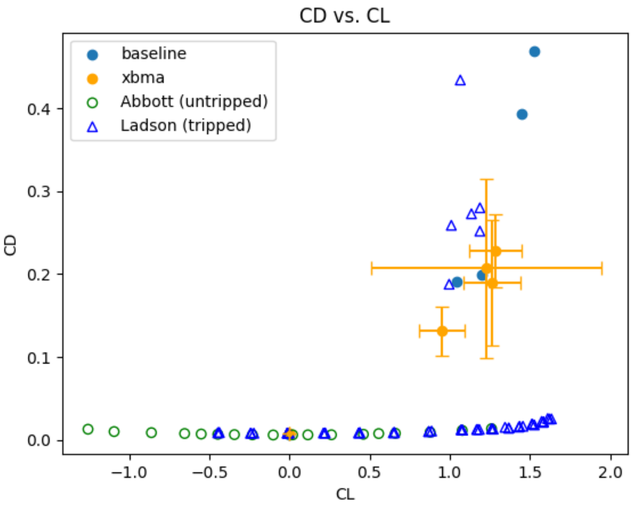

Figure 12: C_D vs. C_L

Case 2DN00: NACA 0012 Airfoil

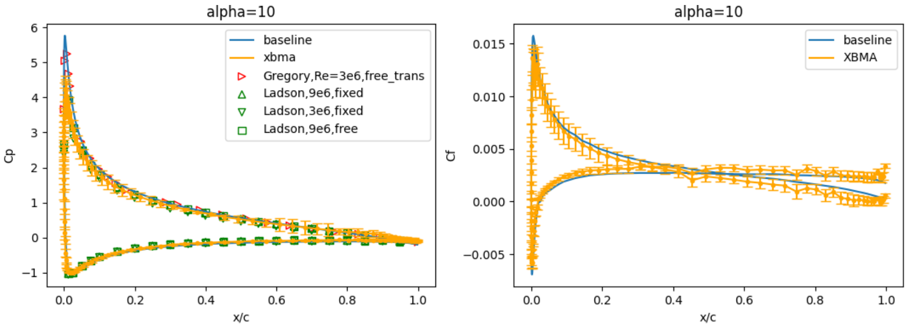

Figure 13: C_p vs. x (left) and C_f vs. x (right) at $\alpha = 10^{\circ}$

Case 2DN00: NACA 0012 Airfoil

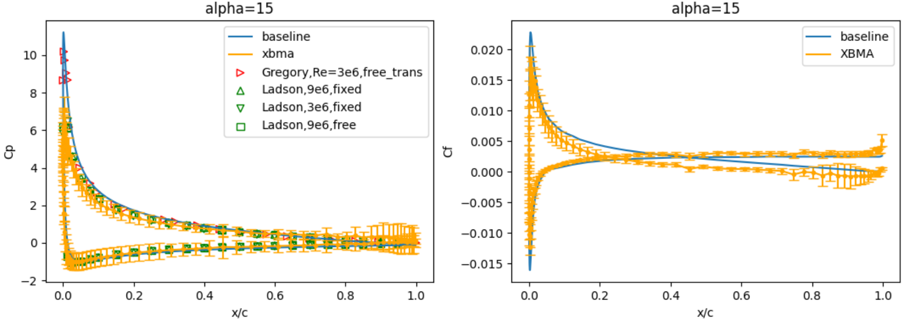

Figure 14: C_p vs. x (left) and C_f vs. x (right) at $\alpha = 15^\circ$

Case 2DN00: NACA 0012 Airfoil

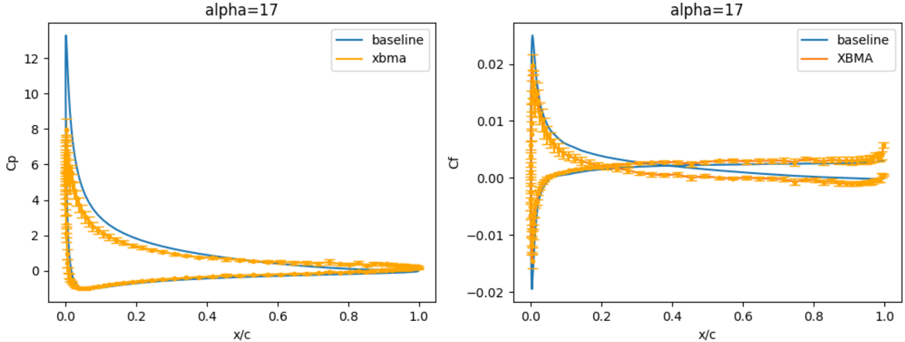

Figure 15: C_p vs. x (left) and C_f vs. x (right) at $\alpha = 17^\circ$

Case 2DN00: NACA 0012 Airfoil

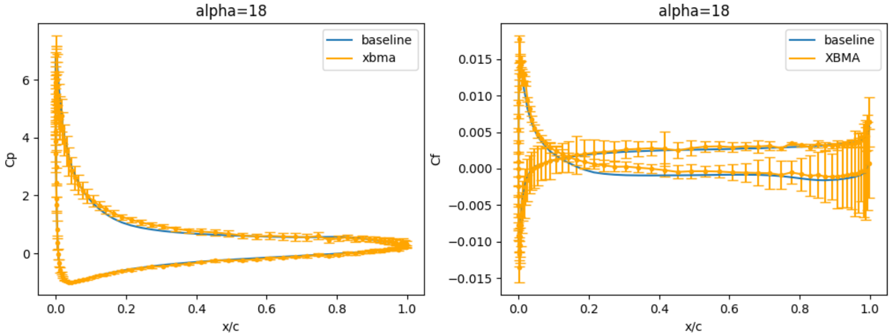

Figure 16: C_p vs. x (left) and C_f vs. x (right) at $\alpha = 18^\circ$

Conclusions and perspectives

- We presented a Sparse Bayesian Learning (SBL) approach for discovering non linear corrections of LEVM with stochastic model parameters
- We explored a method for aggregating, in a **'local'** and **'physics-aware'** manner, predictions of SBL-EARSM models
- X-MA provides estimates of (parametric + model form) uncertainty

→ Future work:

- Derive customized SBL-EARSM for other flow classes
- Relax limitations intrinsic to Pope's representation
- Improve model aggregation algorithm to avoid unphysical wiggles and to return to baseline model for flow regions far apart the training sets

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Training set	Model
(ZPG-TBL)	$\begin{cases} \mathbf{M}^{(1)}_{\mathbf{b}^{\Delta}} = & [(-0.264 \pm 0.1263) + (2.61 \pm 4.55)(I_1 - I_2) + \\ & (-6.19 \pm 12.3)(I_1^2 - I_2^2) + (4.89 \pm 10.0)(I_1^3 - I_2^3)]\mathbf{T}^{(1)} \\ & \pm 0.1647 \\ \mathbf{M}^{(1)}_{\mathbf{b}^{R}} = & [(0.198 \pm 0.0245)I_1^2 + (-0.362 \pm 0.0562)(I_1^3 - I_2^3) + \\ & (3.25 \pm 0.449)(I_1^7 - I_2^7) + (3.13 \pm 0.589)I_1^8 + \\ & +(-0.198 \pm 0.449)I_1 I_2]\mathbf{T}^{(1)} \pm 0.00045 \end{cases}$
(FDC)	$\begin{cases} \mathbf{M}^{(2)}_{\mathbf{b}^{\Delta}} = & [(0.168 \pm 0.0886)]\mathbf{T}^{(1)} \pm 0.893 \\ \mathbf{M}^{(2)}_{\mathbf{b}^{R}} = & [(3.21 \pm 0.361) + (-2.88 \pm 1.24)(I_1^3 - I_2^3) + \\ & (-0.176 \pm 0.32)(I_1^9 - I_2^9)]\mathbf{T}^{(3)} \pm 0.00337) \end{cases}$
(ANSJ)	$\begin{cases} \mathbf{M}^{(3)}_{\mathbf{b}^{\Delta}} = & [(0)] \pm 0.00863 \\ \mathbf{M}^{(3)}_{\mathbf{b}^{R}} = & [(-0.35 \pm 0.0143)]\mathbf{T}^{(1)} + [(-38.476 \pm 2.16)]\mathbf{T}^{(3)} \\ & \pm 0.00241 \end{cases}$

$\mathbf{T}^{(1)} = \frac{1}{\omega} S, \mathbf{T}^{(2)} = \frac{1}{\omega^2}\left(S\Omega - \Omega S\right)$ and $\mathbf{T}^{(3)} = \frac{1}{\omega^2}\left(S^2 - \frac{1}{3}Tr(S^2)I\right)$

Training set	Model
(APG)	$\begin{cases} \mathbf{M}^{(4)}_{\mathbf{b}^{\Delta}} = & [(0.477 \pm 0.259)]\mathbf{T}^{(1)} \pm 0.000626 \\ \mathbf{M}^{(4)}_{\mathbf{b}^{R}} = & [(-0.12 \pm 0.0206) + (0.918 \pm 0.332)(I_1 - I_2)]\mathbf{T}^{(1)} \\ & \pm 0.0000176 \end{cases}$
(SEP)	$\begin{cases} \mathbf{M}^{(5)}_{\mathbf{b}^{\Delta}} = & [(0)] \pm 0.00669 \\ \mathbf{M}^{(5)}_{\mathbf{b}^{R}} = & [(0.382 \pm 0.0184)]\mathbf{T}^{(1)} \pm 0.0385 \end{cases}$
(N4412)	$\begin{cases} \mathbf{M}^{(6)}_{\mathbf{b}^{\Delta}} = & [(-0.39 \pm 0.000214)]\mathbf{T}^{(1)} + [(7.00 \pm 0.00169)]\mathbf{T}^{(2)} + \\ & [(6.00 \pm 0.038)]\mathbf{T}^{(3)} \pm 0.000626 \\ \mathbf{M}^{(6)}_{\mathbf{b}^{R}} = & [(0)] \pm 0.00011 \end{cases}$

$\mathbf{T}^{(1)} = \frac{1}{\omega} S, \mathbf{T}^{(2)} = \frac{1}{\omega^2} (S\Omega - \Omega S)$ and $\mathbf{T}^{(3)} = \frac{1}{\omega^2} \left(S^2 - \frac{1}{3} Tr(S^2) I\right)$

- Let:
  - θ a random variable refering to the generic 'non-infered' model coefficients
  - D^{Calib} a random variable refering to the high-fidelity training data set
- With the SBL framework, we have:

$$\theta | D_k^{Calib} \Leftrightarrow \theta_k^{SBL} | D_k^{Calib}, M_k \tag{6}$$

where:
  - M a random variable refering to the infered form of the SBL correction
  - θ^{SBL} a random variable referinf to the infered model coefficients under the model form M
- We use high-fidelity velocity data to evaluate the relevance of the derived models to each other:
  - D^{Eval} high-fidelity velocity data used to calculate models' weights

- We want to make predictions on an unseen quantity d_t:

$$p(d_t|D^{Eval}) = \sum_{k=1}^{K} p(d_t, D_k^{Calib}|D^{Eval}) \tag{7}$$

$$= \sum_{k=1}^{K} \int p(d_t, D_k^{Calib}, \theta|D^{Eval}) d\theta \tag{8}$$

$$= \sum_{k=1}^{K} \int p(d_t, \theta_k^{SBL}, M_k, D_k^{Calib}|D^{Eval}) d\theta_k^{SBL} \tag{9}$$

$$p(d_t|D^{Eval}) = \sum_{k=1}^{K} \underbrace{p(M_k, D_k^{Calib}|D^{Eval})}_{model-probability} \int \underbrace{p(d_t|M_k, D_k^{Calib}, \theta_k^{SBL})}_{likelihood} \underbrace{p(\theta_k^{SBL}|M_k, D_k^{Calib})}_{posterior} d\theta_k^{SBL} \tag{10}$$

- $p(M_k, D_k^{Calib}|D^{Eval})$ can be calculated using Bayes' theorem:

$$p(M_k, D_k^{Calib}|D^{Eval}) = \frac{p(D^{Eval}|M_k, D_k^{Calib})}{\sum_{l=1}^{K} p(D^{Eval}|M_l, D_l^{Calib})} \tag{11}$$

Spatial Model Aggregation (X-MA)

- We want to make the probability of every model sensitive to local flow features:
  1. We train a CART to identify clusters in the flow and learn the weights of every model using local flow features
  2. Every cluster gives a convex combinaison of the models' weights

$$\boldsymbol{\eta}(\vec{\boldsymbol{x}}) = (\eta_1(x), ..., \eta_{10}(x)) \xrightarrow[w]{CART} \left(p(M_1, D_1^{Calib}|D^{Eval}(x)), ..., p(M_K, D_K^{Calib}|D^{Eval}(x))\right)$$

- The X-MA writes:

$$p(d_t(x)|D^{Eval}) = \sum_{k=1}^{K} w(\boldsymbol{\eta}(\vec{\boldsymbol{x}}))_k \int p(d_t|M_k, D_k^{Calib}, \theta_k^{SBL})p(\theta_k^{SBL}|M_k, D_k^{Calib})d\theta_k^{SBL}$$

- We can proove that:

$$E(d_t(x)|D^{Eval}) = \sum_{k=1}^{K} w(\boldsymbol{\eta}(\vec{\boldsymbol{x}}))_k E(d_t|M_k, D_k^{Calib}) \quad (12)$$

$$Var(d_t(x)|D^{Eval}) = \sum_{k=1}^{K} w(\boldsymbol{\eta}(\vec{\boldsymbol{x}}))_k Var(d_t|M_k, D_k^{Calib}) \quad (13)$$

Grid search

- We performed a preliminary grid search to study the effect of two hyperparameters:
  - The depth of the CART tree: $mdepth$
  - The noise used to model the distribution of high-fidelity data around the SBL-EARSM predictions and that is used to calculate the likelihoods: σ^{CART}
- The choice of the best hyperparameters depend on the velocity predictions of the training set
- Results show that:
  - $\sigma^{CART}_{optim} \simeq 0.01$
  - 2 values of $mdepth_{optim}$ are found:
  - $mdepth_{optim} \simeq 3$ for optimal τ_{xy} predictions
  - $mdepth_{optim} \simeq 10$ for all other Quantities of Interest
- A deeper and more precise grid search around these optimal value is needed for an optimal final result