

Figure A.1: Partition of the spatial grid for the first simulation case.

Appendices

A Computing the CPOD expansion

The driving idea behind CPOD is that a common spatial domain is needed to extract common instabilities over multiple injector geometries, since each simulation run has di erent geometries and varying grid points. We rst describe a physically justi able method for obtaining such a common domain, and then use this to compute the CPOD expansion.

A.1 Common grid

- 1. Identify the densest grid (i.e., with the most grid points) among then simulation runs, and set this as the common reference grid.
- 2. For each simulation, partition the grid into the following four parts: (a) from injector head-end to the inlet, (b) from the inlet to the nozzle exit, (c) the top portion of the downstream region and (d) the bottom portion of the downstream region (see Figure A.1 for an illustration). This splits the ow in such a way that the linearity assumption can be physically justi ed.

- 3. Linearly rescale each part of the partition to the common grid by the corresponding geometry parameters, R_n and L (see Figure A.1).
- 4. For each simulation, interpolate the original ow data onto the spatial grid of the common geometry. This step ensures the ow is realized over a common set of grid points for all n simulations. In our implementation, the inverse distance weighting interpolation method (Shepard, 1968) is used with 10 nearest neighbours.

A.2 POD expansion

After ows from each simulation have been rescaled onto the common grid, the original POD expansion can be used to extract common ow instabilities. Leftx_j $g_{j=1}^{J}$ and f t_m $g_{m=1}^{T}$ denote the set of common grid points and simulated time-steps, respectively, and Nét(x;t;c_i) be an interpolated ow variable for geometric settingc_i, i = 1; ;n (for brevity, assume a single ow variable, e.g.,x-velocity, for the exposition below). The CPOD expansion can be computed using the following three steps.

 For notational convenience, we combine all combinations of geometries and time-steps into a single index. SetN = nT and let I = 1; ;N index all combinations ofn design settings andT time-steps, and let Y₁(x) Y(x; (t; c)₁). De ne Q 2 R^{N N} as the following inner-product matrix:

$$Q_{I;m} = \sum_{j=1}^{X^J} \Psi_I(x_j) \Psi_m(x_j):$$

Such an inner-product is possible because **a**llsimulated ows are observed on a set of common gridpoints set.

First, compute the eigenvectors $a_k 2 R^N$ satisfying:

$$Qa_k = _ka_k;$$

where $_k$ is the k-th largest eigenvalue of Q. Since a full eigendecomposition requires O(N³) work, this step may be intractible to perform when the temporal resolution is dense. To this end, we employed a variant of the implicitly restarted Arnoldi method (Lehoucq et al., 1998), which can e ciently approximate leading eigenvalues and eigenvectors.

2. Compute the k-th mode $_k(\mathbf{x})$ as:

$$\begin{bmatrix} k(\mathbf{x}_1) \\ k(\mathbf{x}_2) \\ \vdots \\ k(\mathbf{x}_J) \end{bmatrix} = \begin{pmatrix} \mathbf{Y}_1(\mathbf{x}_1) & \cdots & \mathbf{Y}_N(\mathbf{x}_1) \\ \vdots & \ddots & \vdots \\ \mathbf{Y}_1(\mathbf{x}_J) & \cdots & \mathbf{Y}_N(\mathbf{x}_J) \end{pmatrix} \mathbf{a}_k:$$

To ensure orthonormality, apply the following normalization:

$$_{k}(\mathbf{x}_{j}) \coloneqq \frac{_{k}(\mathbf{x}_{j})}{\|_{k}(\mathbf{x})\|}; \quad \|_{k}(\mathbf{x})\| = \sqrt{\sum_{j=1}^{J} _{k}(\mathbf{x}_{j})^{2}}$$

3. Lastly, derive the CPOD coe cients $(l_{l,1}; \cdots; l_{l,N})^T$ for the snapshot at indexl (i.e., with design setting and time-step $\boldsymbol{\xi}; \boldsymbol{t}_l$) as:

$$\begin{bmatrix} l,1\\l,2\\\vdots\\l,N\end{bmatrix} = \begin{pmatrix} 1(\mathbf{x}_1) & \cdots & 1(\mathbf{x}_J)\\\vdots & \ddots & \vdots\\N(\mathbf{x}_1) & \cdots & N(\mathbf{x}_J) \end{pmatrix} \begin{bmatrix} \mathbf{Y}_l(\mathbf{x}_1)\\\mathbf{Y}_l(\mathbf{x}_2)\\\vdots\\\mathbf{Y}_l(\mathbf{x}_J) \end{bmatrix};$$

Using these coe cients and a truncation at $K_r < N$ modes, it is easy to show the following decomposition of the ow at the design setting t_i and time-step t_m indexed

by I:

$$\mathsf{Y}(\mathbf{x}_{j};\mathsf{t}_{m};\mathbf{c}_{i})\approx\sum_{k=1}^{K_{r}} \ _{l,k}\mathcal{M}_{i}\{ \ _{k}(\mathbf{x}_{j})\}; \ \mathbf{j}=\mathsf{1};\cdots;\mathsf{J};$$

as asserted in (3).

B Proof of Theorem 2

De ne the map $A : \mathbb{R}^K \times \mathbb{R}^{K \times K} \times \mathbb{R}^p \to \mathbb{R}^K \times \mathbb{R}^{K \times K} \times \mathbb{R}^p$ as a single-loop of the graphical LASSO operator for optimizing T with μ and τ xed, and de ne $B : \mathbb{R}^K \times \mathbb{R}^{K \times K} \times \mathbb{R}^p \to \mathbb{R}^K \times \mathbb{R}^{K \times K} \times \mathbb{R}^p$ as the L-BFGS map for a single line-search when optimizing and τ with T xed. Each BCD cycle in Algorithm 1 then follows the map composition $S = A^M \circ B^N$, where $M < \infty$ and $N < \infty$ are the iteration count for the graphical LASSO operator and number of line-searches, respectively. The parameter estimates at iteration of the BCD cycle can then be given by:

$$_{m+1}$$
 = S($_m$); where $_m$ = (${oldsymbol \mu}_m; {
m T}_m; {oldsymbol au}_m$):

De ne the set of stationary solutions as $= \{ : \nabla I_{\lambda}() = 0 \}$, where ∇I_{λ} is the gradient of the negative log-likelihood $_{\lambda}$. Using the Global Convergence Theorem (see Section 7.7 of Luenberger and Ye, 2008), we can prove stationary convergence:

$$\lim_{m o \infty}$$
 $_m$ = $^* \in$;

if the following three conditions hold:

- (i) $\{m_{m=1}^{\infty}\}_{m=1}^{\infty}$ is contained within a compact subset of $\mathbb{R}^{K} \times \mathbb{R}^{K \times K} \times \mathbb{R}^{p}$,
- (ii) I_{λ} is a continuous descent function on under maps,
- (iii) S is closed for points outside of .

We will verify these conditions below.

- (i) This is easily veried by the fact that $|\boldsymbol{\mu}_m| \leq \left(\max_{i,r,k} \left| \begin{array}{c} {k \choose k} (\mathbf{c}_i) \right| \right) \mathbf{1}_K$, $\mathbf{0} \leq \mathbf{T}_m \leq \left(\max_{k,r} \mathbf{s}^2 \left\{ \begin{array}{c} {k \choose k} (\mathbf{c}_i) \right\}_{i=1}^n \right) \mathbf{I}_K$ and $\boldsymbol{\tau}_m \in [0; 1]^p$, where $\mathbf{s}^2 \{\cdot\}$ returns the sample standard deviation for a set of scalars.
- (ii) To prove that S is a descent function, we need to show that if \in , then $I_{\lambda}{S()} = I_{\lambda}{\{ \}}$, and if \in , then $I_{\lambda}{S()} < I_{\lambda}{\{ \}}$. The rst condition is trivial, since M = 0 and N = 0 when is stationary. The second condition follows from the fact that the maps A and B incur a strict decrease in $_{\lambda}$ wheneverT and $(\mu; \tau)$ are non-stationary, respectively.
- (iii) Note that A^M is a continuous map (since the graphical LASSO map is a continuous operator) and the line-search map ^N is also continuous. Sinc S = A^M ∘ B^N, it must be continuous as well, from which the closedness Soffollows.

C Proof of Theorem 3

Fix some spatial coordinatex and time-stept, and let:

$$\mathbf{y} = (\mathbf{Y}^{(u)}(\mathbf{x}; \mathbf{t}; \mathbf{c}_{new}); \mathbf{Y}^{(v)}(\mathbf{x}; \mathbf{t}; \mathbf{c}_{new}); \mathbf{Y}^{(w)}(\mathbf{x}; \mathbf{t}; \mathbf{c}_{new}))^T$$

be the true simulated ows for x-, y- and circumferential velocities at the new setting pnew,

$$\mathbf{\mathbf{\hat{y}}} = (\mathbf{\hat{Y}}^{(u)}(\mathbf{x}; \mathbf{t}; \mathbf{c}_{new}); \mathbf{\hat{Y}}^{(v)}(\mathbf{x}; \mathbf{t}; \mathbf{c}_{new}); \mathbf{\hat{Y}}^{(w)}(\mathbf{x}; \mathbf{t}; \mathbf{c}_{new}))^T$$

be its corresponding prediction from (9), and

$$\mathbf{y} = (\mathsf{Y}^{(u)}(\mathbf{x}; \mathbf{c}_{new}); \mathsf{Y}^{(v)}(\mathbf{x}; \mathbf{c}_{new}); \mathsf{Y}^{(w)}(\mathbf{x}; \mathbf{c}_{new}))^T$$

be its time-averaged ow. It is easy to verify that, given the simulation data $\mathcal{D} = \{Y^{(r)}(\mathbf{x};t;\mathbf{c}_i)\}$, the conditional distribution of $\mathbf{y}|\mathcal{D}$ is $\mathcal{N}(\mathbf{\hat{y}}; (\mathbf{x};t))$, where:

$$(\mathbf{x}; \mathbf{t}) \equiv \begin{bmatrix} \mathbf{m}^{(u)} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{m}^{(v)} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{m}^{(w)} \end{bmatrix} [\mathbb{V}\{\boldsymbol{\beta}(\mathbf{t}; \mathbf{c}_{new}) | \{\boldsymbol{\beta}(\mathbf{t}; \mathbf{c}_{i})\}_{i=1}^{n} \}]_{uvw} \begin{bmatrix} \mathbf{m}^{(u)} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{m}^{(v)} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{m}^{(w)} \end{bmatrix}^{T};$$

$$(C.1)$$

with:

$$\mathbf{m}^{(r)} = \left[\mathcal{M}_{new} \{ {}^{(r)}_{1}(\mathbf{x}) \}; \mathcal{M}_{new} \{ {}^{(r)}_{2}(\mathbf{x}) \}; \cdots \mathcal{M}_{new} \{ {}^{(r)}_{K_{r}}(\mathbf{x}) \} \right]; \mathbf{r} = \mathbf{u}; \mathbf{v}; \mathbf{w}:$$

Letting (t) = U U^T be the eigendecomposition of (), with = diag{ $_j$ }, it follows that $^{-1/2}U^T(y - y)|\mathcal{D} \stackrel{d}{=} \mathcal{N}(\mu; I_K)$, where $\mu = ^{-1/2}U^T(\mathbf{r} - y)$ and $K = K_u + K_v + K_w$. Denoting $\mathbf{a} = ^{-1/2}U^T(y - y)$, the TKE expression in (13) can be rewritten as:

$$(\mathbf{x}; \mathbf{t}) = \frac{1}{2} (\mathbf{y} - \mathbf{y})^{T} (\mathbf{y} - \mathbf{y}) = \frac{1}{2} (\mathbf{U}^{-1/2} \mathbf{a})^{T} (\mathbf{U}^{-1/2} \mathbf{a})$$

= $\frac{1}{2} (\mathbf{a}^{T-1/2} \mathbf{U}^{T} \mathbf{U}^{-1/2} \mathbf{a})$
= $\frac{1}{2} \mathbf{a}^{T} \mathbf{a} = \frac{1}{2} \sum_{j=1}^{K} {}_{j} \mathbf{a}_{j}^{2}$: (C.2)

Since $\mathbf{a} \sim \mathcal{N}(\boldsymbol{\mu}; \mathbf{I}_K)$, \mathbf{a}_j^2 has a non-central chi-square distribution with one degree-of-freedom and non-centrality parameter $\frac{2}{j}$ (we denote this as $\frac{2}{1}(\frac{2}{j})$). (\mathbf{x} ; t) then becomes:

$$\sum_{j=1}^{K} \frac{-j}{2} \, {}^{2}_{1} ({}^{2}_{j}); \tag{C.3}$$

which is a sum of weighted non-central chi-squared distributions. The computation of the distribution function for such a random variable has been studied extensively, see, e.g., Imhof (1961), Davies (1973, 1980), Castano-Martnez and Lopez-Bazquez (2005), and

Liu et al. (2009), and we appeal to these methods for computing the pointwise con dence interval of (x;t) in Section 4. Speci cally, we employ the method of Liu et al. (2009) through the R (R Core Team, 2015) packageompQuadForm (Duchesne and de Micheaux, 2010).

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