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Maximum Entropy Closure of Galerkin POD models

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Abstract

A maximum entropy closure for Galerkin principal orthogonal decomposition (POD) models of fluid flow systems is developed to examine the triadic interactions between energetic modes, by extension of a previous theoretical treatment of triadic interactions in an incompressible flow system. This closure maximises a relative entropy associated with the uncertainty in the system, subject to constraints arising from conservation of mass, energy and power balance, to infer the probability density function for the mode amplitudes. The framework is applied to the cylinder wake in the oscillatory regime (Re = 100), with important implications for the triadic structure and power balance (energy cascade) in the system.

Introduction

In this work, the MaxEnt method of Jaynes [1] is used to predict the asymptotic state of a low-order Galerkin model of a cylinder wake. The closure maximises a relative entropy associated with the uncertainty in the system, subject to constraints. Several models using constraints arising from conservation of mass and energy have been developed (see [2, 3]). The model presented here also takes into account energy transfers by triadic interactions between the modes, using a theoretical model of these interactions in an incompressible flow system [4].

Theory

Galerkin system

We consider the Galerkin expansion of the velocity field

$$\mathbf{u}(\mathbf{x},t) = \mathbf{u}_0(\mathbf{x}) + \sum_{i=1}^{N} a_i(t)\mathbf{u}_i(\mathbf{x}), \tag{1}$$

where $\mathbf{u}_0$ is the base flow and the functions $\mathbf{u}_i$ are the N first POD modes, forming $L = N/2$ pairs $(\mathbf{u}_{2l-1}, \mathbf{u}_{2l})$ resolving the L first harmonics of the flow.

Projection of the non-dimensional incompressible Navier-Stokes equations

$$\begin{cases} \nabla\cdot\mathbf{u} = 0 \\ \dfrac{\partial\mathbf{u}}{\partial t} + \nabla\cdot(\mathbf{u}\otimes\mathbf{u}) = -\nabla p + \nu\Delta\mathbf{u}, \quad \nu = \dfrac{1}{Re} \end{cases} \tag{2}$$

on the subset $\{\mathbf{u}_i\}_{i\in\{1,\dots,N\}}$ gives the dynamical system

$$\dot{a}_i = c_i + \sum_{j=1}^{N} l_{ij}a_j + \sum_{j,k=1}^{N} q_{ijk}a_j a_k, \quad \forall i \in \{1,\dots,N\}. \tag{3}$$

Assuming the effect of pressure can be neglected, we have

$$\begin{cases} q_{ijk} = \langle \mathbf{u}_i, \nabla\cdot(\mathbf{u}_j\otimes\mathbf{u}_k)\rangle, \\ l_{ij} = \nu^{-1}\langle \mathbf{u}_i, \Delta\mathbf{u}_j\rangle + q_{ij0} + q_{i0j}, \\ c_i = l_{i0} + q_{i00}. \end{cases}$$

Assuming other simplifications, such as symmetries, we assume the system (3) can be simplified under the form

$$\begin{cases} \dot{a}_{2l-1} = \sigma_l a_{2l-1} - \omega_l a_{2l} + \displaystyle\sum_{j,k=1}^{2L} q_{(2l-1)jk}a_j a_k, \\ \dot{a}_{2l} = \sigma_l a_{2l} + \omega_l a_{2l-1} + \displaystyle\sum_{j,k=1}^{2L} q_{(2l)jk}a_j a_k. \end{cases}, \forall\, l \in \{1,\dots,L\}. \tag{4}$$

We denote by $\overline{F}$ the time average of the quantity $F(\mathbf{a})$, with $\mathbf{a}(t)$. Then, we use a Reynolds decomposition, introducing the fluctuation F':

$$\begin{cases} F = \overline{F} + F', \\ \overline{F} := \lim\limits_{T\to\infty} \dfrac{1}{T}\displaystyle\int_0^T F(\mathbf{a})\mathrm{d}t. \end{cases} \tag{5}$$

Introducing this decomposition (5) in the Galerkin system (3) and averaging gives the mean-field equation

$$\dot{\overline{a_i}} = c_i + \sum_{j=1}^{N} l_{ij}\overline{a_j} + \sum_{j,k=1}^{N} q_{ijk}\left(\overline{a_j}\,\overline{a_k} + \overline{a'_j a'_k}\right), \forall i \in \{1,\dots,N\}. \tag{6}$$

Then, multiplying (3) by a'_i and averaging gives the energy equation

$$\begin{cases} \dot{E}_i = \displaystyle\sum_{j=1}^{N} q_{ij}\overline{a'_i a'_j} + \sum_{j,k=1}^{N} q_{ijk}\overline{a'_i a'_j a'_k}, \\ q_{ij} = l_{ij} + \displaystyle\sum_{k=1}^{N} (q_{ijk} + q_{ikj})\overline{a_k}, \end{cases}, \quad \forall\, i \in \{1,\dots,N\}, \tag{7}$$

where the turbulent energy is defined by

$$E_i(t) = \frac{1}{2}\overline{a'_i a'_i}. \tag{8}$$

Then, we obtain 2 sets of N equations (6) and (7), with $2N$ unknowns, the values of interest $\{\overline{a_i}\}_{i=1}^N$ and $\{E_i\}_{i=1}^N$ and the second and third-order moments $\{\overline{a'_i a'_j}\}_{i,j=1}^N$ and $\{\overline{a'_i a'_j a'_k}\}_{i,j,k=1}^N$. These terms have to be modelled to close the problem. We define the triadic interactions by

$$T_{ijk} := q_{ijk}\,\overline{a'_i a'_j a'_k}, \quad \forall\,(i,j,k) \in \{1,\dots,N\} \tag{9}$$

Finite-time thermodynamics model

Noack et al. [4] define the closure assuming that the moments depend only on energy levels:

$$\begin{cases} \overline{a'_i a'_j} = 2E_i\delta_{ij}, \\ T_{ijk} \approx \hat{T}_{ijk} := \alpha\chi_{ijk}\sqrt{E_i E_j E_k}\left(1 - \dfrac{3E_i}{E_i + E_j + E_k}\right), \end{cases} \tag{10}$$

where α is a constant, δ_{ij} is the Kronecker symbol and the triadic function χ_{ijk} is defined by

$$\chi_{ijk} = \frac{1}{6}\Big(|q_{ijk}|+|q_{ikj}|+|q_{jik}|+|q_{jki}|+|q_{kij}|+|q_{kji}|\Big). \quad (11)$$

Using the symmetries and a Krylov-Bogoliugov approximation, it can be shown that most of the possible triadic interactions are zero. Then we define the set

$$\mathcal{T}_N := \Big\{(i,j,k) \in [\![1:N]\!]^3 \ / \ \overline{a_i a_j a_k} \neq 0\Big\}. \quad (12)$$

Equation (7) is then written

$$\dot{E}_i = 2q_{ii}E_i + \sum_{j,k=1}^{N} \hat{T}_{ijk} := \hat{Q}_i + \hat{T}_i = \hat{Q}_i + \alpha\tilde{T}_i, \quad \forall\, i \in \{1,...,N\}. \quad (13)$$

The parameter α is defined using a compatibility condition: we impose that "donor" modes (i.e. the first two modes) tranfer to the dissipative modes all the energy they received from the mean flow, this means

$$\dot{E}_1 + \dot{E}_2 = 0, \quad (14)$$

hence

$$\alpha(E_1,...,E_N) = -\left(\hat{Q}_1+\hat{Q}_2\right)\left(\tilde{T}_1+\tilde{T}_2\right)^{-1}. \quad (15)$$

This obliges to impose in the initial condition the energy of the donor modes in the asymptotic solution.

MaxEnt methodology

We now consider the trajectory of the dynamical system. We define a probability density function (pdf) $p(\mathbf{a})$ on the state space $\mathcal{A} \sim \mathbb{R}^N$, so that $p(\mathbf{a})\mathrm{d}\mathbf{a}$ is the probability to find a point of this trajectory in the hypercube $\prod_{i=1}^{N}[a_i, a_i+\mathrm{d}a_i]$:

$$p(\mathbf{a})\mathrm{d}\mathbf{a} = \mathrm{Prob}\left(a_i \leq \Upsilon_{a_i} \leq a_i + \mathrm{d}a_i \ \ \forall\, i \in \{1,...,N\}\right) \quad (16)$$

This pdf allows the definition of the statistical average of any function $F(\mathbf{a})$:

$$\langle F\rangle := \int_{\mathcal{A}} F(\mathbf{a})p(\mathbf{a})\mathrm{d}\mathbf{a}. \quad (17)$$

The ergodic property requires this average to be equal to the time average for F

$$\langle F\rangle = \overline{F}. \quad (18)$$

We now define on our model the relative entropy, or negative Kullback-Leibler divergence

$$D(p||q) := -\int_{\mathcal{A}} p(\mathbf{a})\ln\left[\frac{p(\mathbf{a})}{q(\mathbf{a})}\right]\mathrm{d}\mathbf{a} := -\left\langle \ln\left[\frac{p(\mathbf{a})}{q(\mathbf{a})}\right]\right\rangle, \quad (19)$$

where $q(\mathbf{a})$ is the "prior pdf", assumed to be the pdf of the system in the absence of any constraint.

The MaxEnt theory developed by Jaynes [1] ensures the most probable choice of p, denoted p^*, maximises the entropy subject to constraints on the system. Assuming that our system reaches an asymptotic state, here a limit circle in each plane (a_{2l-1}, a_{2l}), the pdf is supposed to indicate the position of this attractor. The MaxEnt method then allows the prediction of the asymptotic behaviour of the system without solving the dynamical system.

Constraints, prior and resolution

The constraints on the pdf p are:

- a normalisation constraint:

$$\langle 1\rangle = 1, \quad (20)$$

- N zero-mean constraints :

$$\langle a_i\rangle = 0, \ \ \forall\, i \in \{1,...,N\}, \quad (21)$$

- Constraints on second-order moments: in accordance with (10), we must impose

$$\langle a_i a_j\rangle = 0, \ \ \forall (i,j) \in \{1,...,N\},\ i<j \quad (22)$$

- Energetic constraints: the total energy of the system in its periodic state is constant, giving

$$\left\langle \sum_{i=1}^{L} a_i^2 \right\rangle = 2E, \quad (23)$$

where E is the total energy. Consequently, the total power is zero, with (4) giving

$$\left\langle \sum_{i=1}^{L} \sigma_i a_i^2 \right\rangle = 0 \quad (24)$$

- Constraints on triadic interactions:

$$q_{ijk}\langle a_i a_j a_k\rangle = \hat{T}_{ijk}(E_i,E_j,E_k), \ \ \forall\, (i,j,k) \in \mathcal{T}_N. \quad (25)$$

Since $E_i = \frac{1}{2}\langle a_i^2\rangle$, these constraints are nonlinear, giving

$$q_{ijk}\langle a_i a_j a_k\rangle = \hat{T}_{ijk}(\langle a_i^2\rangle, \langle a_j^2\rangle, \langle a_k^2\rangle) \ \ \forall\, (i,j,k) \in \mathcal{T}_N. \quad (26)$$

- The coefficient α contained in $\hat{T}_{ijk}$ implicates the local power balance (14), equivalent to the energy constraint

$$\langle a_1^2 + a_2^2\rangle = 2(E_1+E_2) = 2\tilde{E}. \quad (27)$$

The prior is chosen to be uniform:

$$q(\mathbf{a}) \equiv 1. \quad (28)$$

This choice is obviously not valid for an infinite domain $\mathcal{A}$, as the prior cannot be normalized. In this case, the prior is not a pdf but a constant used for dimensional purposes, and the Kullback-Leibler divergence (19) is equivalent to the Shannon entropy.

We can then solve the problem using the classical Lagrangian method. The relative entropy (19) subject to the constraints (20)-(27) gives the Lagrangian

$$\begin{aligned} L(p|q) =& D(p||q) - \zeta_0\big[\langle 1\rangle - 1\big] - \zeta_1 \sum_{i=1}^{N} \langle \sigma_i a_i^2\rangle \\ & - \zeta_2\left[\sum_{i=1}^{N}\langle a_i^2\rangle - 2E\right] - \zeta_3\big[\langle a_1^2+a_2^2\rangle - 2\tilde{E}\big] \\ & - \sum_{i=1}^{N} \lambda_i \ \langle a_i\rangle - \sum_{\substack{i,j=1 \\ i<j}}^{N} \theta_{ij} \ \langle a_i a_j\rangle \\ & - \sum_{(i,j,k)\in\mathcal{T}_N} \mu_{ijk}\big[\langle q_{ijk}a_i a_j a_k\rangle - \hat{T}_{ijk}(\langle a_i^2\rangle, \langle a_j^2\rangle, \langle a_k^2\rangle)\big], \end{aligned} \quad (29)$$

where the coefficients ζ_i, λ_i, θ_{ij} and μ_{ijk} are the Lagrange multipliers. We should have cancellation of the functional variation for $p = p^*$, this means

$$\delta L[p = p^*] = \int_{\mathcal{A}} \delta p \frac{\delta L}{\delta p}\bigg|_{p=p^*} \mathrm{d}\mathbf{a} = 0,$$

where $\delta L/\delta p$ is the Frechet derivative, here given by

$$\begin{aligned}\frac{\delta L[p|q]}{\delta p} =& -\ln\left(\frac{p}{q}\right) - 1 - \zeta_0 - \sum_{i=1}^{N} (\zeta_1\sigma_i + \zeta_2)\, a_i^2 \\ & - \zeta_3\left(a_1^2 + a_2^2\right) - \sum_{i=1}^{N} \lambda_i\, a_i - \sum_{\substack{i,j=1 \\ i<j}}^{N} \theta_{ij}\, a_i a_j \\ & - \sum_{(i,j,k)\in\mathcal{T}_N} \mu_{ijk}\Bigg[q_{ijk} a_i a_j a_k \\ & + \frac{3}{\sqrt{2}}\alpha\chi_{ijk}\sqrt{\langle a_i^2\rangle\langle a_j^2\rangle\langle a_k^2\rangle}\,\frac{a_i^2 + a_j^2 + a_k^2}{\langle a_i^2 + a_j^2 + a_k^2\rangle}\Bigg]\end{aligned} \tag{30}$$

This integrand must then vanish, and so:

$$\begin{aligned}p^*(\mathbf{a}) =& q(\mathbf{a})\,\exp\Bigg(-\sum_{i=1}^{N}\lambda_i a_i - \sum_{\substack{i,j=1 \\ i<j}}^{N}\theta_{ij} a_i a_j - \sum_{i=1}^{N} h_i a_i^2 \\ & - \sum_{(i,j,k)\in\mathcal{T}_N}\mu_{ijk} q_{ijk} a_i a_j a_k\Bigg),\end{aligned} \tag{31}$$

with

$$\begin{cases} h_i = e_i - \displaystyle\sum_{(j,k)/(i,j,k)\in\mathcal{T}_N} \mu_{ijk}\,\varphi_{ijk}, \\ e_i = \zeta_1\sigma_i + \zeta_2 + (\delta_{1i} + \delta_{2i})\,\zeta_3, \\ \varphi_{ijk}\left(\alpha, \langle a_i^2\rangle, \langle a_j^2\rangle, \langle a_k^2\rangle\right) = \dfrac{3}{\sqrt{2}}\alpha\chi_{ijk}\dfrac{\sqrt{\langle a_i^2\rangle\langle a_j^2\rangle\langle a_k^2\rangle}}{\langle a_i^2 + a_j^2 + a_k^2\rangle}. \end{cases} \tag{32}$$

Then, the function φ_{ijk} translates the effect of triadic interactions on the Gaussian component of p^*, this means on energy levels. We note that φ_{ijk} is fully symmetric with respect to all variables.

However, the pdf p^* defined by (31) cannot generally be normalised, due to the last term, as the state space $\mathcal{A}$ is not bounded (it is obviously physically bounded, but the bounds are unknown and anyway, a bound-depending solution would not have any sense): it does not *a priori* satisfy the condition

$$p^*(\mathbf{a}) \underset{||\mathbf{a}||\to+\infty}{\longrightarrow} 0, \tag{33}$$

Moreover, the pdf presents a coupling of variables inside the exponential term, requiring computation of the constraints on the whole space, which can be very high-dimensional. This leads us to introduce a simplification.

Linearisation

A solution to avoid these two problems is to assume that the triadic terms are small, as well as the terms $\lambda_i a_i$ and $\theta_{ij} a_i a_j$, introduced to correct perturbations in the means and covariances, and to perform a linearisation of the distribution function. This leads at first order to

$$p^* = \frac{q}{Z} p_0 \left(1 - \sum_{i=1}^{N}\lambda_i a_i - \sum_{\substack{i,j=1 \\ i<j}}^{N}\theta_{ij} a_i a_j - \sum_{(i,j,k)\in\mathcal{T}_N}\mu_{ijk} a_i a_j a_k\right), \tag{34}$$

where the "base pdf" p_0 is the Gaussian function

$$p_0 = \frac{1}{Z_0}\exp\left(-\sum_{i=1}^{N} h_i a_i^2\right) = \prod_{i=1}^{N}\frac{1}{Z_i}\exp\left(-h_i a_i^2\right) := \prod_{i=1}^{N} p_i. \tag{35}$$

A straightforward analytical computation then gives

$$\begin{cases} Z = Z_0 = \displaystyle\int_{\mathbb{R}^N}\exp\left(-\sum_{i=1}^{N} h_i a_i^2\right)\mathrm{d}\mathbf{a} = \pi^L\left(\prod_{i=1}^{N} h_i\right)^{-1/2}, \\ \theta_{ij} = 0, \quad \forall\,(i,j)\in\{1,...,N\}, \\ \langle a_i a_j a_k\rangle = -\dfrac{1}{8 h_i h_j h_k}\mu_{ijk}\left(1 + \delta_{jk}\left(1 - \delta_{ij}\right)\right)\left(1 - \delta_{ij}\delta_{jk}\right), \\ \qquad \forall\,(i,j,k)\in\mathcal{T}_N. \end{cases} \tag{36}$$

The constraints on triadic interactions are then written

$$\begin{aligned} q_{ijk}\langle a_i a_j a_k\rangle\left(h_i, h_j, h_k, \mu_{ijk}\right) &= \hat{T}_{ijk}\left(E_i, E_j, E_k\right) \\ &= \hat{T}_{ijk}\left(h_i, h_j, h_k\right). \end{aligned} \tag{37}$$

The algorithm to compute the Lagrange multipliers is the following:

(a) Initialisation: we start with a non perturbed Gaussian pdf, this means that we have

$$\begin{cases} \forall\,(i,j,k)\in\mathcal{T}_N,\ \mu_{ijk}^{(0)} = 0, \\ \forall\, i\in\{1,...,N\},\ \lambda_i^{(0)} = 0, \end{cases} \tag{38}$$

hence

$$\begin{aligned}\forall\, i\in\{1,...,N\},\ h_i^{(0)} &= e_i^{(0)} \\ &= \zeta_1^{(0)} + \zeta_2^{(0)}\sigma_i + (\delta_{1i} + \delta_{2i})\,\zeta_3^{(0)},\end{aligned} \tag{39}$$

with $\zeta_1^{(0)}, \zeta_2^{(0)}$ and $\zeta_3^{(0)}$ the multipliers obtained with the energetic balances (power, total energy, local energy).

We have with relation (36), for all $(i,j,k)\in\mathcal{T}_N$

$$\langle a_i a_j a_k\rangle^{(0)} = \langle a_i a_j a_k\rangle\left(\mu_{ijk}^{(0)}, h_1^{(0)}, ..., h_N^{(0)}\right) = 0, \tag{40}$$

but obviously, by definition of coefficients $\hat{T}_{ijk}$

$$\hat{T}_{ijk}^{(0)} = \hat{T}_{ijk}\left(h_i^{(0)}, h_j^{(0)}, h_k^{(0)}\right) \neq 0. \tag{41}$$

This leads to the start of the recursive procedure.

(b) Recursive procedure: at step n

1. From constraints on triadic interactions (37), compute coefficients $\mu_{ijk}^{(n+1)}$ for all $(i,j,k)\in\mathcal{T}_N$

$$\begin{aligned} & q_{ijk}\langle a_i a_j a_k\rangle\left(\mu_{ijk}^{(n+1)}, h_i^{(n)}, h_j^{(n)}, h_k^{(n)}\right) \\ & = \hat{T}_{ijk}\left(h_i^{(n)}, h_j^{(n)}, h_k^{(n)}\right)\end{aligned} \tag{42}$$

2. Compute $h_i^{(n+1)}$

$$\begin{aligned} h_i^{(n+1)} &= e_i^{(n)} \\ & - \sum_{(j,k)/(i,j,k)\in\mathcal{T}_N}\mu_{ijk}^{(n+1)}\,\varphi_{ijk}\left(\alpha^{(n)}, h_i^{(n)}, h_j^{(n)}, h_k^{(n)}\right);\end{aligned} \tag{43}$$

3. From power and energy constraints (23) and (24), compute coefficients $\zeta_1^{(n+1)}, \zeta_2^{(n+1)}$ and $\zeta_3^{(n+1)}$;
4. Compute $\lambda_i^{(n+1)} = -\sum_{\substack{j=1 \\ j\neq i}}^{N} \frac{1}{2h_j}\mu_{jji}$ for all i;
5. Compute $\hat{T}_{ijk}^{(n+1)} = \hat{T}_{ijk}\left(h_i^{(n+1)}, h_j^{(n+1)}, h_k^{(n+1)}\right)$ for all i, j, k;
6. Enter loop again at step (1) until convergence of all multipliers.

Results

We present the results for $N = 6$. The set of non-zero triadic interactions (12) is then

$$\begin{aligned}\mathcal{T}_6 = \big\{&(1,1,3),(1,1,4),(1,2,3),(1,2,4),(1,3,5),\\ &(1,3,6),(1,4,5),(1,4,6),(2,2,3),(2,2,4),\\ &(2,3,5),(2,3,6),(2,4,5),(2,4,6)\big\}.\end{aligned} \tag{44}$$

We show on Figure 1 the first component p_1 of the Gaussian function p_0 defined by (35) (note the full pdf is 6-dimensional), in comparison with a case without triadic interactions (this means coefficients φ_{ijk} are set to 0 in equation (32)). Only the donor modes have a real modification, even if quite slight, which is consistent with the linearisation.

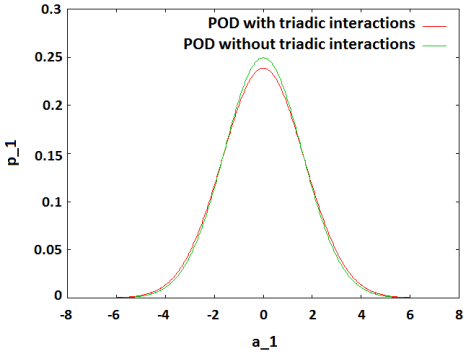

Figure 1: First Gaussian component of p_0, with and without triadic interactions.

We display in Table 1 the values of the μ_{ijk} coefficients for the 14 elements of $\mathcal{T}_6$, showing the symmetry between the interactions:

(i,j,k)	μ_{ijk}	(i,j,k)	μ_{ijk}
$(1,1,3)$	$-6.2041.10^{-2}$	$(2,2,4)$	$6.8900.10^{-2}$
$(1,1,4)$	$-5.9557.10^{-2}$	$(2,2,3)$	$6.07670.10^{-2}$
$(1,2,3)$	-0.197501	$(1,2,4)$	0.120676
$(1,3,5)$	-3.334410	$(2,4,6)$	3.195177
$(1,3,6)$	2.993233	$(2,4,5)$	-3.579895
$(1,4,5)$	-3.054477	$(2,3,6)$	3.651318
$(1,4,6)$	-3.290219	$(2,3,5)$	3.142075

Table 1: Values of the μ_{ijk} multipliers.

The corresponding energy levels are shown on Figure 2. Once again, we show the results given by our model with and without triadic interactions (respectively green and red curves), as well as the exact solution (black) and the solution given by resolution of the FTT model (6)/(7)/(10) using a classical Runge-Kutta algorithm (blue). We can observe a truncation effect for the last two modes due to numerical precision errors.

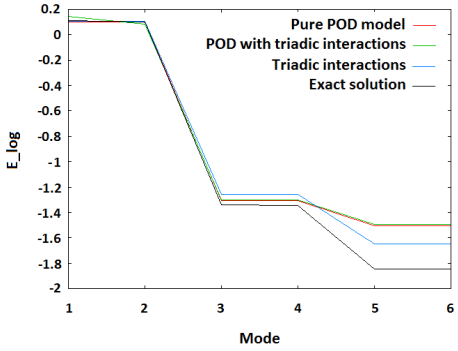

Figure 2: Energy levels in log scaling.

Conclusions

We present a statistical closure of a reduced-order Galerkin model of a cylinder wake in the periodic oscillatory regime, inferred with a MaxEnt method. This method maximises a relative entropy subject to simple physical constraints, and with constraints arising from an efficient modelling of triadic interactions between the Galerkin modes, governing energy transfers between them. Although this leads to an unbounded solution, a linearisation yields a result consistent with the finite-time thermodynamics model and with the results obtained without modelling of energy transfers. This model could be extendable to more complex fluid systems.

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