Application of soft-DTW for Time Series Data Averaging Inside a Rotating Detonation Combustor

Mauro Tagliaferri*
Università degli Studi di Firenze, Florence, 50121, Italy

Provence Barnouin†, Hongyi Wei‡, Eric Bach§, Christian Oliver Paschereit¶, and Myles D. Bohon‖
Technische Universität Berlin, Berlin, 10623, Germany

Applications of high-speed diagnostics can help understand the structure and dynamics of detonation waves in RDCs. Phase averaging can be applied to resolve the circumferential detonation structure. However, a high level of stochasticity has been observed in RDC experimental data. As a result of this variability, when several data samples are averaged using the conventional arithmetic mean, data features can be distorted or overlooked. This can easily lead to an erroneous characterization of the wave structure and flow field inside an RDC. In order to obtain a more accurate representation of the underlying data, this work investigates the application of three different averaging techniques: the Euclidean distance based arithmetic mean, the DTW Barycenter Averaging (DBA) and soft-DTW barycenter. Results show that the Euclidean barycenter does not capture well the sharpness of the detonation front while the DTW Barycenter Averaging absorbs the idiosyncrasies of the data resulting in a discontinuous average that is not characteristic of any of the time series. Soft-DTW based averaging overcomes these limitations through the introduction of a smoothing parameter and yields a more representative average of RDC time series data. In addition, soft-DTW based averaging is less sensitive to small perturbations in the data and can construct a representative average of the data from fewer data samples.

I. Introduction

Rotating detonation combustors (RDC) are a promising candidate in pressure gain combustion (PGC) research, utilizing one or more continuously spinning detonation waves to achieve an increase in stagnation pressure. In an RDC, a detonation wave rotates around the annular combustion chamber at frequencies on the order of 5-6 kHz. Current experimental RDC research mainly depends on the acquisition and processing of high-frequency pressure measurements, high-speed imaging and high-repetition rate laser diagnostics [1–5]. High-speed measurements allow for approximations of the average wave frequency to be made and can shed light on the structure and dynamics of detonation waves inside the combustion chamber. It is often desirable to apply phase averaging of the measured signals over individual wave laps to resolve the circumferential detonation wave structure.

Taking an arithmetic mean of the wave laps is the conventional way to obtain the average distribution of measurable parameters around the combustor annulus. Bohon et al. [1] used the arithmetic mean to average dynamic pressure data from a steady run with a single detonation wave propagating around the annulus. However, the computed average data exhibited significant smoothing of the underlying data, especially for sharp features such as the steep-fronted detonation wave. This is due to lap-to-lap fluctuations observed in high-speed measurements that occur even for cases where stable mode propagation has been successfully established in the RDC. Complex underlying mechanisms may partly account for small variations of the measured properties between individual wave passage. The stochasticity in the measured RDC data is also likely caused by measurement uncertainty, the sensor installation, and sensor noise. In addition, the response time of high-speed diagnostics like piezoresistive pressure sensors has a characteristic response time to the pressure change at the detonation front. This may introduce stochastic artifices in the measurements such as overshoots

*Graduate Student, University of Florence.
†PhD Student, Chair of Pressure Gain Combustion, TU Berlin.
‡PhD Student, Chair of Pressure Gain Combustion, TU Berlin.
§Postdoctoral Researcher, Chair of Pressure Gain Combustion, TU Berlin, AIAA Student Member.
¶Professor, Chair of Fluid Dynamics, TU Berlin, AIAA Associate Fellow.
‖Professor, Chair of Pressure Gain Combustion, TU Berlin, AIAA Member.

and dead time. Furthermore, the sampling rate will affect the stochasticity of the signal when a discrete measurement is used to reconstruct a continuous time stochastic process. To recover a representative average of the measured properties, an effective method must be found to deal with the stochastic RDC data.

Therefore, we pose the following question: How can we best average the high-speed experimental RDC data to resolve the circumferential structure and dynamics of the detonation wave? The arithmetic mean, based on the Euclidean distance, does not always perform well with time series such as time-resolved RDC data because it is not robust to distortions on the time axis. Any shifts in the timing between individual RDC laps results in a distortion of the average. It is therefore preferable to use an averaging approach based on another distance measure that is more robust to time distortions. One candidate is Dynamic Time Warping (DTW). The DTW measure, which seeks a minimum cost alignment matrix, has the ability to deal with local variations in the time axis, allowing a better alignment between the points of time series [6]. In some sense, DTW preserves the human sense of shape-similarity by allowing elastic transformation of time series in order to detect similar shapes across different phases. There are two approaches to averaging based on the DTW metric: DTW Barycenter Averaging (DBA) and the soft-DTW barycenter [7, 8].

The objective of this work is therefore to investigate the application on RDC time series data of three different averaging techniques: the Euclidean distance based arithmetic mean, the DTW Barycenter Averaging and soft-DTW barycenter. The results of this paper are expected to provide guidelines for averaging RDC time series data that future studies can apply to study the detonation wave structure and flow field inside a combustor.

II. Methods

A. Experimental Setup

Data for this study is acquired on the non-premixed RDC geometry at TU Berlin [9], as shown in Figure 1(a). The combustor is composed of an annular chamber with an axial length L of 110 mm, outer diameter D of 90 mm and annulus gap width Δ of 7.6 mm. Hydrogen is injected axially through a fuel plate with a ring of 100 0.7 mm holes, while air is introduced radially through a 1 mm slot and mixes with the fuel in a jet-in-crossflow configuration. A restriction that reduces the outlet area by 16% is also introduced. There are four levels of ports located axially along the combustion chamber wall from which different pressure sensors can be installed. A PCB 112A05 piezoelectric pressure transducer is placed in a flush-mounted configuration on Level 1 to measure the dynamic pressure component as shown in Figure 1(b). Run time is limited to less than 300 ms to mitigate sensor damage. The data are sampled at 500 kHz. In this study, the air mass flow rate is set at 500 $\mathrm{g \cdot s^{-1}}$ and the global equivalence ratio at stoichiometric conditions.

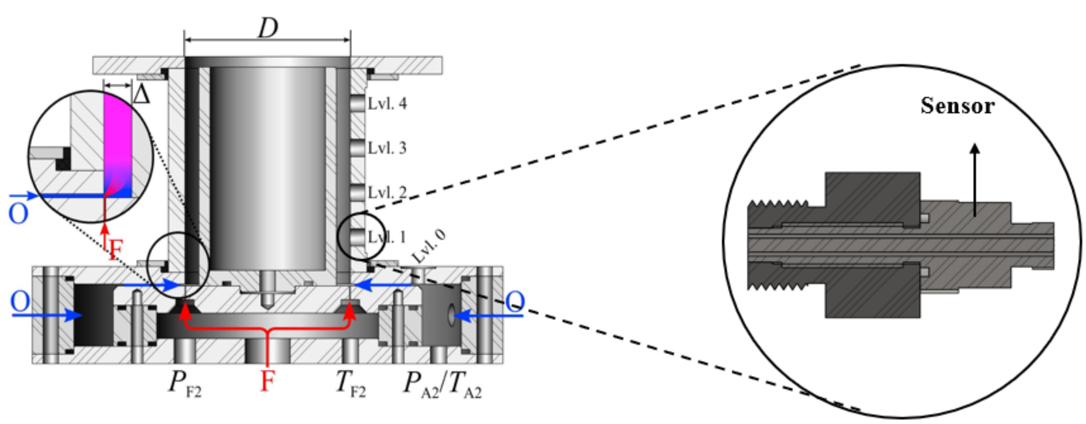

Fig. 1 Experimental setup: (a) Schematic diagram of TU Berlin's RDC, highlighting the reactant injection processes, and (b) pressure sensor in a flush-mounted configuration on Level 1 (detonation region).

B. Averaging Methods

The objective of time series averaging is to construct a single time series $\mathbf{x}$ that is located closest to a given set of time series, $\mathbf{Y} = \{\mathbf{y_1}, \mathbf{y_2}, ..., \mathbf{y_N}\}$, according to a cost-alignment distance. The computed time series $\mathbf{x}$ is referred to as the barycenter of the set $\mathbf{Y}$. Each time series $\mathbf{y_j}$ represents the pressure signal measured at a point by a pressure transducer probe over the detonation wave period. There are different approaches used to compute the average of time series data. Often the average is found by minimizing a cost-alignment problem between time series data using the the Euclidean distance. However, as we will show, the Euclidean distance is not expected to perform well with time series data because it is sensitive to shifts on the time axis. It is therefore preferable to use another measure that is more robust to time distortions. One proposed method is dynamic time warping (DTW). The DTW measure has the ability to deal with local distortions in the time axis, allowing a better matching between the points of a given time series [7]. The Euclidean and DTW distance for two time series are displayed in Figure 2.

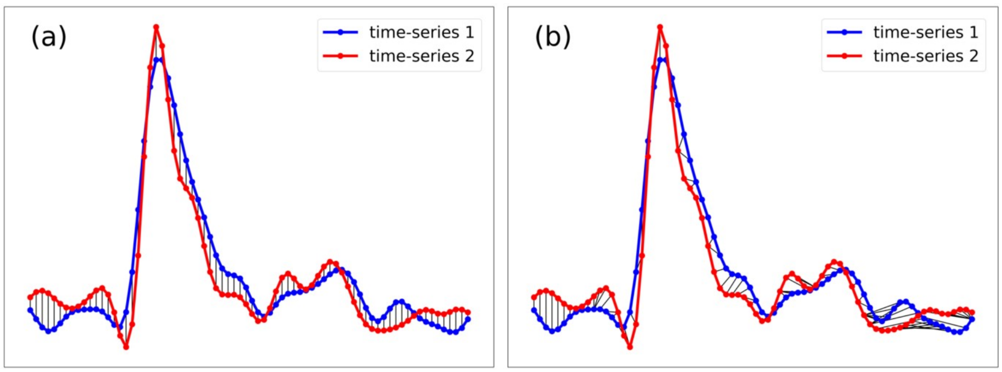

Fig. 2 Alignment of two example RDC time series data using (a) the Euclidean metric, and (b) the DTW metric.

Suppose that $\mathbf{x} \in \mathbb{R}^{m\times d}$ and $\mathbf{y_j} \in \mathbb{R}^{n\times d}$ are two d-dimensional time series of lengths m and n. The cost or distance matrix, $\Delta(\mathbf{x}, \mathbf{y_j}) \in \mathbb{R}^{n\times m}$, can be defined as the squared Euclidean distance between the two time series. $\mathbf{A} \in 0, 1^{m\times n}$ is an alignment matrix between the elements of $\mathbf{x}$ and $\mathbf{y_j}$, where a value of 1 is aligned and 0 is given otherwise. $\mathcal{A}(\mathbf{x}, \mathbf{y_j})$ denotes the number of admissible paths or alignments (coined Delannoy number) between the two time series. Given the cost matrix $\Delta(\mathbf{x}, \mathbf{y})$ and the alignment matrix $\mathbf{A}$, the inner product $\langle\, A, \Delta(\mathbf{x}, \mathbf{y_i})\,\rangle$ is the sum of the costs along the alignment. DTW can then be defined as the minimum cost among all alignments in Equation (1):

$$\mathrm{dtw}_0(\mathbf{x}, \mathbf{y_j}) := \min_{A\in\mathcal{A}_{n,m}} \langle\, A, \Delta(\mathbf{x}, \mathbf{y_j})\,\rangle \tag{1}$$

In soft-DTW the minimum is replaced by a soft minimum described in Equation (2). Soft-DTW introduces a smoothing parameter, γ, which controls a trade-off between smoothness and accuracy.

$$\min{}^{\gamma}(\mathbf{y_1}, \mathbf{y_2}, \ldots, \mathbf{y_N}) = \begin{cases} \min_{i\le N}\mathbf{y_i} & \gamma = 0 \\ -\gamma \log \sum_{j=1}^{N} \exp^{-\mathbf{y_j}/\gamma} & \gamma > 0 \end{cases} \tag{2}$$

As such, soft-DTW as defined in Equation (3), considers all possible alignments weighted by their probability under the Gibbs distribution $\mathbb{P}_\gamma$. When γ is set to 0, the original DTW distance is recovered, and when γ tends to infinity, soft-DTW converges to the sum of all costs [10]. The expected or average alignment matrix $\mathbb{E}_\gamma = \sum_{A\in\mathcal{A}_{n,m}} \mathbb{P}_\gamma \mathbf{A}$ informs for each pair of elements in $\mathbf{x}$ and $\mathbf{y_j}$ how much they will be taken into account in the alignment and is shown in Figure 3.

$$\mathrm{dtw}_\gamma(\mathbf{x}, \mathbf{y}) := \min_{A\in A_{n,m}}{}^{\gamma} \langle\, A, \Delta(\mathbf{x}, \mathbf{y})\,\rangle \tag{3}$$

DTW Barycenter Averaging (DBA) and soft-DTW are two approaches to averaging in the DTW-based space. The average (barycenter) of a set $\mathbf{Y} = \{\mathbf{y_1}, \mathbf{y_2}, \ldots, \mathbf{y_N}\}$ can be found by solving Equation (4). In DBA, an initial series is iteratively refined, in order to minimize the alignment cost matrix with the set of time series considered.

$$\min_{\mathbf{x}\in R^{mxn}} \sum_{i=1}^{N} w_i \mathrm{dtw}_0(\mathbf{x}, \mathbf{y}_j) \tag{4}$$

However, DBA is not differentiable everywhere and can lead to bad local optima when used for averaging [8]. Introducing smoothing can help to avoid bad local optima, as such the soft-DTW barycenter can be defined in Equation 5:

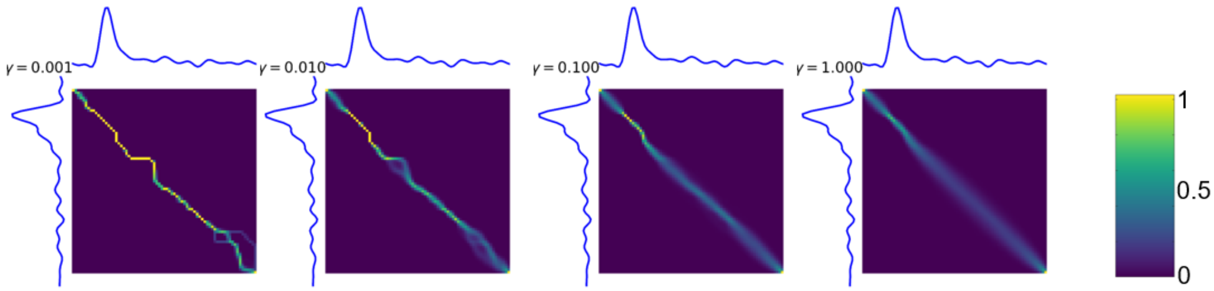

Fig. 3 Expected alignment matrix $\mathbb{E}_\gamma$ for different values of γ.

$$\min_{\mathbf{x}\in R^{mxn}} \sum_{i=1}^{N} w_i \mathrm{dtw}_\gamma(\mathbf{x}, \mathbf{y}_i) \tag{5}$$

The similarity between a set of time series and the calculated barycenter for each method can be quantified using the DTW loss defined in Equation (1) [8]. This measure can be interpreted as the cumulative cost of alignment and will be used as one of the metrics to compare the goodness of fit of the calculated barycenters.

C. Data Pre-Processing

A data pre-processing algorithm is applied on the measured dynamic pressure data shown in Figure 4(a) to obtain N time series over which the averaging methods can be applied. The test case considered in this study is a single rotating detonation wave. From the FFT frequency distribution shown in Figure 4(b), it can be noted this is a fairly stable case with low levels of stochasticity. Pressure data during a stable portion of the run was chosen. Transient behavior between consecutive wave passages from the baseline drift introduced by the PCB sensor was low-pass filtered at 150 Hz.

The pressure traces are then subdivided and aligned into individual time series, with each time series representing a detonation wave passage. There are different ways to align the data set. Two different methods are considered in this paper: one where the mean FFT measured frequency is used to define a window length, from which sequential windows can be taken. Another, where the time-series are aligned according to the pressure peak in an average equal window length. It should be noted that, from prior experience, identifying and aligning individual passages of the detonation wave is not always a trivial process, especially when the data is not as clean as that shown in this dataset. Therefore, the current case in many ways represents a "best case" alignment that may not be achievable in all cases. The N time series are set to have an equal length m based on the average wave period obtained by FFT analysis. This will enable a direct comparison with the Euclidean barycenter, while also minimizing the DTW loss of the DTW and soft-DTW barycenters [7].

The start of the time series is defined to be at 25% of the average period before the maximum pressure rise. This region is chosen as the start because there is relatively little change in pressure per time step. This minimizes the sensitivity of the averaging methods to the input data as DTW and soft-DTW always match the initial and final data points between time series (which is the case for all data points in Euclidean averaging). Calculating the barycenters based on a start point defined in a portion with a high pressure gradient would therefore make the algorithm more sensitive to the subdivision of the time series.

The time series are normalized according to Equation (6). The resulting time series for both alignments are shown in Figures 4(c) and (d). Normalization is not a prerequisite to apply the averaging methods. However, by normalizing the data between [-1 1], similar values of γ can be used in the soft-DTW algorithm for comparable test cases. Although z-normalization is typically used in soft-DTW applications, it normalizes each individual time series and is therefore not suitable for averaging data sets where the amplitude of data is important [6].

$$\tilde{p} = 2\left(\frac{p - \overline{p}_{\max}}{\overline{p}_{\max} - \overline{p}_{\min}}\right) - 1 \tag{6}$$

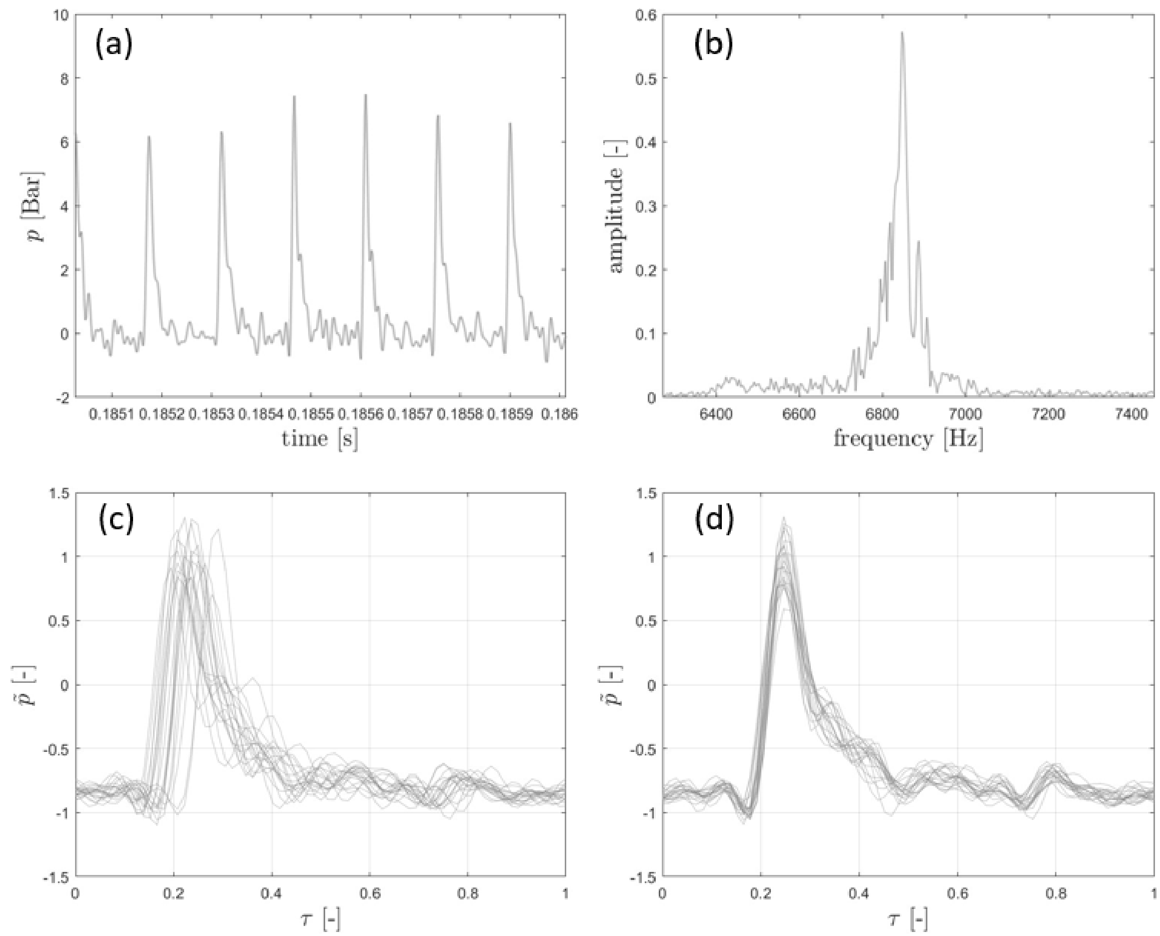

Fig. 4 Data pre-processing procedure: (a) Portion of the dynamic pressure trace considered, (b) FFT analysis of the test case, (c) FFT mean frequency aligned and normalized time series, and (d) peak aligned and normalized time series.

III. Results

The objective of this work is to investigate the averaging of time-dependent measurable parameters inside the RDC such as the pressure in the detonation region. These results will be discussed in two sections. The first section will compare and evaluate the sensitivity of different averaging techniques to demonstrate the practicality of the soft-DTW approach for RDC data averaging. The second section will focus on the soft-DTW averaging method and the effect of soft-DTW parameters will be investigated and recommendations for RDC data application provided.

A. Comparison and Sensitivity of the Averaging Methods

1. Effect of Time Series Alignment

The averaging methods are applied to a data set consisting of dynamic pressure data over one wave period measured by a piezoelectric PCB sensor placed in the detonation region. The data is aligned according to the mean FFT measured frequency and the peak. For both of alignments, 100 time series can be defined, each consisting of 73 data points sampled at a frequency of 500 kHz. The Euclidean, DTW and soft-DTW barycenters are computed for the data set consisting of 20 randomly selected time series and plotted in Figure 7 for both of alignments. Although the results here are given in terms of dynamic pressure, the remaining results will be reported on a normalized axis to allow for comparison with a variety of RDC data types.

It can be observed that for the mean FFT measured frequency based alignment method, the barycenters of each method exhibit different features. The Euclidean barycenter significantly underestimates the peak height and is not representative of any of the individual underlying time series. As the Euclidean barycenter is a point-by-point average, it does not capture well abrupt changes in short time spans, resulting in a flatter slope and rounded peak. The DTW barycenter is able to better capture the peak height, but absorbs the idiosyncracies of the data yielding many small kinks at points such as $\tau = 0.05$, $\tau = 0.65$ and $\tau = 0.82$, that are not representative of any of the time series in the data set. These features of the DTW barycenter were observed across the majority of the RDC pressure data in the detonation zone. Unlike the Euclidean mean, the soft-DTW barycenter is able to capture the sharp change at the detonation front while still yielding a smoother barycenter than the DTW barycenter and that better matches the time series. It can be observed that due to the introduction of the smoothing parameter, γ, the kinks of the DTW barycenter are absent however the variation in the signal in the trailing portion of the pressure trace is retained. In this case, the soft-DTW barycenter better depicts the detonation front and expansion behind the wave.

Unlike for the mean FFT measured frequency based alignment, when using the peak-based alignment, the Euclidean, DTW and soft-DTW barycenters have very similar shapes, although Euclidean and soft-DTW averaging yield smoother barycenters than for DBA. All barycenters are characterized by comparable pressure gradients and peaks at the detonation front, and pressure expansions. It is important to again recall, that this is a particularly well-behaved dataset that lends itself well to this alignment method. Such good alignment is not always achievable, and therefore one could reasonably expect a greater amount of temporal uncertainty and distortion that would prevent an effective use of the Euclidean barycenter. Since all averaging techniques give similar results, the soft-DTW barycenter from the peak-based alignment method is defined as the "true average" of the time series and will be used as a reference to compare against other averages.

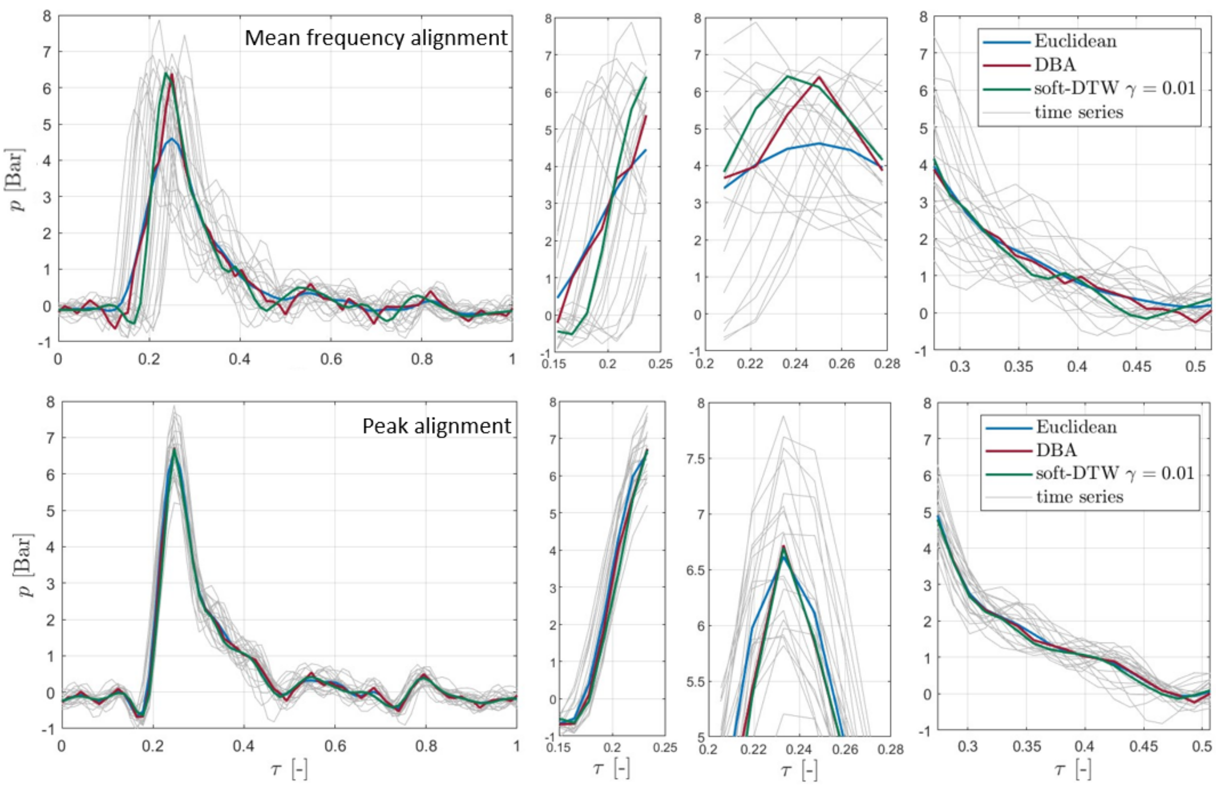

Fig. 5 Barycenters obtained from Euclidean, DBA and soft-DTW for the time series aligned according to the mean FFT measured frequency and peak.

Figure 6 compares the barycenters of each method for each alignment against the "true average" to evaluate their sensitivity to the alignment of the time series. As the Euclidean barycenter is a point-by-point average, it is expected that any small variation in the alignment of the time series will significantly affect the shape of the barycenter. The peak-based Euclidean barycenter closely matches the "true average" only because the time series aligned on the peak are not very stochastic. When the time series are aligned on the mean frequency, the resulting time series are not as neatly arranged. In this case, the Euclidean barycenter significantly minimizes the extremas and is unable to capture the shape of the "true average" even if the data considered exhibits a relatively low level of stochasticity as shown by the FFT analysis in Figure 4.

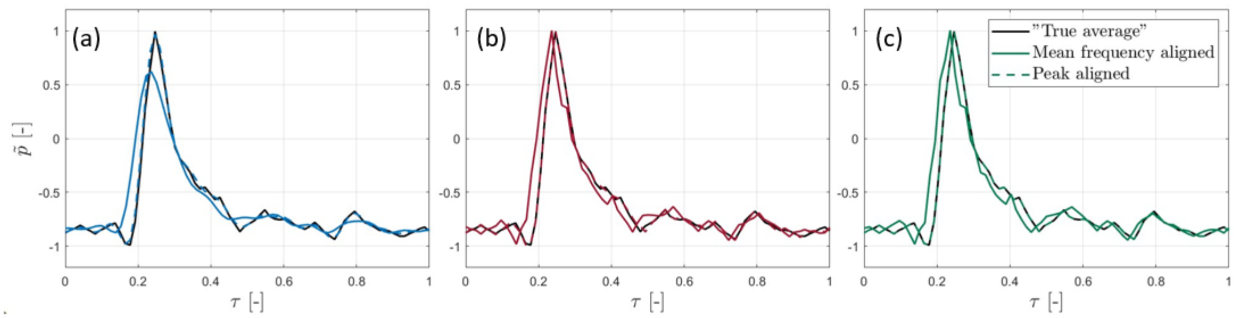

Fig. 6 Comparison of the true average with mean frequency and peak aligned (a) Euclidean barycenters, (b) DBA, and (c) soft-DTW barycenters for $\gamma = 0.01$.

By contrast, the DBA and soft-DTW barycenters are able to better recover the shape of the "true average" even when the underlying time series are more stochastic as in the case of the mean frequency based alignment. However, the DBA falls shorts as it absorbs the idiosyncracies of the underlying time series resulting in different locations of the kinks and a flatter detonation front. The mean frequency aligned soft-DTW barycenter recovers the majority of the shape of the "true average" highlighting the advantage of soft-DTW averaging with stochastic data. For the remaining results, the mean FFT frequency alignment will be used because aligning according to a feature such as the peak forces an assumption on the feature. In particular, this assumption might break down for RDC data sets characterized by higher degrees of stochasticity.

2. Effect of Time Series Sample Size

The effect of the number of the time series on the barycenter calculation is investigated. The Euclidean, DTW and soft-DTW barycenters are computed for the normalized data set consisting of 20, 50, 100 randomly selected time series and plotted Figure 7. It can be observed that the barycenters calculated for 20 time series show similar trends to the ones for 50 and 100 time series. The barycenters for 20, 50 and 100 time series for each methods are compared against the "true average" in Figure 8. For the Euclidean barycenter, the peak height and detonation front slope decrease as the number of time series increases. This behavior is expected as the overall stochasticity of the time series considered in the calculation of the Euclidean barycenter increases with the number of times series.

For the DTW, the barycenter tends to take on a different distribution as the number of time series with which it is calculated changes. With the smoothing parameter γ, the soft-DTW is able to overcome the limitation of the DBA, giving a barycenter that does vary significantly with the number of time series and capture the "true average". It is therefore not necessary to use the entirety of the data to find a representative average. Since the soft-DTW averaging gets comparable results with fewer data sets, an average with a finer temporal resolution could be obtained.

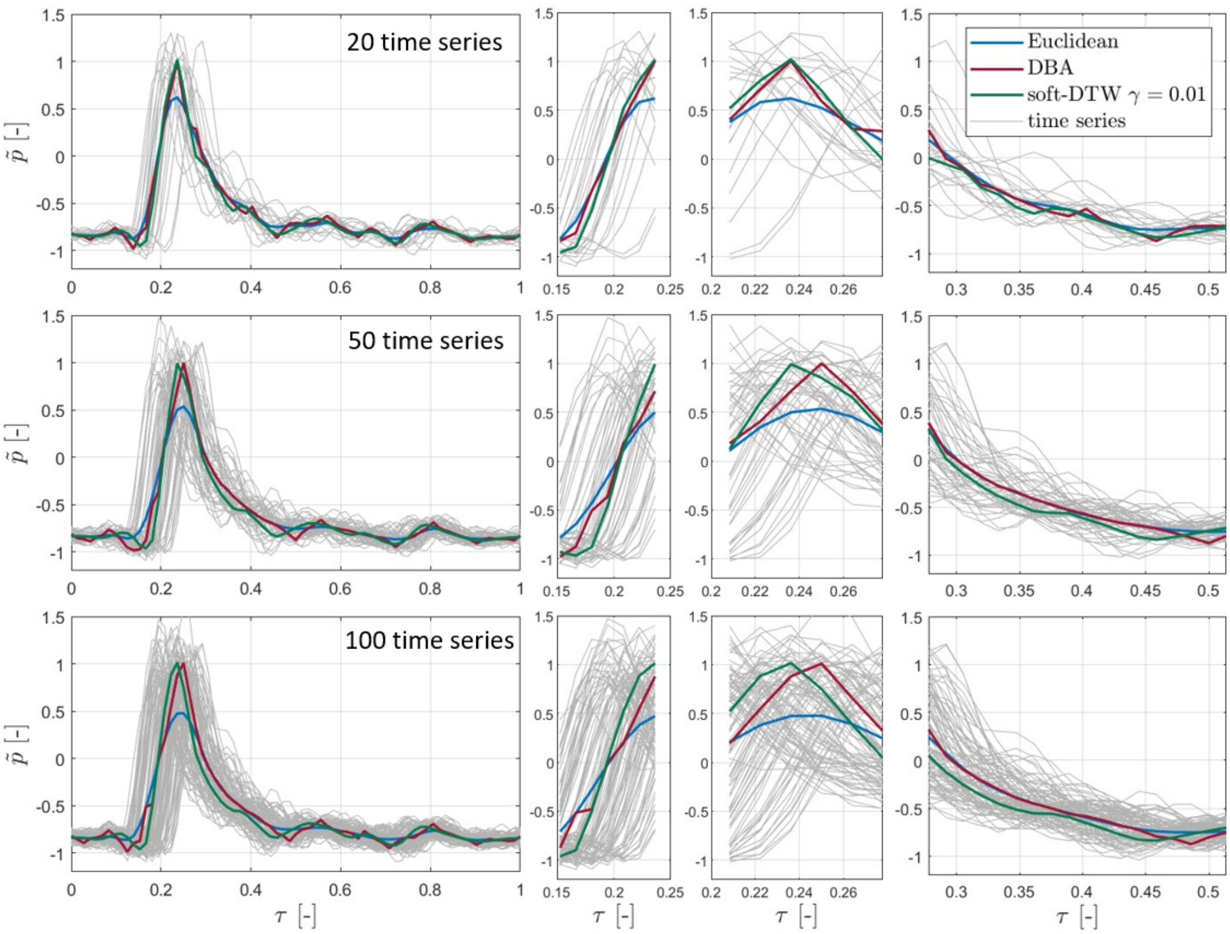

Fig. 7 Barycenters obtained from Euclidean, DBA and soft-DTW for 20, 50 and 100 iterations.

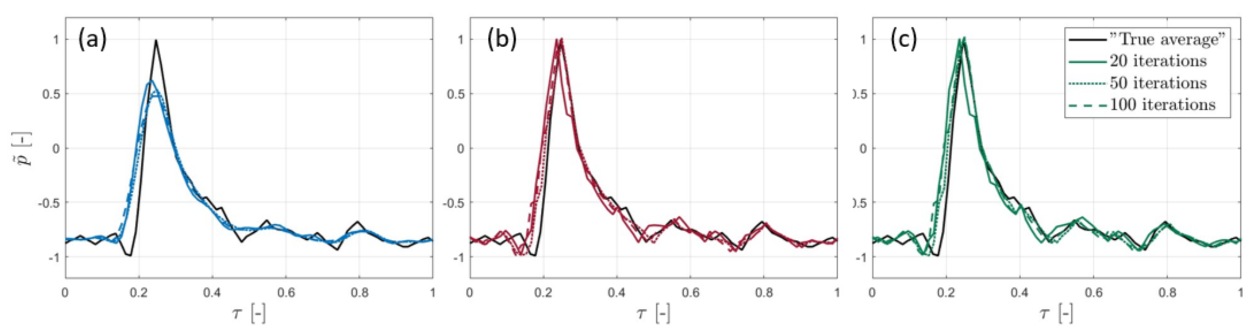

Fig. 8 Comparison of the true average with the (a) Euclidean barycenters, (b) DBA, and (c) soft-DTW barycenters for 20, 50 and 100 iterations.

B. Evaluation of the Soft-DTW Smoothing Parameter γ

In the soft-DTW barycenter algorithm, there are different parameters that can be set such as the smoothing parameter γ, type of initialization, number of time series, weights of the time series λ and type of initialization. In this section, the effects of the smoothing parameter on the soft-DTW barycenter are investigated and recommendations for RDC data applications provided. For the calculations of the barycenter presented in this section, the weight of a time series $\mathbf{y_i}$ is $w_i = \frac{1}{N}$ since all N time series have an equal length m. In addition, the barycenter is initialized from the soft-DTW initialization, itself initialized from a Euclidean mean. Such an initialization scheme yields lower DTW loss in accordance with the results presented in the literature [7, 10]. For each method, the maximum number of iterations is set to 100. To minimize the proposed soft-DTW barycenter objective, the L-BFGS optimization procedure is used.

In soft-DTW, γ is a parameter that controls the trade-off between accuracy and smoothness [8, 10]. Figure 9 shows the variation of the soft-DTW barycenter with γ. For very low values of the smoothing parameter (such as $\gamma = 0.001$), there are jagged features in the barycenter, which are not representative of the underlying data similarly to DBA. In particular, when γ is set to 0, the original DTW distance is recovered. For higher values such as $\gamma = 1$ local minima or maxima are attenuated. In order to select a γ that best represents the main features of the data and smooths out the idiosyncrasies of the data, the main features of the data for different values of γ were evaluated.

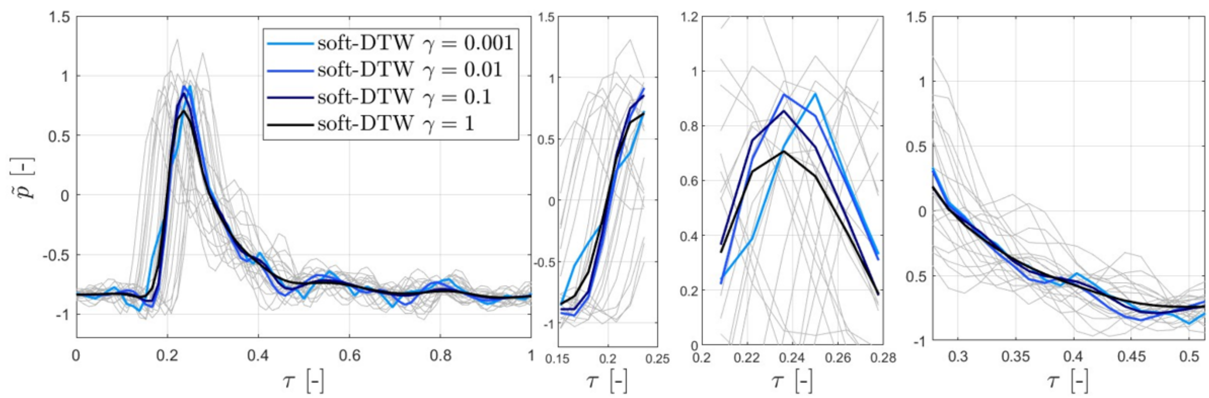

Fig. 9 Comparison of the soft-DTW barycenter for different values of γ.

The peak height, full width half maximum (FWHM) and slope of the soft-DTW barycenters are compared against the corresponding average values of all the time series as shown in Figure 10. The DBA and Euclidean barycenters are plotted for reference. It can be observed that for insufficient smoothing at $\gamma = 0.001$, the slope of the barycenter is underpredicted as the barycenter absorbs the idiosyncracis of the underlying data similarly to DBA. For over smoothing, the peak and the slope are underpredicted due to the attenuation of extrema similarly to the Euclidean barycenter. For $\gamma = 0.01$ the average peak, FWHM slope of the time series are well captured by the soft-DTW barycenter. While the FWHM is slightly underpredicted for the soft-barycenter with $\gamma = 0.01$, this can be neglected as it is most likely due to the temporal resolution on the order of $\tau = 0.02$, set by the sampling rate. A soft-DTW barycenter with a smoothing parameter such that $\gamma = 0.1$ seems to be an appropriate candidate for representing the chosen time series as the main features of the time series are preserved.

The DTW loss parameter can provide further confirmation for an appropriate choice of the smoothing parameter. The DTW loss parameter is calculated according to the procedure presented by Cuturi et al. [8]: The barycenter is computed for 20 randomly selected time series and from Equation (1), the DTW loss is calculated between barycenter and all the time series. This procedure is repeated 10 times and the averaged results are reported in Table 1. It can be observed that on average the lowest DTW loss is achieved for $\gamma = 0.01$. For DBA or soft-DTW with too low γ parameters, the DTW loss increases as the obtained barycenters get stuck in local minima resulting in kinks, which are not present in any of the underlying time series. For barycenters with higher values at γ and the Euclidean barycenter, the local extrema such as the peak pressure are smoothed out which contributes to a higher DTW loss. For this data and other similar data sets, a soft-DTW barycenter with a value of $\gamma = 0.01$ is a good candidate for the representation of the average time series as it preserves the main features of the underlying data and yields a low DTW loss. That said, users may need to fine tune the value of γ in order to preserve specific features of the underlying dataset or suppress numerical artifacts.

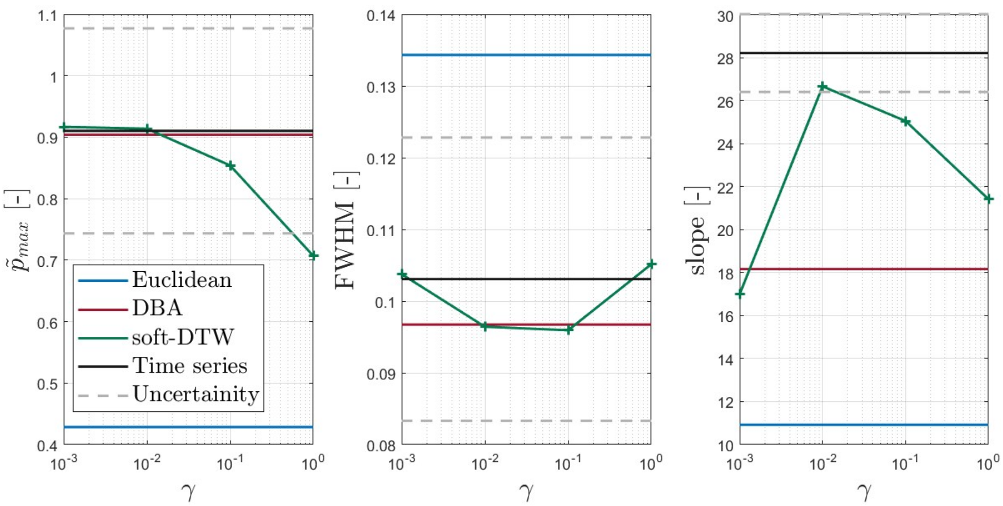

Fig. 10 Comparison of (a) the peak, (b) full width half maximum, and (c) slope obtained from Euclidean, DBA, and soft-dtw averaging.

Method	Euclidean	DBA	Soft-DTW $\gamma = 0.001$	Soft-DTW $\gamma = 0.01$	Soft-DTW $\gamma = 0.1$	Soft-DTW $\gamma = 1$
DTW loss	1.43	0.79	0.78	0.72	0.86	1.03

Table 1 Mean DTW loss calculated from Equation (1) for the different averaging methods.

IV. Conclusion

The study investigated the application on RDC time series data of three different averaging techniques: the Euclidean distance based arithmetic mean, the DTW Barycenter Averaging and soft-DTW barycenter. Results show that the Euclidean barycenter is very sensitive to the quality of the alignment and repeatability of the underlying dataset, and for noisy data does not capture well the sharpness of detonation front. Meanwhile, the DTW barycenter Averaging absorbs the idiosyncracies of the data resulting in a jagged average that is not characteristic of any of the time series. Soft-DTW based averaging overcomes these limitations through the introduction of a smoothing parameter without distorting the rapid pressure rise in the detonation front and yields a more representative average of RDC time series data. In addition, soft-DTW based averaging is less sensitive to small perturbations in the data and can construct a representative average of the data from few data samples. The results of this paper are expected to provide guidelines for averaging RDC time series data that future studies can apply to study the detonation wave structure and flow field inside a combustor and could provide reliable characteristic parameters for CFD simulations. Future work will focus on linking parameters of soft-DTW averaging to experimental variables and different wave modes.

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