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Unsteady simulation of quasi-periodic flows in Organic Rankine Cycle cascades using a Harmonic Balance method

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Abstract

Currently, turbomachinery design optimization methodologies are mainly restricted to steady state approaches, due to the high computational cost associated with time-accurate shape optimization algorithms. However, the possibility to include unsteady effects in turbomachinery optimization can significantly increase the level of accuracy of the design predictions, leading to a more realistic representation of the actual performance and ultimately to a substantial increase in operating efficiency. Unsteady effects are particularly relevant in Organic Rankine Cycle turbines. A trade-off between high-fidelity time-accurate unsteady simulations of the flow solution and computational cost is therefore needed at design level. In this paper, a first application of the harmonic balance method to non-ideal compressible flows is presented. The methodology allows to solve the unsteady flow equations for a set of specified frequencies only, with significant computational time savings. An algorithm is proposed for non uniform time sampling in order to resolve frequencies that do not need to be integral multiple of one fundamental harmonic. This enables the solution of quasi-periodically forced non-linear flow problems, in combination with complex fluid models based on accurate equations of state. The method is applied to the unsteady analysis of a supersonic Organic Rankine Cycle stator with quasi-periodic inlet operating conditions, showing about one order magnitude lower computational cost compared to time-accurate simulations.

Keywords: CFD; Unsteady; Harmonic Balance; NICFD; Turbomachinery; Time Sampling; Quasi-periodic

1. Introduction

The increasing spread of renewable energy power systems operating with non conventional fluids (e.g. ORC [1], scCO2 [2], refrigeration cycles [3]), has led to a renewed interest in design methods to provide a step change in components performance. Among the various cycle components, turbomachinery design optimization is not only beneficial from the efficiency point of view, but it also offers a cost-effective solution compared to the re-design of other components. Given the current lack of established design guidelines, optimal design can be accomplished only through automated procedures using high-fidelity computational fluid dynamic tools able to accurately model non-ideal fluid flows. Recently, work has been done to apply CFD-based optimization to single cascades of ORC turbines in steady-state conditions [4–6]. Nonetheless, due to the inherently unsteady nature of turbomachinery flows, steady state assumption may not only lead to different, and possibly less realistic [7], performance predictions but also to the

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impossibility of taking into account phenomena that are intrinsically related to unsteady effects (e.g. variable blade load, noise). More in particular, recent work has outlined the relevance of unsteady effects in the design of Organic Rankine Cycle (ORC) turbines [8]. Furthermore, unsteady design methodologies would effectively model external sources of time-varying effects, such as fluctuations in the operating conditions. This aspect, often neglected at design level, is of particular concern in renewable energy applications which are likely to be operated continuously at part loads. Considering that time-accurate design is still computationally prohibitive for industrial applications, reduced-order models have been proposed to reach a suitable compromise between accuracy and computational efficiency [9]. In particular, the harmonic balance (HB) method allows to solve unsteady problems for a specific set of frequencies only, reducing the computational cost of at least one order of magnitude compared to time-accurate non-linear solvers [10]. In this work the time-domain harmonic balance [11–13] is applied to simulate unsteady flows past ORC cascades with the aim of showing the capability of the method to predict unsteady effects at reduced computational cost. Furthermore, a non-uniform time sampling algorithm is proposed to ensure convergence of the method when a set of non-harmonically related frequencies are specified. This is considerably relevant to simulate turbomachinery stator-rotor interaction and random time-dependent operating conditions. The exemplary application considers a supersonic ORC stator subject to varying inlet conditions.

2. Method

2.1. Time Discretization

The semi-discrete form of the Navier-Stokes equations in Cartesian coordinates, for a generic cell volume Ω, is given by

$$\Omega\frac{\partial \mathbf{U}}{\partial t} + \mathcal{R}(\mathbf{U}) = 0\,, \tag{1}$$

in which $\mathbf{U} = (\rho, \rho v_1, \rho v_2, \rho v_3, \rho E)$ is the vector of conservative variables, with ρ the density and E the total specific energy. $\mathcal{R}$ is the spacial operator of the convective and dissipative fluxes. Applying a time discretization yields

$$\Omega\mathcal{D}_t(\mathbf{U}^{q+1}) + \mathcal{R}(\mathbf{U}^{q+1}) = 0\,, \tag{2}$$

with q the physical time step index. In Eq.2, the operator $\mathcal{D}_t$ was introduced. Finally, considering a dual-time step approach [14,15] with pseudo-time τ

$$\Omega\frac{\Delta\mathbf{U}^{q+1}}{\Delta\tau} + \Omega\mathcal{D}_t(\mathbf{U}^{q+1}) + \mathcal{R}(\mathbf{U}^{q+1}) = 0\,. \tag{3}$$

2.2. Harmonic Balance Operator

Applying the discrete Fourier transform (DFT) [12] to $\mathbf{U}$, the corresponding Fourier coefficients are given by

$$\hat{\mathbf{u}}_k = \frac{1}{N}\sum_{n=0}^{N-1}\mathbf{U}_n e^{-i\omega_k t_n}\,, \tag{4}$$

where $\tilde{\mathbf{U}} = [\mathbf{U}_0, \mathbf{U}_1, ..., \mathbf{U}_{N-1}]$, is the vector of the conservative variables evaluated at N time instances

$$\mathbf{t} = [t_0, t_1, ..., t_{N-1}] \tag{5}$$

and

$$\hat{\mathbf{u}} = [\mathbf{u}_0, \mathbf{u}_1, ..., \mathbf{u}_{K-1}]\,, \tag{6}$$

the corresponding Fourier coefficients, with $N = 2K + 1$, $\omega_k = 2\pi k f_k$ and K the number of frequencies . The vector of the K resolved frequencies can be the expressed as $\boldsymbol{\omega} = [0, \omega_1, ..., \omega_K, \omega_{-K}, ..., \omega_{-1}]$, with $\omega_{-k} = -\omega_k$.

Introducing the Fourier transform (DFT) matrix

$$E_{k,n} = \frac{1}{N} e^{-i\omega_k t_n}\,, \tag{7}$$

and the inverse IDFT

$$E^{-1}_{k,n} = e^{i\omega_k t_n}\,. \tag{8}$$

The Fourier coefficients can be calculated as

$$\hat{\mathbf{u}} = \mathbf{E}\tilde{\mathbf{U}}\,, \tag{9}$$

and the vector of the conservative variables

$$\tilde{\mathbf{U}} = \mathbf{E^{-1}}\hat{\mathbf{u}}\,. \tag{10}$$

It is important to notice that, if the frequencies f_k (and hence ω_k) are not multiple of f_1, once constructed either the DFT matrix from Eq.7 or the inverse Fourier transform (IDFT) matrix from Eq.8, it is not possible to have an analytical expression for the corresponding inverse matrix.

The time operator of Eq. 2 can be approximated using spectral interpolation. Applying the spectral operator to the vector of conservative variables $\tilde{\mathbf{U}}$, evaluated at N time instances, yields

$$\mathcal{D}_t(\mathbf{U}) \approx \mathcal{D}_t(\tilde{\mathbf{U}}) \tag{11}$$

Using Eq. 10 and Eq.9, since $\hat{\mathbf{u}}$ is independent from time, it can be written

$$\mathcal{D}_t(\tilde{\mathbf{U}}) = \mathcal{D}_t(\mathbf{E^{-1}}\hat{\mathbf{u}}) = \frac{\partial \mathbf{E^{-1}}}{\partial t}\hat{\mathbf{u}} = \frac{\partial \mathbf{E^{-1}}}{\partial t}\mathbf{E}\tilde{\mathbf{U}}\,. \tag{12}$$

From Eq.8

$$\frac{\partial \mathbf{E^{-1}}}{\partial t} = \mathbf{E^{-1}}\mathbf{D}\,, \tag{13}$$

where

$$D_{k,n} = i\omega_k \delta_{k,n}\,. \tag{14}$$

D is the diagonal matrix given by

$$\mathbf{D} = \mathrm{diag}\,(0, i\omega_1, ..., i\omega_K, i\omega_{-K}, ..., i\omega_{-1})\,. \tag{15}$$

Combining Eq.12 with Eq.13 and defining the spectral operator matrix **H** as

$$\mathbf{H} = \mathrm{Re}\left(\mathbf{E^{-1}DE}\right)\,, \tag{16}$$

it follows

$$\mathcal{D}_t(\tilde{\mathbf{U}}) = \mathbf{H}\tilde{\mathbf{U}}\,. \tag{17}$$

2.3. Time-domain harmonic balance

Considering $\tilde{\mathbf{U}}$, the set of the conservative variables evaluated at N time instances, Eq. (3) can be written as

$$\Omega \frac{\Delta \mathbf{U}^{q+1}_n}{\Delta \tau} + \Omega \mathcal{D}_t(\mathbf{U}^{q+1}_n) + \mathcal{R}(\mathbf{U^{q+1}_n}) = 0\,. \tag{18}$$

Linearising the residual, yields

$$\mathcal{R}(\mathbf{U}_n^{q+1}) = \mathcal{R}(\mathbf{U}_n^q) + \frac{\partial \mathcal{R}(\mathbf{U}_n^q)}{\partial \mathbf{U}_n^q}\Delta \mathbf{U}_n = \mathcal{R}(\mathbf{U}_n^q) + \mathbf{J}\Delta \mathbf{U}_n\,. \tag{19}$$

Since, from Eq.17, $\mathcal{D}_t$ is a linear operator

$$\mathcal{D}_t(\Delta \mathbf{U}_n) = \mathcal{D}_t(\mathbf{U}_n^{q+1} - \mathbf{U}_n^q) = \mathcal{D}_t(\mathbf{U}_n^{q+1}) - \mathcal{D}_t(\mathbf{U}_n^q)\,. \tag{20}$$

$$\mathcal{D}_t(\mathbf{U}_n^{q+1}) = \mathbf{H}\Delta \mathbf{U}_n + \mathbf{H}\mathbf{U}_n^q\,. \tag{21}$$

Substituting the linearised expressions, Eq.18 becomes

$$\left(\frac{\Omega \mathbf{I}}{\Delta\tau} + \mathbf{J} + \Omega\mathbf{H}\right)\Delta \mathbf{U}_n + \mathcal{R}(\mathbf{U}_n^q) = -\Omega \mathbf{H}\mathbf{U}_n^q\,. \tag{22}$$

The system of PDE, which holds for either laminar or turbulent flow problems, is solved within the open-source code SU2 [16,17]. A previous implementation of the time-domain harmonic balance method in SU2 [18] is used for this work. Compared to the original implementation [18], the possibility to specify non-uniform spaced time instances, i.e. for frequencies that are not commensurable, is added in SU2. This is done to enhance the convergence and the accuracy of the HB solver, see thereafter. Furthermore, in order to perform simulations of the testcase proposed in this work, SU2 was extended with time-varying HB boundary conditions, the capability to calculate proper turbomachinery performance for the HB resolved time instances and spectral interpolated performance averages. It is finally worth mentioning that in SU2 is possible to perform turbulent Non-Ideal Compressible Fluid Dynamics (NICFD) simulations [19].

2.4. NUOPT - Non Uniform time sampling OPTimization algorithm for convergence improvement

For quasi-periodic flows the DFT matrix and its inverse can be ill-conditioned, since the rows of $\mathbf{E}^{-1}$ are not necessarily orthogonal, as opposed to the case in which harmonically related frequencies are resolved. The high condition number leads to severe convergence problems [20,21]. In order to guarantee convergence for quasi-periodic forced flows, an algorithm is proposed to minimize the condition number of the IDFT matrix, $\kappa(\mathbf{E}^{-1})$. From Eq. 8, the selection of the time instances is a degree of freedom thus, in order to reduce the condition number of the IDFT matrix, three alternatives can be envisaged: 1. using a uniform time sampling and varying the period [18]; 2. using an non-uniform time sampling [20–22]; 3. oversampling over a uniform time distribution [20,22].

In the algorithm proposed in this work (NUOPT), the time instances of Eq. 5 are parametrized using a non-uniformly distributed set of time samples

$$t_n = \sum_{j=0}^{j=n} t_j + \alpha_n\, T_0 \qquad n \in [0, N-1]\,, \tag{23}$$

with $\alpha_n \in [0, 1]$ and for a fixed period T_0 corresponding to the minimum input frequency. The selection of T_0 is done in order to minimize aliasing errors [18]. According to this parametrization, the condition number $\kappa(\mathbf{E}^{-1})$ can be expressed as a function of the time sampling parameters only, i.e. $\kappa(\alpha)$. A differential evolution [23] method, in combination with the SLSQP gradient-based optimization algorithm [24], is used to obtain the global solution of the following minimization problem

$$\begin{aligned}
&\underset{\alpha_n\in[0,1]}{\text{minimize}} && \kappa(\alpha_n) && n \in [0, N-1]\,,\\
&\text{subject to} && \sum_{n=1}^{i} \alpha_n < 1 && i \in [1, N-2]\,,\\
& && \sum_{n=0}^{N} \alpha_n = 1\,.
\end{aligned} \tag{24}$$

3. Results

This section presents a first application of the time-domain harmonic balance method to non-ideal compressible flows. First, a verification of the proposed NUOPT algorithm is discussed. Subsequently, the harmonic balance method is applied to a supersonic cascade. All the results are obtained with the open-source code SU2 [16–19].

3.1. Time sampling algorithm verification

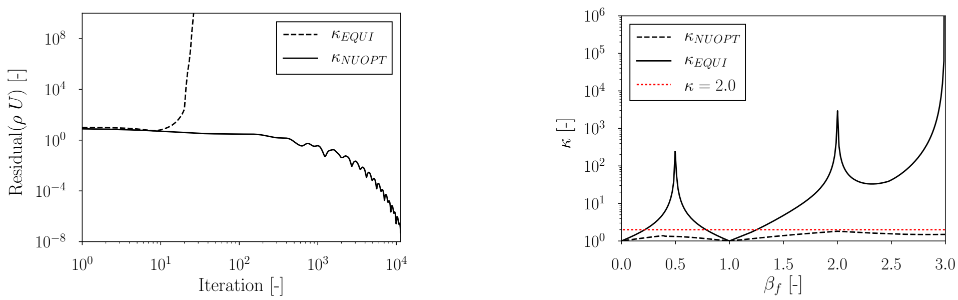
In order to verify the NUOPT algorithm, an unsteady total pressure is assigned at the inlet of a two-dimensional converging subsonic nozzle (outlet Mach number $Ma = 0.7$)

$$\tilde{P}_{tot} = P_{tot}\left[1 + A sin(\omega_1 t) + A sin(\omega_2 t)\right], \tag{25}$$

in which $A = 0.05$ and $\omega_2/\omega_1 = 15.1$. Inviscid calculations over a 5000 elements mesh are performed using MM as working fluid. Time discretization is applied using a second-order dual-time stepping approach [15], whereas a second-order accurate generalized Roe scheme [19,25] is adopted for convective fluxes discretization, based on the Monotone Upstream-centered Schemes for Conservation Laws (MUSCL) approach. Fig. 1a shows the convergence history of the nozzle for the optimized set of non-uniform time samples. Convergence is achieved with the optimized time instances ($\kappa_{NUOPT} = 1.3$) whereas the computation diverges for the original equispaced time set ($\kappa_{EQUI} = 1022.1$). The root-mean-square error (RMSE) between the HB converged solution and the time-accurate unsteady simulation is about 0.08%; the RMSE is calculated for a set of ten equispaced pressure probes along the nozzle axis. A further verification of the capability of the method is performed for a larger range of frequency ratios by defining the frequency parameter

$$\beta_f = \frac{\omega_2 - \omega_1}{\omega_1}. \tag{26}$$

The condition number of the IDFT matrix is calculated with both an equispaced approach (κ_{EQUI}) and with the non-uniform time sampling using the NUOPT algorithm (κ_{NUOPT}). In Fig.1b it is possible to see that, for the selected values of β_f, the IDFT matrix condition number calculated with the NUOPT algorithm is always lower than two. It is worth noting that in Fig.1b a minimum value of $\kappa = 1.0$ is obtained by both algorithms for $\beta_f = 1$ and $\omega_2 = 2\,\omega_1$, because the frequencies are harmonically related.



(a) Convergence history.

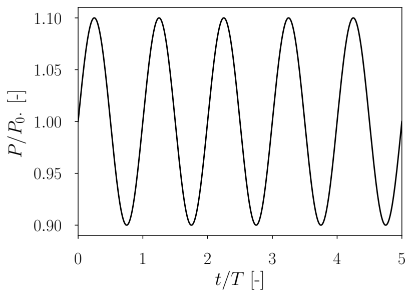
(b) Condition number.

Fig. 1: Verification results for the NUOPT algorithm.

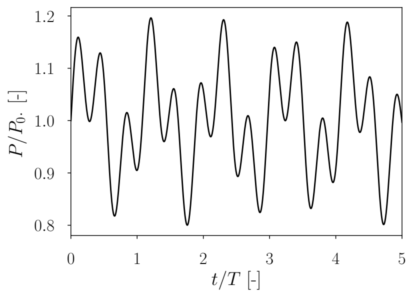
3.2. Supersonic stator cascade

The time-domain HB method is applied to perform Reynolds-averaged Navier-Stokes (RANS) simulations of an ORC supersonic cascade, operating under a time-varying inlet pressure. The working fluid is the siloxane MDM, modelled with a polytropic Peng-Robison equation of state [26]. The two-dimensional flow domain is discretized with an unstructured grid of about 40000 elements; a generalized Roe scheme [19,25] is used for the convective fluxes discretization and turbulent computations are carried out using the SST turbulence model [27]. Second order accuracy is obtained with MUSCL approach and gradient limitation. Tab. 1 summarizes the main simulation parameters. A time-dependent total pressure is imposed at the cascade inlet according to Eq.25 and two different operating conditions are considered, namely TC1 and TC2 (Tab.2).

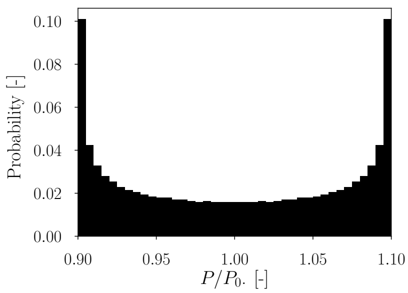
For the test-case TC1, an input signal characterized by a single frequency is assigned (Fig. 2a) whereas, for TC2, the signal is composed by two harmonics that are not commensurable (Fig. 2b). The time-varying operating conditions are imposed in order to test the HB method for unsteady effects caused by the variability of external flow quantities. For the sake of clarity, the probability corresponding to TC1 and TC2 are depicted in Fig. 2c and Fig. 2d, respectively. The combination of the HB method and the NUOPT algorithm can allow the selection of a random set of frequencies, enabling the possibility to resolve arbitrary probability density functions deriving from randomly variable operating conditions.



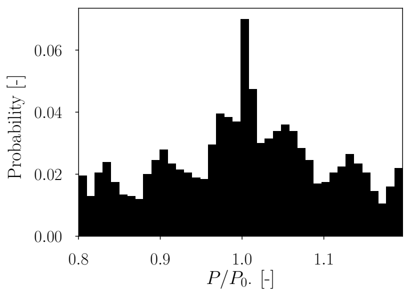
(a) TC1 input.



(b) TC2 input.



(c) TC1 input probability.



(d) TC2 input probability.

Fig. 2: Total pressure inlet for the stator cascade and corresponding probability histogram.

Fig. 3a shows the geometry and the density gradient for the TC1 test-case, normalized with respect to the inlet density. A normalized static pressure distribution is reported in Fig. 3b. Notice that the flow field is characterized by strong shock waves in the diverging section of the blade row, with non-linear effects predicted by the algorithm. The capability of predicting non-linear forced flows is one of the feature of the proposed time-domain HB formulation.

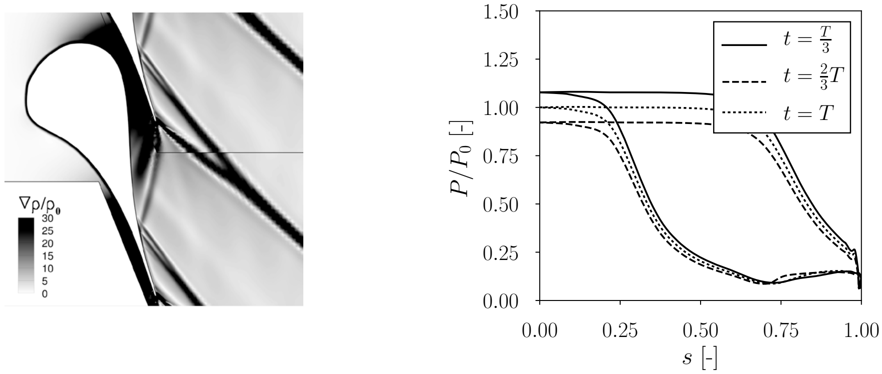
Table 1: Input parameters for supersonic ORC cascade .

Working fluid	MDM
Inlet compressibility factor	0.72
Total inlet temperature	545 K
Nominal Pressure ratio	8.
Background turbulence level	3%

Table 2: Simulation parameters for total pressure inlet (Eq. 25) .

Test-case	A [-]	ω_2/ω_1 [-]
TC1	0.10	0
TC2	0.04	2.7

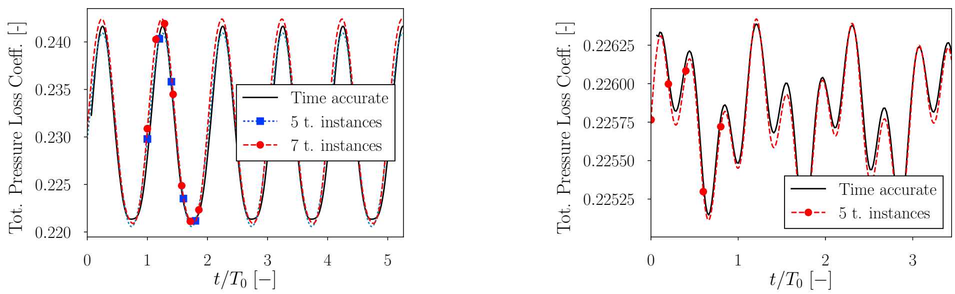
Finally, for both test cases, the total pressure loss coefficient of the cascade is calculated with a second-order accurate in time simulation using a dual-time step approach [15] and compared with the one obtained from the HB simulations (RMSE lower than 2%). For the time-accurate simulation the total number of time-steps, time-step size



(a) $t = \frac{1}{3}T_0$. (b) Pressure distribution.

Fig. 3: Results of the TC1 test-case. (a) Geometry and normalized density gradient contour calculated for one time instance ($t = 1/3T$). (b) Normalized static pressure distribution along the blade length for three time instances.

and number of internal iterations, are chosen as a trade-off between computational cost and accuracy evaluated on the total pressure coefficient. The HB results, obtained for different set of time instances, are spectrally interpolated and shown in Fig. 4. Furthermore, the computational cost of the HB simulation is found to be about one order of magnitude lower than that of the time-accurate unsteady.



(a) TC1. (b) TC2.

Fig. 4: Total pressure loss coefficient for the TC1 (a) and the TC2 testcase (b).

4. Conclusions

In this paper, a first application of the time-domain harmonic balance (HB) method to non-ideal compressible flows is presented and applied to a supersonic ORC stator. A non-uniform time sampling is proposed in order to ensure convergence for non harmonically related frequencies. This opens the possibility of considering intrinsic and extrinsic unsteady effects in the design optimization of turbomachines, and especially of ORC turbines. The results highlighted that the method is about one order of magnitude faster than time-accurate unsteady simulations, while showing an adequate level of accuracy for design purposes. Furthermore, the governing equations assume a form similar to the steady-state formulation. By leveraging on these features, ongoing work is focusing on the development of an HB adjoint-based shape optimization method.

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