Response to referees:

HarmonicBalance.jl: A Julia suite for nonlinear dynamics using harmonic balance

First, we would like to thank the referees for their detailed and thorough reviews of our manuscript. We are glad that Referee 1 recognizes the clarity and significance of our work. We also appreciate that Referee 1 finds the results of high practical contribution, and gives valuable, detailed suggestions. The referees' comments allowed us to significantly clarify and improve our manuscript. In the following, we answer (in blue text) to each of the points raised by the referees (in black), and highlight the corresponding changes in the revised manuscript (in red).

Response to Referee 2:

The authors present and discuss an open-source software package that allows to analyze nonlinearly coupled driven resonators. Specifically, this package aims at offering a tool for analyzing the steady state of the oscillations using the method of the Harmonic Balance. The latter method allows, provided a suitable ansatz, to reduce the problem of the time-dependent equations of motion of N driven nonlinear resonators to the problem of nonlinearly coupled equations for the amplitudes (with first derivative in time). This method is well known and widely used by the community working in this field. The paper is well written and it is a good pedagogical introduction to the topic of nonlinear coupled resonators.

At the introduction, the authors give a narrow overview of the literature who tackles the problems of nonlinear resonators and missed books and relevant references, as for example:

- A. H. Nayfeh and D. T. Mook, Nonlinear Oscillations (2008);

- H.G. Schuster, Reviews of Nonlinear Dynamics and Complexity (2009);

- M.I. Dykman, "Theory of nonlinear nonequilibrium oscillators interacting with a medium",

Zh. Eksp. Teor. Fiz. 68, 2082 (1975) [Soviet Physics JETP 41, 1042 (1975)];

and some recent and relevant works as for example: - PloS One 9, e0162365 (2016);

- Appl. Phys. Lett. 114, 103103 (2019);

- Phys. Rev. Applied 13, 014049 (2020);

- Nature Nanotechnology 12, 631 (2017);

- Nature Communications 8, ncomms15523 (2017).

We thank the Referee for their appreciation of our work. The principal intention of our manuscript was to illustrate the functionalities of the library and exemplify its usage with simple canonical problems. We did our best to cover important references in the various disciplines dealing with nonlinear dynamics (nonlinear electronics, photonics, topological bosonic phases, cavity optomechanics). Alas, we omitted the proposed citations and gladly refer to them in the revised manuscript.

Action taken:

We have included the proposed citations in our revised version.

In some interesting cases, the steady state solution can correspond to limiting cycles of the slow varying amplitude, see for example: Phys. Rev. Lett. 118, 033903 (2017), Phys. Rev. Lett. 121, 244302 (2018), Phys. Rev. Lett. 122, 254301 (2019, generating frequency comb. In this case, these variables are not described by fixed (time independent) points but they can have very different frequencies from the drive (not commensurate and different in scale). This possibility is not covered by the present package which makes uses of the ansatz based on the Harmonic Balance.

We thank the Referee for their essential comment, which also resonates with a comment raised by Referee 1. We summarise our reply above also here: limit cycles may be simulated using the time-dependent functionality of the package, see https://nonlinearoscillations.github.io/HarmonicBalance.jl/dev/examples/time_dependent/ Yet, the adaptation of the package to this purpose is straightforward. As the Referee rightly highlights, zero-dimensional fixed points do not describe a limit cycle in a rotating frame, and limit cycles appear at incommensurate frequencies with the drives in the system. These manifesting frequencies, however, can in some cases be estimated in the vicinity of a Hopf bifurcation. Once such frequencies are known to exist, their oscillation amplitudes can be found by applying the harmonic balance method within an increased (truncated) Fourier expansion. We are currently not aware of similar other approaches to this problem and believe this is an exciting avenue with fundamental interest beyond the scope of the current version of the library.

Action taken:

We plan to expand our support to limit cycles in future work. Please see “Action Taken” from the first point in response to the other Referee.

Another interesting case is the subharmonic resonance response. For a single resonator, this occurs when the drive frequency is close to a multiple of the bare frequency. For example, for the Duffing resonator, the drive frequency can be 3 times the harmonic frequency. In this case, the system can oscillate to a fraction of the drive frequency and, this case cannot be addressed by the package, as I understood. The two effects mentioned are theoretically interesting as they are due to the breaking of the discrete time translational symmetry on which is based the Harmonic Balance method.

We agree with the Referee that subharmonic responses of nonlinear oscillators are of great interest, but we point out that these can be already treated with the package. A particular example is the parametrically driven Duffing resonator which can sustain a subharmonic, period-doubling response, see https://nonlinearoscillations.github.io/HarmonicBalance.jl/stable/examples/single_parametron_1D/.

Action taken:

The parametrically driven Duffing oscillator example has been added to the manuscript. In the corresponding text, we included the following new references:

[Ref. 1] E. Goto, The parametron, a digital computing element which utilizes parametric oscillation, Proc. IRE **47**, 1304 (1959).

[Ref. 2] J. v. Neumann, Non-linear capacitance or inductance switching, amplifying and memory devices, U.S. Patent 2, 815,v488 (1959).

[Ref. 3] F. Sterzer, Microwave parametric subharmonic oscillators for digital computing, Proc. IRE **47**, 1317 (1959).

[Ref. 4] M. Hosoya, W. Hioe, J. Casas, R. Kamikawai, Y. Harada, Y. Wada, H. Nakane, R. Suda, and E. Goto, Quantum flux parametron: A single quantum flux device for Josephson supercomputer, IEEE Trans. Appl. Supercond. **1**, 77 (1991).

[Ref. 5] I. Mahboob and H. Yamaguchi, Bit storage and bit flip operations in an electromechanical oscillator, Nat. Nanotechnol. **3**, 275 (2008).

Since it is not discussed, I assumed that the package cannot address the problem of the ring-down dynamics of the nonlinear resonators which is an important and relevant problem in the field. The ring-down measurement is valuable experimental way to reveal nonlinear effects affecting the system, see for instance for example Scientific Reports 7, 18091 (2017).

Time-dependent scenarios such as ring-down are already included in the package, as described in Section 3.4, `Time-dependent simulations'. Namely, our tool receives both the original differential equations, solvable via DifferentialEquations.jl, and derives the approximate harmonic equations symbolically, which can be subsequently solved via our interface. Specifically, the insets in Figure 3 contain concrete examples, whereas Section 5.2, `Navigating involved solution landscapes', employs time-dependent simulations to adiabatically follow stable solution branches.

Action taken:

To further emphasise the time-domain simulation capabilities of the package, we incorporated in the manuscript a link to an example in the online documentation:

> To include additional frequencies, the harmonic ansatz must be expanded. To illustrate the interface to time-dependent solvers, we provide a simple example in the online documentation [link].

It is also worthy to mention the switching processes induced by the noise between the stable solutions that generates a slow dynamics that is not related to the drive frequency, see for example: Phys. Rev. Lett. 65, 48 (1990), Phys. Rev. E 49, 1198 (1994), Phys. Rev. E 57, 5202 (1998), Phys. Rev. E 74, 061118 (2006), Phys. Rev. Lett. 100, 130602 (2008), Phys. Rev. E 92 050903 (2015). But I understand that the inclusion of the noise is beyond the scope of the present software as well as the possibility to calculate theoretically the power spectrum which gives essential information about the nonlinear systems, see for instance Nature Nanotechnology 11, 552 (2016), and Nature Communication 5, 5819 (2014). In this sense, the scope of this package looks quite modest as it does not address essential aspects of the nonlinear physics.

The current package functionality focuses on deterministic nonlinear dynamics. Noise-activated processes are in our scope for future development, cf. preliminary steps in this direction in other works from our group [Ref. 76, http://arxiv.org/abs/2112.03357 , https://arxiv.org/abs/2203.05577]. On the other hand, the small-amplitude (linear) noisy response around attractors and the related power spectral density follows from the sole knowledge of the Jacobian eigenspectrum for a given solution.

Action taken

We now provide a LinearResponse module to calculate linear response, as documented in [https://nonlinearoscillations.github.io/HarmonicBalance.jl/stable/examples/linear_response/].

We added a comment in the revised manuscript regarding the focus on deterministic dynamics. Within the comment, we refer to the effects that are currently not covered by our software and add citations to the references mentioned above, as well as highlighting the said LinearResponse module:

As the system is coupled to dissipative baths, it will be also subject to fluctuations. While the current focus of our package is deterministic dynamics, analysis of weak fluctuations around a stable fixed point is included. The linear response of a stable, steady state to an additional oscillatory force, caused by weak probes or noise, is often observed in experiments [97]. It can be calculated by adding a small driving term δf cos(ΩdT) to the harmonic Eq. (8). To account for the time dependence of the perturbation, linearisation around u0 should retain the previously-dropped higher-order time derivatives. While implemented in the package, we leave a thorough discussion of this topic, as well as noise-activated dynamics, to future work.

But the most critical question is the following: for which experimental systems this tool can be useful? I mean the following. The authors report the example of two linearly coupled Duffing resonators and I agree that a such kind of system can represent many experimental systems, from nanomechanics to optomechanics, and so on. Indeed, this problem has been studied theoretically by many theoreticians, at least for the fundamental harmonics. Naturally, one can analyze the role of other harmonics and this is, in some sense, equivalent to increase the number of harmonic components. The authors present a table with maximum N=5 resonators. From my knowledge, most of the experiments studying nonlinear resonators are confined to investigate a very limited numbers of coupled modes and the majority of these studies focus on a few modes (N=2 or N=3). When we increase this number, one has to face a "zoo" of solutions from which it is in general difficult to gain some physical insight, unless one wants to merely compare theoretical points with experimental data.

We appreciate many experiments in nonlinear oscillators focus on a minimal number of modes, where theoretical insight is straightforward. Indeed, once the number of solutions increases, we have to deal with the complexity of deciphering the manifesting phenomena of each solution. Note that until recently, even the mere access to the plethora of solutions of larger systems was considered to be computationally intractable and was commonly relegated to the "cascade to chaos". For the first time, our package offers access to this so-called "zoo" of solutions. This also gives the ability to propose qualitatively new protocols by which to reach these new solutions.

An exciting research avenue where our toolbox could be helpful is coherent Ising machines, which use nonlinear oscillator networks as solvers of combinatorial optimisation problems (e.g. number partition and MAX CUT problems, see Inagaki, et.al (2016). *Science*, *354* (6312), 603-606), by exploiting the mapping of the optimisation solution to the ground state of spin models (Refs [65-70]). As shown in Ref. [70], even for systems with a minimal number of modes, the underlying mapping of spins to nonlinear oscillator states is a strong approximation, to be tested on each region of parameter space. Having the knowledge of the complete steady-state landscape and the ability to visualise solutions is thus essential for characterising an Ising machine's functionality, and assist in designing Ising networks from networks of nonlinear resonators.

Action taken

We shaped the discussion in section 5.4, "Increasing computational complexity: performance scaling" by highlighting some example experimental directions where our library can be most appropriate.

> Here, we will shortly illustrate the performance of HarmonicBalance.jl for varying system sizes. We consider a chain of linearly coupled Duffing oscillators, each with nonlinear damping (amplitude η, other parameters defined above Eq. 6.
> —-(Eq. 17)
> Similar systems have been explored in the context of combinatorial optimisation machines based on the mapping of effective spins to parametron networks [65-70].

In unison, we stressed the potential impact in other research areas in the conclusions:

(..) Ising machines [65–70], and many-body light-matter systems [71–77].

The ability to explore the complete solution landscape with an ansatz that has a tunable level of complexity makes our tool ideal for working alongside experiments. Specifically, high-order processes (e.g., up-conversion) can be readily accounted for through the progressive addition of harmonic frequencies. We hope that the free availability (...)

On the other hand, if one increases the size (for example a long chain of couple Duffing resonator with tens of resonators) then one has to solve a fully many-body (classical) problem. In this context, the method presented here should be compared with other more sophisticated techniques as Molecular Dynamics and must demonstrate its advantages. Furthermore, when we have a long chain, one could attack the problem from a different point of view, namely by using the linear modes of the coupled particles: the chain's modes. In this case, I expect that the effective nonlinear coupling between the several chain's modes is only relevant when we have internal resonances between these modes and this should restrict, again, the study to a few modes.

We acknowledge real-time evolution approaches to find steady states which also encompass Molecular Dynamics (see Allen, M. P., & Tildesley, D. J. (2017). *Computer simulation of liquids*. Oxford university press.). As described in Sec. 3.4, our functionality does include time-dependent solving. However, our main focus is strikingly different, namely finding *all* possible steady states of a nonlinear, driven dissipative system, which to our knowledge, cannot be managed in generic problems by direct time propagation methods, hence precluding a direct comparison.

The second point raised by the Referee mentions using normal modes rather than point-like coordinates to describe large systems. This is indeed standard practice when dealing with many coupled oscillator normal modes of continuous structures [Ref. 45 from the manuscript]. In such cases, instead of modelling the entire system, one only uses a set of discrete coordinates to describe a subset of the normal modes. The resulting equations of motion are identical to those of coupled oscillators and can be plugged into HarmonicBalance.

Action taken

To further establish the different capabilities of our methodology and time evolution toward the steady-state, we revised the Introduction slightly:

(...) is not analytically tractable in most cases. Hence, one often resorts to using numerical ODE solvers, e.g. as in molecular dynamics simulations [Ref. 1]. These usually focus on initial value problems, where the system's state is advanced from a set of initial conditions.

Including the textbook reference listed above:

[Ref. 1] Allen, M. P., & Tildesley, D. J. *Computer simulation of liquids*. Oxford university press. (2017)

In other words, from a point of view of basic research (and not for engineering) it is not clear to me what is the fascinating and new physics that would emerge by analyzing an increasing number of resonators or only two modes but with many harmonics. Of course, this package offers a useful tool for having (in a fast time) solutions for problems who have been already addressed and investigated theoretically and experimentally. Therefore I am not fully convinced for its publication.

We hope our argumentation has convinced the Referee that intermediate-size systems and their intricacies are still not well understood, despite a significant body of work in few-mode nonlinear networks and many-body states. Such small networks bear interest in many current experimental activities that explore so-called noisy intermediate-scale quantum (NISQ) systems applications. Beyond its pedagogical nature and interest as a complementary practical tool, our work can inspire a bottom-top development of theory for these systems. In line with the last comment of Referee 1, we have decided to proceed with a resubmission to SciPost Codebases.