Answers to Referee #1

We thank Referee #1 for his/her valuable comments and criticism on the manuscript that helped to clarify and improve it. We addressed all the issues raised by him/her in the revised version of the manuscript. Our detailed answers, point-by-point, are below.

Referee #1 general comments

Referee #1 general comment (1): "This paper is primarily an evaluation of a method of achieving end to end modelling of marine ecosystems using Ecopath and Ecosim written in FORTRAN and a biogeochemical model. As such it should be accepted, it provides a generally clear exposition of a conceptually simple way of linking models, a series of test of reproducibility and a worked example of the method being discussed. However, the paper is over glib in places (particularly about the results) and overstates the value of the FORTRAN method compared to others whilst failing to mention that the choice of approach is very much dependent on system organisational and objective considerations and by no means the only or indeed always the best approach. There needs to be more comparison and evaluation of the quality of the results.

Author's response: Above considerations were mostly addressed with our quick response to **Referee #1**. In addition to that, we modified the introduction in order to explicitly acknowledge possible approaches for coupling other than Fortran recoding of EwE (page #3 lines 21-25). Moreover, this manuscript was not meant to be an end-to-end (E2E) paper, but the releasing of a Fortran recoding of Ecopath with Ecosim (EwE-F). In order to emphasize this, we explicitly stated the possibility of EwE-F integration with many other models in the introduction (page #3 lines 29-31). Please also refer to the introductory comment by **Referee #2** that understood the broad scope of the EwE recoding and of the paper. Furthermore on this line, we did not mean to provide an ecologically validated E2E model, nor to draw ecological conclusion from our example, but we simply wanted to show that and how the coupling can be done and some first insights on its implications. Therefore, we believe that a comparison of our approach against other existing E2E methodologies (see also **comment (C) and comment (7)** below of the same **Referee #1**), while clearly of great interest, is far beyond the scope of our paper.

Referee #1 general comment (2): I suggest that the authors change the emphasis of the introduction and particularly the discussion. I am happy for the model and results section to be kept substantially as is – except for one or two specific comments.

Author's response: We believe that in addition to the changes in the introduction section, with further amendments detailed below, the introduction and discussion sections of the paper now explicitly and clearly state the intention and motivation of the manuscript.

Referee #1 specific comments

Referee #1 comment (A): The sentence 'Ecopath is also characterized by a top-down assumption' is not strictly true Ecopath finds equilibrium for a moment in time and do there is no regulation per se.

Author's response: We intended to refer here to the fact that the solution of the system of linear equations of Ecopath is obtained using a top-down approach (solving starting from top-predators), as mentioned by Steele (2009) (cited). This of course has nothing to do with the "top-down" and "bottom-up" regulation that, we agree, is regarding system dynamics. We rephrased the text in order to be clearer and avoid confusion (added text in bold) on page #5 lines 5-7:

"Ecopath is also characterized by top-down ***solution of the system of equations****, i.e. consumption on a group is a function of predator biomass, which differs from bottom-up approaches used in other inverse modelling approaches (Steele, 2009)."*

Referee #1 comment (B): When the authors move from Ecopath to Ecosim they do not discuss the additional model parameters. Although some of these are beyond the scope of the current paper they omit the discussion of the vulnerability parameter which defines how bottom-up versus top-down the model is and affects model stability. It is possible that some aspects of the LTL and physical models may affect this so it should not be ignored.

Author's response: Without doubt, the vulnerability parameters are crucial for any time dynamic simulation with Ecosim, as their value can very much influence results. However, the scope of the work here was not to contrast simulations with data for which the vulnerability setting would be fundamental but to contrast the effects of linking. Thus, we tested performances using the default value of vulnerability (v_{ij}=2), that is considered as an intermediate effect (referred as mixed control in Christensen et al., 2005). This is now mentioned in the main text (added text in bold) on page #11 lines 26-27 as:

"The coupled simulation was run ten years, two of which were for spin-off. ***In the simulations we used default values for vulnerabilities (v_{ij}=2) that represent a mixed control (Christensen et al., 2005)****."*

Further, earlier in the manuscript, we added a brief explanation concerning how the consumptions of state variables are calculated following the foraging arena concept utilising vulnerability parameters (page #5 lines 18-23) and referred to respective literature as:

*"****Q_{ij} is defined on the basis of biomasses of predator and prey in a form that represents a slightly modified version of Holling Type II functional response in order to consider only the part of the biomass of the prey i that is accessible to the predator j (foraging arena theory; Ahrens et al., 2012). For each trophic interaction, the accessible biomass is dynamically defined on the basis of a parameter called "vulnerability" (for details refer to Walters et al., 1997; Walters et al., 2000; Ahrens et al., 2012).****"*

Referee #1 comment (C): The authors should point out that there are at least three possible approaches to reconciling EwE with FORTAN biogeochemical models: 1.) Keeping everything as a single model – but using both languages and using a Thunking or data translation layer between the VB and FORTRAN components (Visual studio does this by using mixed native and managed code in C++, and copying across between arrays and similar. In a Unix environment f2c can be used 2.) Using inter-process communication such as pipes or sockets –could work across sockets or mechanisms 3.) The approach used here. We should probably discount the reverse approach of writing biogeochemical models in Visual Basic.

Author's response: We acknowledge the existence of alternative methodologies for coupling and now we explicitly stated this in the revised version of the MS (page #3 lines 21-25) as (added text in bold):

*"**One possible solution is the offline coupling of EwE and Fortran-coded models via two-way data transfer between the models at predefined time intervals while pausing the other model (i.e. turn-based run). Another solution could be utilising inter-process communications such as pipes and/or sockets between EwE and the model to be coupled while simultaneously running the model.** However, E2E model construction will benefit from a Fortran version of EwE that will permit direct integration of the EwE modelling approach with physical and biogeochemical models in Fortran, and will allow a straightforward and two-way propagating feedback between high trophic level (HTL) and low trophic level (LTL) models. **Furthermore, the development of a Fortran version of EwE will also be useful for integration of HTL food web models with potentially any other model written in Fortran which simulates, for example, socioeconomic, bioenergetic dynamics.**"*

Referee #1 comment (4): The ecology results are a mixed bag and should be stated as such. In particular a lot of things are dying and it would be interesting to know why they are dying (starvation, predation, fishing etc.) and what can be done about this. Given we are starting with existing models what we most need to know is whether we can fix this kind of thing in model or will need to add a lot more code.

Author's response: We did not include much interpretation about the ecological results of the coupled model since the objective of the paper is to represent the Fortran version of EwE and provide a working example of coupling. Nevertheless, we added a brief explanation for the dying groups, which is an important effect of coupling and explicit representation of biogeochemical cycles. Please see page #12 lines 10-13:

*"**However, while most of the bottom-associated groups decreased, by the incorporation of the biogeochemical model in the coupled scheme, pelagic-associated groups increased due to the explicit representation of resuspension of detritus and remineralisation that favoured plankton.**"*

Referee #1 comment (5): The authors quite rightly allude to the different time scales of the two models and how they have been reconciled but should focus more on the implications of time on the problem of marrying two such different models, especially given the long-term nature of Ecosim.

Author's response: We tested Ecosim using different time steps and it proved to perform good enough even using daily time steps in comparison with the default monthly time step. Therefore, to clarify this issue, we added an additional explanation at page #13 lines 27-28 as:

*"**Although Ecosim, by default, works with monthly time steps it is capable of simulating high frequency dynamics using shorter time steps.**"*

Referee #1 comment (6): The authors allude to Ecospace as somewhat beyond the scope of this paper but this seems to be the main *raison d'etre* of the FORTRAN translation. A platform independent EwE model would have the advantage of being able to run on UNIX clusters which is going to be a requirement if large scale spatial models are to be run.

Author's response: We fully agree with Referee #1 and we thank him/her for reminding us this important point. Hence, for discussing this potentiality of EwE-F, we added a new subsection (5.1.3.) under discussions section on <u>page #15 lines 1-11</u> as:

*"**5.1.3. Spatial simulations***

***Another area where having EwE-F may play a substantial role is spatial simulations. Given the current experience with biogeochemical models coupled with hydrodynamic models e.g. Lazzari et al., 2012), explicit accounting for spatial variability would be important for any assessment of marine ecosystem dynamics. Future efforts would be required to add spatial simulation capabilities to EwE-F, either by implementing Ecospace in Fortran or by direct integration of Ecosim-F in a spatially explicit coupled hydrodynamic-biogeochemical model. Due to high computational costs required for such representations, we foresee that EwE-F could better exploit the power of high performance computing clusters via parallelisation to significantly decrease simulation times.**"*

Referee #1 comment (7): There is currently a fluidity of model and approaches to E2E modelling, it would be helpful if the authors could carry out some kind of compare and contrast exercise.

Author's response: As stated previously and also in our quick response to Referee #1, we think that including a comparison of our approach against other existing E2E methodologies is out of the scope of the paper. Furthermore, calibrating each end-to-end scheme for the same test case and running simulations to compare them against each other would constitute a distinctive research by itself. Our main aim was not to delineate a specific application of E2E but simply to present EwE-F. Hence, we presented a simple example of coupling to show one potential application and how the coupling can be done. Therefore, we believe that a comparison of our approach against other existing E2E methodologies, while clearly of great interest, is beyond the scope of our paper.

Referee #1 comment (8): Similarly it would be helpful if the usefulness of Ecosim as the HTL component could be evaluated. The impression I get is that Ecosim adds more to the biogeochemical models than the biogeochemical models add to Ecosim at the moment – not sure if that is a fair evaluation.

Author's response: We included in the introduction a brief justification on the use of EwE as the HTL model (please see <u>page #2 lines 30-32 and page #3 lines 1-2</u>) as:

*"**The availability of numerous ready-to-use HTL models built with EwE in various aquatic ecosystems makes it a strong candidate as the HTL model in coupling schemes. In situations where an EwE model is available, the development of a integrated approach would only require minimal work concerning the HTL model and remove the burden of starting from scratch.**"*

If we understood correctly, the referee's comment concerning to the two-way propagating effects between HTL and LTL models, we disagree with him/her. We consider the benefits of coupling EwE with a biogeochemical model as mutual. Please refer also to our response to **Referee #1 comment (4),** which briefly explains the existence of both bottom-up and top-down propagating effects. However, if the issue raised by Referee #1 is more general and is with respect to the benefits of coupling, we think that both models contribute to ecosystem dynamics with important and peculiar processes so as to provide benefits to the whole coupling scheme. A very simplified example of benefits is depicted in Fig. 6. But we foresee important application and implications when future works permit explicit spatial representation.

Referee #1 comment (9): The move away from EwE databases and front ends towards namelist and HDF files may be seen as a usability disadvantage, the authors should consider how usable EwE-F is for an experienced EwE developer.

Author's response: In contrast to the stock EwE, the introduction of namelist and HDF files to be used for the operation of EwE-F may create a hindrance to its users. However, it is not necessarily more complicated than the current EwE database files (MS Access). EwE-F requires an HDF5 database file only when transferring information from Ecopath-F to Ecosim-F, and output to and input from this file does not require any user intervention. In addition, the results of both Ecopath-F and Ecosim-F models are output into TAB-delimited ASCII files, which are quite similar to the EwE's output files, i.e. comma-separated value (CSV) ASCII files. These TAB-delimited files can easily be opened with spreadsheet programs similar to EwE's CSV files. The only hindrance for the user could be the preparation of the TAB-delimited ASCII input files for Ecopath-F and Ecosim-F. This is not much different from the experience which common EwE users need for preparing inputs for Ecosim. Moreover, how to prepare these files is explained in detail in the EwE-F User's Manual. Therefore, considering an experienced EwE user, we believe that the learning curve to use EwE-F is not steep.

Referee #1 comment (10): The authors have a big wish list and because they have in effect created a fork will always to an extent be playing catch up with the official EwE release. Which of these improvements are most critical to the model's role in end to end modelling?

Author's response: Of course, another important consideration to be discussed is to maintain EwE-F updated with EwE releases. With every new release of EwE software, many things are prone to change. However, the majority of these changes are related to the ancillary functionalities (graphical user interface, network analysis routines etc. but NOT to the core state equations and its related calculations) that are not included in EwE-F at the moment. Considering that EwE-F is a bare-bones implementation of EwE and does not include the sophisticated analysis capabilities of EwE package, it is believed that the core structure of EwE-F (state equations and other related calculations) can be kept on par with the original EwE with little effort. Moreover, this work is a result of co-development with the Ecopath Research Consortium that is consisting of several experts that have joined their efforts for developing the EwE approach; hence, this guarantees the consistent development of EwE-F at the very least case of maintenance for compliance with EwE.

Answers to Referee #2

We thank Referee #2 for his/her valuable comments and criticism. Further, we appreciate the technical comments provided by Referee #2. We tried to do our best to address all the issues related to the manuscript as well as the ones related to the technical concerns raised by him/her in the revised version of the manuscript. We hope that we could meet his/her expectations. Our detailed answers, point-by-point, are as follows.

Referee #2 general comments

The paper presents a novel tool that has the potential of substantially enhancing the capability of the marine ecosystem modelling community. EwE-F enables the application of a well-established and tested food-web modelling framework (Ecopath with Ecosim, EwE) to questions that go beyond the immediate scope of the original EwE software, such as end-to-end modelling from biogeochemical to socioeconomic concerns, multiple run analyses to study structural uncertainty or policy optimizations, and enhanced physiological or demographic detail where needed, while safeguarding the tested and proven EwE concept. This capability is well illustrated by the exemplary application provided, which can additionally serve as an inspiration or guideline for future coupling of EwE with biogeochemical models. The translation of EwE into Fortran is not the only endeavour to allow such coupling, it will, however, be amongst the most straight forward attempts to do so with the publication of the current paper and code.

Author's response: We thank Referee #2 for his/her quite positive appraisal of our work. We are delighted to see that our opinions and future prospects related to this work are also hold by Referee #2. Feedback as such strengthens our motivation and determination for our commitment related to the work.

Referee #2 specific comments

Referee #2 comment (A): The title is a suitable representation of the study, however, given the potential significance of the work also for a less technical audience, the term 'for coupling' may benefit from increased clarity for scientists less familiar with geoscientific modelling.

Author's response: We agree with Referee #2 about the possible ambiguity of the term "for coupling" may create for less-technical audience of the manuscript. Hence, we assessed two alternatives: i) to remove "for coupling", and ii) to accompany it with short explanatory words. We think that the first option causes a drawback with respect to our aim to be explanatory about the motivation of the paper inferred from its title. Therefore, we opted for the latter option and we appended explanatory words to the title as "…for coupling **and integration with other models.**" (added text in bold).

Referee #2 comment (B): The abstract represents a complete, yet brief summary of the content. However, I perceive the attribute 'great' in p. 1512, line 7, as too judging.

Author's response: Abstract has been amended in order to consider this comment and the word "great" was removed.

Referee #2 comment (C): The introduction presents a clear and shortest appropriate presentation of the study's background, motivation and approach. I would have appreciated references that underpin the claim that 'Oceanographic models [. . .] have mostly been written in Fortran' (p. 1514, line 1).

Author's response: We added appropriate references to support our statement as (<u>page #2 lines 9-13</u>, added text in bold):

"Oceanographic models, particularly computationally intensive hydrodynamic and biogeochemical models, have mostly been written in Fortran ***(e.g. hydrodynamic models: NEMO (Madec 2008), ROMS (Shchepetkin and McWilliams, 2005), POM (Blumberg and Mellor, 1978), MITGCM (Adcroft et al., 2004, MOM (Stock et al., 2014); and biogeochemical models: ERSEM (Blackford et al., 2004), BFM (Vichi et al 2015), ERGOM (Neumann, 2000)).****"*

Referee #2 comment (D): A description of the time-dynamic Ecosim module prior to outlining the stationary state Ecopath in Sect. 2 is unusual. Most published descriptions of the EwE model follow the logic that the earlier is based on the latter. Also the following description of the implementation of both modules in EwE-F in Sect. 3.1 and 3.2 follow this principle, potentially hindering the understanding for a reader new to the concept of EwE. Else, the paper is conclusive structured and references to the respective sections throughout the text facilitate its comprehension.

Author's response: As suggested by Referee #2, we moved the explanations so that Ecopath is explained first and then Ecosim explanations are reported so that the flow is consistent with the general logic present in the available literature related to EwE and with the rest of the manuscript.

Referee #2 comment (E): I agree with Rev. #1 that the concepts of vulnerabilities and Foraging Arena have to be outlined at first mentioning (Sect. 3.2, p. 1518, line 5).

Author's response: This issue is addressed with a short explanation of the two concepts and the reader is referred to related literature. Please see answer to Referee #1 comment (B) for details. For Referee #2's quick reference, we added the below text where the Ecosim master equation is explained in order to briefly introduce the foraging arena and vulnerability concepts (please see page #5 lines 18-23):

*"****Q_{ij} is defined on the basis of biomasses of predator and prey in a form that represents a slightly modified version of Holling Type II functional response in order to consider only the part of the biomass of the prey i that is accessible to the predator j (foraging arena theory; Ahrens et al., 2012). For each trophic interaction, the accessible biomass is dynamically defined on the basis of a parameter called "vulnerability" (for details refer to Walters et al., 1997; Walters et al., 2000; Ahrens et al., 2012).****"*

Referee #2 comment (F): It has not become clear to me whether Ecosim-F at the current state allows the inclusion of fishing effort time series or fishing mortalities only, as my interpretation of p. 1518, lines 6-7 go. If efforts cannot be included yet, I regard that as a considerable drawback of the method that should be discussed.

Author's response: It should be noted that changes in fishing mortality is the most general way to include fishing changes over time. The original Ecosim, in fact, utilises fishing effort time series as normalised multipliers to the Ecopath-calculated initial exploitation rate ($Catches_i/Biomass_i$) of group *i* to produce time series of fishing mortalities to be used as forcing for this group in an Ecosim simulation. The same is true for Ecosim-F and it can use fishing effort time series provided that a single fleet exploits the stocks. However, in the case of multiple fleets, Ecosim-F requires that the time series of fishing mortalities are calculated externally using the time series of fishing efforts and the Ecopath-calculated initial exploitation rates by fleet. These are simple calculations that will result in the fishing mortality time series by species to be used in Ecosim-F. Therefore, the absence of possibility for directly importing fishing effort time series for multiple fleets in Ecosim-F should not be considered as a drawback for EwE-F, given that user can simulate whatever complicate fisheries dynamics using fishing mortalities estimated offline. However, we acknowledge that this is not a straight forward method and, hence, we amended the EwE-F manual, p. 45 (please see supplementary materials) in order to explicit this fact to the EwE-F users.

Referee #2 comment (G): The exploration of EwE-F's flexibility in the coupling exercise, else a well readable demonstration of the tool's capabilities, lacks detail on the sensitivity experiments mentioned in p. 1521, line 7, which appears to affect the reproducibility of the study. Also, having both an EwE and EwE-F version of the Northern Adriatic model at hand offers, a priori to the coupling exercise, another opportunity to evaluate the skills of EwE-F by comparing both runs. Given the prospect of the procedure outlined in Sect. 4 of this study to become state of the art when coupling biogeochemical models with EwE-F, reporting differences in model results depending on the version used is supposedly good advice.

Author's response: We agree with Referee #2 and would like to state that our prescription in the manuscript is misleading. What we carried out was to tune the mortality coefficients of phytoplankton and zooplankton groups in order to have a seasonal cycle of these state variables similar to the ones observed in the standalone LTL model. However, we observed that without adjusting their respective mortalities, the plankton dynamics in the coupled model simulation were qualitatively comparable to the standalone biogeochemical model and missed only the second peak observed in the mesozooplankton group. In order to be able to simulate this second peak, we reduced the mortality coefficient of this group with steps of -10%, -30%, -50% only to see that such a peak was not simulated. After this attempt, considering that our research was not an idealised case study and the seasonality observed in the plankton groups were acceptable, we concluded not to perform any further fine-tuning and kept the closure parameters untouched as they were in the standalone biogeochemical model. We amended the respective section of the manuscript as (added text in bold and removed text in strikethrough):

"The final step in the harmonisation process ~~was~~ ***would be*** *to adjust the closure terms of the biogeochemical model (mortality rates of zooplankton and phytoplankton groups) so as to compensate the additional losses through explicit predation of these groups by the HTL state variables. ~~Hence, in the coupled scheme, the mortality rates of the LTL variables that were predated by HTL groups were decreased by sensitivity experiments to the extent to satisfy the seasonality in the original biogeochemical model.~~* ***However, for our specific application, we decided to keep these values identical to the standalone biogeochemical model as it produced similar seasonal cycles observed in the standalone biogeochemical model except the missing second cycle in mesozooplankton (Figure 6). Considering that our research was not an idealised case study, our aim was to have plankton dynamics qualitatively comparable to the biogeochemical model, therefore, further fine-tuning was avoided.****"*

The second issue on the comparison between EwE-F and EwE for the Northern Adriatic Sea was already included in Fig. 6. However, we realised that was a bit unclear and therefore we now clarify in the revised version with the following text (page #11 line 28, added text in bold):

"Comparison of uncoupled ***EwE*** *and coupled* ***EwE-F*** *model results (Figure 6) demonstrated that the coupling scheme worked successfully…"*

The third issue of reporting differences depending on the model version used, we added a sentence to warn the readers (page #8 lines 17-18) as:

*"****It is worth noting that other EwE versions may produce slightly different results compared to EwE-F v1.0.****"*

Referee #2 comment (H): The real-time coupling method sketched in Sect. 5.1.1 is not exclusive to a Fortran version of EwE, as might be perceived from p. 1524, line 16.

Author's response: We removed the sentence.

Referee #2 comment (I): Examples of an implicit representation of nutrient limitations in food-webs modelled with EwE, as mentioned in p. 1524, line 24, could be interesting for a reader to be referred to.

Author's response: We added references to related literature for the interested readers' attention as (added text in bold, page #14 lines 13-14):

"*…although implicit nutrient-based limitations can be represented in EwE* ***(Araujo et al., 2006; Christensen et al., 2005)***."

Referee #2 comment (J): Sect. 5.2, in p. 1527, line 1, could awake the impression that vulnerability search and time series fitting are independent affairs, which they are not. Besides, the lack of a such fitting routine in EwE-F (p. 1527, line 5) is probably less of an obstacle than the implementation of those elements that enable a one-to-one representation of normal Ecosim runs: mediation function, consumer and producer forcing function, egg production and, if not yet implemented, fishing effort time series.

Author's response: Yes, we agree with Referee #2 that "vulnerability search" and "time series fitting" are not independent. To remedy this, first we modified the text to avoid such impression as (page #16 lines 24-27, added text in bold and removed text in strikethrough):

"Therefore, analyses requiring the aforementioned specific routines (e.g. Monte-Carlo analysis, ***Network Analysis*** *~~vulnerability search, time-series fitting~~ etc.) in uncoupled or coupled EwE-F simulations can be done by coding the required specific routines or alternatively EwE could be employed for such purposes."*

Second, because primary producer forcing functions, fishing effort and mortality forcing, nutrient forcing, which are the most commonly-used forcing time series in EwE, have already been implemented in EwE-F v1.0, we explicitly stated our aim to implement mediation function and vulnerability search in further versions of EwE-F as (page #16 lines 29-30 and page #17 line 1), added text in bold):

"However, these technical shortcomings and the lack of aforementioned tools ***including mediation function and time series fitting via vulnerability parameter search*** *are planned to be addressed in the future by incorporating these routines…"*

Referee #2 technical comments

Referee #2 technical comment (1): De facto should be set in italic type (p. 1513, line 9).

Author's response: It was typeset to italic.

Referee #2 technical comment (2): Multi-stanza should be consistent, best with a hyphen (p. 1515, line 12 & p. 1516, line 18).

Author's response: All occurrences of multistanza were set to "*multi-stanza*" throughout the manuscript.

Referee #2 technical comment (3): The second sentence in Sect. 3.2 (p. 1518, line 2) requires to be either set plural ('output files from Ecopath-F run S ') or lacks an article ('from the Ecopath-F run').

Author's response: The missing article was added (in bold) so the text now reads: *"...from **the** Ecopath-F run...*"

Referee #2 technical comment (3): The relaxation parameter mentioned in p. 1518, line 10, and why it is 'necessary to initialise the simulation' are not intuitive to every reader and might better be explained.

Author's comment: Because the details of the requirement of this parameter for the Ecosim simulation is out of the scope of the paper, the reader is now referred to the relevant literature for the explanation as (page #8 lines 6-7, added text in bold):

"*...nutrients, relaxation parameter and simulation end time in years, to prepare the Ecosim simulation **(see Christensen et al., 2005, p. 78)***."

Referee #2 technical comment (4): It could be beneficial to refer to Fig. 2 and 3 already when describing what is visualized in p. 1581, line 22.

Author's response: The figures are referred in the amended text as (added text in bold):

"*The residuals for each state variable in the respective simulations were visualised with box-whisker plots showing the minimum value, 25th percentile, median, 75th percentile and maximum values respectively **(Figs. 2 and 3).***"

Referee #2 technical comment (5): Mind tense in p. 1519, line 8; p. 1520, line 16; p. 1522, line 12; and p. 1523, line 21.

Author's response: The tenses in the respective lines were corrected as (added text in bold, removed text in strikethrough):

"*In fact, the direct integration of these two models ~~require~~ **required** to address, and subsequently solve a number of problems.*"

"*For simplicity, the HTL and LTL groups ~~were~~ **are** not given in detail in the figure, however, sources and sinks of the whole HTL compartment and the linkages between the HTL and LTL domains and state variables ~~were~~ **are** shown.*"

"*...the ecological interpretations of these results are not the focus of this work and thus ~~were~~* ***are*** *only briefly discussed here.*"

"*In addition, the EwE-F ~~has generated~~* ***enables*** *significant opportunities for integrating it with any kind of Fortran models as depicted in Figure 7.*"

Referee #2 technical comment (6): Tautology in p. 1521, line 18: 'aforementioned above'.

Author's response: "*aforementioned above*" is removed.

Referee #2 technical comment (7): The abbreviation 'ODE' is not introduced in p. 1524, line 15.

Author's response: Modified as (added text in bold):
"*...to conform to the time step of the biogeochemical model (one hour) in order to render the use of one common* ***ordinary differential equation*** *(ODE) solver...*"

Referee #2 technical comment (7): Potentially revise articles in p. 1512, line 18; p. 1513, line 9; p. 1516, lines 17, 18 and 24; p. 1517, line 1; p. 1520, line 26; p. 1524, line 15; and p. 1527, line 11.

Author's comment: The articles in the mentioned lines are modified as (added text in bold, removed text in strikethrough):

"*In the present work, first ~~the~~ fundamentals of EwE-F are introduced, followed by validation of...*"

"*...changing demands enabled this it to remain as ~~the~~ de facto standard for writing...*"

"The EwE software was translated to ~~the~~ Fortran 95/2003 language in its core architecture and kept limited to; i) ***the*** *Ecopath mass-balance routine including multi-stanza calculations, and ii)* ***the*** *Ecosim time-dynamic simulation including multi-stanza calculations. Due to modularity considerations, EwE-F was implemented under two separate components; i) Ecopath-F: the Ecopath mass-balance algorithm, and ii) Ecosim-F: the Ecosim time-dynamic simulation algorithm. EwE-F v1.0 includes only core routines of Ecopath and Ecosim: complementary routines for calculation of indicators for Network Analysis, as well as routines for Monte-Carlo Simulation, Time Series Fitting and Ecospace are not included. Also* ***the capability to define*** *mediation functions is not yet implemented in EwE-F v1.0, although is planned to be addressed in future versions."*

"~~The~~ ***A*** *schematic view of the..."*

"*...state variables with faster dynamics compared to ~~the~~ HTL model, it...*"

"*...common ordinary differential equation (ODE) solver solver (***the*** *Runge-Kutta 4th order) possible.*"

"*...developing EwE-F may also focus on incorporating ~~the~~ 2D spatial dynamics by implementing the Ecospace module.*"

EwE-F 1.0: An implementation of Ecopath with Ecosim in Fortran 95/2003 for coupling and integration with other models

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Abstract

Societal and scientific challenges foster the implementation of the ecosystem approach to marine ecosystem analysis and management, which is a comprehensive means of integrating the direct and indirect effects of multiple stressors on the different components of ecosystems, from physical to chemical and biological and from viruses to fishes and marine mammals. Ecopath with Ecosim (EwE) is a widely used software package, which offers ~~great~~ capability for a dynamic description of the multiple interactions occurring within a food web, and potentially, a crucial component of an integrated platform supporting the ecosystem approach. However, being written for the Microsoft .NET framework, seamless integration of this code with Fortran-based physical oceanographic and/or biogeochemical models is technically not straightforward. In this work we release a re-coding of EwE in Fortran (EwE-F). We believe that the availability of a Fortran version of EwE is an important step towards setting-up integrated end-to-end (E2E) modelling schemes utilising this widely adopted software because it i) increases portability of the EwE models, ii) provides ~~greater~~ additional flexibility towards integrating EwE with Fortran-based modelling schemes. Furthermore, EwE-F might help modellers using Fortran programming language to get close to the EwE approach. In the present work, first ~~the~~ fundamentals of EwE-F are introduced, followed by validation of EwE-

F against standard EwE utilising sample models. Afterwards, an E2E ecological representation of the Trieste Gulf (Northern Adriatic Sea) ecosystem is presented as an example of online two-way coupling between an EwE-F food web model and a biogeochemical model. Finally, the possibilities that having EwE-F opens up for are discussed.

1 Introduction

Oceanographic models, particularly computationally intensive hydrodynamic ~~models~~ and biogeochemical models, have mostly been written in Fortran (e.g. hydrodynamic models: NEMO (Madec 2008), ROMS (Shchepetkin and McWilliams, 2005), POM (Blumberg and Mellor, 1978), MITGCM (Adcroft et al., 2004), MOM (Stock et al., 2014); and biogeochemical models: ERSEM (Blackford et al., 2004), BFM (Vichi et al 2015), ERGOM (Neumann, 2000)). In fact, Fortran was the first programming language specifically designed for solving engineering and scientific computing problems (Backus et al., 1957) and proved to be one of the most efficient for performing complicated mathematical tasks with its collection of predefined high-level mathematical functions. Over the years, frequent revision of the Fortran ~~language~~ standard and the addition of new capabilities to the language to meet changing demands enabled ~~this language~~it to remain as ~~the~~ *de facto* standard for writing computationally intensive scientific and engineering applications.

Ecopath with Ecosim (hereinafter EwE) (Christensen and Walters, 2004; Christensen et al., 2005) is the most widely adopted tool for building models of marine and freshwater ecosystems, and possibly the first choice for analysis of food web dynamics. Freely available at www.ecopath.org, EwE has long been used for scientific studies related to fisheries, and also including some aspects of aquaculture, marine ecology, climate and pollution. There are thousands users of the software worldwide (last record in 2008, reported 5649 users; www.ecopath.org) and more than 400 scientific publications utilising EwE as a modelling tool have been published only in the last two decades (search on Web of Science on 29/09/2014 for “Ecopath with Ecosim” or “Ecospace” or “Ecopath” resulted in 469 items published between 1997 and 2014). ~~EwE has a spreadsheet-based user-friendly graphical interface that facilitates its adoption.~~ The availability of numerous ready-to-use HTL models built with EwE in various aquatic ecosystems makes it a strong candidate as the HTL model in coupling schemes. In situations where an EwE model is available, the development of a

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integrated approach would only require minimal work concerning the HTL model and remove the burden of starting from scratch. ~~However, being written for the Microsoft .NET framework constrains this software's ability to integrate with models written in Fortran language.~~ EwE is designed for interoperability with other models, which is crucial considering that ecological modelling is facing an important challenge to set a basis for the comprehensive description of marine ecosystems through what are called End-to-End (hereinafter E2E) models (Fulton, 2010). This interoperability leads to insightful linking of primary production into EwE models (e.g. Christensen et al., 2014) and EwE flexibility already permits to link physical/biogeochemical oceanographic models with EwE (e.g. Libralato and Solidoro, 2009). Linking permits exchanges of information between models that are run separately (one-way coupling) and is valid, robust and usually faster to implement than a two-way coupling. In spite of the interesting results obtained, however, linking lacks a complete representation of feedbacks that propagate two-ways between the coupled models. These feedbacks were proven to be important and reveal important ecological mechanisms (Kearney et al., 2012) that need to be accounted explicitly for a full representation of ecosystem effects due to climatic changes, aquaculture, socioeconomic changes and other important drivers (Fulton, 2010). The scientific requirements for the so-called E2E models, therefore, mandate two-way coupling with existing oceanographic models which are mostly written in Fortran. Because these models and EwE use different programming languages, the technical differences complicate the coupling task more than anticipated (Beecham et al., 2010). One possible solution is the offline coupling of EwE and Fortran-coded models via two-way data transfer between the models at predefined time intervals while pausing the other model (i.e. turn-based run). Another solution could be utilising inter-process communications such as pipes and/or sockets between EwE and the model to be coupled while simultaneously running the models. ~~Overall~~However, E2E model construction will benefit from a Fortran version of EwE that will permit direct integration of the EwE modelling approach with physical and biogeochemical models in Fortran, and will allow a straightforward and two-way propagating feedback between high trophic level (HTL) and low trophic level (LTL) models. Furthermore, the development of a Fortran version of EwE will also be useful for integration of HTL food web models with potentially any other model written in Fortran which simulates, for example, socioeconomic, bioenergetic dynamics.

In this work, we present (Section 3) the first version of EwE re-coded in Fortran 95/2003 language standard (EwE-F, version 1.0). In Section 3.3, we provide evidence of the full reliability of the code by comparing EwE-F with standard EwE (version ~~6.4~~6.5) utilising sample food web models. In Section 4, we present how EwE-F allows for easy coupling with other models, by providing an example of integration with a biogeochemical model of the Gulf of Trieste in the Northern Adriatic Sea. Finally, in the same section, we discuss the possibilities opened up by the availability of EwE-F. We believe that EwE-F will appeal also to the scientific community previously sceptical to the EwE approach (usually more confident with Fortran programming) and provide the possibility of both easy modification of the EwE-F structure and parameterisation for specific cases and easy integration with other biogeochemical, population dynamics, individual-based and/or any type of ecological model written in Fortran.

2 A brief description of the EwE Model

EwE modelling software includes a suite of modules that enables the building and analysis of food web models. EwE includes three main modules; i) Ecopath; the mass-balance representation, ii) Ecosim; the time-dynamic simulation, and iii) Ecospace; the 2D spatial-temporal dynamics, plus other complementary routines: Network Analysis (Ulanowicz, 1986), Monte-Carlo Simulation and Time Series Fitting. EwE-F comprises only Ecopath and Ecosim modules thus only these two are briefly summarised here.

The Ecopath module comprises a series of linear equations that defines a mass-balance stationary state of the food web. The functional groups are regulated by gains (consumption, production, and immigration) and losses (mortality and emigration), and are linked to each other by predatory relationships. Fisheries extract biomass from the targeted and by-catch groups. In Ecopath, a set of linear equations describes flows of mass into and out of discrete biomass pools of the form

$$B_i * \left(\frac{P}{B}\right)_i - \sum_{j=1}^{n} B_j * \left(\frac{Q}{B}\right)_j * DC_{ji} - B_i * \left(\frac{P}{B}\right)_i * (1 - EE_i) - Y_i - E_i - BA_i = 0 \qquad (1)$$

where, for each functional group *i*, *B* stands for biomass, *(P/B)* stands for the production rate per unit of biomass, *(Q/B)* stands for the consumption rate per unit of biomass of predator *j*, DC_{ji} is the fraction of prey *i* in the average diet of predator *j*, *Y* is the landings, *E* is net emigration rate, and *BA* is the biomass accumulation rate (Christensen et al, 2005). *EE* is the ecotrophic efficiency representing the proportion of mortality of a group that is not attributable to predators or fishing activities. As it can be seen, Equation (1) is quite simple as a result of the fact that it represents the budget of biomass fluxes in a given time window and within an ecosystem. Ecopath is also characterized by a top-down solution of the system of equations, i.e. consumption on a group is a function of predator biomass, which differs from bottom-up approaches used in other inverse modelling approaches (Steele, 2009).

In the time-dynamic module of EwE (Ecosim), dynamics of a state variable are defined with a differential equation composed of sources and sinks terms. Each state variable represents the biomass of a functional group representing species and/or groups of species or populations split into age-size categories (multi-stanza). The definition of such differential equation in Ecosim is as follows:

$$\frac{dB_i}{dt} = \gamma_i * \sum_{j=1}^{n} Q_{ji} - \sum_{j=1}^{n} Q_{ij} + I_i - (M_i + F_i + e_i) * B_i \tag{2}$$

where dB_i/d_t is the rate of change of biomass *(B)* of group *i* over time *t*, □ is the growth efficiency of group *i*, $\sum Q_{ji}$ is the sum of the consumptions of group *i* over all of its preys, $\sum Q_{ij}$ is the sum of the predation on group *i* by all of its predators, *I* is the immigration, *M* is the non-predation mortality, *F* is the fisheries mortality and *e* is the emigration rate of group *i* (Walters et al., 1997). Q_{ij} is defined on the basis of biomasses of predator and prey in a form that represents a slightly modified version of Holling Type II functional response in order to consider only the part of the biomass of the prey *i* that is accessible to the predator *j* (foraging arena theory; Ahrens et al., 2012). For each trophic interaction, the accessible biomass is dynamically defined on the basis of a parameter called "*vulnerability*" (for details refer to Walters et al., 1997; Walters et al., 2000; Ahrens et al., 2012). This system of differential equations is numerically integrated over time under the influence of forcing functions (typically fishing mortalities and/or efforts, changes in primary productivity) starting from the initial condition settings defined by the Ecopath module.

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~~where, for each functional group *i*, *B* stands for biomass, *(P/B)* stands for the production rate per unit of biomass, *(Q/B)* stands for the consumption rate per unit of biomass of predator *j*, DC_{ji} is the fraction of prey *i* in the average diet of predator *j*, *Y* is the landings, *E* is net emigration rate, and *BA* is the biomass accumulation rate (Christensen et al, 2005). *EE* is the ecotrophic efficiency representing the proportion of mortality of a group that is not attributable to predators or fishing activities. As it can be seen, Equation (2) is quite simple as a result of the fact that it represents the budget of biomass fluxes in a given time window and within an ecosystem. Ecopath is also characterized by a top-down assumption, i.e. consumption on a group is a function of predator biomass, which differs from bottom-up approaches used in other inverse modelling approaches (Steele, 2009).~~

3 The EwE-F Software

The EwE software was translated to ~~the~~ Fortran 95/2003 language in its core architecture and kept limited to; i) the Ecopath mass-balance routine including multi-stanza calculations, and ii) the Ecosim time-dynamic simulation including multi-stanza calculations. Due to modularity considerations, EwE-F was implemented under two separate components; i) Ecopath-F: the Ecopath mass-balance algorithm, and ii) Ecosim-F: the Ecosim time-dynamic simulation algorithm. EwE-F v1.0 includes only core routines of Ecopath and Ecosim: complementary routines for calculation of ~~indices~~ indicators ~~and~~ for Network Analysis, as well as routines for Monte-Carlo Simulation, Time Series Fitting and Ecospace are not included. Also the capability to define mediation functions is not yet implemented in EwE-F v1.0, although is planned to be addressed in future versions. ~~The~~ A schematic view of the EwE-F components and the input/output (I/O) files necessary for information exchange are given in Figure 1~~Figure 1~~. In the following two sections 3.1 and 3.2), the structure and functioning of the components in Figure 1~~Figure 1~~ are described in detail.

3.1 Ecopath-F

Ecopath-F is the component of EwE-F that carries out mass-balance calculations given in Equation (1)~~(2)~~. Similar to stock Ecopath, it requires the same fundamental input parameters to be entered via four tab-delimited ASCII (American Standard Code for Information Interchange) encoded text input files; i) a scenario file containing the basic input and multi-stanza parameters and landings, ii) a file comprising the diet composition matrix of the state variables, iii) a file comprising the detritus fate of the state variables and, iv) if applicable, a file including the growth parameters of the multi-stanza groups. Furthermore, Ecopath-F requires a Fortran "namelist" file that includes the full path names of the above-mentioned four input files and, in addition, the path to the output HDF5 (Hierarchical Data Format version 5, www.hdfgroup.org/HDF5) file where the mass-balance calculation results will be output and be used to initialise and run Ecosim-F (Figure 1~~Figure 1~~).

An Ecopath-F run produces two output files; i) an ASCII file which includes the summary of estimated parameters and basic statistical information, and ii) an HDF5 file specifically formatted to define the initial conditions for the Ecosim-F simulation (Figure 1~~Figure 1~~). The output HDF5 file includes all the parametric details about the state variables of Ecopath run and further comprises the diet composition matrix, detritus fate matrix and multi-stanza group parameters.

Ecopath-F is independent of the Ecosim-F ~~implementation,~~implementation; however, Ecosim-F requires output data from Ecopath-F plus additional parameter settings. The data transfer from Ecopath-F to Ecosim-F is carried out via the intermediary HDF5 data file.

3.2 Ecosim-F

Ecosim-F is the component of EwE-F that carries out time-dynamic simulation calculations given in Equation (2)~~(1)~~. Ecosim-F requires the HDF5 output file from the Ecopath-F run and three additional tab-delimited ASCII encoded text input files; i) a scenario file containing group information of state variables, ii) a file comprising the vulnerability matrix between predator-prey pairs, and iii) a file comprising the monthly fishing mortality/effort time series forcing functions for all state variables (Figure 1~~Figure 1~~). Similar to Ecopath-F, Ecosim-F also requires a namelist file that includes the full paths to the input files as well as the values of some particular variables; i.e. number of time steps per month, base proportion of free nutrients, relaxation parameter~~,~~ and simulation end time in years, ~~necessary~~ to ~~initialise~~ prepare the Ecosim simulation (see Christensen et al., 2005, p. 78).

Once completed, Ecosim-F simulation produces four tab-delimited ASCII coded text files comprising the annual and monthly absolute and relative biomass values of the state variables throughout the simulation in the model directory (Figure 1~~Figure 1~~).

3.3 The skill assessment of EwE-F

In order to assess the skill of EwE-F with respect to EwE, two test case simulations, "Generic 37" and "Tampa Bay", which are distributed with the installation of the EwE software were used. The test case simulations were run both with EwE version ~~6.4~~6.5 and EwE-F version 1.0 and the residuals between simulated absolute biomasses of state variables were used to evaluate the performance of EwE-F. It is worth noting that other EwE versions may produce slightly different results compared to EwE-F v1.0. The residuals for each state variable in the respective simulations were visualised with box-whisker plots showing the minimum value, 25th percentile, median, 75th percentile and maximum values respectively (Figs. Figure 2 and Figure 3).

The residuals between the simulated biomass values of EwE-F and EwE ranged from 10^{-8} to 10^{-5}, with the maximum difference found to be on the order of 10^{-5}. The residuals calculated from the comparison of the simulations justified that EwE-F possessed the necessary skill to reproduce the results of EwE for the Generic 37 ~~(Figure 2)~~ and Tampa Bay ~~(Figure 3)~~ simulations. The magnitude of the misfits concluded that EwE-F was capable of being used in conjunction with other models without introducing significant sources of error to the resulting modelling scheme.

4 Exploring EwE-F flexibilities: example from a complex coupling exercise

The Fortran recoding of EwE creates great flexibility for customization, modification or coupling to different models written in Fortran. An example, which will illustrate the potential of such flexibility, came from the integration of EwE-F to a biogeochemical Fortran model. In fact, the direct integration of these two models required to address, and subsequently solve a number of problems. These include defining the links between the two models and modifying them accordingly, exchanging information between the two models, dealing with different model time steps, and accounting for different model currencies.

The HTL model is an updated version of the EwE model of the Northern Adriatic Sea originally developed by Coll et al. (2007). The original model composed of 40 functional groups (FG) has been updated by i) removing discards and by-catch FGs, ii) splitting phytoplankton and zooplankton in two FGs each to represent small and large taxa; iii) adding bacteria to explicitly represent the microbial loop; iv) adjusting diet of plankton feeders to split the diet into the new plankton FGs. The updated model has 44 FGs and parameters for the plankton groups were updated considering literature information (see Cossarini and Solidoro, 2008 and references therein). The model currency is wet weight. The time step of the model is one month, the default time step of the EwE software.

The biogeochemical model is a Fasham-like (Fasham et al., 1990) 0D box model of the Northern Adriatic Sea (Cossarini and Solidoro, 2008) and consists of phytoplankton, zooplankton, and heterotrophic bacteria groups, one pool of inorganic phosphorus (PO_4^{3-}); one dissolved organic matter compartment in terms of phosphorus (DOP) and carbon (DOC), and one particulate organic matter compartment in terms of phosphorus (POP) and carbon (POC) (Figure 4~~Figure 4~~). The model is a multi-currency model calculating the biomasses of its particular state variables (sediment, dissolved organic matter, particulate organic matter) both in terms of carbon and phosphorus. The time step of the model is one hour. Full description of the biogeochemical model is reported in Cossarini and Solidoro (2008).

For the harmonisation of both models in an E2E coupled scheme, first, the state variables that were already present in the LTL model were removed from the HTL model as well as their links (grey-shaded area and links in Figure 4~~Figure 4~~). Then the linkages between the state variables of the HTL model and the state variables of the LTL model were set-up in accordance with the removed state variables as shown in Figure 4~~Figure 4~~ (links in dashed and continuous black lines). In this way, a coupled model scheme that ~~comprised~~ consisted of 44 functional groups was set up: 9 FG represented the state variables of the biogeochemical model, i.e., plankton groups plus inorganic and organic nutrient forms (Figure 4~~Figure 4~~). For simplicity, the HTL and LTL groups ~~were~~ are not given in detail in the figure, however, sources and sinks of the whole HTL compartment and the linkages between the HTL and LTL domains and state variables ~~were~~ are shown.

The second step in the harmonisation of models consisted of accounting for the different currencies used. Considering the multiple currency utilisation of the biogeochemical model for some of its state variables and the fact that the application of a similar principle in the HTL model would require the modification of the various calculations in the state equation of the original EwE software, the state variables of the HTL model, which were in wet weight (tons), were converted to phosphorus (μmol P) weight utilising C:N:P ratios taken from literature.

The third step in the harmonisation procedure was to reconcile the differences in the integration time step between the two models. Considering that the biogeochemical model ~~comprised~~ consisted of state variables with faster dynamics compared to ~~the~~ HTL model, it was convenient to make the HTL model comply with the integration step of the biogeochemical model. For this purpose, the rates of the HTL model, which were “per year (yr^{-1})”, were converted to “per hour (h^{-1})” by simply dividing the rates by 8760 (365 d^{-1} x 24 h^{-1}) so that the HTL variables could be integrated with the same time step of the biogeochemical model.

The final step in the harmonisation process ~~was~~ would be to adjust the closure terms of the biogeochemical model (mortality rates of zooplankton and phytoplankton groups) so as to compensate the additional losses through explicit predation of these groups by the HTL state variables. However, for our specific application, we decided to keep these values identical to the standalone biogeochemical model as it produced similar seasonal cycles observed in the standalone biogeochemical model except the missing second cycle in mesozooplankton (Figure 6). Considering that our research was not an idealised case study, our aim was to have plankton dynamics qualitatively comparable to the biogeochemical model, therefore, further fine-tuning was avoided. ~~Hence, in the coupled scheme, the mortality rates of the LTL variables that were predated by HTL groups were decreased by sensitivity experiments to the extent to satisfy the seasonality in the original biogeochemical model.~~

The technical overview of the coupling scheme is given in Figure 5~~Figure 5~~. As shown in the figure, the coupled simulation was carried out in four consecutive stages. In the first stage, a static mass-balance model of the whole system, which comprised all the HTL and LTL state variables in the ecosystem, was set-up utilising Ecopath-F. In this stage, the LTL state variables were ordered in advance of the HTL state variables so that the LTL state variables were numbered from 1-9 and the HTL state variables from 10-35 in the resulting scheme. Following this procedure, Ecopath-F was run to calculate the basic parameters and exchange rates between the state variables of the HTL and LTL compartments which were necessary to perform a dynamic simulation after completing all of the harmonisation steps ~~aforementioned above~~. In the second stage, utilising the calculations from the previous stage, the HTL and LTL models were initialised by calculating initial conditions for each of their respective state variables utilising their specific internal routines. In the third stage, the sources and sinks of HTL and LTL state variables were computed via utilising their respective derivative functions during the whole simulation period. The selection of the derivative function to be used to calculate the differentials of the state variables depended on the rank of the state variables determined during the Ecopath-F set-up in the first stage. This stage continued iteratively until the end of the simulation and at the end of each time step, stage four was executed so that the results calculated at each time step were, if required, post-processed and then written to the results file. Post-processing of LTL results might not be necessary in all cases but only if the LTL model is a multi-currency model and calculates its variables in more than one currency. In our example, because the LTL model represented some of its state variables both in carbon and phosphorus but the coupled HTL model only in phosphorus, a post-processing step was necessary to compute the corresponding phosphorus values of variables that were in carbon units while interchanging information between the HTL and LTL derivative functions as well as before writing the results into the output files. The coupled simulation was run ten years, two of which were for spin-off. In the simulations, we used default values for vulnerabilities (v_{ij} = 2) that represent a mixed control (Christensen et al., 2005).

Comparison of uncoupled EwE and coupled EwE-F model results (Figure 6~~Figure 6~~) demonstrated that the coupling scheme worked successfully and highlighted the effects of integration of LTL and HTL models. Because the aim of this exercise was only to demonstrate the capability of EwE-F to be used in integration with other models, the ecological interpretations of these results are not the focus of this work and thus ~~were~~ are only briefly discussed here. Comparing the seasonal dynamics of LTL state variables before and after coupling showed that explicit addition of HTL dynamics influenced the seasonality of the LTL state variables (grey-shaded plots in Figure 6~~Figure 6~~). It is worth noting that presence of several detrital and predatory links between HTL and LTL models (as shown in Figure 4~~Figure 4~~) resulted in clear top-down impacts on the LTL variables, particularly in non-living and bacteria. Furthermore, the comparison between the simulation results of HTL model forced with primary productivity changes (green lines in Figure 6~~Figure 6~~) in stock EwE and the fully coupled HTL/LTL models (black lines) showed that changes in the biogeochemical dynamics, namely nutrient recycling, not only impacted the LTL groups but also propagated up through the food web (bottom-up) to impact the biomasses of HTL organisms. However, while most of the bottom-associated groups decreased, by the incorporation of the biogeochemical model in the coupled scheme, pelagic-associated groups increased due to the explicit representation of resuspension of detritus and remineralisation that favoured plankton. Thus as evidenced in Figure 6~~Figure 6~~, the consequences of two-way coupling were not only one directional. These proved that the proper exchange of ~~information,~~information and the establishment of successful interaction between the two models were realised in the final coupled scheme.

5 Discussions and conclusions

5.1 Potential and flexibility of the application

In this work, the reliability of EwE-F was proven by utilising two sample models as test cases and comparing the absolute biomass values simulated by EwE-F against the simulated absolute biomass values by stock EwE version ~~6.4~~6.5. Further, the applicability of EwE-F in an E2E modelling framework was exemplified with a test case for the Gulf of Trieste ecosystem. This example proved the adaptability of EwE-F for coupled modelling frameworks, facilitating its coupling with other hydrodynamic and biogeochemical Fortran models for aquatic ecosystems in E2E ecosystem research. The scheme used in this work successfully conveyed two-way dynamics of HTL and LTL domains along the whole food web. As a step forward, this opened up the opportunity for using EwE, by utilising EwE-F implementation, as an HTL component of E2E ecosystem representations in various ecosystems.

According to Rose et al. (2010), the main difficulty encountered in coupling models of different realms lies in the reconciliation of the differences in time and spatial resolutions. However, difficulties may extend beyond these two areas, e.g. differences in model currencies. The coupling scheme used in this work is able to provide solutions to overcome such constraints highlighted by Rose et al. (2010) and others (Fulton, 2010; Kearney et al., 2012; Salihoglu et al., 2013) via its simplistic but ecologically capable approach to form end-to-end representations of aquatic ecosystems through the incorporation of EwE- F. In addition, the EwE-F ~~has generated~~enables significant opportunities for integrating it with any kind of Fortran models as depicted in Figure 7~~Figure 7~~. The figure represents a typical EwE food web model in the middle rectangular box and elaborates the possibilities of modifying EwE-F in different ways by replacing different components with sophisticated model representations for selected state variables or incorporating additional Fortran models to enhance the applicability of the original EwE approach. These solutions and possibilities are explored in detail in the following sections; i) reconciling different integration steps (Section 5.1.1), ii) dealing with models that use multiple currencies (Section 5.1.2), iii) other possibilities: incorporation of population demographic structure, physiological processes, socioeconomical frames (Section 5.1.4~~5.1.3~~).

5.1.1 Reconciling different integration steps

There are two possibilities when combining two models with different integration (time) steps; i) keeping the integrator function of the two models intact and averaging the outputs of the model with faster dynamics (high turnover rate) over the time frame of the model with slower dynamics (low turnover rate) and vice versa when exchanging information (time-averaged coupling), and ii) utilising a common integrator for both models and adjusting the rates of the model with slower dynamics to comply with the time window of the model with faster dynamics (real-time coupling). Although Ecosim, by default, works with monthly time steps it is capable of simulating high frequency dynamics using shorter time steps. In the present work, we opted for the latter to showcase the possibility of harmonisation in terms of integration step size when using EwE-F in coupled modelling schemes. The difference in the time resolution of both models was remedied by adjusting the HTL model's time step (one month) to conform to the time step of the biogeochemical model (one hour) in order to render the use of one common ordinary differential equation (ODE) solver (the Runge-Kutta 4th order) possible. ~~This was applicable since both models were written in Fortran.~~ Furthermore, due to this change in the time step of the HTL model, the annual rates of the HTL groups were converted to hourly rates by simple arithmetic calculations.

5.1.2 Dealing with models that use multiple currencies

Some biogeochemical models may carry out their computations in more than one currency for explicit representation of the ratios of fundamental nutrients in the system and their rate limiting conditions on nutrient uptake and primary productivity that can vary in space and time. The multiple currency approach, however, is usually not applied in HTL models, although implicit nutrient-based limitations can be represented in EwE (Araujo et al., 2006; Christensen et al., 2005). Hence, the coupling exercise presented here provided a simple solution for such situations. In order to reconcile the currency differences, one may opt to pick one of the currencies utilised in the biogeochemical model as the one considered to be the limiting nutrient, use it for the final coupled scheme incorporating the EwE-F model and post-process the derivative function outputs of the two models when exchanging information. In the coupling example given in this work, the difference in the currencies of the models was adjusted by converting the currency of the HTL model from wet weight to phosphorus (PO4) utilising the conversion rates and equations available in the literature for HTL groups (stage 1 of the coupling scheme in Figure 5~~Figure 5~~). In addition, the simulated results of the biogeochemical model (which were in dual currency, phosphorus and carbon) were post-processed prior to output and transferred to EwE-F so as to comply with the currency of the HTL compartment (stage 4 in Figure 5~~Figure 5~~). The approach used in this work proved to be a practical resolution for the issue in cases where there is no particular consideration to have simultaneously tracking multiple currencies in the HTL food web. However, with the availability of EwE-F, HTL models with computations of multiple model currencies can even be set-up if desired, although this will require significant modification of various calculations in the EwE state equations.

5.1.3 Spatial simulations

Another area where having EwE-F may play a substantial role is spatial simulations. Given the current experience with biogeochemical models coupled with hydrodynamic models e.g. Lazzari et al., 2012), explicit accounting for spatial variability would be important for any assessment of marine ecosystem dynamics. Future efforts would be required to add spatial simulation capabilities to EwE-F, either by implementing Ecospace in Fortran or by direct integration of Ecosim-F in a spatially explicit coupled hydrodynamic -biogeochemical model. Due to high computational costs required for such representations, we foresee that EwE-F could better exploit the power of high performance computing clusters via parallelisation to significantly decrease simulation times.

5.1.4 Other possibilities: population demographic structure, physiological processes, socioeconomical frames

Similar to the flexibility of EwE provided by its plugin system, EwE-F gives broad possibilities for interconnecting HTL models with other Fortran models sophisticating and/or incorporating HTL processes. Examples span from fish population to socioeconomic dynamic models.

For instance, EwE-F permits incorporating sophisticated population dynamic models written in Fortran within the EwE-F scheme (Figure 7~~Figure 7~~, C). These population models can be of any kind, including population's demographic structure (age/size classes) used for stock assessment and account for differences in fecundity by ages or size (Hilborn and Walters, 1992).

Moreover, EwE-F allows for parameterising various rates for HTL groups (e.g. assimilation efficiency, respiration) under the influence of various environmental factors (e.g. temperature, pH, light) that is not always straightforward otherwise (Figure 7~~Figure 7~~, D). In addition, EwE-F allows for replacing the growth of certain state variables in the food web with sophisticated bioenergetics models coded in Fortran. In this way, various physiological processes of the selected HTL organisms can be related directly and explicitly to the ambient physical factors such as light, temperature and nutrient availability (Figure 7~~Figure 7~~, B). With EwE-F, in fact, as demonstrated in this work, the dynamics of any desired additional state variable in the final coupled scheme could be resolved using derivative functions defined in other models during run-time. This allows for a two-way coupling of, potentially, any number of models (including earth system ones) in one coupling scheme.

Given the calls for ecosystem-based management for marine ecosystems, one can also incorporate socioeconomical dynamics on E2E ecosystem representations that deal with fisheries on top of EwE-F. Considering its modular structure and ease of integration with other models as demonstrated in this work, such holistic representations of ecological and socioeconomical systems have been significantly improved also including frameworks that involve integration of multiple models written in Fortran (Figure 7~~Figure 7~~, A).

5.2 Other practical considerations and future development

Through its simple input/output scheme utilising ASCII encoded text files, the availability of EwE-F provides a further opportunity by giving Fortran modellers the possibility to perform detailed sensitivity and uncertainty analyses using hundreds of ensemble scenarios that can easily be prepared also by using modern high-level languages (e.g. Perl, Python, NCL) in addition to Fortran. For their convenience, users of EwE-F are advised to set-up, test and fit their models to time series data using EwE also benefiting of the several routines included in EwE and, thereafter, transfer their models to EwE-F.

Ecospace (Walters et al., 1999) and other complementary routines aforementioned (see section 3) were not implemented considering that EwE-F was not designed to be a EwE replacement but a bare-bones incarnation that can be used easily for purposes summarised in Section 5.1.4~~5.1.3~~. Therefore, analyses requiring the aforementioned specific routines (e.g. Monte-Carlo analysis, Network Analysis~~vulnerability search, time series fitting~~ etc.) in uncoupled or coupled EwE-F simulations can be done by coding the required specific routines or alternatively EwE could be employed for such purposes. The current lack of such useful tools that are present in EwE ~~6.4~~6.5 is considered as a drawback for the EwE-F v1.0, which may represent an obstacle for some users. However, these technical shortcomings and the lack of aforementioned tools including mediation function and time series fitting via vulnerability parameter search are planned to be addressed in the future by incorporating these routines in EwE-F and developing a Visual Basic plug-in for stock EwE which will prepare input files required by EwE-F through EwE's graphical user interface in a straightforward way. Furthermore, considering advancements for coupling in the spatial scale, future efforts of developing EwE-F may also focus on incorporating ~~the~~ 2D spatial dynamics by implementing the Ecospace module of EwE to facilitate the use of EwE-F in schemes that require spatial-temporal dynamics to be resolved.

6 Code availability

The source code of EwE-F version 1.0 detailed in the present work and the corresponding User's Manual can be obtained as supplementary material to this article. In the User's Manual, detailed instructions to obtain the current and future versions of EwE-F along with building and running EwE-F on different platforms are described. Further versions of EwE-F model and their respective documentations can be obtained on Bitbucket.org (https://bitbucket.org/ewe-f). The system requirements, license and other basic information regarding EwE-F version 1.0 are given in Table 1~~Table 1~~.

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Table 1. General system and software related requirements of EwE-F v1.0.

Name	EwE-F (Ecopath with Ecosim in Fortran)
Operating Systems	Unix-like operating systems (Linux, *BSD, Mac OS X) and Microsoft Windows
Processor	Intel or AMD x86 processor
Disk Space	30 MB
Compiler	Fortran 95/2003 standards compliant compiler (e.g. GNU Fortran, Intel® Fortran Compiler, PGI® Fortran, Oracle® Solaris Studio, Absoft® Pro Fortran Compiler)
Version Control System	GIT (optional, for version controlled development)
Building	GNU Make (only required for building on Unix-like systems)
Required External Libraries	HDF5 version 1.8.11 or above
License	GNU Public License (GPL) version 2
Homepage	https://bitbucket.org/ewe-f
Obtaining and Documentation	supporting information (SI) "EwE-F User's Manual"

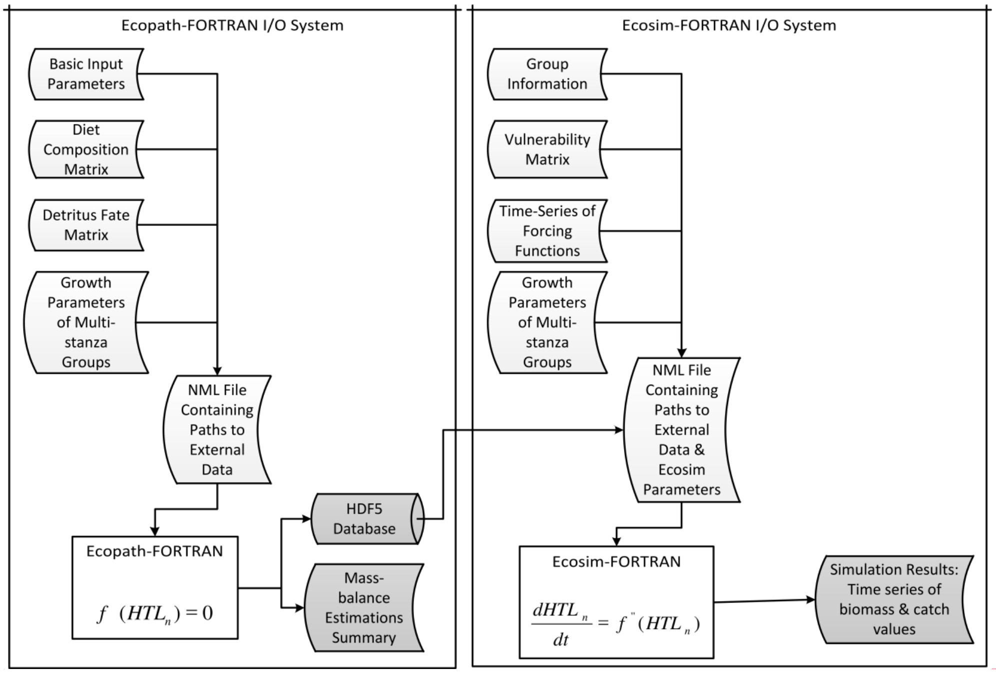

Figure 1. The EwE-F data input/output scheme. Curved white rectangular boxes denote tab-delimited ASCII files providing external data input to the EwE-F models (rectangles). Curved grey-shaded rectangles and the cylindrical box denote the model output via tab-delimited ASCII and HDF5 files respectively. For details see sections 3.1 and 3.2.

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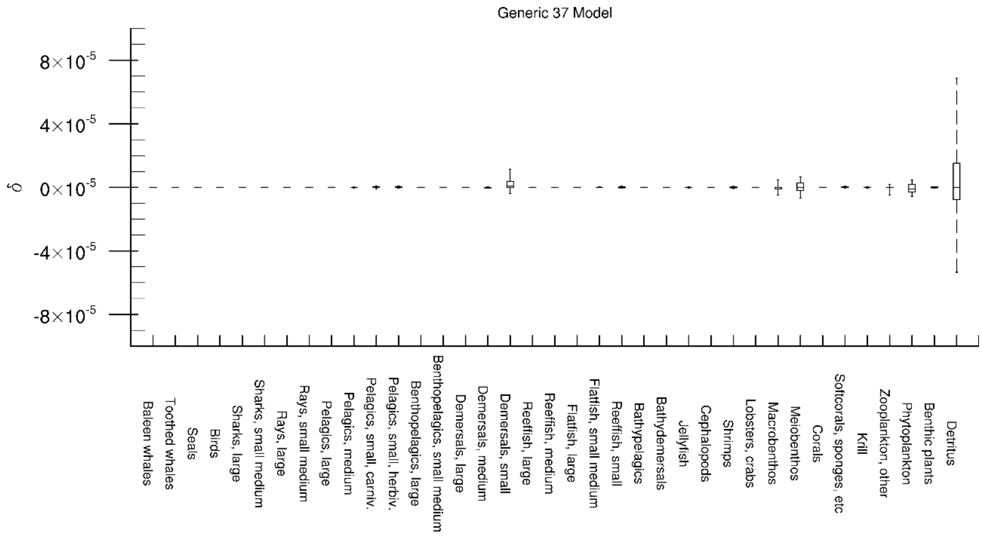

Figure 2. The residuals between absolute biomasses simulated by EwE ~~6.4~~6.5 and EwE-F 1.0 for the Generic 37 model. X-axis denotes all state variables in the model.

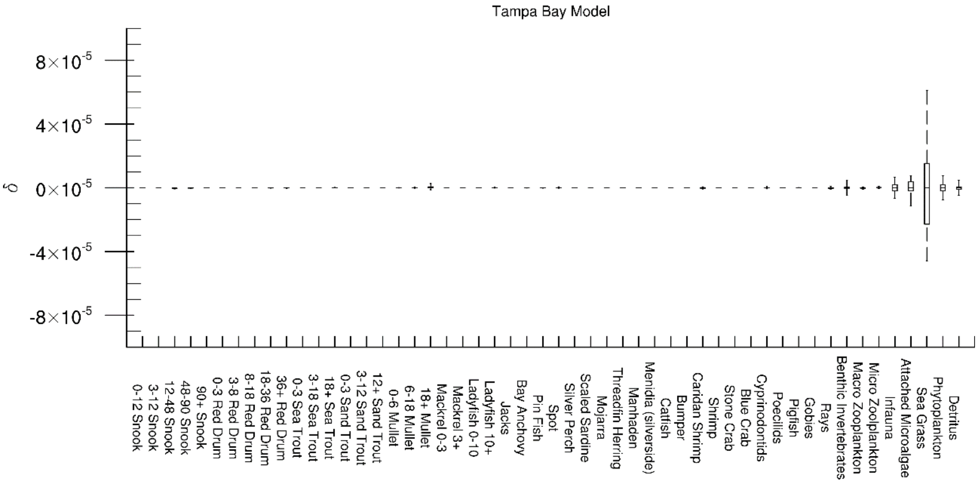

Figure 3. The residuals between absolute biomasses simulated by EwE ~~6.4~~6.5 and EwE-F 1.0 for the Tampa Bay model. X-axis denotes all state variables in the model.

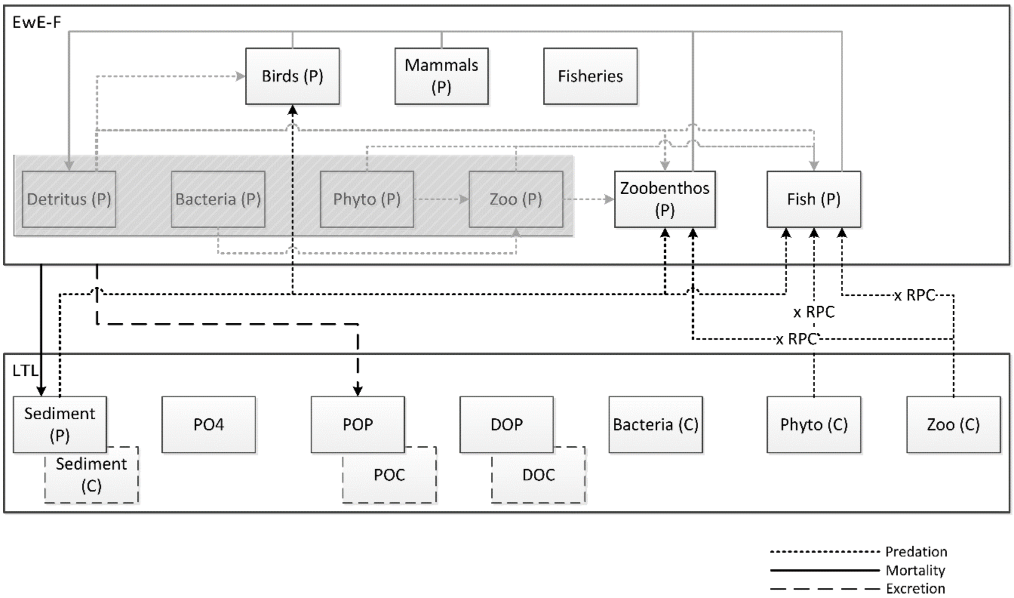

Figure 4. Coupled trophodynamic model scheme of the Gulf of Trieste (Northern Adriatic Sea) showing the linkages between the HTL and LTL models. Phosphorus (denoted with P) was used as the currency for all of the HTL state variables and flows linking the two models. Flows originating from the state variables of the LTL model which were expressed in carbon (denoted with C); i.e. phytoplankton and zooplankton, to the HTL model were converted to phosphorus (by multiplying variable-specific phosphorus to carbon (RPC) ratios) before being transferred. Grey-shaded state variables and flows in the HTL model were replaced by the LTL model's corresponding state variables and the new linked flows shown in black dashed and continuous lines. Abbreviations: Zoo (small and large zooplankton groups), Phyto (small and large phytoplankton groups), PO4 (phosphate), POP (particulate organic phosphorus), DOP (dissolved organic phosphorus).

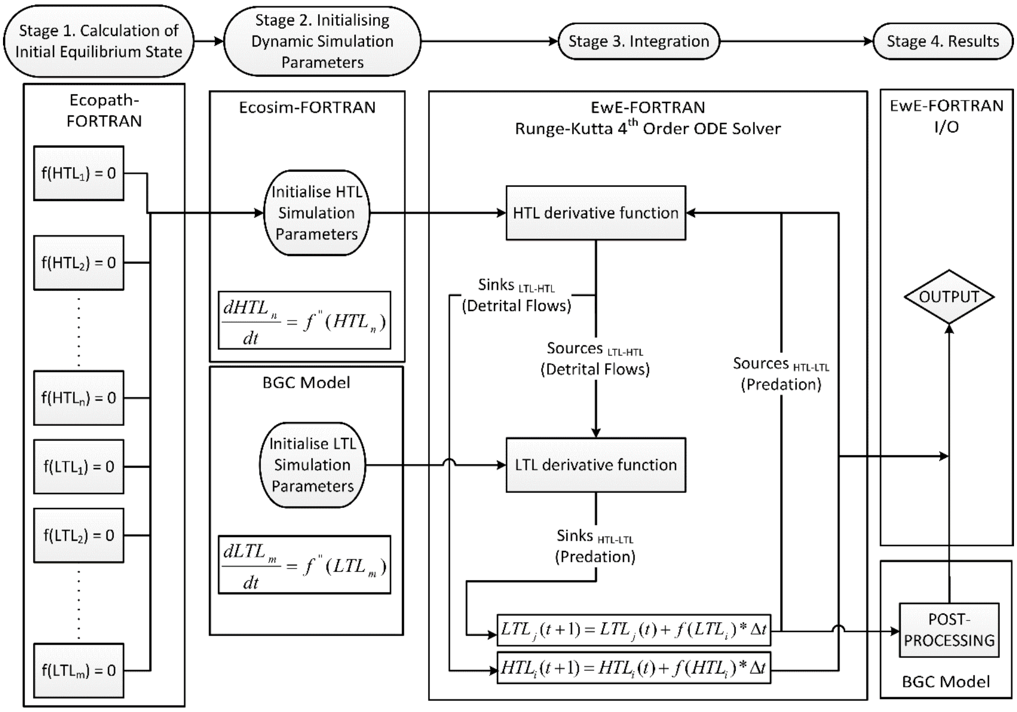

Figure 5. The technical overview of the coupling scheme. ODE stands for "Ordinary Differential Equation", I/O stands for "Input/Output", and BGC stands for "Biogeochemical Model" used in the present work.

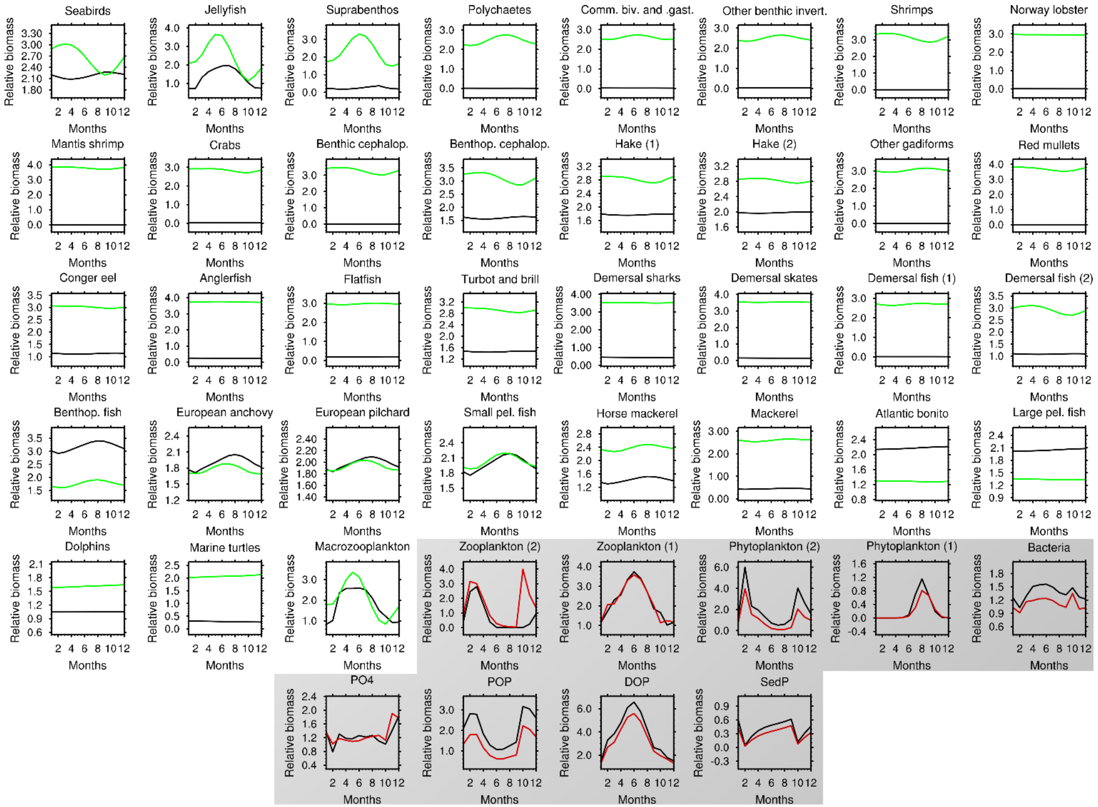

Figure 6. Monthly results of the final year in a 10-year simulation of the coupled (black lines) model versus simulations of uncoupled EwE ~~6.4~~6.5 (green lines for HTL variables) and biogeochemical (red lines for grey-shaded LTL variables) models.

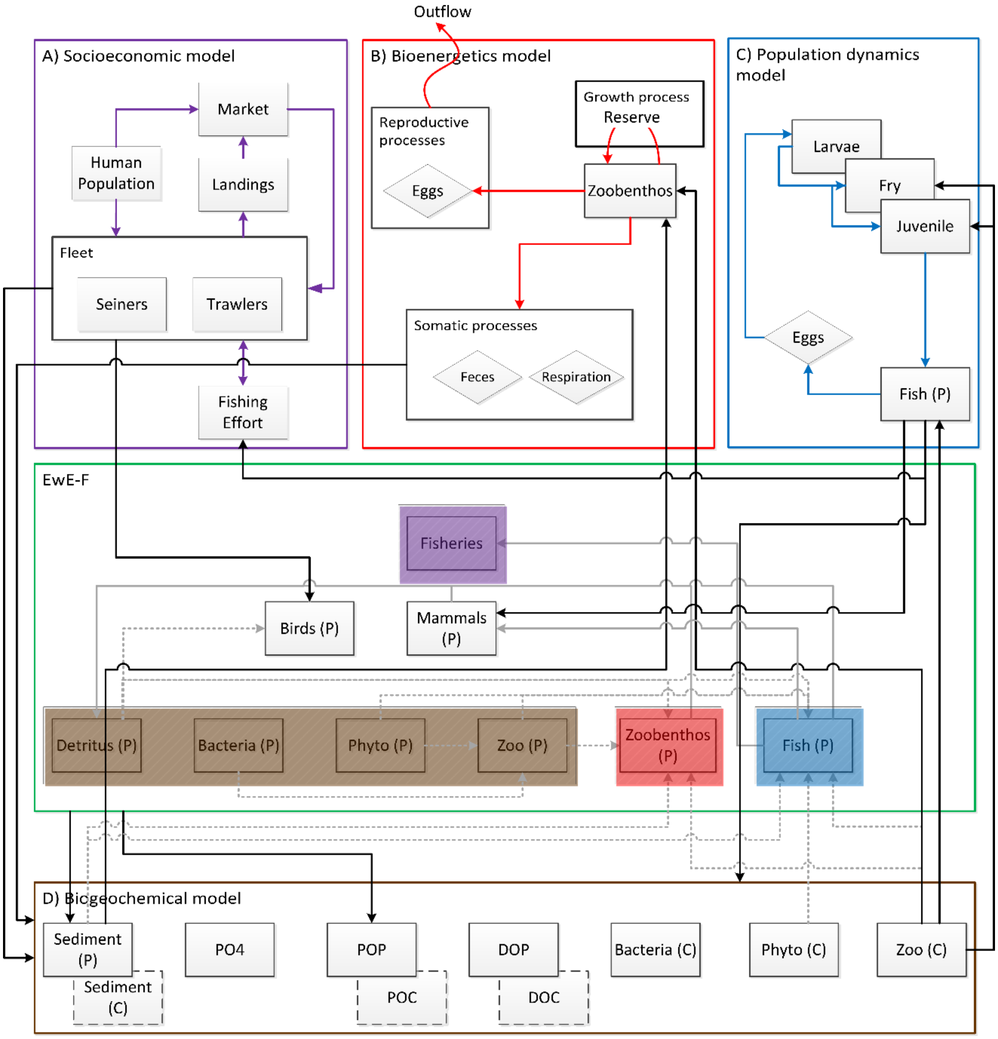

Figure 7. Potentialities provided by the EwE-F approach. Coloured arrows denote flows specific to the integrating Fortran models. Black arrows denote linking flows and grey-shaded arrows denote flows replaced/augmented by the linking flows. Boxes denoted by the letters A, B, C and D and bordered by coloured lines replace the respective colour-shaded regions in the EwE-F box (bordered green) under the integration scheme.