

The manuscript has been improved in several areas, but especially the mathematical description needs improvement.

MP1 and MP2:

The discussion issue (MP1, PK1.1) has been solved in the revision and the manuscript has been much improved, both by toning down the introduction and by expanding section 5. The same applies to MP2.

MP3:

This issue is not solved sufficiently and needs improvement prior to publication.

RC1.4: Still unclear why the term numerical approximator and not integrator or solver is used (as in the math-lit), but an improvement is available.

RC1.5: This was not meant as an implementation question: In cases of rapid, non-linear changes (eg Power-Law-Equation with an exponent  $> 4$ ), implicit solvers often fail to converge for a specific time step – even A-stable solvers like the implicit Euler. Complex solvers (eg. RKF 45, CVODE and many others) use an adaptive time stepping scheme, which is, as the authors explain in their answer to RC1.8, not suitable for SuperFlexPy. This is important information and should be mentioned in the section 4.3

RC1.6: Reference is provided now, but the properties of the algorithm should be stated in the supplemental material (limits and speed of convergence). The algorithm is not explained or just described as a mixture of regula falsi with the secant method.

RC1.7: After careful reading of Supl-Section 5.1, I cannot find the information from this answer. The need for smoothing when using the implicit solver must be mentioned as a one-liner in the main text.

RC1.8: My concerns about numerical errors by the operator split are explained in the answer to the reviewers (RC1.8), but have not made it in the manuscript – neither in the main text nor in the supplemental material. In fact, both m/s and supplement are plainly wrong: m/s l. 514 suggest a free choice for the selected numerical solver and the supplement mat 5.1 suggests RK-solvers as an additional (not yet used) choice. However, RC1.8 explains me (but not the readers), that only single step Euler solvers are suitable to solve the system as other solvers would introduce the need for a formal integration of the fluxes over the (outer) timestep:

“When fixed-step solvers are used, this "one-element-at-a-time" strategy is equivalent to applying the same (fixed-step) solver to the entire ODE system simultaneously (i.e., no additional approximation error is introduced). “ (from answer to RC1.8)

This section needs to make it in the main text of the manuscript, together with a reference for the claim.

RK-solvers of  $n$ th order use  $n-1$  (or more) substeps to predict the final state at the output timestep by fitting an  $n$ th-order polynom into these substeps. Using the flux at  $Y(t, S(t))$  or  $Y(t+1, S(t+1))$  is not the correct number, as the solver calculates the ODE between these timesteps and introduces an uncaught numerical error into the system. While the user is free to use any Jacobian-free root finder, the choice of the ODE-solver is (obviously) limited to implicit and explicit Euler methods (PECE methods might also an alternative). There is no interface to calculate the Jacobian matrix of an Element, hence Newton-like root finding algorithms are not suitable. The freedom of the solver choice is quite limited by the use of the sequential solution of the DAG approach – this is of course valid, but should be made explicit.

MP4:

The classical structure of scientific writing is of course not directly fitting with a model description paper. However, I would see the choice of math, programming language and design principles rather as the methods of a model implementation and the resulting code and use examples as the results section. The new, frequent links to other sections, are a poor surrogate for a cleaner structure but are an improvement over the original manuscript.

Additional issues:

Section 4.2:

The m/s mentions 8 times the object oriented design of the implementation and but does not feature the object oriented design choices at a prominent place. The UML-diagram is now hidden in the last section of the supplemental material. The UML-like diagram should be moved to the main text in section 4.2, as it is essential for the understanding of the object oriented design. Now section 4.2 lists, how the OO-design helps to accomplish certain goals, but we, as the readers, can only guess what that OO-design is.

Fig 12: I am familiar with most services and software mentioned in Fig 12 (except binder), however, I had a hard time to understand it. Mixing cloud services like github, binder, zenodo, and read the docs with a file format (Jupyter-Notebooks) on an equal level does not help to understand any of these services. Having the developer and the user as the same person (symbol) complicates the understanding with the blue and black lines. The authors state, that explaining the ecosystem around SuperflexPy is important – while I do not follow the premise, explaining the services is possibly better done with text. But if the ecosystem is important enough for a large figure in the main text (while omitting the UML-Diagram), then the importance should be highlighted throughout the paper, as the object oriented design is. I still recommend to delete this figure. If the authors are absolutely sure, this figure is needed, they need to a) redraw the figure using two persons and kicking out Jupyter-Notebooks (as they are not a web service themselves) and test the figure with friends from the intended audience, b) explain the figure in much more detail and the role of every mentioned service therein, and c) introduce throughout the paper the importance of a webservice ecosystem for modern model development (eg. mention in section 1.2, practical criteria). However, as of now, this figure is hardly explained, and someone who is not familiar with these services will not profit from it. Even worse, the figure in its current state is prone to misunderstandings and does a disservice to the paper. Moving the figure as is to the supplement material does not solve the issues mentioned above.

Jansen et al (2020) reference: This is unpublished work, and I as a reviewer am unable to check the content of this reference and review its role in the paper. The author's claim about its content might be wrong. As such, the reference needs to be removed. If a public preprint had been cited, this problem would not exist.