

¹ TransiFlow: A Python package for performing bifurcation analysis on fluid flow problems

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⁷ Summary

⁸ Dynamical systems derived from models of fluid flow show transition behaviors associated with ⁹ fluid flow instabilities ([Wubs & Dijkstra, 2023](#)). For example, dynamical systems from ocean ¹⁰ models in which transition behavior is caused by slow changes in parameters representing the surface forcing ([Westen et al., 2024](#)). A flow transition is a qualitative change in the flow ¹¹ when a specific parameter is varied, e.g. a transition from a no-flow heat-conducting fluid to ¹² a heat-transporting flow (as in Rayleigh-Bénard convection), or a steady flow which has a ¹³ steady forcing and steady boundary conditions that turns into a transient flow which may even ¹⁴ produce sound (as in the von Kármán vortex street). In both these examples the qualitatively ¹⁵ different solutions do not appear out of the blue.

¹⁶ If one perturbs a steady solution before the transition point then the perturbation will die out ¹⁷ and recover to the steady solution. This means that the steady solution is stable. However, this ¹⁸ perturbed flow already reveals the shape that will occur after the transition point. For forcing ¹⁹ beyond this point that shape will grow into a new steady flow (the stable solution becomes ²⁰ unstable) for Rayleigh-Bénard convection and into a transient flow for the von Kármán vortex ²¹ street (the stationary flow becomes unstable). The parameter value for which the transition ²² occurs is called a bifurcation point, sometimes also referred to as a transition or tipping point.

²³ Studying these phenomena (bifurcation analysis) can be done by performing numerical ²⁴ simulations and observing transient behavior after a certain time. This is, however, ²⁵ computationally expensive and in many cases infeasible. Instead, so-called continuation ²⁶ methods are able to trace stable and unstable steady states in parameter space, obviating ²⁷ expensive transient simulations ([Dijkstra, 2005](#)). The TransiFlow Python package implements ²⁸ a continuation framework in which fluid flow problems can be studied with the help of several ²⁹ computational back-ends that can, based on the needs of the user, be easily switched between.

³⁰ One motivation behind TransiFlow is that writing research software that works efficiently on a ³¹ parallel computer is a challenging task. Numerical models are often developed as a sequential ³² code with parallelization as an afterthought, making them difficult to parallelize, or as a parallel ³³ code from the start, making them complicated to work with. This is especially problematic ³⁴ since people that work with these codes generally only use them for the duration of ³⁵ a project. If there is insufficient documentation and continuity between the projects then ³⁶ knowledge of how to use or develop the codes may get lost, rendering the software useless.

³⁷ In climate modelling, this is a prominent issue, since the models are complex, are usually ³⁸ intercoupled with other models (e.g., ocean, atmosphere, ice), take a very long time to run (i.e., ³⁹ multiple months) and require large amounts of parallelism to reach a sufficient resolution (i.e., ⁴⁰ using thousands of cores for a single run) ([Mulder et al., 2021](#); [Thies et al., 2009](#)). Therefore, ⁴¹ ease of developing and using the parallel software is crucial.

43 We achieve this by abstracting away the computational back-end, which allows the user to
 44 adjust a model to their own needs on their own machine (e.g., a laptop) in Python using the
 45 SciPy back-end. Assuming it is implemented on a Cartesian grid, the user can then run a
 46 large-scale simulation on an HPC system using, e.g., the Trilinos back-end, which can use a
 47 combination of OpenMP, MPI, and potentially GPUs, without requiring any changes to the
 48 model code. The computationally expensive parts of the program are implemented by these
 49 libraries so one does not have to worry about the efficiency of the Python implementation of the
 50 model. Initial tests indicate that the overhead of using Python is small when compared to the
 51 expensive linear system solves that are handled by the external libraries that are implemented
 52 in e.g. C++.

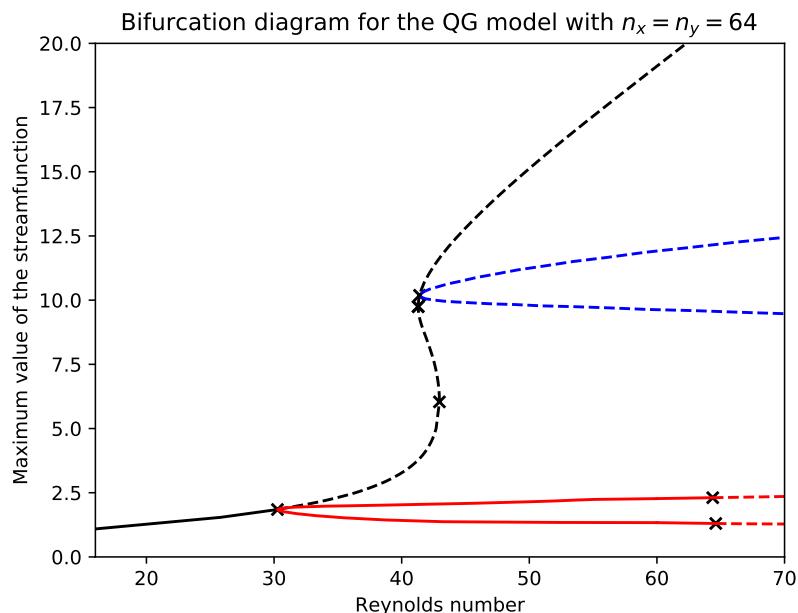


Figure 1: Bifurcation diagram of the double-gyre wind-driven circulation configuration that is included in TransiFlow. The markers indicate pitchfork, Hopf and saddle-node bifurcations that were automatically detected by the software. Solid lines indicate stable steady states of the system; dashed lines indicate unstable steady states. A more extensive description of the bifurcation diagram and steps to reproduce it can be found in (Sapsis & Dijkstra, 2013).

53 Statement of need

54 TransiFlow aims to be an easy-to-use tool for performing bifurcation analysis on fluid flow
 55 problems that can be used in combination with fast parallel solvers with minimal additional effort.
 56 TransiFlow implements pseudo-arclength continuation and implicit time integration methods,
 57 as well as finite-volume discretizations for the incompressible Navier-Stokes equations with
 58 optional heat and salinity transport. We also provide implementations of various canonical fluid
 59 flow problems such as lid-driven and differentially heated cavities, Rayleigh-Bénard convection
 60 and Taylor-Couette flow, a feature none of its competitors provide.

61 The main competitors are [AUTO](#) (Doedel et al., 2007), [MatCont](#) (Dhooge et al., 2008)
 62 [BifurcationKit.jl](#) (Veltz, 2020) and [pde2path](#) (Uecker, 2014). These packages are widely
 63 used, and they are much more feature complete in terms of bifurcation analysis. However, they
 64 lack the discretized fluid flow models and parallel solver interfaces that make TransiFlow easy
 65 to use.

⁶⁶ A continuation package that allows for easy coupling with parallel solvers is the [LOCA](#) package in
⁶⁷ [Trilinos](#) ([The Trilinos Project Team, 2024](#)). Using LOCA, however, requires a vast knowledge
⁶⁸ of C++ and any change to the continuation algorithm requires a full stack of C++ templates
⁶⁹ to be reimplemented. Moreover, LOCA has not seen any active development in over 10 years.
⁷⁰ An alternative Python package for performing bifurcation analysis is [PyNCT](#) ([Draelants et al., 2015](#)). It is,
⁷¹ however, difficult to extend, the latest version of the software is not freely available,
⁷² and it can only be used for systems that are symmetric positive-definite.

⁷³ Past and ongoing research

⁷⁴ [TransiFlow](#) has been used to generate results in ([Wubs & Dijkstra, 2023](#)) and ([Bernuzzi et al., 2024](#))
⁷⁵ and has been used in courses at Utrecht University and the University of Groningen (NL).
⁷⁶ Earlier versions have also been used to generate results in ([Song, 2019](#)) and ([Baars et al., 2020](#)).
⁷⁷ The code is currently being used in various projects at Utrecht University, such as a project
⁷⁸ for coupling climate models and a project for studying transitions in the Atlantic Meridional
⁷⁹ Overturning Circulation. There is also ongoing work on adding 3D ocean and atmosphere
⁸⁰ discretizations to [TransiFlow](#). [TransiFlow](#) is also used by several external researchers.

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