Numerical methods for studying transition probabilities in stochastic ocean-climate models

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PUBLICATIONS AND PREPRINTS

S. Baars, J. Viebahn, T. Mulder, C. Kuehn, F. Wubs, and H. Dijkstra. Continuation of Probability Density Functions Using a Generalized Lyapunov Approach. *Journal of Computational Physics*, 336:627–643, May 2017. doi: 10.1016/j.jcp.2017.02.021.

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SOFTWARE

This chapter contains a list of software that has been developed, or has been contributed to, as part of this work.

FVM A finite volume package which contains implementations of a lid-driven cavity, a differentially heated cavity, Rayleigh-Bénard convection, and convection in a differentially heated rotating cavity. https://bitbucket.org/hymls/hymls/src/master/fvm

HYMLS A Hybrid direct/iterative solver for the Jacobian of the incompressible Navier-Stokes equations on structured grids. The implementation of the preconditioner and the domain decomposition are described in this thesis. https://github.com/nlesc-smcm/hymls

I-EMIC An Implicit Earth System Model of Intermediate Complexity. The I-EMIC contains a number of implicit submodels coupled through a modular framework. At the center of the coupled model is the implicit primitive equation ocean model THCM that has been used in the past to study bifurcations in the thermohaline circulation. This package interfaces to parallel C++ versions of RAILS and the methods for computing transition probabilities that were discussed in this thesis. https://github.com/nlesc-smcm/i-emic

JDQZ++ A templated C++ implementation of the JDQZ generalized eigenvalue problem solver. https://github.com/erik808/jdqzpp

MOxUnit A lightweight unit test framework for Matlab and GNU Octave. https://github.com/MOxUnit/MOxUnit

OpenBLAS An optimized BLAS library based on GotoBLAS2 1.13, BSD version. http://www.openblas.net

PHIST A Pipelined Hybrid Parallel Iterative Solver Toolkit. PHIST provides implementations of and interfaces to block iterative solvers for sparse linear and eigenvalue problems. https://bitbucket.org/essex/phist

RAILS An implementation of the Residual Approximation-based Iterative Lyapunov Solver as described in this thesis in Matlab and a parallel implementation in C++. https://github.com/Sbte/RAILS

Transitions A Matlab implementation of the methods for computing transition probabilities as described in this thesis. https://github.com/Sbte/transitions

Trilinos The Trilinos Project is an effort to develop algorithms and enabling technologies within an object-oriented software framework for the solution of large-scale, complex multi-physics engineering and scientific problems. A unique design feature of Trilinos is its focus on packages. https://trilinos.org

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SUMMARY

There is a strong variability in the everyday weather related to the development of high- and low-pressure fields. These developments do not have anything to do with the external solar forcing, but are due to the internal variability of the atmospheric flow. The time scale of this variability of 3-7 days is determined by the nonlinear processes in the atmosphere itself. Similar processes happen in every part of the climate system on varying time scales. A high-frequency process is the weather as described above; a low-frequency process is the change in land-ice distribution. In the ocean, internal variability causes formation of ocean eddies and the meandering of ocean currents such as the Gulf Stream. Interaction between all the different processes on different time scales may result in internal variability on other time scales that is not present in decoupled systems. This makes such processes very challenging to study, and difficult to understand. Therefore it is often a good idea to take a step back, and look at a more simplified model to make sure one is at least able to understand the results, and then apply this newly acquired knowledge to the fully coupled system.

We work with such a simplified model of the Meridional Overturning Circulation (MOC). The MOC consists of a global 'conveyor belt' of ocean currents, which are driven by wind stress forces and fluxes of heat and freshwater at the surface. In the Atlantic ocean, it consists of surface currents that transport relatively light water toward high latitudes, deep water currents going in the opposite direction, and sinking and upwelling processes that connect these two. The circulation system contains two overturning cells: one in the north with North Atlantic Deep Water (NADW) and one in the south with Antarctic Bottom Water (AABW).

Since the first model proposed by Stommel, many model studies have

shown that the MOC may be sensitive to variability in the freshwater forcing. In a global coupled climate model by Vellinga and Wood the NADW circulation collapses and recovers after 120 years. This is because weakening the MOC by introducing more freshwater in the North Atlantic (melting of the Greenland ice sheet) leads to a reduced northward saltwater transport, which in turn amplifies the freshwater perturbation.

A state of the MOC with a strongly reduced heat transport may have large consequences for the global climate. Cooling of a few degrees may be observed in Europe, which in turn may lead to growing glaciers and then global cooling. Therefore, an estimate of the probability of MOC transitions is crucial for prediction of a collapse of the MOC and with that a rapid climate change.

This collapse may occur due to the existence of a tipping point associated with the salt-advection feedback. Tipping points exist due to the presence of multiple stable steady states for the same parameter values. Due to unresolved small-scale variability, however, transitions may even be observed before a tipping point is reached. This unresolved variability is often represented as noise. We aimed to develop methods which can be used for studying transition behavior in the MOC.

To be able to observe these transitions between stable steady states, we first need to be able to compute the steady states themselves. They can be computed by using time integration, which is often expensive, especially if steady states have to be computed for multiple parameter values. Instead one can apply a method called (pseudo-arclength) continuation, which can compute the steady states directly by applying Newton's method. This can speed up the computation of steady states considerably. Pseudo-arclength continuation is especially useful for computing unstable steady states, i.e. steady states for which a small disturbance causes the state to converge to a different steady state. Time integration methods are usually incapable of computing these unstable steady states.

During the application of Newton's method, many linear systems of equations have to be solved. For the MOC, these are specifically equations that include the Navier–Stokes equations discretized on a staggered grid. Direct (sparse) solvers are not practical since a typical ocean model involves millions of unknowns leading to a huge memory requirement for storing the factorization and an enormous amount of time to compute it. For such problems, iterative methods are preferred, e.g. Krylov subspace methods with suitable preconditioning to ensure robustness, fast convergence and accuracy of the final approximate solution.

Preconditioners that are often advocated include standard additive Schwarz domain-decomposition, multigrid with aggressive coarsening and strong smoothers (e.g. ILU), and 'block preconditioners' that use an approximate block LU factorization and some approximation of the Schur complement associated with the pressure unknowns, e.g. SIMPLEC, LSC, and PCD.

Another class of Schur complement methods is obtained when eliminating the interior of geometric partitions (or subdomains) and constructing a suitable approximation of the reduced system on the separator. In this class of methods, we presented a multilevel preconditioner for the Navier–Stokes equations discretized on a staggered grid. The resulting operator acts in the divergence-free space, which allows the method to handle the saddle-point structure of the system in a natural way.

After computing steady states of the MOC, we are interested in its sensitivity to noise. The sensitivity around a steady state can be determined from the probability density function. It is well known that this probability density function can be computed from the solution of a generalized Lyapunov equation. Direct methods for solving a generalized Lyapunov equation such as Bartels–Stewart algorithm are based on dense matrix solvers and hence inapplicable for large systems. Other existing methods which use low-rank approximations might also become expensive for high-dimensional problems, particularly when trying to use previous initial guesses along a continuation branch. We, therefore, presented a novel method for computing the solution of generalized Lyapunov equations that is particularly well suited for our ocean problem in a continuation context. The method works by applying a Galerkin type projection with the space built from the eigenvectors belonging to the largest eigenvalues of the residual at every iteration of the method. Most important is that the method can be restarted, which allows for less memory usage, faster iterations, and recycling of previous solutions. We showed that for an idealized 2D MOC model, our method is the most efficient method in terms of both memory usage and time.

A shortcoming to this above approach is that it only describes the sensitivity to noise around a steady state. To study the more global phenomenon of transitions between steady states, stochastic time integration is required. Applying a standard Monte Carlo method, however, is way too expensive, especially for high-dimensional systems and when the probability of a transition is small. Multiple methods exist to work around this problem by applying some form of resampling. To improve on these methods, we came up with a projected time stepping method, which reduces the memory usage for our idealized 2D MOC model with 96%, and the time consumption by 30%. We showed that the probability of a transition increases drastically when getting closer to a bifurcation point, and that the projected method is able to obtain the same results as standard methods.

Since we only looked at an idealized 2D MOC model, we can not really say anything about the transition probabilities of the MOC in the actual Atlantic ocean, but we did provide methods with which this becomes feasible.

SAMENVATTING

Ontwikkelingen van hoge- en lagedrukgebieden zorgen voor een sterke variabiliteit van het weer. Deze ontwikkelingen worden niet veroorzaakt door stralingsenergie afkomstig van de zon, maar zijn te wijten aan de interne variabiliteit van de atmosferische stroming. De tijdschaal van 3 tot 7 dagen van deze variabiliteit wordt bepaald door niet-lineaire processen in de atmosfeer zelf. Soortgelijke processen vinden op verschillende tijdschalen plaats in elk deel van het klimaatsysteem. Een hoogfrequent proces is het weer zoals hierboven beschreven; een laagfrequent proces is de verandering in de dekkingsgraad van ijs op land. In de oceaan veroorzaakt interne variabiliteit vorming van wervels en het meanderen van oceaanstromingen zoals de Golfstroom. Interactie tussen alle verschillende processen op verschillende tijdschalen kan leiden tot interne variabiliteit op andere tijdschalen die niet aanwezig is in de afzonderlijke systemen. Dit maakt dergelijke processen zeer lastig om te bestuderen en moeilijk om te begrijpen. Daarom is het vaak een goed idee om een stap terug te doen en te kijken naar een eenvoudiger model om er zeker van te zijn dat men in ieder geval in staat is om de resultaten te begrijpen, en om deze nieuw verworven kennis vervolgens toe te kunnen passen op het volledig gekoppelde systeem.

We werken met een dergelijk vereenvoudigd model van de meridionale omwentelingscirculatie (MOC). De MOC bestaat uit een mondiale 'transportband' van zeestromingen, die wordt aangedreven door windspanningskrachten en fluxen van warmte en zoet water aan het oppervlak. In de Atlantische oceaan bestaat het uit oppervlaktestromen die relatief licht water naar hoge breedtegraden transporteren, diepe waterstromen die in de tegenovergestelde richting gaan en zink- en opwellingprocessen die deze twee verbinden. Het circulatiesysteem bevat twee omwentelingscellen: één in het noorden met

Noord-Atlantisch diep water (NADW) en één in het zuiden met Antarctisch bodemwater (AABW).

Sinds het eerste door Stommel voorgestelde model hebben veel modelstudies aangetoond dat de MOC gevoelig kan zijn voor variabiliteit in de zoetwaterforcering. In een gekoppeld klimaatmodel van Vellinga en Wood stort de NADW-circulatie in en herstelt zich na 120 jaar. De verzwakking van de MOC door de introductie van meer zoet water in de Noord-Atlantische oceaan (het smelten van de Groenlandse ijskap) leidt namelijk tot een verminderd zoutwatertransport naar het noorden, wat op zijn beurt de zoetwaterverstoring versterkt.

Een toestand van de MOC met een sterk gereduceerd warmtetransport kan grote gevolgen hebben voor het mondiale klimaat. In Europa kan een afkoeling van enkele graden worden waargenomen, die op haar beurt kan leiden tot groeiende gletsjers en vervolgens tot wereldwijde afkoeling. Daarom is een schatting van de kans op MOC-transities cruciaal voor het voorspellen van een ineenstorting van de MOC en daarmee een snelle klimaatverandering.

Deze ineenstorting kan optreden vanwege het bestaan van een kantelpunt die gerelateerd is aan de zout-advectieterugkoppeling. Kantelpunten bestaan vanwege de aanwezigheid van meerdere stabiele evenwichtstoestanden voor dezelfde parameterwaarden. Vanwege kleinschalige variabiliteit die niet in het model wordt gevangen kunnen echter transities worden waargenomen zelfs voordat een kantelpunt wordt bereikt. Deze kleinschalige variabiliteit wordt vaak beschreven door middel van ruis. Ons doel was om methoden te ontwikkelen die kunnen worden gebruikt voor het bestuderen van transitiegedrag in de MOC.

Om deze overgangen tussen stabiele evenwichtstoestanden te kunnen waarnemen, moeten we eerst de evenwichtstoestanden zelf kunnen berekenen. Ze kunnen worden berekend met behulp van tijdsintegratie, wat vaak duur is, vooral als evenwichtstoestanden berekend moeten worden voor meerdere parameterwaarden. In plaats daarvan kan men een methode toepassen genaamd (pseudo-arclength) continuatie, die de evenwichtstoestanden rechtstreeks kan berekenen door de methode van Newton toe te passen. Dit kan de berekening van evenwichtstoestanden aanzienlijk versnellen. Pseudo-arclength continuatie is vooral nuttig voor het berekenen van onstabiele evenwichtstoestanden, d.w.z. evenwichtstoestanden waarbij een kleine verstoring ervoor zorgt dat de toestand convergeert naar een andere evenwichtstoestand. Tijdsintegratiemethoden zijn meestal niet in staat om deze onstabiele evenwichtstoestanden te berekenen.

Bij de toepassing van de methode van Newton moeten veel lineaire stelsels van vergelijkingen worden opgelost. Voor de MOC zijn dit specifiek vergelijkingen die de Navier-Stokes-vergelijkingen omvatten, gediscretiseerd op een versprongen rooster. Directe (ijle) oplossingsmethoden zijn niet praktisch, omdat een typisch oceaanmodel miljoenen onbekenden omvat, wat leidt tot een grote geheugenvereiste voor het opslaan van de factorisatie en een enorme hoeveelheid tijd die nodig is om deze te berekenen. Voor dergelijke problemen wordt de voorkeur gegeven aan iteratieve methoden, bijvoorbeeld de Krylov-deelruimtemethoden met geschikte preconditionering om de robuustheid, snelle convergentie en nauwkeurigheid van de uiteindelijke benaderende oplossing te garanderen.

Preconditioneerders die vaak worden bepleit zijn standaard additieve Schwarz domein-decompositie, multigrid met agressieve verruwing en sterke gladstrijkers (bijv. ILU), en 'blok-preconditioneerders' die een benaderende blok-LU-factorisatie en een benadering van het Schur-complement geassocieerd met de druk-onbekenden gebruiken, bijvoorbeeld SIMPLEC, LSC en PCD.

Een andere klasse van Schur-complementmethoden wordt verkregen wanneer het interieur van geometrische partities (of subdomeinen) wordt geëlimineerd en een geschikte benadering van het gereduceerde systeem op de separator wordt geconstrueerd. In deze klasse van methoden stelden we een meerlaagse preconditioneerder voor de Navier–Stokes-vergelijkingen die gediscretiseerd zijn op een versprongen rooster. De resulterende operator werkt in de divergentievrije ruimte, waardoor de methode de zadelpuntstructuur van het systeem op een natuurlijke manier kan behandelen.

Na het berekenen van evenwichtstoestanden van de MOC zijn we geïnteresseerd in de gevoeligheid voor ruis. De gevoeligheid rond een evenwichtstoestand kan worden bepaald aan de hand van de kansdichtheid. Het is algemeen bekend dat deze kansdichtheid kan worden berekend uit de oplossing van een gegeneraliseerde Lyapunov-vergelijking. Directe methoden voor het oplossen van een gegeneraliseerde Lyapunov-vergelijking zoals het Bartels–Stewart-algoritme zijn gebaseerd op solvers voor volle matrices en zijn daarom niet toepasbaar voor grote systemen. Bestaande methoden die gebruik maken van benaderingen met een lage rang kunnen ook duur worden voor hoogdimensionale problemen, met name bij het gebruik van eerdere initiële schattingen langs een continuatietak. We ontwikkelden daarom een nieuwe methode voor het berekenen van de oplossing van gegeneraliseerde Lyapunov-vergelijkingen die bijzonder goed geschikt is voor ons oceaanprobleem in een continuatiecontext. De methode werkt door een Galerkin-type projectie toe te passen met de ruimte die is opgebouwd uit de eigenvectoren die behoren tot de grootste eigenwaarden van het residu in elke iteratie van de methode. Het belangrijkste is dat de methode kan worden herstart, wat zorgt voor minder geheugengebruik, snellere iteraties, en wat hergebruik van eerdere oplossingen toestaat. We hebben laten zien dat voor een geïdealiseerd 2D MOC-model onze methode de meest efficiënte methode is in termen van zowel geheugengebruik als tijd.

Een tekortkoming van deze aanpak is dat deze alleen de gevoeligheid voor ruis rond een evenwichtstoestand beschrijft. Om het meer globale fenomeen van transities tussen evenwichtstoestanden te bestuderen, is een stochastische tijdsintegratie nodig. Het toepassen van een standaard Monte Carlo methode is echter veel te duur, vooral voor hoogdimensionale systemen en wanneer de kans op een transitie klein is. Er bestaan meerdere methoden om dit probleem te omzeilen door een of andere vorm van resampling toe te passen. Om deze methoden te verbeteren, hebben we een geprojecteerde tijdstapmethode bedacht, die het geheugengebruik voor ons geïdealiseerde 2D MOC-model met 96% en het tijdsverbruik met 30% vermindert. We toonden aan dat de kans op een transitie drastisch toeneemt wanneer we dichter bij een bifurcatiepunt komen, en dat de geprojecteerde methode in staat is dezelfde resultaten te verkrijgen als standaardmethoden.

Omdat we alleen naar een geïdealiseerd 2D MOC-model hebben gekeken, kunnen we niet echt iets zeggen over de transitieskansen van de MOC in de werkelijke Atlantische oceaan, maar we hebben wel methoden ontwikkeld waarmee dit haalbaar wordt.

SOAMENVATTING

Klaainschoalege veranderlekhaid ien t klimoat kin grode effecten hebben op mondioale oceoancirculoatsie. Veurbeelden van zukke klaainschoalege veraanderns binnen schommelingen ien houveulhaid zuit wotter deur t smelten van t ies op Gruinlaand. Dizze schommelingen kinnen aanlaaiden wezen tot n òfnoame van haile globoale oceoancirculoatsie, wat op zien beurt òfkouln van n poar groad kin geven ien Uropoa. Om der achter te kommen houveul kaans wie moaken op zo'n klimoatomslag, mouten der berekens doan wòrren mit grootschoalege oceoanmodèllen. Jammer genog binnen bestoande rekentechnieken nait vlug genog en doarom mouten der nije technieken bedòcht wòrren. Ien dit proufschrift stellen wie drij veur. Eerste is n methode om grode systemen van vergeliekens op te lössen, twijde n methode om gevuileghaid veur schommelingen wied genog vot van t omslaggebied te bepoalen, en leste methode berekent waarkelke kaans op n klimoatomslag ien grootschoalege modèllen. Wie loaten zain hou dizze methoden waarken op n idealiseerd twijdimensionoal oceoancirculoatsiemodèl. Ien toukomst kinnen dizze methoden bruukt wòrren om echte omslagkaansen ien realistische drijdimensionoale klimoatmodèllen mit n hoge rezeluutsie te bereken. Veur n oetgebraaidere soamenvatting verwiezen wie joe geern deur noar Nederlandse soamenvatting.

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Welcome to the acknowledgments, which is very likely to be one of the very few parts of my thesis that you will ever read, maybe together with the summary. I do not mind this at all, since I am also guilty of this habit, especially when receiving a thesis that is unrelated to my field of research. For this reason, I also provide the summary not only in Dutch, as seems to be common, but also in English and Gronings.

First and foremost, I would like to thank my supervisor Fred Wubs. I do not think that any PhD student could ever wish for a better supervisor. You gave me full freedom to pursue my own interests, even if they did not fully overlap with your initial plans for this project, and were always interested in the progress that I made. And whenever I had any questions, you were there in your office, ready to answer them. I also enjoyed the travels we made together to conferences and to Jonas in Cologne, especially the cycling trip we made to Bonn and back.

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Curriculum vitae

Sven Baars was born on August 15, 1990 in Eenrum, The Netherlands. After completing his primary education in Eenrum, he attended secondary education at the Praedinius Gymnasium in Groningen. From 2008 to 2014 he was a student at the University of Groningen, where he obtained his bachelor's and master's degree (cum laude) in the field of numerical mathematics. During this time, he also did an internship at the German Aerospace Center in Cologne.

From 2015 to 2019, Sven was a PhD student at the university of Groningen in the group of prof. dr. ir. R.W.C.P. Verstappen under the supervision of dr. ir. F.W. Wubs. The topic of his research was numerical methods for studying transition probabilities in stochastic ocean-climate models.