Universiteit Utrecht

Faculty of Geosciences
Department of Earth Sciences

Review of the PhD thesis:
"A numerical study of subduction zone dynamics using linear viscous to thermo-mechanical model setups including (de)hydration processes" by Matthieu Quinquis.

This thesis deals with numerical modelling experiments of convective flow in the Earth's mantle. Numerical modelling has developed into a major tool in geodynamics where a main application has become the testing of conceptual ideas about dynamical evolution scenario's based on geological and geophysical observations.

An important part of the thesis work has been the validation of modelling outcome by critical comparison of the results of alternative approximations for the physical boundary conditions. This is the focus of Chapter 3 that has been published in *Tectonophysics*. Here an important result is obtained in the conclusion that an Eulerian spatial grid with a free-slip impermeable top surface can be applied succesfully when combined with a thin weak top layer mimicking a basaltic oceanic crust. It is shown that results modelling the evolution of subducting lithospheric slabs in this way compare well with those of more complex models including a stress free top surface. This is an important finding that jusitfies the application of the simpler Eulerian models.
Validation of complex geodynamical modelling methods was further obtained in a bechmark comparison for an oceanic subduction model with complex non-linear rheology. This is the subject of Chapter 4 where a series of models of increasing complexity are investigated. The results of up to 7 different authors that apply different numerical methods are compared here. It is found that differences in the results are small and mainly occur in the early and final stages of the subduction sequence, when the effects of mechanical interaction of the lithospheric parts or the impermeable bottom boundary are maximum.
Chapter 5 deals with subduction models including the effects of both free and bound water on the viscous rheology. Maximum bound water content is modelled by using pressure,temperature tables calculated by thermodynamic modeling methods. Several transport schemes for free water are compared here and results indicate that these produce basically similar results. Another important finding is that although significant the effect of the water distribution on dynamics of the mantle wedge is small. The results of this chapter have been published in *Solid Earth*.

In summary this thesis represents a significant contribution to the field of Geodynamics. The results of the various investigations will be helpful for subsequent model development by the broader geodynamics community. With this work the author has demonstrated his ability to do creative scientific work and I therefore recommend that it is accepted as a PhD thesis.

Below is a list of comments and questions concerning the thesis that I would like to be discussed by M. Quinquis during the defence. These are mainly aimed at exploring possible implicationts of choices in the model representations and opportunities for future extensions and applications of the methods presented.

1. *Question on aspects of mechanical boundary conditions*
   Chapter 3 of your thesis is devoted to an investigation of the role of boundary conditions on the results of numerical modelling. A particularly useful outcome of your work comes from comparing the dynamic effect of a stress free surface, implemented with a moving boundary, with an approximate model applying an eulerian computational grid with a free-slip impermeable top surface. You have shown that including a weak basaltic crust in the eulerian model will

produce very similar dynamics as in the more complex model with stress-free moving boundary. You consider two types of models in Chapter 3: the first type has closed, free-slip, lateral boundaries, the second type has a prescribed fluid flux on one of the two lateral boundaries while the opposite boundary is closed. Uniform inflow of 5 cm/yr is prescribed at lithospheric levels (depth $<$ 100 km). Zero fluid-flux is obtained by balanced (sub-lithospheric) uniform outflow. A thin transition (10 km or 5 elements) between in-outflow boundary segments to smoothen the vertical profile of the flow (page 42).
An alternative way of approximating open boundaries was investigated by (Chertova et al., 2012). They use so called *fully developed flow* conditions, corresponding to a 1-D approximation with a zero normal component of the velocity gradient. This is a more flexible condition that allows for example the boundary in-out flow to adapt to changing dynamical conditions. **Could you discuss the differences between your approximation and the approach followed by (Chertova et al., 2012). Do you expect any differences in the subduction dynamics between both approaches?**

2. *Questions on the choice of approximation in the model equations*
You use the standard Boussinesq approximation (BA) in your thermal convection models, instead of the so called extended (EBA) approximation (Steinbach et al.,1989, Ita and King, 1994). As a consequence terms describing heating due to adiabatic (de)compression and viscous dissipation are dropped from the energy transport equation.

   - In particular the effect of adiabatic heating seems important in modelling thermal evolution of subducting lithospheric slabs. This may cause a temperature increase of over 100 K in a slab sinking through the upper mantle. In your work you have compensated for the absence of adiabatic heating in the energy equation by enforcing a pseudo-adiabatic temperature gradient by specifying a high value for the thermal conductivity (Pysklywec and Beaumont ,2004). Your choice of k $100 \mathrm{Wm}^{-1}\mathrm{K}^{-1}$, is about 20-30 times higher than expected values for a representative mineralogy under upper mantle conditions.
This approach implies replacing an equilibrium thermodynamic process, heating by adiabatic compression, by the non-equilibrium process of thermal diffusion. This introduces characteristic thermal diffusion time scales that seem relevant when modelling thermal evolution of slabs.
Could you discuss the impact of this artificial conductivity method in your results of thermal modelling?
   - An other implication of the Boussinesq model is the assumption of incompressibility of the medium. Together with a constant gravity acceleration this implies the use of a constant gradient of the lithostatic pressure.
In Chapter 5 of your thesis you model the effects of dehydration on subducting slabs. Here you apply a mineral phase diagram and a corresponding 2-D pressure-temperature table of the maximum weight fractions of bound water. This table has been calculated thermodynamically for assemblages of compressible mantle silicates, with a phase dependent density corresponding to a non-uniform pressure gradient.
What impact do you expect on your results from the 'pressure-mismatch' between Boussinesq models based on a uniform pressure gradient and thermodynamically consistent P,T tables?

- In the description of your application of the incompressible Boussinesq model (Chapter 2, p.19) you assume a zero Eulerian time derivative of the density. While you refer to the implied neglect of density variation due to thermal expansion (except in the buoyancy) you do not consider compositional density variation here. At the same time composition dependent density contrasts of several percent occur in your models equivalent to large temperature contrasts of around 1000 K.
  Could you discuss how the compositional density variations in your models can be reconciled with the proper continuity equation for the Boussinesq-approximation?

3. *Questions concerning models including effects of water*
   In Chapter 5 you deal with the effect of water on the dynamics of subduction models through the impact of water on the viscosity of mantle rock material and you show the effect on the convection dynamics of the mantle wedge to be small but non-negligable.
   Could you speculate on the possible further extension of your 'water model' so that it will become applicable to assess the details of the effect of water on the distribution of partial melting?
   This seems relevant because of the importance of partial melting and on the impact of water on the melting phase diagram of mantle silicates.
   Could you discuss what will be needed for such a model extension in your computer codes?

4. *Questions concerning the implementation of thermodynamic data in the models*
   Three different lithologies are considered in the modelling: Bulk Oceanic Crust (BOC), Serpentinized Harzburgite (SHB) mantle and pyrolitic mantle peridotite, each characterized by a unique mineral assemblage with contrasting material properties like density and water solubility.
   In a convecting mantle system mechanical mixing will occur and in the numerical model this may be reflected in the mixing of tracer particles near the lithological boundaries. The physical effect of this mixing can be accounted for in model calculations by using proper expressions for effective material properties like density and water content.
   Could you discuss how such mechanical mixing is accounted for in your convection model dealing with density and water solubility?

Finally I would like to pass my congratulations to Matthieu for the accomplishment of his doctoral thesis and wish him succes in his further career.

Utrecht, October 31, 2014

Dr. A.P. van den Berg
Dept. Theoretical Geophysics
Institute of Earth Sciences
Utrecht University
Budapestlaan 4
3584 CD Utrecht
The Netherlands