

Workshop Report: Implementing Solvers in CitcomCU and CitcomS

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1 Overview

Members of the [Computational Science Working Group](#) recently organized a small workshop on implementing solvers in CitcomCU and CitcomS. The goal was to have members of the CIG Computational Science Working Group meet with CIG staff and several members of the mantle convection community to address specific avenues for furthering the solver capabilities of several CIG community codes, with a focus on CitcomCU and CitcomS in particular. The workshop was a combined onsite and virtual meeting hosted at the CIG facilities on the UC Davis campus, September 16-17, 2013. Approximately 16 participants attended, with 11 people onsite and 5 connecting through Adobe Connect. A group size of less than 20 was targeted, as the goal was to have a hands on meeting with ample time spent in the code and focused code implementation. The list of participants and workshop agenda is included in Section 4.

This meeting was motivated by the need for more robust solvers in mantle convection codes, so that the computational software keeps pace with the increasing complexity in the science and the advances in hardware and computational facilities. For example, previous work has shown that large viscosity variations occurring over short distances pose a challenge for computational codes, and models with complex 3D geometries require substantially greater numbers of elements, increasing the computational demands ([Moresi and Solomatov, 1995](#); [Moresi et al., 1996](#); [Tackley, 1996](#); [May and Moresi, 2008](#); [Geenen et al., 2009](#); [Burstedde et al., 2009](#); [Jadamec and Billen, 2010](#); [Furuichi et al., 2011](#); [Jadamec et al., 2012](#)). In addition, for complex time-dependent problems, the computational runs often face temperature overshoots. Thus, there are immediate computational challenges facing the mantle convection community in terms of the capabilities of the Stokes solvers and solver for the energy equation.

Therefore, this workshop was convened to gather both computational scientists and several members of the mantle convection community to work out the details of the specific code modifications that would be required. This work session follows from goals identified in the workplan, “Prioritized List of Proposed Work Related to CitcomS/CitcomCU”, that was drafted in September 2012, and compiled by the [Mantle Convection Working Group](#). A copy of the workplan is attached as Appendix A.

2 Outcomes

The workshop comprised of two days of short presentations, with the presentations followed by lengthy discussion, and examination of the CitcomCU and CitcomS source code. The three primary categories covered were the Stokes Solvers, the energy equation solver, and mantle convection/subduction benchmarks. The implementation of the energy equation solver in the CIG supported code Aspect was also discussed at length. The workshop outcomes are described in the sections that follow. See Section 4 for the meeting agenda.

2.1 Stokes Flow

Margarete Jadamec presented an overview of the scientific drivers and motivation for increasing the solver functionality in CitcomCU and CitcomS. She showed results from her recent study optimizing the full multigrid parameters in CitcomCU for 3D subduction models with a non-Newtonian viscosity, and hence large viscosity variations ([Jadamec et al., 2012](#)). Improvements on runtime by up to 30% were achieved, which is significant for models run on hundreds to thousands of cores

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(Jadamec et al., 2012). In addition, the initial code performance and sensitivity results for Citcom from Moresi and Solomatov (1995) and Moresi et al. (1996) for models with large viscosity variations were summarized. Shijie Zhong presented a review of the Citcom, CitcomCU, and CitcomS architecture and a description of how the Stokes flow problem is solved including the pressure equation and the conjugate gradient method and the Uzawa algorithm which uses the geometric multigrid on the inner solve (Moresi and Solomatov, 1995; Moresi et al., 1996; Zhong et al., 2000; Zhong, 2006; Zhong et al., 2008). Recommendations for improvements were suggested including using a non-linear solver for better convergence, improving the Stokes solver for models using weak zones, and improving the energy equation to reduce the overshoot problems.

2.1.1 Nonlinear Solvers

Matt Knepley discussed the inclusion of a nonlinear solver in Citcom. Nonlinear solvers, such as Newton’s method, perhaps preconditioned with the nonlinear Generalized Minimum Residual Method (NGMRES), could greatly improve the convergence for difficult viscosity distributions, such as those seen in subduction models (Jadamec and Billen, 2010). A trial implementation is available on Bitbucket which used PETSc. A model of the data distribution in Citcom was made using the PETSc DMDA class, which handles Cartesian grids, so that the communication pattern could be replicated. Then a routine was added to calculate the full residual, for velocity and pressure. This residual routine could be used by the PETSc SNES solver for nonlinear equations. In future work, an analytic Jacobian routine could also be added, although PETSc currently uses graph coloring to construct one automatically. There appeared to be a small discrepancy between the boundary values on different processes during the Citcom linear solve, and during the nonlinear solver update, which is being investigated.

2.1.2 Linear Solvers

Dave May presented his work on robust solvers for the variable viscosity Stokes equation, which is summarized in May and Moresi (2008). He showed a series of benchmarks, culminating in a challenging problem with many small sinking blocks. He showed that a stable element is necessary for the Schur complement to have a condition number independent of the system size, meaning that the number of linear solver iterations can remain constant with increasing system size. Details of stable element types, both macro elements and the stabilized element mentioned by Shijie, are given in Elman et al. (2005). It also contains a large amount of information about Krylov methods and block preconditioners for Stokes. The spectral equivalence between the pressure Schur complement and the scaled mass matrix is proved in Grinevich and Olshanskii (2009). Moreover, using a scalar multigrid solve on each component of the Stokes system, while fine for the iso-viscous case, show notable growth in the number of iterations for these complex variable-viscosity test cases. This kind of component-split preconditioning is used in both Rhea (Burstedde et al., 2009) and Aspect (Kronbichler et al., 2012), which therefore do not solve the variable viscosity problem scalably.

Rajesh Kommu presented his work on introducing PETSc into CitcomS. He put a wrapper around the vector and matrix data structures with PETSc Vec and Mat objects, which then allowed the PETSc linear solvers to be used. He has replicated the existing Citcom linear solver using PETSc classes. Since all PETSc configuration is done dynamically, at runtime, solver optimization should now be possible without much more effort. However, improvements are limited by the current discretization scheme, and scalability is limited by the current parallel communication scheme. We discussed the changes necessary in order to implement these scalable Stokes solvers in Citcom. It would involve a substantial rewrite in that all the element routines would have to be changed, which would mean also changing all the parallel code. Thus, the end product would be largely a completely new code. A possible alternative would be addition to the code used by Dave May to accommodate Citcom input and produce Citcom output.

2.2 Energy Equation and Composition

The challenges for the energy solver in the mantle convection codes, CitcomCU, CitcomS and Aspect were discussed. In particular, the problems for temperature dependent viscosity with oscillations and overshoots. There was a discussion of monotone integrators and the problems with the current discretization for the diffusion equation. Gerry Puckett and student Ted Studley presented work on the energy equation in Aspect. The possibility of working on a general solution for the problems with the energy solver in both CitcomCU/S and Aspect was recommended, as there are commonalities for the implementation in both codes.

It was agreed that it was important to formulate a discontinuous space in which finite volume or DG methods could be used. Gerry and Ted were interested in pursuing the use of monotone FV methods defined on embedded subgrids. Recent methods for positivity- and maximum principle-preserving limiters for DG and (W)ENO methods are also available (Zhang and Shu, 2011). A modest amount of refinement (internal to Stokes elements) appears to be computationally affordable and may be important to resolve fine-scale features over the domain, though a transport method that is nominally higher than second order is also likely to be important. In case of a Cartesian grid, (W)ENO methods with limiters are straightforward to implement and the action of the limiters is more localized than with high-order DG. With all these methods, it is important

to have a velocity field that is discrete divergence-free, otherwise overshoots can arise even for the exact solution of the transport equation. This can be achieved by using a discontinuous pressure space in the Stokes solve.

As an advection-dominated process (high cell Péclet number), the energy equation is very similar to methods for tracking composition, for which particles are popular. We discussed whether field-based methods could be used for composition, as an alternative to the challenges of using particles. Moment of Fluid methods (Schofield et al., 2010) have been enjoying popularity lately, though they are complicated to implement and the computational cost depends on the factorial of the number of materials in a given cell. Several participants stated that most science could be accomplished with two or perhaps three materials, although others wanted at least ten. Since it is unlikely that many materials would be present in the same cell, moment of fluid methods appear to be viable, though nobody has leapt to the task of implementing. The alternative of simply using a monotone transport scheme (a strict maximum principle is crucial) was discussed, though it would require a filter to ensure that the fractions of all materials sum to 1 and would require increased subgrid resolution to control numerical diffusion.

2.3 Benchmarking and Uncertainty Quantification

As several options for implementing solver flexibility into the CitcomCU and CitcomS codes were presented, each varying in the degree of modifications of the existing source code, the topic of benchmarks was discussed. The importance of adequately benchmarking the individual codes as changes occur was emphasized as well as options for benchmarks across codes to compare code performance and usability. In particular, two kinds of benchmarks were highlighted: (a) benchmarks for accuracy in geophysical problems and (b) benchmarks for scaling. Shijie Zhong gave a presentation summarizing the benchmarking results for CitcomCU and CitcomS. Specifically, a series of benchmarks for CitcomCU are given in Zhong (2005, 2006), and Zhong et al. (2000, 2008) contain benchmarks for CitcomS, including scaling information for models run on up to 3072 cores run on Ranger. In addition, a benchmark comparison for six mantle convection codes is given in King et al. (2010) and subduction benchmarks are given in van Keken et al. (2008). Pierre Arrial presented recent work on benchmarking a new mantle convection solver in collaboration with Louise Kellogg and the group at NCAR. In addition, Matthew Knepley suggested the exact solutions from Mirko Velic at Monash University.

With models increasing in complexity and grid size, the group discussed obtaining scaling information for up to 10K cores or larger 50K or 100K(?). It was recommended to start with the benchmarks from Zhong (2006) and Zhong et al. (2008). In addition, it was recommended to generate a new benchmark for a 3D subduction model with large viscosity variations, although this would be difficult to test for accuracy without an analytic solution, but would be useful for comparison of code performance. The general agreement was to start with about 5 benchmark cases, consisting of a few Stokes solver cases for convection and a couple temperature dependent viscosity cases for testing the energy equation.

Jed Brown presented the advantages and several approaches to better constraining the uncertainty of the convection solutions, quantification of the fit between model predictions and observational constraints, and quantifying the information value of different types of observations. This was agreed as an area of important research in the convection community, especially with the wealth of observational data now being acquired. It was emphasized to keep code modifications open, where possible, to further development in order to incorporate uncertainty quantification algorithms. The methods used by the seismic tomography community are seen as being relatively mature and worth emulating where possible, though this is challenging since the models are nonlinear and data sources relevant to mantle convection and subduction are more diverse and tend to have poorly-understood and/or poorly-documented errors and correlations.

3 Summary

It was recommended to pursue the two levels of code modifications to improve the Stokes solvers in CitcomCU and CitcomS. Rajesh Kommu and Eric Heien will continue the implementation of solver functionality without changing the CitcomCU and CitcomS internal data structures. Matt Knepley and Margarete Jadamec will explore the degree of code modifications required in changing the internal data structures and testing its implementation. Shijie Zhong will consult on this effort. Contributions from other members of the mantle convection group/community are welcome. Advantages of not changing the CitcomCU/S data structures included that users want to default to the old code, may not want to read the new code, and do not want to change the build system. Advantages of the deeper level code changes are the flexibility of interchanging solvers because, it was discussed that the experience with the codes thus far has shown that different solvers are optimal for different kinds of scientific problems. Thus, the less intrusive changes are limited in that sense. However, with the changes required to convert the data structures in CitcomCU/CitcomS to take advantage of the PETSc solver options, it may be worth exploring using Dave May's new code for very complex rheological problems. There is no answer for which is best.

It was recommended that the Ted Studley and Gerry Puckett pursue the work on the energy equation in Aspect with cognizance of how to extend the modifications to the energy solver implementation in CitcomCU and CitcomS. This work will be done as a part of CIG in collaboration with Wolfgang Bangerth. Jed Brown and Matt Knepley will be available to consult on the solver options.

It was recommended that the benchmarking cases (~ 5) be identified by the 2013 Fall AGU meeting or in the early spring of 2014.

It was recommended to convene online meetings monthly or every fortnight during the fall of 2013 and assess/discuss progress on the code implementations. It was also recommend to meet in person at the CIG Business meeting at the AGU Fall 2013 meeting in San Francisco.

A temporary code repository was set up on Bitbucket that will be migrated to the CIG hosted repository. In addition, it was recommended to move the main CIG CitcomCU and CitcomS repositories to Git due to the improved functionality of Git over the older SVN method for version control.

4 Workshop Information: Participant List and Workshop Agenda

Attendees

- Katrina Arrendondo (UC Davis)
- Pierre-Andre Arrial (CIG)
- Jed Brown (ANL/PETSc)
- Adam Holt (USC)
- Eric Heien (CIG)
- Lorraine Howang (CIG)
- Margarete Jadamec (Brown Univ.)
- Louise Kellogg (UC Davis)
- Scott King (Virginia Tech., via email)
- Rajesh Kommu (CIG)
- Matt Knepley (Univ. Chicago, CIG, PETSc)
- Dave May (ETH)
- Gerry Puckett (UC Davis)
- Alex Rice (Univ. Hawaii)
- Ted Studley (UC Davis)
- Matt Weller (Rice Univ.)
- Shijie Zhong (CU Boulder)

Implementing Solvers in CitcomCU and CitcomS

Workshop at UC Davis, Sept. 16-17, 2013

Organizers: [Margarete Jadamec](#) and [Matthew Knepley](#)

Workshop Agenda

Time (Pacific Time Zone)	Session	Monday, Sept. 16 th : CitcomCU	Tuesday, Sept. 17 th : CitcomS
9:00 a.m. - 9:40 a.m.	Talks	Getting Started with CitcomCU: Science Drivers: M. Jadamec Perspective from CIG: L. Kellogg Architecture and Algorithms: M. Knepley	Solvers in CitcomCU and CitcomS: Block Solvers and Multigrid for Citcom: D. May Implementation in CitcomS: R. Kommu Work on Energy and Aspect: Ted Studley
9:40 a.m. - 10:00 a.m.	Discussion	Getting Started with CitcomCU: Discussion Leader: S. Zhong	Commonalities in CitcomCU & CitcomS: Discussion Leader: D. May
10:00 a.m. - 12:30 p.m.	Work Session	Delving into CitcomCU/S, Stokes Solvers: Work Session Leader: M. Knepley	Citcom, Aspect and Energy Solvers: Work Session Leader: Gerry Puckett
12:30 p.m. - 2:00 p.m.	Lunch	Walk to Silo and/or Memorial Union	Walk to Silo and/or Memorial Union
2:00 p.m. - 2:20 p.m.	Talks	Simulation Workflow and Analysis: Applications and Benchmarking: S. Zhong Inv. Problems & Uncert. Quantification: J. Brown	CitcomCU, CitcomS Development Plans: Mantle Convection Benchmarking: Pierre Arrial CitcomCU Workplan: M. Jadamec
2:20 p.m. - 3:00 p.m.	Discussion	Simulation Workflow and Analysis: Discussion Leader: J. Brown	Extending CitcomCU and CitcomS Discussion Leader: M. Jadamec
3:00 p.m. - 5:30 p.m.	Work Session	More time in the CitcomCU Code: Work Session Leader: M. Knepley	Round Table Discussion: Work Session Leader: M. Knepley
5:30 p.m. - 7:00 p.m.	Dinner	Dinner in downtown Davis	Dinner in downtown Davis

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Prioritized List of Proposed Work Related to CitcomS/CitcomCU

This document is a request from the Mantle Convection Working Group and members of that community for CIG to dedicate programmer resources to improving the Stokes solver and energy solver in CitcomS/CitcomCU. The details in this document and attached documents are included as a starting point for the software engineers/programmers in determining the best approach to take. Suggestions are provided, as well as names of researchers to include in discussions before a solution is agreed upon and implemented. These researchers are also willing to help develop appropriate benchmarks and test cases for the new solvers.

This document was prepared with input by:

- Shijie Zhong (U. of Colorado, Boulder)
- Scott King (Virginia Tech)
- Thorsten Becker (USC)
- Clint Conrad (U. of Hawaii)
- Allen McNamara (ASU)
- Garrett Ito (U. of Hawaii)
- Margarete Jadamec (Brown Univ.)
- Magali Billen (UC Davis)
- Eh Tan (Institute for Earth Sciences, Taiwan)
- Tobias Hoeink (Rice University)
- Wei Leng (Caltech)
- Louis Moresi (Monash Univ.)
- Matt Knepley (ANL)
- Adrian Lenardic (Rice Univ)

A. Issue to be improved (in order of priority)

1. Stokes Solver:
 - a. Pre-conditioner: relatively slow convergence as viscosity contrast increases, or dynamics or geometry becomes more complex.
 - b. Non-linear rheology: relatively slow convergence as viscosity contrast increases or model includes more geometric complexity.
2. Energy solver:
 - a. Temperature overshoots occur when advection is strong.
3. Add checking for correct/consistent parameter usage (e.g., multigrid mesh size)
4. New more realistic and illustrative cookbook/tutorial problems

We would like to emphasize that these improvements need to be done in such a way as to preserve the ability to use the current solvers, and are therefore implemented as input file options. In addition, as you will see from the attached e-mail discussion, there is some apprehension in the community about using PETSc, mainly stemming from worries that the code might be difficult to compile on different systems, however others have found that this is not an issue. We also see that implementing the Stokes solver suggested here using PETSc will open up the door to experiment with other solver/preconditioner options, and its important for the programmers to keep these possible future uses in mind.

B. Technical details for current solver implementation in CitcomS/CitcomCU.

Stokes Solver:

- Uses Q1P0 element is used.
- local stiffness matrix and local divergence matrix are assembled in each process.
- local preconditioner is computed in each process.
- global Stokes problem is solved by the Uzawa iterations, a Conjugate Gradient type iteration preconditioned with the local preconditioner.
- Within each iteration:
 - whenever a vector in the velocity space (ie. the velocity residual, the velocity solution, gradient(pressure), ...) is updated, communication with neighboring processes is required.
 - inversion of the stiffness matrix is done by a custom MG solver, which has custom projector and injector, and a custom Gauss-Seidel-type smoother.
 - Jacobi iteration is used for the boundary nodes, while Gauss-Seidel is used for the interior nodes.
 - every Gauss-Seidel iteration requires a communication with neighboring processes.
- For non-linear rheology (depends on the velocity through the stress or strain-rate)
 - Solved with a Picard iteration
- See also references listed below.

Energy Solver:

- Uses a streamline upwind Petrov-Galerkin (SUPG) Formulation
 - The same elements as for the Stokes' flow equation.

Relevant publications and technical issues:

- Moresi & Solomatov, Phys. Fluids, 1995, for the first 2-D Cartesian Citcom variable viscosity calculations, 2-D Stokes' benchmark, and general Uzawa algorithm.
- Moresi & Gurnis, EPSL, 1996, for the first 3-D Cartesian Citcom calculation.
- Moresi, Zhong & Gurnis, PEPI, 1996 for extensive 2-D Stokes' benchmarks using 2-D Cartesian Citcom.
- Zhong, Gurnis and Moresi, JGR, 1998, for the first MPI-parallel version of 3-D Citcom and the first 2-D and 3-D calculations using non-linear rheology.
- Zhong et al., JGR 2000 for the first description of spherical shell convection code CitcomS (mesh, parallel, consistent projection, and full multi-grid).
- Zhong, JGR 2006 for extensive benchmark calculations in 3-D Cartesian and regional spherical models using CitcomCU.
- Zhong, Yuen & Moresi, Treatise on Geophysics, 2007 for detailed descriptions of Uzawa and SUPG algorithms used in Citcom family of codes.
- Zhong et al., G-cubed, 2008 for extensive benchmark calculations using

CitcomS.

C. Suggested Modifications to CitcomS/CitcomCU

Stokes Solver and Preconditioner

- a. Suggested change:
 - i. Implement modified preconditioner following Dave May's implementation using PETSc
- b. Some notes from the e-mail discussion (see appendix):
 - i. Dave May has a modified version of CitcomS (called CitcomSX) which implements the modified preconditioner using calls into PETSc FieldSplit preconditioner.
 - ii. See attached document from Dave May providing overview of CitcomS and provides very useful perspectives on how to improve the Stokes Solver, and limitation.
 - iii. Knepley: In order to convert the linear solver, you would replace the communication in assembly with a PETSc VecScatter, and you would assemble the full residual and Jacobian, rather than the pieces. FieldSplit would pull apart the pieces it needs for the given solver. The MG can be wrapped in the PCMG preconditioner exactly the same way that we wrap up ML from Sandia.
- c. Testing and Benchmarks:
 - i. Efficiency of new methods can be demonstrated by comparing with the existing CitcomCU/CitcomS code by computing the same problems with variable viscosity.
 1. Zhong et al. (G-cubed, 2008) has some large viscosity contrast cases for a full-earth mantle convection (e.g., cases A9 or B9 in Table 5 with 10^7 viscosity variations).
 2. Billen and Jadamec (G-cubed, 2012) has some idealized, regional subduction cases with large viscosity variations.
 3. Jadamec and Billen (XSEDE Conference, 2012) also presents some nice convergence testing of the multigrid solver options using an idealized vertical slab and weak zone.
- d. Contact Researchers:
 - i. Magali Billen, Eh Tan, Margarete Jadamec and Shijie Zhong.

Stokes Solver and Non-linear Rheology

- a. Suggested change: modify the code to use a Newton solver.
 - i. At the CIG meeting, Matt Knepley suggested that this change to the solver could be done by modifying the code to use PETSc
 - ii. Recommend working with Matt to implement this change.
- b. Testing and Benchmarking:
 - i. Use 2D and 3D subduction models, which have had problem converging. Could also use model configuration in Billen and Jadamec, (G-cubed,

- 2012). These did not converge at all for larger viscosity variations given the element size.
- ii. Prepare cookbook/tutorial for these examples that teaches new users how to understand if their model is converging properly (how to interpret, understand convergence output).
- c. Contact Researchers:
- i. Magali Billen (and her group) has volunteered to help test this in CitcomS.
 - ii. Margarete Jadamec may be willing to test this CitcomCU as she has had problems with the solver.
 - iii. Shijie Zhong

Energy Solver.

- a. Suggested change:
 - i. Semi-Lagrangian Methods: these are effectively particle tracking schemes between two regular meshes that preserve the regularity of the mesh between time-steps (Speigelman and Katz, 2006). At each time step, a discrete set of particles arriving at the grid points is tracked backward over a single time step along its characteristic line up to its departure points. The solution value at the departure points is then obtained by interpolation (Staniforth and Cote, 1991; Xiu and Karniadakis, 2001). Advantages: does not have a CFL stability criterion allowing the time-step to be decoupled from spatial resolution. Is stable and can (depending on interpolation scheme) reduce interpolation artifacts for sharp features without introducing numerical diffusion.
- b. Testing and Benchmarks:
 - i. Comparing the existing CitcomS/CitcomCU for the same problems with strong advection (e.g., rapid plume rising or strongly temperature-dependent viscosity cases, e.g., cases A9 or B9 in Table 5 of Zhong et al., G-cubed, 2008)
 - ii. Billen's group also have some 2D subduction models which end up with temperature overshoots in front of the sinking slab and are currently using the filtertemp function to remove these.
- c. Contact Researchers:
 - i. Shijie Zhong, Magali Billen, OTHERs??

E. References

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