The Overshoot Problem in Mantle Convection Models

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CIG COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

Introduction and Background

The overshoot/undershoot problem in computational modeling is a numerical artifact that occurs in models of fields with sharp or discontinuous gradients.

Overshoot in a 2D FDM code for modeling advection causes the data to exceed its maximum T=1 and minimum T=0 values in the direction of advection, namely the positive x direction, v=(1,0) .

The overshoot problem is characterized by oscillatory behavior along sharp gradients, causing the data to exceed its maximum and minimum values.

Here we consider the overshoot problem in the finite element (FEM) mantle convection code **ASPECT** (**A**dvanced **S**olver for **P**roblems in **E**arth's **C**onvec**T**ion) as well as in a small finite difference (FDM) test code written explicitly to study the overshoot phenomenon. Both codes are available online upon request.

Overshoot in Mantle Convection Codes

Overshoot/umdershoot may occur in mantle convection simulation in a number of different situations. For example, models of subducting slabs or hot upwelling mantle plumes may result in the sharp gradients which cause overshoot.

While moderate (±9%) overshoot/undershoot may not be an issue for some codes, certain postprocessing techniques, such as melt calculations, rely nonlinearly upon certain values which may cause drastic differences in the exact and approximate calculated values if they fall outside of the appropriate range.

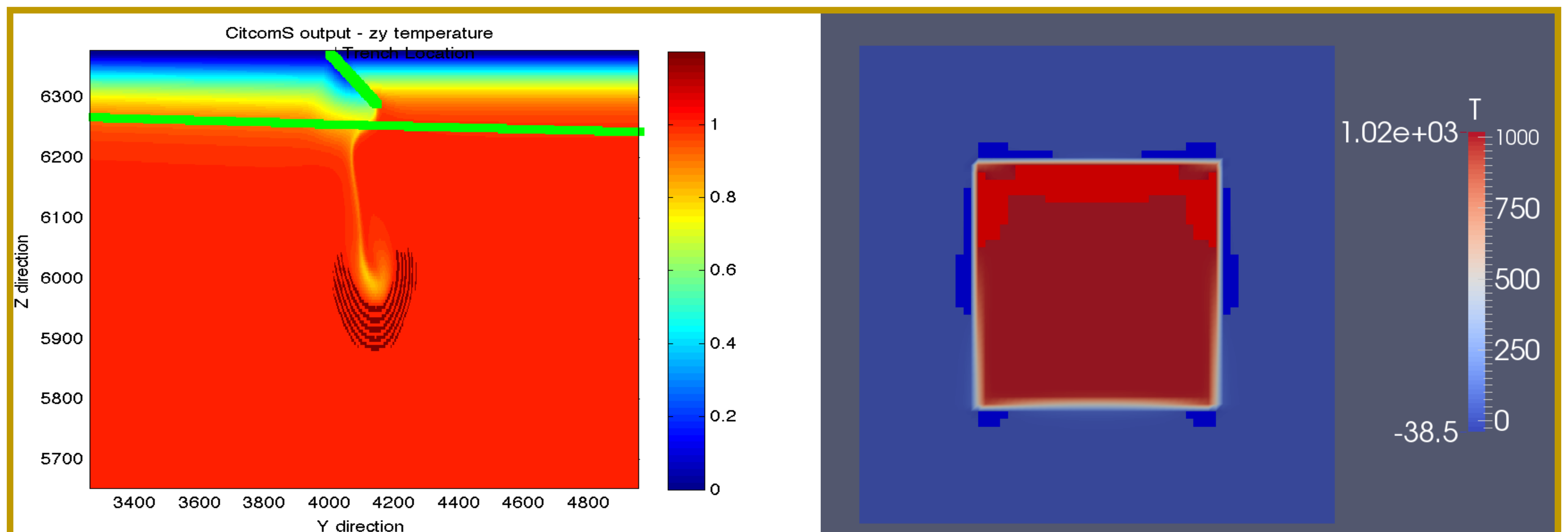
These effects have been observed in the FEM mantle convection codes ConMan, Citcom and ASPECT and will occur in any high-order accurate FEM mantle convection code. The overshoot/undershoot problem is an inherent problem in all high-order FEM and FDM methods. To the best of our knowledge, this issue has not be addressed within the mantle convection community.

Overshoot in Finite Difference Codes

We developed a simple FDM method for modeling 1D and 2D advection in order to study the effects of various numerical methods on the overshoot problem. Thus, our method approximates solutions of the advection equation

$$u_t + v \cdot \nabla u = 0 \qquad (1)$$

for the scalar u.



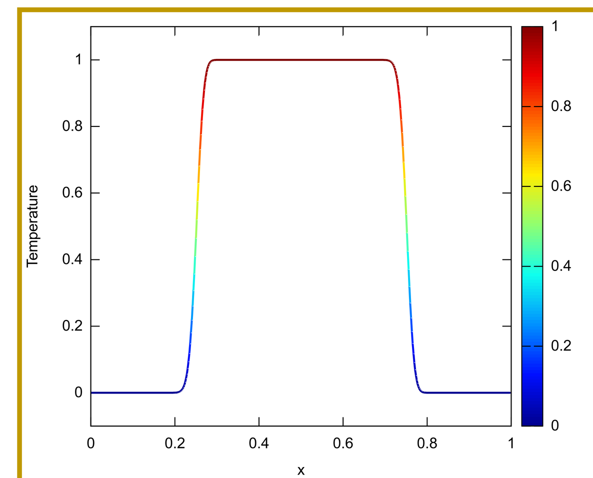
Examples of overshoot from CitcomS and ASPECT, two FEM mantle convection codes. Overshoot can be seen below a falling plume in a subducting slab simulation from CitcomS (left), causing a nonphysical oscillation that appears to "push" the colder falling material back upwards. The initial temperature was strictly between 0 and 1, and physically should remain so. In a simulation from ASPECT (right), a rising hot box-shaped blob has overshoot trailing the leading edge and undershoot along all sides of the blob. The initial temperature was strictly between 0 and 1000, and should remain between these values.

Given the temperature u_j^n at time $t^n = n\Delta t$ and position $x_j = j\Delta x$, we may discretize the 1D version of equation (1) with the first-order upwind method to obtain

$$u_j^{n+1} = u_j^n + \frac{v\Delta t}{\Delta x}\left(u_{j-1}^n - u_j^n\right) \qquad (2)$$

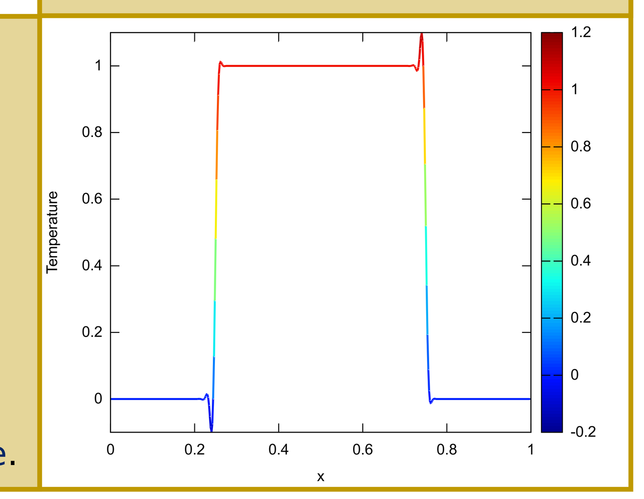
or the second-order Fromm's method to obtain

$$u_j^{n+1} = u_j^n + \frac{v\Delta t}{\Delta x}\left(u_{j-1}^n - u_j^n\right) + \left(\frac{v\Delta t}{2\Delta x} - \frac{v^2\Delta t^2}{4\Delta x^2}\right)\left(u_{j+1}^n - u_j^n - u_{j-1}^n + u_{j+2}^n\right) \qquad (3)$$



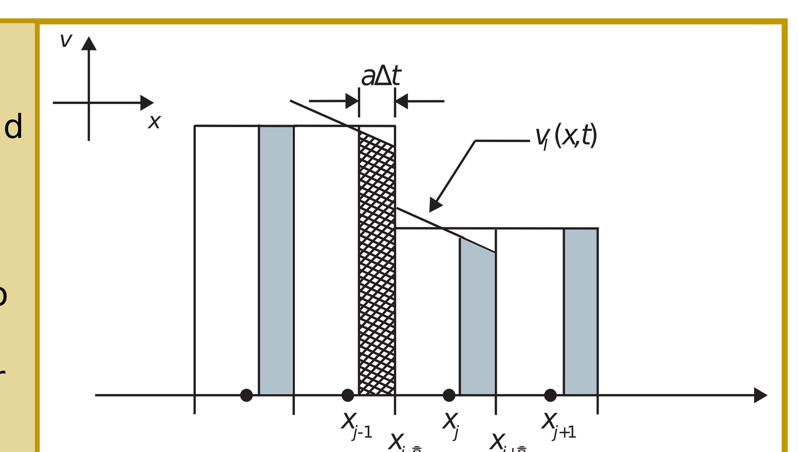
The upwind method does not overshoot, but has an only first-order rate of convergence, as evidenced by the rounded corners of the advected square wave. As a result, the computation requires a much finer spatial discretization to achieve the same level of accuracy as a higher-order method.

Fromm's method has a second-order rate of convergence, resulting in the sharper corners visible in this figure, but overshoots the maximum value u=1.0 and undershoots the minimum value u=0.0. In both plots, the initial conditions were a square wave with 256 subdivisions, advected in the positive x direction for one cycle.



The cause of the overshoot is directly related to the accuracy of the method. By Godunov's Theorem, all linear methods with second-order or higher accuracy will overshoot. In a first-order method, the flux is approximated to be constant across the width of each cell, whereas in a second-order method, the flux is refined using an additional linear term across the width of the cell. This linear term is the cause for the overshoot/undershoot, as it may over or under-estimate the flux along a cell containing a steep gradient.

The use of a piecewise linear flux approximation may lead to non-physical overshoots and undershoots along sharp gradients, due to the tendency of these approximations to over or under-estimate the flux across a sharp edge



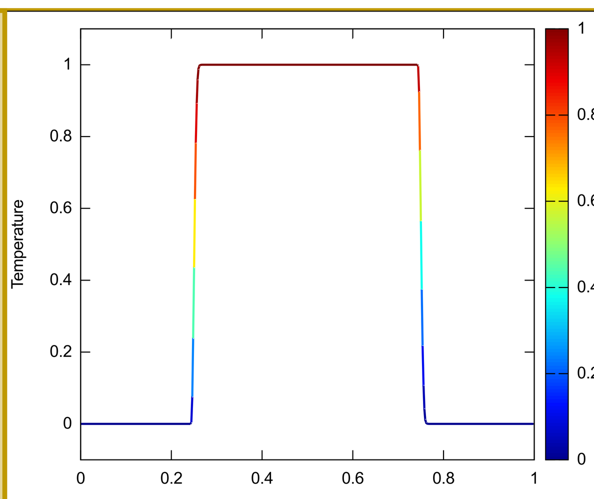
One way to address this overshoot/undershoot problem is to use a flux-limiter, which enforces the use of upwind (i.e., lower-order) fluxes in neighborhoods of sharp gradients in u and high-order fluxes (e.g. Fromm's Method) in smooth regions of u, since the Upwind Method does not overshoot near large gradients in u, while Fromm's Method is more accurate elsewhere.

To this extent, we arrive at a new solution to the problem, given by the equation

$$u_j^{n+1} = u_j^n + \frac{v\Delta t}{\Delta x}\left(u_{j-1}^n - u_j^n\right) + \left[\left(\frac{v\Delta t}{2\Delta x} - \frac{v^2\Delta t^2}{4\Delta x^2}\right)\left(u_{j+1}^n - u_j^n - u_{j-1}^n + u_{j+2}^n\right)\right]\phi(\theta_j)$$

Where θ_j is an approximation to the "smoothness" of the data at the point x_j and ϕ is a function which varies between 0 and 1 depending upon the value of θ_j. This yields an entire family flux-limiter methods depending upon the choice of θ_j and ϕ. Similar approaches have been successfully developed for Runge-Kutta Discontinuous Galerkin Finite Element methods (RKDG), although they have not yet been implemented in mantle convection codes

Fromm's method with Van-Leer flux limiters yields almost-second-order accuracy with discontinuous initial data, while preserving sharp corners much more accurately than upwind method. The initial conditions for this plot were the same as those shown previously.



Results and Conclusions

While the introduction of a nonlinear flux-limiting term is suficient to fix the overshoot problem in finite-difference codes, initial inquiries into a similar solution for finite element codes have been unsuccessful. To this end, we hope to approach the same resolution of the overshoot problem by using discontinuous Galerkin elements to prevent the same sort of over-estimation along sharp gradients that we have seen in the finite-difference case. For more information, see "Addressing the Overshoot Phenomenon in Geodynamic Codes" (DI31A-2199) by Rajesh Kommu.

For more information on ASPECT visit: www.dealii.org/aspect
For more information on CIG visit: www.geodynamics.org

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