The Overshoot Problem in Mantle Convection Models

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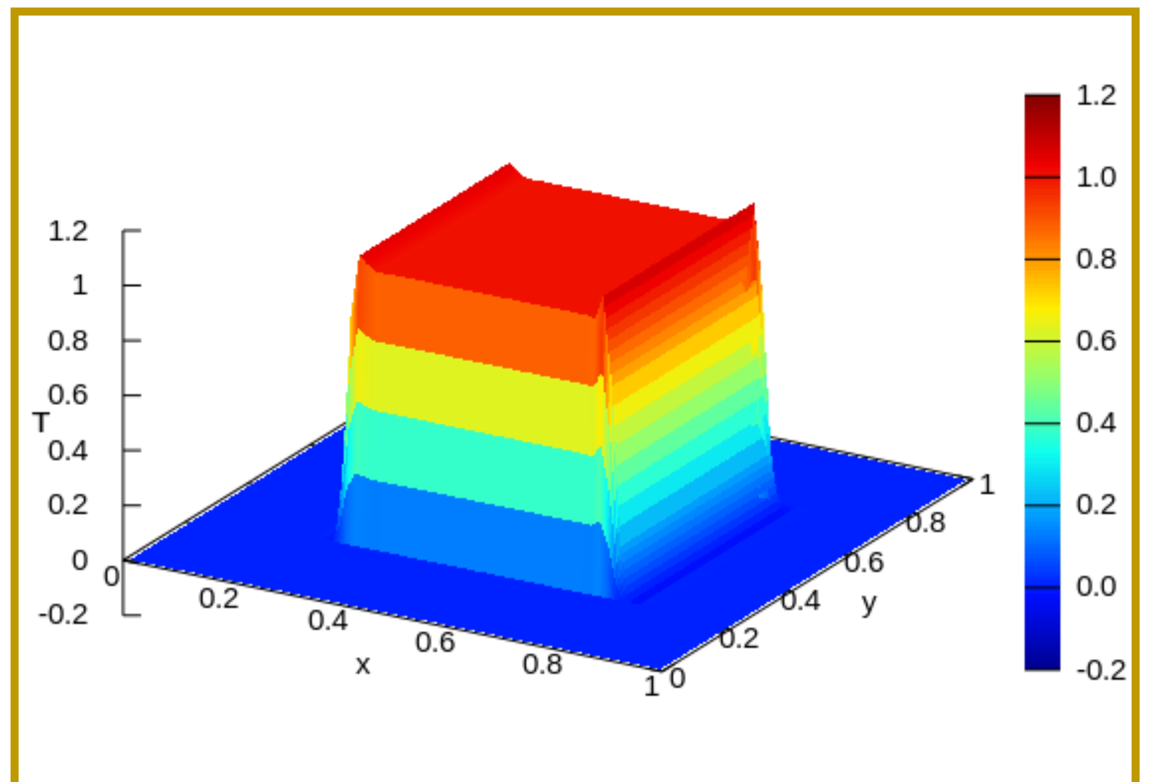
Introduction and Background

The overshoot/undershoot problem in computational modeling is a numerical phenomenon 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) .

Overshoot is characterized by oscillatory behavior along sharp gradients, causing the data to exceed its physically correct values.

These effects have been observed in the Finite Element (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 inherent to any high-order FEM or FDM method. To our knowledge, this issue has not be addressed within the mantle convection community.

Overshoot in Mantle Convection Codes

Overshoot/undershoot may occur in, 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 is not an issue for some scientific problems, certain postprocessing calculations, such as melt volume, are strongly sensitive to temperature, so that overshoot may cause drastic differences between the true and approximate values.

Overshoot in Finite Difference Codes

We developed a simple FDM code 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

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

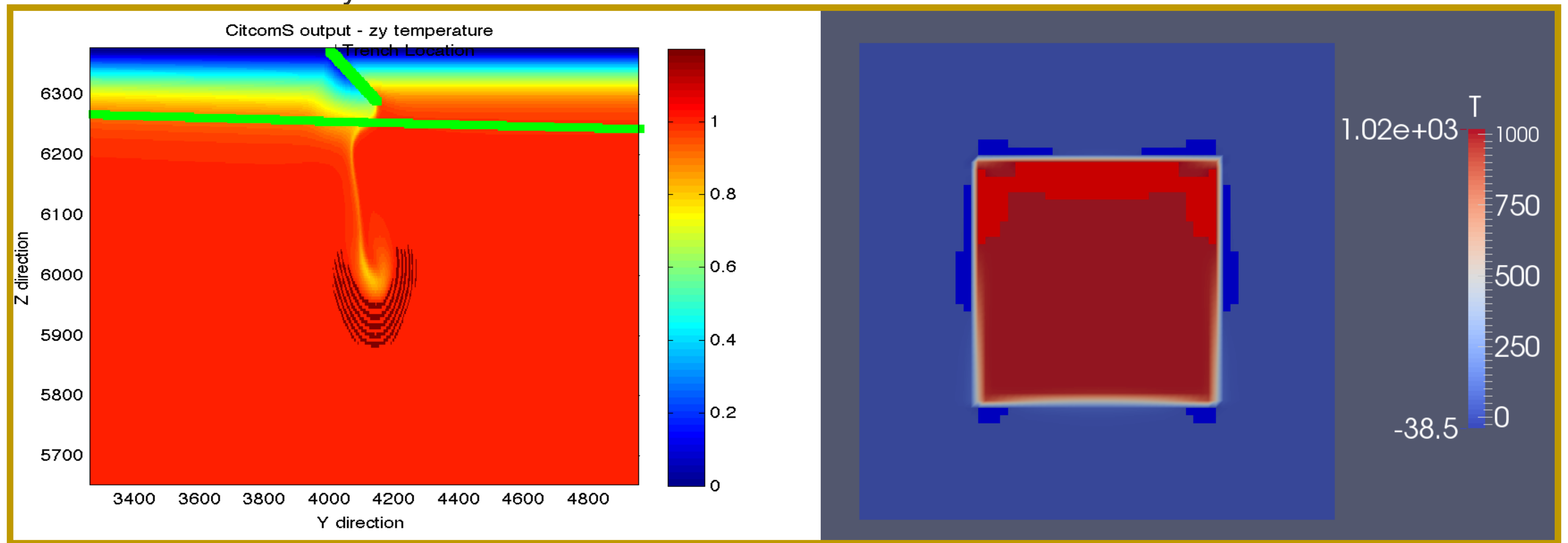
for the arbitrary scalar u.

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

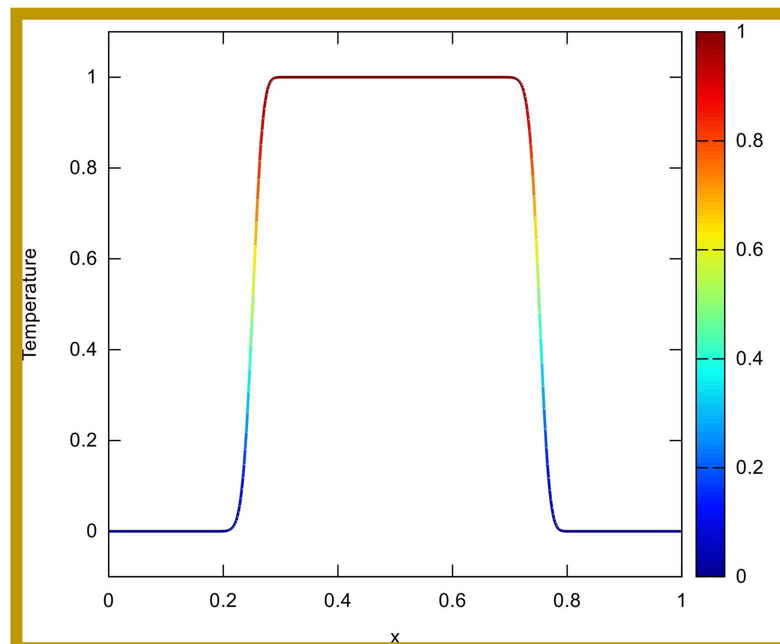
$$u_j^{n+1} = u_j^n + \frac{v\Delta t}{\Delta x}\left(u_{j-1}^n - u_j^n\right) \qquad (2)$$

or the second-order Fromm's method to obtain

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

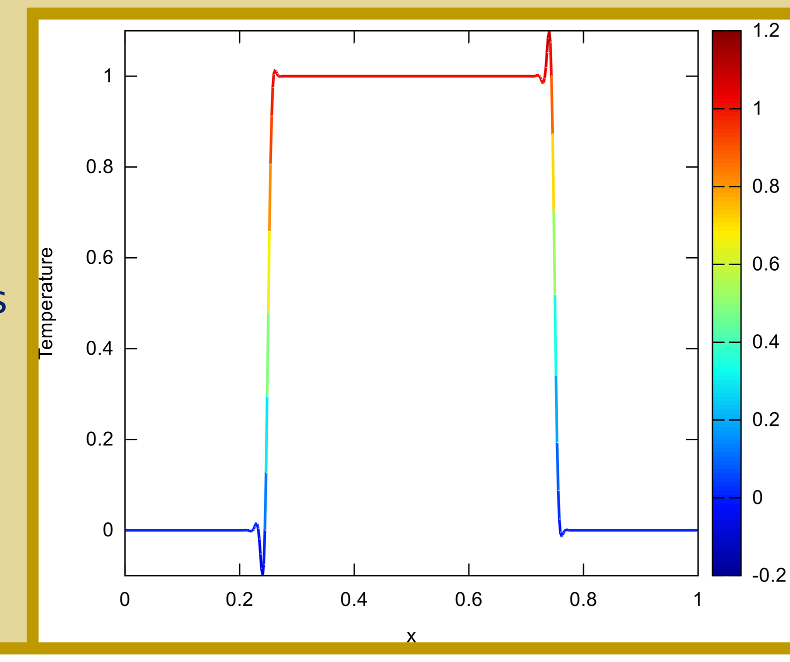


Overshoot/undershoot in CitcomS and ASPECT, two FEM mantle convection codes. Left: overshoot can be seen in a CitcomS model of a subducting slab, causing a nonphysical oscillation. The initial temperature was strictly between 0 and 1, and physically should remain so. Right: a rising hot square blob in ASPECT exhibits 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 so.



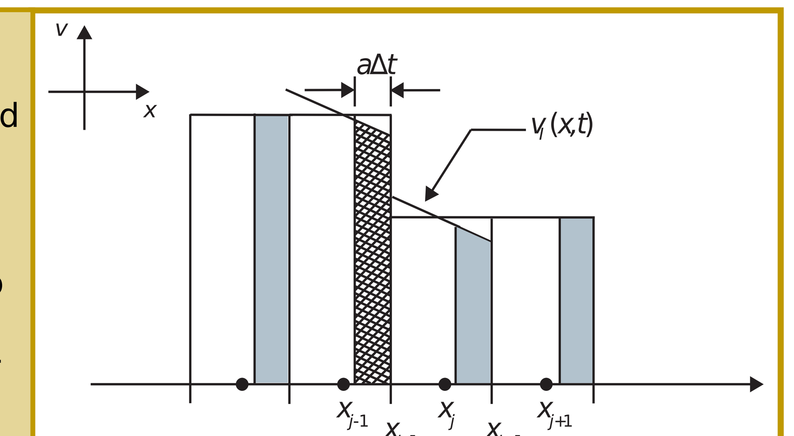
The Upwind Method (left) does not overshoot, but has an only first-order rate of convergence, as evidenced by the rounded corners of the advected square wave. As a result, the computation requires a much finer spatial discretization to achieve the same level of accuracy as a higher-order method.

Fromm's method (right) 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 tundershoots he minimum value u=0.0. Both plots had square-wave initial conditions 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 as constant across 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



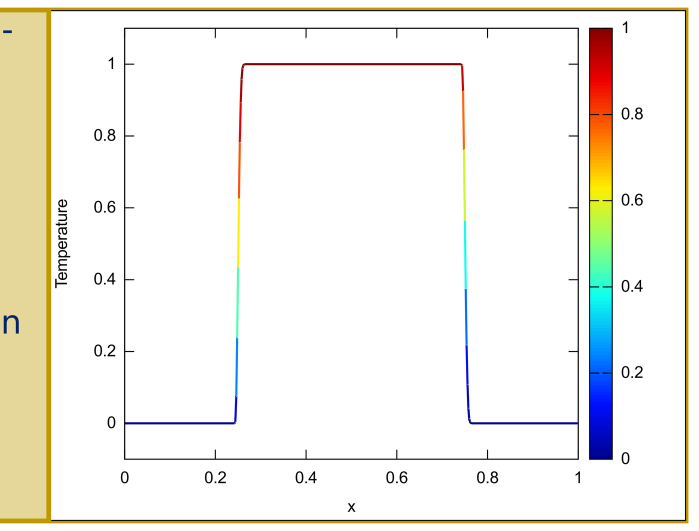
One way to address this overshoot/undershoot problem is to use a flux-limiter that enforces the use of upwind (i.e., lower-order) fluxes in neighborhoods of sharp gradients in u and high-order fluxes (e.g. Fromm's Method) in smooth regions of u. This is because the Upwind Method does not overshoot near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

The flux-limited version of (3) is thus,

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

where θ_j is a measure of the "smoothness" of u in a neighborhood of 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 of flux-limiter methods depending upon the choice of θ_j and ϕ [1,2]. Similar approaches have been successfully developed for Runge-Kutta Discontinuous Galerkin (RKDG) FEM although, to the best of our knowledge, they have not yet been implemented in mantle convection codes.

Fromm's Method with Van-Leer flux-limiters yields nearly second-order accuracy in the L^1 and L^2 norms with discontinuous initial data, while preserving sharp corners with greater accuracy than the Upwind Method. The initial conditions for this plot are identical to those shown previously.



Results and Conclusions

The introduction of nonlinear flux-limiting has adequately addressed the overshoot/ undershoot problem in FDM. However, attempts to use techniques based on artificial viscosity or "clipping" in FEM models of mantle convection have proven to be inadequate. We plan to address the overshoot/undershoot problem by using RKDG FEM in mantle convection codes. For more information, see the poster "Runge-Kutta Galerkin Method for the Advection-Diffusion Equation"(DI31A-2199) by Rajesh Kommu.

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

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