Treatment of Compressibility in TERRA

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Strategy for Implementing the Anelastic Approximation for Infinite Prandtl Number Flow in TERRA

In place of enforcing incompressibility $\nabla \bullet \mathbf{u} = 0$, let us instead enforce the anelastic approximation

$$\nabla \bullet [\rho_0(r)\mathbf{u}] = 0. \qquad (1)$$

where $\rho_0(r)$) is a radially varying reference density.

Let us define a diagonal matrix $\mathbf{R} = \rho_0(r)\mathbf{I}$, where $\mathbf{I}$ is the identity tensor, and also define a new variable q that will substitute for the pressure p such that

$$\mathbf{RG}q = \mathbf{G}p. \qquad (2)$$

where $\mathbf{G}$ is the gradient operator. Note that with this notation (1) becomes

$$\mathbf{G}^T\mathbf{R}u = 0. \qquad (3)$$

In terms of the new variable q, the momentum equation

$$\mathbf{A}u - \mathbf{G}p = b$$

then becomes

$$\mathbf{A}u - \mathbf{RG}q = b. \qquad (4)$$

Multiplying (4) by $\mathbf{G}^T\mathbf{R}\mathbf{A}^{-1}$, we obtain

$$\mathbf{G}^T\mathbf{R}\mathbf{u} - \mathbf{G}^T\mathbf{R}\mathbf{A}^{-1}\mathbf{R}\mathbf{G}q = \mathbf{G}^T\mathbf{R}\mathbf{A}^{-1}b. \qquad (5)$$

Note that $\mathbf{G}^T\mathbf{R}\mathbf{A}^{-1}\mathbf{R}\mathbf{G}$ is positive definite and we can therefore apply a conjugate gradient method to find a q* such that

$$-\mathbf{G}^T\mathbf{R}\mathbf{A}^{-1}\mathbf{R}\mathbf{G}q^* = \mathbf{G}^T\mathbf{R}\mathbf{A}^{-1}b, \qquad (6)$$

which implies the anelastic approximation (3) is satisfied.

The only changes in converting an incompressible code to this anelastic formulation involve replacing $\mathbf{G}p$ with $\mathbf{R}\mathbf{G}q$ and $\mathbf{G}^Tu$ with $[\mathbf{R}^{-1}]^2\mathbf{G}^T\mathbf{R}u$. The only place the pressure p is used explicitly is in computing boundary deflections. Since $\mathbf{R}$ does not vary rapidly at the boundaries, it is reasonable to approximate p as $\mathbf{R}^{-1}q$ for purposes of computing boundary deflections.

The Energy Equation for Compressible Convection in TERRA

Let us first derive the equation for internal energy by subtracting the rate of change of kinetic energy from the rate of change of total energy. The rate of change of total energy is given by

$$\rho D(\tfrac{1}{2}u^2 + i)/Dt = \rho \mathbf{g}\cdot\mathbf{u} + \nabla\cdot(\mathbf{u}\cdot\boldsymbol{\sigma}) + \nabla\cdot(k\nabla T) + Q, \qquad (1)$$

where ρ is density, $\mathbf{u}$ is velocity, i is internal energy, $\mathbf{g}$ is gravitational acceleration, $\boldsymbol{\sigma}$ is the total stress, k is thermal conductivity, T is temperature, and Q is specific heat production.

If we take the inner product of velocity and the momentum equation, we get the equation for the rate of change of kinetic energy as follows:

$$\mathbf{u}\cdot[\rho D\mathbf{u}/Dt = \rho\mathbf{g} + \nabla\cdot\boldsymbol{\sigma}] \quad \Rightarrow \quad \tfrac{1}{2}\rho Du^2/Dt = \rho\mathbf{g}\cdot\mathbf{u} + \mathbf{u}\cdot(\nabla\cdot\boldsymbol{\sigma}).$$

Subtracting rate of change of kinetic energy from rate of change of total energy yields the following equation for the rate of change of internal energy:

$$\rho Di/Dt = \nabla\cdot(\mathbf{u}\cdot\boldsymbol{\sigma}) - \mathbf{u}\cdot(\nabla\cdot\boldsymbol{\sigma}) + \nabla\cdot(k\nabla T) + Q.$$

But since $\nabla\cdot(\mathbf{u}\cdot\boldsymbol{\sigma}) = \mathbf{u}\cdot(\nabla\cdot\boldsymbol{\sigma}) + \boldsymbol{\sigma}:\nabla\mathbf{u}$, we have $\rho Di/Dt = \boldsymbol{\sigma}:\nabla\mathbf{u} + \nabla\cdot(k\nabla T) + Q.$

Expressing total stress in terms of pressure p and deviatoric stress $\boldsymbol{\tau}$, $\boldsymbol{\sigma} = -p\mathbf{I} + \boldsymbol{\tau}$, we obtain

$$\rho Di/Dt = -p\nabla\cdot\mathbf{u} + \boldsymbol{\tau}:\nabla\mathbf{u} + \nabla\cdot(k\nabla T) + Q. \qquad (2)$$

As a next step let us rewrite this equation in terms of entropy s instead of internal energy. From mass conservation, $\partial\rho/\partial t + \nabla\cdot(\rho\mathbf{u}) = 0$, we have $\partial\rho/\partial t + \mathbf{u}\cdot\nabla\rho + \rho\nabla\cdot\mathbf{u} = Dr/Dt + \rho\nabla\cdot\mathbf{u} = 0$, which implies

$$\nabla\cdot\mathbf{u} = -1/\rho\; D\rho/Dt = \rho Dv/Dt,$$

where v is specific volume. Hence (2) may be rewritten as

$$\rho[Di/Dt + pDv/Dt] = \boldsymbol{\tau}:\nabla\mathbf{u} + \nabla\cdot(k\nabla T) + Q.$$

Since Tds = di + pdv, we get

$$\rho T[Ds/Dt] = \boldsymbol{\tau}:\nabla\mathbf{u} + \nabla\cdot(k\nabla T) + Q. \qquad (3)$$

Let us now employ various thermodynamics relationships to rewrite (3) in terms of temperature alone, instead of temperature and entropy. We can proceed either of two ways, using either the relation

$$ds = (\partial s/\partial T)_v\, dT + (\partial s/\partial v)_T\, dv \qquad (4)$$

or the relation

$$ds = (\partial s/\partial T)_p\, dT + (\partial s/\partial p)_T\, dp. \qquad (5)$$

Let us choose the first approach. Using the definitions of thermodynamic quantities $c_v = T(\partial s/\partial T)_v$, $\alpha = (\partial s/\partial v)_T/K_T$, and $\gamma = aK_T/(\rho c_v)$, where c_v is specific heat at constant volume, α is the volume coefficient of thermal expansion, K_T is the isothermal bulk modulus, and γ is the Grüneisen ratio, we can express (4) as

$$Tds = c_v dT + aK_T Tdv = c_v dT - \alpha K_T T/\rho^2 d\rho = c_v dT - c_v \gamma T/\rho d\rho.$$

Therefore (3) can be rewritten as

$$\rho c_v[DT/Dt - gT/\rho\ D\rho/Dt] = \boldsymbol{\tau}\mathbf{:}\boldsymbol{\nabla}\mathbf{u} + \boldsymbol{\nabla}\bullet(k\boldsymbol{\nabla}T) + Q. \qquad (6)$$

But since, as we showed earlier, $-1/\rho\ D\rho/Dt = \boldsymbol{\nabla}\bullet\mathbf{u}$, and since $DT/Dt = \partial T/\partial t + \mathbf{u}\bullet\boldsymbol{\nabla}T$ and $\mathbf{u}\bullet\boldsymbol{\nabla}T = \boldsymbol{\nabla}\bullet(T\mathbf{u}) - T\boldsymbol{\nabla}\bullet\mathbf{u}$, we can express (6) as a time rate of change in temperature as

$$\partial T/\partial t = -\boldsymbol{\nabla}\bullet(T\mathbf{u}) - (\gamma-1)T\boldsymbol{\nabla}\bullet\mathbf{u} + 1/(\rho c_v)[\mathbf{t}\mathbf{:}\boldsymbol{\nabla}\mathbf{u} + \boldsymbol{\nabla}\bullet(k\boldsymbol{\nabla}T) + Q]. \qquad (7)$$

This is the version of the energy equation used in TERRA.

We can also proceed using (5) instead of (4) and employ the definitions $c_p = T(\partial s/\partial T)_p$ and $\alpha = -\rho(\partial s/\partial p)_T$ to express (5) as

$$Tds = c_p\, dT - \alpha T/\rho\, dp.$$

In this case (3) may be rewritten as

$$\rho c_p DT/Dt - \alpha T Dp/Dt = \boldsymbol{\tau}\boldsymbol{:}\boldsymbol{\nabla}\mathbf{u} + \boldsymbol{\nabla}\bullet(k\boldsymbol{\nabla}T) + Q, \qquad (8)$$

which is identical to eq. 6.9.7 in Schubert, Turcotte, and Olson (2001).

Let us consider the term $Dp/Dt = \partial p/\partial t + \mathbf{u} \bullet \boldsymbol{\nabla}p$. If we neglect the term $\partial p/\partial t$ (consistent with the anelastic approximation) and make the approximation that $\boldsymbol{\nabla}p = -\rho g\mathbf{r}$, where $\mathbf{r}$ is the unit radial vector, we can approximate Dp/Dt as $-\rho g u_r$, with u_r the radial velocity. As above, with $DT/Dt = \partial T/\partial t + \mathbf{u}\bullet\boldsymbol{\nabla}T$ and $\mathbf{u}\bullet\boldsymbol{\nabla}T = \boldsymbol{\nabla}\bullet(T\mathbf{u}) - T\boldsymbol{\nabla}\bullet\mathbf{u}$, we have $DT/Dt = \partial T/\partial t + \boldsymbol{\nabla}\bullet(T\mathbf{u}) - T\boldsymbol{\nabla}\bullet\mathbf{u}$. Equation (8) can then be rewritten as

$$\partial T/\partial t = -\boldsymbol{\nabla}\bullet(T\mathbf{u}) + T\boldsymbol{\nabla}\bullet\mathbf{u} - \alpha g T u_r/c_p + 1/(rc_p)[\boldsymbol{\tau}\boldsymbol{:}\boldsymbol{\nabla}\mathbf{u} + \boldsymbol{\nabla}\bullet(k\boldsymbol{\nabla}T) + Q]. \qquad (9)$$

Next, making use of the anelastic approximation, we find we can express $\nabla \cdot \mathbf{u}$ in terms of the radial velocity u_r. Given the fact that the hydrostatic pressure gradient is given by $\partial p/\partial r = -\rho g$, the adiabatic bulk modulus, defined $K_s = \rho(\partial p/\partial \rho)_s$, can be written in terms of the hydrostatic pressure gradient as $K_s = \rho[(\partial p/\partial r)(\partial r/\partial \rho)]_s = -\rho^2 g(\partial r/\partial \rho)_s$. Under the anelastic approximation, with $\partial \rho/\partial t = 0$, the continuity equation becomes $\nabla \cdot (\rho \mathbf{u}) = \rho \nabla \cdot \mathbf{u} + \mathbf{u} \cdot \nabla \rho = 0$, and so

$$\nabla \cdot \mathbf{u} = -(1/\rho)\mathbf{u} \cdot \nabla \rho.$$

Neglecting horizontal spatial variations in ρ relative to the radial hydrostatic compression, we have $\mathbf{u} \cdot \nabla \rho \approx u_r(\partial \rho/\partial r)$. In terms of the adiabatic bulk modulus, we note that $(\partial \rho/\partial r) = \rho^2 g/K_s$ and obtain the result that

$$\nabla \cdot \mathbf{u} \approx \rho g u_r/K_s. \qquad (10)$$

Recalling that $\gamma = \alpha K_T/(\rho c_v)$ and using the fact that $K_T = (c_v/c_p)K_s$, we have $\gamma = \alpha K_s/(\rho c_p)$ and can rewrite (9) as

$$\partial T/\partial t = -\nabla \cdot (T\mathbf{u}) - \rho g(\gamma - 1)T u_r/K_s + 1/(\rho c_p)[\boldsymbol{\tau} : \nabla \mathbf{u} + \nabla \cdot (k \nabla T) + Q]. \qquad (11)$$

Note that when the approximation (10) is used in (7), the resulting energy equation

$$\partial T/\partial t = -\boldsymbol{\nabla}\bullet(T\mathbf{u}) - \rho g(\gamma - 1)Tu_r/K_s + 1/(\rho c_v)[\boldsymbol{\tau}:\boldsymbol{\nabla}\mathbf{u} + \boldsymbol{\nabla}\bullet(k\boldsymbol{\nabla}T) + Q]. \qquad (12)$$

is similar to (11).

$$\partial T/\partial t = -\boldsymbol{\nabla}\bullet(T\mathbf{u}) - \rho g(\gamma - 1)Tu_r/K_s + 1/(\rho c_p)[\boldsymbol{\tau}:\boldsymbol{\nabla}\mathbf{u} + \boldsymbol{\nabla}\bullet(k\boldsymbol{\nabla}T) + Q]. \qquad (11)$$

The sole difference is that c_v occurs in (12) in place of c_p in (11). One difference in the derivation was that in the second case, the anelastic approximation was invoked before approximation (10) was applied, while in the first case, it was not. Note that $c_p = (1 + \alpha\gamma T)c_v$ and that the quantity $\alpha\gamma T$ is typically everywhere smaller than 0.01.

Momentum Equation in TERRA

The equation used for conservation of momentum in the infinite Prandtl number limit is

$$\nabla \bullet \boldsymbol{\tau} = \nabla(p - p_0) - (\rho - \rho_0)\mathbf{g}, \quad (1)$$

where $\boldsymbol{\tau}$ is devatoric stress, p is pressure, p_0 is a radially varying reference pressure, ρ is density, ρ_0 is a radially varying reference density, and $\mathbf{g}$ is gravitational acceleration. The deviatoric stress is given by

$$\boldsymbol{\tau} = \mu[\nabla\mathbf{u} + (\nabla\mathbf{u})^T] - \tfrac{2}{3}\mu\mathbf{I}\nabla \bullet \mathbf{u}, \quad (2)$$

where μ is the dynamic viscosity, **u** is velocity, **I** is the diagonal identity tensor, and the bulk viscosity is assumed to be zero. The solution is linearized about a radially symmetric adiabatic reference state (ρ_0, p_0,T_0) such that

$$\rho = \rho_0[1 + (p - p_0)/K_T + \alpha(T - T_0)], \quad (3)$$

where T_0 is the reference temperature, K_T is the isothermal bulk modulus, and α is the volume coefficient of thermal expansion.

An equation of state is employed using suitable material parameters (typically uncompressed density, uncompressed isothermal bulk modulus, pressure gradient of isothermal bulk modulus, and Grüneisen ratio) to obtain density from a given pressure and temperature. An iterative procedure is then applied to find the self-consistent radially symmetric adiabatic reference state.

In TERRA there is a choice among a third-order Eulerian Birch-Murnaghan EOS, a Morse EOS, or a simple Murnaghan EOS.

With built-in material parameter choices for the upper mantle, upper transition zone, lower transition zone, and lower mantle, a reference state relatively close to that of PREM can be realized.

The following are the parameters for the upper mantle, upper transition zone, lower transition zone, and lower mantle required to match the PREM density profile for the third-order Eulerian Birch-Murnaghan EOS given by

$$p(\rho,T) = 1.5K_o(\rho/\rho_0)^{5/3})[(\rho/\rho_0)^{2/3} - 1]\{1 + 0.75(K_o' - 4)[(\rho/\rho_0)^{2/3} - 1]\} + \alpha K(\rho)T$$

where $K(\rho) = K_o(\rho/\rho_0)^{5/3}\{1 + (1.5K_o' - 2.5)[(\rho/\rho_0)^{2/3} - 1]\}$

rhor(1) = 3425.
rhor(2) = 3695.
rhor(3) = 3760.
rhor(4) = 4245.

bmod(1) = 1.40e11
bmod(2) = 1.60e11
bmod(3) = 1.60e11
bmod(4) = 2.70e11

dbmd(1) = 4.00
dbmd(2) = 4.00
dbmd(3) = 4.00
dbmd(4) = 3.65

cvref = 1371.
gamref = 1.05
t0adbt = 1900.

TERRA Radially Varying Parameters and Adiabatic Reference State

radius	density	tmprf	avg temp	pressure	gravity
6.3700E+06	3.3993E+03	1.9000E+03	3.0000E+02	0.0000E+00	9.8218E+00
6.3047E+06	3.3300E+03	1.9311E+03	1.2289E+03	2.1669E+09	9.8401E+00
6.2352E+06	3.3157E+03	1.9659E+03	1.8191E+03	4.4280E+09	9.8649E+00
6.1617E+06	3.3540E+03	2.0031E+03	2.0031E+03	6.8580E+09	9.8937E+00
6.0841E+06	3.4108E+03	2.0416E+03	2.0416E+03	9.4476E+09	9.9247E+00
6.0027E+06	3.4693E+03	2.0810E+03	2.0810E+03	1.2241E+10	9.9577E+00
5.9176E+06	3.7785E+03	2.1204E+03	2.1204E+03	1.5270E+10	9.9839E+00
5.8291E+06	3.9064E+03	2.1600E+03	2.1600E+03	1.8742E+10	9.9998E+00
5.7373E+06	3.9705E+03	2.2005E+03	2.2005E+03	2.2296E+10	1.0014E+01
5.6425E+06	4.4242E+03	2.2362E+03	2.2362E+03	2.6282E+10	1.0014E+01
5.5452E+06	4.4839E+03	2.2667E+03	2.2667E+03	3.0683E+10	9.9992E+00
5.4454E+06	4.5422E+03	2.2971E+03	2.2971E+03	3.5117E+10	9.9844E+00
5.3438E+06	4.6023E+03	2.3275E+03	2.3275E+03	3.9818E+10	9.9707E+00
5.2405E+06	4.6607E+03	2.3575E+03	2.3575E+03	4.4520E+10	9.9585E+00
5.1360E+06	4.7204E+03	2.3873E+03	2.3873E+03	4.9464E+10	9.9484E+00
5.0307E+06	4.7780E+03	2.4165E+03	2.4165E+03	5.4370E+10	9.9410E+00
4.9250E+06	4.8366E+03	2.4453E+03	2.4453E+03	5.9489E+10	9.9370E+00
4.8193E+06	4.8928E+03	2.4734E+03	2.4734E+03	6.4529E+10	9.9370E+00
4.7140E+06	4.9497E+03	2.5008E+03	2.5008E+03	6.9751E+10	9.9416E+00
4.6095E+06	5.0038E+03	2.5275E+03	2.5275E+03	7.4849E+10	9.9514E+00
4.5062E+06	5.0584E+03	2.5534E+03	2.5534E+03	8.0100E+10	9.9670E+00
4.4046E+06	5.1101E+03	2.5785E+03	2.5785E+03	8.5180E+10	9.9889E+00
4.3048E+06	5.1620E+03	2.6027E+03	2.6027E+03	9.0383E+10	1.0018E+01
4.2075E+06	5.2106E+03	2.6259E+03	2.6259E+03	9.5369E+10	1.0053E+01
4.1127E+06	5.2594E+03	2.6483E+03	2.6483E+03	1.0045E+11	1.0096E+01
4.0209E+06	5.3047E+03	2.6696E+03	2.6696E+03	1.0527E+11	1.0146E+01
3.9324E+06	5.3500E+03	2.6900E+03	2.6900E+03	1.1016E+11	1.0204E+01
3.8473E+06	5.3918E+03	2.7094E+03	2.7094E+03	1.1475E+11	1.0269E+01
3.7659E+06	5.4334E+03	2.7278E+03	2.7278E+03	1.1938E+11	1.0340E+01
3.6883E+06	5.4713E+03	2.7453E+03	2.7453E+03	1.2367E+11	1.0417E+01
3.6148E+06	5.5082E+03	2.7617E+03	2.7789E+03	1.2800E+11	1.0500E+01
3.5453E+06	5.5353E+03	2.7772E+03	2.9381E+03	1.3194E+11	1.0587E+01
3.4800E+06	5.5573E+03	2.7918E+03	3.2000E+03	1.3590E+11	1.0679E+01

radius	alpha	cv	bulk modulus	gamma
6.3700E+06	3.6026E-05	1.3710E+03	1.3583E+11	1.0500E+00
6.3047E+06	3.8381E-05	1.3710E+03	1.2490E+11	1.0500E+00
6.2352E+06	3.8899E-05	1.3710E+03	1.2271E+11	1.0500E+00
6.1617E+06	3.7536E-05	1.3710E+03	1.2863E+11	1.0500E+00
6.0841E+06	3.5660E-05	1.3710E+03	1.3769E+11	1.0500E+00
6.0027E+06	3.3895E-05	1.3710E+03	1.4735E+11	1.0500E+00
5.9176E+06	3.1119E-05	1.3710E+03	1.7479E+11	1.0500E+00
5.8291E+06	3.0249E-05	1.3710E+03	1.8590E+11	1.0500E+00
5.7373E+06	2.8885E-05	1.3710E+03	1.9788E+11	1.0500E+00
5.6425E+06	2.0327E-05	1.3710E+03	3.1332E+11	1.0500E+00
5.5452E+06	1.9266E-05	1.3509E+03	3.2852E+11	1.0449E+00
5.4454E+06	1.8295E-05	1.3319E+03	3.4374E+11	1.0395E+00
5.3438E+06	1.7358E-05	1.3127E+03	3.5981E+11	1.0338E+00
5.2405E+06	1.6506E-05	1.2947E+03	3.7580E+11	1.0280E+00
5.1360E+06	1.5686E-05	1.2767E+03	3.9255E+11	1.0218E+00
5.0307E+06	1.4943E-05	1.2598E+03	4.0910E+11	1.0156E+00
4.9250E+06	1.4232E-05	1.2430E+03	4.2631E+11	1.0092E+00
4.8193E+06	1.3589E-05	1.2273E+03	4.4318E+11	1.0029E+00
4.7140E+06	1.2975E-05	1.2118E+03	4.6062E+11	9.9647E-01
4.6095E+06	1.2423E-05	1.1974E+03	4.7758E+11	9.9021E-01
4.5062E+06	1.1895E-05	1.1831E+03	4.9501E+11	9.8383E-01
4.4046E+06	1.1421E-05	1.1700E+03	5.1182E+11	9.7772E-01
4.3048E+06	1.0969E-05	1.1571E+03	5.2901E+11	9.7154E-01
4.2075E+06	1.0565E-05	1.1452E+03	5.4544E+11	9.6570E-01
4.1127E+06	1.0179E-05	1.1335E+03	5.6216E+11	9.5982E-01
4.0209E+06	9.8350E-06	1.1229E+03	5.7798E+11	9.5432E-01
3.9324E+06	9.5062E-06	1.1124E+03	5.9401E+11	9.4881E-01
3.8473E+06	9.2152E-06	1.1029E+03	6.0901E+11	9.4372E-01
3.7659E+06	8.9361E-06	1.0937E+03	6.2417E+11	9.3864E-01
3.6883E+06	8.6908E-06	1.0853E+03	6.3817E+11	9.3400E-01
3.6148E+06	8.4602E-06	1.0773E+03	6.5196E+11	9.2949E-01
3.5453E+06	8.2961E-06	1.0715E+03	6.6217E+11	9.2618E-01
3.4800E+06	8.1651E-06	1.0669E+03	6.7056E+11	9.2348E-01

The mean mantle density is 4.4520E+03 kg/m3.**