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C Last change: 3 April 2014 by M. Fernandez
C Version adapted to sbr-ATTEN, TAST and ABAST
C Synthetic tomography and reference model
C delete line 4 entry mater
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
CCC
C *****
C * PROGRAM "LITMOD_v4.0" for Lithospheric Modelling *
C *****
C
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C
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C
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C
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C
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C Sydney, Australia. All rights reserved.
C
C Main Reference: Afonso et al., 2008, G-3, 9, doi:10.1029/2007GC001834
C Based on program CAGES by Zeyen and Fernandez (1994)
C
C *****
C
C LitMod is a self-consistent geophysical-petrological approach in which
C most of the rock physical properties are derived from EOS. These
C properties are externally calculated by the 'GENERATOR' code which after
C reading the main oxides composition (given by the user) calculates the
C mineral assemblages according to P-T conditions and the physical
C properties according to EOS via PERPLEX. GENERATOR provides a set of tables
C with the relevant properties (Vp, Vs, density, thermal conduct., thermal
C expansion, etc.) at different P-T. These tables are used by LitMod as inputs.
C
C The use of GENERATOR is mandatory for mantle bodies whereas for crustal
C bodies is optional (i.e., crustal properties may be introduced in LitMod.inp
C independently on rock composition.
C
C The model extends down to 400 km depth (d410) and bodies can be coupled or
C decoupled in calculating isostatic elevation to take into account processes
C like subduction, slab detachment, etc. These decoupled bodies do not have
C effects on calculated topography but they do on gravity/geoid calculations.
C The lowermost point of the 'lithosphere model' should be ALWAYS at < 400 km
C since the level of compensation is taken at 400 km (~d410).
C
C The program solves the (heat) flux equation in 2D using "simplex" finite
C elements assuming steady state. Temperature is fixed at the base of the model
C (400 km) with a default values of 1520 °C. Temperature is also fixed at the
C base of lithosphere at 1320 °C and below the LAB temperature evolves with an
C adiabatic gradient between 0.35 and 0.5 °C/km. To avoid unrealistic
C discontinuities in the thermal gradient at the base of the lithosphere, a
C temperature buffer is applied between the lithospheric and sublithospheric
C domains (Afonso et al., 2008). With the calculated temperature and apriori
C pressure the code reads the properties of each material, particularly
C density, from GENERATOR and then calculates elevation, gravity, geoid and
C synthetic tomography.
C
C For topography below sea level the gravity effect before Bouguer reduction
C is calculated at sea level. No water body must be defined. Gravity
C calculations include Bouguer, Free Air and a combination of both.

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C The Bouguer anomaly is calculated with a reduction density of  
C 2670 kg/m<sup>3</sup> after having calculated the total 2D effect of the model  
C mass below every surface node. The reduction is a full topographical  
C one. A reference model which occupies the same space below sea level  
C is subtracted from the calculated anomalies in order to reduce  
C border effects. The resulting anomaly is shifted so that the mean  
C difference with the measured data becomes zero.

C  
C The geoid is calculated in 2D based on a formula for 3D rectangular prisms  
C (the triangles of the FE grid are converted by pairs to best fitting  
C rectangles), developed by HZ in

C Zeyen et al., 2005, TECTONICS, 24, doi:10.1029/2004TC001639.

C A 1D geoid calculation is also added following the formulas given by  
C Turcotte & Schubert 1982 (Geodynamics), p. 225-226, i.e. taking all  
C distances from sea level and integrating  $\rho(z) \cdot z \cdot dz$  from topo to  
C depth of compensation (Caution: in Turcotte & Schubert, topography  
C has a different sign than depth, which is not the case in LitMod).

C  
C \*\*\*\*\*List of main changes\*\*\*\*\*

C  
c Beginning of LitMod generation: TO BE CHECKED (MF\_15aug2012)

c  
C

c 01.Jan.2007: First thermodynamically self-consistent version of LitMod.

C It works with self-consistent thermodynamic databases for mantle  
C domains and with petrological models of oceanic lithosphere.

C Thermal conductivities and seismic velocities are calculated  
C with newer models of composites. The thermal conductivity of all  
C mantle bodies are explicitly modelled as a function of pressure  
C (strictly, depth) and temperature, but not as a function of  
C composition. The code works together with Perple\_x, which is  
C used in a pre-modelling stage to obtain thermodynamic info  
C for different lithospheric bodies. (JCA)

c Dec 2010: Now the code can be used to model crustal bodies with the  
c same thermodynamic formalisms as for the mantle. Although  
c not strictly necessary, these crustal bodies should be identified  
c with LITHO numbers  $1 < \text{LITHO} < 10$  in the Litmod.inp file. (JCA)

C June 2012: Thermal conductivity is now calculated as function of composition,  
c temperature, and pressure following the newest models of Anne  
c Hofmeister (parameterised by Chirs Grose). This version is really  
c messy in the way it does it... to be improved. (JCA)

c May 2013: Cleaning the code and subroutines. This new version does not  
c incorporate calculations in 2.5D, rheology (strength envelopes)  
C and some input and boundary conditions are fixed

c The following variables have been deleted: MODGRA, XW, XE,  
C NCOLUMN, ICOLUMN, COMSTR, EXTSTR, SSSTR, TOTCOM, TOTEXT, TOTSS,  
C U0, XL0. The following subroutines have been deleted: GRAV25,  
C DENINP, NUDTOT, CALGEO2D (MF)

C Input parameters in litmod.inp have been changed! (MF)

C Mar 2014: Incorporation of perturbations within the sublithospheric mantle.  
C Perturbations can be introduced by:

C 1.- An external file 'tomo1level.dat' where seismic velocities  
C are given for up to 4 depth levels. Seismic data can be either  
C  $V_p(\%)$ ,  $V_s(\%)$ ,  $V_p$ -absolute or  $V_s$  absolute. See sbr-TAST.

C 2.- Anomalous sublithospheric bodies. In this case, bodies can  
C have anomalous composition (C), temperature (T) or seismic  
C velocity (V). In each body, a combination of C-T or C-V can be  
C given. Any combination of C-T-V is allowed for different bodies.  
C see sbr-ABAST

C When sublithospheric mantle perturbations are given, the code  
C calculates both, coupled elevation (i.e. considering that density  
C anomalies beneath LAB are transmitted to surface elevation) and  
C decoupled elevation (i.e., when these anomalies are not

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C      transmitted to surface elevation but to potential fields and
C      seismic velocities). (MF)
C
C      Incorporation of attenuation through subroutine ATTENU (MF)
C      Calculation of synthetic tomography relative to a thermodynamic
C      reference model (Pr-2). (MF)
C
C      New SUBROUTINES: TAST, ABAST, ATTENU (MF)
C
C
C*****
C
C      PARAMETERS TO BE READ BY THE INPUT FILE (ALL MANDATORY)
C
C
C 0. INPUT AND OUTPUT FILE NAMES
C
C      If a file name is blank, this file is not used (read or written)
C
C      1. Input file elevation data (1st line is interpreted as header).
C          Ideally points must coincide with nodes.
C      2. Input file gravity data (1st line is interpreted as header)
C          Ideally points must coincide with nodes.
C      3. Input file free air data (1st line is interpreted as header)
C          Ideally points must coincide with nodes.
C      4. Input file geoid data (1st line is interpreted as header)
C          Ideally points must coincide with nodes.
C      5. Output file elevation result (1 header line)
C      6. Output file Bouguer gravity result (1 header line)
C      7. Output file free air (1 header line)
C      8. Output file free air offshore, Bouguer onshore (1 header line)
C      9. Output file geoid results in 2D and 1D (1 header line)
C      10. Output file temperatures (1 header line)
C      11. Output file surface and asthenospheric heat flow (1 header line)
C      12. Input file 'tomo1level.dat' with
C          line #1 NLEVELS (max. 4) and ISEIS (code for seismic data)
C          line #2 ZLEVEL. Depth in m (negative downwards) of the anomalous level
C          line #3-n Seismic perturbation in each node of ZLEVEL (10F6.3). NX data.
C          lines #2 and #3-n repeat NLEVELS times.
C          level at -400000 m is mandatory (including perturbations at that depth)
C      13. Output file FREE for future use
C      14. Output file FREE for future use
C      15. Output file with results of special material boundaries
C          (ok for "TMOHO") ADD PRESSURE AND AVERAGE DENSITY
C      16. Output file with body limits
C      17. Output file with element boundaries
C      18. Output file FREE for future use
C      19. Output file with P,T at every node (1 header line?)
C      20. Output file for densities
C      21. Output file which serves as input file for Transient-LitMod
C      22. Index of Thermodynamic database used (see Generator.exe)
C
C 1. TITLE          FORMAT 72A1      SUBROUTINE INPUT
C
C 2. MATER,NCORP,IEL_C,DSIZE,IOSPE,IPRINT
C      FREE FORMAT      SUBROUTINE INPUT
C      MATER: Number of different materials (Last material must be
C              asthenospheric material!)
C      NCORP: Number of different bodies
C      IEL_C: Control on density variations within the sublithospheric
C              mantle due to thermal or compositional anomalies.
C              = 0: Sublithospheric mantle homogeneous and without thermal
C              anomalies.

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= 1: Sublithospheric mantle affected by anomalies of thermal and/or compositional origin. Anomalies can be prescribed in given nodes over given depth levels via external file (only seismic perturbations), or defining anomalous bodies within the sublithosphere, thus requiring either thermal or seismic perturbations to be prescribed. Both coupled (anomalous asthenosphere influences elevation) and decoupled (elevation is not affected by sublithospheric perturbations) elevations are calculated.

DSIZE: Mantle grain size (mm). Recommended value = 5.0 Range = 3. - 15.

IOSPE: Oscillation period. Chose among 50, 75 and 100 seconds.

IPRINT: Parameter for the print of entries and results:  
 IPRINT = 0: Results are printed for all nodes, entries are not printed  
 > 0: Results for all nodes and entries are printed  
 < 0: Results are printed only for interfaces and special columns (surface and base in any case), not for all nodes. Entries are not printed.

3. 3xMATER lines (see 2.) with the description of the materials:

3.1 Identification: NCAPA,LITHO

3.2 Thermal parameters: HPA,HPB,C1,C2,AL2,TCT,TCD

3.3 Density parameters: RHO,FACRHO,ITDEP,DILAT

FREE FORMAT SUBROUTINE INPUT

NCAPA: Identification number of the material  
 The asthenospheric mantle has to be the last material entered.

LITHO < 0: Sedimentary layer. Density is read in for every column (see below: 6.)  
 = 0: General layer (no associated thermodynamic table)  
 1 <= LITHO <= 10: Crustal layer with a thermodynamic table  
 > 20: Lithospheric mantle bodies: a thermodynamic table must be associated with this body (same number).  
 =99: Ashtenosphere (needs thermodynamic table)

HPA,HPB HPA = Parameter A0 of the heat production (W/m3)  
 HPB = Reference thickness B for the exponential term of heat production. [m]  
 IF HPB = 0.: Constant production (= HPA)

C1,C2,AL2: Description of the conductivity tensor for the solution of the transport equation [W/m K]. Conductivity for mantle materials comes from thermodynamic table and values are not used but needed.

TCT: Temperature dependence of the thermal conductivity  
 If TCT=0: No temperature dependence  
 ELSE: for the crust:  
 $C = C_0 / (1 + TCT * T)$   
 For mantle bodies a thermodynamic table is used unless TCT=0 and then is constant.

TCD: Depth dependence of thermal conductivity  
 IF TCD=0., No depth (pressure) dependence  
 For mantle bodies a thermodynamic table is used unless TCT=0 and then is constant. In this case TCD is irrelevant.  
 Depth coordinates are metres

Recommended values:  
 Sediments:  $C_0 = 1.3$  TCT=0. TCD=0.7D-4  
 Upper crust: 3.0 1.55D-3 0.  
 Lower crust: 2.5 0.80D-3 0.

RHO: Reference density in kg/m\*\*3. Requires (LITHO=0)  
 Normally this number is the density at the surface (zero presure and zero temperature).  
 Mantle materials read density from thermodynamic table.

C      FACRHO: Is thought for use in the upper crust, but can be  
 C              used anywhere else (even for the sediments).  
 C              Density is then:  $\text{RHO} \cdot (1 + \text{FACRHO} \cdot P)$ , being:  
 C               $P$  = Pressure at the node in Pa [ $\text{Pa}^{**} \cdot 1$ ]  
 C      ITDEP:    = 0: Density is independent of temperature  
 C              (mainly for the crust)  
 C               $< > 0$ : Density depends on temperature  
 C      DILAT:    Coefficient of thermal expansion (valid only for the crust)  
 C  
 C      FOR ANOMALOUS BODIES WITHIN THE ASTHENOSPHERE (IEL\_C=1)  
 C  
 C      RHO < 0    Denotes that this body is anomalous in composition, or  
 C              temperature, or seismic velocities  
 C      FACRHO: denotes DT in K or C-degree (needs ITDEO < 0)  
 C      ITDEP: Type of anomaly  
 C              > 0 denotes VTOMO code for v-anomaly  
 C                  (1) Tomography referred to Vp(%)  
 C                  (2) Tomography referred to Vs(%)  
 C                  (3) Tomography referred to Vp(>6.5), Vs(<6.5)  
 C              = 0 denotes no T- or v- anomaly  
 C              < 0 denotes T-anomaly  
 C      DILAT: Average VTOMO values according to ITDEP  
 C  
 C      4. This group is given NCORP times, describing the different bodies  
 C  
 C      4.1 NMAT      FREE FORMAT      SUBROUTINE CUERPO  
 C              NMAT: Identification number of the material forming  
 C              the body.  
 C  
 C      4.2 XC(I),ZC(I),I=1,4    FORMAT 8F8.0    SUBROUTINE CUERPO  
 C              Coordinates of the corners of the bodies (X,Z)  
 C              In every line 4 corners are defined. The last corner  
 C              given has to have the same coordinates as the first one.  
 C              Z is positive upwards.  
 C  
 C      In subroutine MATERI the bodies to which the elements belong  
 C      are calculated, taking as reference the mass center of the  
 C      element.  
 C  
 C      5. Boundary conditions and dimensions of the net  
 C  
 C      5.1 - 5.3: 3 lines with five numbers each, describing the default  
 C              boundary conditions. The order of these five values is:  
 C                  1. General condiciones  
 C                  2. Conditions at the upper limit  
 C                  3. Conditions at the lower limit  
 C                  4. Conditions at the left border  
 C                  5. Conditions at the right border  
 C  
 C      5.1 ICOD      FREE FORMAT      SUBROUTINE NUDXZ  
 C              ICOD: Code for the fixed conditions:  
 C                  = 0: Fixed heat flux  
 C                  = 1: Fixed temperature  
 C                  usually (0,1,1,0,0) -> fixed T at surface and LAB  
 C  
 C      5.2 HEAT      FREE FORMAT      SUBROUTINE NUDXZ  
 C              HEAT: Fixed heat flux (W/m) integrated over half of the  
 C              contiguous element boundaries for border nodes  
 C              where ICOD=0. For nodes at the four corners, this  
 C              value is automatically reduced to one half.  
 C              However, if the grid spacing is not regular, the  
 C              heat flux has to be defined manually for every  
 C              corresponding node (see 5.7). This is especially

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C         the case if non-zero horizontal heat flow is
C         defined at the vertical model boundaries.
C         usually (0.,0.,0.,0.,0.) -> no heat flow is imposed at any
C         boundary
C
C 5.3 TEMP          FREE FORMAT          SUBROUTINE NUDXZ
C     TEMP: Fixed temperature for border nodes where ICOD=1
C           usually (0.,15.,1320.,0.,0.) -> only Tsup and Tlab are
C           imposed
C
C 5.4 DIMENSIONS OF THE NET:
C     X0,DX,NX,NZ  FREE FORMAT          SUBROUTINE NUDXZ
C     X0:  Origin of the net (meters).
C     DX:  Distance between two horizontal nodes (meters)
C     NX:  Number of nodes in X direction
C     NZ:  Must be set to 96 ALWAYS.
C
C     ATTENTION!!! VERY IMPORTANT:
C           NX > 96 (or > NZ) ALWAYS. Then, the nodes are numbered by
C           columns, e.g.:
C           1  4  7 10
C           2  5  8 11
C           3  6  9 12
C
C 5.5 Z(I), I=1,NZ  FORMAT 8F8.0  SUBROUTINE NUDXZ
C     Z-coordinates of the rows (from top to down)
C     Z(I) are not taken as fixed values, but the column between
C     Z(1) and Z(NZ) is fitted between the surface and base level of
C     every column (calculated from the body limits).
C
C 6. Mean sediment density for every column if LITHO<0 (FORMAT(10F6.0))
C     SUBROUTINE INPUT
C     The densities must be given for all columns, not only where they are
C     needed (i.e., bodies containing LITHO < 0). Densities in kg/m3.
C
C 7. Description of output of special material limits.
C
C 7.1 NLIMIT,ILIMIT(1,...,2*NLIMIT)  FREE FORMAT  SUBROUTINE INPUT
C     NLIMIT = Total number of material limits for which the
C               resulting temperature, horizontal and vertical heat
C               flow are outputted to print.
C     ILIMIT = Two numbers for every material limit indicating the
C               codes (= NCAPA, see 3.) of the materials which
C               contact at the desired limit.
C
C *****
C INPUT FILE WITH SEISMIC PERTURBATIONS (file='tomo1level.dat')
C   line #1 nlevels, nrem: number of levels (<5) and reference earth model
C   line #2 ZLEVEL(nlevels). Depth (negative downwards) of vtomo-level
C   line #3-n vtomo(nl,j): vtomo values for each level (j=1,nx) (10F6.3).
C   lines #2 and #3-n repeat NLEVELS times.
C   level at -400000 m is mandatory (including perturbations at that depth)
C   nrem:
C     case (1). Tomography referred to Vp(%)
C     case (2). Tomography referred to Vs(%)
C     case (3). Tomography referred to Vp(>6.5), Vs(<6.5)
C *****
C THERMODYNAMIC DATA
C Thermodynamic calculations of material properties at different P-T

```

C conditions are performed by GENERATOR.FOR  
 C LITMOD requires to know with which thermodynamic database GENERATOR  
 C calculated the thermodynamic tables for each body (composition).  
 C The thermodynamic database is identified by an index (integer\*2) in  
 C line 22 of Input/output filenames.  
 C The thermodynamic tables for each material (composition) are identified  
 C by LITHO in each body. These tables contains the following parameters:  
 C R1:T(K); R2:P(bar); R9:Vp(km/s); R10:Vs(km/s); R12:RHO(kg/m3);  
 C R25:dVp/dT; R26:dVs/dT; R28:dVp/dP; R29:dVs/dP; R50: k(W/m K).  
 C  
 C Presently GENERATOR generates thermodynamic phases within the T range  
 C of 250 to 1800 C, which results in DT of +/-280 C or a DVp of +/- 1.3%  
 C and DVs of +/- 2.5%. Larger DV need modification of GENERATOR.  
 C  
 C\*\*\*\*\*  
 C  
 C Logical units (LU ASSIGNED NUMBER):  
 C  
 C INELE (1): Input of measured topography data (read in subr. OUTPUT)  
 C TEMOUT (2): Output of calculated temperatures  
 C FLUOUT (3): Output of surface and LAB heat flow  
 C ELEVUT (4): Output of calculated topographic elevation  
 C INP (5): Input of program parameters  
 C OUTP (98): Control output (PRINT)  
 C STCOUT (7): Output file set FREE for future use  
 C STEOUT (8): Output file set FREE for future use  
 C COLOUT (9): Output file set FREE for future use  
 C COROUT (10): Output of the corner coordinates of the bodies  
 C GINP (11): Input of Bouguer gravity data  
 C GOUT (12): Output of calculated gravity  
 C MATOUT (13): Output of results along special material boundaries  
 C ELEMUT (14): Output of element boundaries  
 C STROUT (15): Output file set FREE for future use  
 C POUT (16): Output of Pressure and Temperature for every node for  
 C VELPREP. To be set FREE  
 C IOUT (17): Output of material, body, node and element specifications  
 C for RECAGES  
 C DINP (18): Input file set FREE for future use  
 C DOUT (19): Output of densities  
 C FREOUT (20): Output of free air anomaly  
 C FREINP (21): Input of free air data  
 C FBOUT (22): Output of combined free air and Bouguer anomalies  
 C GEOIN (23): Input of geoid data  
 C GEOUT (24): Output of geoid data  
 C  
 C\*\*\*\*\*  
 C  
 C Minimum dimensions of the vectors and arrays used in the programs  
 C  
 C If the net consists of NX\*NZ nodes:  
 C MAXNX = NX  
 C MAXNZ = NZ  
 C MAXNUD = NX \* NZ  
 C MAXELE = (NX-1) \* (NZ-1) \* 2  
 C MAXBAN = MIN(NX+2,NZ+2)  
 C MAXPAR = 4 \* MAXNUD: Maximum number of non zero elements in the  
 C matrix to be inverted.  
 C MAXMAT Maximum number of materials  
 C MAXCOR Maximum number of bodies  
 C MAXNC Maximum number of corner points for any body  
 C  
 C MEMTOT=277\*MXNUD+8\*MXBAN\*MXNUD-152\*MXNZ-116\*MXNX+152+100\*MXMAT+  
 C (16\*MXNC+8)\*MXCOR+50K (for the rest of used variables)

[illegible]