On computation of atmospheric chemical potential in MALO software package

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1 Algorithm for computation of the atmospheric chemical potential

Input: T — air temperature in K, P_w — partial pressure of water vapor in Pa. First, we compute dew point temperature T_d :

$$T_d(T, P_w) = T_0 + b_1 \ln \frac{\frac{\ln P_w}{c_1}}{a_1 - \frac{\ln P_w}{c_1}}$$
(1)

Then we compute relative humidity ρ :

$$\rho(T, T_d) = \exp^{-\frac{L_v}{R_v} \left(\frac{1}{T} - \frac{1}{T_d}\right)} \tag{2}$$

Finally, we compute atmospheric chemical potential A_c :

$$A_c(T,\rho) = a_0 T^2 \ln \frac{1}{\rho} \tag{3}$$

If, by chance, the atmospheric chemical potential becomes less than 0.0001, it is replaced with value 0.0001.

Here are numerical values of used constants:

 $T_0 = 273.16$

 $a_0 \quad 2.32 \cdot 10^{-7}$

 a_1 17.625

 b_1 243.04

 c_1 610.94

 $L_v = 2.5 \cdot 10^6$

 R_v 461.5

Software package MALO computes for each epoch the 2D field of the atmospheric chemical potential in the following way:

- 1. Parses the 3D output of numerical weather models at native resolution and extracts layer pressure thickness, air temperature, and specific humidity for mid-layer points.
- 2. For each epoch, each longitude and latitude extracts a a column of layer pressure thickness, air temperature, and specific humidity for mid-layer points at native, non-uniform, irregular grid. Then it solves hypsometric differential equation and computes total atmospheric pressure, partial pressure of water vapor on a uniform grid that runs from -1000 to 90,000 meters. The initial conditions are defined by the ground geopotential used by the numerical weather model.
- 3. Using these three variables of state of the atmosphere, for each element of the 3D grid it computes the atmospheric chemical potential following expression 3.
- 4. It expands the atmospheric chemical potential over a 3D B-spline basis.
- 5. Using these expansion coefficients, the atmospheric chemical potential is computed on another grid with resolution D1023 (2048×4096) at the specified height above the surface that is defined by G3TOPO model. At the moment, this height is set to 100 m.
- 6. The 2D gridded atmospheric chemical potential is written in the output files in HEB format, one grid per epoch.

2 Data flow

Steps 1 are done at the massloading.net host. That hosts checks remote servers with numerical weather model outputs on hourly basis. When the new data become available, it downloads them, parses, extracts the necessary datasets, writes them in HEB format, and stores at the directory that is publicly accessible via ftp protocol.

Host at ertha.org checks the public ftp directory at massloading.net and when it finds new parsed datasets from numerical weather models, it downloads them and initiates the procedure that executes steps 2–6.

At the moment data from two numerical weather models are processed:

- 1. ertha.org:/d3/merra_acp/. Reanalysis MERRA model that runs from 1979.01.01 and is the most stable. It has resolution $0.666^{\circ} \times 0.5^{\circ} \times 72 \times 6^{h}$. It is updated on a monthly basis and has latency 25–60 days. Host ertha.org holds the series of atmospheric chemical potential since 1998.01.01.
- 2. ertha.org:/d4/geosfp_acp/. Operational GEOS-FP model that runs from 2011.09.01 and is updated approximately annually. Discontinuities may occur as a result of updates. It has resolution $0.3125^{\circ} \times 0.25^{\circ} \times 72 \times 3^{h}$. It is updated 4 times a day and has latency 7–16 hours. Host ertha.org holds the series of atmospheric chemical potential since 2013.06.13.