CHESS: HWSD soil data

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Abstract

This document describes the creation of two new soil datasets for CHESS, derived from the Harmonized World Soil Dataset, and using methods from the CAP 6.1.

1 HWSD data

The HWSD data are provided as a MS Access database (`HWSD.mdb`), associated with a binary map file (`hwsd.bil`). I have saved these files to `/prj/chess/emrobi/data/hwsd/data_orig`.

The values in the map file are integer soil mapping units, each unique mapping unit has an entry in the Access database, with associated soils and soil parameters. In order to read the data into my Fortran script, it was necessary to export the data from the table `HWSD_DATA` to a CSV file using **External Data** ⇒ **Text File**. On the first page of the Wizard, I chose to untick **Export data with formatting and layout**. On the second page I picked the **Delimited** option. On the third page I chose the **Comma** delimiter and to use double quotes to signify strings. On the final page I picked the destination `/prj/chess/emrobi/data/hwsd/data_orig/HWSD_DATA.txt`. Each soil mapping unit may have more than one soil (or non-soil) type associated with it – each of these (non-)soil types has an entry in the exported CSV file.

2 Working directory

The working directory is `/users/global/emrobi/Data-Area/projects/CHESS/soils`. All scripts are in the scripts directory, and they call source code in the src directory. Input files that give options to the various programs are in the input directory. The following descriptions give paths relative to the working directory.

3 Remapping

In order to do the remapping from the HWSD grid (30 arcsec resolution lat/lon grid) to the CHESS grid (1km resolution British National Grid), we require the map as a netCDF files. In order to speed up the remapping, I also decided to extract only the UK from the global map file. This was done using the script `scripts/extract_uk.sh`, which extracts data between latitudes 49.5N – 60.0N and longitude 8.0W – 2.0E (This includes the mainland UK on the current CHESS grid. In future we may include Northern Ireland and the Scottish islands, as well as the Republic of Ireland). Figure 1 shows these data plotted using the script `scripts/plot_maps.sh`.

The remapping requires grid files containing the latitude and longitude coordinates at the centres and corners of each grid square, which are used as input to the SCRIP function. These grid files were created with `scripts/create_grid_files.sh` and are stored in the directory `grid_files/`. The HWSD grid file (`hwsd_uk_30arcsec.nc`) corresponds to the extracted data for the UK, while the CHESS grid file

(chess_1km_land.nc) corresponds to the CHESS land vector. Note that this will have to be recreated if we include Northern Ireland and/or the Scottish islands at some point.

The next step was to use SCRIP [6] to create remapping files, using the script scripts/create_scrip_remap_files_land.sh. SCRIP takes the information from the grid files and uses it to create links between the two grids. Then the remapping script makes use of these links to do the remapping. SCRIP provides several options for calculating the remapping. In this case, since the mapping unit index is not a continuous variable, we needed to use a largest area fraction (LAF) method. That is, we pick the value which covers the largest area of the destination grid square. Unfortunately , this is not implemented in SCRIP, however the conservative remapping option does calculate the area of overlap between the two grids, so I used this option to create the remap files. The version of SCRIP used is /prj/arcc/emrobi/data/src/SCRIP/scrip and the input file is input/140211_regrid_scrip_elr_land.in. The remap files are stored in remap_files/ and the file used to remap from the HWSD grid to the CHESS land vector is rmp_hwsd_uk_30arcsec_TO_chess_1km_land.nc.

Finally, the remapping was carried out by the script scripts/remap_soil_land.sh. The remapping code used was regrid_scrip_elr_3d_unwanted/regrid_scrip_3d, with input input/140211_regrid_scrip_elr_land.in. Conservative remapping can usually be first or second order (first order weights the values by the overlapping area, while second order also includes a calculation of the gradient). In the code, this is selected using the mapOrder input parameter. In order to carry out LAF remapping, I edited the code to have an extra mapOrder value of 3, which used the weights to select the largest area fraction. It should be noted that if there is more than one possible largest area value, the code currently just selects the first one found (the selection is done by the Fortran intrinsic function MAXLOC, which just gives the position of the first appearance of the maximum value in an array). It may be desirable to do something more sophisticated, but I have not done yet.

Some of the mapping units in the HWSD data are non-soil types (eg, urban, inland water) and some are sea points. These are listed in Table 1. I have masked all of these values with the result that, if the destination grid contains only sea or non-soil then it will be missing value, otherwise it will take the value of the soil type covering the largest area. In urban areas in particular (but also apparently along some rivers, eg the Thames around Oxford), there are several points that do not overlap with any soil type, so these are output as missing on the CHESS grid.

The remapped data with missing values are output to /prj/chess/emrobi/data/hwsd/1km/data/hwsd_uk_1km_land.nc. Figure 2a shows the remapped data.

4 Replacing missing data

As the HWSD missing data do not necessarily correspond to non-soil (ie. urban, inland water) landcover in CHESS, we must provide some kind of soil parameters even within these areas. One option is to simply replace missing data with an average soil type, however this can end up with large differences between the replaced data and adjacent squares. Therefore, I decided to instead replace missing data with the nearest (dominant) soil type after remapping.

This was carried out by the script scripts/replace_missing.sh, which called src/replace_missing.py. For each grid box containing missing data the script first finds closest point(s). If any of these closest points are not missing, then it finds the most commonly occurring value and replaces the missing data with it. If all of the closest points are also missing data, then the script looks to the next closest point(s) instead and will recurse until it finds some non-missing data. Note that these tests of missing/non-missing are carried out on the input data, so are not affected by any points that have already been replaced with non-missing values. Note also that, in the event of a tie between two values, the one which occurs first in the array is chosen, due to the use of the numpy.argmax function to find the maximum. This is consistent with the LAF remapping described above, but it may be possible to do something more sophisticated.

Since the most computationally intensive part of the process is calculating the distances between points, we don't need to calculate the distance between each missing value and all of the other points in

MU_GLOBAL	Symbol	Land cover type
7000	NI	No data
7001	UR	Urban
7003	WR	Inland water
10800	NI	No data
10802	NI	No data

Table 1: Non-soil types included in the UK soil map. During remapping these are masked, with the effect that the dominant soil type present in the grid box will be used, even if the dominant type is non-soil. For any grid boxes which are entirely non-soil, we fill in the missing areas after remapping by replacing them with the nearest soil type.

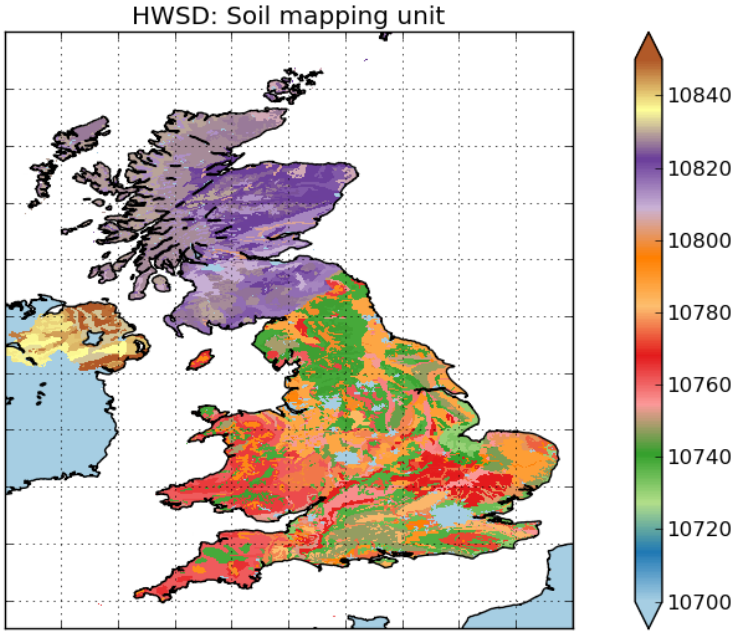
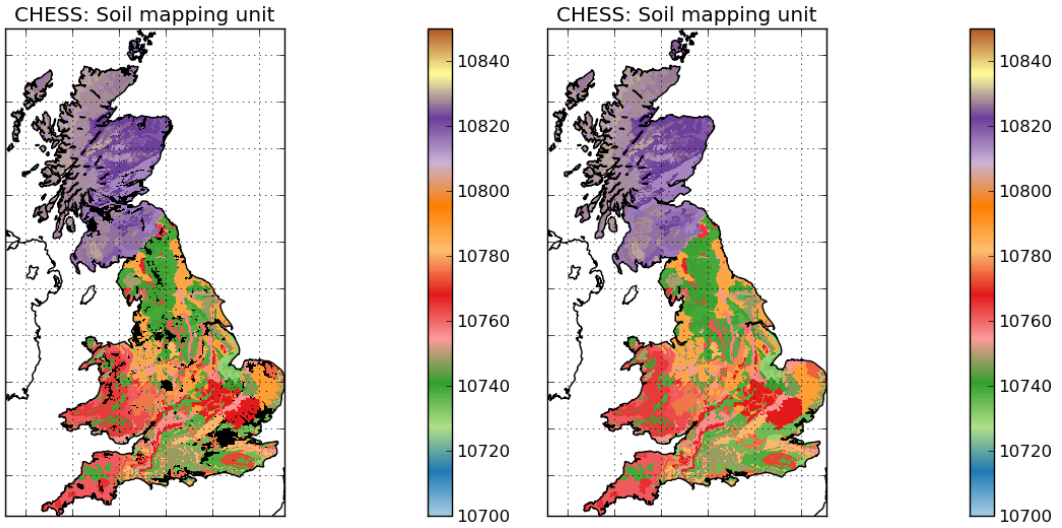


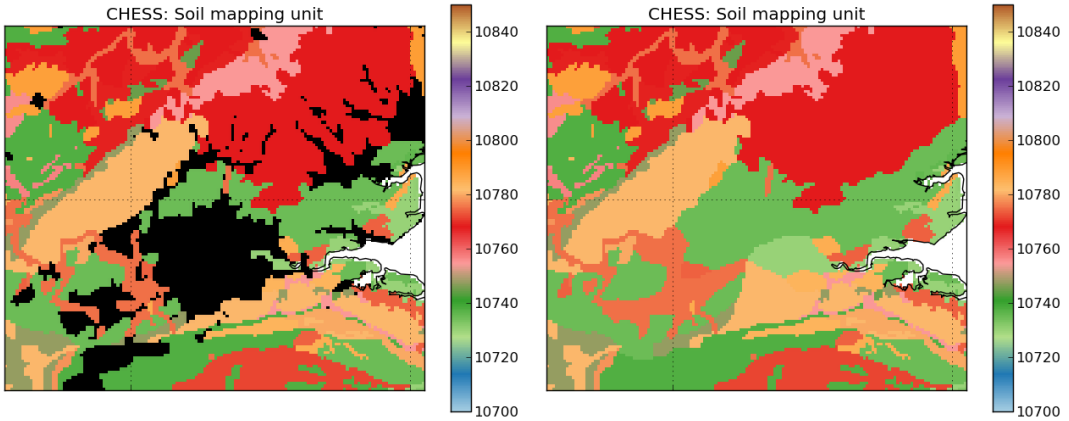
Figure 1: HWSD soil mapping units over the British Isles at 30 arcsec resolution. The unit IDs seem to cluster so that there are noticeable boundaries that correspond to political borders (emphasised by my choice of colorbar), however it should be remembered that these numbers do not correspond to any continuous variable.



(a) Soil mapping units with missing data shown in black.

(b) Soil mapping units when the missing data have been replaced with the nearest dominant soil type.

Figure 2: Soil mapping unit after 2a remapping to the CHESS grid and 2b replacing missing data with the nearest soil type.



(a) Soil mapping units with missing data shown in black.

(b) Soil mapping units when the missing data have been replaced with the nearest dominant soil type.

Figure 3: Soil mapping unit after 3a remapping to the CHESS grid and 3b replacing missing data with the nearest soil type. Zoomed in to have a clearer view of how this worked round London.

the vector. So we set a threshold distance within which to calculate the distances. This is chosen to be a 0.5 degree square, based on the identified size of areas of missing data.

The data are saved to `/prj/chess/emrobi/data/hwsd/1km/data/hwsd_uk_1km_soil_land.nc`. Figure 2b shows the data after the missing data have been replaced with the nearest soil types.

5 Making the ancillaries

To run JULES we require several parameters for each soil type. In JULES we can use either the van Genuchten or the Brooks and Corey methods for solving the Darcy equation. Previously in CHESS, we were using the van Genuchten method, so we required values of the van Genuchten parameters α and n (in fact, we input these as $\frac{1}{\alpha}$ and $\frac{1}{n-1}$. However, there's no reason why we shouldn't also use Brooks and Corey, in which case we require the saturated soil water suction, Ψ_s, and the Clapp and Hornberger soil exponent, b.

We also require values of the volumentric soil moisture concentration at saturation θ_s, at the critical point (-33 kPa) θ_c, and at the wilting point (-1500 kPa) θ_w. In the van Genuchten formulation, these are actually defined relative to the residual soil moisture θ_r. (Note that in the original CHESS LUT file, it lists the critical point as -40kPa.).

Finally, we require two thermal parameters; the heat capacity, C_s, and the thermal conductivity, λ, of the soil. These can also be calculated in a variety of ways from the soil texture properties.

These can be calculated from a selection of the parameters provided by the HWSD data set. Table 2 shows the parameters required for JULES [2] and the HWSD parameters required to calculate them. Table 3 shows the HWSD parameters that we use [1].

5.1 Hydrological parameters: van Genuchten

In order to obtain the van Genuchten hydrological parameters, we must first find the parameters α, n, θ_r, θ_s and K_s from the soil texture. We use the method of the CAP6.1, in that we use the input sand, silt, clay and organic carbon fractions to determine the texture class (very fine, fine, medium-fine, medium, coarse or organic).

Once we have the soil textures, we use a look up table to get the values of α, n, θ_r, θ_s and K_s for that soil texture. These parameters are different for topsoil and subsoil (except for organic soils, which do not distinguish the two). We use the values from Table 4 of [4], reproduced in part here as Table 5

For each of the soil textures, we can calculate θ_c and θ_w by calculating the hydraulic conductivity using van Genuchten's equations. The critical point is defined to be when the matrix potential is $\Psi_p = -33$kPa and the wilting point when it is $\Psi_p = -1500$kPa. We first convert these values to head/suction Ψ in units of m, such that

$$\Psi = -1000\frac{\Psi_p}{g\rho_w}, \tag{1}$$

where $g = 9.80665\text{ms}^{-2}$ is acceleration due to gravity and $\rho_w = 1000\text{kgm}^{-3}$ is the density of water.

The suction can then be used in the van Genuchten equation

$$\frac{\theta - \theta_r}{\theta_s - \theta_r} = \frac{1}{[1 + (\alpha\Psi)^n]^m}, \tag{2}$$

where $m = 1 - 1/n$ [5]. Note that we actually use the values of soil moisture with respect to the residual, so we return $\theta'_s = \theta_s - \theta_r$ etc.

5.2 Hydrological parameters: Brooks and Corey

In this method, we find the parameters b, Ψ_s, K_s and θ_s as continuous functions of the sand and clay fractions (no organic soils). The Cosby et al paper does linear regressions of b, θ_s, $\log \Psi_s$ and $\log K_s$, but it is apparently ambiguous as to whether they meant log in base e or log in base 10, so there are two options for the Ψ_s and K_s parameters.

Parameter	units	description
van Genuchten		
$\frac{1}{\alpha}$	m	Reciprocal of the α van Genuchten parameter
$\frac{1}{n-1}$	none	Function of the n van Geunuchten parameter
Brooks and Corey		
Ψ_s	m	Soil water suction
b	none	Clapp and Hornberger soil exponent
Always required		
K_s	ms^{-1}	Hydraulic conductivity of saturated soil
θ_c	$\mathrm{m}^3\mathrm{m}^{-3}$	Soil moisture concentration at critical point (-33kPa)
θ_s	$\mathrm{m}^3\mathrm{m}^{-3}$	Soil moisture concentration at saturation
θ_w	$\mathrm{m}^3\mathrm{m}^{-3}$	Soil moisture concentration at wilting point (-1500kPa)
C_s	$\mathrm{Jm}^{-2}\mathrm{K}^{-1}$	Heat capacity
λ	$\mathrm{Wm}^{-1}\mathrm{K}^{-1}$	Thermal conductivity

Table 2: Parameters required for JULES. The first two are only required for van Genuchten, the next two for Brooks and Corey, and the rest are always required

Parameter	units	description
MU_GLOBAL	none	Soil mapping unit index
ISSOIL	none	Flag indicating soil or non-soil
SEQ	none	Index indicating dominance of soil type
SU_SYM90	none	Soil mapping unit symbol (from [3])
T_SAND	% wt.	Topsoil sand fraction
T_SILT	% wt.	Topsoil silt fraction
T_CLAY	% wt.	Topsoil clay fraction
T_BULK_DENSITY	kg dm^3	Topsoil bulk density
T_OC	% wt.	Topsoil organic carbon fraction
S_SAND	% wt.	Subsoil sand fraction
S_SILT	% wt.	Subsoil silt fraction
S_CLAY	% wt.	Subsoil clay fraction
S_BULK_DENSITY	kg dm^3	Subsoil bulk density
S_OC	% wt.	Subsoil organic carbon fraction

Table 3: Parameters used from the HWSD data set. Note thate we must convert the soil percentages to fractions (in the range 0-1) and the bulk densities to kg m^{-3}.

Class	definition
Very fine	$f_{\mathrm{clay}} \geq 60\%$
Fine	$35\% \leq f_{\mathrm{clay}} < 60\%$
Medium-fine	$f_{\mathrm{silt}} > 50\%$ and $f_{\mathrm{clay}} < 0.35$
Medium	$18\% \leq f_{\mathrm{clay}} < 35\%$ or $f_{\mathrm{clay}} < 35\%$ and $f_{\mathrm{sand}} < 65\%$ or $f_{\mathrm{sand}} \geq 65\%$ and $f_{\mathrm{clay}} < 18\%$ and $f_{\mathrm{OC}} \geq 3\%$
Coarse	$f_{\mathrm{sand}} \geq 65\%$ and $f_{\mathrm{clay}} < 18\%$
Organic	$f_{\mathrm{OC}} \geq 10\%$

Table 4: Definition of soil textures. Note that I'm assuming that the organic values are % but it's not really clear from the documentation. It may be that they should be masses (per m2) instead.

For b and θ_s, the equations are

$$b = 3.10 + 15.70 f_{\text{clay}} - 0.3 f_{\text{sand}} \quad (3)$$
$$\theta_s = 0.505 - 0.037 f_{\text{clay}} - 0.142 f_{\text{sand}} \quad (4)$$

For the other two parameters, the equations are either

$$\Psi_s = 0.01 e^{2.17 - 0.63 f_{\text{clay}} - 1.58 f_{\text{sand}}} \quad (5)$$
$$K_s = e^{-5.55 - 0.64 f_{\text{clay}} + 1.26 f_{\text{sand}}} \quad (6)$$

or

$$\Psi_s = 0.01 \times 10^{2.17 - 0.63 f_{\text{clay}} - 1.58 f_{\text{sand}}} \quad (7)$$
$$K_s = 10^{-5.55 - 0.64 f_{\text{clay}} + 1.26 f_{\text{sand}}} \quad (8)$$

The code has a flag to pick which base to use, for now I am using base 10.

5.3 Heat capacity

There are two methods provided to calculate heat capacity, the first is used with the Brooks and Corey scheme and linearly combines the values for clay, sand and silt such that

$$C_s = (1 - \theta_s)(f_{\text{clay}} C_{\text{clay}} + f_{\text{sand}} C_{\text{sand}} + f_{\text{silt}} C_{\text{silt}}), \quad (9)$$

where $C_{\text{clay}} = 2.373 \times 10^6$ Jm^{-3}K^{-1}, $C_{\text{sand}} = 2.133 \times 10^6$ Jm^{-3}K^{-1} and $C_{\text{silt}} = 2.133 \times 10^6$ Jm^{-3}K^{-1} (the silt values are copied from the sand values).

In the second method, the Johansen method, heat capacity is calculated from an average soil heat capacity, $\hat{C}_s = 1.942 \times 10^6$, and the saturated soil moisture with respect to the residual, θ_s, such that

$$C_s = (1 - \theta_s)\hat{C}_s. \quad (10)$$

This is usually used with the van Genuchten hydraulic properties.

5.4 Thermal conductivity

There are three ways provided to calculate the thermal conductivity. The first is the Farouki method and is usually used with the Brooks and Corey hydraulic parameters. In this the thermal conductivity is calculated from the clay, sand and silt fractions and the soil moisture at saturation, such that

$$\lambda = \lambda_{\text{air}}^{\theta_s} \lambda_{\text{clay}}^{f_{\text{clay}}(1-\theta_s)} \lambda_{\text{sand}}^{f_{\text{sand}}(1-\theta_s)} \lambda_{\text{silt}}^{f_{\text{silt}}(1-\theta_s)}, \quad (11)$$

where $\lambda_{\text{air}} = 0.025$ Wm^{-1}K^{-1}, $\lambda_{\text{clay}} = 1.16$ Wm^{-1}K^{-1}, $\lambda_{\text{sand}} = 1.57$ Wm^{-1}K^{-1}, $\lambda_{\text{silt}} = 1.57$ Wm^{-1}K^{-1}.

The second method is the Peters Lidard (Johansen) method and we use this with the van Genuchten hydraulic parameters. The thermal conductivity is calculated from the soil bulk density, ρ_s, such that

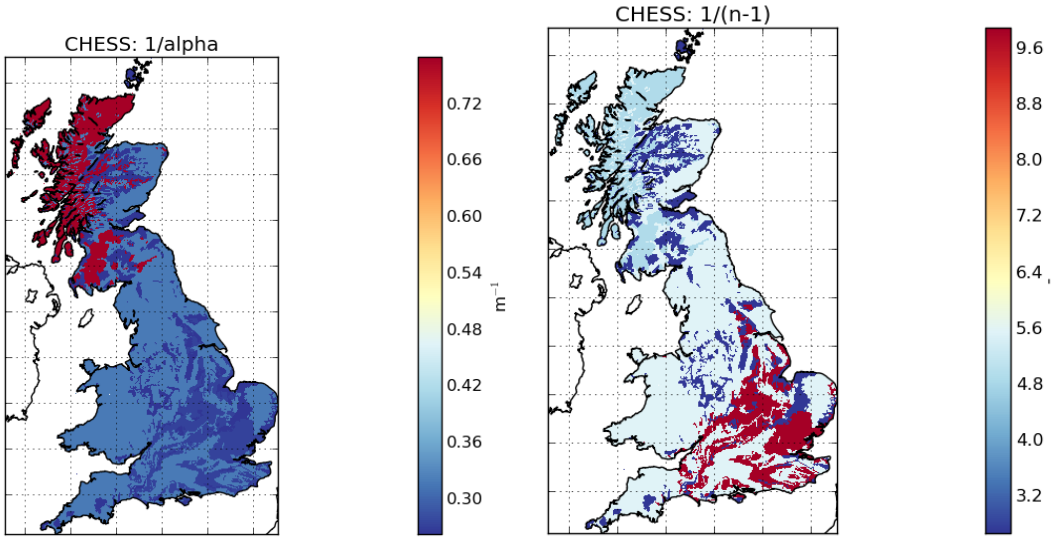
$$\lambda = \frac{0.135\rho_s + 64.7}{\rho_r - 0.947\rho_s}, \quad (12)$$

where $\rho_r = 2700$kgm^{-3} is a standard value for the density of rock.

The third is the Lu method and thermal conductivity is a regression function of porosity, such that

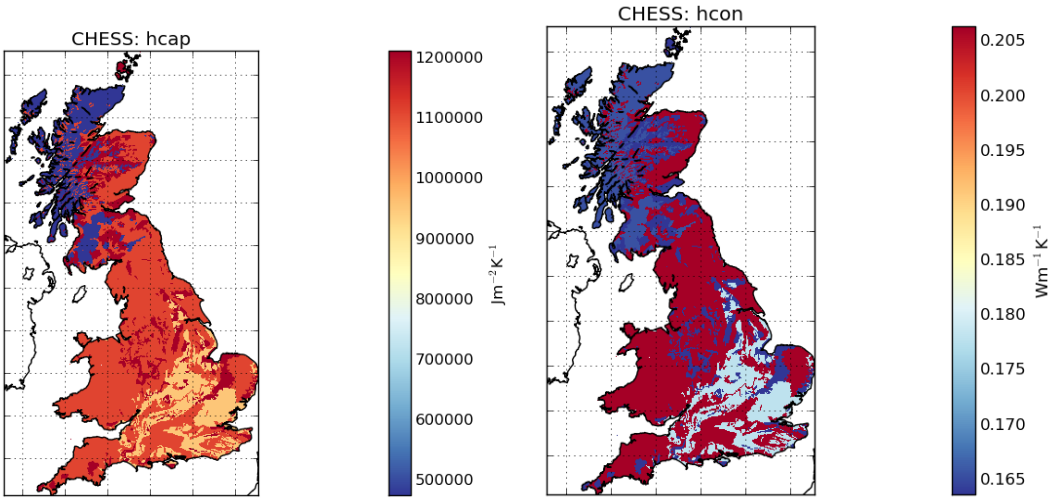
$$\lambda = -0.56\theta_s + 0.51. \quad (13)$$

This is included for completeness, but I haven't used it to calculate any parameters (yet).



(a) Map of $\frac{1}{\alpha}$

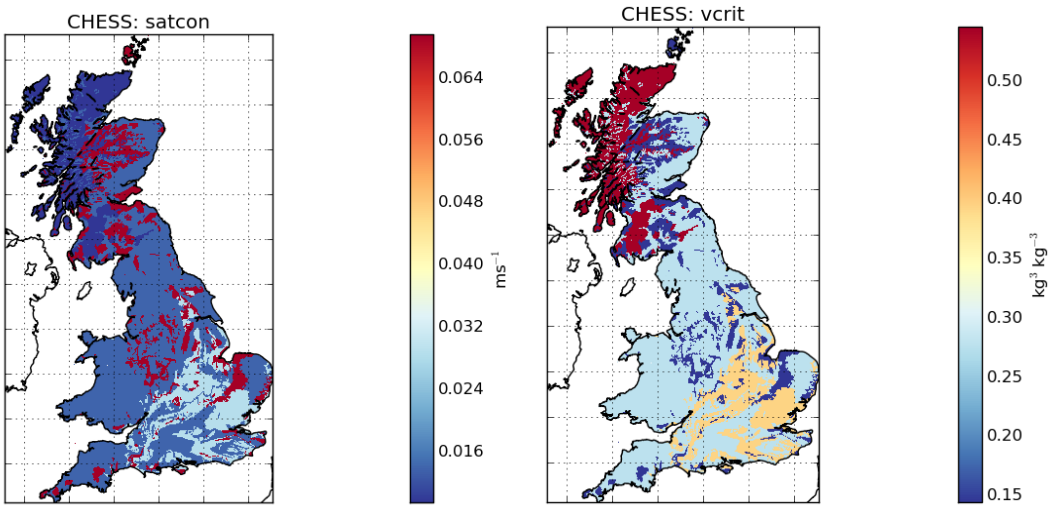
(b) Map of $\frac{1}{n-1}$



(c) Map of heat capacity

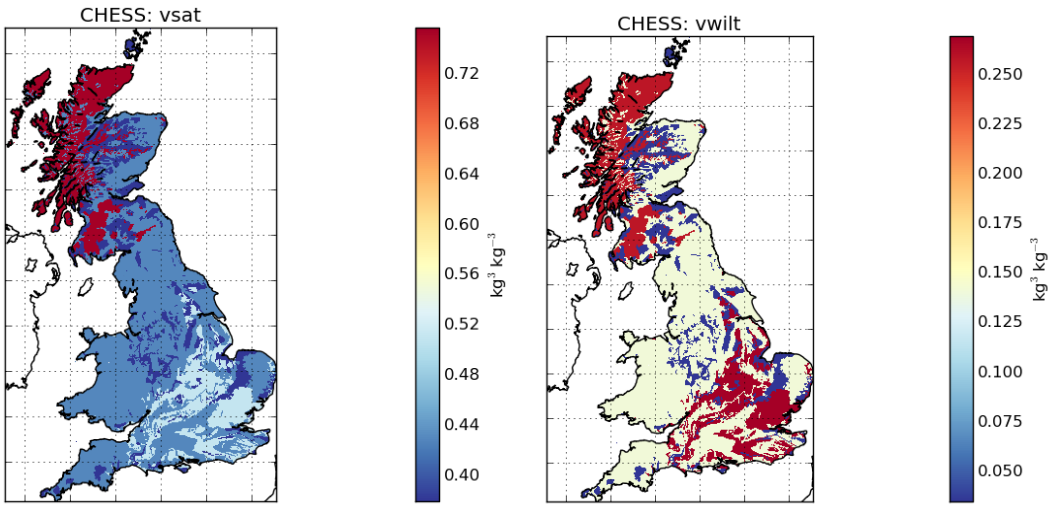
(d) Map of thermal conductivity

Figure 4: van Genuchten topsoil parameters



(a) Map of K_s

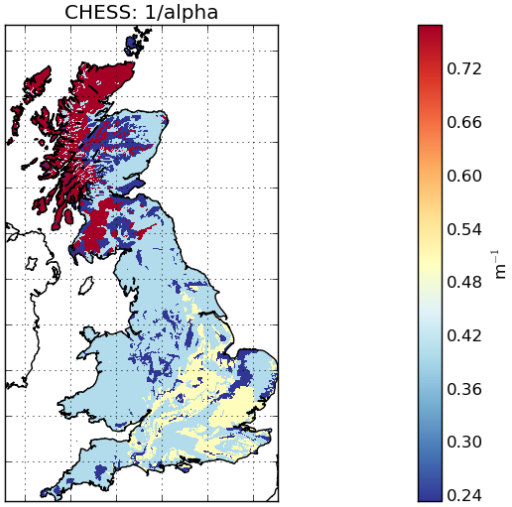
(b) Map of θ_c



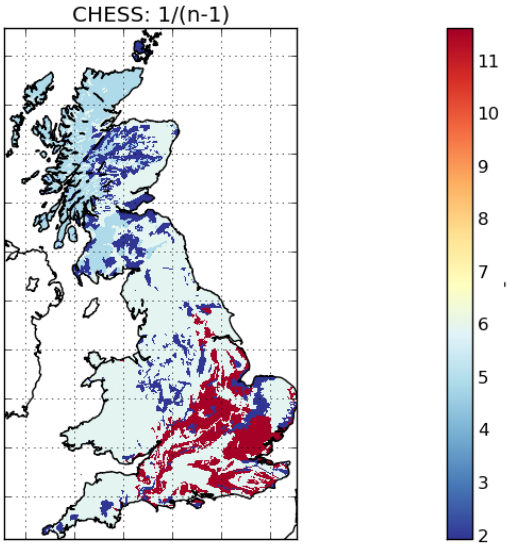
(c) Map of θ_s

(d) Map of θ_w

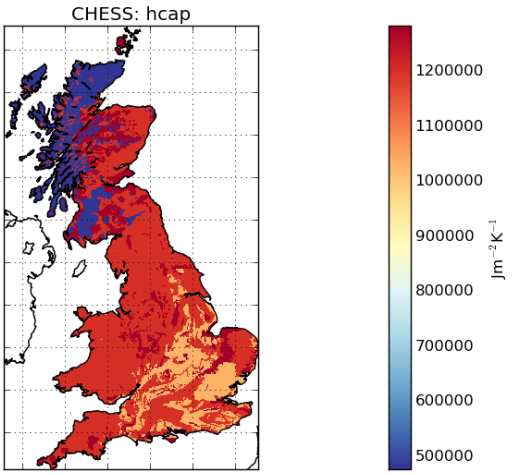
Figure 5: van Genuchten topsoil parameters



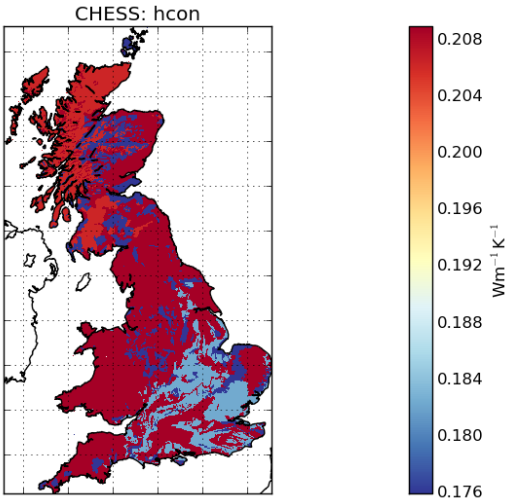
(a) Map of $\frac{1}{\alpha}$



(b) Map of $\frac{1}{n-1}$

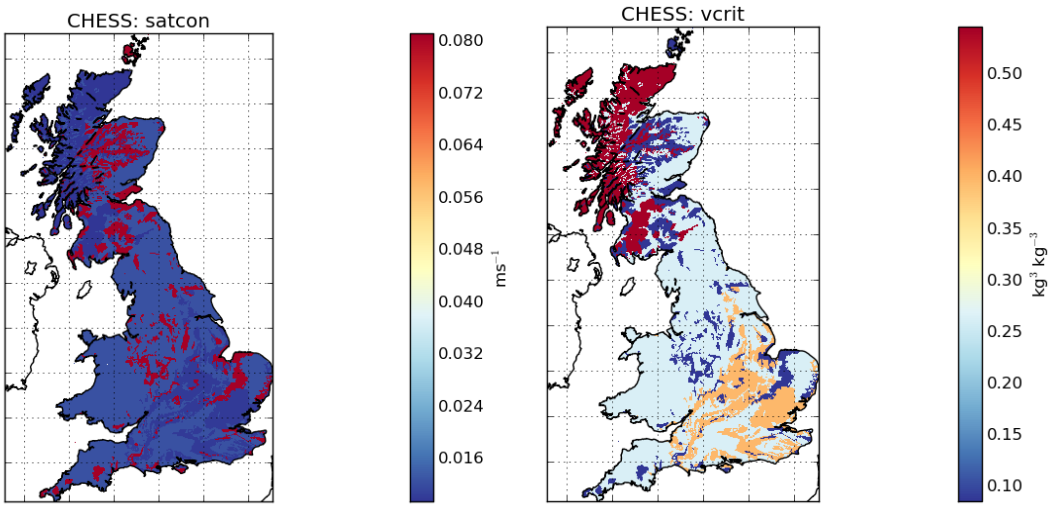


(c) Map of heat capacity



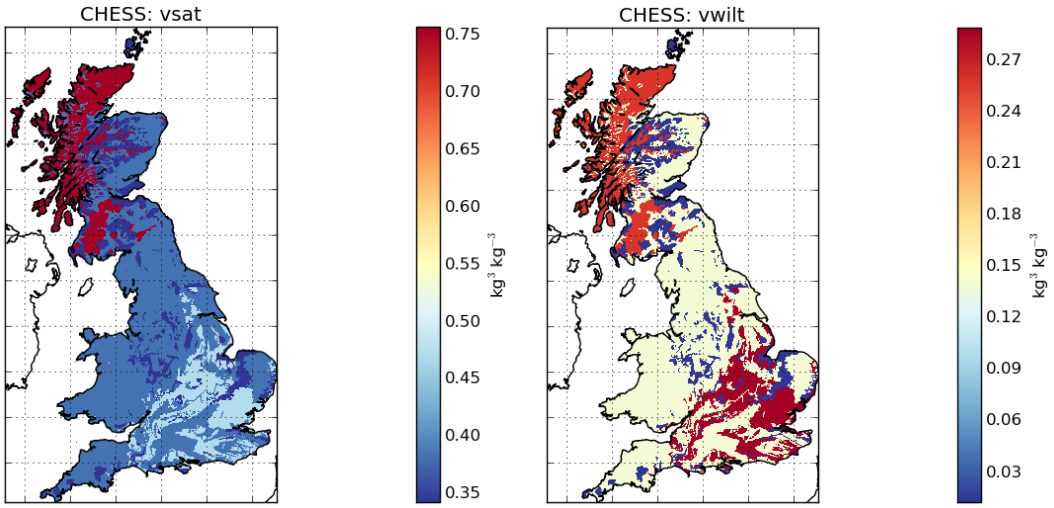
(d) Map of thermal conductivity

Figure 6: van Genuchten subsoil parameters



(a) Map of K_s

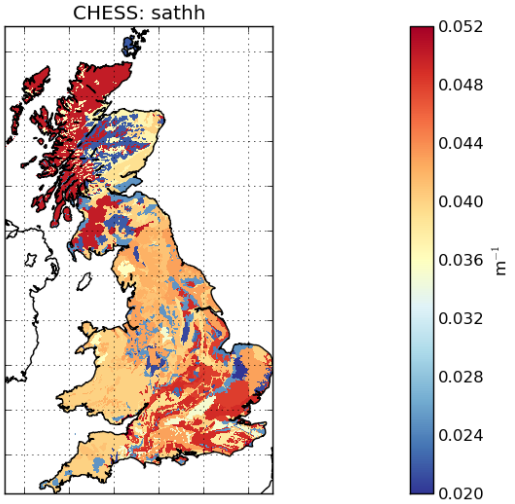
(b) Map of θ_c



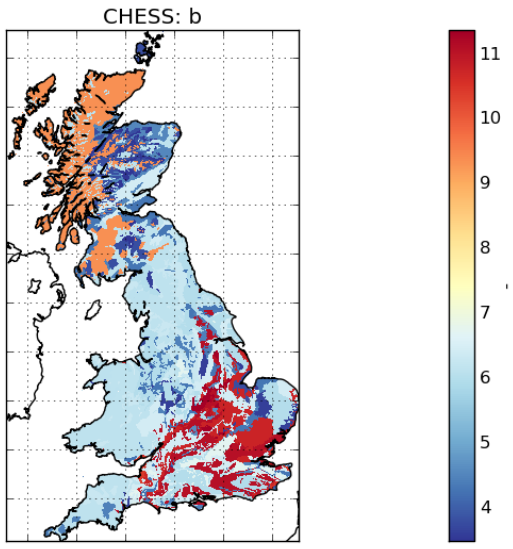
(c) Map of θ_s

(d) Map of θ_w

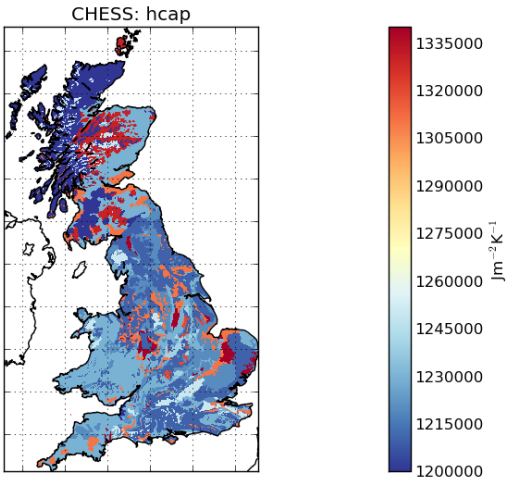
Figure 7: van Genuchten subsoil parameters



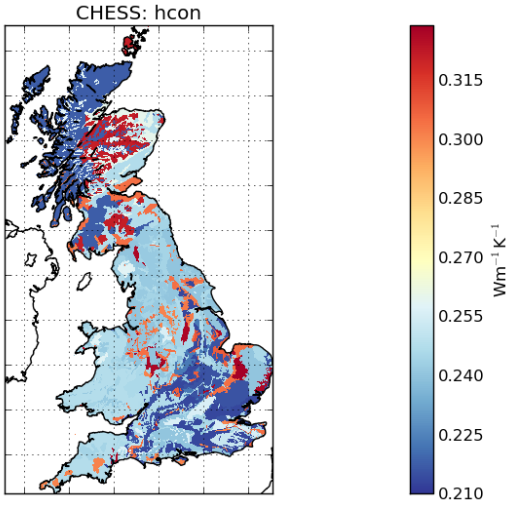
(a) Map of Ψ_s



(b) Map of b

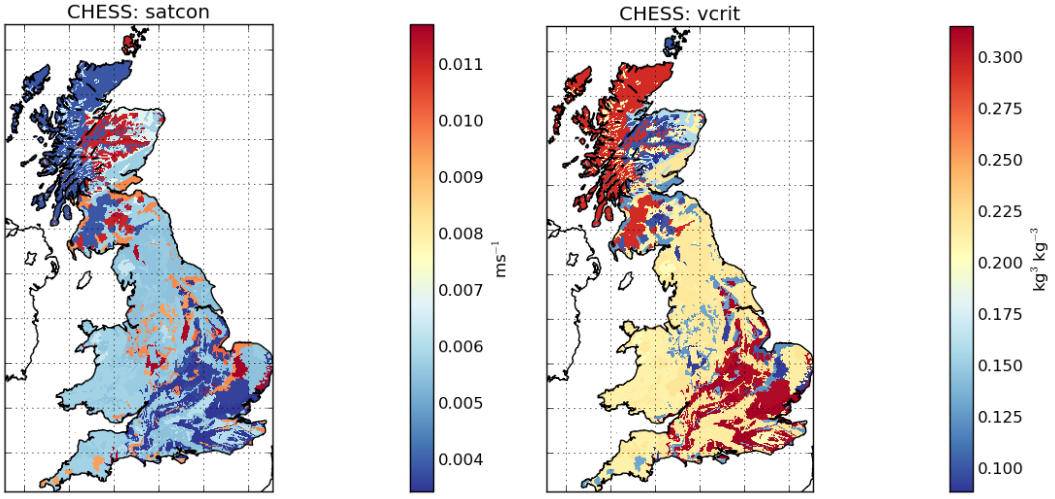


(c) Map of heat capacity



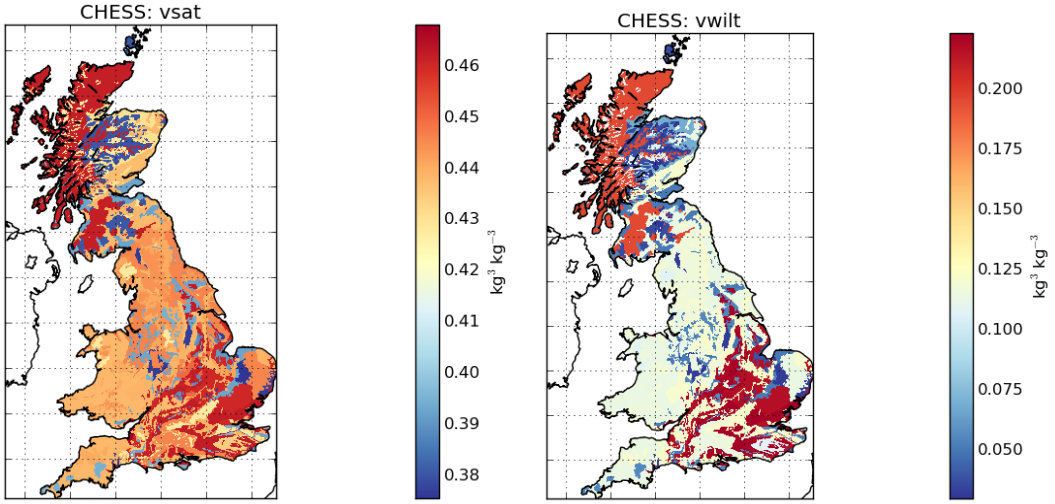
(d) Map of thermal conductivity

Figure 8: Brooks and Corey topsoil parameters



(a) Map of K_s

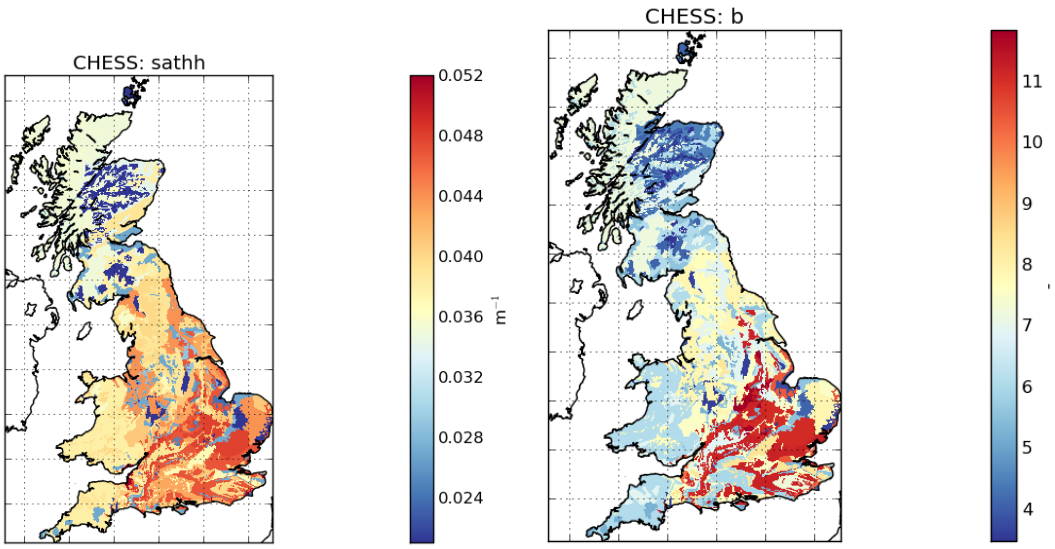
(b) Map of θ_c



(c) Map of θ_s

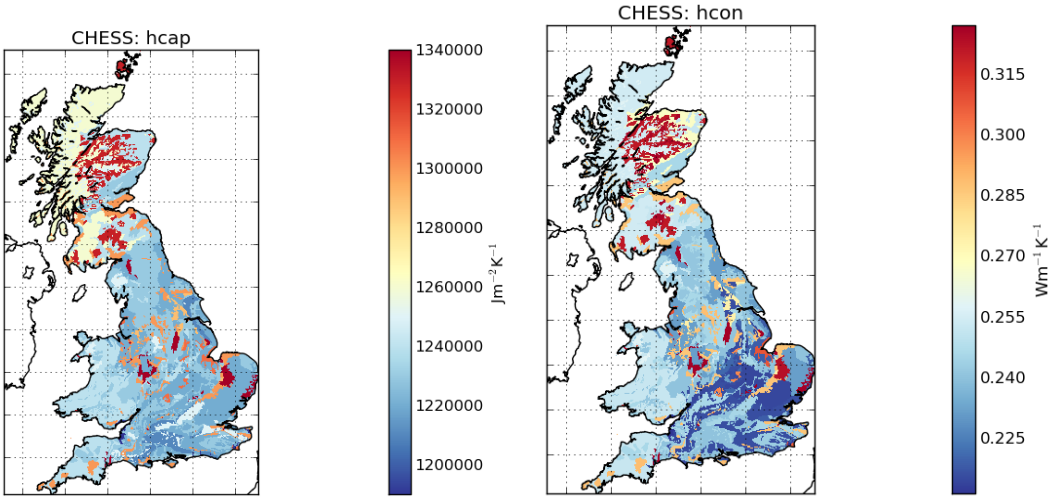
(d) Map of θ_w

Figure 9: Brooks and Corey topsoil parameters



(a) Map of Ψ_s

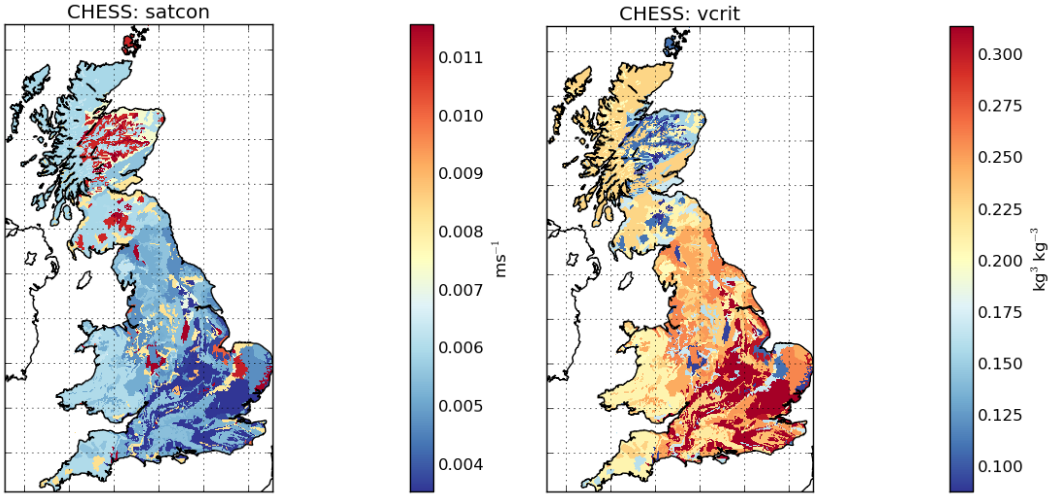
(b) Map of b



(c) Map of heat capacity

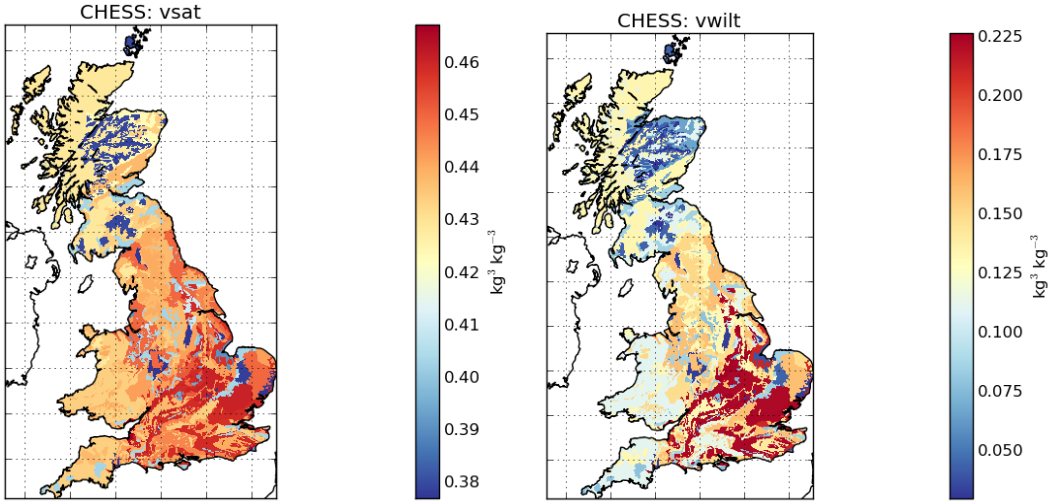
(d) Map of thermal conductivity

Figure 10: Brooks and Corey subsoil parameters



(a) Map of K_s

(b) Map of θ_c



(c) Map of θ_s

(d) Map of θ_w

Figure 11: Brooks and Corey subsoil parameters

5.5 Output files

I have used the code to create two netCDF files containing 1 km resolution maps of the parameters for four soil layers over GB. One file contains van Genuchten hydraulic properties, the Johansen heat capacity and the Peters Lidard (Johansen) thermal conductivity and the other contains Brooks and Corey hydraulic properties, the first (texture based) heat capacity method and the Farouki thermal conductivity.

References

[1] FAO/IIASA/ISRIC/ISS-CAS/JRC, 2012. *Harmonized World Soil Database (version 1.2)*. FAO, Rome, Italy and IIASA, Laxenburg, Austria.

[2] M. J. Best et al, 2001: *The Joint UK Land Environment Simulator (JULES), model description - Part 1: Energy and water fluxes*. Geosci. Model. Dev., 4, 677-699.

[3] FAO/Unesco/ISRIC, 1990. *Revised Legend of the Soil Map of the World*. World Soil Resources Report, FAO, Rome, Italy

[4] J. H. M. Wösten et al, 1999. *Development and use of a database of hydraulic properties of European soils*, Geoderma 90 169-185

[5] M. Th. van Genuchten, 1980. *A Closed-form Equation for Predicting the Hydraulic Conductivity of Unsaturated Soils*. Soil Science of Americal Journal, 44, 5.

[6] P. W. Jones. *A User's Guide for SCRIP*. Los Alamos National Lab.

	θ_r kg^{3}kg^{-3}	θ_s kg^{3}kg^{-3}	α cm^{-1}	n -	K_s cm[day]$^{-1}$
Topsoils					
Coarse	0.025	0.403	0.0383	1.3774	60.000
Medium	0.010	0.439	0.0314	1.1804	12.061
Medium-fine	0.010	0.430	0.0083	1.2539	2.272
Fine	0.010	0.520	0.0367	1.1012	24.800
Very fine	0.010	0.614	0.0265	1.1033	15.000
Subsoils					
Coarse	0.025	0.366	0.0430	1.5206	70.000
Medium	0.010	0.392	0.0249	1.1689	10.755
Medium-fine	0.010	0.412	0.0082	1.2179	4.000
Fine	0.010	0.481	0.0198	1.0861	8.500
Very fine	0.010	0.538	0.0168	1.0730	8.235
Organic	0.010	0.766	0.0130	1.2039	8.000

Table 5: van Genuchten parameters from [4]. Note that we actually need α in units of m^{-1} and K_s in units of ms^{-1}.