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EASYMORE: A Python package to streamline the remapping of variables for Earth System models

Shervan Gharari[a,*], Kasra Keshavarz[b], Wouter J.M. Knoben[c], Gouqiang Tang[d], Martyn P. Clark[b]

[a] Centre for Hydrology, University of Saskatchewan, Saskatoon, Saskatchewan, Canada
[b] Department of Civil Engineering, University of Calgary, Alberta, Canada
[c] Centre for Hydrology, University of Saskatchewan, Canmore, Alberta, Canada
[d] Climate and Global Dynamics, National Center for Atmospheric Research, Boulder, Colorado, United States

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ABSTRACT

The Earth System modeling community uses different methods to discretize a landscape in model elements, such as square grids, triangles, or irregular shapes. Mapping data from one spatial configuration to another is an essential part of environmental modeling, and can be time-consuming and cumbersome. In this work, we present a Python package called EASYMORE. EASYMORE stands for EArth SYstem MOdeling REmapper and enables users to quickly and efficiently remap variables, such as precipitation or temperature, from one spatial representation (e.g., unstructured grids) to another (e.g., sub-basins). The package is aimed to increase the efficiency of data preparation for Earth System modeling in a reproducible and transparent manner. The remapped variables, provided in netCDF or CSV formats, can then be used directly or changed to the format needed for intended uses. This manuscript presents examples that show various applications of EASYMORE.

Code metadata

Current code version	1.0.0
Permanent link to code/repository used for this code version	https://github.com/ElsevierSoftwareX/SOFTX-D-23-00264
Permanent link to Reproducible Capsule	
Legal Code License	GNU General Public License v3.0 (GPL3)
Code versioning system used	git
Software code languages, tools, and services used	Python
Compilation requirements, operating environments & dependencies	Python
If available Link to developer documentation/manual	For example: https://github.com/ShervanGharari/EASYMORE
Support email for questions	shervan.gharari@usask.ca; sh.gharari@gmail.com

1. Motivation and significance

Process-based models developed across different areas of the environmental sciences are now converging to the interdisciplinary "Earth Systems" modeling paradigm. For example, the traditional land-surface models used in numerical weather prediction and climate models have evolved from providing lower boundary conditions for the atmosphere to simulating the dynamics of terrestrial systems. These models now include many above-ground and below-ground processes – e.g., vegetation dynamics, and sub-surface lateral flow – that are needed to predict water, energy, and biogeochemical cycles. As another example, traditional hydrology models now include more sophisticated representations of ecological processes – e.g., carbon assimilation and photosynthesis – that are needed to improve simulations of transpiration. Similarly, ecological models now include more sophisticated representations of hydrological processes – e.g., lateral flow – that are needed to

* Corresponding author.
E-mail address: shervan.gharari@usask.ca (Shervan Gharari).

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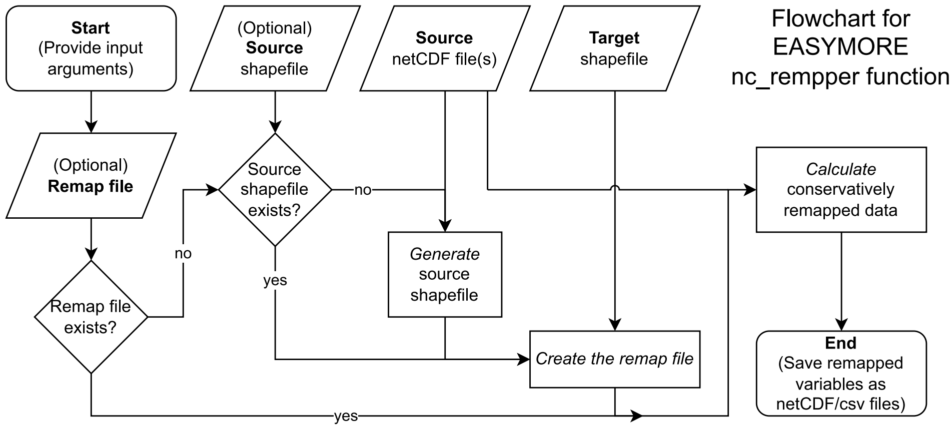

Fig. 1. EASYMORE `nc_remapper` function flowchart.

improve simulations of water stress on plants. Such terrestrial systems models require expertise from scientists across multiple disciplines, including hydrologists, biogeochemists, ecologists, geologists, atmospheric scientists, social scientists, computer scientists, and applied mathematicians.

A key task in complex environmental models is preparing the necessary geospatial and meteorological data used to force models. For example, station and gridded data (reanalysis, remotely sensed, dynamically or statistically down-scaled products) that define the atmospheric variables often needed to be remapped from their native spatial resolution to the modeling elements used in terrestrial systems models, such as grids, subbasins, or any other hypothetically define boundaries (hydrological response units, HRUs). Based on extensive hands-on experience with different Earth System models, we identified some of the main common tasks that are part of remapping variables in an Earth System modeling context. These tasks can be summarized as follows:

- Remapping variables from one spatial representation (e.g., regular grids, rotated grids, or non-regular shapes such as Thiessen polygons or Voronoi diagrams) to another spatial representation (e.g., subbasins, a different grid, or any other shape). Examples of this can be named (but not limited): (1) The transformation of gridded precipitation data to subbasins (where the simulation of the Earth System models take place), (2) remapping of temperature field to shapes with different elevations and accounting for the impact of elevation (called lapsing the temperature), (3) regridding variables from grids such as cubed-sphere or tri-polar to regularly spaced lat/lon grids, and (4) remapping of model output such as runoff field from gridded format to subbasins for river routing models.
- Extraction of data for a given point, such as extraction of temperature or precipitation from a gridded dataset at station locations for comparison or bias correction.
- Generating summary metrics for a region of interest. For example, average precipitation over a province or state.
- Visualization of variables in various configurations, original or remapped to any spatial configuration, to visually check the integrity of the original and remapped variables.

Usually, research groups and model developers use in-house scripts that are tuned for their modeling approach purposes. A part of the community uses packages that might need extensive training (for example, Earth System Modeling Framework, ESMF, https://github.com/esmf-org/esmf, [1]). Additionally, more attention is given to tasks and techniques for re-gridding of gridded dataset [2–4]. A pressing need for a package to fulfill the above-mentioned bullet points is apparent. In this study, we introduce EASYMORE: an easy-to-use Python package designed for these tasks in a generalized form. In the following, the EASYMORE package is explained, a few examples are provided and its impact on the Earth System modeling community and ongoing research is presented.

2. Software description

2.1. Software access, requirements and community

EASYMORE is a Python package available on the Python Package Index, PyPI repository https://pypi.org/project/easymore/. It can therefore be installed using package installer, `pip`, by using `pip install easymore`. EASYMORE is designed for Python 3 and its source code is available on the following GitHub repository https://github.com/ShervanGharari/EASYMORE. The package dependencies are described in `setup.py` file and installed upon the packaged installation. The main packages that provide the functionality of EASYMORE are netCDF4, xarray, numpy, pandas, and geopandas among others (and their underlying code and modules such as gdal and netcdf). The contribution guidelines for EASYMORE are described in `CONTRIBUTING.md` file on the EASYMORE GitHub repository.

2.2. Software architecture and functionality

EASYMORE functions are prepared in an `easymore` class of functions in a file called `easymore.py`. The core functionality of EASYMORE is the function `nc_remapper`. `nc_remapper` calls any other functions in the `easymore` class depending on the case the user specifies. All other functions in the `easymore` class, such as the function to create point shapefiles, `make_shape_point`, from the pandas dataframe, or from the netCDF or CSV files that contain latitude and longitude variables of station data (e.g, `dataframe_to_netcdf_xr` can be used to create a netCDF file from station data that is saved as CSV file), can also be called individually and directly.

EASYMORE's core function `nc_remapper` takes the following inputs (see Fig. 1 for an overview of the full remapping procedure):

- A (collection of) source netCDF file(s), which contain data values for specified latitude/longitude coordinates;
- (Optionally) a source shapefile, which includes polygons to describe the spatial area of each latitude/longitude coordinate in the source netCDF file;
- A target shapefile, which includes polygons to describe the spatial area for which representative data is desired, i.e., the polygons we want to map the data in the source netCDF file(s) onto;
- (Optionally) a remap file, which describes the areal overlap between the source and target shapefiles.

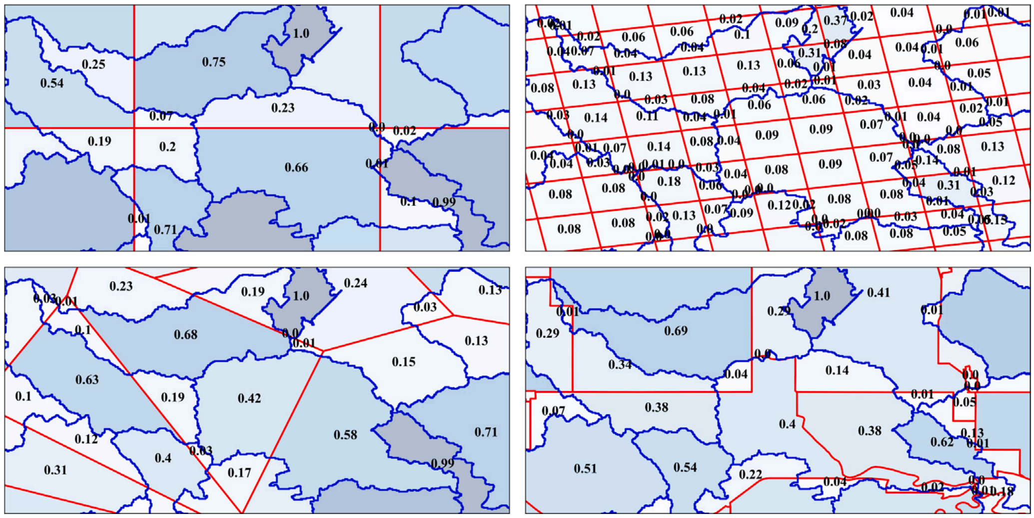

Fig. 2. Visualization of weights (expressed as numbers) from source shapefile (red outlines) to target shapefile (blue outlines) for four different types of source shapefiles: (top left) regularly spaced latitude/longitude grid of ERA5, (top right) the rotated grids of WRF-CONUS-I, (bottom left) Thiessen or Voronoi polygons of stations presence in SCDNA dataset, and (bottom right) irregular shapes showing the dissemination area for Canadian census. The target shapefile in all cases shows the river basins that make up the South Saskatchewan River at Medicine Hat, Alberta, Canada. These examples are discussed in more detail in Section 3. Note that the weight might not sum to 1.00 due to rounding of values for visualization purposes. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

When provided with a source netCDF and a target shapefile, EASYMORE `nc_remapper` first checks if the data in the source netCDF follow a regular or rotated grid. If this is not the case, EASYMORE assumes that each data-point at a specific latitude/longitude coordinate is representative of an area around these coordinates and EASYMORE will automatically create Thiessen polygons (also known as Voronoi diagrams) based on the latitude/longitude coordinates in the source netCDF file. Data values are then assumed to be representative values for Thiessen polygon areas. This behavior can be overridden if the user provides a "source shapefile", that contains the polygons for which each data value is considered to be representative. Providing a custom source shapefile (rather than relying on the built-in Thiessen polygons) can, for example, be helpful in cases of rapid topographic change, where real-world mountain ranges dictate to a large extent the regions in which data points are representative. EASYMORE `nc_remapper` then calculates the areal overlap between each source polygon (created either internally or taken from the source shapefile) and each polygon in the target shapefile and saves this information in a so-called remap file. The user can short-circuit this procedure by specifying an existing remap file as an input to the `nc_remapper` function. If such a remap file is provided EASYMORE `nc_remapper` will skip all GIS-based processing steps. This can be beneficial in cases where multiple source netCDF files with the same spatial organization need to be remapped repeatedly. Finally, EASYMORE uses the areal overlaps to remap values in the source netCDF onto the polygons in the target shapefile and saves the results as a new netCDF file (and optionally CSV files). An example of various source-to-target configurations for subbasins of the South Saskatchewan River up to Medicine Hat in Alberta, Canada, is provided in Fig. 2.

It is noteworthy to mention that the internal remapping weights are first-order conservative [5]. This means the weights used for remapping are based on the fraction of areas from the source shape in the target shape. However, the remap file and its weight can be created outside of `nc_remapper` to emulate second-order conservative remapping, or Kriging with any type of semivariogram [6]. Examples of such cases are presented on EASYMORE GitHub repository https://github.com/ShervanGharari/EASYMORE while examples that are presented in this study follow first-order conservative assumptions as depicted in Fig. 2.

EASYMORE's `nc_rempper` has the capability to rescale the remapping weights and normalize them in two steps (by default). The first normalization of weights is when the source and target shapes do not fully overlap. The second layer of normalization of weights is based on the existing missing values in the source netCDF files and it is performed per time step. A hypothetical example is provided in Fig. 3. The top left panel provides the source and target shapes with their IDs. The target shapefile includes multi-polygons with an IDt of 23 or outside of the boundaries of source shapes with an IDt of 25. The top right panel provides the weight of source shapes in the target shapes. The sum of weights for each overlapping target shape with source shapes is one (normalized). The bottom panels provide the source and remapped values for the two different time steps without and with missing values (identified by nan in the figure). When the source shape includes no data for a specific time, `nc_remapper` by default rescales the weight to unity. This can be seen for shapes with IDt of 21 and 22 (the missing values are ignored and the remapping weights are normalized to ignore missing values). This rescaling of the weights results in the estimation of values for target shapes with new weights from the source that is conserved (not affected by weights that are not summing to unity due to missing values). This is important for Earth System modeling as it preserves the mass or energy during the remapping from source to target shapes.

2.3. Input and output formats

EASYMORE uses two file formats as its main input and output files. These two formats are netCDF and ESRI shapefile. NetCDF, or Network Common Data Form; with the typical extension of .nc, is a set of software libraries and machine-independent data formats that support the creation, access, and sharing of array-oriented scientific data. NetCDF is self-describing and scalable which makes it suitable for spatial and temporal storage of Earth System data [7].

A shapefile, with the typical extension of .shp, is a widely used format to represent spatial data or features as a vector of point(s), multi-point(s), polygon(s), multi-polygon(s), and line(s). The shapefile format was developed by the Environmental Systems Research Institute [8, ESRI], and is now commonly used with open-source software and packages. Data is typically distributed over multiple files with different extensions (.shp, .dbf, .shx, .prj). The file with the extension .shp is the file that includes the geometry of the shape. Each element in the file with the .shp extension identifies whether the shape is (multi-)point(s), (multi-)line(s), (multi-)polygon(s) as well as the coordinates of those shapes. dBASE files with the .dbf extension contain any feature

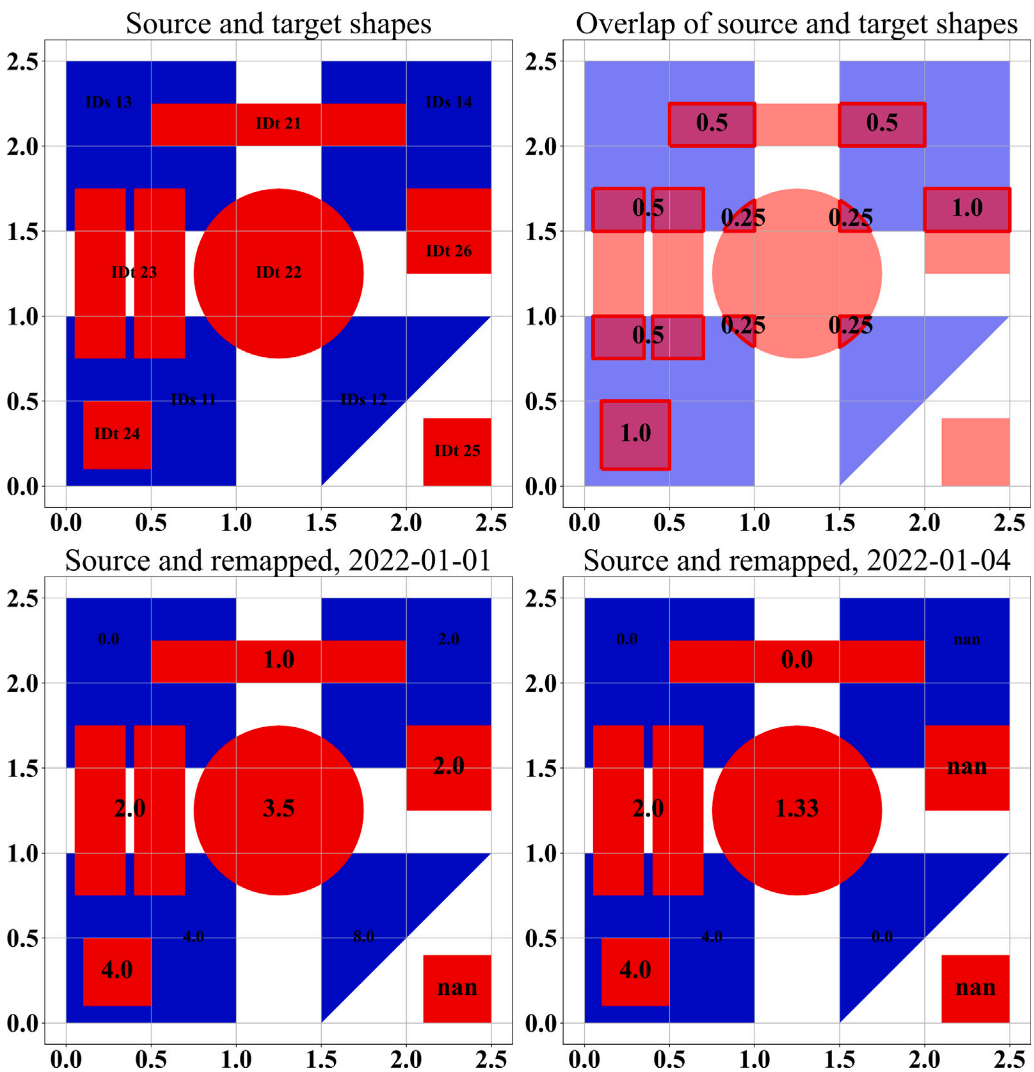

Fig. 3. A Hypothetical example of a source and target shapefile and variables. (Top left) Source (blue) and target (red) shapefile IDs are represented by IDs and IDt respectively. In this case, one wants to compute the currently unknown data values of the red shapes from the known data values in the blue shapes based on their overlapping areas. (Top right) Normalized weights show how much each source shape contributes to the computation of target values. Weights are determined based on the relative overlap of source shapes for a given target shape. For example, the top horizontal red bar overlaps equally with both the top left and top right blue squares. The normalization procedure assigns weights of 0.50 (50%) to each overlap, and so accounts for the middle part of the red shape that does not overlap with any blue shapes. (Bottom left) Source (blue) and remapped (red) values. Data values in the red shapes are derived from the known values in the blue shapes and the weights shown in the top right plot. This example assumes values are known for all source shapes. (Bottom right) Source and remapped values for a case with missing values (nan) in the source netCDF file (blue shapes). In this case, weights are adjusted to exclude the source shapes with nan values. For example, the top horizontal red bar overlaps equally with both the top left and top right blue squares but its value is determined solely from the top left square, because no data value is known for the top right square. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

attributes and their keys for each shape. .shx files are index files and files with extension .prj define the spatial projection of vectors that are held in the geometry of the shapefile.

3. Examples

The examples in the following sections are presented under the examples folder on the EASYMORE GitHub repository. These examples are intended to highlight EASYMORE's remapping functionality and focus on specific aspects that are common to Earth System modelers. The target shapefile in all cases contains polygons of irregular shape. There is no fundamental difference between remapping to regular grids or rotated grids compared to irregular shapes in terms of the requirements imposed on EASYMORE's `nc_remapper` function.

3.1. Remapping of ERA5 data on a regularly spaced grid to sub-basins of the South Saskatchewan River

ERA5, a meteorological reanalysis product by [9], provides an example of remapping the variables from a netCDF file with regularly spaced grids into the subbasins of the South Saskatchewan River up to the city of Medicine Hat, in Alberta, Canada. This example is based on the remapping of the temperature field from grids to subbasins (Fig. 4).

There might be cases in which the target shapefile and the domain of the source netCDF file(s) do not overlap. As an example, a gridded source netCDF file containing precipitation values may be limited to an administrative border that does not overlap with all the subbasins of a major river basin. EASYMORE allows the user to keep the non-overlapping shapefile values as nan or fully remove them from the remapped file based on the needs without manually selecting or preparing overlapping shapes. Fig. 5 depicts an example in which the source

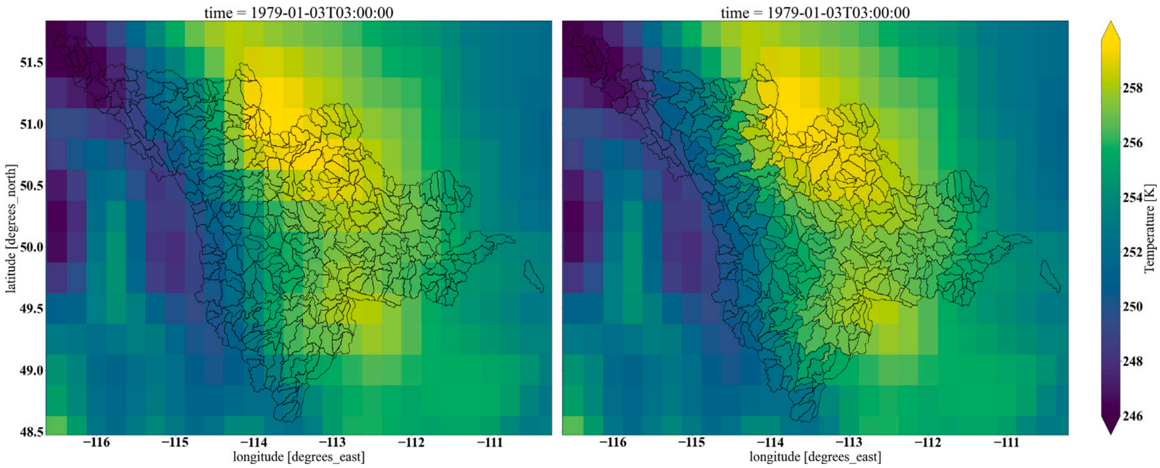

Fig. 4. Visualization of temperature field for ERA5 dataset from (left) the original grids to (right) remapped variables at subbasins.

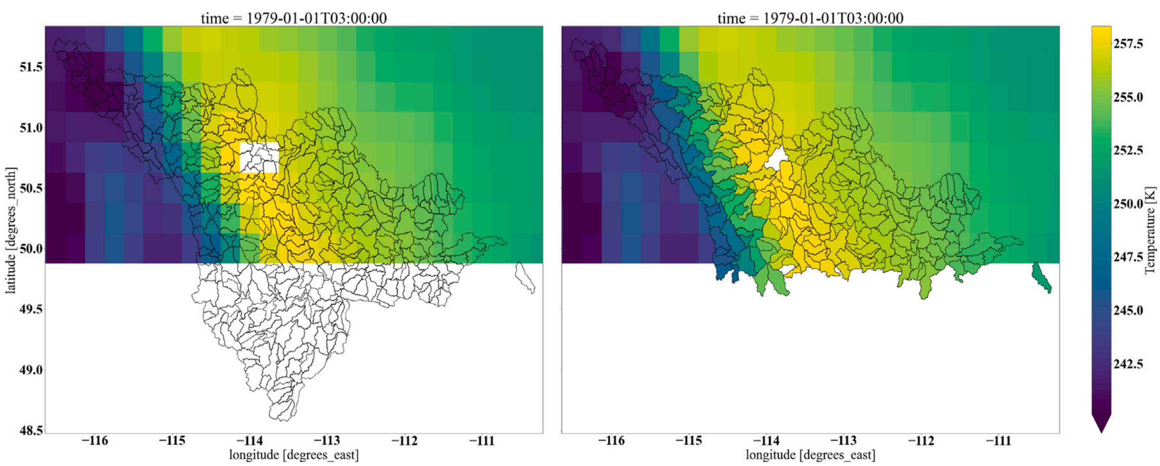

Fig. 5. Visualization of temperature field from ERA5 dataset with missing values for two grids and non-overlapping areas from (left) the original grids to (right) remapped variables at subbasins. Shapes with nan values are not shown in the right panel.

netCDF files extent does not overlap with the target shapefile and values of a few grids do not exist for a few time steps (nan). EASYMORE can rescale weights for the non-overlapping shape or grids without values and provide conserved remapped variables at target shapes that are comparable to other overlapping target shapes from Fig. 5.

3.2. Remapping of WRF-CONUS-I to sub-basins of the South Saskatchewan River

The second example provides the remapping of rotated coordination for netCDF file(s) in which each grid has a different latitude and longitude (not uniformly spaced). WRF-CONUS-I by [10] which is a dynamically downscaled atmospheric variable product from NCAR, National Center for Atmospheric Research of the United States, is selected for this example. Similarly to regularly spaced grids of ERA5, EASYMORE can remap the temperature variables to the subbasins of the South Saskatchewan River (Fig. 6).

3.3. Remapping of SCDNA to sub-basins of the South Saskatchewan River

SCDNA by [11] provides a serially complete station dataset for approximately 26000 stations across the North American domain. EASYMORE package can create the Voronoi diagram or Thiessen polygons for stations based on the latitude and longitude provided in the netCDF file. EASYMORE uses the created Thiessen polygons, or any other shapefile which might be provided as a source shapefile alongside the netCDF files, and creates the remapping file. The remapping file is then used, similar to earlier examples, to remap the variables from stations' locations to sub-basin shapes (Fig. 7).

3.4. Population density of subbasins of the South Saskatchewan River

This example focuses on the capabilities of creating a netCDF file from an external source, alongside its shapefiles, to remap specific variables. The Canadian census of 2016 and its dissemination area, which is the delineated areas that account for 400 to 700 inhabitants on average, are used for remapping the population density to subbasins of south Saskatchewan regions. First, the census data alongside its IDs (that correspond to the dissemination areas) are converted into a netCDF file from CSV files using EASYMORE `dataframe_to_netcdf_xr`. Then the `nc_remapper` is called using the created netCDF file as the source file and its associated shapefile is used to ramp the population density to the subbasins of the South Saskatchewan River (Fig. 8). Note, for this example, we used an area-independent variable such as population density for the average rather than absolute population.

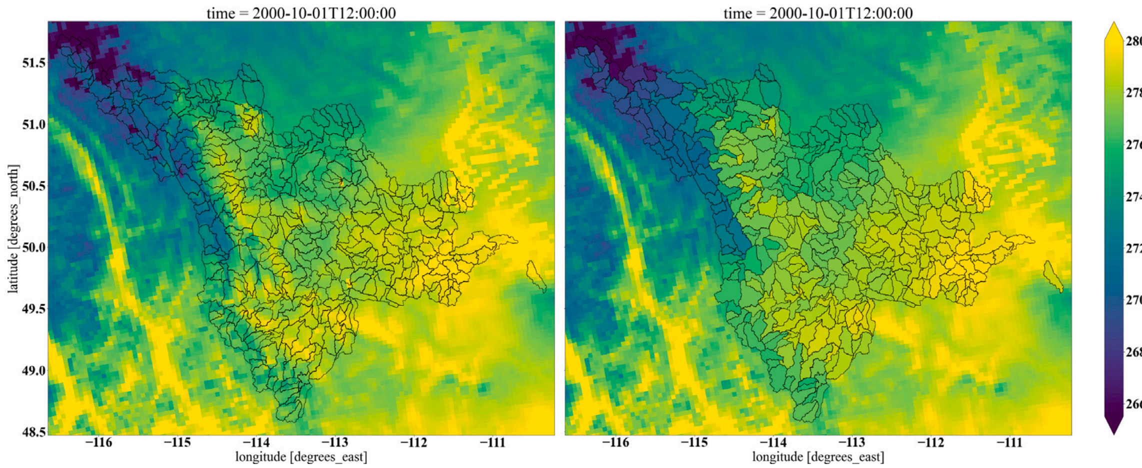

Fig. 6. Remapping of WRF-CONUS-I temperature field from (left) original rotated grids to (right) remapped variable at South Saskatchewan sub-basins.

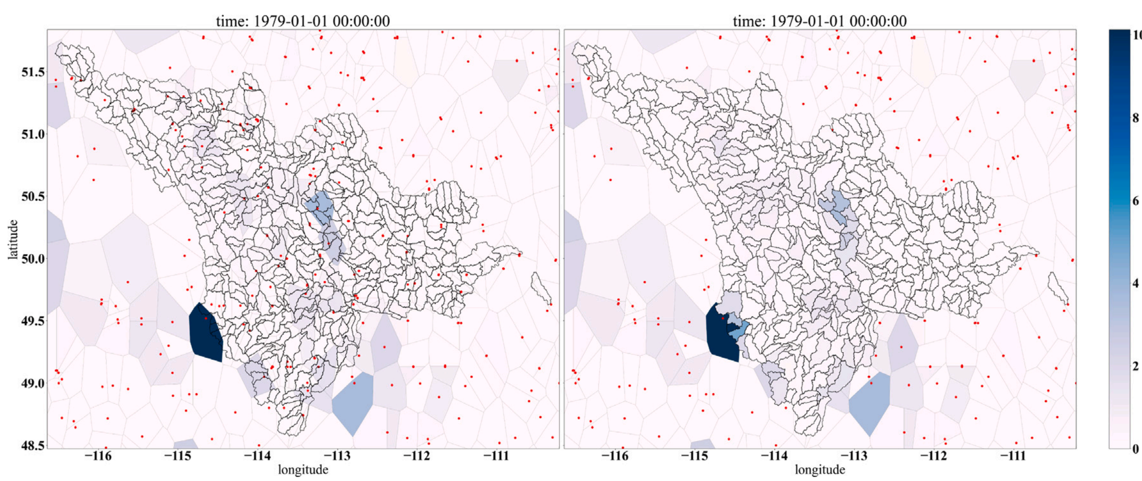

Fig. 7. Remapping of precipitation field for SCDNA dataset from (left) Voronoi diagram or Thiessen polygons to (right) subbasin of South Saskatchewan River. Red dots indicate locations of stations for which the Thiessen polygons are created.

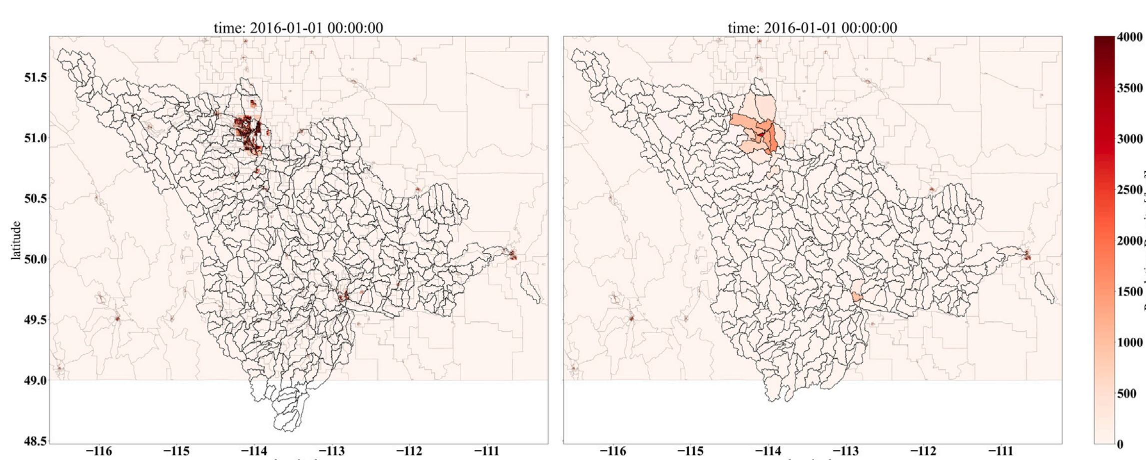

Fig. 8. Remapping of population density from (left) dissemination areas to (right) subbasin of South Saskatchewan River. Shapes with nan values are not shown in the right panel.

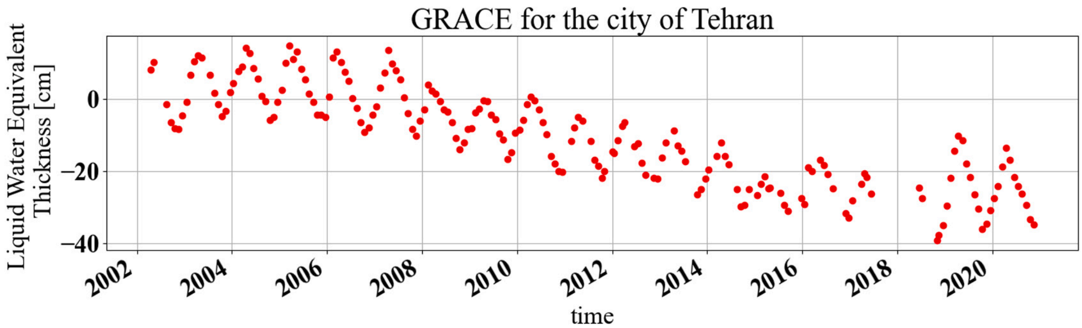

Fig. 9. Change in GRACE reading of terrestrial water for the City of Tehran over the past two decades.

3.5. Extracting the GRACE dataset for the capital cities

The last example in this work is reading the GRACE dataset [12, Gravity Recovery and Climate Experiment]. GRACE is a space-born product that provides an understanding of freshwater changes over the world at a resolution of 1 degree (approximately grids of 100 kilometers at equators). The GRACE dataset is provided with a longitude of 0 to 360 while the target shapefile for capitals of the world is given with a longitude between −180 to 180 degrees. EASYMORE can recognize this difference and correct the shapefile so they can read the right values from the source netCDF file. The GRACE anomaly is extracted for the point shapefile of all the capital cities around the world. The data for the grid where the city of Tehran is located is plotted in Fig. 9.

4. Impact

Our goal with EASYMORE is to reduce the time costs needed to prepare inputs for Earth System Models. A notable use of EASYMORE in Earth System modeling is given in the CWARHM initiative, which is focused on reproducible science and transparent modeling workflows [13, CWARHM: Community Workflows to Advance Reproducibility in Hydrologic Modeling]. EASYMORE plays a critical role in the remapping of meteorological and geospatial data in this project. Recent studies using CWARHM, and its EASYMORE component, to study the impact of meteorological forcing uncertainty on hydrological processes are published or under review [14]. These studies are easier to carry out because the remapping of many ensemble members and databases is streamlined within the single EASYMORE package. EASYMORE is currently seeing uptake beyond the original group of developers. This is evidenced by the use of EASYMORE for more flexible model configuration for Earth System legacy models [15, CREST-VEC], and the numerous downloads through PyPI (https://pypistats.org/packages/easymore).

As mentioned in the introduction, other tools can be used for remapping purposes such as ESMF. These tools are often very comprehensive on the scientific and computational fronts. However, users may experience a steep learning curve. EASYMORE is a focused tool that provides easy-to-use remapping capabilities commonly needed in Earth System Modeling and catchment hydrology. Additional examples of EASYMORE capabilities beyond those discussed in Section 3 are presented on the GitHub repository (https://github.com/ShervanGharari/EASYMORE) as Jupyter notebooks. These provide a clear starting point for novice users and cover the most common remapping cases.

5. Conclusions

EASYMORE provides a Python package for remapping variables from netCDF file(s) to any desired shape provided within a shapefile. The package is part of the Python indexing package and is open-source and available to the public on GitHub. We look forward to more use of this package and improvement in the future both in the sense of efficiency and complexity of cases that the package can handle. We would like to emphasize that the accuracy of remapping is based on `nc_remapper` workflow in creating the remapping file, its assumptions, and underlying packages and libraries. A careful assessment and comparison of generated grids, Thiessen polygons, the remapping file, and remapped values with other similar packages is necessary in the future.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

No data was used for the research described in the article.

Acknowledgment

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