Supplement 1: MATLAB® Data Import

There are several ways to import data into the MATLAB workspace. See topic ‘Using Import Functions with Text Data’ in the online help for an overview concerning text data. There are special commands for importing spreadsheet data (\texttt{csvread}); there is even a special command for importing from Microsoft EXCEL: \texttt{xlsread}.

It is not the intention here to go into details. We demonstrate a user-friendly tool, which provides a data preview and several data manipulation tools during importing. The ‘Open Import Wizard’ interface is called by \texttt{uiimport}

from the MATLAB® command window. The functionality is exemplified on one of the most cited data sets, showing the increase of atmospheric CO\textsubscript{2} concentrations within almost 50 years. The data-set, which is measured at the Mauna Loa Observatory in Hawai’i at a height of 3400 meters above sea-level, can be obtained from the internet. For monthly recorded data see: http://www.seattlecentral.org/qelp/set78/078.html. All data are given in a single ASCII text file. Typical content is depicted after calling \texttt{uiimport} from the command window and opening the file (see Fig. S.1).

\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{fig_s1.png}
\caption{Data import, 1st screen}
\end{figure}
After pressing the ‘Next’ button another similar window appears, which allows some manipulations on the data file. Here it is important to increase the number of text header lines to 15. After that in the right data window the data matrix appears, as depicted in the Fig. S.2.

The year is given in the first column; 14 following columns show month related concentrations, the annual mean and a fitted annual mean. As we liked to take the monthly measurements only, we highlight the corresponding 12 columns by mouse-click in the right data window. Use the right mouse button to obtain a pop-up window, including a copy button. After copying the highlighted columns, use the ‘Back’ button to return to the first window; and select ‘Clipboard’ using the corresponding radio button. Now the carbon-dioxide values appear in the data blocks; years are omitted.

Click two times ‘Next’ to move to the final window. Here, choose only to re-name the data variable (use again right mouse button) to ‘CO2’. The final ‘Finish’ (button!) creates a new variable with the chosen name in the workspace (see Fig. S.3). With that operation the command is finished and the wizard disappears.
In the next step we manually change ‘-99.99’ entries in the data set that is used in the data set for missing values, to ‘NaN’, which fits with the MATLAB\textsuperscript{®} convention (using copy and paste operations in the array editor. There are only few missing values, which allow the manual operation. For more complex data sets one has to utilize some MATLAB\textsuperscript{®} commands as demonstrated in the following.

In order to plot the data, the matrix is transformed into a row vector. This can be done using the following command sequence:

```matlab
for i=1:47
    for j = 1:12
        co2(12*(i-1)+j)=CO2(i,j);
        t(12*(i-1)+j)=datenum(1957+i,j,15)
    end
end
```

The 2D data set in the variable ‘CO2’ is converted to a row in the variable ‘co2’. In addition another row vector with corresponding times is created. We use the serial date number, which is one of several MATLAB\textsuperscript{®} alternatives to represent date and time (for more information see the online help index ‘dates and times’). The `datenum` command converts a date into the serial date number. Called with three numbers, these correspond to year, month and day. There are several more alternative calls of the command, which the user may look up in the help. The aimed plot is finally created by the commands:

```matlab
plot (t,co2)
datetick ('x',11)
xlabel (year); ylabel('Atmospheric CO\textsubscript{2} [ppm]');
```

The following figure results. Corresponding to the time format the datetick command offers several options to display time. There is a list of 28 alternatives which can be applied by the `datetick` command. Here we choose to show the year only. The result is shown in Fig. S.4.
Supplement 2: Data Export

Data are exported by using the `save` command. Let us take the calculated `co2` data from Supplement 1 as an example. The command

```
save ('co2.mat', 'co2')
```

stores the values in the file `co2.mat` in the working directory. Make sure that the user has write-permissions on that file. Otherwise change the directory by using the `cd` (change directory) command. Note that MATLAB® has its own data storage format that is the default here. Usually the extension `.mat` is used for files with that data format.

Other data formats can also be stored. Most important is the ASCII format, which is obtained by using:

```
save ('co2.mat', 'co2','-ascii')
```

Also important is the `-append` option for the data to be appended at the end of an existing file.
Supplement 3: Data Presentation in a Histogram

There are various ways to represent environmental data using MATLAB®. The reader may have a look in MATLAB® online command index for the `hist`, `bar` and `bar3` commands.

As an example we show a histogram of concentration measurements of different chemical species at various observation points. Six species were measured at 13 positions. The entire data-set is stored in a matrix \( C \).

The histogram is then produced by the `bar` command:

```matlab
bar(C);
```

The code can be found on the CD under the name ‘`bardemo.m`’

![Histogram of concentration measurements](image)

**Fig. S.5.** Example data representation in a histogram
The result of the M-file is depicted in Fig. S.5. Further commands concern the labels of the axes and the legend. Note how greek characters are introduced in the text, by using the \ operator.

```m
xlabel ('observation points');
ylabel ('C [\ mug/l]');
title ('measured concentrations');
legend ('Na','Cl','B','HCO3','F','TOC');
```
In twenty chapters, the book shows various applications of MATLAB® in the field of environmental modeling. Numerous MATLAB® commands are introduced and their use demonstrated. Various fields of environmental modeling have been touched.

After twenty chapters, the book remains incomplete. Neither the entire field of environmental modeling is covered, nor is the entire capability of MATLAB® exploited. Of course, either of the mentioned tasks would be too ambitious to be worked out, even within several book volumes.

Is something missing that is important? Probably everyone working in the field of environmental modeling, who does not find her/his special problem set-up, will say, yes. It was already mentioned that the entire field is too vast. Concerning MATLAB®, the important application field of numerical methods for 2D and 3D applications is missing. MATLAB® can be used to implement important numerical approaches, like finite differences, or finite elements. These methods were omitted as a consequence of the decision to focus on core MATLAB®. The easiest way to apply such numerical techniques is to use the partial differential toolbox of MATLAB®. Core MATLAB® could also be used to implement higher-dimensional numerical models, but manual programming skills are required. Only the advanced user would be addressed by this topic, to whom the recently published book of Danaila et al. (2007) can be recommended. Among other numerical topics Quarteroni (2003) outlines methods for the advection diffusion equation using advanced Finite Element modeling techniques and presents MATLAB® source code for the solution of the 1D steady state.

Concerning the environment, the hydrosphere is surely over-represented in the book, while the atmosphere and the pedosphere appear only sporadically. Among the hydrosphere topics, groundwater has the biggest share. The choice of the topics is surely due to the background of the author, who in the past mainly worked in the favored fields. However, the mathematical concepts that were introduced are mostly independent from the environmental compartment
and thus applicable in several environmental areas. The given applications should be viewed as examples for the mathematical techniques.

It was the purpose of the book to give a first introduction. I hope that goal is reached. Aside from that, some novel approaches have been introduced and examined which are beyond state-of-the-art. Some of these approaches turn out to be simple and useful and will hopefully find their way into the practice of environmental modeling. If that really happens, is due to the reader and her/his conception of the book. In that sense, I wish the book to find understanding readers who make these concepts work.

References

Quarteroni A., Modellistica Numerica per Problemi Differenziali, Springer Publ., Milan, 332p, 2003 (in Italian)
The following list gathers the MATLAB® commands, which are mentioned in the book. For each command find the corresponding chapter and sub-chapter numbers within the book. For frequently appearing commands the most important occurrences are listed, only.

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Companion Software List

The accompanying CD contains the M-files which are described in the book, sometimes extended versions. The files can also be downloaded from the MATLAB® central file exchange (www.mathworks.com/matlabcentral/fileexchange).

advection.m  MichaelisMenten.m
analtrans.m  newtondemo.m
analtrans_s1.m  nuclides.m
analtrans_s2.m  OpenChannel.m
analtrans_s3.m  par_est.m
analtrans_s4.m  par_esta.m
analtransnodim.m  par_estb.m
AnElements.m  par_estc.m
animation.mpg  par_est2.m
bardemo.m  par_est2a.m
boudreau_westrich.m  pdepetrans.m
comparts.m  phasediag.m
compspec.m  predprey.m
cplxPot.m  re toxsteady.m
diffusion.m  retention.m
dipole.m  richards.m
DischargePotential.m  simpletrans.m
GaussianPlume.m  slowsorp.m
GaussianPuff.m  Speciation.m
GdDTPA.m  StreeterPhelps.m
georef.m  strtransanal.m
gw_flow.m  thiem_test.m
histogram.m  ThreeD_flow.m
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