PEcAn v1.4.7 Hands-On Demo

In the following demos, URL is the web address of a PEcAn server and will refer to one of the following:

- If you are doing a live demo with the PEcAn team, URL was provided
- If you downloaded the PEcAn VM, URL = localhost:6480
- If you are running PEcAn on Amazon AWS, URL is the Public IP
- If you installed PEcAn on your server, URL is your server’s IP

Demo 1: Single-site model run

Objective:

We will begin by exploring a set of web-based tools that are designed to run single-site model runs. A lot of the detail about what’s going on under the hood, and all the outputs that PEcAn produces, are left to Demo 2. This demo will also demonstrate how to use PEcAn outputs in additional analyses outside of PEcAn.

1. Start PEcAn: Enter URL/pecan in your web browser

Click the ‘Next’ button to move to the “Site Selection” page.
2. Site Selection

1. **Host**: Select the local machine “pecan64” Other options exist if you’ve configured PECaN to run models on remote servers.
2. **Model**: Select SIPNET from the available models because it is quick & simple.
3. **Site Group**: To filter sites, you can select a specific group of sites. For this tutorial we will use Ameriflux.
4. **Conversion**: Select the conversion check box, to show all sites that PECaN is capable of generating model drivers for automatically. By default (unchecked), PECaN only displays sites where model drivers already exist in the system database.
5. **Site**: For this tutorial, type US-NR1 in the search box to display the Niwot Ridge Ameriflux site (US-NR1), and then click on the pin icon. When you click on a site’s flag on the map, it will give you the name and location of the site and put that site in the “Site:” box on the left hand site, indicating your current selection.
6. **Click “Next”**
3. Run Specification

Next we will specify settings required to run the model. Be aware that the inputs required for any particular model may vary somewhat so there may be addition optional or required input selections available for other models.

1. **PFT (Plant Functional Type):**
   Niwot Ridge is temperate conifer. Available PFTs will vary by model and some models allow multiple competing PFTs to be selected.

2. **Start/End Date:** Select 2004/01/01 to 2007/12/31. In general, be careful to select dates for which there is available driver data.

3. **Weather Data:** Select “Use Ameriflux” from the available meteorological drivers.

4. **Optional Settings:** leave all blank for demo run
   1. **Email** sends a message when the run is complete.
   2. **Use Brown Dog** will use the Brown Dog web services in order to do input file conversions. *(Note: Required if you select Use NARR for Weather Data)*
   3. **Edit pecan.xml** allows you to configure advanced settings via the PECan settings file.
   4. **Edit model config** pauses the workflow after PECAn has written all model specific settings but before the model runs are called and allows users to configure any additional settings internal to the model.
   5. **Advanced Setup** controls ensemble and sensitivity run settings discussed in Demo 2.
   6. **Click Next** to start the model run.

6. You will see a data policy statement if you selected a data source with a policy. Agreeing to the policy is required prior to starting the run.

**If you get an error in your run today** it is probably simplest to start over and try changing options and re-running (e.g. with a different site or PFT), as time does not permit detailed debugging.
4. Model Run Workflow

1. **MET Process**: First, PEcAn will download meteorological data based on the type of the Weather Data you chose, and process it into the specific format for the chosen model.

2. **TRAIT / META**: PEcAn then estimates model parameters by performing a meta-analysis of the available trait data for a PFT. TRAIT will extract relevant trait data from the database. META performs a hierarchical Bayes meta-analysis of available trait data (1). The output of this analysis is a probability distribution for each model parameter. PEcAn selects the median value of this parameter as the default, but in Demo 2 we will see how PEcAn can use this parameter uncertainty to make probabilistic forecasts and assess model sensitivity and uncertainty. Errors at this stage usually indicate errors in the trait database or incorrectly specified PFTs (e.g. defining a variable twice).

3. **CONFIG**: writes model-specific settings and parameter files

4. **MODEL**: runs model.

5. **OUTPUT**: All model outputs are converted to **standard netCDF format**

6. **ENSEMBLE & SENSITIVITY**: If enabled post-process output for these analyses

**Congratulations!** If you got this far, you have managed to run an ecosystem model without ever touching a line of code! Now it’s time to look at the results. When the workflow is done click Finished.

FYI, **adding a new model** to PEcAn does not require modification of the model’s code, just the implementation of a wrapper function.
5. Output and Visualization

For now focus on graphs, we will explore all of PEcAn’s outputs in more detail in Demo 2.

1. Graphs
   1. Select a Year and Y-axis Variable, and then click 'Plot run/year/variable'. Initially leave the X-axis as time.
   2. Within this figure the points indicate the daily mean for the variable while the envelope encompasses the diurnal variability (max and min).
   3. Variable names and units are based on a standard netCDF format.
   4. Try looking at a number of different output variables over different years.
   5. Try changing the X-axis to look at bivariate plots of how different output variables are related to one another. Be aware that PEcAn currently runs a moving min/mean/max through bivariate plots, just as it does with time series plots. In some cases this makes more sense than others.

2. Alternative Visualization: Shiny
   1. Open another window to URL/shiny
   2. Click on workflowPlot.

The shiny app will automatically access your run’s output files and allow you to visualize all output variables as a function of time. Use the pull down menu under Variable Name to choose whichever output variable you wish to plot.

6. Model Run Archive
   Return to the URL/pecan window and Click on the HISTORY button. Click on any previous run in the “ID” column to go to the current state of that run's execution -- you can always return to old runs and runs in-progress this way. The run you just did should be the more recent entry in the table. For the next analysis, make note of the ID number from your run.
7. Analyzing model output

In this final section we will compare model outputs to data outside of the PEcAn web interface. The goal of this is to demonstrate that it is straightforward to perform additional analyses using PEcAn’s outputs. To do this you can download each of the Output files, and then perform the analyses using whatever software you prefer, or you can perform analyses directly on the PEcAn server itself. Here we’ll be analyzing model outputs in R using a browser-based version of RStudio that’s installed on the server.

1. Open RStudio Server in a new window at URL/rstudio

![Image of RStudio interface]

1. The username is *carya* and the password is *illinois*.

2. To open a new R script click File > New File > R Script

3. Use the Files browser on the lower right pane to find where your run(s) are located
   1. All PEcAn outputs are stored in the **output** folder. Click on this to open it up.
   2. Within the outputs folder, there will be one folder for each workflow execution. For example, click to open the folder PEcAn_99000000001 if that’s your workflow ID.
   3. A workflow folder will have a few log and settings files (e.g. pecan.xml) and the following subfolders:
      - *run* contains all the inputs for each run
      - *out* contains all the outputs from each run
      - *pft* contains the parameter information for each PFT

   Within both the run and out folders there will be one folder for each unique model run, where the folder name is the run ID. **Click to open the out folder.** For our simple case we only did one run so there should be only one folder (e.g. 99000000001). Click to open this folder.

4. Within this folder you will find, among other things, files of the format `<year>.nc`. 
Each of these files contains one year of model output in the standard PEcAn netCDF format.

2. Load and plot the model output

```r
library(PEcAn.utils)
arun <- read.output(99000000001, "output/PEcAn_99000000001/out/99000000001/",2006,2006,c("time","NEE"))
plot(arun$time,arun$NEE,type="l",ylab="kg ha-1 yr-1",xlab="day of year")
```

The arguments to `read.output` are the run ID, the folder where the run is located, the start year, the end year, and the variable being read.

3. Compare model to flux observations

**First** load up the observations and take a look at the contents of the file

```r
library(PEcAn.assim.batch)
names(obs)
```

Here 0-722 is the database site ID, a folder that was created when you selected the site and PEcAn downloaded the Ameriflux NetCDF (.nc) file from the Ameriflux website.

**Second**, change all missing values from -9999 to not a number (NA) and also u* filter the fluxes. Here we will apply a conservative u* of 0.2.

```r
obs[obs==-9999]=NA
obs$NEE[obs$UST<0.2]=NA
```

**Third**, convert the model to have the same units as the data

```r
modNEE <- ud.convert(arun$NEE,"kg ha-1 yr-1","ug m-2 s-1")/12.0 #12 g C per mol
```

**Fourth**, plot model predictions vs. observations and compare this to a 1:1 line

```r
plot(modNEE,obs$NEE)
abline(0,1,col="red") # intercept=0, slope=1
```

**Fifth**, calculate the Root Mean Square Error (RMSE) between the model and the data

```r
rmse = sqrt(mean((modNEE-obs$NEE)^2,na.rm = TRUE))
```

**Finally**, plot time-series of both the model and data together

```r
plot(arun$time,modNEE,type='l',ylab="umol m-2 s-1",xlab="day of year")
lines(arun$time,obs$NEE,col="green")
```
DEMO 2: Ensemble & Sensitivity Analyses

In Demo 2 we will be looking at how PEcAn can use information about parameter uncertainty to perform three automated analyses:

- **Ensemble Analysis:** Repeat numerous model runs, each sampling from the parameter uncertainty, to generate a probability distribution of model projections. Allows us to put a confidence interval on the model.
- **Sensitivity Analysis:** Repeats numerous model runs to assess how changes in model parameters will affect model outputs. Allows us to identify which parameters the model is most sensitive to.
- **Uncertainty Analysis:** Combines information about model sensitivity with information about parameter uncertainty in order to determine the contribution of each model parameter to the uncertainty in model outputs seen in the Ensemble Analysis. Allow us to identify which parameters are driving model uncertainty.

1. Return to the main menu for the PEcAn web interface: URL/pecan
2. Repeat the steps for site selection and run specification, however this time click to turn on “Edit pecan.xml” and also “Advanced setup”
3. By clicking Advanced setup, PEcAn will first show an Analysis Menu, where we are going to specify new settings.

1. For an ensemble analysis, increase the number of runs in the ensemble, in this case to 100. In practice you would want to use a larger ensemble size (100-5000) than we are using in the demo. The ensemble analysis samples parameters from their posterior distributions to propagate this uncertainty into the model output.

2. PEcAn's sensitivity analysis holds all parameters at their median value and then varies each parameter one-at-a-time based on the quantiles of the posterior distribution. PEcAn also includes a handy shortcut, which is the default behavior for the web interface, that converts a specified standard deviation into its Normal quantile equivalent (e.g. 1 and -1 are converted to 0.157 and 0.841). In this example set Sensitivity to -2, -1, 1, 2 (the median value, 0, occurs by default).
We also can tell PEcAn which variable to run the sensitivity on. Here, replace NPP with NEE, so we can compare against flux tower NEE observations.

Click **Next**

3. Advanced Edit (optional)

Advanced Edit lets you edit the **pecan.xml settings file**, which lets you control additional parameters not enabled on the web interface and turn on additional analyses, such as state and parameter data assimilation and benchmarking. For example, the Ensemble and Sensitivity settings the XML let your control variables such as start and end year of the analysis separately from the years of the run itself.

“Save” any changes then click “**Continue**”

4. Additional Outputs:
The PEcAn workflow will take considerably longer to complete since we have just asked for over a hundred model runs. Once the runs are complete you will return to the output visualization page were there will be a few new outputs to explore, as well as outputs that were present earlier that we’ll explore in greater details:

1. **Run ID**:
   While the sensitivity and ensemble analyses synthesize across runs, you can also select individual runs from the Run ID menu. You can use the Graphs menu to visualize each individual run, or open individual runs in URL/shiny/workflowPlot/

2. **Inputs**:
   This menu shows the contents of /run which lets you look at and download:
1. A summary file (README.txt) describing each run: location, run ID, model, dates, whether it was in the sensitivity or ensemble analysis, variables modified, etc.
2. The model-specific input files fed into the model
3. The jobs.sh file used to submit the model run

3. Outputs:
   This menu shows the contents of /out. A number of files generated by the underlying ecosystem model are archived and available for download. These include:
   1. Output files in the standardized netCDF ([year].nc) that can be downloaded for visualization and analysis (R, Matlab, ncview, panoply, etc)
   2. Raw model output in model-specific format (e.g. sipnet.out).
   3. Logfile.txt contains job.sh & model error, warning, and informational messages

4. PFTs:
   This menu shows the contents of /pft. There is a wide array of outputs available that are related to the process of estimating the model parameters and running sensitivity/uncertainty analyses for a specific Plant Functional Type.
   1. TRAITS: The Rdata files trait.data.Rdata and madata.Rdata are, respectively, the available trait data extracted from the database that was used to estimate the model parameters and that same data cleaned and formatted for the statistical code. The list of variables that are queried is determined by what variables have priors associated with them in the definition of the PFTs. Priors are output into prior.distns.Rdata. Likewise, the list of species that are associated with a PFT determines what subset of data is extracted out of all data matching a given variable name. Demo 3 will demonstrate how a PFT can be created or modified. To look at these files in RStudio click on these files to load them into your workspace. You can further examine them in the Environment window or accessing them at the command line. For example, try typing names(trait.data) as this will tell you what variables were extracted, names(trait.data$Amax) will tell you the names of the columns in the Amax table, and summary(trait.data$Amax) will give you summary data about the Amax values.

2. META-ANALYSIS:
   1. *.bug: The evaluation of the meta-analysis is done using a Bayesian statistical software package called JAGS that is called by the R code. For each trait, the R code will generate a [trait].model.bug file that is the JAGS code for the meta-analysis itself. This code is generated on the fly, with PEcAn adding or subtracting the site, treatment, and greenhouse terms depending upon the presence of these effects in the data itself. If the <random.effects> tag is set to FALSE then all random effects will be turned off even if there are multiple sites.
   2. meta-analysis.log contains a number of diagnostics, including the summary statistics of the model, an assessment of whether the posterior is consistent with the prior, and the status of the Gelman-Brooks-Rubin convergence statistic (which is ideally 1.0 but should be less than 1.1).
   3. ma.summaryplots.*.pdf are collections of diagnostic plots produced in R after the above JAGS code is run that are useful in assessing the statistical model. Open up one of these pdfs to evaluate the shape of the posterior distributions (they should generally be unimodal), the convergence of the
MCMC chains (all chains should be mixing well from the same distribution), and the autocorrelation of the samples (should be low).

4. **traits.mcmc.Rdata** contains the raw output from the statistical code. This includes samples from all of the parameters in the meta-analysis model, not just those that feed forward to the ecosystem, but also the variances, fixed effects, and random effects.

5. **post.distns.Rdata** stores a simple tables of the posterior distributions for all model parameters in terms of the name of the distribution and its parameters.

6. **posteriors.pdf** provides graphics showing, for each model parameter, the prior distribution, the data, the smoothed histogram of the posterior distribution (labeled `post`), and the best-fit analytical approximation to that smoothed histogram (labeled `approx`). Open **posteriors.pdf** and compare the posteriors to the priors and data.

3. **SENSITIVITY ANALYSIS**
   1. **sensitivity.analysis.[RunID].[Variable].[StartYear].[EndYear].pdf** shows the raw data points from univariate one-at-a-time analyses and spline fits through the points. [Open this file](#) to determine which parameters are most and least sensitive.

4. **UNCERTAINTY ANALYSIS**
   1. **variance.decomposition.[RunID].[Variable].[StartYear].[EndYear].pdf**, contains three columns, the coefficient of variation (normalized posterior variance), the elasticity (normalized sensitivity), and the partial standard deviation of each model parameter. [Open this file and answer the following questions](#):

   2. The Variance Decomposition graph is sorted by the variable explaining the largest amount of variability in the model output (right hand column). From this graph identify the top-tier parameters that you would target for future constraint.

   3. A parameter can be important because it is highly sensitive, because it is highly uncertain, or both. Identify parameters in your output that meet each of these criteria. Additionally, identify parameters that are highly uncertain but unimportant (due to low sensitivity) and those that are highly sensitive but unimportant (due to low uncertainty).

   4. Parameter constraints could come from further literature synthesis, from direct
measurement of the trait, or from data assimilation. Choose the parameter that you think provides the most efficient means of reducing model uncertainty and propose how you might best reduce uncertainty in this process. In making this choice remember that not all processes in models can be directly observed, and that the cost-per-sample for different measurements can vary tremendously (and thus the parameter you measure next is not always the one contributing the most to model variability). Also consider the role of parameter uncertainty versus model sensitivity in justifying your choice of what parameters to constrain.

5. **PEcAn Files:**
   This menu shows the contents of the root workflow folder that are not in one of the folders indicated above. It mostly contains log files from the PEcAn workflow that are useful if the workflow generates an error, and as metadata & provenance (a detailed record of how data was generated).
   1. **STATUS** gives a summary of the steps of the workflow, the time they took, and whether they were successful
   2. **pecan.*.xml** are PEcAn settings files
   3. **workflow.R** is the workflow script
   4. **workflow.Rout** is the corresponding log file
   5. **samples.Rdata** contains the parameter values used in the runs. This file contains two data objects, sa.samples and ensemble.samples, that are the parameter values for the sensitivity analysis and ensemble runs respectively
   6. **sensitivity.output.[RunID].[Variable].[StartYear].[EndYear].Rdata** contains the object sensitivity.output which is the model outputs corresponding to the parameter values in sa.samples.

7. **ENSEMBLE ANALYSIS**
   1. **ensemble.Rdata** contains the object ensemble.output, which is the model predictions at the parameter values given in ensemble.samples.
   2. **ensemble.analysis.[RunID].[Variable].[StartYear].[EndYear].pdf** contains the ensemble prediction as both a histogram and a boxplot.
   3. **ensemble.ts.[RunID].[Variable].[StartYear].[EndYear].pdf** contains a time-series plot of the ensemble mean, median, and 95% CI
6. **Global Sensitivity**: Shiny

   Navigate to URL/shiny/global-sensitivity.

   ![Global sensitivity analysis](image)

   This app uses the output from the ENSEMBLE runs to perform a global Monte Carlo sensitivity analysis. There are three modes controlled by **Output type**:

   1. **Pairwise** looks at the relationship between a specific parameter (X) and output (Y)
   2. **All parameters** looks at how all parameters affect a specific output (Y)
   3. **All variables** looks at how all outputs are affected by a specific parameter (X)

   In all of these analyses, the app also fits a linear regression to these scatterplots and reports a number of summary statistics. Among these, the slope is an indicator of **global sensitivity** and the $R^2$ is an indicator of the contribution to **global uncertainty**

   The next set of tutorials will focus on the process of data assimilation and parameter estimation. The next two steps are in “.Rmd” files which can be viewed online at:

   [https://github.com/PecanProject/pecan/tree/master/documentation/tutorials](https://github.com/PecanProject/pecan/tree/master/documentation/tutorials)
Additional material

In addition to the materials below you are encouraged to take a look at the Site-Level Runs section on the PEcAN wiki (https://github.com/PecanProject/pecan/wiki/Getting-started#site-level-runs) which describes the process of setting up a new site, new meteorology, new PFT, etc.

Additional useful information on the wiki includes: how to report bugs, how to sync your PEcAn database with others, how to grab the latest “development” branch of the PEcAn code, how to install PEcAn on a server, how to add new models and data processing modules, and how to add new code to PEcAn.

Currently, the web interface does not have access to all of PEcAn’s functionality. For additional tasks we will need to work in the statistical programming language R. To make this easier we have installed a browser-based R interface, RStudio Server (http://rstudio.org), on the VM.

1. Open RStudio Server:
   1. Open up a second window on your web browser to URL/rstudio
      If you closed your previous PEcAn session, make sure the first window is open and points to URL/pecan
   2. The username for the VM is carya and the password is illinois.
   3. You do not need to do this now, but FYI it is also possible to ssh into the virtual machine using the following command in terminal:
      ssh -l pecan -p 6422 localhost
2. Open PECaN settings file
   1. Go back to URL/pecan and note the Run ID for your model run.
      In the visualization window this is listed in the top left pull-down menu

3. PECaN Workflow
   1. In the Files window, go to the Home > pecan > web directory
   2. Open the file workflow.R. This script provides an example of some of the high-level modules within PECaN and we will use it to run the meta-analysis, sensitivity analysis, ensemble analysis, and variance decomposition.

1. Re-run the sensitivity analysis and variance decomposition for a different output variable, time period, site, or PFT and compare results with first site.
   1. If you are only changing the output variable or time period, you don't need to re-run the whole workflow since all the output variables are in the model output files. You can modify the pecan.xml settings object within R and run the workflow from the extraction of the output from the model runs onward (from get.model.output on)
   2. If you are running a new site, it is generally a good idea to do a single test run first to make sure the model behaves sensibly before conducting hundreds of (potentially uninformative) runs.

2. Use the web database interface to change priors, define a new site, or define a new PFT
   1. Open up a new browser window to URL/bety. This page is the web-interface to the database underlying PECaN – it started as an independent project as part of our biofuel work, hence the name BETY-db, but is now much more generic (apologies for the fact that web design has not kept up). For those that are interested the full version of the database is at betydb.org.
   2. To modify or add a new Plant Functional Type (PFT), or to change a PFT's priors, navigate on the grey menu bar to Data > PFTs
      1. To add a new pft, click “new PFT” at the top and enter a name and description.
      2. To add new species to a PFT click on [+] View Related Species and type the species, genus, or family you are looking for into the Search box. Click on the + to add.
      3. To remove a species from a PFT, click on [+] View Related Species and click on the X of the species you want to remove from the PFT.
      4. To remove a prior, click [-] View Related Prior and click on the X of the variable who's prior you want to remove. This will cause the parameter to be excluded from all analyses (meta-analysis, sensitivity analysis, etc) and revert to its default value.
      5. To add a prior, choose one from the white box of priors on the right to choose.
      6. To view the specification of a prior, or to add a new prior, click BETY-DB > Priors and enter the information on the variable, distribution name, distribution parameters, etc. N is the sample size underlying the prior specification (0 is ok for uninformative priors).
      7. You can also got to Data > Variables in order to use the search function to find an existing variable (or create a new one). Please try not to create new variables unnecessarily (e.g. changes of variable name or units to what your model uses is handled internally, so you want to find the trait with the correct MEANING).
   3. To add a new site
      1. The database currently requires that a site be associated with a citation. Navigate to > CITATIONS and select a reference for the study site by clicking the check mark, or
create a new citation (creating a 'pers. communication' or 'unpublished data' citation IS allowed)

2. Click on the **New Site** button. Fill out at least a name and lat/lon (which can be done by hand or by clicking on the map).

3. To upload model driver data [or any other input data] for the site (currently required in order to run the model at a site)
   1. Select RUNS > INPUTS
   2. At the bottom of the page click on New Input
   3. Choose your site from the pulldown menu
   4. Set the date range, file format, and other meta-data
   5. Click “Create”
   6. To associate the Input record in the database, click “Edit” and then “New File”
   7. Select the machine that the file is on (pecan32 is the VM itself) and fill in the directory path where the file is located and the file name
   8. Click Update

Citation: