

BioNumerics Tutorial:

Setting up a BioNumerics database with levels

1 Aims

The database levels in BioNumerics form a powerful concept that allows users to structure information in a hierarchical way. Each database level reflects the physical entity from which information is collected, thereby avoiding information duplication that would occur in a "flat" table. It also provides a convenient framework to deal with replicate experiments.



This tutorial starts from following situation: A culture collection is responsible of maintaining a large number of microbial strains. Each strain is assigned a strain number and stored as a freeze-dried culture in air-tight vials. Whenever a batch of such vials is running out or when a certain amount time has passed, a single vial is resuscitated and a subculture started to prepare a new batch of vials. For the curators of the culture collection, it is very important to confirm the integrity of their strains. Therefore, they perform a high resolution DNA fingerprint on each batch of vials as a quality check. The patterns are then compared with the original DNA fingerprints from the strains and should of course match 100%.

In this use scenario, setting up a database with three levels (respectively "Strain", "Batch" and "Profile") allows the users to:

- Assign specific information fields to the corresponding database level, avoiding unnecessary duplication of information.
- Deal with replicate measurements.
 - Summarize experiments from the "Profile" to the "Batch" and "Strain" level.
 - Provides an easy way to approve experiments, without the need to actually delete sub-optimal fingerprints from the database.

In this tutorial, we discuss the necessary steps to set up levels in a new, empty database.

2 Creating a new BioNumerics database

1. Double-click on the BioNumerics icon () on the desktop.
2. In the *BioNumerics Startup* window, press the  button to enter the *New database* wizard.
3. Enter a database name, e.g. "Culture collection".
4. Click *<Next>* and then *<Finish>*.

A new dialog box pops up, asking whether to create a new relational database for data storage or to use an existing one.

5. Leave the default option *Create new* enabled and press *<Next>*.

The next dialog asks which database engine should be used for storing data.

6. Select the *Use default (SQLite)* option and press <**Finish**>.

The *Plugins* dialog box pops up which allows you to install additional functionality.

7. Press <**Proceed**> to start BioNumerics.

The *Main* window opens with an empty database.

3 Configuring the Main window

When working with levels in a BioNumerics database, the *Database design* panel is frequently needed. Therefore, we will change the layout of the *Main* window so that this panel is always in view.

1. Click on the tab from the *Database design* panel (bottom left of the *Main* window in default configuration). While keeping the mouse button pressed, drag the mouse over the *Database entries* panel and release it over the top part of the docking guide.

This results in a window configuration as displayed in Figure 1, allowing easy access to the *Database design* panel.

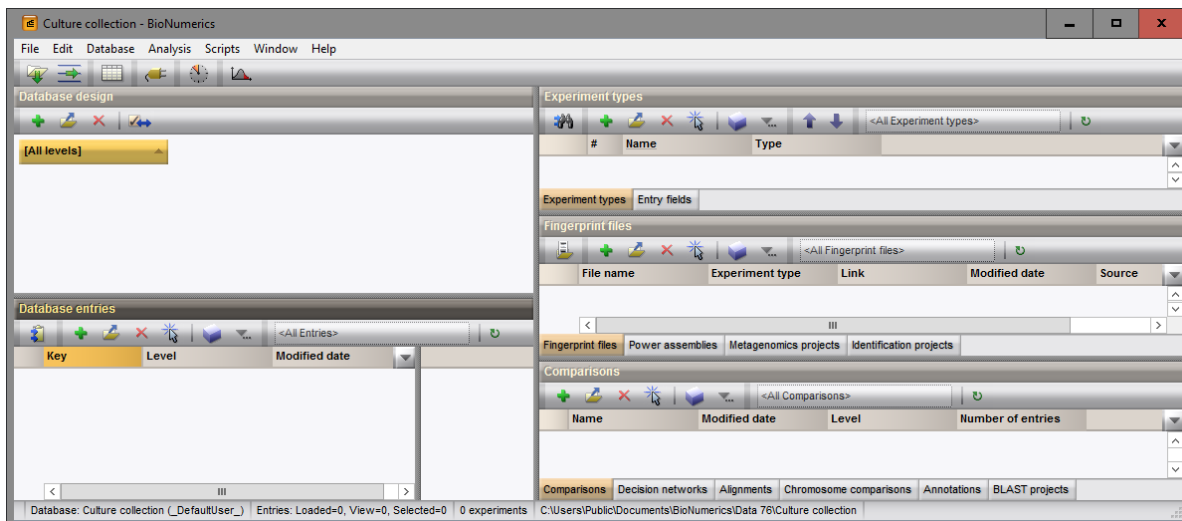


Figure 1: The *Main* window with the *Database design* panel shown.

4 Creating database levels

By default, the *Database design* panel shows only [All levels]. We will create three hierarchical levels in this example database:

1. **Strain:** A level that will contain all strains (sometimes also referred to as "accessions") available from the culture collection. Each strain has a unique strain number and additional descriptive information (e.g. Genus and Species).
2. **Batch:** This level holds information about the batches of preservation vials. A batch is always prepared from a single strain. From any given strain in the database, multiple batches can be prepared.

3. **Profile:** This level corresponds to individual DNA fingerprint profiles. A profile originates from a single batch. Typically, one profile would be prepared per batch, but replicates are needed when the generated profile does not meet the quality criteria.

Proceed as follows to create the **Strain** level:

1. Highlight [All levels] in the *Database design* panel and select *Database* > *Levels* > *Add new level...* (+).
2. Enter “Strain” as *Name* for the level and optionally a *Description*, e.g. “Contains strains available from our culture collection”. Press <OK>.

The level **Strain** is created as a child level from [All levels]. We will now create the **Batch** level:

3. With the **Strain** level highlighted, select *Database* > *Levels* > *Add new level...* (+) again.
4. This time, enter “Batch” as *Name* for the level and optionally a *Description*, e.g. “Contains preservation batches for a given strain”. Press <OK>.

The level **Batch** is created as a child level from **Strain**. Finally, we will create the **Profile** level:

5. With the **Batch** level highlighted, select *Database* > *Levels* > *Add new level...* (+) once more.
6. Enter “Profile” as *Name* for the level and optionally a *Description*, e.g. “Contains Profile profiles”. Press <OK>.

The *Database design* panel should now look like in Figure 2.



Although in theory an unlimited number of levels can be created, it is advisable to limit the number of levels to the minimum necessary.

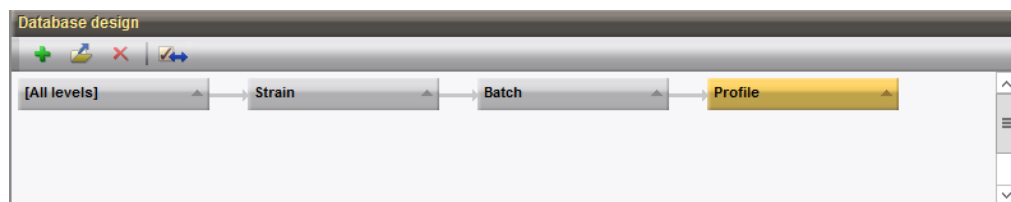


Figure 2: The *Database design* panel with three levels defined.

5 Level-specific information fields

As soon as levels are present in a database, creating entry information fields is specific for the active level, i.e. the level that is highlighted in orange in the *Database design* panel.

Proceed as follows to create the Strain-specific entry field **Strain number**:

1. Click on **Strain** in the *Database design* panel to make **Strain** the active database level.
2. In the *Entry fields* panel, select *Edit* > *Create new object...* (+).
3. Enter “Strain number” as *Name* for the new information field, check *Calculate field content from other fields* and press <Edit>. Press *Add information field*, select *Key* and press <OK> twice.

Using these settings, BioNumerics will create a text field in the database that is specific for the **Strain**. The content of the field will be derived from the **Key** field.

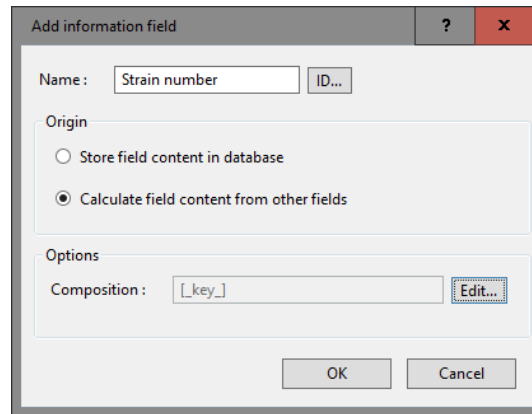


Figure 3: Strain number.

Proceed as follows to create a new field, specific to the **Batch** level:

4. Click on **Batch** in the *Database design* panel to make **Batch** the active level.
5. In the *Entry fields* panel, select *Edit* > *Create new object...* (+).
6. Enter “Preservation date” as *Name* for the new information field and press <OK>.

Similarly, we can create a new field in the **Profile** level:

7. Highlight the **Profile** level in the *Database design* panel, select *Edit* > *Create new object...* (+) in the *Entry fields* panel, and enter “Run number” as field name. Press <OK>.

Finally, we will create a field in the **Profile** level that will hold the information whether or not a curator has approved the DNA fingerprint profile:

8. Make sure **Profile** is still the active level, in the *Entry fields* panel, select *Edit* > *Create new object...* (+).
9. Enter “DNA fingerprint approved” as *Name* for the new information field and press <OK>.

The *Database design* panel should now look like in Figure 4.

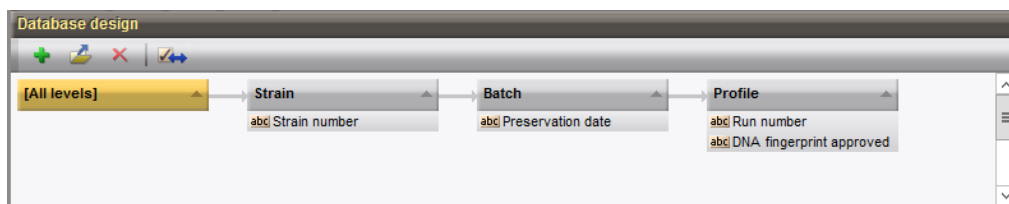


Figure 4: Level-specific information fields.

10. In the *Entry fields* panel, double-click on *DNA fingerprint approved* to open the *Database field properties* dialog box.

Since the profile is either approved or not, we will add two field states (i.e. **Yes** and **No**) with color coding and will prevent the input of any other text than specified in the field states:

11. Press the <Add> button, enter “Yes” and press <OK>.
12. Repeat the previous step to add a second field state “No”.

13. Check **Restrict content to states** and **Use colors**. Optionally, enter “No” as **Default content** (see Figure 5).

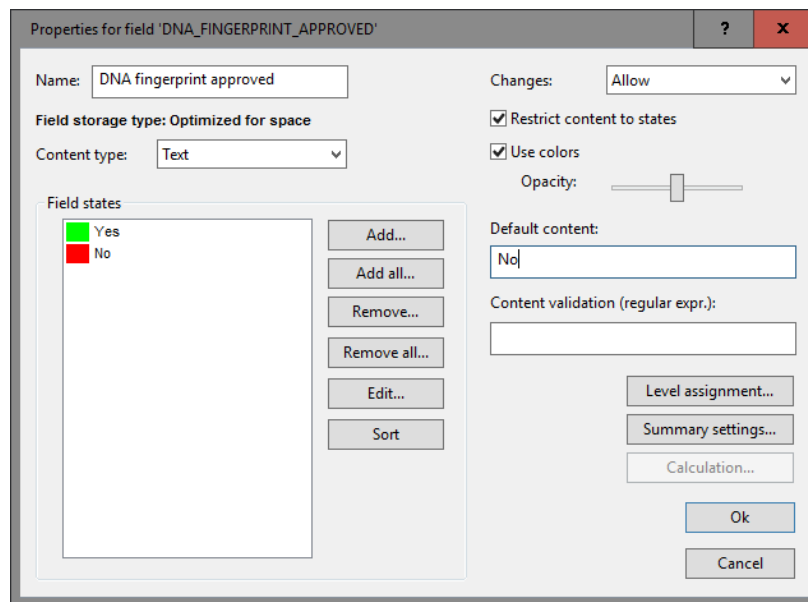


Figure 5: DNA fingerprint approved: settings.


14. Press **<OK>** to save the information field settings.



When information fields are created in a database without levels or with [All levels] highlighted, by default a fixed entry information field will be created that occurs on all levels. If the information is level-specific, a new flexible field should be created and the information copied over for the selected entries via **Edit > Information fields > Edit field in selection...** (**Ctrl+M**). The original fixed field can then be deleted.

Information that is defined at a certain level will be displayed when this level is the active one, and can be edited there if needed. Some information needs to be displayed at other levels than the level at which it is defined. The information will simply be replicated there and cannot be edited.

In this example, the **Strain number** is a good example of information that needs to be shown at all three levels.

15. Click on **Strain** in the *Database design* panel to make **Strain** the active database level.
16. In the *Entry fields* panel, click on **Strain number** and select **Edit > Open highlighted object...** (, **Enter**). Alternatively, simply double-click on **Strain number**.
17. In the *Database field properties* dialog box, press the **<Level assignment...>** button to display the *Level assignment* dialog box (see Figure 6).
18. Change the **Assignment** from “Not used” to “Replicated” for the **Batch** and **Profile** level (see Figure 7).
19. Press **<OK>** to accept the level assignment settings and **<OK>** once more to close the *Database field properties* dialog box.

Now the strain number will be displayed in each level. It will be shown in grey at the **Batch** and **Profile** levels to indicate that it is not defined there and that it cannot be modified there.

Similarly, it might be useful to display the profile **Run number** of a profile at the **Batch** level.

20. Click on **Profile** in the *Database design* panel to make **Profile** the active database level.

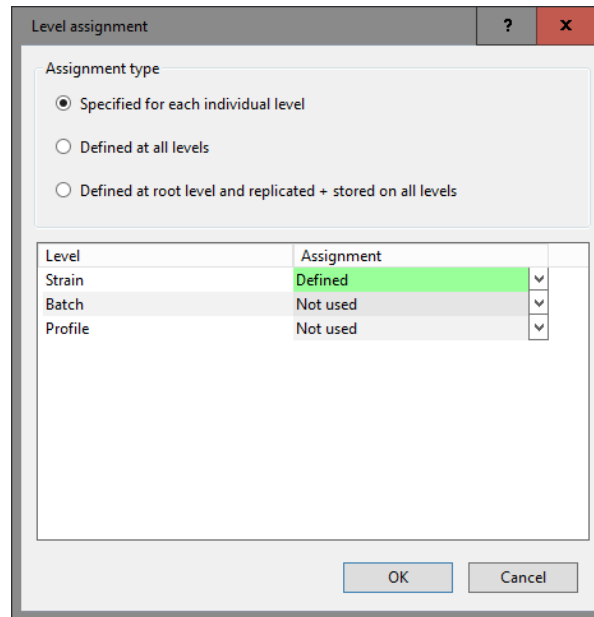


Figure 6: Initial level assignment for the *Strain number* entry field: defined at the **Strain** level and not used at the other levels.

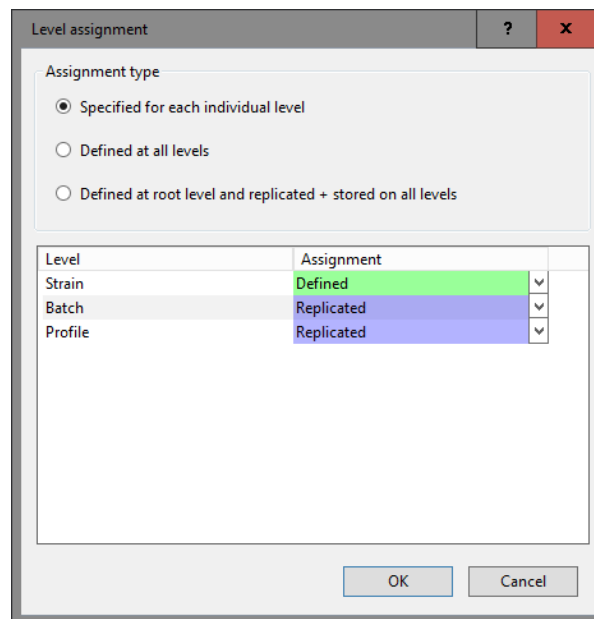


Figure 7: Updated level assignments for the *Strain number*.

21. In the *Entry fields* panel, click on **Run number** and select *Edit > Open highlighted object...* (🔗, Enter). Alternatively, simply double-click on **Run number**.
22. Press the <*Level assignment...*> button to display the *Level assignment* dialog box.
23. Change the *Assignment* from “Not used” to “Replicated” for the **Batch** level and press <*OK*> (see Figure 8).

Since we are now replicating information from a child level to a parent level, we need to define how the information is summarized:

24. Press the <*Summary settings...*> button to show the *Field summary method* dialog box (see Figure 9).

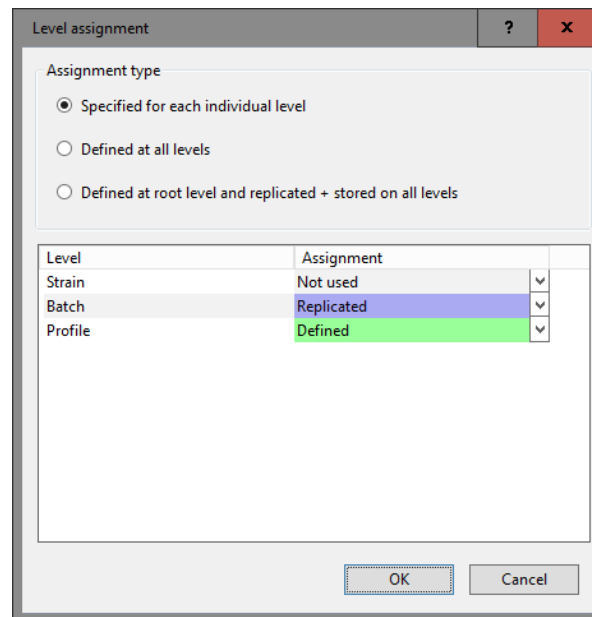


Figure 8: Level assignment for the *Run number*.

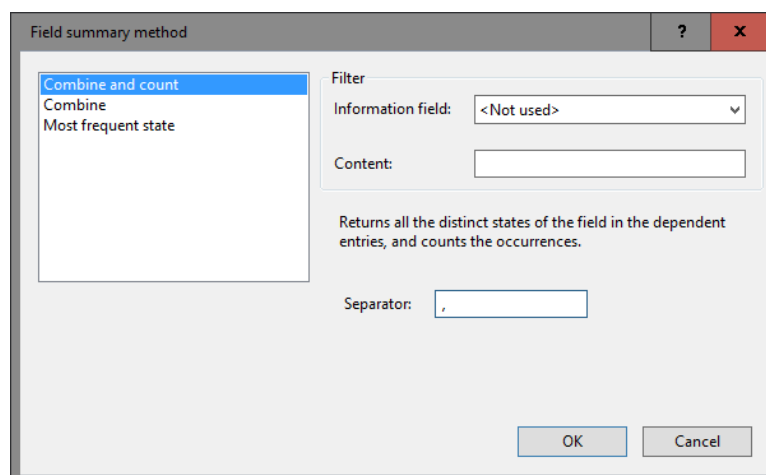


Figure 9: Summary settings for *Run number*.

The default method *Combine and count* will work fine for our purposes, so we will leave this enabled.

25. Press <OK> to accept the summary settings and <OK> once more to close the *Database field properties* dialog box.

6 Level-specific experiment types

Similar to information fields (see 5), experiment types can also be defined at a specific database levels and replicated over other levels if desired. Below the steps are listed to define a new experiment type and to replicate the data over different levels. In the tutorial "Importing information in a database with levels" these steps are illustrated using a fingerprint type experiment, created during import of the data.

- Before launching the *Create a new experiment type* dialog box (in the *Experiment types* panel, select *Edit > Create new object...* (+)), make sure the correct level is selected in the *Database design*

panel. The created experiment type will be defined at the selected level. Alternatively, the experiment type can be created during import of the data.

- The experiment type can be replicated to other levels with the level assignment options present in the *Level assignment* dialog box. This dialog can be called from very experiment type window with the command *Settings > Level assignment...*
- The method used to replicate the experimental information can be specified in the *Experiment summary method* dialog box. This dialog can be called from very experiment type window with the command *Settings > Summary replication settings...*

7 Importing information in a database with levels

When importing data (descriptive information and/or experimental data) in a database with levels, it is important to highlight the corresponding level first. Typically, information will most often be imported at the deepest child level (i.e. **Profile**). In such case, all entries will be correctly linked if the **Batch** key and **Strain** key are specified during import. For more instructions, see our separate tutorial on "Importing information in a database with levels".