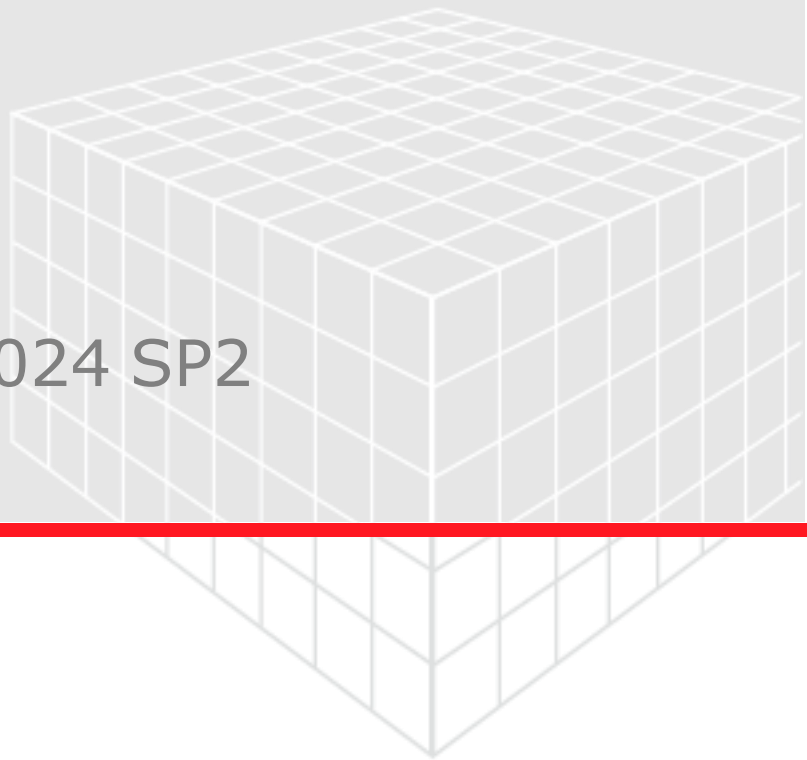


DIGITAL BATTERY CHARGING WITH **GEO**DICT

Tutorial

GeoDict release 2024 SP2

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GEODICT

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DIGITAL BATTERY CHARGING

INTRODUCTION

MOTIVATION

The success of electromobility and the widespread interests in electric vehicles (EVs) significantly depends on increasing their transporting distance as well as the charging rate of their batteries. To increase both of the charging speed and capacity, understanding the processes on a microstructural level inside the electrodes is imperative.

Unfortunately, the processes occurring in the electrodes are rather complicated and have not been suitably understood. Hence, employing powerful simulation software like **GeoDict** is indeed a fruitful tool in this issue. **GeoDict** for battery material design offers several features like:

- Visualize 3D scans of real electrode materials, create detailed 3D models from scans, and analytical identification of the components of the materials, such as active material and binder.
- Generate a statistical digital twin, and interactively change the material components and parameters, e.g. the binder content in an electrode.
- Simulate the charging and discharging of a digital battery starting from real electrode materials. Predict the effect of modifying the microstructure of the digital electrode model and the conditions on the charging process.
- Complement or replace costly and time-consuming experiments that need sophisticated interpretations to study the influence of a certain parameter(s) on a complex battery system.

The powerful **GeoDict** tools offer various insightful opportunities and possibilities to develop and optimize battery materials. For example, it would be very easy to optimize the binder content of electrode materials and investigate their effects on the charging behavior in a short time.

This tutorial is the last part of the **Digital Battery Design** tutorial series:

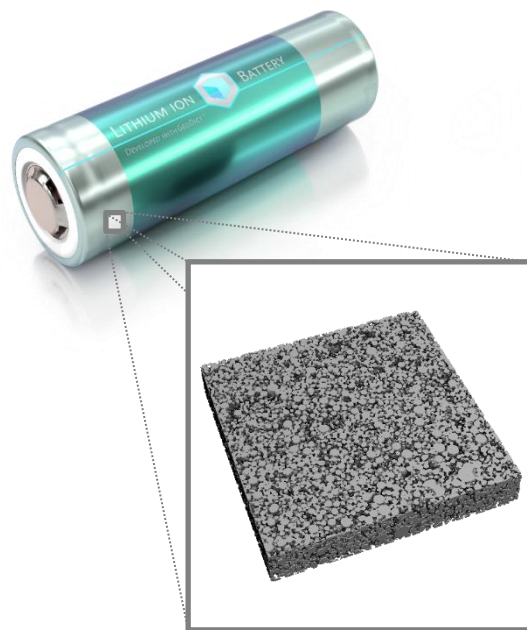
1. **Import and quality control of a cathode material:** This tutorial guides the user stepwise analyzing, post-processing and finally segmenting a 3D-scan of an NMC-cathode.
2. **Standardized microstructure analysis of a cathode material:** This tutorial shows how to analyze the segmented scan regarding transport properties and pore size distribution.
3. **Building a statistical digital twin of a cathode material:** In this tutorial a statistical digital twin is built and validated by employing the results obtained from the second part of this tutorial series.
4. **Digital battery charging:** The charging behavior analysis in a digital battery consisting of bimodal electrodes is also described here.

In detail, this tutorial teaches the user to do the following:

- Set up a digital battery in the **BatteryDict** environment using predefined materials
- Charge the digital battery fully resolved and accurately using **BatteryDict** LIR
- Charge the digital battery on the meso-scale using BESTmeso
- Lithiation of a cathode using **BatteryDict** LIR
- Compare the charging behavior.

BACKGROUND OF THE SAMPLE

In this study, we use the Electrochemistry 3D data set **NMC_94wt_600bar** from the Laboratory for Nanoelectronics, ETH Zurich, that was used for the publication [1]. It stems from the project *X-ray Tomography of Porous, Transition Metal Oxide Based Lithium Ion Battery Electrodes*. Find the cropped, segmented structure with binder identified in the **Input-Data** folder of this tutorial folder. The structure **ETH-NMC-Cathode_Binder_Cropped.gdt** is a result of the previous part of this tutorial series **Building a statistical digital twin of a cathode material**.



The sample is used to illustrate the capabilities of **GeoDict**, and its module **BatteryDict** to simulate the charging of an electrode but the results are not meant to judge in any way the quality of the data set or physical material.

Disclaimer:

The work for this tutorial was not endorsed nor funded by ETH Zurich

HOW TO USE THIS TUTORIAL

All operations described in this tutorial are based on the supplied files. The essential capabilities of **BatteryDict** are described in easy-to-follow steps and figures.

We build a battery from bimodal electrodes and perform two charging simulations on this battery. The first one is a fully resolved method to ensure gaining accurate results, and the other one is relatively faster on the meso-scale.

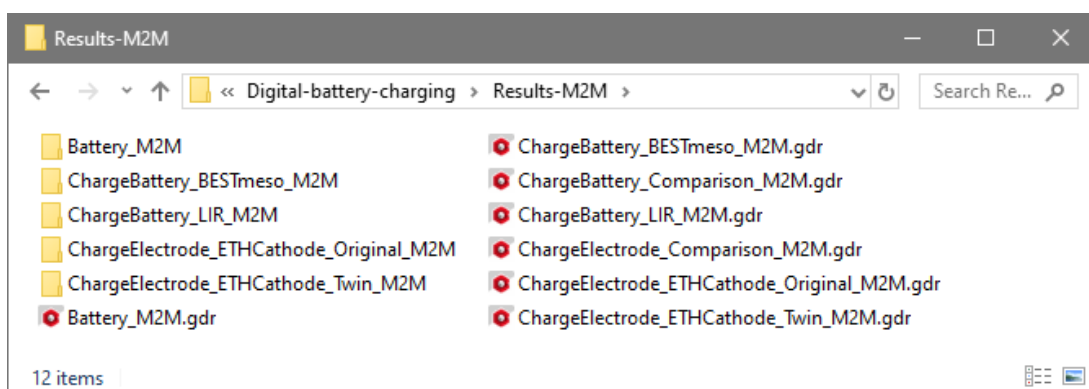
Afterwards, we compare the results and show when to use the faster simulation on the meso-scale.

Finally, an electrode charging simulation is done on the previously mentioned cathode and its digital twin to show how to analyze the performance for only one electrode without having to build a battery.

Modules needed to follow this tutorial:
BatteryDict

The **Digital-battery-charging** tutorial folder contains three folders and this PDF file.

- The **Input-Data** folder contains the predefined data that you need to follow this tutorial:
 - One predefined anode material: **BimodalAnode.gdt**, in **GeoDict** geometry file format.
 - One predefined cathode material: **BimodalCathode.gdt**, in **GeoDict** geometry file format.
 - The cropped structure file from the previous tutorial part **ETH-NMC-Cathode_Binder_Cropped.gdt** and ...
 - ...its digital twin **StatisticalTwin_Cropped.gdt** designed in the previous tutorial part.
- The **Results-User** folder is empty and will be filled with the user's test results derived from this tutorial.
- The **Results-M2M** folder contains the results that M2M obtained by following this tutorial which are 5 folders and 7 files. These results (as always in **GeoDict**) consist of **GeoDict** result files (*.gdr) and their corresponding folders with the same names as following:



- A **GeoDict** result file of a battery designed from two bimodal electrodes, **Battery_M2M.gdr**. The corresponding structure file can be found in the folder **Battery_M2M**.
- A **GeoDict** result file of the charged battery using the **BESTmeso** solver, **ChargeBattery_BESTmeso_M2M.gdr**, and the folder **ChargeBattery_BESTmeso_M2M**, containing detailed information about the computation.
- A **GeoDict** result file of the charged battery using the **LIR** solver, **ChargeBattery_LIR_M2M.gdr**, and the folder **ChargeBattery_LIR_M2M**, containing detailed information about the computation.
- A **GeoDict** result file of the lithiated cathode using the **LIR** solver, **ChargeElectrode_ETHCathode_Original_M2M.gdr**, and the folder **ChargeElectrode_ETHCathode_Original_M2M**, containing detailed information about the computation.
- A **GeoDict** result file of the lithiated cathode of the digital twin using the **LIR** solver, **ChargeElectrode_ETHCathode_Twin_M2M.gdr**, and the folder **ChargeElectrode_ETHCathode_Twin_M2M**, containing detailed information about the computation.
- A **GeoDict** result file **ChargeBattery_Comparison_M2M.gdr** that combines the result files **ChargeBattery_LIR_M2M.gdr** and **ChargeBattery_BESTmeso_M2M.gdr**.
- A **GeoDict** result file **ChargeElectrode_Comparison_M2M.gdr** that combines the result files **ChargeElectrode_ETHCathode_Original_M2M.gdr** and **ChargeElectrode_ETHCathode_Twin_M2M.gdr**.

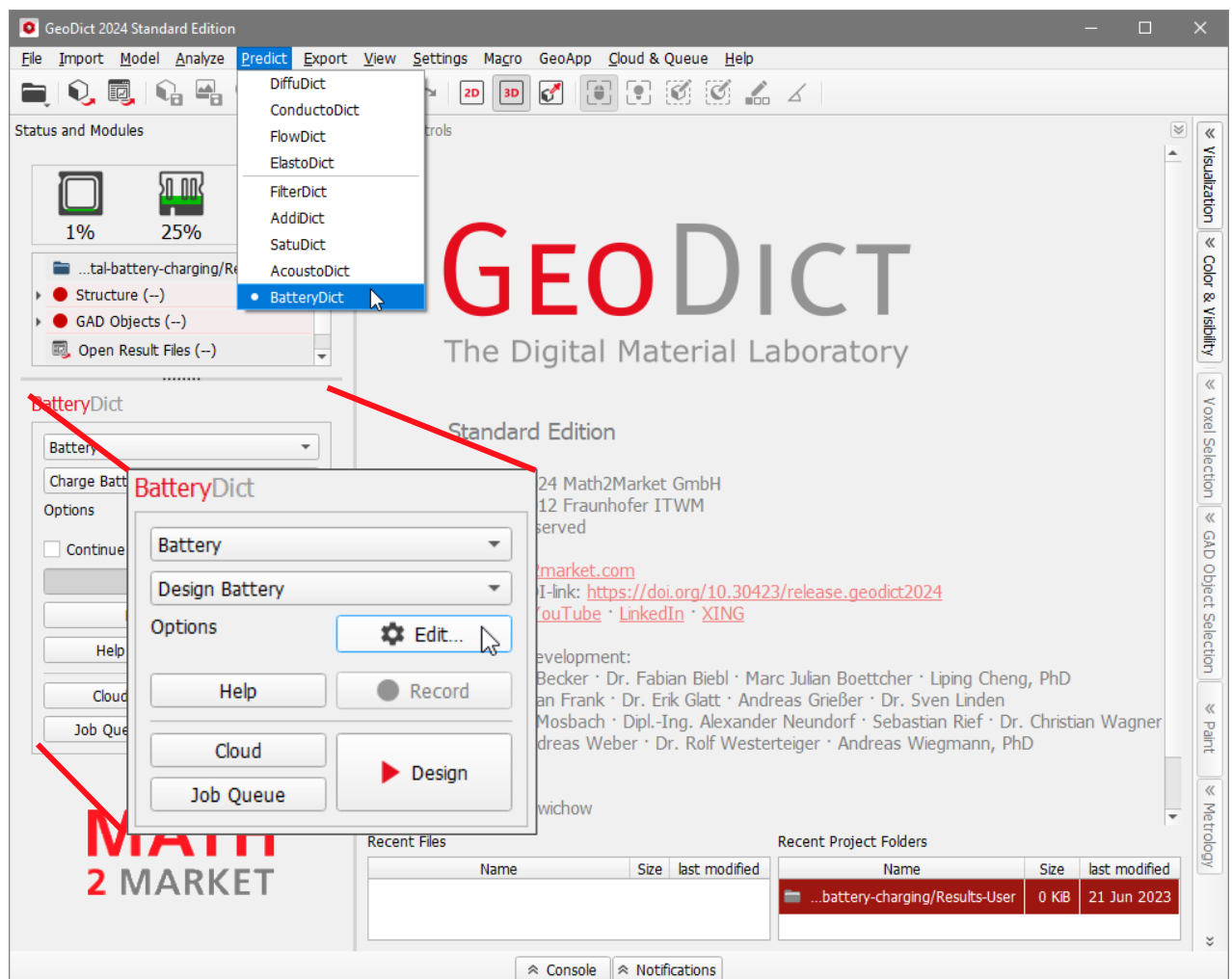
We recommend that before starting to work through this tutorial, you set the folder **Results-User** as the project folder. To do so, in the **GeoDict** GUI select **File** → **Choose Project Folder** → **Select Project Folder** and navigate to **Results-User**.

1. CREATING A DIGITAL BATTERY

Before starting the tutorial, it is recommended to change the **GeoDict** project folder as described on page 4.

The first step is to build a digital battery from two electrodes, i.e. add separator and current collectors. In this tutorial, we use electrodes generated with the Bimodal Anode and Bimodal Cathode **GeoApps** to be found when selecting **GeoApp** → **Battery** → **Electrode Generation**. How to use these apps is described in the [GeoApp](#) handbook of the User Guide and in two YouTube tutorials ([Creating a digital bimodal cathode](#) and [Creating a digital bimodal anode](#)). With these apps, electrodes are generated to match the same loading.

1. Select **Predict** → **BatteryDict** in the menu bar of the **GeoDict** GUI.
2. Select **Battery** from the first and **Design Battery** from the second pull-down menu in the **BatteryDict** section on the bottom left side.
3. Click **Edit ...** to open the **Design Battery** dialog.



4. Change the **Result File Name** to **Battery.gdr**.

Under the **Geometry** tab, a 3D scheme of a typical battery is shown. Below the Anode and Cathode sections, click the **Browse...** buttons to navigate to the **Input-Data** folder and load the predefined electrode materials into the battery designer.



Select **BimodalAnode.gdt** for the anode and **BimodalCathode.gdt** for the cathode.

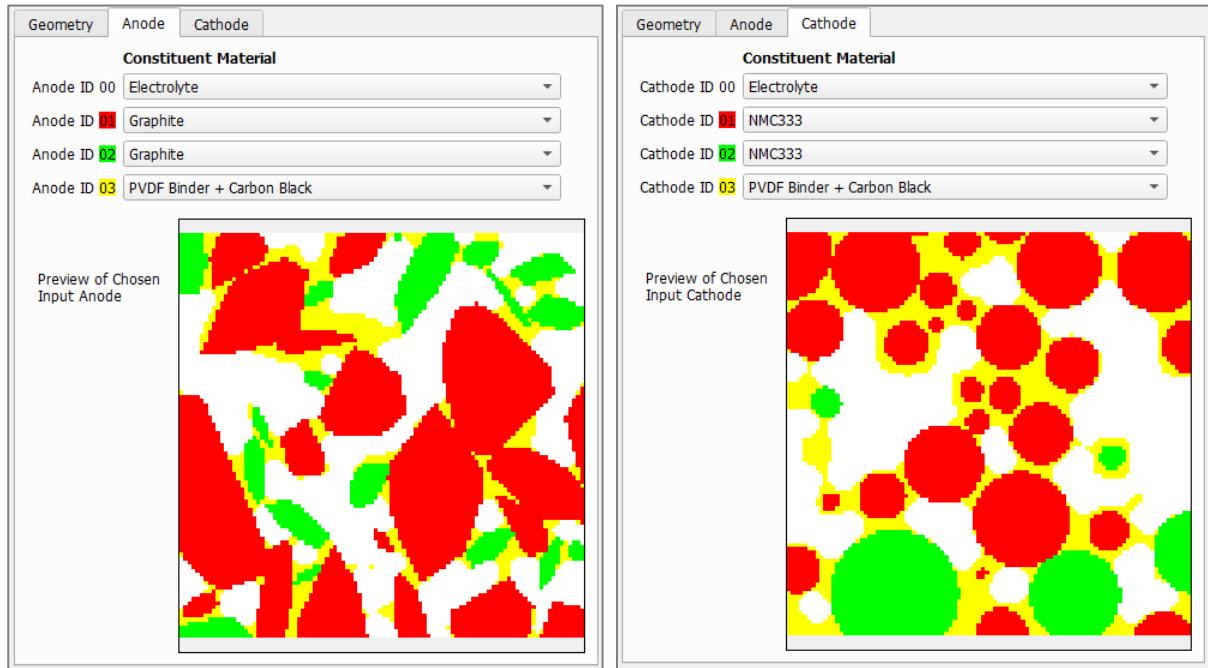
5. In the **Anode** and **Cathode** tabs, the constituent materials are controlled. Check that the selected materials for the battery are the following:


■ Anode:

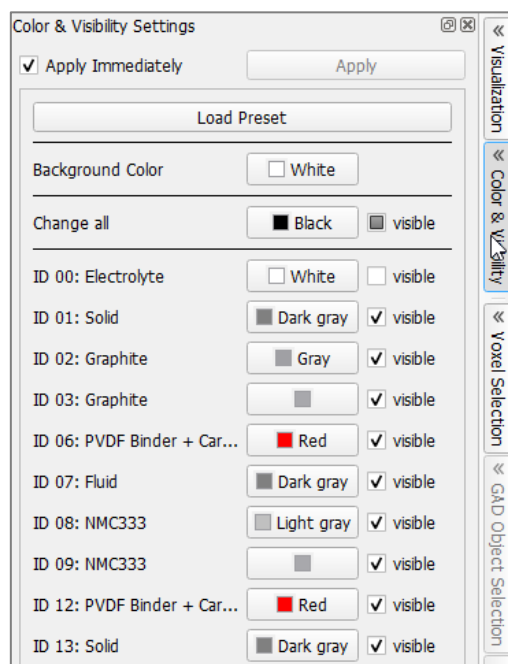
- Anode ID 00: Electrolyte
- Anode ID 01: Graphite (as active material)
- Anode ID 02: Graphite (as active material)
- Anode ID 03: PVDF Binder + Carbon Black (as binder)

■ Cathode:

- Cathode ID 00: Electrolyte
- Cathode ID 01: NMC333 (as active material)
- Cathode ID 02: NMC333 (as active material)
- Cathode ID 03: PVDF Binder + Carbon Black (as binder)



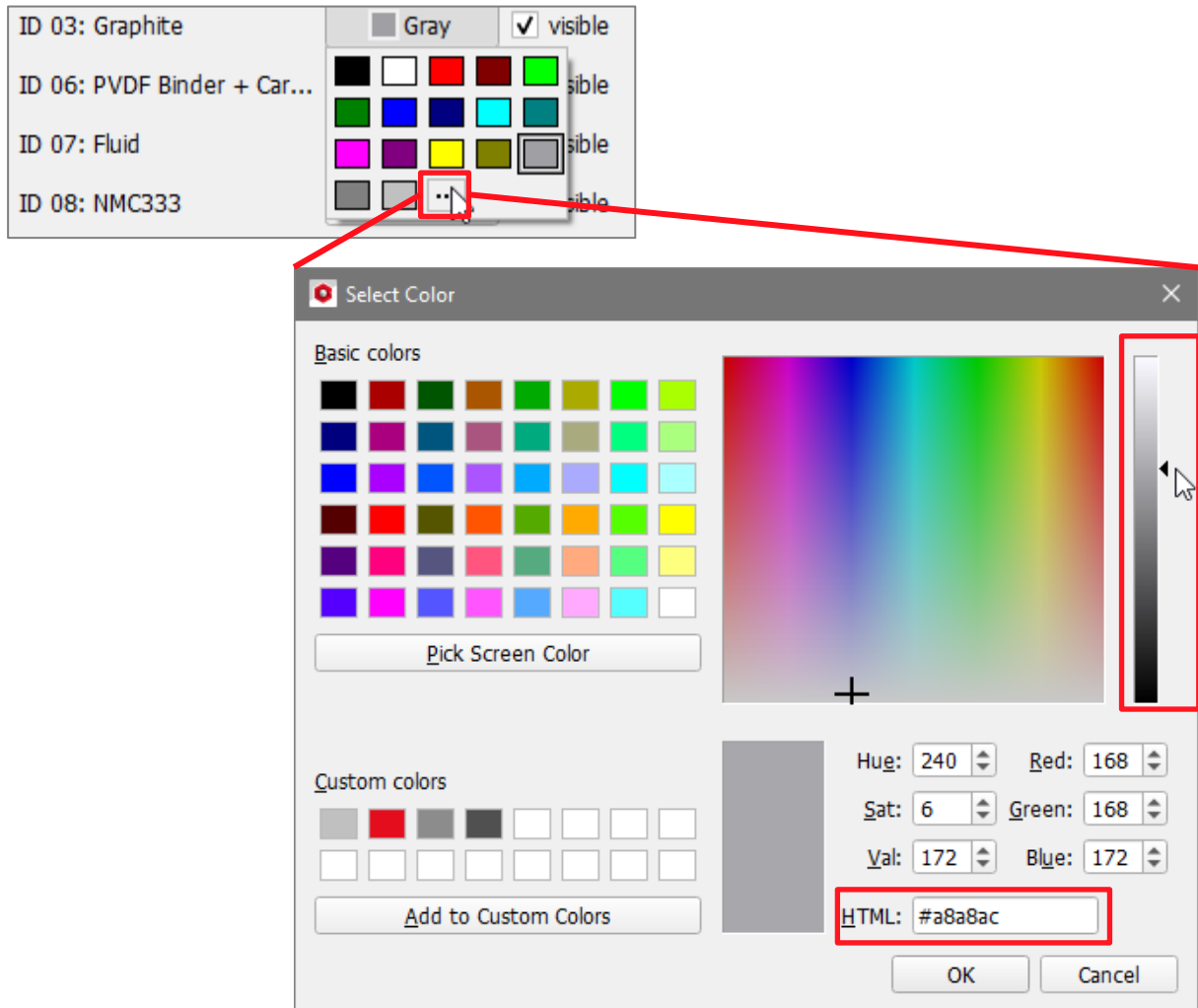
6. Click **OK** to close the **Design Battery** dialog and then, click **Design** in the **BatteryDict** section. When it is finished, the structure is generated accompanied by the **Result Viewer** window, which open automatically. The **Result Viewer** window shows the volume fractions of the constituent materials.
7. In the visualization area, a 3D-view of the battery can be seen. To see the 3D view of the generated structure, click on the 3D icon  in the toolbar.
8. The colors of the materials can be adjusted through the **Color & Visibility** tab located on the right side bar. Herein, the following colors are selected to get our desirable material visualization.



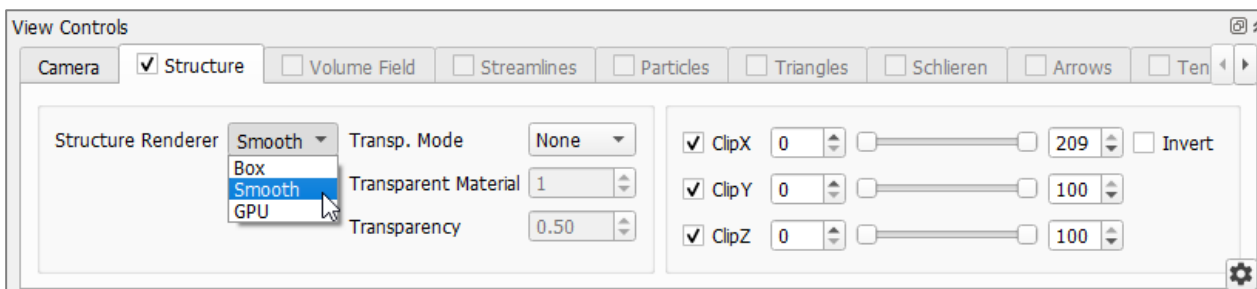
The colors intensity for ID 03 and ID 09 are slightly lighter than the Gray (ID 02) and Light gray (ID 08).

To obtain these colors, that are not predefined as basic colors, do the following: Set the color of ID 03 to **Gray** by clicking on the color button. Then, click again on this color button and expand the color menu by clicking on the three dots.

Adjust the gray color by pulling up the triangle slider on the right, next to the gray scale bar and see the color changes. To reproduce the same color for ID 09, copy the HTML code from ID 03 (we chose #a8a8ac) and paste it for ID 09.



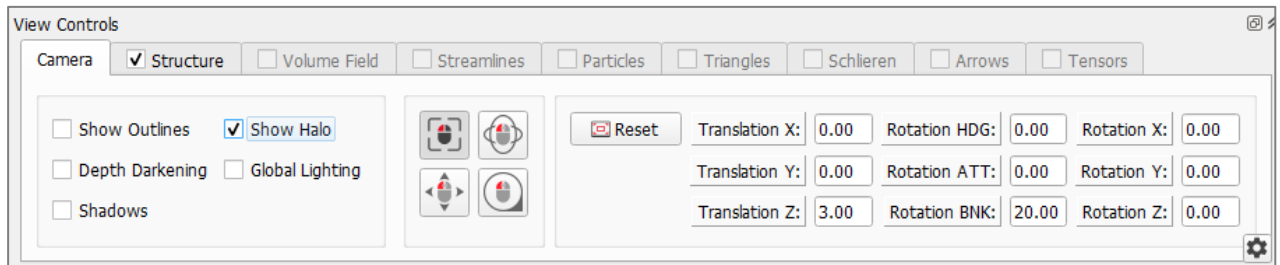
9. In the **View Controls**, go to the **Structure** tab and choose **Structure Renderer** as **Smooth**.



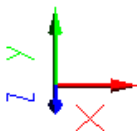
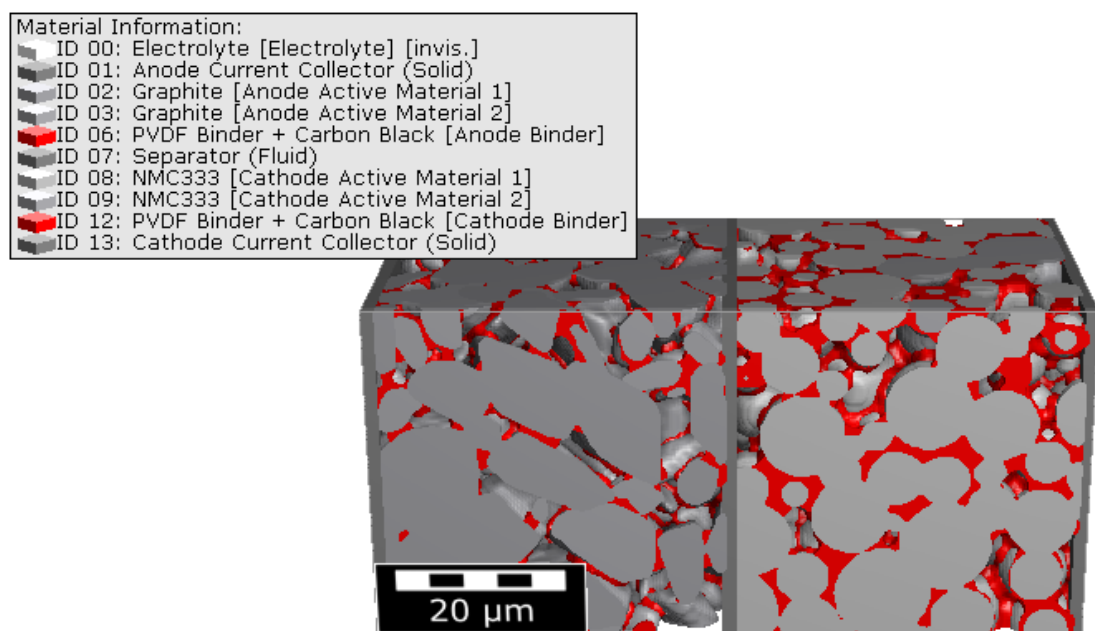
10. Switch to the **Camera** tab and make the following settings:

- **Rotation BNK: 20**
- **Translation Z: 3**

- Set the rest to: **0**
- Check **Show Halo**



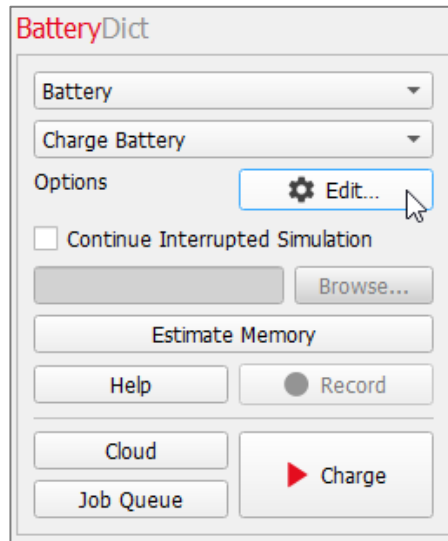
The digital battery is now functional and ready to charge with a very nice visualization.



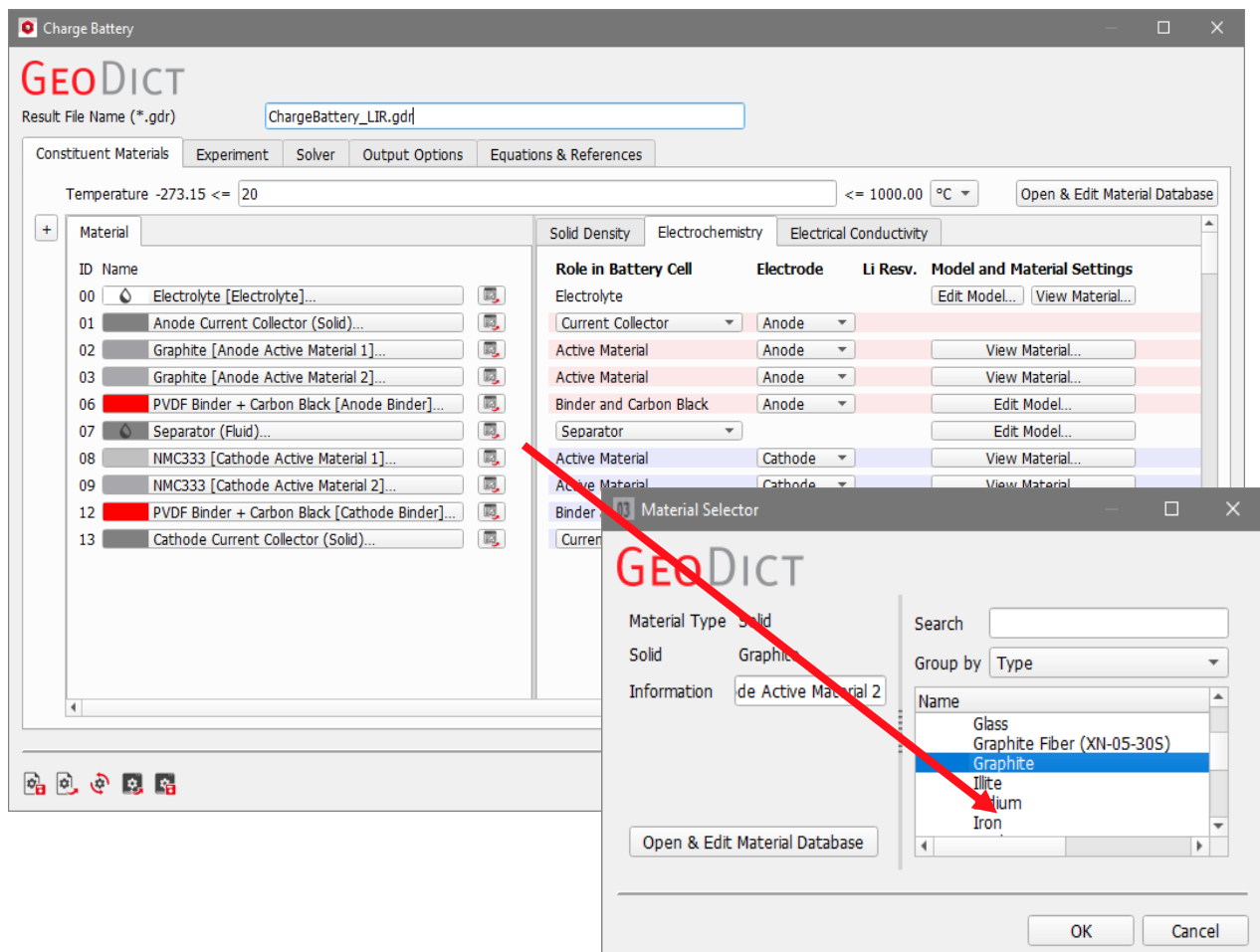
2. CHARGING THE DIGITAL BATTERY

In this section, a charging simulation is carried out on the digital battery using **BatteryDict LIR**. The **LIR** solver is a very fast solver for a fully resolved simulation, which leads to a very accurate charge curve and resolved solution outputs.

In the **BatteryDict** section select **Charge Battery** from the second pull-down menu. Click **Edit...**



1. In the opened **Charge Battery** dialog, set **ChargeBattery_LIR.gdr** as **Result File Name**.



- In the **Constituent Materials** tab, check that the materials are set correctly. Otherwise, you can change the constituent materials by clicking on the material name and selecting the correct material.
- In the **Experiment** tab, set the **Range of the Cell State of Charge** to be from 40.00% to 60.00%.

The screenshot shows the 'Experiment' tab with the following settings:

- Experiment Type: Charge Battery Cell
- Boundary Conditions in Through Direction: Charge Rate
- Charge Rate / (1): 1
- ☐ Use Upper Cut-Off Voltage / (V): 4.3
- Start and End Condition: Minimum and Maximum Cell SOC
- Range of the cell state of charge / (%): 40.00 to 60.00 (highlighted with a red box)
- Boundary Conditions in Tangential Direction: Symmetric
- ☐ Max. Simulated Time / (s): 3600

With these settings, the battery will be charged with a charge rate of 1 starting with an SOC of 40% and ends at SOC of 60%. Charging means lithiation of the anode and delithiation of the cathode.

- Change to the **Solver** tab and select **LIR** as **Solver Type**.

The screenshot shows the 'Solver' tab with the following settings:

- Simulation Type: Fully Resolved Simulation
- Solver Type: LIR
- Parallelization: <local max. - 8x> Edit...
- Time Step: Time-Step Input Mode Automatic
- LIR sub-tab: BESTmicro, BESTmeso
- ☒ Error Bound: 0.01
- ☐ Maximal Iterations: 100000
- ☐ Maximal Run Time / (h): 240
- Advanced Options: (collapsed)

- Click **OK** to close the dialog and then click **Charge** in the **BatteryDict** section.

The screenshot shows the 'BatteryDict' dialog box with the following elements:

- Battery: (dropdown menu)
- Charge Battery: (dropdown menu)
- Options: Edit... (gear icon)
- ☐ Continue Interrupted Simulation
- Browse... (button)
- Estimate Memory (button)
- Help (button)
- Record (radio button)
- Cloud (button)
- Job Queue (button)
- Charge (button, highlighted with a mouse cursor)

It takes around 1 hour to complete the simulation on 8 processing cores.

At the end, the **ChargeBattery_LIR.gdr** file is generated together with the folder **ChargeBattery_LIR** in the **Results-User** project folder. The results will be discussed on page [17](#).

For detailed information about all options of the **Charge Battery** dialog, refer to the [BatteryDict](#) handbook of the User Guide.

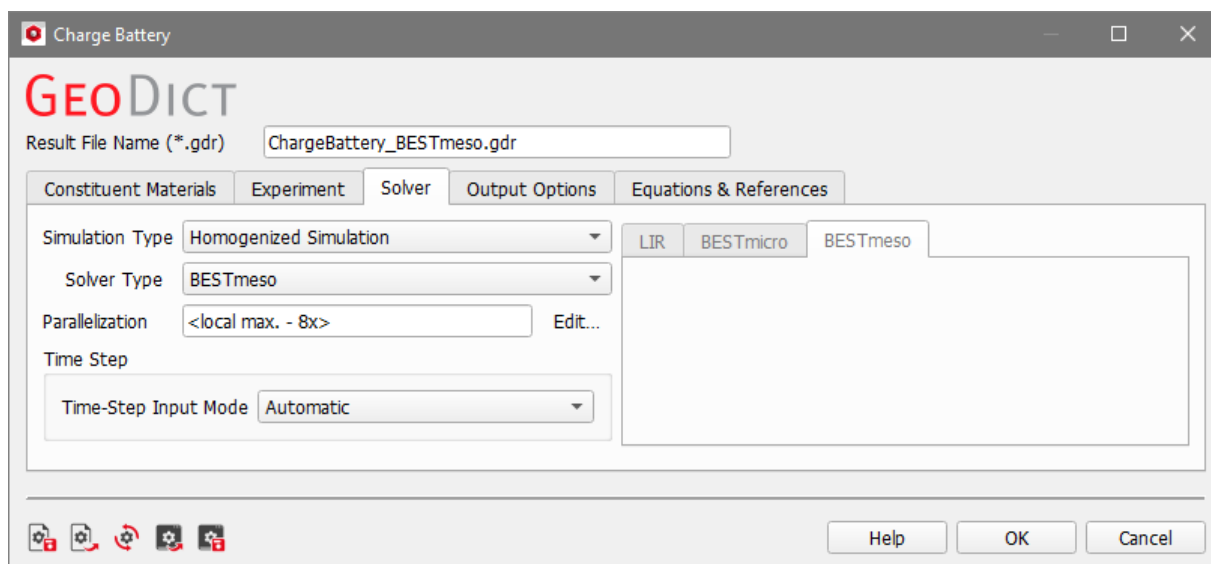
3. CHARGING THE DIGITAL BATTERY ON A MESO-SCALE

The previous charging computation was based on the voxel geometry and thus fully resolves the battery. We also provide a pseudo-2D Newman Model Simulation with the **BESTmeso solver**. Although it does not fully resolve the structures within the battery cell, it can provide a reasonable approximation for the charging-curve and takes relatively shorter calculation time.

In this model, **BatteryDict** first calculates geometry dependent input parameters, such as ionic diffusivity and ionic conductivity in the different materials. With these effective parameters, this method is able to consider various characteristics of anode and cathode.

In the next step, the battery structure is then composed of representative effective voxels. These voxels are arranged in 1D in the X-direction. Each of these voxels contains a sphere-shaped representative active particles for each active material. The effective radius of these spheres is calculated using the effective parameters and gives a second degree of freedom. This has no spatial dimension and is thus called "pseudo-dimension". Therefore, the method is called pseudo-2D. With the effective active material particles, it is possible to simulate the amounts of lithium diffusion into or out of the active material. This means, the battery equations are solved on the simplified structure with less computational effort compared to the fully resolved simulation. Additional information is found in the [BatteryDict](#) handbook of the User Guide.

1. In the **BatteryDict** section, click **Edit...** to open the **Charge Battery** options dialog. The settings for the materials and the experiment are the same as described in the previous chapter starting on page [10](#).
2. Change the **Result File Name** to **ChargeBattery_BESTmeso.gdr**.



3. In the **Solver** tab, change the **Simulation Type** to **Homogenized Simulation**. Then, the **BESTmeso** solver is selected automatically for the **Solver Type**.
4. Click **OK**, and in the **BatteryDict** section click **Charge** to start the simulation.

The simulation will be performed far faster (in about 1 minute on 8 processing cores) benefitting from similar results that are obtained from the **LIR** solver, as is shown in the result analysis chapter on page [17](#).

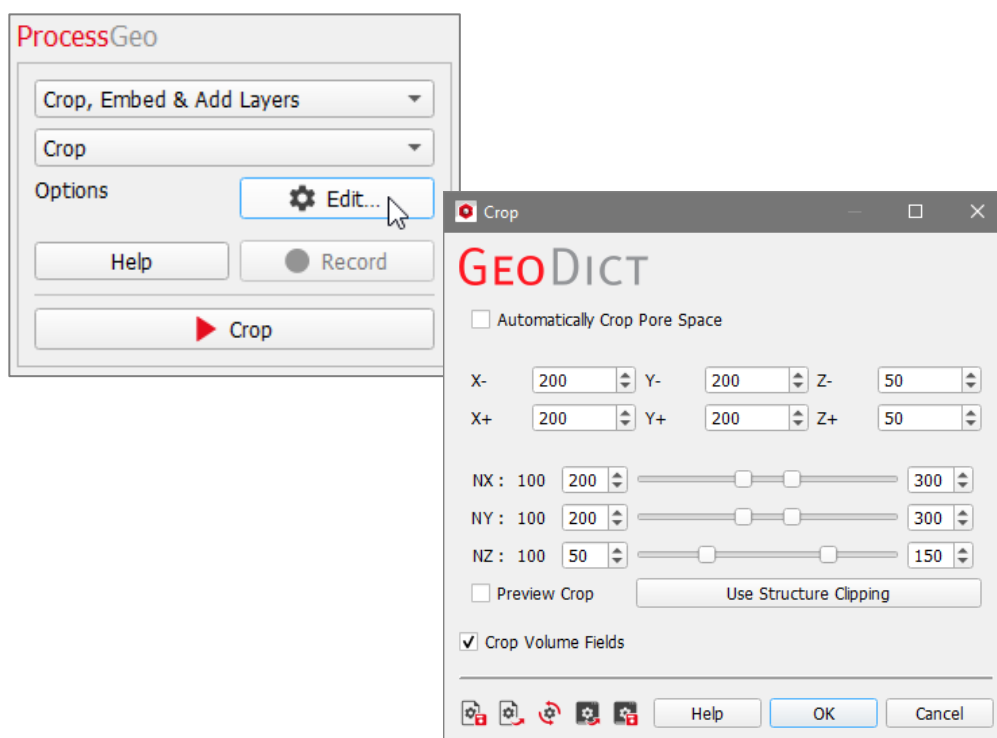
4. LITHIATION OF A CATHODE

In this section, we show how to simulate only one electrode, e.g. the NMC-cathode. For this purpose, the lithiation of the NMC-cathode, which takes place during discharge of the full battery, is investigated. This is very useful, if only one electrode should be analyzed instead of a whole battery cell.

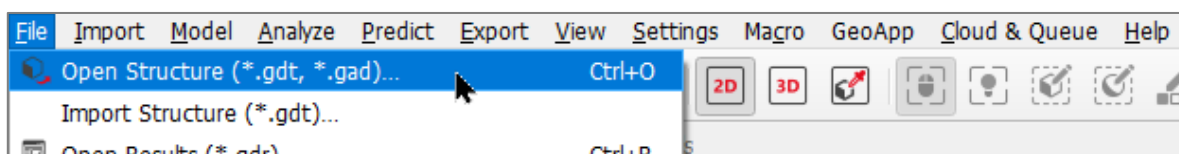
In addition, it is not necessary to use Design Battery for this purpose. **BatteryDict** adds separator, current collectors and a lithium reservoir as an anode as its default geometry. Electrochemically, the investigated electrode is always considered as cathode.

We use the cathode structure and its digital twin created in part 3 of the **Digital Battery Design** tutorial series. Provided in the **Input-Data** folder is the cropped original cathode structure and the cropped digital twin of the cathode.

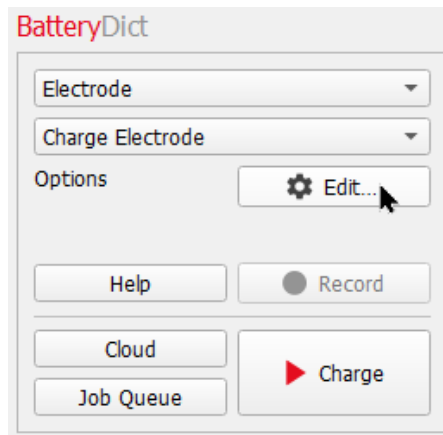
If you worked through the previous tutorials of this series, you may also crop these structures manually. For this select **Model** → **ProcessGeo** and in the **ProcessGeo** section, select **Crop, Embed & Add Layers** from the first pull-down menu. Select **Crop** from the second and click **Edit....** Enter the settings shown here and click **OK** and then **Crop**.



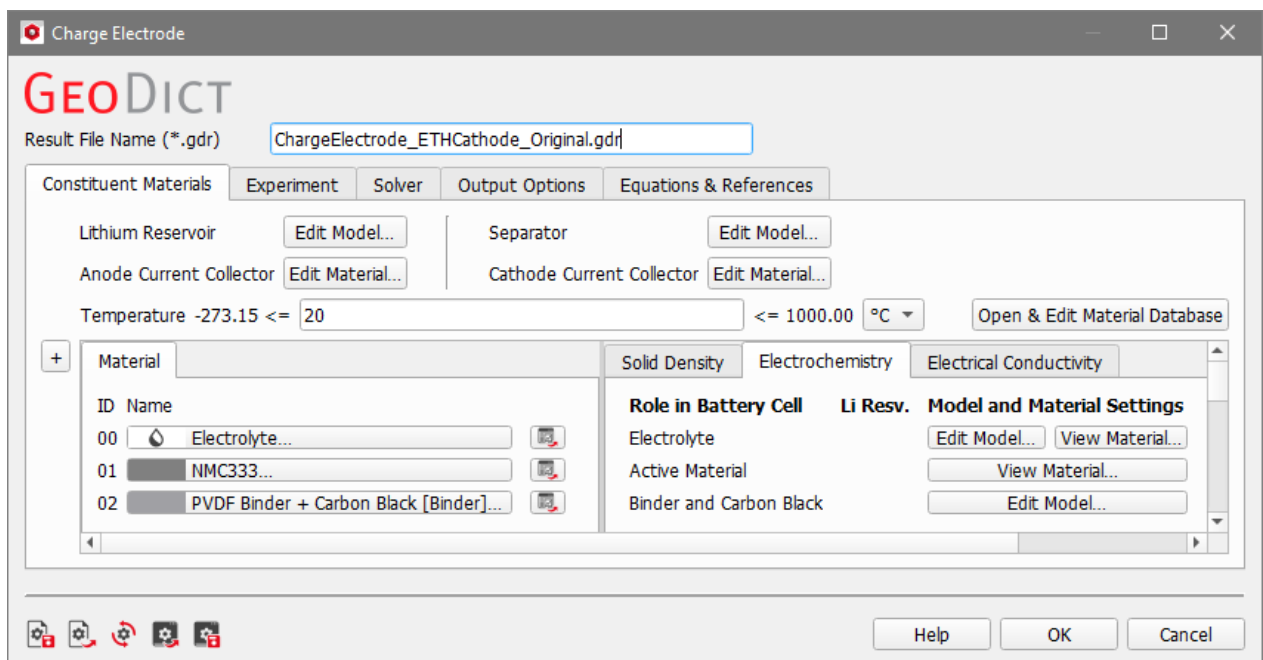
1. Click **File** → **Open Structure (*.gdt, *.gad) ...** in the menu bar. Choose the file **ETH-NMC-Cathode_Binder_Cropped.gdt** from the **Input-Data** folder to be loaded into **GeoDict**.



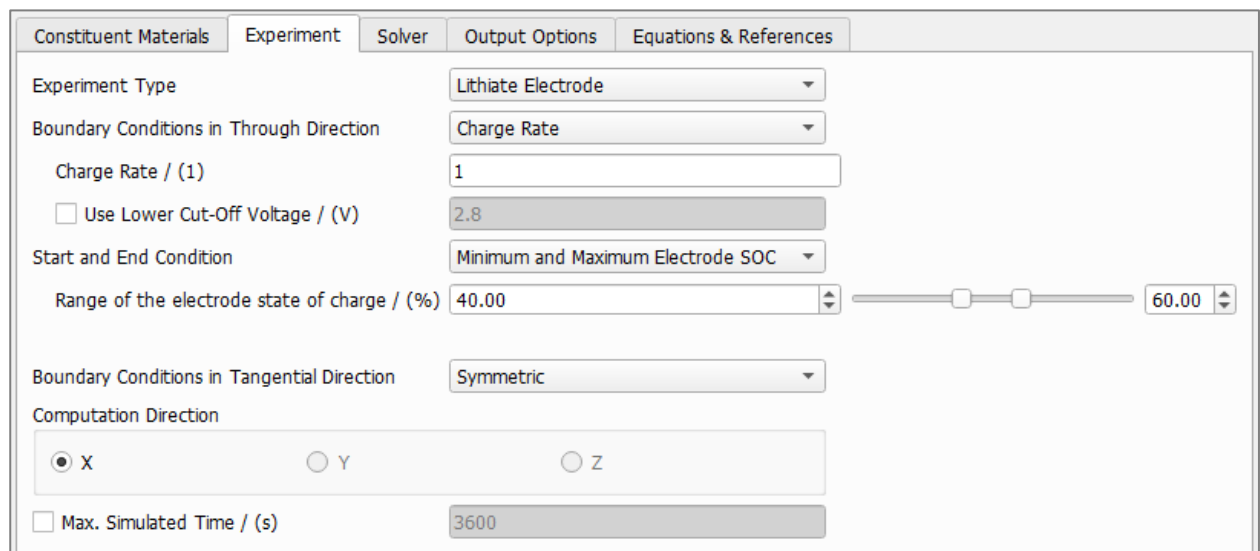
2. Choose **Electrode** from the first pull-down menu and **Charge Electrode** from the second in the **BatteryDict** section. Then, click **Edit....**



3. Change the **Result File Name** to **ChargeElectrode_ETHCathode_Original.gdr**.



4. In the **Experiment** tab, choose **Lithiate Electrode** as **Experiment Type**. Set the **Range of the electrode state of charge** to be from 40.00% to 60.00%.



- Go to the **Solver** tab and select **LIR** as the **Solver Type**.

The screenshot shows the 'Solver' tab in the GeoDict GUI. The 'Simulation Type' is set to 'Fully Resolved Simulation'. The 'Solver Type' is set to 'LIR'. The 'Parallelization' is set to '<local max. - 8x>'. The 'Time Step' section has 'Time-Step Input Mode' set to 'Automatic'. On the right, the 'LIR' sub-tab is active, showing 'Error Bound' at 0.01, 'Maximal Iterations' at 100000, and 'Maximal Run Time / (h)' at 240. There is an 'Advanced Options' link.

- Click **OK** and then **Charge** in the **BatteryDict** section to run the simulation.
The simulation finishes in about 30 minutes on 8 processing cores.
- Then, load the **StatisticalTwin_Cropped.gdt** file in the **GeoDict** GUI (**File** → **Open Structure (*.gdt, *.gad)** ... in the menu bar).
- In the **Charge Electrode** dialog, change the **Result File Name** to **ChargeElectrode_ETHCathode_Twin.gdr**. The other settings are the same as for the previous run.

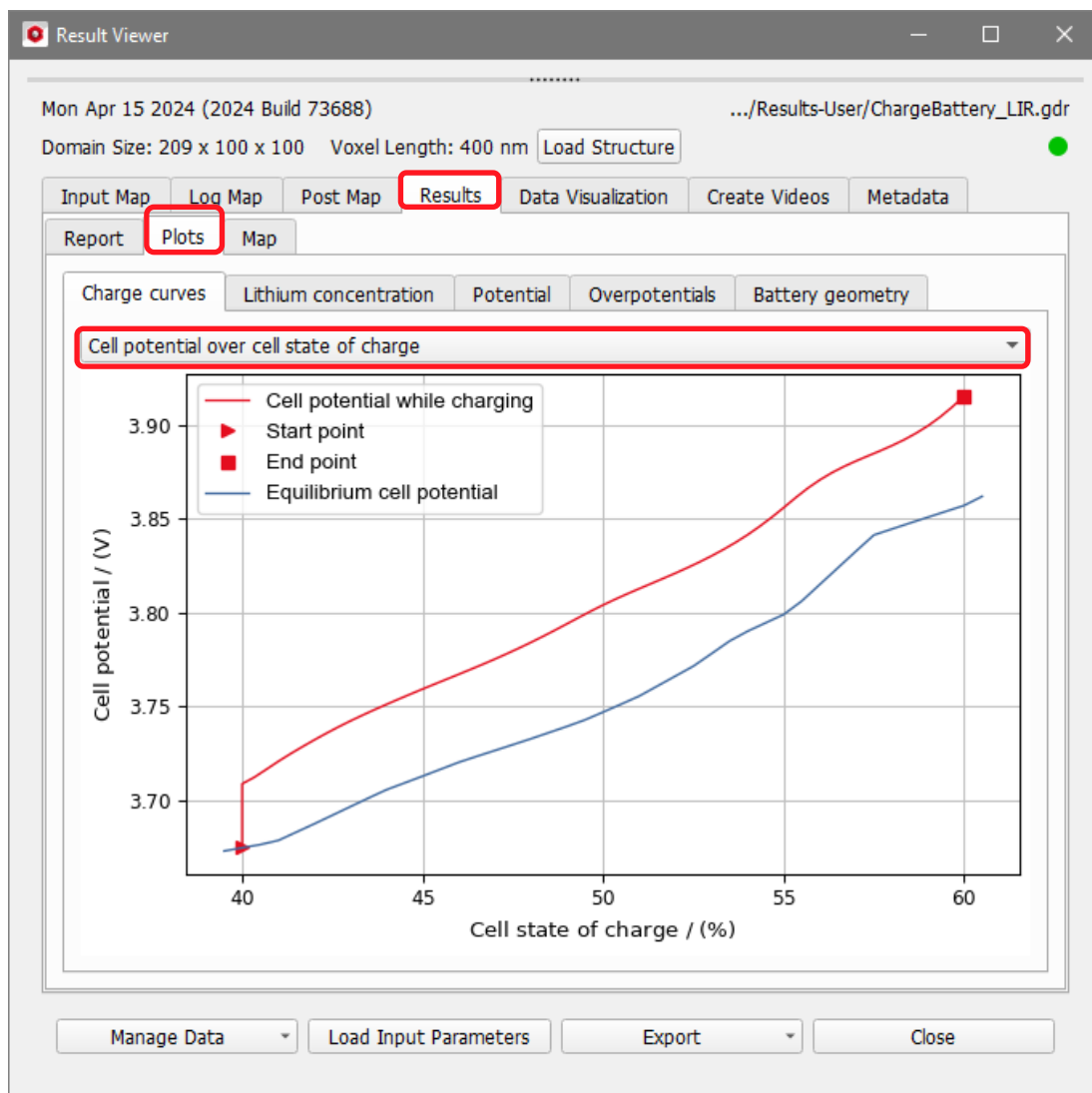
The screenshot shows the 'Charge Electrode' dialog box. The 'Result File Name (*.gdr)' is set to 'ChargeElectrode_ETHCathode_Twin.gdr'. The 'Constituent Materials' tab is active, showing a table of materials: ID 00 is 'Electrolyte...', ID 01 is 'NMC333...', and ID 02 is 'PVDF Binder + Carbon Black [Binder]...'. The 'Temperature' is set to 20 °C. The 'Solid Density' tab is also visible, showing 'Role in Battery Cell' and 'Li Resv.' columns. The 'Electrochemistry' and 'Electrical Conductivity' tabs are also present. At the bottom, there are 'Help', 'OK', and 'Cancel' buttons.

- Click **OK** and then **Charge** in the **BatteryDict** section to start the simulation.
The simulation finishes in about 30 minutes on 8 processing cores.

5. RESULT ANALYSIS

For each completed simulation, the corresponding result file is opened in the **Result Viewer** of the .gdr result file.

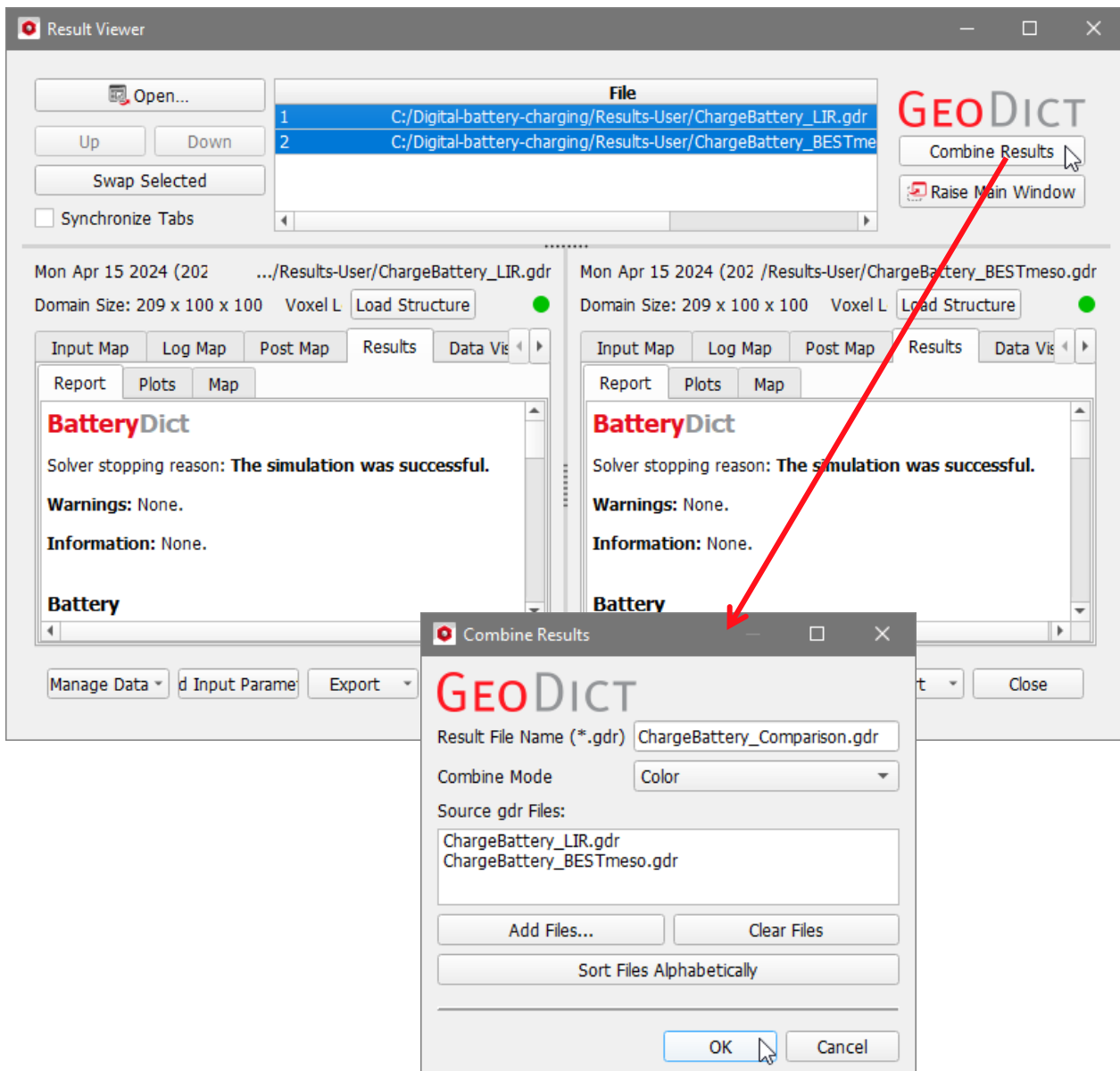
1. Go to the **Results** → **Plots** subtab, to observe the **Charge curves**.
2. Select the **Cell potential over cell state of charge** from the pull-down menu to see the following curves:
 - Cell potential while charging (red curve).
 - Evolution of the equilibrium cell potential (blue curve).



CHARGE BATTERY RESULT ANALYSIS

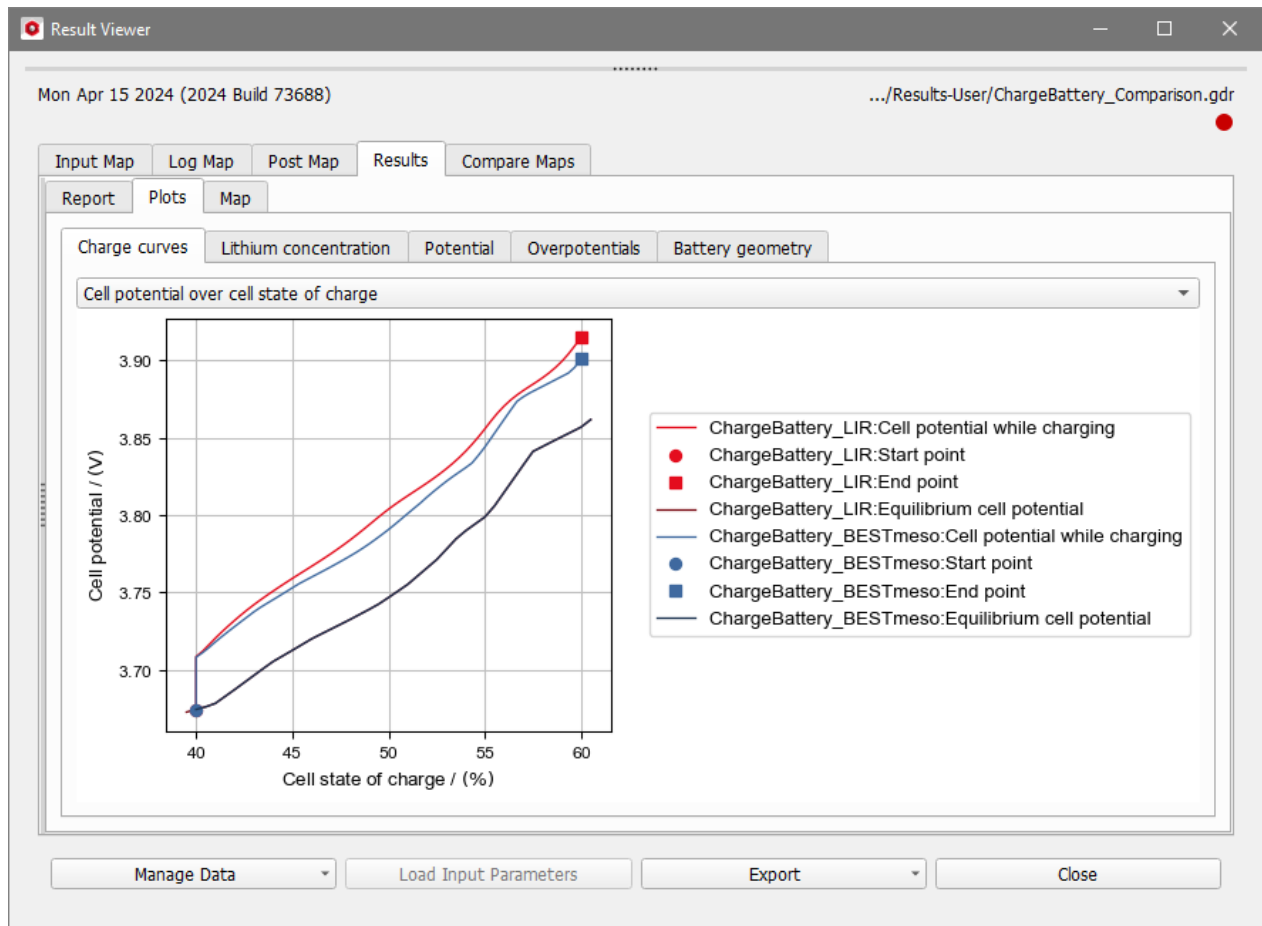
Use the combine .gdr functionality of the **Result Viewer** to compare the results of the **BatteryDict** with **LIR** and **BESTmeso** solvers simultaneously.

1. Press and hold CTRL-key.
2. Select the **ChargeBattery_LIR.gdr** and **ChargeBattery_BESTmeso.gdr** result files and then, click **Combine Results**.
3. In the **Combine Results** dialog, change the **Result File Name** to **ChargeBattery_Comparison.gdr** and then, click **OK**.



4. Go to the **Plots** subtab of the combined .gdr files to observe the combined charging curves.

The curve resulting from the simulation with the **LIR** solver is shown in blue and the one from the **BESTmeso** solver is in red.



See how the result of the **BESTmeso** solver is relatively similar to the fully resolved simulation with a significantly faster calculation time (1 minute vs. 1 hour!).

Consequently, as an example case of the bimodal electrodes, choosing the pseudo-2D Newman model simulation is preferred.

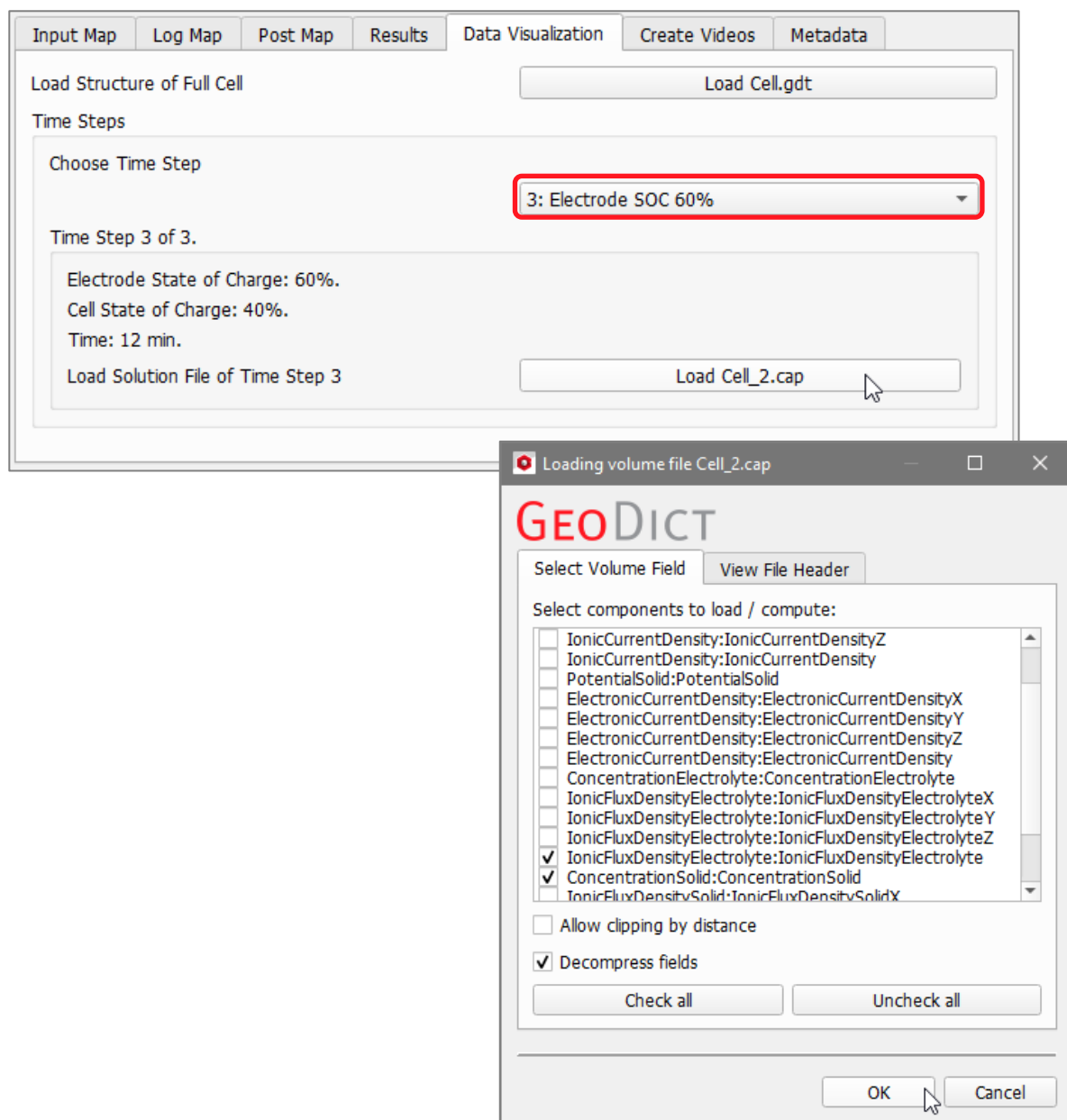
However, if you want to visualize the 3D result fields such as the lithium ion concentration or the ionic diffusion for several intermediate charging steps, choose the fully resolved model.

CHARGE ELECTRODE RESULT ANALYSIS

In the next steps, we carry out the 3D visualization of the results from the Charge Electrode simulation.

For this purpose, select the result file **ChargeElectrode_ETHCathode_Twin.gdr**.

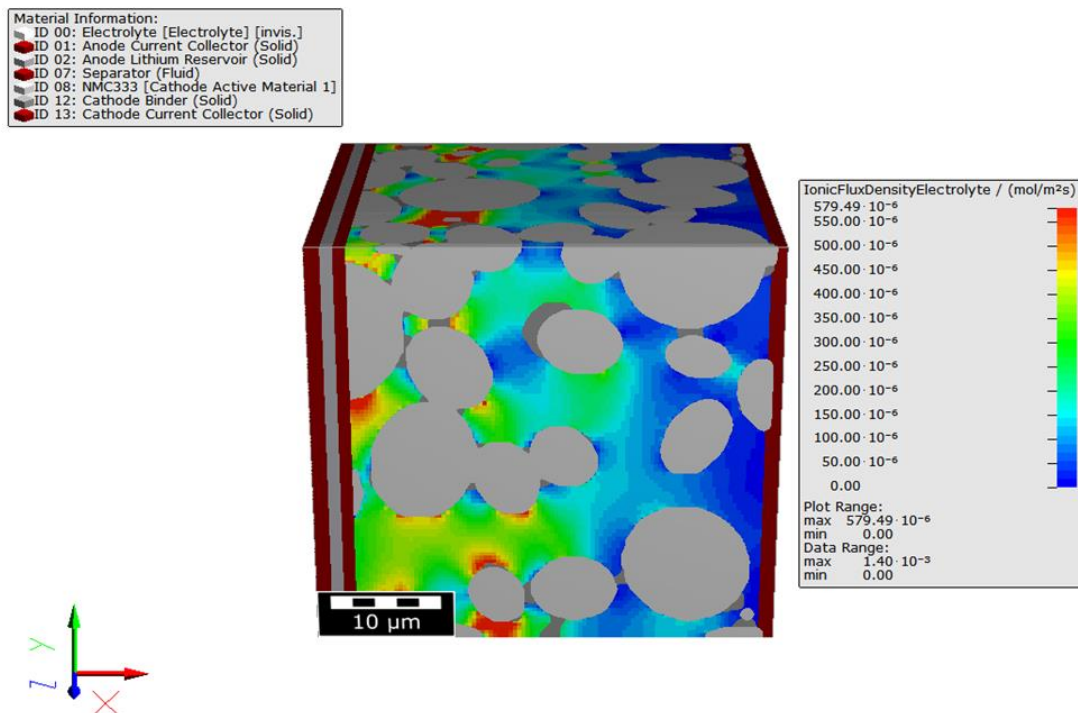
1. Visualize the results for the third time step by going to the **Data Visualization** tab, choosing **3: Electrode SOC 40%** from the pull-down menu, and clicking **Load Cell_2.cap**.



Now, select only the components that you wish to visualize. Here, the **DiffusionFlux** that is visualized as a default volume field, as well as the Lithium-Ion concentration in the solid materials are chosen.


In the dialog, click **Uncheck all** to de-select all components and then, select **ConcentrationSolid:ConcentrationSolid** and **IonicFluxDensityElectrolyte:IonicFluxDensityElectrolyte**. Click **OK**.

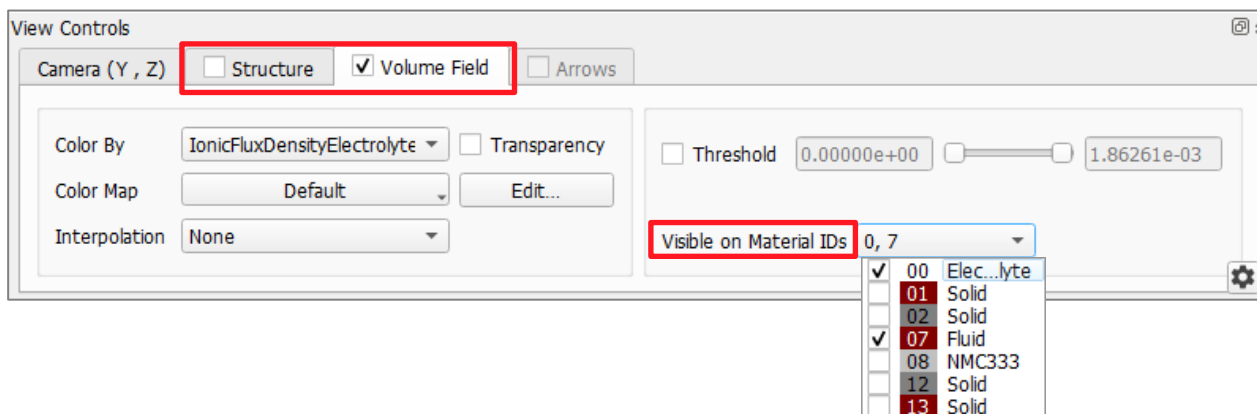
As it is shown here, the battery cell microstructure generated in GeoDict contains a separator, lithium reservoir anode, NMC cathode, and current collectors.



In the above picture, the colors are selected as following:

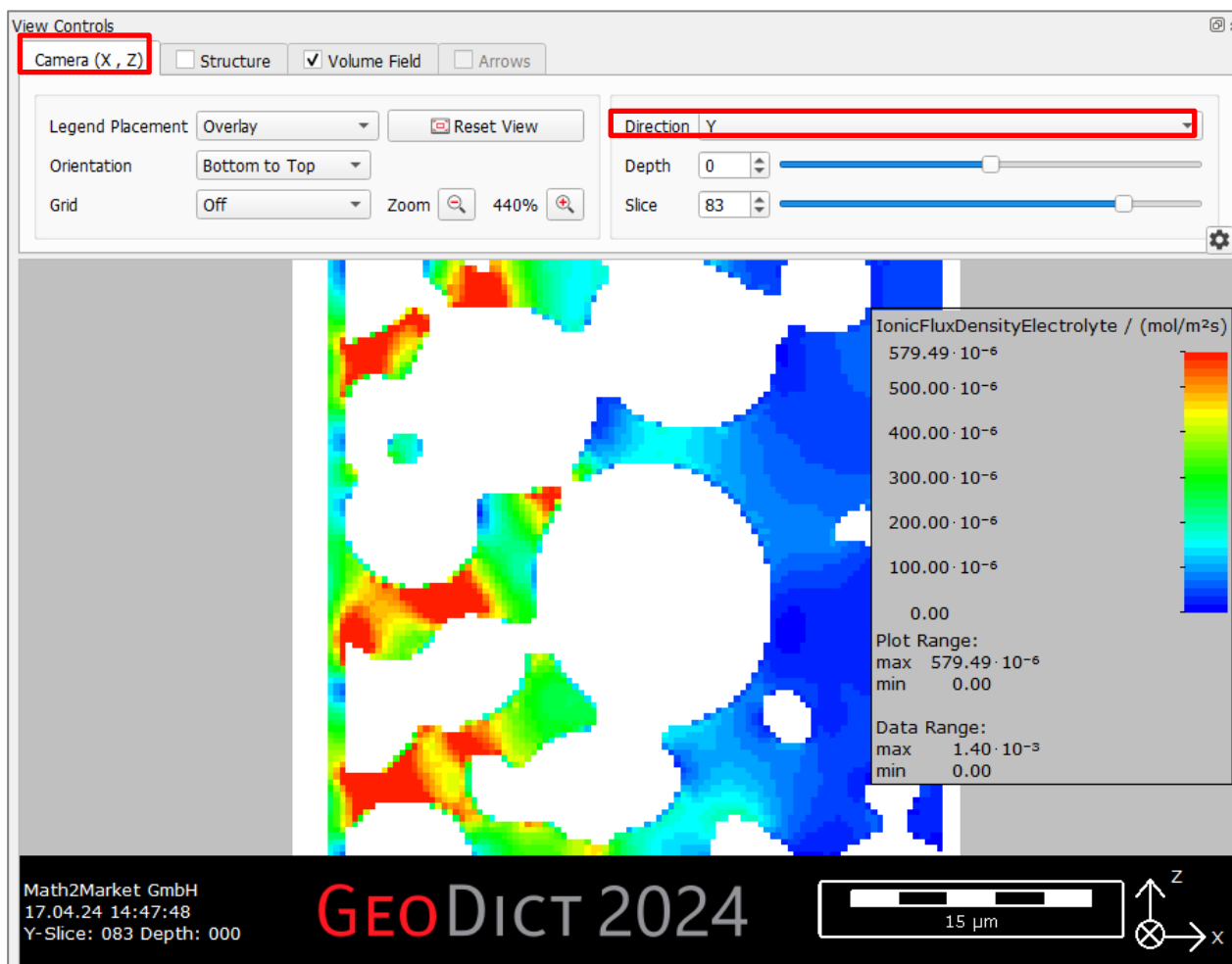
ID 00: Electrolyte	<input type="checkbox"/> White	<input type="checkbox"/> visible
ID 01: Solid	<input checked="" type="checkbox"/> Dark red	<input checked="" type="checkbox"/> visible
ID 02: Solid	<input checked="" type="checkbox"/> Dark gray	<input checked="" type="checkbox"/> visible
ID 07: Fluid	<input checked="" type="checkbox"/> Dark red	<input checked="" type="checkbox"/> visible
ID 08: NMC333	<input checked="" type="checkbox"/> Light gray	<input checked="" type="checkbox"/> visible
ID 12: Solid	<input checked="" type="checkbox"/> Dark gray	<input checked="" type="checkbox"/> visible
ID 13: Solid	<input checked="" type="checkbox"/> Dark red	<input checked="" type="checkbox"/> visible

- To see the 2D view, click the 2D icon  in the toolbar.
- Select **View** → **Legends / Overlays** from the menu bar. In the opened window, deselect **Material Legend**.
- Uncheck the **Structure** tab in the Visualization panel above the Visualization area and go to the **Volume Field** tab. From the pull-down menu for **Visible on Material IDs**, uncheck Material IDs 01, 02, 08, 12 and 13 to only visualize the diffusion in the electrolyte and the separator, as the diffusion is 0 mol/m²s in all other materials.

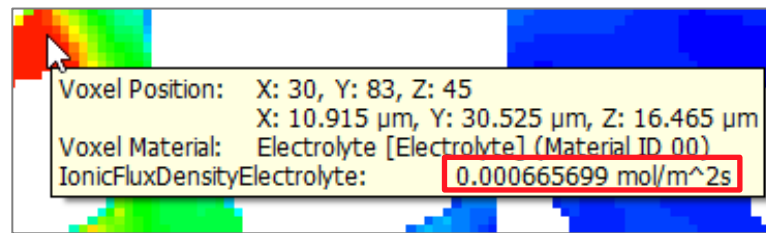


- Go to the **Camera** tab and select **Y** as **Direction**. Scroll through the slices with the mouse wheel or with the slider in the Visualization panel.

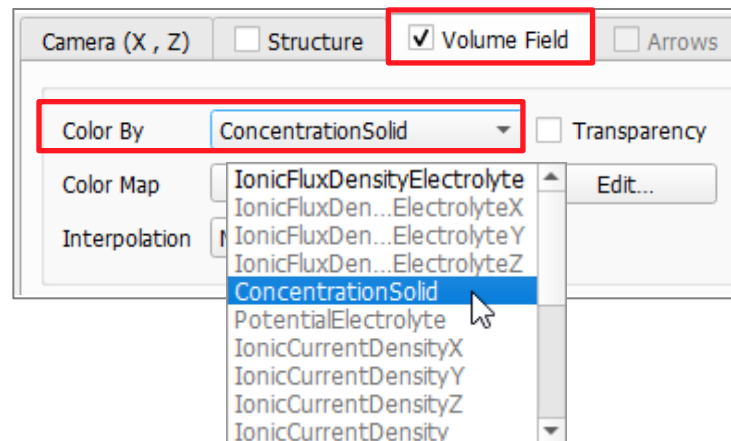
The results indicate that in all slices, the diffusion values near to the separator are higher than those around the cathode current collector.



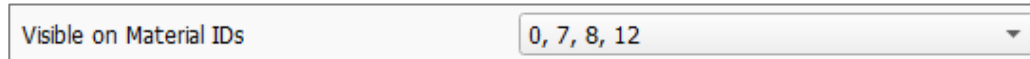
- Hover the cursor over the volume field to see the exact diffusion flux values and the materials in the corresponding voxels.



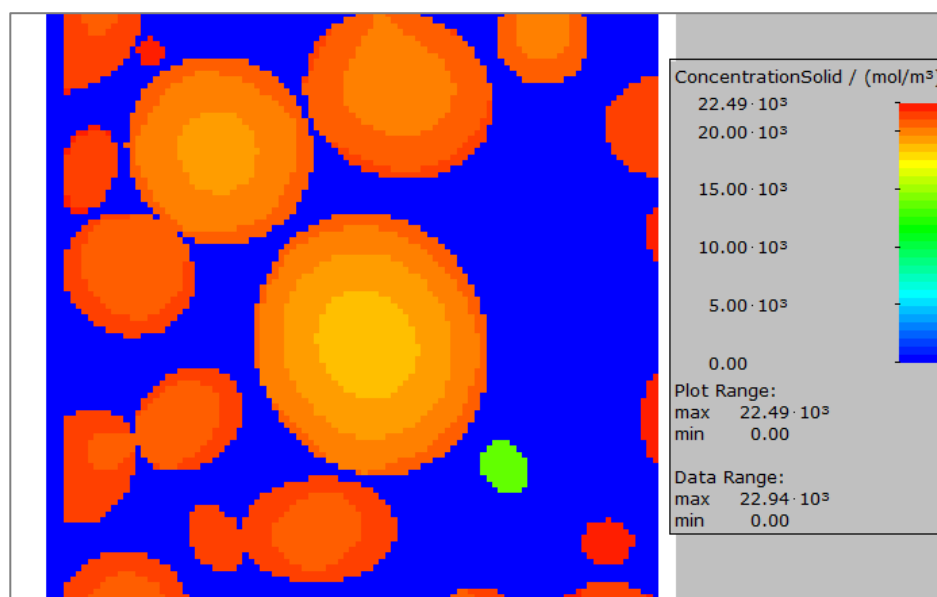
- Go to the **Volume Field** tab. In the **Color By** option, select **ConcentrationSolid** to view the ion concentration of the solid in the battery structure.



- Select ID 08 and 12 again for **Visible on Material IDs** to visualize the ion concentration in the NMC particles and the binder phase.



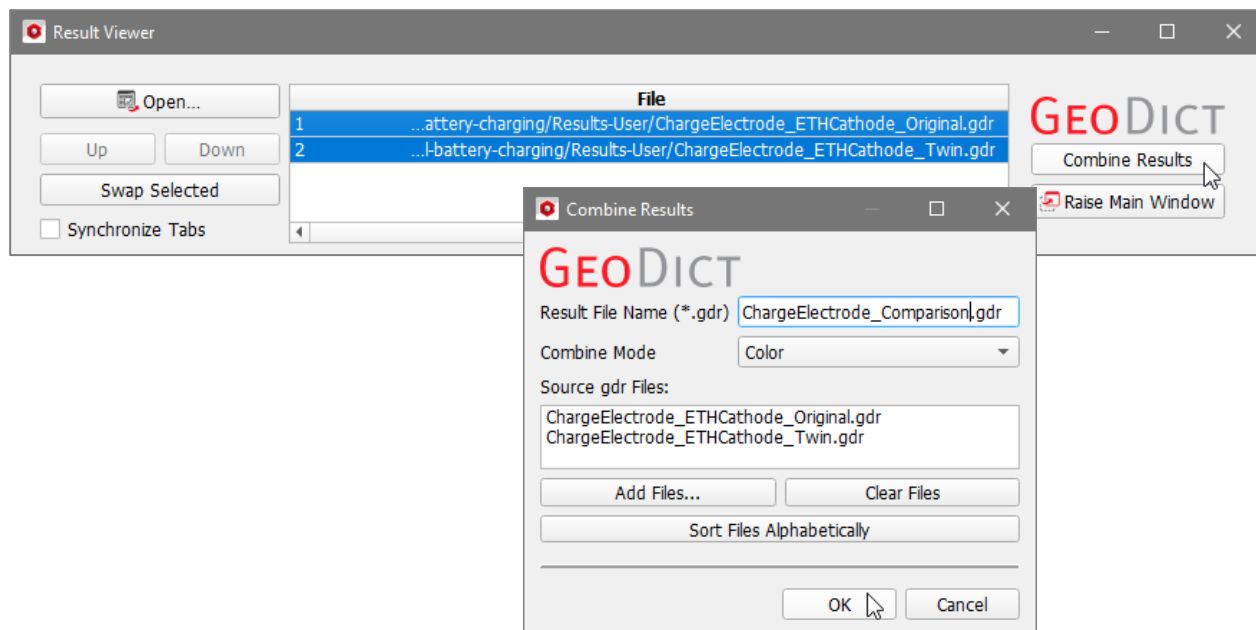
The colors indicated that the local concentration in the electrolyte is low, while in the NMC particles is in the highest value. In addition, the larger grains have a lower concentration than the smaller particles. The binder phase has the same concentration as the electrolyte, due to its porous model.



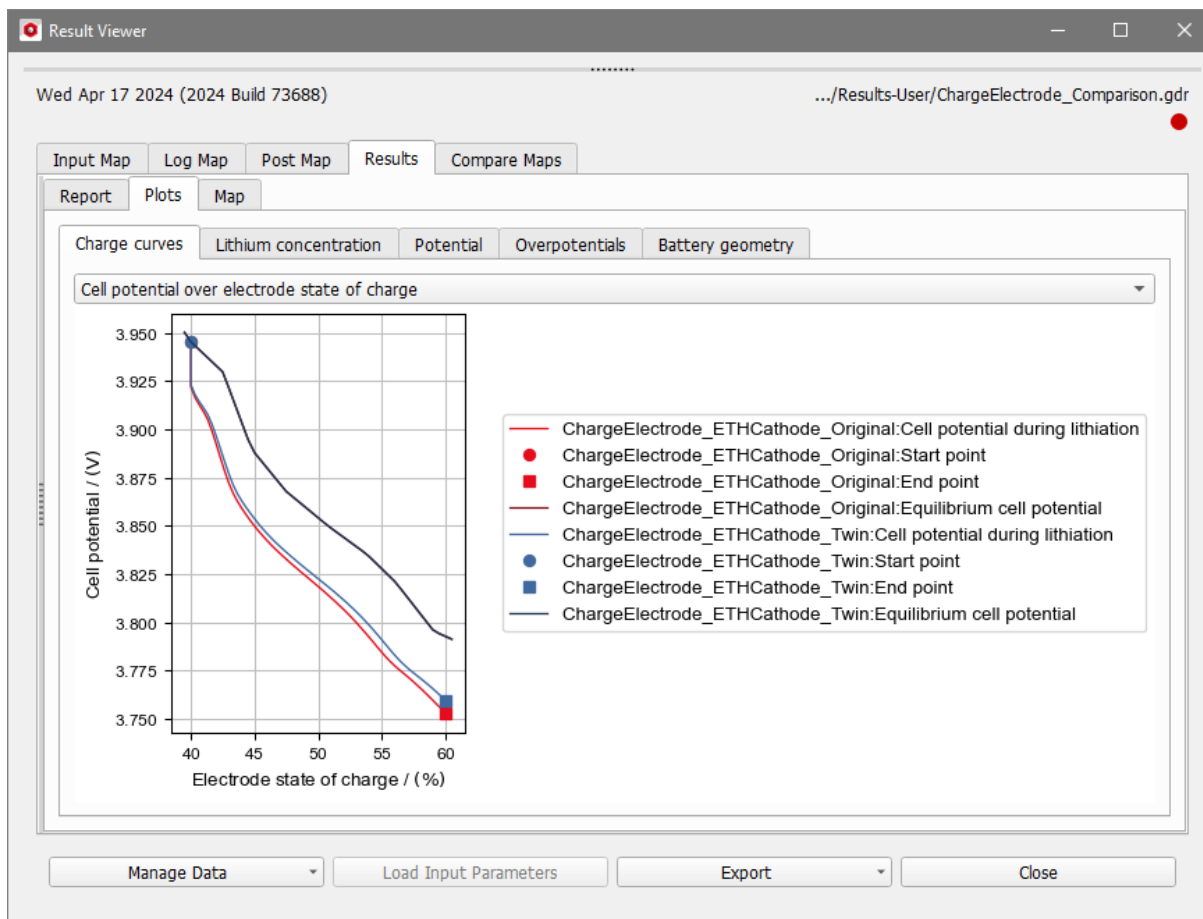
- To compare the results of the Charge Electrode simulations, load the **ChargeElectrode_ETHCathode_Original.gdr** and

ChargeElectrode_ETHCathode_Twin.gdr files and combine them in the Result Viewer as shown previously.

Click **Combine Results** and select the **Result File Name** to be **ChargeElectrode_Comparison.gdr**



As was shown before, compare the charging curves for the original cathode and its digital twin. They are fairly similar.



CONCLUSION

In this tutorial, we have shown how to simulate and analyze the charging behavior of a digital battery consisting of bimodal electrodes.

For the digital battery used in this tutorial, the resulting charging curve from the **BESTmeso** solver is very close to the charging curve obtained with the **LIR** solver.

When no result fields or slice mean plots are needed, the **BESTmeso** is a good and fast tool to analyze the performance of a battery with these materials.

To find out whether this finding holds for your own setup, test the simulation with cropped (but still representative) electrodes and compare the results of the **LIR** and the **BESTmeso** solver according to this tutorial. If the results are close, simulating on larger cutouts may be performed using the **BESTmeso** solver with high accuracy.

The [tutorial series Digital Battery Design](#) enable the users to import and segment scans from a real electrode microstructure to create, charge, and analyze a statistical Digital Twin in **GeoDict**. The series consists of the following tutorials:

1. **Import and quality control of a cathode material**: stepwise guide to analyze, post-process and segment a 3D-scan of a NMC-cathode.
2. **Standardized microstructure analysis of a cathode material**: stepwise guide to analyze the segmented scan regarding transport properties and pore size distribution.
3. **Building a statistical digital twin of a cathode material**: building of a statistical digital twin and validation using the results from the **Standardized microstructure analysis of a cathode material** tutorial.
4. **Digital battery charging**: Learn how to analyze the charging behavior of a digital battery consisting of bimodal electrodes.

*Our Electrochemistry - Batteries Team is eager to help you discover the features of **GeoDict** and of **BatteryDict** for the design of battery materials.*

Contact us: [Ilona Glatt](#) and [Roman Buchheit](#).

REFERENCES

- [1] M. Ebner, D.-W. Chung, R.E. García, V. Wood,
Tortuosity Anisotropy in Lithium-Ion Battery Electrodes, Advanced Energy
Materials, Vol. 4, 2014, 1301278
<https://doi.org/10.1002/aenm.201301278>.

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