GeoDict

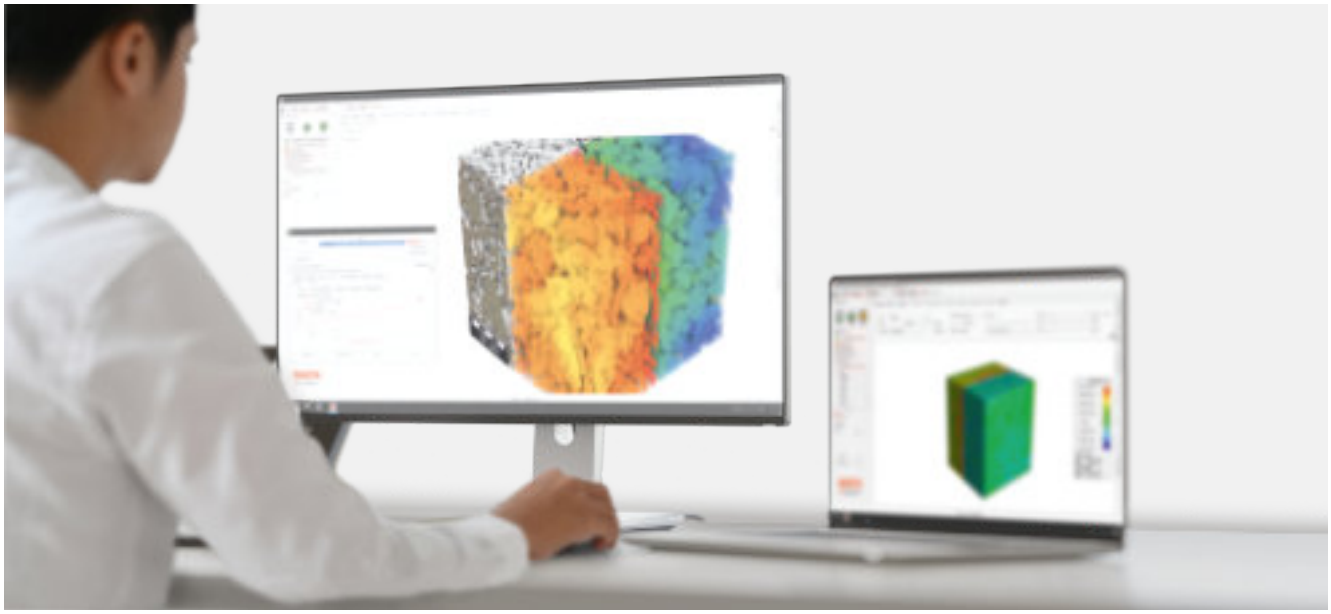
The Digital Material Laboratory

Battery Material Development

for Electrode and Cell Design

MATH
2 MARKET

GeoDict: Revolutionizing Battery Analysis, Research & Development

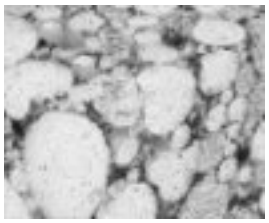
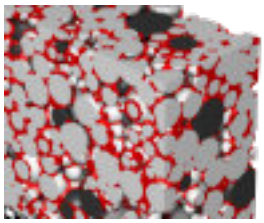
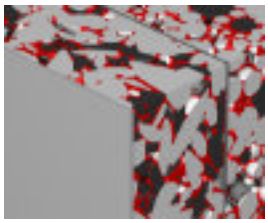


GeoDict stands as a pioneering digital platform in materials science and engineering, delivering unique problem-solving capabilities and innovative insights through microscale analysis and modeling of complex materials.

The GeoDict software, Math2Market's solution for digital material design and analysis, represents an integrated platform that revolutionizes materials science by way of microscale visualization, modeling, and analysis of complex material structures.

GeoDict's robust simulation capabilities offer precise predictions of the performance of designs under various conditions. GeoDict facilitates efficient modeling of material properties and phenomena, and fosters innovation in materials science, with a userfriendly interface and powerful algorithms.

GeoDict bridges the gap between theoretical principles in mathematics and physics and practical applications in material sciences and engineering, enhancing precision and reliability. GeoDict provides a key toolset for those in materials science research & development, to drive forward their work and projects.

Digitalize »	Analyze »	Validate »	Design »	Next Generation Material
				
Model a material from scratch or import scans of an existing material to understand and improve it. Create a digital material model.	Analyze the material geometry and compute physical properties of the material. Extract statistical data to create a digital twin.	Replicate the material and its properties in the computer through a digital twin. Validate the digital twin by comparing with real experiments on the existing material	Modify the digital twin to create a variety of digital prototypes and compute their properties. Loop and optimize to find the new material with the desired properties.	Manufacture the next generation material based on the digital design. The materials of the future are within reach. We help you develop them faster.
Digital Material	Statistical Model	Digital Twin	Digital Prototypes	This is innovation through simulation

The Material Design Process

The interplay between the geometry of the microstructure, properties of the constituent materials, and properties of the resulting materials forms a fundamental nexus in materials science and engineering. This intricate relationship serves as the cornerstone for advanced material design and optimization in GeoDict.

The geometry of the microstructure, such as the arrangement of phases, pores, and interfaces, critically influences a material's performance. GeoDict's expertise lies in the potential to harness this geometry as a lever to tailor material properties. By manipulating microstructural features, the tool enables the design of materials with specific electrochemical or morphological properties, or other attributes.

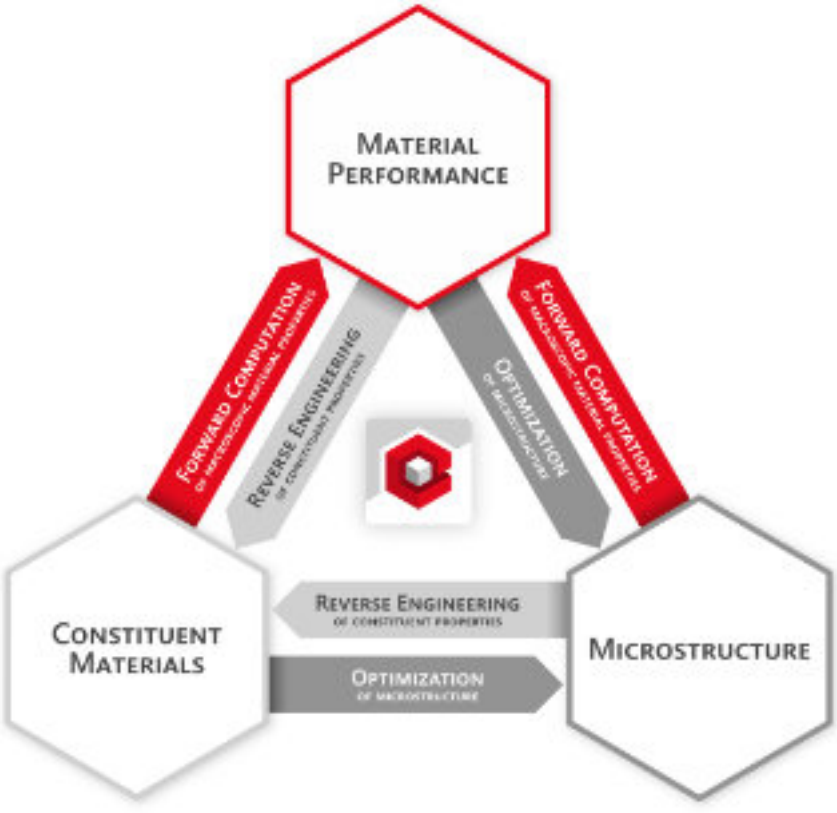
Equally pivotal are the properties of the constituent materials. GeoDict empowers researchers to input these properties from its database and predict resulting material behaviors. This predictive capability opens avenues to choose optimal constituent materials for a desired outcome, thus circumventing exhaustive and costly trial-and-error approaches.

Moreover, GeoDict opens the door to the reverse approach: deriving constituent material properties based on the material characteristics and geometry from its results. This reverse inference unlocks insights into the underlying composition of complex materials, accelerating the understanding of intricate systems.

In certain cases, GeoDict even enables the estimation of geometrical properties from known material properties and from the properties of the constituent materials. This versatile bi-directional prediction transforms the way new materials may be conceptualized and designed.

In essence, GeoDict's unique capability to interrelate microstructure, constituent materials, and resultant properties empowers materials engineers to innovate with unprecedented precision and efficiency. It transforms the field by enabling systematic exploration, efficient optimization, and the modeling of materials with tailored functionalities, all while unraveling the intricate threads that weave materials science together.

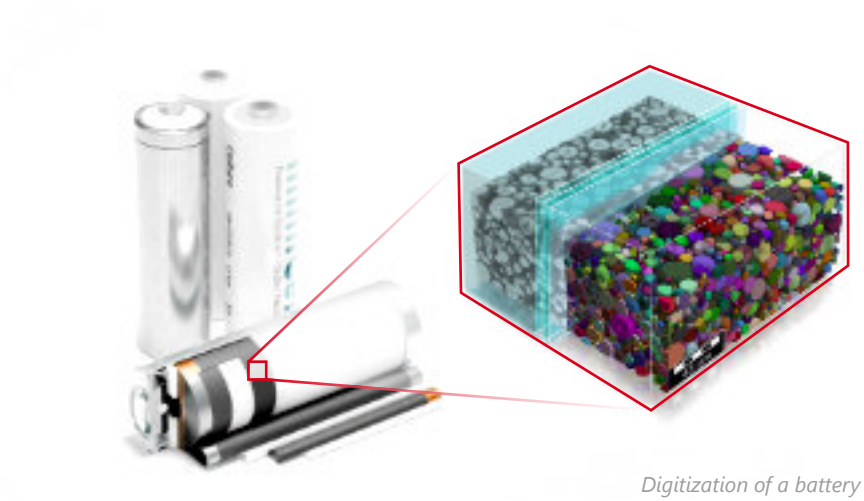
The GeoDict Triangle



Exploring the relations between microstructure, constituent properties, and material performance

Innovation through Simulation

GeoDict, by Math2Market, offers tailored solutions for R&D professionals in materials science. Among its features, the detailed material analysis, specialized applications, a user-friendly interface, and true-to-life 3D modeling are standing out. Advantages encompass high precision, easy integration, comprehensive scientific support, and continuous innovation, providing benefits such as improved efficiency, data-driven decision making, scalability, and cost-effectiveness.



Digitization of a battery

GeoDict Features

GeoDict offers a robust suite of features tailored to the requirements of R&D professionals working with battery design, electrode materials, electrolytes, separators, all solid-state batteries, lithium-ion technology, thermal management systems, and battery safety testing.

- **Detailed Material Analysis:** GeoDict provides in-depth analysis capabilities to investigate key material characteristics, such as grain sizes, conductivity, surface areas, diffusivity, tortuosity, and pore size analysis.
- **Specialized Application:** GeoDict is designed specifically for the simulation of materials such as batteries, electrodes, electrolytes, separators, and delivers precise, reliable results.
- **User-friendly Interface:** GeoDict offers an intuitive interface, simplifying navigation and operation and enhancing user productivity.
- **True-to-Life Material Modeling:** Build 3D material models with GeoDict to create accurate simulations for reliable, practical outcomes.

Why choose GeoDict?

GeoDict offers several key advantages over other material simulation software options:

- **Precision:** Advanced algorithms confer GeoDict unique accuracy in data interpretation and modeling.
- **Easy Integration:** GeoDict integrates seamlessly with existing software tools, enhancing workflows and reducing time spent on configuration and data preparation.
- **Support and Training:** Our commitment to our clients extends beyond providing a superior software solution. We offer ongoing scientific support and training to ensure maximal benefits from GeoDict.
- **Continual Innovation:** GeoDict remains a leading solution for simulations in materials science by continually fine-tunning the software based on user feedback and industry advancements.

Benefits of GeoDict

Investing in GeoDict is more than a software decision; it's a strategic move towards better efficiency, informed decision-making, scalability, and cost-effectiveness.

- **Improved Efficiency:** GeoDict reduces time spent on data analysis and simulation, leading to increased productivity and faster turnaround times.
- **Better Decision-Making:** With its precise and detailed material analysis, GeoDict supports data-driven decision-making processes.
- **Scalability:** No matter the size of the project, GeoDict can handle it, providing a reliable tool for all material development needs. We offer efficient cloud solutions for further scalability.
- **Cost-Effective:** GeoDict's comprehensive capabilities and seamless integration make it a cost-effective solution that provides a significant return on investment.

GeoDict Workflow for Battery Development

Easy-to-use

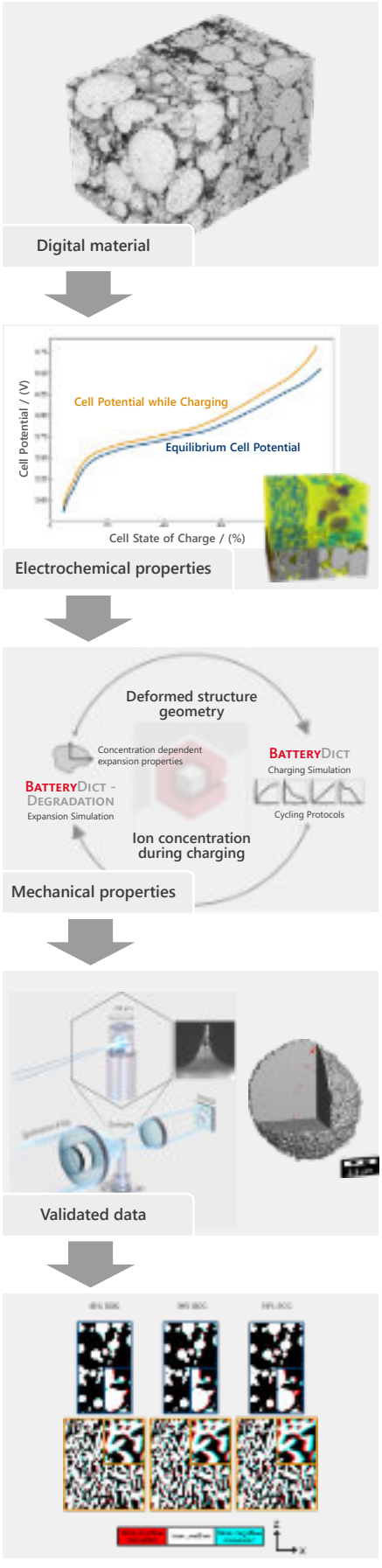
- User-friendly, intuitive graphical user interface
- Seamless integration into existing IT infrastructure
- Complete automation and replication - thanks to Python
- Voxel grid-based simulation eliminates the need for complex meshing

Advanced and powerful features

- Analysis, property prediction, and visualization directly on computed tomography (CT) scans, focused ion beam-scanning electron microscopy (FIB-SEM) scans, and synchrotron scans.
- Structure generators: realistic modelling of microstructures with random elements for fast digital experiments
- Artificial Intelligence for identification of binder and grains, and grain distribution analysis
- High storage efficiency: simulations on structures of 64 billion voxels and more are possible on single computers or in clusters

Accurate property prediction

- Accurate prediction of battery performance characteristics, such as ion transport efficiency, overpotentials or thermal and electrical conductivity, degradation mechanisms, and overall energy density
- Unmatched range of physical parameters predicted by GeoDict.
- Prediction of complex material behaviors, such as individual contributions to cell overpotential, battery degradation, local lithium concentration changes, and mechanical stresses from volume changes due to electrochemical reactions.



Example of GeoDict workflow for experimentally validated simulation of strain-induced battery aging

1. Data acquisition

Import: Import and segment µCT und FIB-SEM 3D-scans of existing materials. Handling and processing of 3D material models.

Modeling: Develop 3D models of granular material microstructures by incorporating geometric and granular parameters (e.g., particle size distribution, shape, packing density, porosity). Construct advanced material models by integrating and merging multiple phases (e.g., pores, inclusions, binder phases).

2. Electrochemical Simulation

This process models battery charging to analyze electron and ion movement and the resulting cell voltage, considering equilibrium cell voltage and overpotentials under various conditions like constant charge rates or constant current/voltage.

It offers insights into the processes inside the battery, such as lithium concentration changes and ion fluxes, and identifies origins of overpotential, like the kinetics of ion exchange or diffusion. These simulations facilitate pinpointing and optimizing battery performance bottlenecks.

3. Mechanical Simulation

Battery degradation is linked to microstructural changes caused by mechanical stress and strain in electrode materials due to lithium intercalation. Using GeoDict software, local volumetric changes are simulated based on lithium concentration changes, integrating electrochemical and mechanical simulations.

The result is a detailed analysis of stress, strain, and displacement, indicating cell damage during battery cycling, offering insights into improving battery durability and performance.

4. Measurements

The SOLVED![1] project used in-operando XTM at the TOMCAT beamline to track battery microstructure changes during cycling, extracting expansion coefficients for anodes and cathodes for simulation.

Validated against in-operando XTM data and refined with electrochemical characterization, the project produced a validated dataset, advancing battery performance understanding.

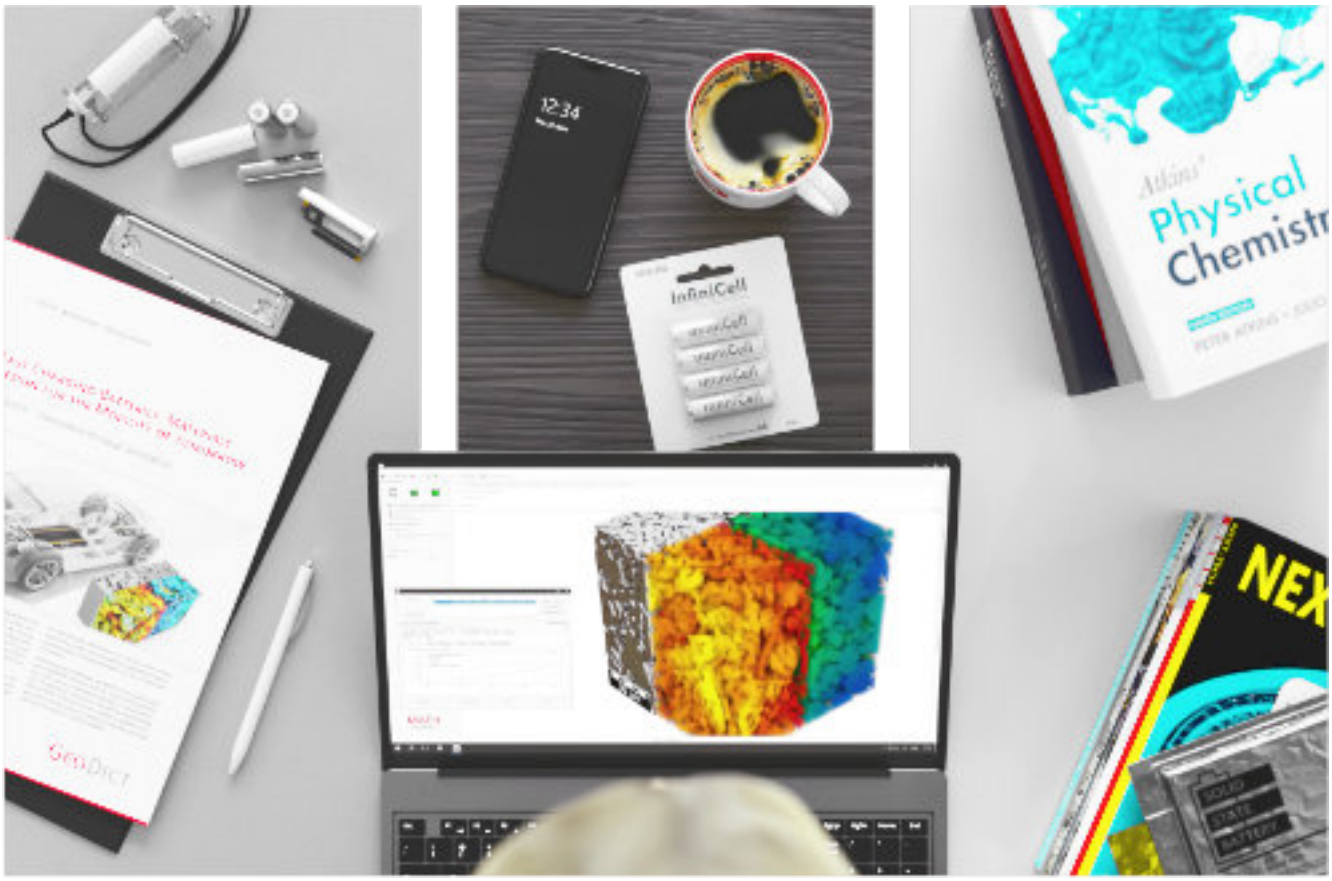
[1] Studying battery aging with quantitative simulation in the SOLVED! project

5. Validation

The simulation of a battery with a graphite anode and NMC811 cathode was validated against in-operando measurements, showing well-matching expansions of 10% and 9.8%.

The agreement was quantified through voxel congruence, with 2D cross-sections overlaid to visualize matching areas, highlighted by white voxels for agreement. This validation confirms the effectiveness of digital simulations in battery R&D, enhancing design and performance analysis.

GeoDict in Industrial and Academic Settings



R&D Professionals

As an R&D professional, challenges often involve developing innovative materials while reducing the time and cost of experimentation. GeoDict, with its advanced simulation capabilities, allows to create and test materials in a digital environment. It provides in-depth material analysis, speeding up the process of fine-tuning material properties. It's a reliable partner to enhance innovation and reduce time-to-market in material development.

All the desired properties of the material are simulated from the desk. No need to purchase small quantities of sample materials, to setup large production machines for small test quantities and to evaluate properties with the usual experimental deviations.

GeoDict qualifies and quantifies the needed material properties with rigorous precision.

Production Managers

In production, efficiency, quality, and cost-effectiveness are key. Using GeoDict's simulations, manufacturers can identify potential problems early on.

GeoDict helps to optimize the use of raw materials, minimize waste, and improve quality control. It's a powerful tool to achieve the required production efficiency and sustainability goals.

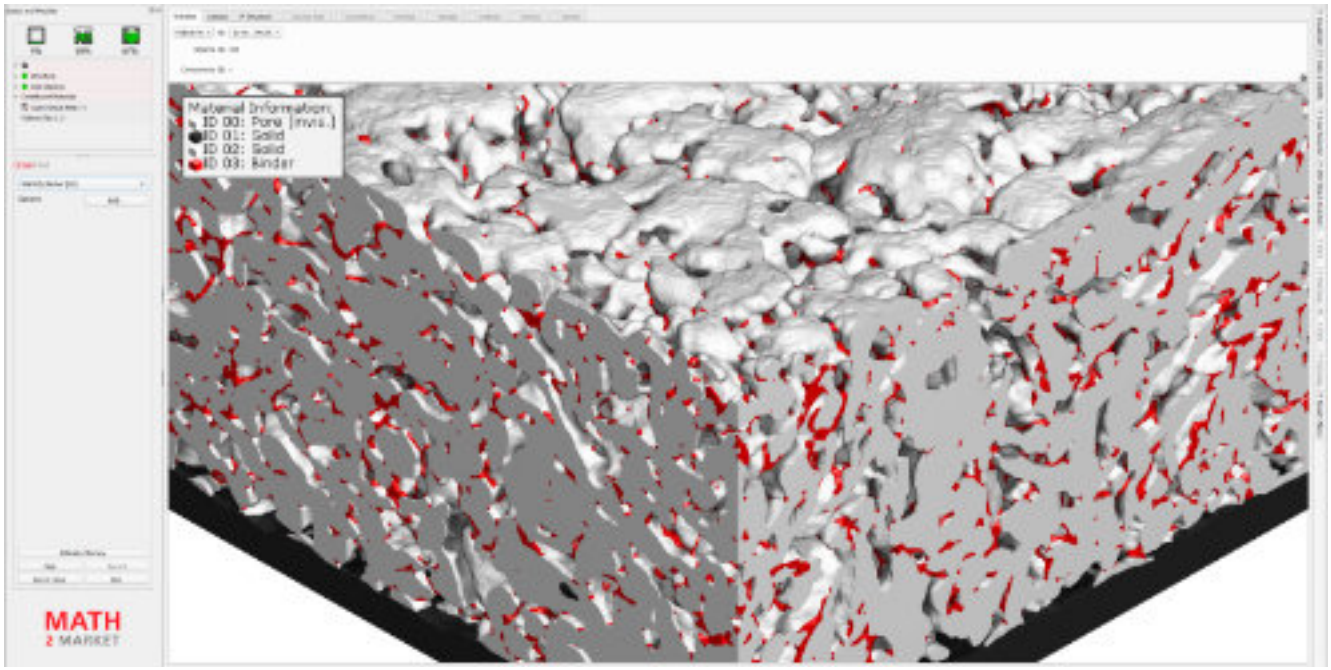
As you know, errors in production quickly develop into large costs. Before even encountering any of these errors, GeoDict is brought into play to conduct studies using design of experiments methods and estimate the impact of these errors on product quality. Moreover, GeoDict is a great tool for quality control and helps to effectively monitor particular relevant parameters.

Academic Researchers

In the world of academic research, the boundaries of material science are continuously pushed and tested. GeoDict supports research studies with its true-to-life 3D material modeling and its precision in the analysis of numerous material characteristics. Its ability to handle complex simulations allows exploring novel research areas and deepen the understanding of material behavior. GeoDict, with its ongoing updates and enhancements, is a powerful and reliable tool in the pursuit of academic excellence.

By calculating material properties using physical models on microstructures, GeoDict is a crucial tool for all material scientists. The relevant parameters for the design of novel materials are easily determined and optimized for future usage cases while maintaining full control of all related input values.

Usability: A Core Strength of GeoDict



GeoDict has gained notable acclaim due to its unique fusion of advanced simulation capabilities and an exceptionally intuitive user interface. This software has been purposefully crafted to clarify the intricacies of complex material simulations and analyses, presenting itself as an accessible and userfriendly tool suitable for individuals of all skill levels. Whether you're a novice venturing into the world of simulations or a seasoned expert, GeoDict's user-centric approach ensures effortless navigation through sophisticated simulations, seamlessly translating complex data into valuable insights.

The coupling of sophistication and simplicity within GeoDict delivers a powerful material simulation tool that prioritizes usability. This steadfast commitment to user-friendly design underscores Math2Market's unwavering dedication to providing accessible solutions to the materials science community, enabling the realization of advanced simulations without the typical steep learning curve. GeoDict empowers a diverse user base by striking the perfect equilibrium between technical prowess and an approachable interface, making it a cornerstone in the realm of material science innovation.

User-friendly Interface

One of the fundamental aspects of GeoDict's usability lies in its intuitive interface. A clean, organized layout facilitates easy navigation through its comprehensive suite of features. The process to set up, run simulations, and interpret results has been streamlined, reducing the learning curve and enhancing productivity.

Interoperability

GeoDict has been built with interoperability as a key feature. It seamlessly integrates with other software tools commonly used in material development and research, creating a unified workflow. This simplifies data management and enhances efficiency.

Comprehensive Support

GeoDict's usability extends beyond its software design. Math2Market provides robust customer support, including detailed user manuals, video tutorials, and access to our team of experts for more complex scientific queries. We offer dedicated training courses to master GeoDict and exploit its full potential.

Customization

The flexibility of GeoDict allows for customization to meet individual project needs. Users choose from a wide array of parameters and settings to tailor their simulations, offering a personalized experience.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OVATION
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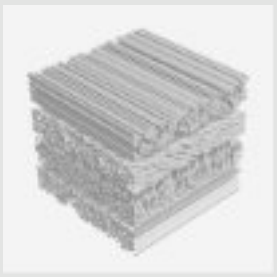
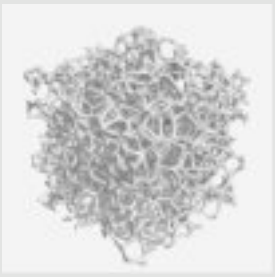
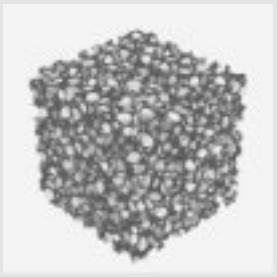
ImportGeo


FiberGeo

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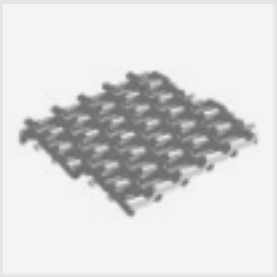
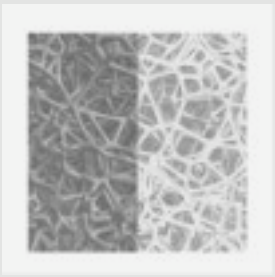
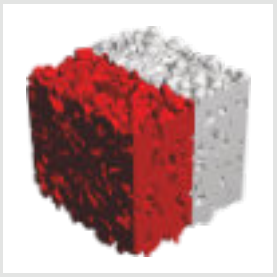



WeaveGeo

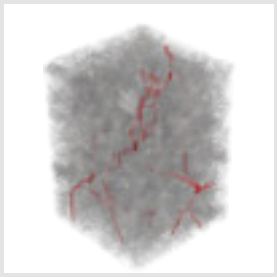
GridGeo



MeshGeo

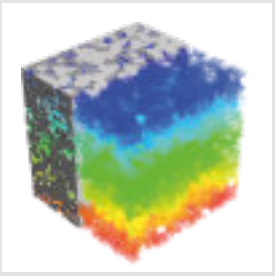


ExportGeo

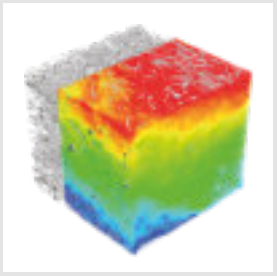


PoroDict

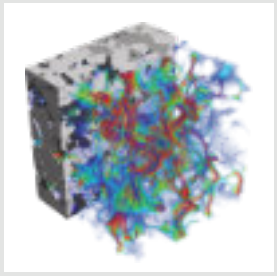
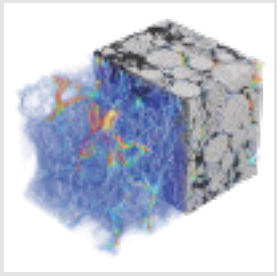
This is **Innovation** through **Simulation**



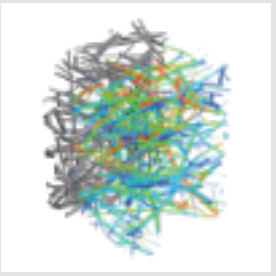
DiffuDict



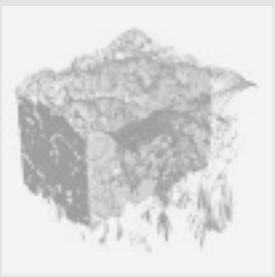
ConductoDict

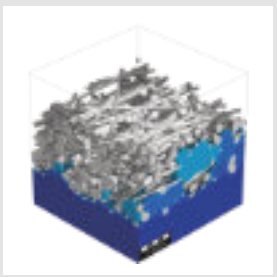
FlowDict



ElastoDict



AddiDict



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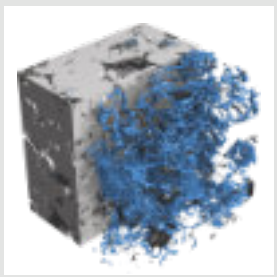
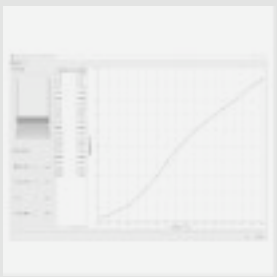
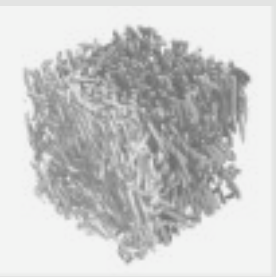



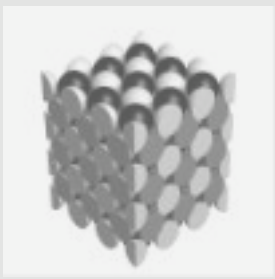
AcoustoDict

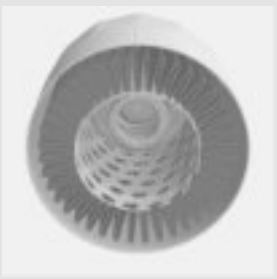


FiberFind AI

PaperGeo

GrainGeo





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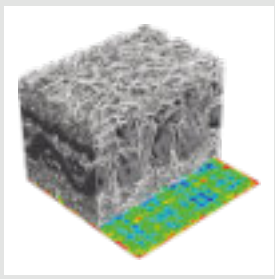
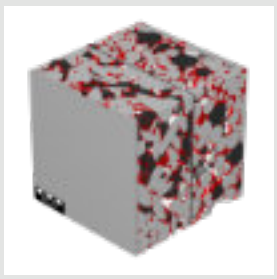
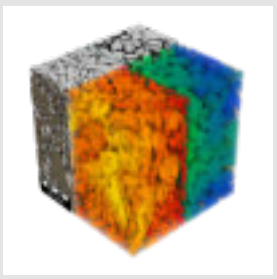
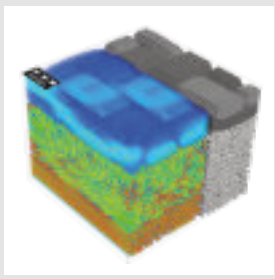


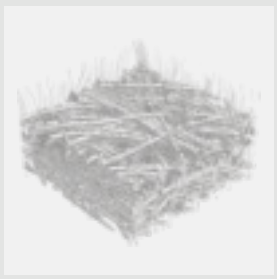
MatDict



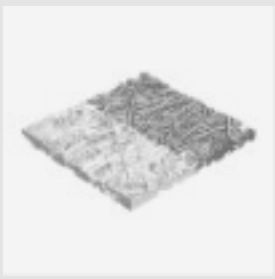


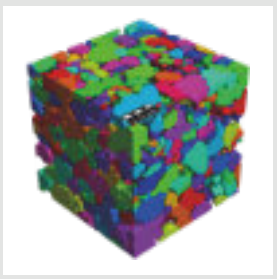
BatteryDict





FilterDict Media & Element





GrainFind

GeoDict Modules

GeoDict is used worldwide for R&D and production in industrial and academic settings mainly in the fields of batteries, fuel cells, electrolyzers, Digital Material R&D, filtration, and digital rock physics.

The modular setup of the GeoDict software is essential to its versatility and adaptability to the specific requirements of diverse applications. In this way, GeoDict is a customized solution, tailored to the development or research task of the user.

GeoDict Modules

GeoDict Base

The GeoDict Base package contains the basic features and modules of the GeoDict software. It includes a graphical user interface, advanced visualization capabilities, and tools for fine-tuning and transforming 3D images and material models. Also included are a Python integration for workflow automation and modules for interface with Matlab® and Microsoft Excel®. Overall, the Base package provides a comprehensive set of tools to create, analyze, and manipulate 3D images and material models.

GeoDict's Base Package comes fully equipped with the following essential modules:

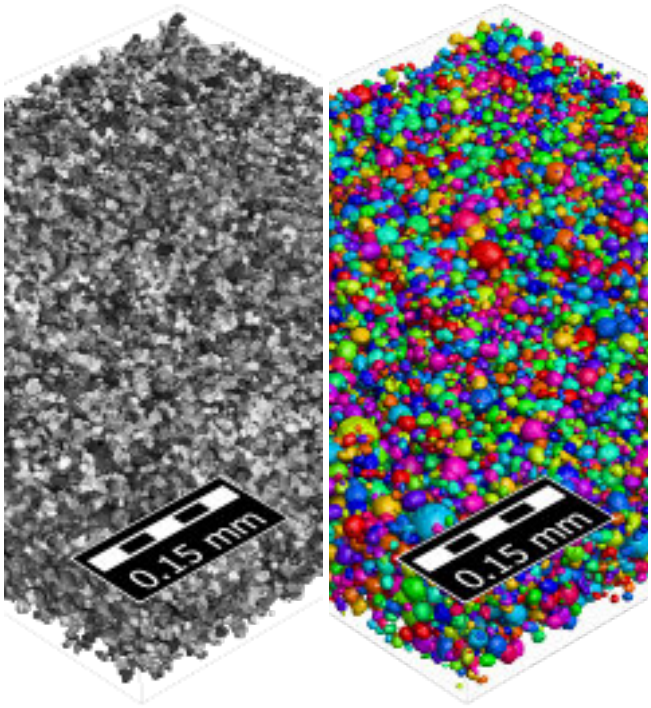
- **GeoLab**: Matlab® interface for GeoDict.
- **GeoDexcel**: Analyze GeoDict results with Microsoft Excel®.
- **ProcessGeo**: Powerful 3D image and material model processing tools.
- **LayerGeo**: Combine and layer segmented 3D images and models.
- **ImportGeo-Base**: Import data in various GeoDict formats.
- **ExportGeo-Base**: Export to GeoDict and other formats (*raw, *png, *am).
- **GadGeo**: Create and manipulate 3D material models with ease.

GrainFind

The GrainFind module is designed for analyzing µCT- or FIB-SEM scanned granular structures, such as those found in battery electrodes. It features the Identify Grains algorithm, which calculates the best-fit shape for each grain, recognizing individual grains and their spatial orientation. This information can be seamlessly integrated into GrainGeo to create detailed microstructure representations or to consider anisotropic material properties, facilitating the modeling of statistical Digital Twins of the scanned microstructure.

A common challenge in µCT scans is distinguishing between binder and grains due to similar gray values. To address this, the "Identify Binder (AI)" module employs Artificial Intelligence to differentiate between the two based on shape. GeoDict includes neural networks for identifying binders in NMC and graphite structures, with the capability to train additional networks for varied particle shapes and distributions through GeoDict-AI.

GrainFind streamlines material analysis with AI, automating grain and binder identification for applications in battery development offering insights through 3D visualization.



Identified grains are displayed as an index image on the 3D model.

ImportGeo-Vol

Import

GeoDict offers the option to import / load a variety of file formats. Its ImportGeo-Vol module handles the following file formats: *.raw, *.vol, *.rek, *.vox, *.vgi,*.iass, *.am, *.txm, *.bmp, *.gif, *.jpg, *.mng, *.pbm, *.pgm, *.png, *.ppm, *.tif, *.tiff, *.xbm, *.xpm, and GeoDict specific formats. The add-on ImportGeo-CAD module is required for the import of *.stl files.

3D Image Processing

GeoDict's ImportGeo-Vol module offers various image editing and processing features, including file import and domain editing tools such as rotation, cropping, and slice extraction.

The module includes a variety of image filters e. g. for denoising, edge detection, and contrast enhancement, all of which run in 3D on both CPU and GPU.

Specific tools for microCT and FIB-SEM scans are also available, such as ring-artifact removal and slice alignment. GeoDict provides several tools for image segmentation, including user-defined thresholds, threshold filters like the Phansalkar filter, and automated segmentation methods such as k-means and Otsu clustering algorithms, as well as Artificial Intelligence-based methods.

AI-Powered Labeling with Magic Brush

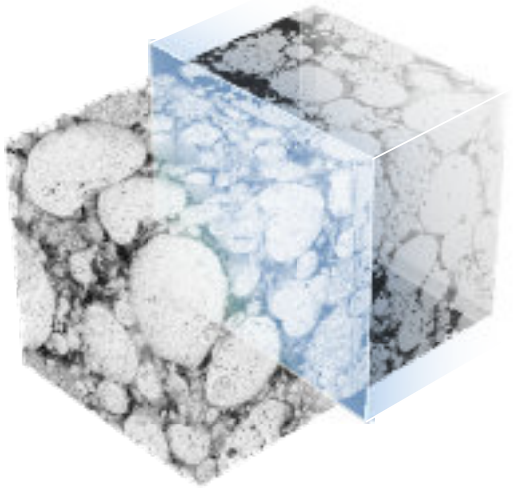
The Magic Brush for AI Labeling makes labeling of gray scale image data easy for users by offering a clustered selection tool for efficient labeling of segmented areas.

Enhanced Multi-Channel AI Segmentation

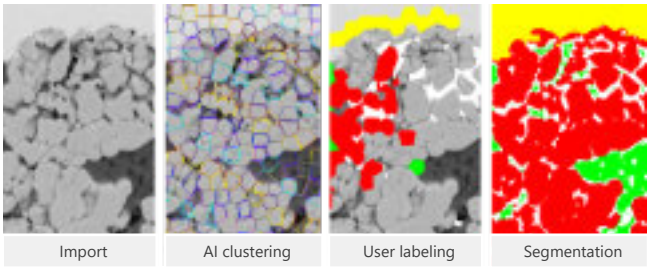
Multi-channel AI segmentation within ImportGeo-Vol allows to integrate multiple image stack data sets, e.g. recorded by different detectors, to use the maximum available information for the µCT or FIB-SEM segmentation. When segmenting a FIB-SEM scan it combines the SE2 detector's ability to identify the scan's focus plane and the ESB detector's material contrast clarity. This integration results in superior segmentation outcomes compared to conventional single-image methods.

Deep Learning for Image Quality Enhancement

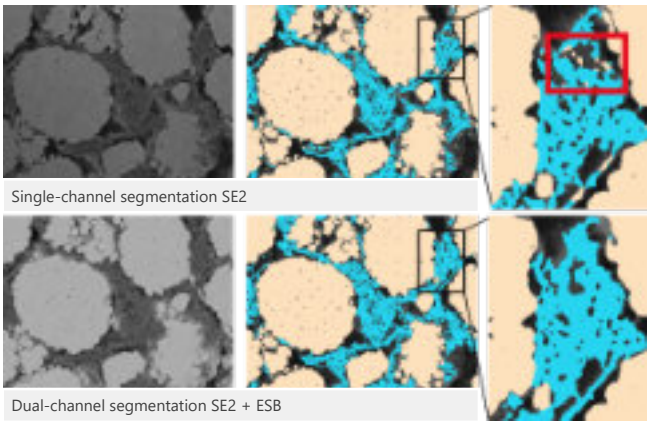
Deep learning advancements enable GeoDict to transform quickly captured, low-resolution images into high-quality versions by training a neural network with pairs of low and high-quality images. This process reduces noise and enhances resolution, saving time and costs in scanning your sample while ensuring detailed structure import.



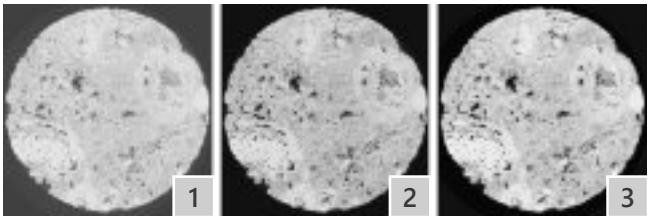
CT-scan of LiFePO4 cathode provided
by KIT (Karlsruhe Institute of Technology)



Magic Brush segmentation of a FIB-SEM scan of a NMC532 cathode



Comparison of single-channel segmentation and
dual-channel segmentation



Comparison of **fast-scan (1)**, **quality-scan (2)**, and **AI-enhanced-scan (3)**

GeoDict Modules

GrainGeo

GrainGeo is a GeoDict module designed to create digital 3D models of various granular microstructures such as

- electrode materials,
- sintered materials,
- grain packings,
- and powders.

GrainGeo inputs are user-defined parameters like

- grain size,
- pore size distribution,
- and grain shapes

to generate detailed microstructure models for visual analysis, comparable to what one might achieve through µCT-scans.

In GrainGeo, these parameters might be modified to design new material structures and compute their properties, facilitating the optimization of material performance by comparing new designs with existing products.

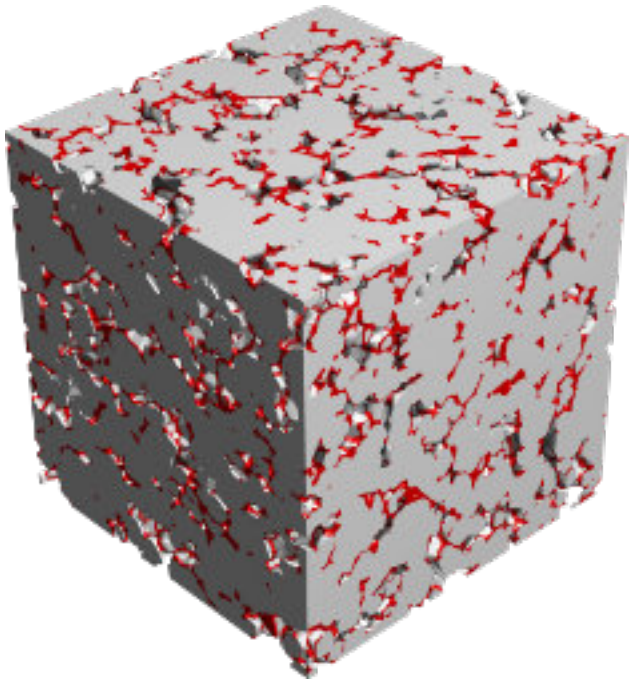
Applications of GrainGeo include the modeling of

- battery electrodes,
- secondary active material particles made up of primary particles,
- sintered structures,
- and components of other electrochemical devices, such as PEM fuel cells and electrolyzers,

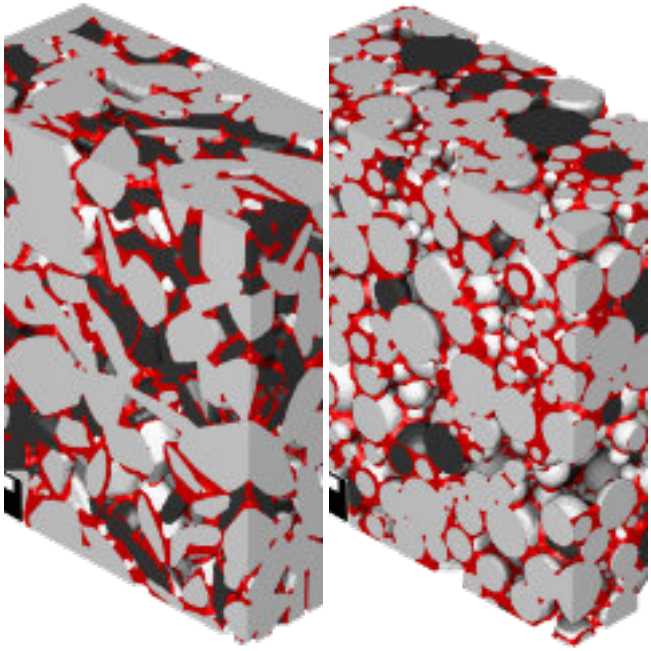
focusing on target parameters such as

- certain porosity,
- grain size distribution,
- grain shapes,
- or achieving high packing densities.

GrainGeo models various states of the sintering process and can handle objects of different shapes and sizes, including spheres, ellipsoids, polyhedra, and fibers, with the capability to model both open and closed porosities as well as sintered composites without porosity.



3D microstructure model of a Lithium-Ion electrode



Anode and cathode designed with GrainGeo

BatteryDict

BatteryDict is a specialized module within GeoDict designed for the detailed modeling and simulation of Li-ion battery cells. It supports the comprehensive analysis of electrochemical cycling, integrating advanced solvers for both fully resolved (detailed) and homogenized (fast) simulations. Key solvers include the LIR solver developed by Math2Market and the BEST solver from the Fraunhofer Institute for Industrial Mathematics (ITWM), enhancing the module's simulation capabilities.

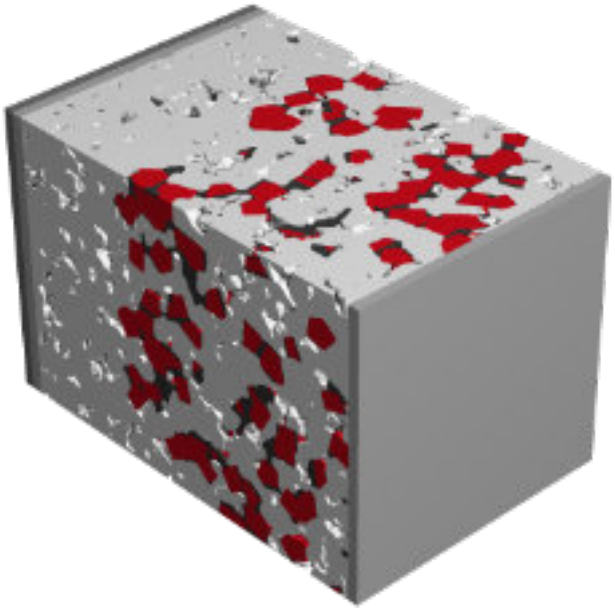
Simulation and Analysis Features:

- **Electrochemical Cycling Analysis:** Simulation and comparison of charge curves at specific charging rates or potentials against equilibrium curves. Crucial for evaluating battery performance under various conditions.
- **Microstructure Analysis:** Identifies inactive regions within battery materials and electrolyte, aiding in the optimization of battery efficiency and longevity.

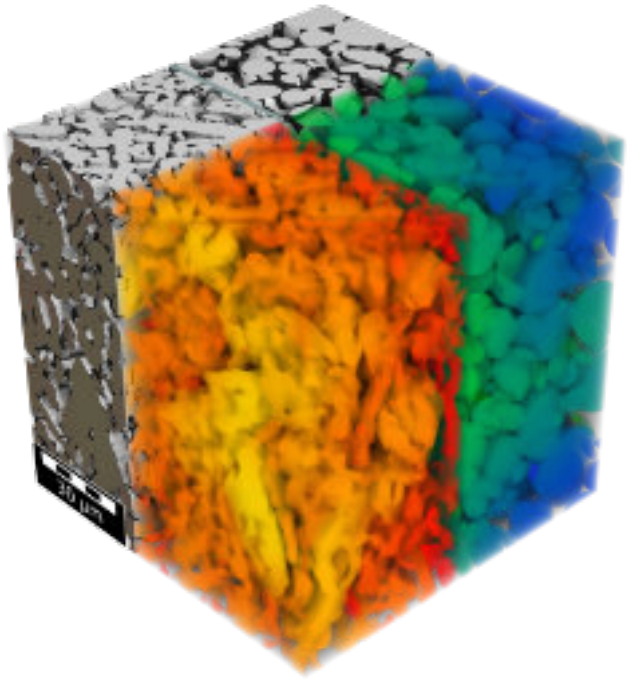
Core Functionalities:

- **Design Battery:** Facilitates the digital modeling of battery structures, enabling users to specify electrode orientation, material models, and component placement for optimal cell geometry.
- **Analyze Battery:** Evaluates digital models for connectivity and material distribution, aiming to reduce unconnected material and ensure balance between the cathode and anode.
- **Charge Battery:** Features three sophisticated solvers for micro-scale battery charging simulations, prioritizing efficiency and detail with concentration-dependent parameters.
- **Degradation Analysis:** Utilizes the FeelMath solver in the BatteryDict-Degradation add-on to compute mechanical stress and strain from lithium intercalation, highlighting potential mechanical degradation and guiding structural optimization for extended electrode lifespan.

BatteryDict offers a unique blend of detailed modeling capabilities, efficient simulation tools, and comprehensive analysis options. It stands as an indispensable tool for researchers and engineers focusing on the development and optimization of Li-ion batteries, ensuring high performance, durability, and efficiency in battery design and analysis.



All-Solid-State-Battery microstructure model



An electrode with a 70 percent charge, displaying the lithium ion concentration within both the anode and cathode

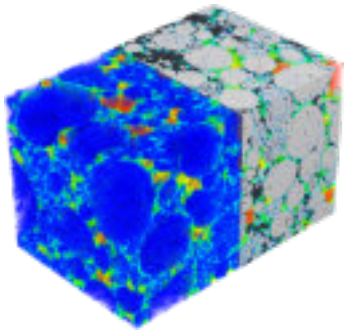
GeoDict Modules

PoroDict + MatDict

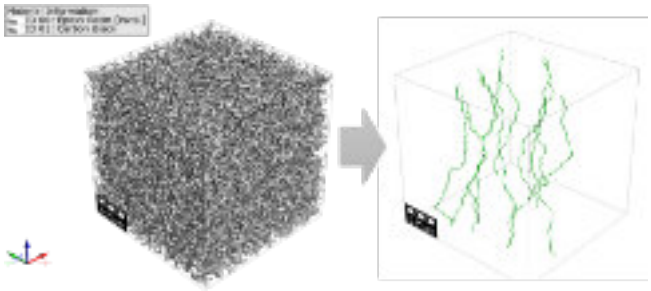
Geometrical characterization of the pore-space is carried out in GeoDict within the PoroDict module. The PoroDict module determines total porosity, connected and isolated porosity, pore size and pore throat size distributions, the surface area, and computes percolation paths (connectivity) through the pore space. When determining the pore characteristics of 3D functions, other CT, µCT or FIB-SEM image data as well as model functions generated with PoroDict can be used.

Furthermore, PoroDict can identify individual pores by a specialized watershed algorithm, to perform shape characterization (e.g. sphericity), and determine pore volume, orientation, coordination number, pore cluster sizes, Minkowski parameters, etc.

The MatDict module examines the solid material distribution in segmented 3D images or models. It determines the spatial heterogeneity, density, structure information, connected components, percolation paths (connectivity), etc.



Pore size analysis of a LiFePO4 cathode (PoroDict).



Paths of electrical percolation in an epoxy resin filled with carbon black (MatDict).

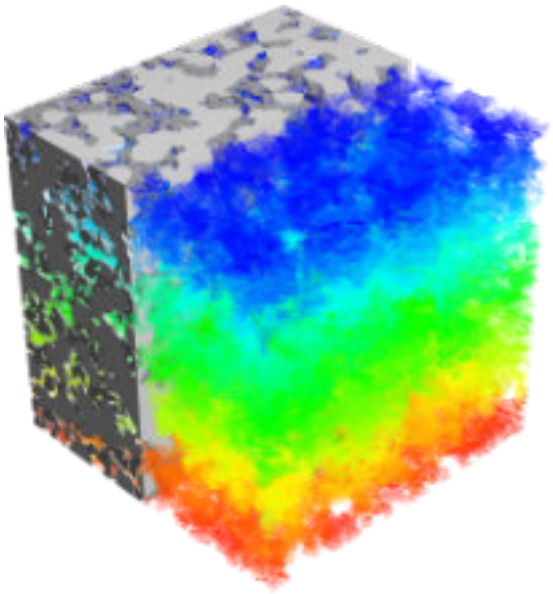
DiffuDict

DiffuDict computes the tortuosity factor and effective diffusivity of porous media. Depending on the pore size, the diffusing fluid is treated as a continuum or as single molecules reflecting off pore walls. The dominant model is determined by the Knudsen number (Kn), which compares the pore diameter to the mean path length of fluid molecules.

For small Knudsen numbers, the fluid is treated as a continuum, and the concentration distribution follows Laplace's equation. Effective diffusivity is determined from the resulting concentration flux using Fick's first law. The relative diffusivity and tortuosity factor are obtained by comparing the effective diffusivity with the bulk diffusivity of the fluid.

For large Knudsen numbers, the simulation includes the reflection of single molecules at the pore walls, calculating their mean squared displacement over time. The effective diffusivity is computed based on this value.

For intermediate Knudsen numbers, Bosanquet's approximation is employed to find the effective diffusivity by averaging between the two cases.

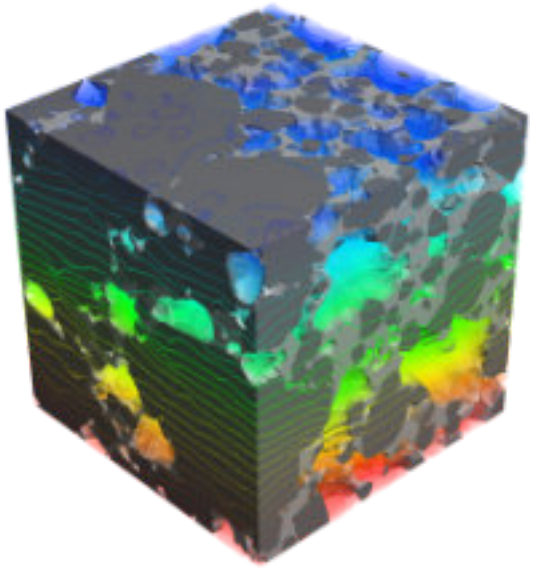


Bulk diffusion in lithium electrode

ConductoDict

ConductoDict is dedicated to simulating electrical and thermal properties of materials. Within ConductoDict, effective conductivity computations are performed for porous and composite materials. This module encompasses two solvers: EJ (Explicit Jump) and LIR, which facilitate the calculation of electrical and thermal conductivity tensors, formation factor, as well as potential, temperature, current density, electric field, and heat flux fields.

ConductoDict offers flexibility in assigning different conductivity values to segmented phases and varying contact resistivity between different phases. Additionally, it supports the assignment of non-isotropic material properties, such as transverse-isotropic or orthotropic properties. This capability allows for accurate modeling of materials with varied conductivity and complex structural configurations, providing insights into their electrical and thermal behavior.



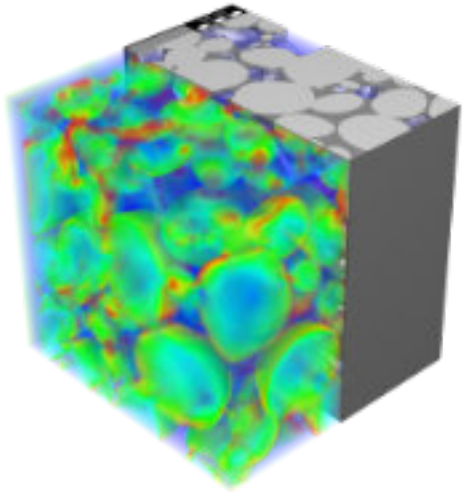
Determination of thermal conductivity of a lithium ion cathode

ElastoDict

ElastoDict in GeoDict revolutionizes the characterization of complex materials by enabling direct calculations on segmented CT scans, eliminating the need for meshing. With ElastoDict, you can analyze anisotropic stiffness, elastoplastic deformation, damage, and material failure directly on the 3D microstructure, even visualizing these properties on CT images. It offers three powerful options:

- **ElastoDict-AF**: This option provides fast analytic approximations and bounds for the linear elastic properties of complex microstructures. It efficiently computes a first approximation of the material behavior without solving partial differential equations, making it ideal for quick assessments.
- **ElastoDict-VOX**: This option accurately computes the linear elastic properties of complex microstructures by solving the corresponding partial differential equation on the 3D image or model. It provides detailed results, including the local von Mises stress, the complete stiffness tensor, and information about the material's orthotropic, transversal isotropic, or isotropic character, which indicates directionally dependent properties. Additionally, extensive post-processing steps can be performed on the VOX results.
- **ElastoDict-LD**: This option enables the simulation of nonlinear large deformations. It allows you to set up standard tensile experiments in arbitrary directions of the 3D microstructure. By incorporating advanced material models, such as damage, failure, plastic deformation, and viscous effects, it provides comprehensive insights. With ElastoDict-LD, you can obtain strain-stress curves, identify regions where damage occurs and the material fails, and conduct cyclic load experiments, bending tests, and shear experiments. Furthermore, the LD simulation generates deformed 3D structures from each computed deformation step, facilitating visualization and further analysis.

By leveraging the microstructure scale, ElastoDict empowers engineers and researchers to improve component simulations and optimize material designs, all while directly utilizing segmented CT scans without the need for meshing. It represents a significant advancement in accurately characterizing and understanding the mechanical properties of complex materials.



Von Mises stress from a degradation simulation of a NMC811

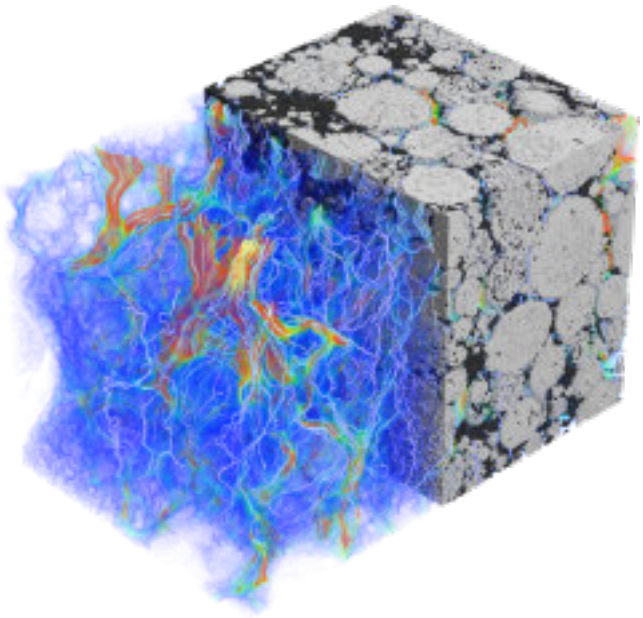
GeoDict Modules

FlowDict

FlowDict in GeoDict enables simulation of single-phase flow, offering three solvers (SimpleFFT, LIR, Explicit Jump) to compute permeability and fluid flow fields by solving the (Navier-)Stokes(-Brinkman) equations using finite volume approaches. Its capabilities encompass predicting mean flow velocity for a given pressure drop, estimating pressure drop for a given mean flow velocity, and determining the full or partial permeability tensor.

LIP and SimpleFFT have been demonstrated to handle geometries with 109 cells and more, as documented in Saxena et al., 2017, and Menke et al., 2018. The LIR solver's methodology, published by Linden et al., 2015, has also been cited in these studies.

GeoDict provides visualizations and exports of pressure and velocity fields in *.raw file format. Additionally, it reports key values such as absolute permeability, pressure drop, mean velocity, and the complete permeability tensor.

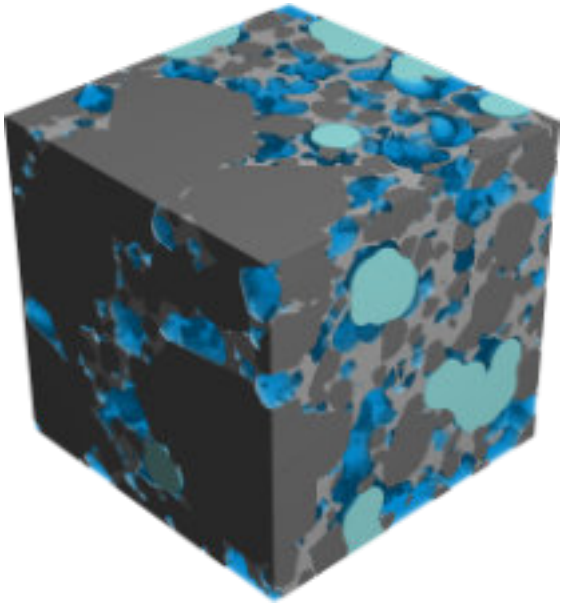


Flow inside an imported LiFePO4 cathode

SatuDict

SatuDict in GeoDict analyzes the distribution of two fluid phases (gas or liquid) within porous materials, affecting properties like permeability, diffusivity, thermal conductivity, and electrical conductivity. For example, it can track down the electrolyte filling process during battery fabrication.

It computes capillary pressure curves using the pore morphology (PM) method, enabling calculation for imbibition and drainage. Schulz et al. (2015) extended the PM method to accommodate different wettability conditions. The PM method considers fluid properties by adjusting interfacial tension and derives actual fluid distributions in the pore space. Berg et al. (2016) compared PM-generated distributions with computed tomography measurements. Combining with FlowDict determines effective and relative permeability, while combining with ConductoDict computes resistivity index, saturation exponent, cementation exponent, and relative diffusivity as in DiffuDict.



Capillary pressure in a lithium ion cathode

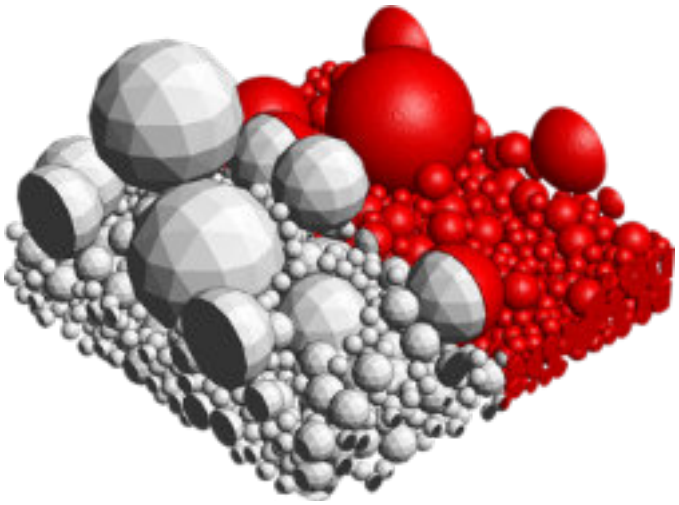
ExportGeo-CAD

ExportGeo-CAD exports structures from GeoDict formats to generic surface representation formats or generic CAD formats, enabling the integration of GeoDict-modelled structures into pre-established workflows.

ExportGeo supports a variety of surface description formats like *.stl, *.wrl, *.obj.

It also can be used in combination with CADlook (only available on Windows) to export CAD formats e.g. *.x_t, *.stp, *.igs, *.sat.

ExportGeo-CAD enables e.g. 3D printing, visualization using an external render software and integration into a simulation workflow.



Preview of the surface triangulation of a sphere cluster

Customer Service & Support

An intensive exchange of information, trainings, workshops and our annual **GeoDict Innovation Conference** ensure for our customers and partners the transfer of know-how and the same high-service standard for all GeoDict users.

For complex projects and applications, Math2Market offers consulting and carries out project work for our customers.

GeoDict User Guide

A comprehensive User Guide is available to all GeoDict users. The User Guide handbooks, for all GeoDict modules, describe all parameters in the Graphical User Interface for the modules, with images and explanations of their options.

The User Guide handbooks are reachable with 1-click directly from the GeoDict GUI and available as PDFs from the Math2Market website.

Training offers

Online or in person, our application specialists use practical examples to show the functionality and the possibilities of GeoDict simulations.

The content is oriented towards your level of experience with GeoDict and tailored to your application area.

Self Learning 24/7

Our written and short video tutorials provide a step-by-step introduction, followed by advanced knowledge in the functionality and possibilities of GeoDict. All are advantages: decide when and where, and learn at your own pace.

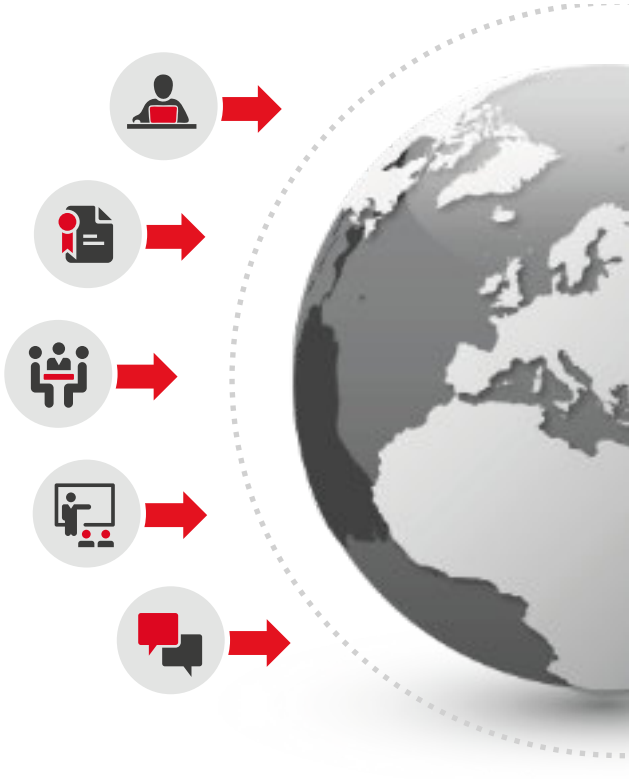
The range of topics is regularly revised and expanded.

Electrochemistry team
Individual trainings onsite and online, individual consulting, and industry-specific support

GeoDict Consulting and Projects team
Individual automation, app engineering, validation projects, and customization projects

GeoDict Development team
Annual software releases, regular Service Pack updates, and individual software development projects

Customer Support team
Professional support on technical and scientific questions related to GeoDict



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GeoDict - Licensing flexibility

For the versatile fields of application of GeoDict, we offer a flexible range of licenses to provide an attractive price-performance ratio to our customers.

GeoDict is the complete solution for multi-scale digital research and development of materials in academic and industrial settings. GeoDict's modular structure makes possible to adapt the software package to the customer requirements at any time and to find a customized solution for every application. All modules are completely integrated into GeoDict and, thus, guarantee a smooth simulation workflow.

Purchase of a GeoDict license

When purchasing a GeoDict license, a license package is built according to the requirements of the application. The license price depends on the selected license model, the modules included in the package, and the required computing speed.

We help in selecting a license package fitting your application and your working situation by choosing the most useful customizable combination of GeoDict modules. An overview of the available modules is found in pages 8-9. Individual modules may be varied in a package at any time.

License Type	Description	Maintenance (Updates and Support)
Purchase	unlimited time license	1 year included, afterwards cost-effective renewal
or		
Lease	limited time license	defined by lease period

Start with a validation project!

Want to see convincing results and customer-fitted simulation requirements before (or instead of) ordering?

Choose a pay-for validation project run by Math2Market for your specific application. The validation project brings solution-oriented information on a GeoDict configuration that works for you.

Furthermore, we train you specifically for your application case with GeoDict.

The simulation requirements for the application of the customer are analyzed in a pay-for validation project that provides solution-oriented information on the best GeoDict configuration for you. Contact us about your particular material development or analysis needs!

License Options

Remote Access

From mobile office
always included

Node Locked

One on-site computer,
one user at a time

One Site

All employees employed at
one designated site

No Cloud

Physical machines

Floating

Any computer, one user
at a time per license

One Site

All employees employed at
one designated site

Local

Physical machines
Virtual machines

Multiple Sites

All employees employed at
all sites

Cloud

GeoDict pay-per-use
clouds, all other clouds

GeoDict: Q&A

What is GeoDict ?

GeoDict is a comprehensive simulation software suite developed by Math2Market for digital material analysis, research, and development. It allows users to generate, edit, and visualize complex material models and prepare results for presentations.

Who typically uses GeoDict?

GeoDict is typically used by researchers, scientists, and developers in the field of materials science, including those working in academia, industry, and research institutions.

How does GeoDict help with material analysis and research?

GeoDict offers a range of tools and features that assist in digital material analysis and research. These include modules for image processing, material modeling, property computation, and prediction. It also provides advanced options to import and export data in various formats.

How does GeoDict integrate with existing workflows?

GeoDict seamlessly integrates with established workflows through its interfaces to Python, MATLAB®, and Microsoft Excel®. This allows for efficient automation and deep analysis of results within these well-known environments.

What are the key features of GeoDict?

Key features of GeoDict include a highly user-friendly graphical interface, fast 3D visualization of material models and simulation results, voxel and analytic object-editing tools, image and video capturing and processing tools, and scripting interfaces to Python and MATLAB®.

How do I customize GeoDict to meet my specific needs?

GeoDict is designed with a focus on flexibility and adjustment to your precise requirements. This can be optimally achieved by selecting from its dedicated modules designed for various tasks, including image processing, material analysis, material modeling, and property prediction. Refer to pages 10 - 19 for an in-depth overview of the modules that are particularly relevant for digital Research & Development in material sciences.

What data types may I import into and export from GeoDict?

GeoDict supports import and export of data in various formats. It imports files in GeoDict formats and exports to both GeoDict and non-Geo-Dict formats, including RAW Data, VOL Data, Avizo Binary Files, and 2D Image Stack. See details in page 12.

How does GeoDict handle 3D material models?

GeoDict includes tools to construct any geometry from analytic objects and modify 3D material models. These features allow detailed exploration and analysis of the data.

How does the post-processing and analysis in GeoDict work?

GeoDict provides detailed post-processing and analysis capabilities through its GeoDexcel module. GeoDict result files are automatically loaded into Microsoft Excel® spreadsheets for further analysis and comparison.

How does GeoDict benefit my work in materials science or material development?

GeoDict serves as an innovation catalyst, fostering a space where creativity thrives. Its flexible environment allows experimenting with diverse scenarios regarding materials and conditions, facilitating rapid iteration and exploration of new ideas. With GeoDict as your ally, be ready to push the boundaries of possibility, bringing novel materials to market faster and staying ahead of the competition.

What kind of support and resources are available to learn how to use GeoDict?

Math2Market offers various resources to quickly learn how to use GeoDict, including tutorials, user guides, and a highly skilled support team that assists if technical issues or queries arise.

How is GeoDict licensed and what are the costs associated with using it?

Specific licensing information and costs associated with GeoDict may be obtained by contacting Math2Market directly as these details might vary based on the intended use, number of users, and the specific modules needed.

Empowering Your Vision: Your Success, Our Priority

Online Scheduling

We understand that your time is precious, and we are committed to making your communication with us as convenient as possible. We offer a hassle-free online booking system to streamline the scheduling process.

The journey towards innovation, collaboration, and success starts with a single step. Use our online system to schedule a query or consultation, and let us guide you on this exciting path. We are ready to provide insights, offer solutions, and work alongside you to achieve your goals. Don't miss out on the opportunity to connect with our experts at your convenience. Book your consultation today and take the first step towards unlocking digital innovation.

Make an apointment with our **Electrochemistry** team

Website

Explore our comprehensive website. Find detailed information about our services, case studies highlighting success stories, and a contact form to reach us conveniently.

www.math2market.com

Email

Prefer to communicate via email? Drop us a message. We direct your inquiry to the right team and promptly address your needs.

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Stay Connected

We are dedicated to sharing valuable insights, thoughts, and inspiring content with the simulation community. Connect with us and do not miss out on the latest updates and engaging discussions.

Linkedin.com

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Math2Market - The Company

GeoDict combines cutting-edge scientific advances and powerful software development into a user-friendly solution for innovative digital material analysis, research, and development in industrial and academic settings.

Math2Market GmbH was founded in September 2011 by three members of the GeoDict software development team as a spin-off from the Fraunhofer Institute for Industrial Mathematics (ITWM, Institute für Techno- und Wirtschaftsmathematik) in Kaiserslautern, Germany. Some of the founders had been working on the software since its inception in 2001. Today, Math2Market has a workforce of over 60 employees at its Kaiserslautern site and, with GeoDict, is one of the worldwide leading providers of digital solutions in the field of material analysis, research, and development.

„Thanks to the analysis of microstructures, GeoDict helps you to significantly increase the performance of your batteries."

Dr. Ilona Glatt
Business Manager Electrochemistry / Math2Market GmbH

TOYOTA VOLKSWAGEN HYUNDAI HONDA CELLFORCE BYD

Over 500 universities, research institutes, and large companies from various industries worldwide use GeoDict to develop innovative materials and optimize their material analysis and development processes. With our unique pool of top mathematicians, physicists, geologists, chemists, biologists, engineers, and computer scientists, we believe in making available the benefits of cutting-edge, university-level research to our clients, to be applied by non-experts using our software GeoDict.

Our customers also benefit from the comprehensive services of Math2Market, including regular updates of GeoDict, intensive customer assistance and consulting, as well as training and reliable support by our experts in their respective fields.

Math2Market cooperates in diverse ways with international partners from industry and academia and participates regularly in scientific congresses and technical trade fairs with innovative scientific contributions.

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