Continuum Modelling with QuickWave Software: Extensions & Applications in H2020 NanoBat project

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NanoBat project aims to develop a novel nanotechnology toolbox for **quality testing of Li-ion and beyond Lithium batteries** with the potential to redefine battery production in Europe and worldwide. The targeted radio frequency **(RF)-nanoscale techniques** will be faster and more accurately calibrated than existing methods. The project will significantly reduce the costs of battery production thus greatly benefiting the evolving **clean energy and e-mobilit**y transition in Europe.

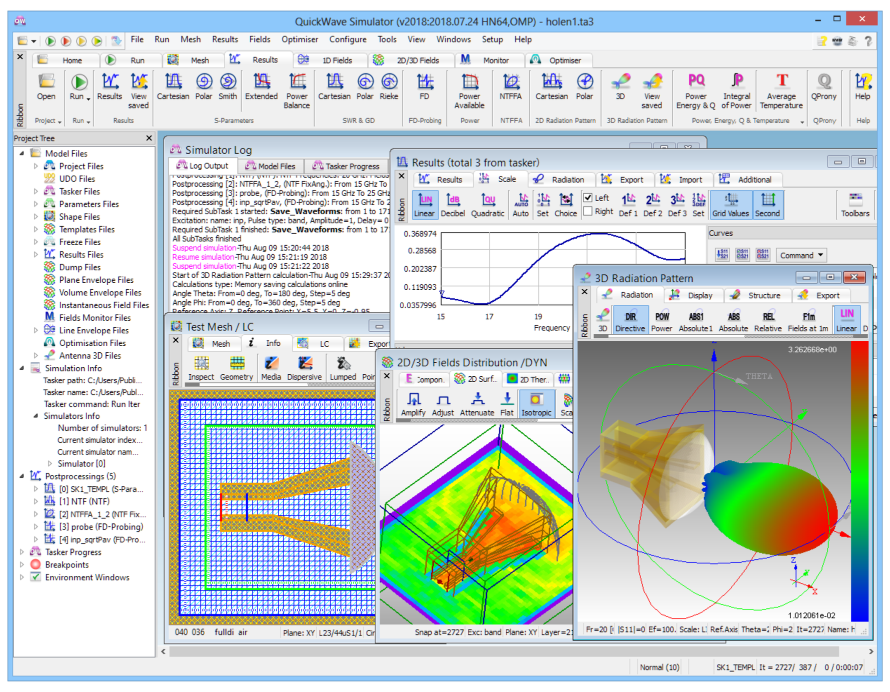
Background: QuickWave Software

Electromagnetic & Multiphysics simulation software accounting for **materials modelling at the continuum level, utilising conformal FDTD method.**

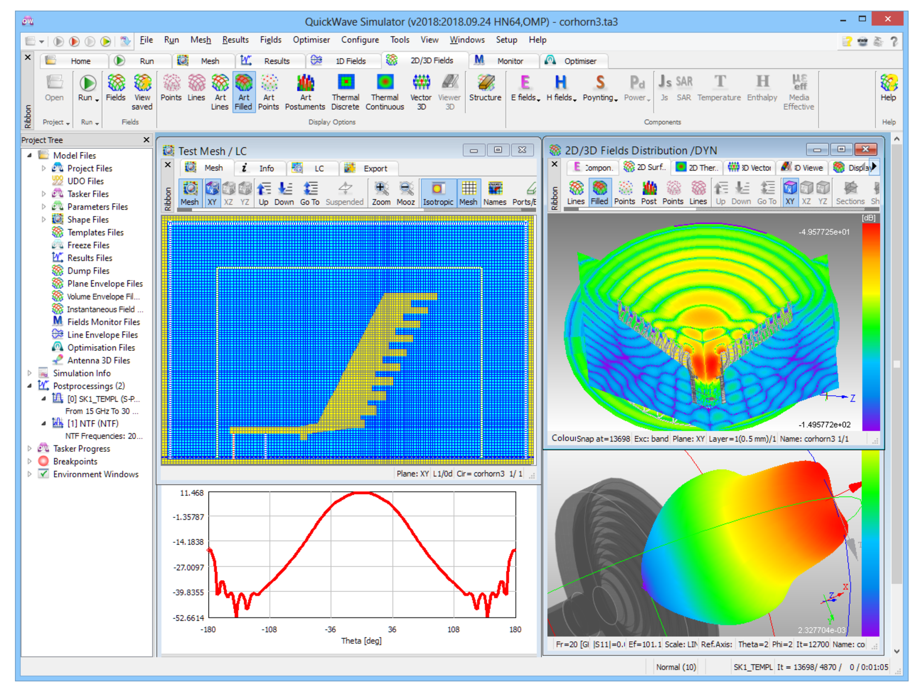
It has a well-established position on the world's market due to approaching specific, challenging problems (often associated with consultancy by QWED's specialists).

Major packages:
- **QuickWave 3D**
- **QuickWave V2D**
- **Multiphysics 3D**

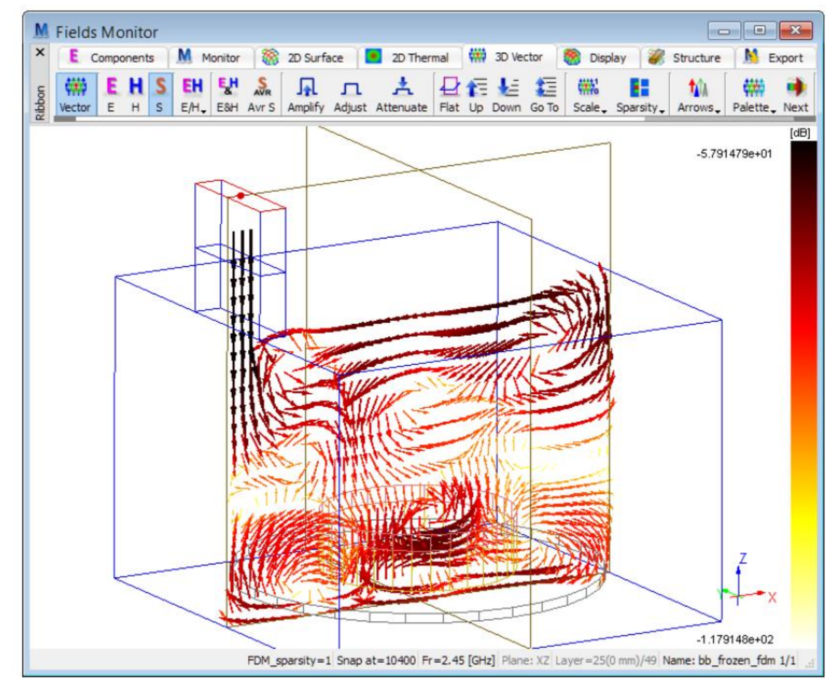
QuickWave 3D - universal general purpose software for electromagnetic design and simulations based on the conformal FDTD method, supplemented with a range of unique models for curved boundaries, media interfaces, modal excitation, and parameter extraction.



QuickWave V2D - ultra-fast Vector 2D (V2D) solver for axisymmetrical structures (BOR - Body of Revolution) including antennas, circular waveguides discontinuities, and resonators S-parameters, radiation patterns, etc. calculations structures as large as 2000 wavelengths.



QW-BHM - 3D & BOR <ultiphysics (coupled EM, thermodynamic, mechanical models) – allows modelling of microwave heating applicators for materials processing – from domestic microwave ovens through plastics, metallurgy, and biomaterials, down to microwave pharmacy.

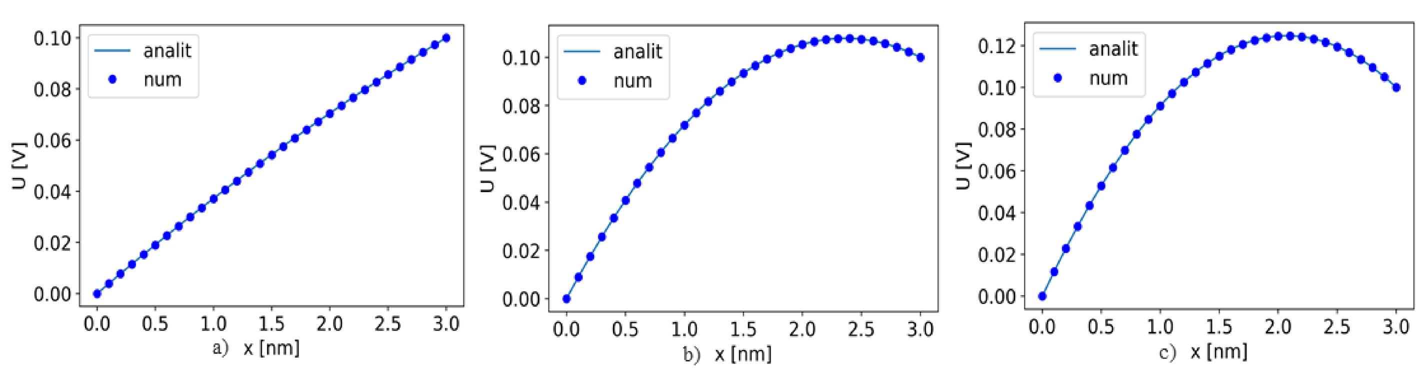


Software Extensions in NanoBat

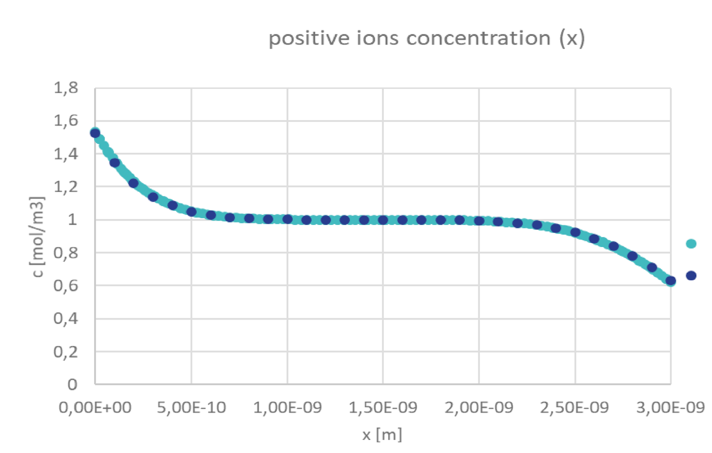
Modelling of coupled electrochemical phenomena occurring at **electrolyte/electrode interfaces**.

The problems are solved using **coupled Laplace / Poisson and drift-diffusion equations**, which create a basic model of **ion transport process in the electrolyte**, as in e.g. popular Li-ion batteries.

The developed coupled FDTD solver is validated against analytical solutions for the electrostatics and independent FEM solutions for the electrochemistry.



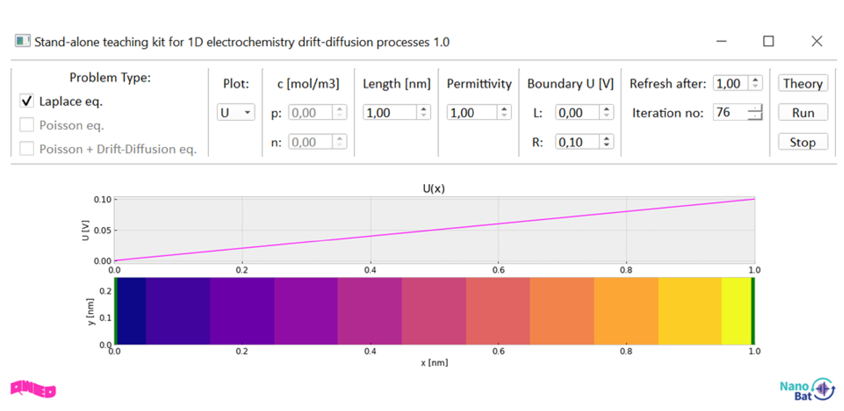
Comparison of FDTD solution and analytical solution of the Poisson equation. Electric potential (U) distribution in 3 nm space limited by electrodes of 0.1 V potential difference, filled with electrolyte of εr = 2.82 and static positive charges of molar concentration: (a) 1 mol/m3, (b) 10 mol/m3, and (c) 15 mol/m3. The ions are assumed to be static, which has the physical sense of zero diffusivity and mobility

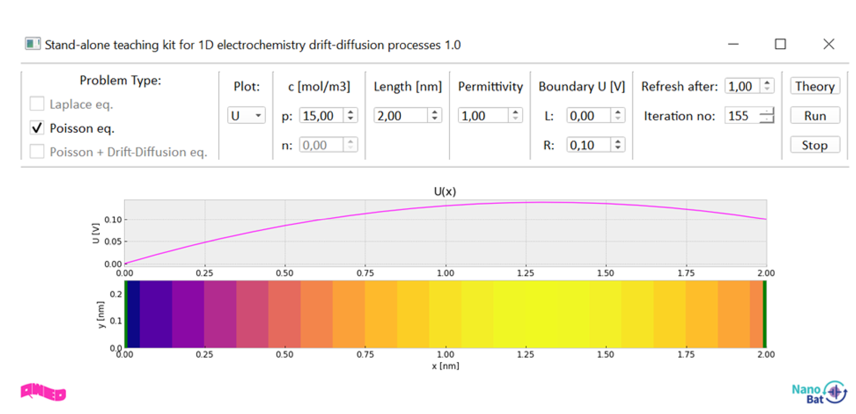


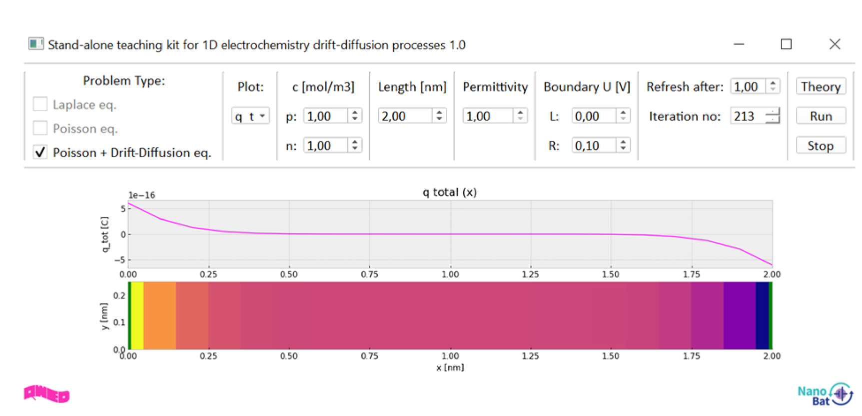
Comparison of FDTD solution (new in NanoBat) and FEM solution (COMSOL). Positive ions concentration distribution in space limited by electrodes of 0.1 V potential difference, filled with electrolyte of εr = 2.82, with initial uniform concentration of positive and negative ions of 1 mol/m3 and Dc=10-9 m2/s**.** A perfect agreement between the FDTD and FEM solutions is demonstrated.

Example teaching kit for 1D electrochemistry

The application is prepared to be openly used for the modeling of industrially representative test-fixtures for battery materials, such as those defined in the H2020 NanoBat project. It can be used to **visualize three different User Cases** of increasing complexity. In future work, the models will be coupled to high-frequency electromagnetic models.





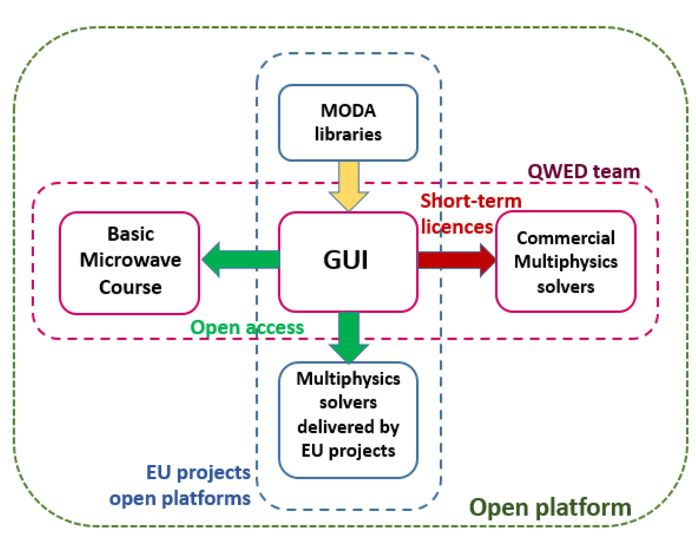


The User Cases are modelled using **Laplace, Poisson, and coupled Poisson-drift-diffusion equations**, which are solved by a novel FDTD scheme

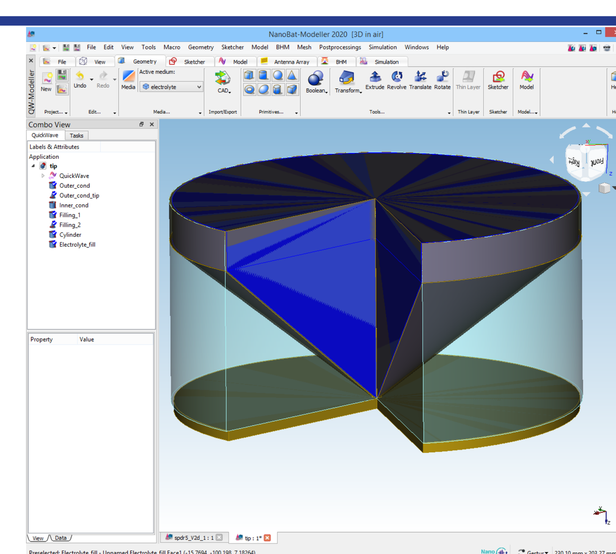
NanoBat Concept of Open Platform

Open Modelling Platforms are expected to **deliver the results of research for the usage by a wide scientific community as well as for the teaching.** They will deliver a complete solution allowing for **multi-scale multi-physics material analysis from the electronic level, through atomistics and mesoscale to continuum modelling** (and possibly also data-based modelling).

- Common GUI
- Interfaces to various solvers
- Assuring FAIR data
- Enabling modelling at different levels
- Various access rights (open access, licensed access to commercial tools, etc.)



Modelling platform with exemplary commercial contribution of QWED tools



Open platform GUI workbench

Facilitating:

- ✓ Interoperability
- ✓ Software deployment
- ✓ Model development
- ✓ Enhancing industry impact

Acknowledgement

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