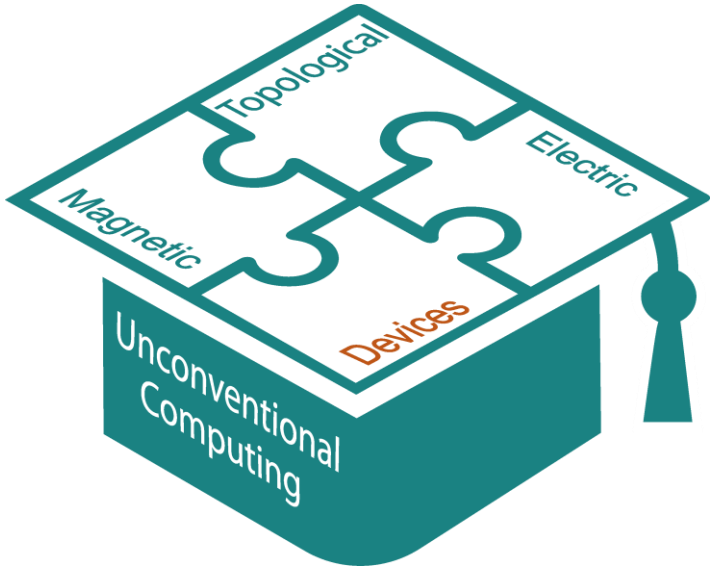
TOPOCOM

Petaspin Microelectric Solver



Installation and Usage Guide

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What Is the Petaspin Microelectric Solver?

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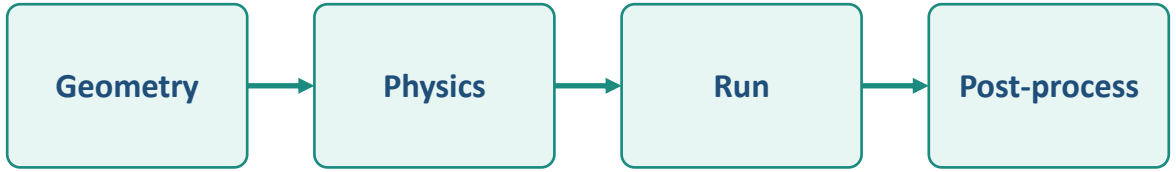
- A PyQt5 desktop GUI for a high-performance CUDA™ (Compute Unified Device Architecture) C/C++ phase-field solver for ferroelectric materials.
- Configure geometry, physics, and excitations, then run and visualize output, without editing files by hand.
- Two physical models in one solver: Relaxation (TDGL) and Dynamics (LKT).
- GPU (Graphics Processing Unit) or a CPU (Central Processing Unit) backends, selectable from the interface.
- Developed under TOPOCOM (NTNU) with the PETASPIN group (University of Messina).



A typical session moves left to right through these four stages.

Two interchangeable backends:

GPU (CUDA)	CPU
fast, needs NVIDIA GPU	runs anywhere

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Installation

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1. Run the Windows installer (topocom_simulator_setup.exe).
2. Choose a setup language and installation folder.
3. The installer creates C:\MicroElectricTemplate with both solver executables (GPU + CPU) and default configuration files.
4. Launch from the Start Menu or desktop shortcut.

Minimum System Requirements

- Windows 10/11, 64-bit
- 8 GB RAM (16 GB recommended)
- 1 GB disk space
- NVIDIA GPU + CUDA 6.0+ (GPU backend only)
- CPU backend: no GPU needed

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Getting Started

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- Launch Petaspin Simulator from the Start Menu or desktop shortcut.
- Choose New Project to start fresh, or Open Project to resume existing work.
- A new project copies default configuration files as an example and both solver executables into your chosen folder.
- The current project directory is always shown in the toolbar.

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The Main Window

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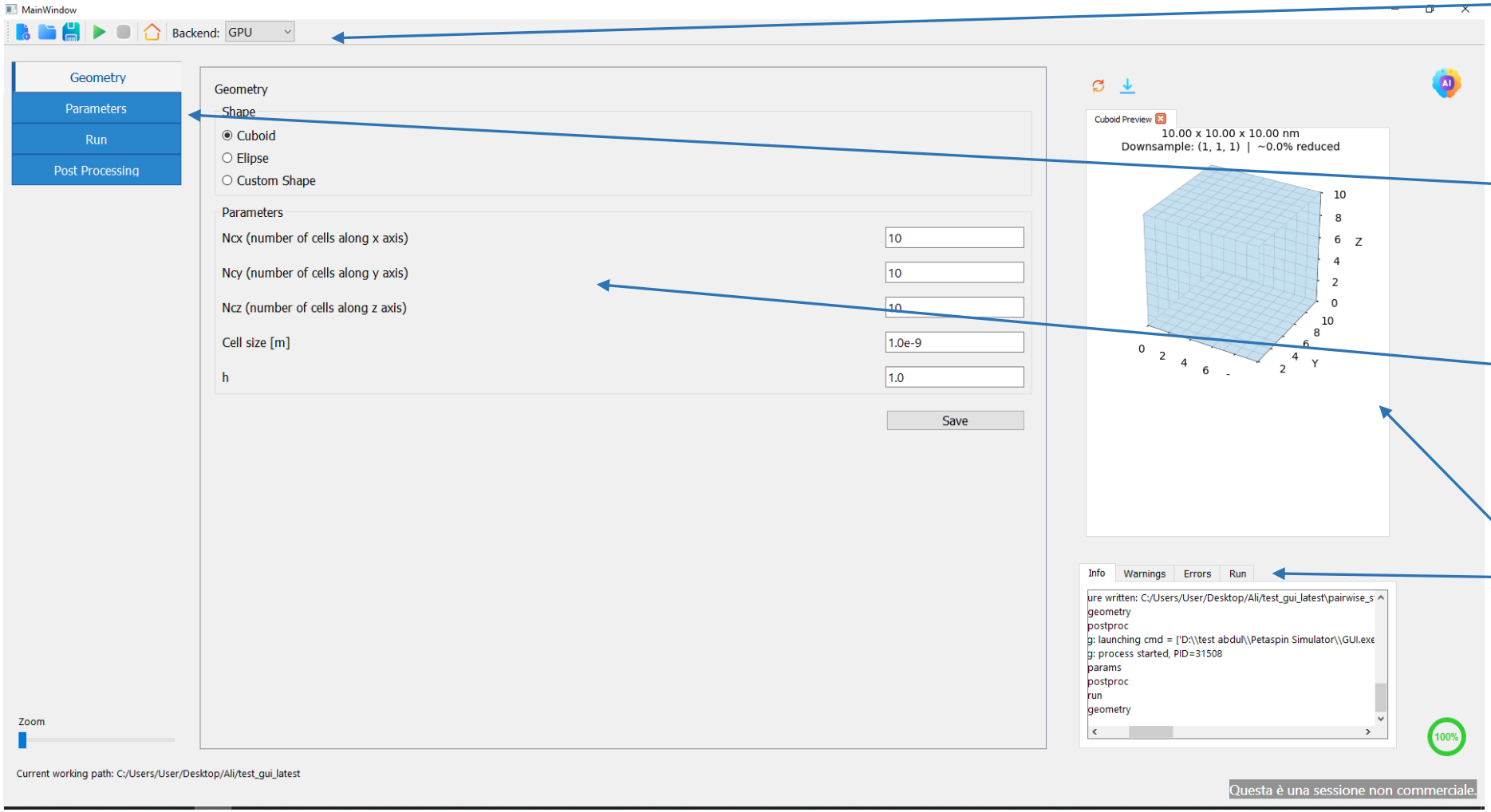

Toolbar
New / Open / Save / Play / Stop / Home + backend selector

Left navigation
Geometry, Parameters, Run, Post-Processing

Center panel
Settings for the selected page

Preview / log panel
Geometry preview, equations, run log

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Constitutive Parameters

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Seven sub-pages, each with rendered equations for reference

Landau	Gradient	Electrostatic	External Field	Strain	Run Parameters	Output

- Landau: Landau-Devonshire free-energy coefficients.
- Gradient: Domain-wall (gradient energy) coefficients.
- Electrostatic: Permittivity, padding.
- External Field: DC, AC, pulse, and sinc excitation.
- Strain: Under development (placeholder).
- Run Parameters: Integrator, run mode, initial polarization, damping and inertia.
- Output: Which output files to write, and how often.

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Landau Field

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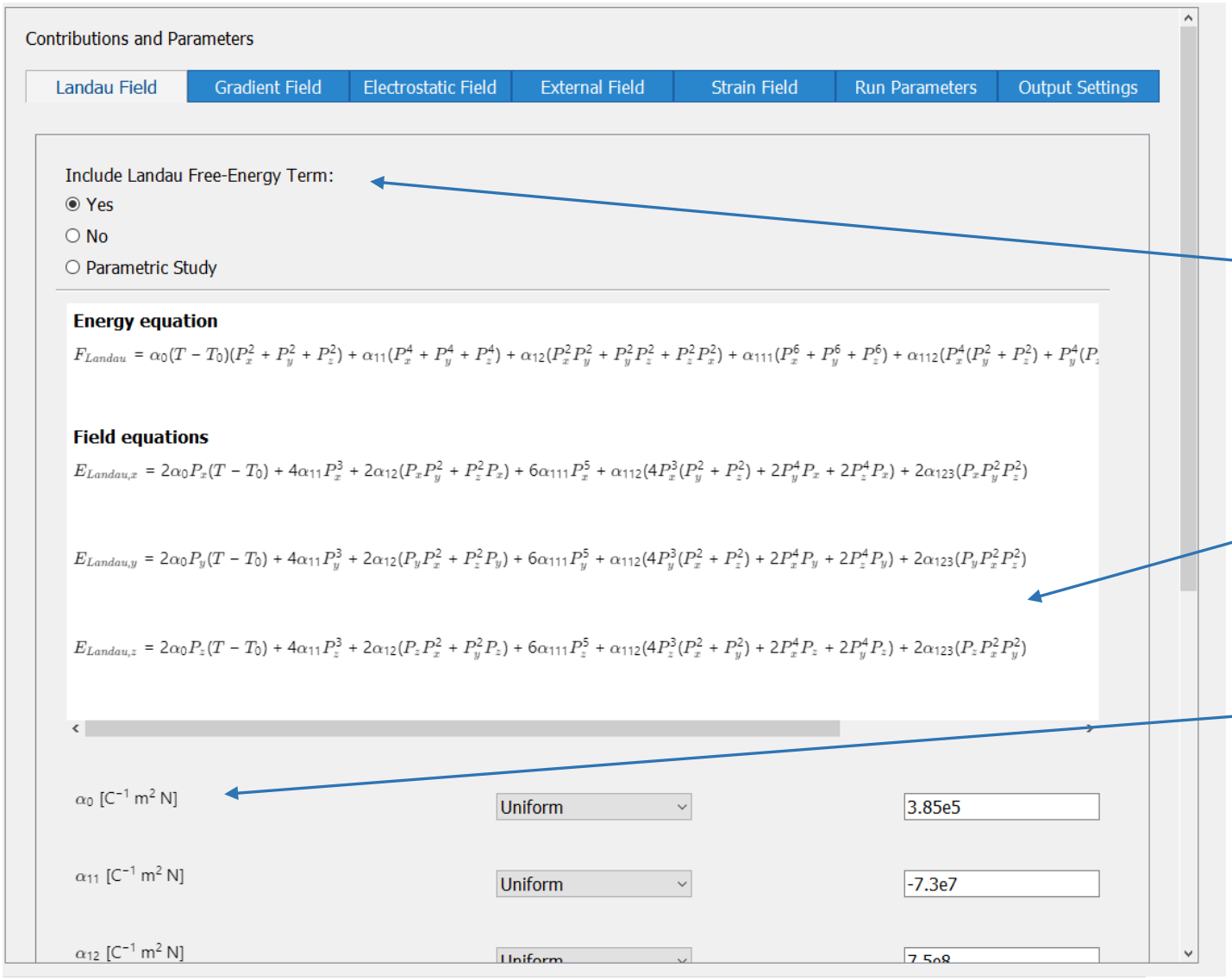
Landau-Devonshire free energy coefficients



Enable toggle
Yes / No / Parametric Study

Reference equations
Rendered energy and field equations

Coefficients
$\alpha_0 \ldots \alpha_{123}$, each Uniform / Thickness / Spatially dependent

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Gradient Field

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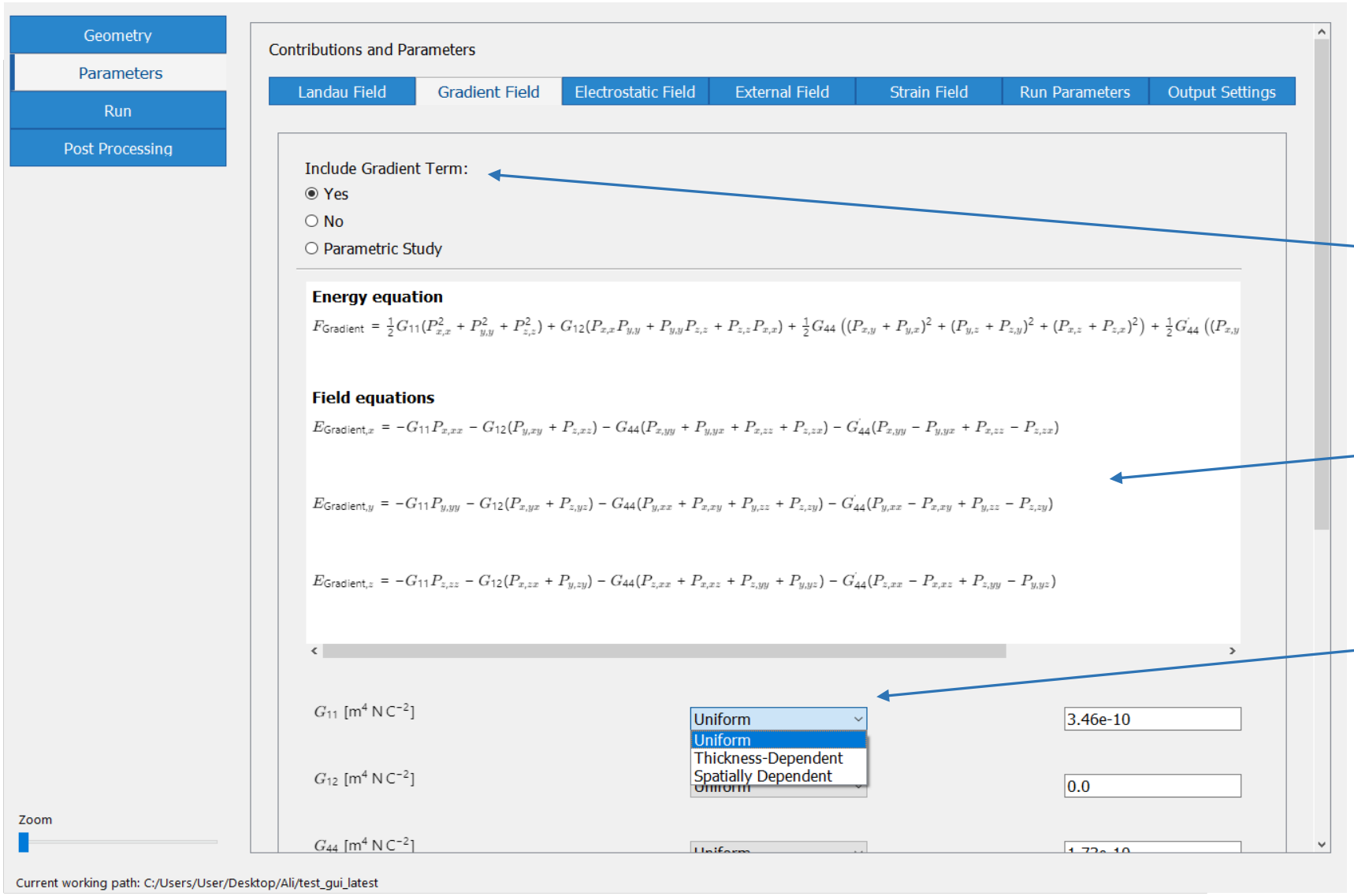
Domain-wall energy coefficients



Enable toggle
Yes / No

Reference equations
Gradient energy and field equations

Uniformity dropdown
Uniform / Thickness-Dependent / Spatially Dependent

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Electrostatic Field

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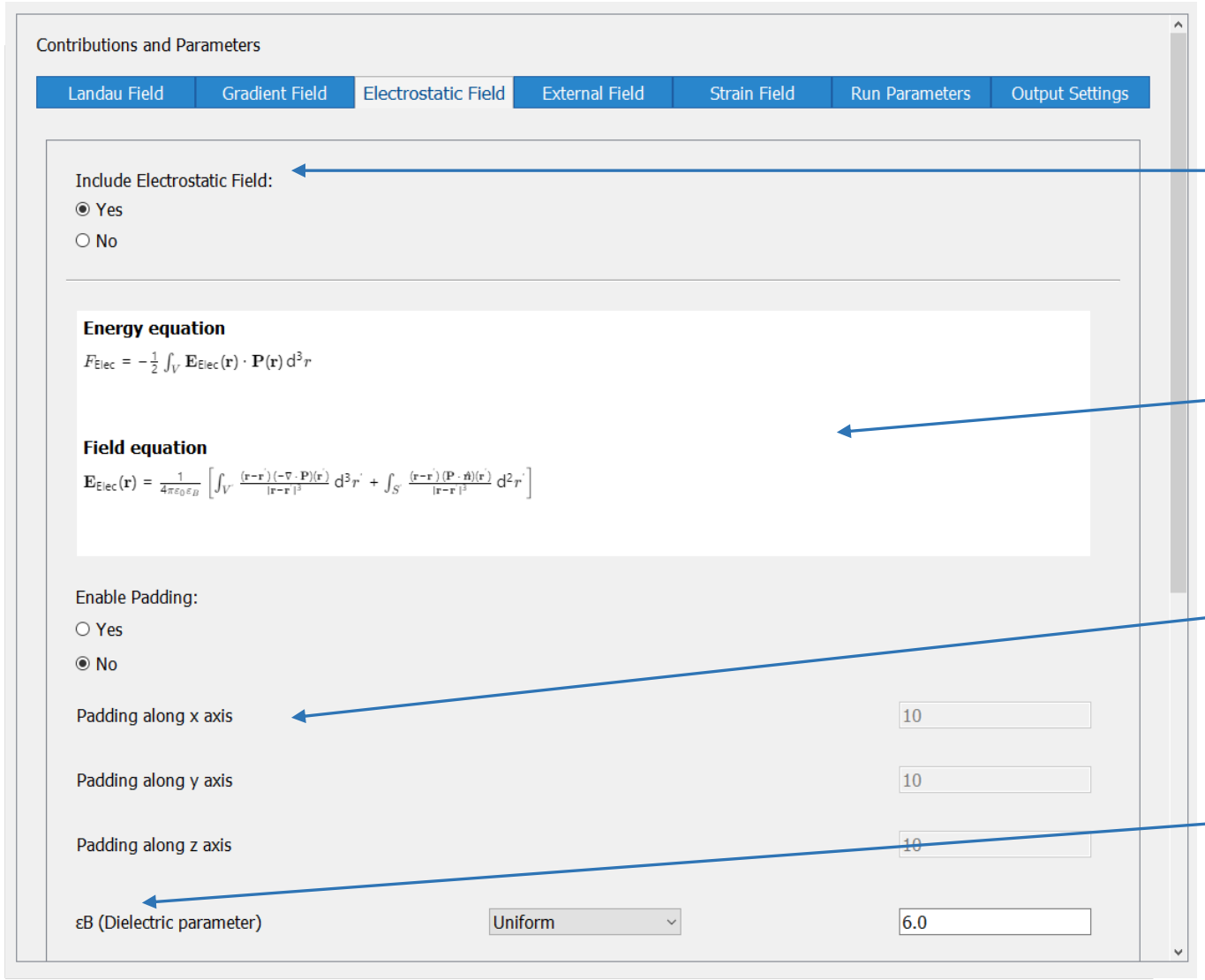
Permittivity and padding settings



Enable toggle
Include Electrostatic Field: Yes / No

Reference equations
Energy and field equations

Padding
Recommended default padding

Permittivity
Background dielectric parameter

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External Field

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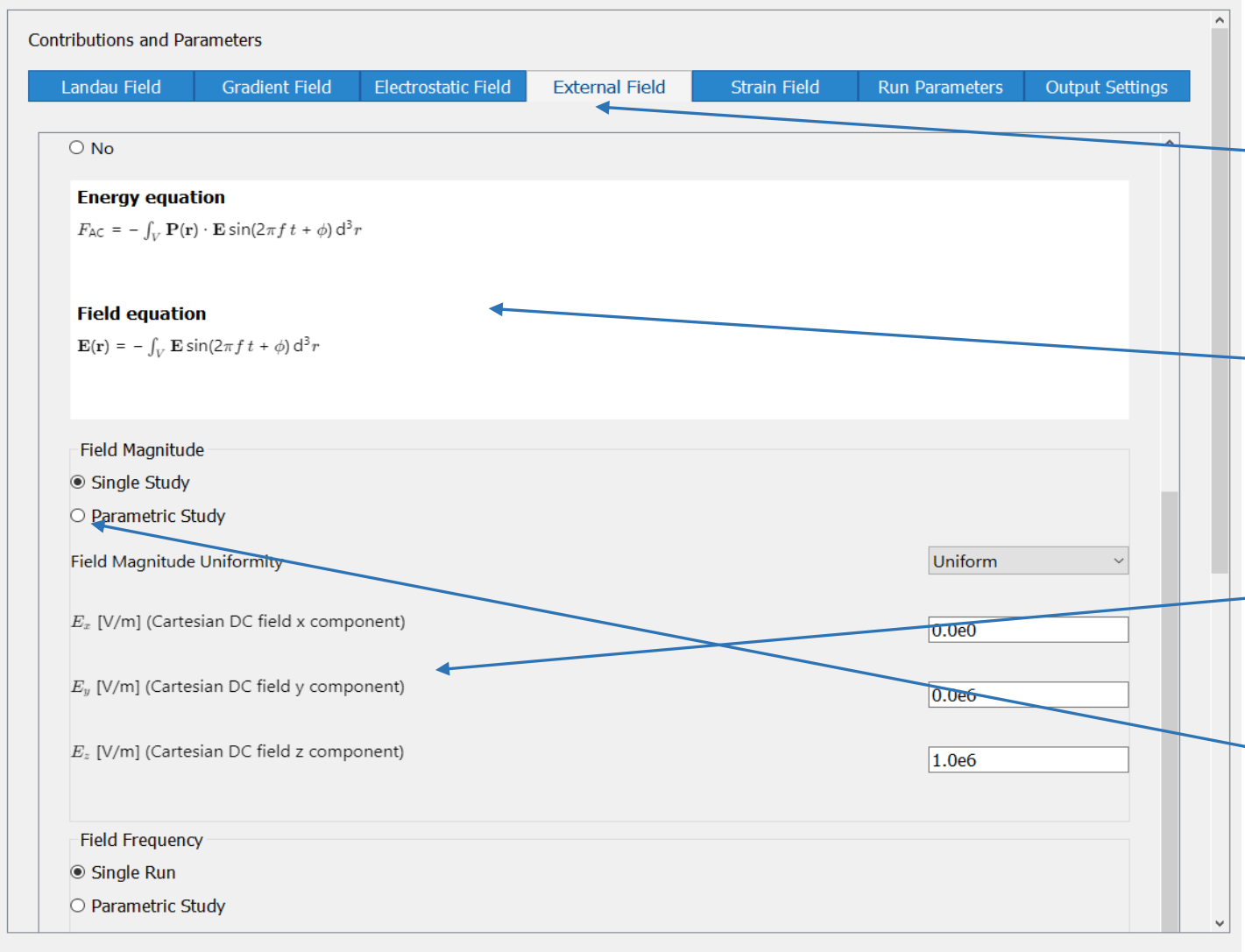
DC, AC, phase, pulse, and sinc excitation



Field type
DC / AC / Pulse / Sinc, each independently toggled

Reference equations
Energy and field equations per excitation type

DC field components
E_x, E_y, E_z in V/m

Study mode
Single value or parametric sweep

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Strain Field

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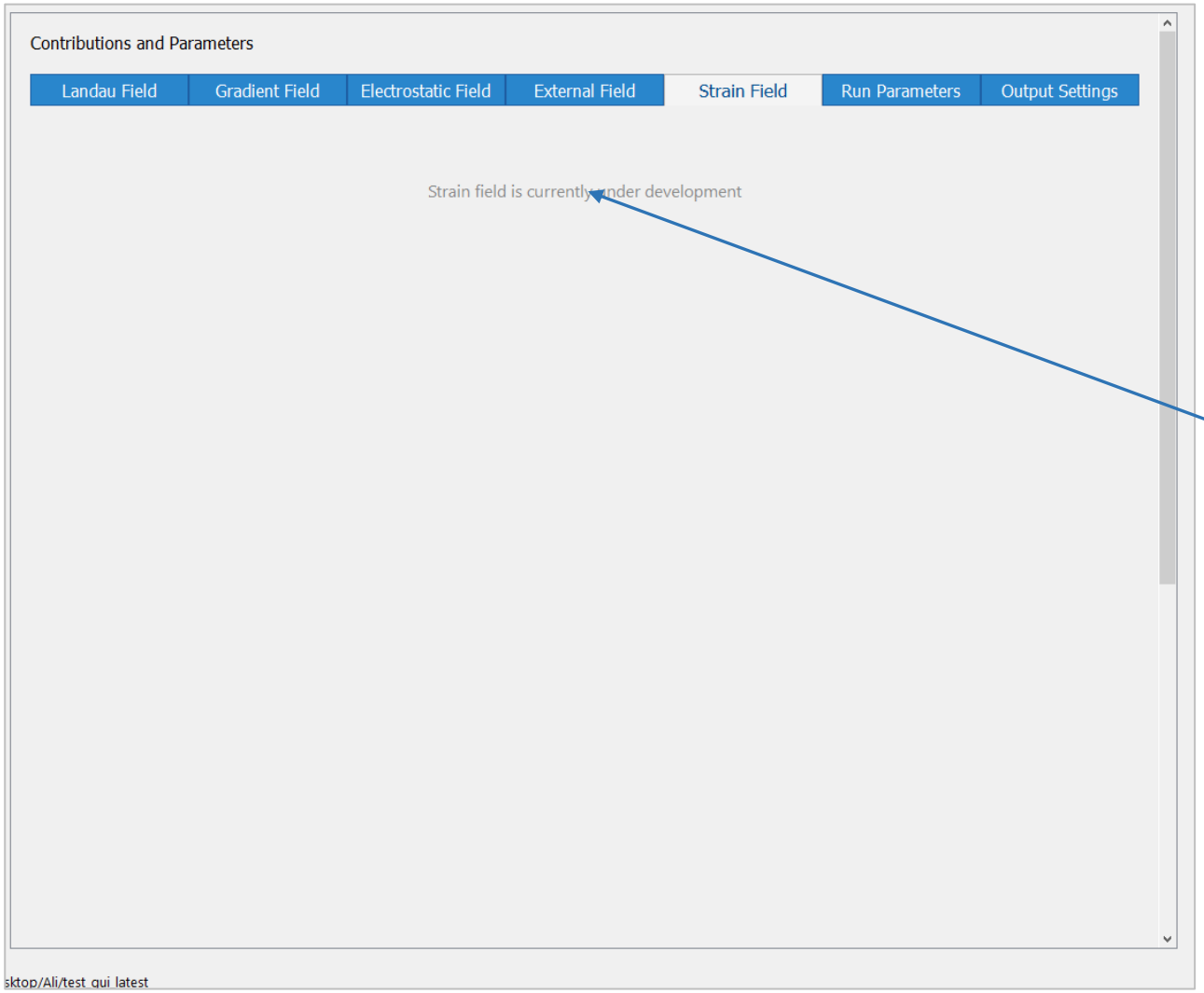
Currently under development



Placeholder

This tab is reserved for a future elastic/strain module

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Run Parameters

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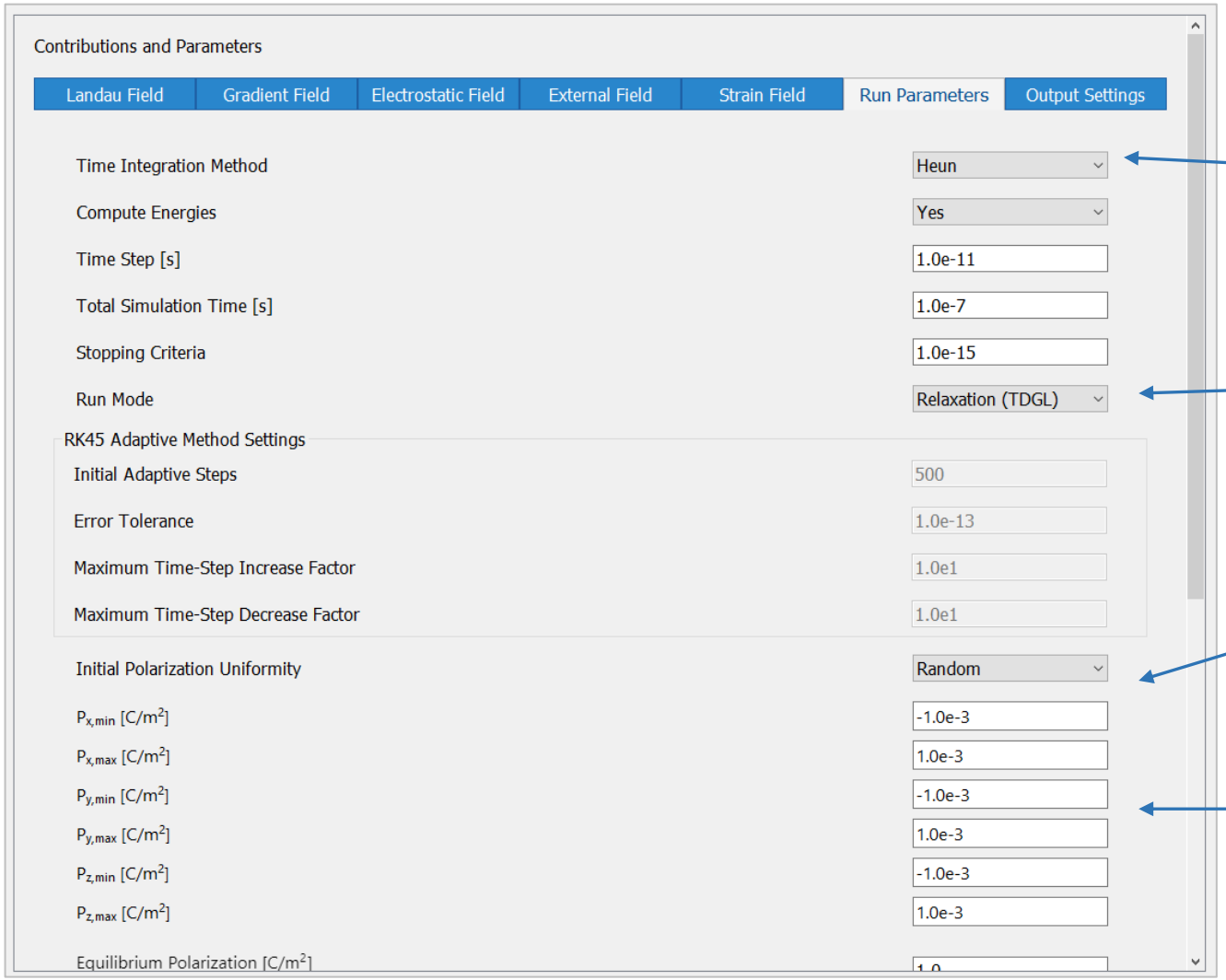
Integrator, run mode, initial polarization, damping and inertia



Time integrator
Heun / RK45 fixed / RK45 adaptive / AB3M2

Run mode
Relaxation (TDGL) or Dynamics (LKT)

Initial polarization
Uniform / Thickness / Spatially dependent / Random

Random bounds
Per-axis min/max, only active in Random mode

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Output Settings

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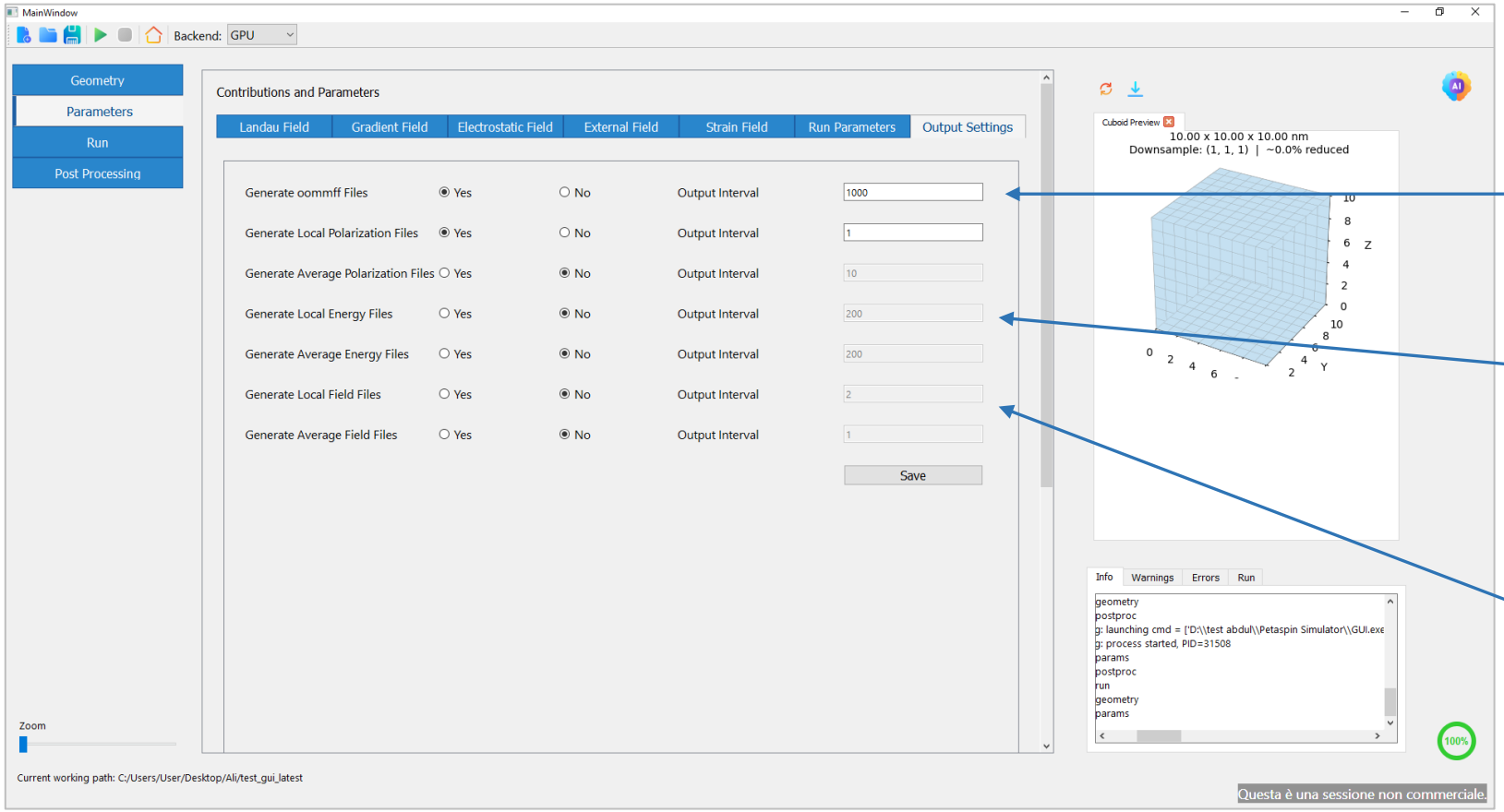
Choose which output files to generate, and how often



OOMMF / polarization
Local and average polarization output

Energy output
Local and average energy, each with an interval

Field output
Local and average effective field

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Running a Simulation

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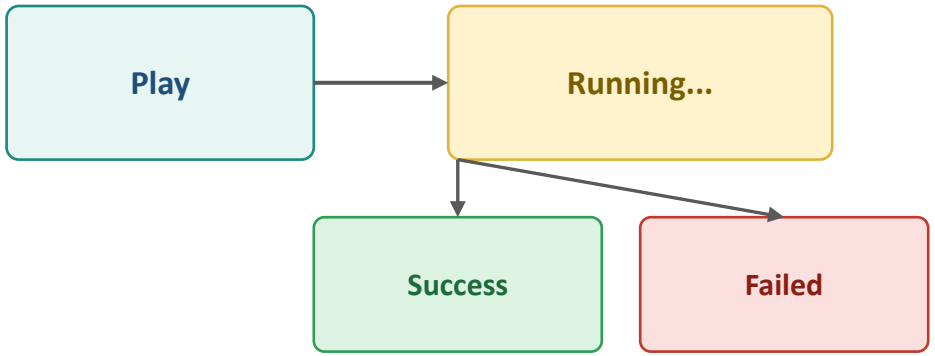
- Choose GPU (default) or CPU from the toolbar backend dropdown.
- Click Play. Unsaved changes are saved automatically first.
- Solver output streams live into the Run log tab.
- Click Stop at any time to terminate a running simulation.



Progress indicator: yellow while running, green on success, red on failure.

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Post-Processing

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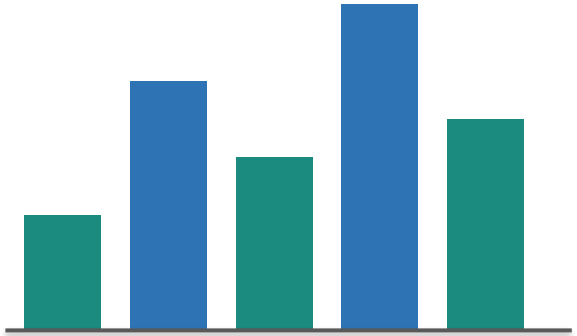
- Draw Final Polarization 3D Graph opens a 3D vector-field plot of polarization output, sliced along all three axes once the simulation completes.
- A live file list monitors the output folder, refreshing every 5 seconds as the simulation writes new snapshots.
- Select any snapshot and click Plot selected file to inspect an intermediate state without waiting for the run to finish.



Live snapshot list + 3D plot viewer

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Example: Spontaneous Domain Formation in $PbTiO_3$

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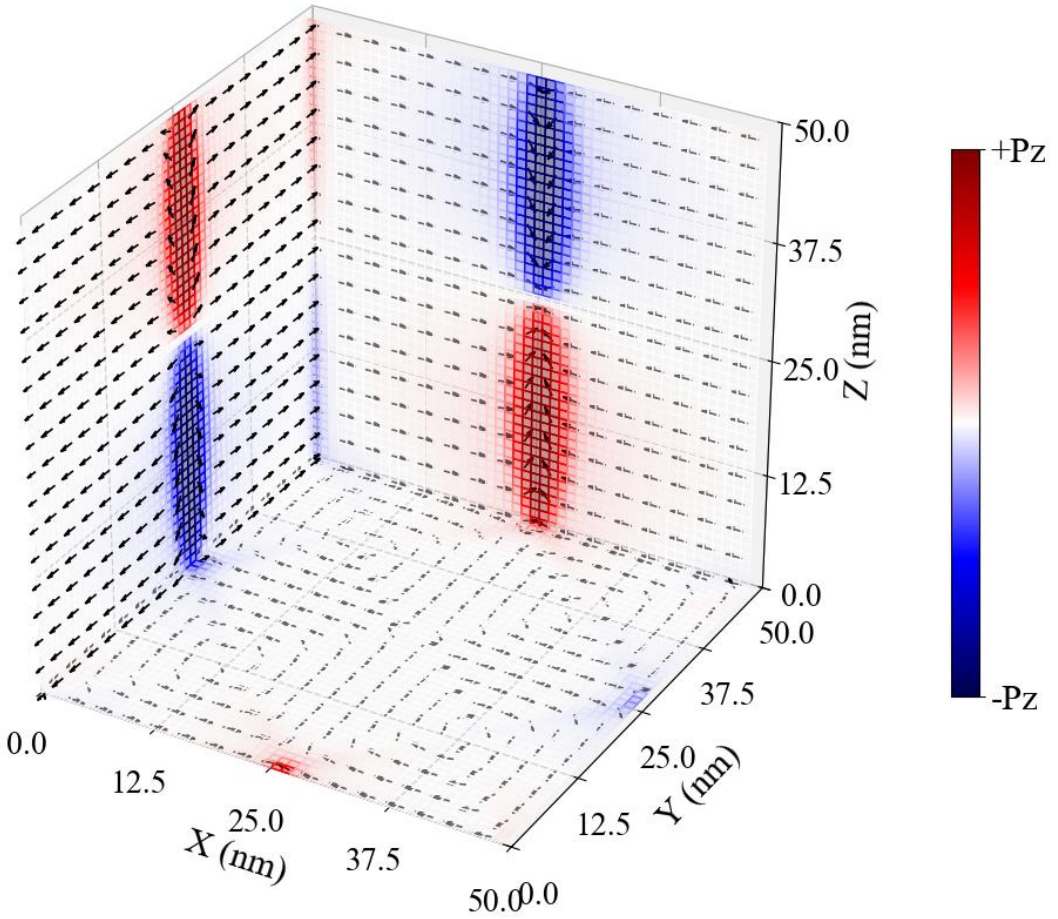
Random initial polarization, relaxation (TDGL) only, no field or elastic coupling

One ready-to-run example included with the solver for new users

- Material: PbTiO3 (Parameters are summarized in Table 1 in README)
- Grid: 50 × 50 × 50 cells, 1.0 nm cell size
- Initial polarization: random, $\pm 1.0 \times 10^{-3}$ C/m² per component
- No external field, no elastic coupling, no thermal noise
- Run mode: Relaxation (TDGL), 1.0×10^{-6} s total



Result

Four alternating 180° polarization domains form spontaneously, with vortex-like in-plane patterns at each x-y cross-section. For comparing the results, the exact output folder can be found together with the README file.

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Authorship and Acknowledgement

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Prof. Giovanni Finocchio and Prof. Davi Rodrigues

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How to Cite This Code

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If you use this solver or publish results obtained with it, please cite the following work.

[1] A. Hasan et al., A GPU-based Solver for Polarization Dynamics in Ferroelectric Materials, arXiv:2605.28800 (2026).

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Where to Learn More

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- The full README (Word document) covers every page and setting in detail: project file structure, the .dat configuration format, backend comparison, tips, and troubleshooting.

- Both solver executables (GPU and CPU) and default configuration templates install automatically.

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