Building Open and Reproducible Geospatial Simulations with Python

DisSModel — Discrete Spatial Modeling Framework

Sérgio Souza Costa · LambdaGeo / UFMA

Cellular Automata | System Dynamics | LUCC · Mangroves | LUCC · CLUE

UFMA · INPE · Brazil Data Cube

AGENDA

What we will cover today

01 - CONTEXTUALIZATION

Career and Research Evolution

- Research Projects
- Academic & Professional

Research Projects

- 2002 — **Data Exchange** — Terra Trans.
- 2006 — **Prototyping** — TerraHS
- 2008 — **ABM — LUCC** — TerraME
- 2013 — **LBS Apps** — OCM
- 2016 — **Linked Data** — DBCells
- 2024 — **RDF Cube** — SPARQL
- 2025 — **Dyn Models** — DisSModel
- 2027 — **LUCC** — LuccME++

Academic & Professional

- 2000 — **Undergraduate** — Data Proc.
- 2004 — **Master's** — INPE
- 2007 — **PhD** — INPE
- 2010 — **Teaching** — UNIFEI
- 2013 — **Teaching** — UFMA
- 2027 — **Collab.** — INPE

Focus on Spatial Modeling and Geographic Data (Open Science)

01 - CONTEXTUALIZATION

Geospatial Simulations

Land Use and Cover Change (LUCC)

LUCC models how and why the land surface changes over time. It is the mathematical language of human consequences on the territory.

Deforestation

Conversion of native forest to agricultural use.

Coastal Dynamics

Mangroves vs. urbanization and sea level rise.

Urban Expansion

Growth of cities over rural and natural areas.

Agricultural Frontier

Agribusiness advance over the Cerrado and the Amazon.

FOCUS: PROCESS-BASED GEOSPATIAL MODELING

Expectation Alignment

This presentation focuses exclusively on **Geospatial Models** instead of general-purpose Machine Learning models.

Key Brazilian Geospatial Tools

Dinamica EGO

UFMG · since 2002

Visual GUI platform for spatially explicit LUCC modeling.

STRENGTHS

- No-code visual interface
- Academic benchmark

LIMITATIONS

- Manual reproducibility
- Scalability issues

TerraME

INPE · since 2005

Lua simulation framework for cellular automata models.

STRENGTHS

- Native Agent/Space logic
- PostGIS integration

LIMITATIONS

- High technical barrier
- No BDC/STAC support

LuccME

INPE · built on TerraME

Modular framework based on Demand/Allocation architecture.

STRENGTHS

- Interchangeable parts
- CLUE methodology

LIMITATIONS

- Inherits Lua constraints
- Weak Python link

02 — THE PROBLEM

The reproducibility crisis in computational science

Baker (2016), Nature · NAS (2019) · Stodden et al. (2016), Science · Krafczyk et al. (2021)

Baker, Nature 2016

70%

of researchers could not reproduce experiments from other groups.

NAS, 2019

National Academies, commissioned by the U.S. Congress. Formal report defining computational reproducibility as a pillar of modern science and establishing institutional recommendations.

Code doesn't run

Undocumented dependencies, incompatible versions, **implicit environments** — the experiment only works on the author's machine.

Inaccessible data

Input data not versioned or not published. **Without original data,** the result cannot be audited or replicated.

Opaque parameters

Critical model configurations are in ad hoc scripts or in the researcher's memory, not in formal auditable records.

Baker (2016) Nature 533:452 · NAS (2019) doi:10.17226/25303 · Stodden et al. (2016) Science 354:1240 · Krafczyk et al. (2021) Phil.Trans.R.Soc. 379:20200069

02 — THE PROBLEM

Challenges in Dynamic Geospatial Modeling

Spatial simulations have additional challenges beyond general computational reproducibility

01 Geospatial data is large and volatile

Rasters and vectors with specific CRS, varying resolutions and version history. A different GeoTIFF silently masks calibration errors.

02 Models couple science and infrastructure

The CA or LUCC logic gets mixed with file I/O, visualization and loop control — impossible to reuse without rewriting.

03 Experiments are not traceable

Which model version? Which parameters? Which input dataset? Without formal records, the result is irreproducible by design.

04 Scale breaks the scientific workflow

The researcher calibrates in the notebook, but running scenarios at scale requires rewriting the code — or abandoning production execution.

Why doesn’t LambdaGEO propose modernizing TerraME?

Historical Data	LUCC Classification	Future Simulation	Scenarios & Policies	Decision
MapBiomas, Census	SITS, BDC, STAC	Bottleneck in modern stack	Env. Planning	

	TerraME / LuccME	DisSModel (The Proposal)
Language	Lua + TerraLib (no longer maintained)	**Pure Python (Geopandas, NumPy)**
Reproducibility	No formal record	**Git + SHA-256 per execution**
Cloud Integration	Isolated local execution	**Cloud Native (API, Minio, Docker)**

DisSModel preserves the TerraME modeling philosophy in a modern ecosystem.

DisSModel

Building the Solution

MVP — Initial Version

Reproducible

Every experiment is an immutable and auditable artifact.

Native Python

Integrates with the existing scientific ecosystem.

No Rewrite

The same code runs in the notebook and on the cluster.

"Science should not need to be rewritten to go into production." — **DisSModel Principle**

DisSModel

Main Repositories

Modules of the @dissmodel Organization

Base

3 repositories

Provides the model's core engine, platform infrastructure, and official catalog.

Lab Models

2 repositories

Focused on cellular automata and dynamic systems for testing, teaching, and learning.

Empirical Models

3 repositories

Containing high-fidelity models for real-world use cases and land cover analysis.

Interfaces

1 repository

Interface repository with plugin code (e.g., QGIS) to demonstrate data consumption.

Visit our documentation at: **https://dissmodel.github.io/**

DisSModel

The Researcher's Journey: End-to-End Workflow

Modules of the @dissmodel Organization

PHASE 1 DEVELOPMENT & PACKAGING

1. Creation

Model design using the base library (model, environments, geo models, rules).

2. Packaging

Logic is fully encapsulated in *executors* (validate, load, execute, save).

3. Tests

The model is validated locally in an incredibly agile way via CLI tool.

4. Publishing

Library source code made available in independent GitHub repositories.

PHASE 2 INTEGRATION & EXECUTION

5. Integration

Researcher creates a .toml manifest and submits a PR to the catalog.

6. Curation

Maintainers review compliance and security before official incorporation.

7. API Execution

Platform manages dependencies and exposes results via dynamic API.

"Science should not need to be rewritten to go into production." — **DisSModel Principle**

DisSModel

Core Principles

The fundamental pillars for robust and scalable scientific modeling.

Reproducible Research

Data & code sharing for third-party verification.

IMPLEMENTATION:

- Executor + TOML + Docker
- Auditable Record (SHA-256)
- Code/Parameter separation

Claerbout (1992) · Victoria Stodden (2016), Science

FAIR for Software

Findable, Accessible, Interoperable, and Reusable.

KEY PILLARS:

F: DOI + Metadata
A: API + S3/MinIO
I: GeoTIFF + Xarray
R: TOML Versioning

Wilkinson et al., 2016

Software Engineering

Bridging the gap: Scientists vs. Production Engineers.

LAYER SEPARATION:

Science: logic is kept pure.
Platform: APIs & infrastructure.
SimOps: Scientific SimOps.

Baxter et al. (2012) · Wilson (2017) PLOS Comp. Bio.

"Science should not need to be rewritten to go into production." — **DisSModel Principle**

DisSModel

System Components

🧩 dissmodel

LIBRARY (Core Framework)

Central simulation engine for local scientific model development and execution.

github.com/DisSModel/dissmodel

`pip install dissmodel`

⚙️ dissmodel-platform

PLATFORM (Cloud-Native)

Open and scalable infrastructure for distributed cloud experiment execution.

github.com/DisSModel/...-platform

`docker compose up --build`

📁 dissmodel-configs

MODEL CATALOG

The single source of truth. Centralizes configuration files (manifests in .toml).

github.com/DisSModel/...-configs

`pull requests`

"Science should not need to be rewritten to go into production" — ***dissmodel*** *runs the same code locally and on the remote* ***platform****.*

Core Framework

core

Simulation Engine

Discrete clock + execution cycle via Environment & Model.

Environment, Event dispatch, step control.

geo

Spatial Substrate

Dual design: Vector (GeoDataFrame) + Raster (NumPy).

Queen/Rook and Moore/Von Neumann neighborhoods.

executor

Execution Layer

ModelExecutor ABC + SimulationRegistry.

Local CLI and Remote Workers — same code.

io

Storage I/O

Local file and MinIO/S3 read/write operations.

Checksums and provenance.

vis

Visual Observers

Chart, Map, RasterMap, display_inputs.

Decoupled Observer pattern.

"Science should not need to be rewritten to go into production" — **DisSModel Principle**

Server Side

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FastAPI Gateway

API-Driven Execution

- Programmatic REST calls
- Legacy dashboard integration
- Validation via Pydantic

Docker Workers

Subprocess Isolation

- Jobs in isolated containers
- No dependency conflicts
- Redis Queue scalability

Jupyter Lab

Experiment Service

- Interactive experimentation
- Direct data visualization
- Rapid model prototyping

MinIO Storage

Agnostic Storage

- S3-compatible integration
- Unified spatial writing
- Zarr and GeoTIFF support

The infrastructure orchestrates **FastAPI, Redis, and Docker** *to ensure science does not need to be rewritten for production.*

Architecture deployable via **Docker Compose** in Cloud environments.

DisSModel

The Central Catalog: dissmodel-configs

Single Source of Truth

To keep the ecosystem scalable and secure, we separate the model code from its publication.

The catalog stores only declarative manifests, ensuring full traceability and governance.

Manifestos .toml
Each model has a centralized configuration file.

Versioning
Points to the specific *release* or *tag* on GitHub.

Parameterization
Defines default limits consumed by the API.

configs/models/coastal_raster.toml

```toml
[model]
executor_module = "br-mangue.executor"
name = "br-mangue"
package = "git+https://github.com... "

[model.parameters]
end_time = 88
taxa_elevacao = 0.5
altura_mare = 6.0
acrecao_ativa = false
resolution = 100.0
crs = "EPSG:31984"
```

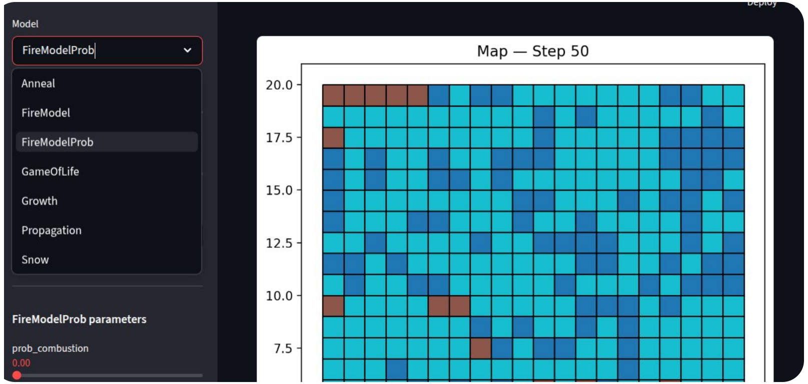
Declarative configurations ensure exact simulation reproducibility.

Classical Models (SysDyn and CA)

DisSModel

⬡ dissmodel-ca

CELLULAR AUTOMATA



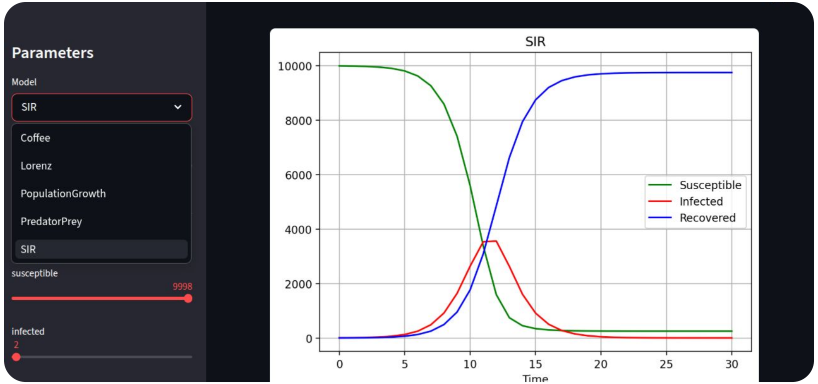
Spatial Modeling

Complex systems through local interactions in spatial grids.

- Game of Life & Forest Fire
- Substrate: GeoDataFrame
- Processing via NumPy

~ dissmodel-sysdyn

SYSTEM DYNAMICS



Temporal Dynamics

Focus on flows, stocks, and feedback loops for temporal behavior.

- SIR, Lorenz, Predator–Prey
- Streamlit Explorers
- CLI Interface

Cellular Automaton: Game of Life

DisSModel

Model Implementation

- Inherits from **CellularAutomaton**
- **setup()**: Uses Queen neighborhood via libpysal
- **initialize()**: Initial random state fill
- **rule(idx)**: Implementation of Conway's rules
- Supports: glider, pulsar, blinker patterns
- Includes Streamlit Explorer integration

```
class GameOfLife(CellularAutomaton):
def setup(self) -> None:
# Queen neighborhood
self.create_neighborhood(strategy=Queen)

def rule(self, idx) -> int:
state = self.gdf.loc[idx, 'state']
n = self.neighbor_values(idx).sum()
if state == 1:
return 1 if 2 <= n <= 3 else 0
return 1 if n == 3 else 0
```

Dynamic Systems: SIR Model


```python
from dissmodel.core import Environment
from dissmodel.sysdyn import SIR
from dissmodel.visualization import Chart

env = Environment()
SIR(susceptible=9998, infected=2,
contacts=6, probability=0.25)
Chart(show_legend=True)
env.run(30)
```

Concept Mapping

Environment:
Global simulation clock

SIR (Model):
Model inherits from Model ABC

Chart:
Observer decoupled from the model

env.run(30):
30 discrete timesteps

DisSModel in Real-World Scenarios

🌿 brmangue-dissmodel

REFERENCE

Coastal Case Study

- Flooding and Mangroves
- Based on Bezerra et al. (2014)
- Focus Area: Maranhão Coast

🌍 DisSLUCC-Cont.

REFERENCE

Land Use and Cover

- Demand + Potential + Allocation
- CLUE and LUCCME Structure
- INPE/Brazil Methodology and Expertise

Coastal Case Study: brmangue-dissmodel

📍
Study Area
Maranhão Coast, Brazil. Vector spatial grid.

📄
Scientific Basis
Bezerra et al. (2014).

🌊
FloodModel
Flooding due to sea level rise scenarios.

🌿
MangroveModel
Migration by tide and soil type dynamics.

```
env = Environment(start_time=2008, end_time=2030)

# Add specialized models
FloodModel(gdf=gdf, elevation_rate=0.5,
use_attr='usage')
MangroveModel(gdf=gdf, tide_height=6.0,
soil_attr='soil')

env.run()
```

Performance Benchmark

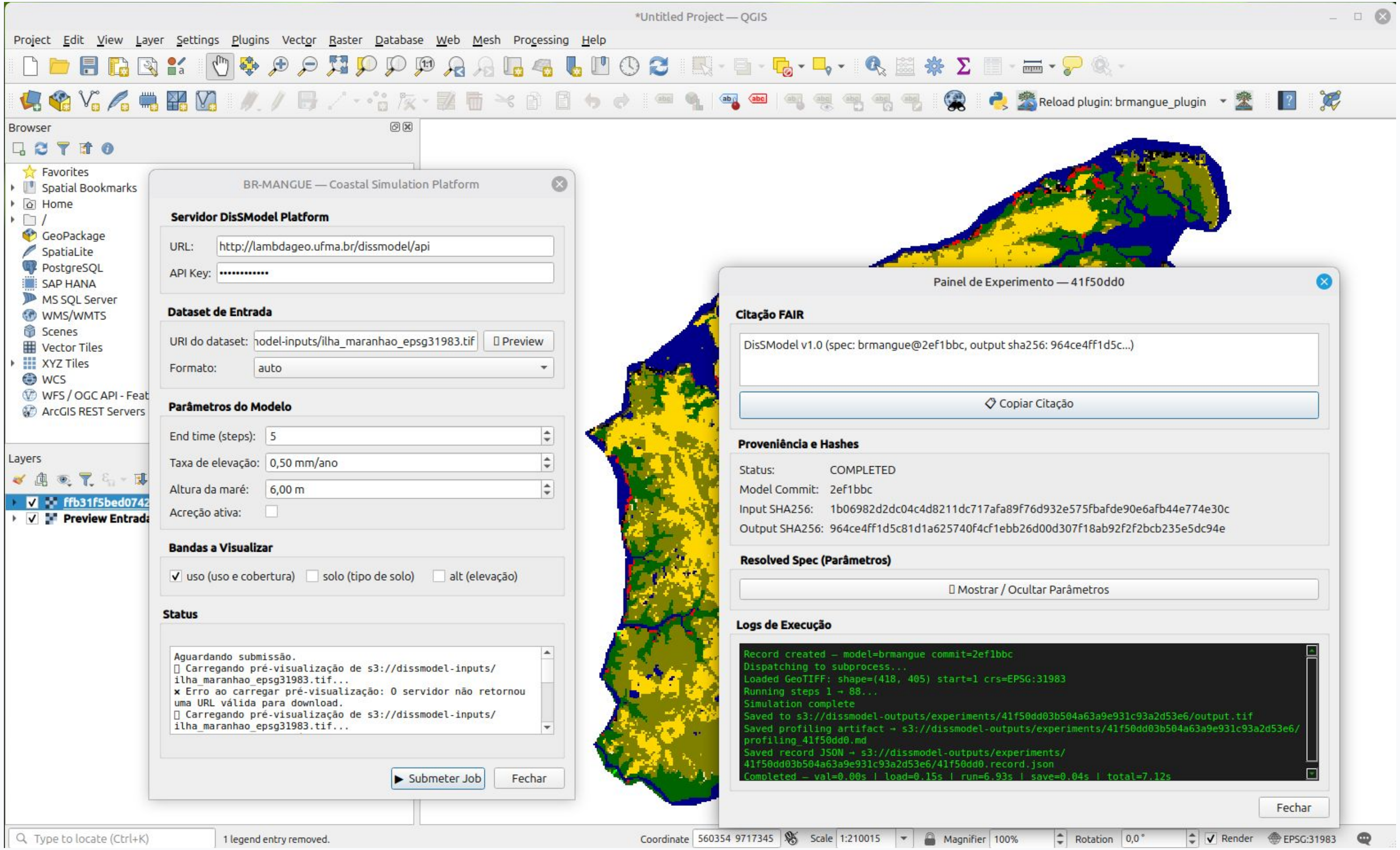
SUBSTRATE | MS/STEP | SPEEDUP

Vector: **1241.7** (1.0x)

Raster: 31.5 (39.4x ⚡)

Accuracy vs TerraME: **99% match**

Coastal Case Study: brmangue-dissmodel



Plugin Feature

QGIS Integration

Dedicated plugin for the brmangue model, enabling streamlined simulation and visualization of coastal dynamics within the QGIS environment.

- Intuitive interface for parameter input
- Direct visualization of model outputs
- Seamless integration with vector grids

DisSLUCC-Continuous: Land Use & Cover

Continuous Modeling

The package implements the CLUE-type allocation algorithm (Veldkamp & Fresco, 1996). Cells receive *fractional proportions* instead of discrete classes.

Evaluation Metric

For continuous outputs, the **MAE (Mean Absolute Error)** was adopted to directly evaluate modelling error (Willmott, 2005).

1. Demand

Magnitude of change per timestep. Pre-computed via historical CSV.

```
DemandPreComputedValues(
  annual_demand=load_csv(...)
)
```

2. Potential

Change suitability via linear regression with driver variables.

```
PotentialLinearRegression(
  gdf=gdf, drivers=[...]
)
```

3. Allocation

CLUE-like distribution based on potential and constraints.

```
AllocationClueLike(
  demand, potential
)
```

Experimental Setup

Dataset
LucccME Package - AC (2008-2014)

Time Steps
6 Steps

Resolution
6,574 cells

DisSLUCC - Validation and Performance Results

Performance (6 steps · 6,574 cells)

3.9×

SPEEDUP RASTER VS VECTOR
(31.6 ms vs 122.5 ms)

Accuracy vs TerraME

0.002276

MAE VS TERRAME · BOTH SUBSTRATES
97.09% match · Vector = Raster · MAE 0.002276

Technical Highlight: Raster substrate achieves 3.9× speedup over Vector (31.6 ms vs 122.5 ms/step). Both substrates match TerraME at 97.09% — and produce identical output (MAE = 0.000), confirming the raster optimisation preserves full algorithmic correctness.

Dataset: LuccME Package - AC - 2008–2014 · 6 steps · 6,574 cells · tolerance 0.01

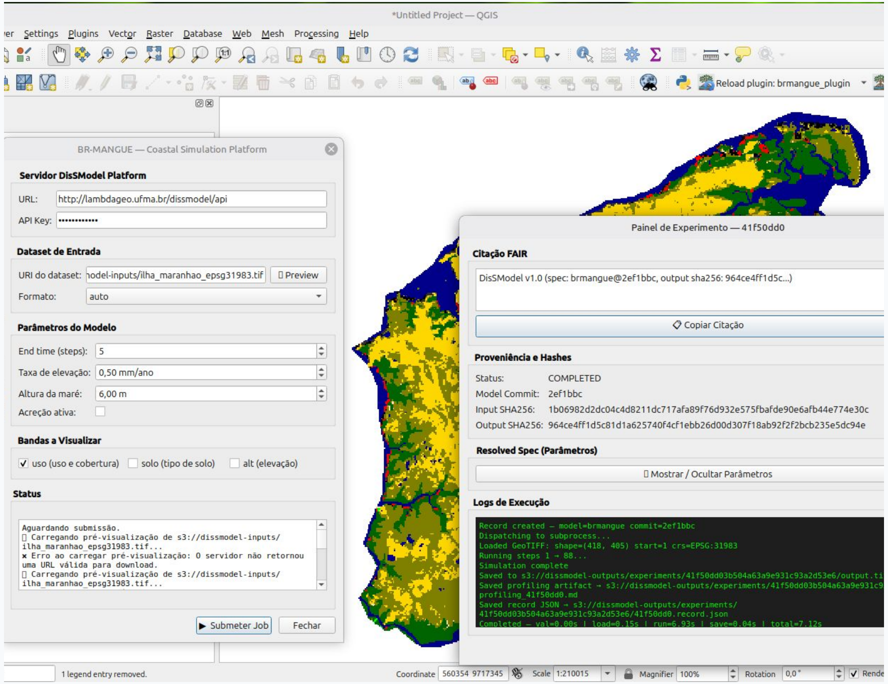
TRANSFORMING GEOSPATIAL SCIENCE

Hidden Engineering
The complex cycle of data orchestration runs seamlessly.

Full Traceability
Guaranteed data provenance for every simulation stage.

Direct Delivery
Dynamic results delivered directly within GIS tools.

End-to-End Focus
Researchers focus on science, users on decisions.



DisSModel Roadmap 2026–2028

2026 S1	2026 S2	2027 S1	2027 S2	2028
JOSS Submission	**DisSLUCC focus**	**BDC Integration**	**Dask / Ensemble**	**Book + Community**
Repo organisation & PyPI v0.5	CLUE & CLUE-S (PIBIC)	STAC source reader	Lazy eval (Pangeo)	Geospatial DS book
Formalisation at UFMA	LUCC Scholars (PIBIC)	Xarray (time, y, x)	Parallel scenarios	PT-BR Edition
Research plan submissions	BRMangue JOSS	ExpRecord → MinIO	Native Zarr output	Workshop INPE/SBSR
	DisSModel v1.0			

** QGIS plugins (qgisparql-triple2layer / layer2triple): joint JOSS submission under evaluation.*

08 — NEXT STEPS

Strategic Partnership: DisSModel & LuccME++

2027/28 — DisSModel will serve as the innovation laboratory for the evolution of **LuccME** at CCST/INPE.

DisSModel

Partnership & Evolution →

Future of LUCC

TerraME was the starting point — **DisSModel advances as the foundation for LuccME++**

Thank you!

DisSModel — open source, open science

GitHub	Docs	PyPI	Contact
dissmodel.github.io	dissmodel.github.io/dissmodel/	pip install dissmodel	sergio.costa@ufma.br

> *"Science should not need to be rewritten to go into production."*
> — DisSModel Principle

dissmodel	dissmodel-ca	dissmodel-sysdyn	brmangue-dissmodel	DisSLUCC-Cont.

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Modeling

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