

# One-Week PINN Project — Checklist & Repo Layout (Denmark Soil Moisture)

A tight, printable 1-page checklist to run a full-time PINN MVP in 5 days. No code—just the playbook.

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## Snapshot

- **Goal:** Fit a PINN that reconstructs  $\theta(z,t)$  at one Danish site (multi-depth sensors) with 1-D Richards + van Genuchten–Mualem; free-drainage bottom; flux top (rain – evap).
  - **Outputs:** Cleaned dataset + data card, diagnostics, bucket baseline, PINN fit & learned params, 5–7 page report.
  - **Cadence:** Hourly (preferred) or daily; Europe/Copenhagen timezone.
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## Day-by-Day

**Day 1 — Data & EDA** - [ ] Select station & season ( $\geq 3$  depths,  $\geq 3$ –5 rain events). - [ ] Acquire  $\theta(z,t)$ +QC (ISMN/HOBE), meteo (DMI), optional soils (SoilGrids/OpenLandMap). - [ ] Harmonize: timezone, cadence, units ( $\theta$  m<sup>3</sup>/m<sup>3</sup>; precip mm/step; depth m). - [ ] QC: drop bad flags; mask long  $\theta$  gaps; smooth met spikes only. - [ ] Plots:  $\theta(z,t)$  heatmap; event-aligned  $\Delta\theta$ ; rough water balance ( $P - ET_0$  vs  $\Delta S$ ).

**Day 2 — Problem Spec** - [ ] Freeze physics (1-D Richards; van G-M; bare soil or fixed shallow uptake). - [ ] Boundary conditions: top flux (rain – evap), bottom unit gradient; initial  $\theta$  profile. - [ ] Non-dimensionalization ( $z$ ,  $t$ , head); write scales in spec. - [ ] Decide learned params: ( $\alpha$ ,  $n$ ,  $K_s$ ,  $\theta_r$ ,  $\theta_s$ ) global; (optional) two-layer. - [ ] Losses: data, PDE residual, BC/IC, parameter-prior penalties. - [ ] Collocation sampling plan (densify near surface & rain windows). - [ ] Time splits (Train 70% / Val 15% / Test 15%, keep events intact).

**Day 3 — First Training Pass** - [ ] Initialize params within pedotransfer bounds. - [ ] Curriculum: start data-heavy; ramp PDE/BC weights. - [ ] Track: per-depth RMSE (Train/Val), water balance, parameter ranges. - [ ] Early stop on Val; save best checkpoint.

**Day 4 — Tighten & Compare** - [ ] Build simple bucket baseline; calibrate 1–2 knobs. - [ ] Add small top-flux correction term (L2-penalized) if met forcing imperfect. - [ ] Ablation: remove parameter priors once; note  $\Delta$  in metrics. - [ ] Choose best PINN variant by Test RMSE + physical plausibility.

**Day 5 — Package & Report** - [ ] Compute deep drainage  $q_{\text{bottom}}(t)$ ; cumulative drainage. - [ ] Compare learned ( $\alpha$ ,  $n$ ,  $K_s$ ,  $\theta_r$ ,  $\theta_s$ ) to soil-class ranges. - [ ] Quick LOEO (leave-one-event-out) sanity check. - [ ] Finalize artifacts (data, figs, config) + short report.

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## Data Prep & QC (Quick Checks)

- [ ]  $\theta$  within  $[\theta_r, \theta_s]$ ; no long saturation plateaus unless justified.
  - [ ] Rain events list (thresholds:  $\geq 2$  mm/hr or  $\geq 5$  mm/day) for sampling/plots.
  - [ ]  $ET_0$  (FAO-56) computed once; used for sanity only.
  - [ ] Soil texture by depth extracted; pedotransfer  $\rightarrow$  **wide** bounds for  $(\alpha, n, K_s, \theta_r, \theta_s)$ .
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## Training & Evaluation

- [ ] Non-dimensional inputs/targets; gradient clipping enabled.
  - [ ] Collocation resampling where PDE residual high (fronts, surface).
  - [ ] Metrics: RMSE per depth; event timing (wetting-front lag); mass balance drift.
  - [ ] Compare vs bucket baseline on Val/Test.
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## Success Criteria

- **Fit:** Test RMSE  $\leq 0.03$ – $0.05$  m<sup>3</sup>/m<sup>3</sup> per depth; plausible wetting-front timing.
  - **Physics:** No  $\theta > \theta_s$ ; reasonable drainage; learned params within soil-class ranges.
  - **Beat baseline:** PINN improves RMSE and event timing vs bucket.
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## Risks & Fast Mitigations

- **Training instability:** data-first curriculum; normalize; clip grads.
  - **Bad top flux:** enable small trainable correction (strongly penalized).
  - **Heterogeneity:** defer layering unless Day 3 already stable.
  - **Time sink:** keep MLP+tanh (5–8 layers); one file + config.
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## Repo Layout (barebones)

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pinndk/
├─ README.md           # What/why; quickstart; reproduction steps
├─ config.yaml         # Paths, cadence, hyperparams, loss weights
├─ spec.md             # Physics, BCs, scales, losses, splits
├─ data/
│   ├─ raw/            # Original downloads (ISMN, DMI, soils)
│   ├─ clean/          # siteX.parquet/CSV + event_list.csv
│   └─ meta/           # soil_priors.yaml; station_metadata.json
├─ figs/               # Heatmaps, event stacks, fits, balance, tables
├─ src/
│   └─ pipeline.py|jl  # Single entry: load-QC-EDA-train-eval-export
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|   └─ utils.py|jl           # Minimal helpers (I/O, plots). Keep tiny.
└─ report/
   └─ report.md             # 5-7 pages w/ figures (or .tex/.docx)
   └─ tables.xlsx           # Metrics, learned parameters, comparisons
```

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## “Data Card” Template (fill once)

- **Site & Period:** name, lat/lon, start–end dates, timezone.
  - **Sensors:** depths (m), sampling cadence, QC flags used, outages.
  - **Meteo:** source(s), variables, cadence, missing intervals.
  - **Soils:** texture by depth; source & date; pedotransfer used; parameter bounds.
  - **Preprocessing:** resampling rules, unit conversions, filters.
  - **Events:** detection thresholds; number of events; notable extremes.
  - **Splits:** train/val/test dates; rationale.
  - **Known Issues:** rain gauge gaps, sensor drift, site notes.
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## Notes

- Keep all plots legible in grayscale for printing.
- Log every assumption in `spec.md`; do not change mid-week without noting.