

MAT4EU: Phase-Change Evidence

CONFIRMED: working-grid numerical screening; rejected coarse grid retained; no experimental material validation

Plain-English Summary

The model can calculate heat storage through melting and freezing and share the calculation across graphics processors. The attached example is a small assumed sample using published property inputs. It is not a measured device or a qualified alloy batch.

Proposal Text

A three-dimensional conduction-based phase-change model has been implemented with CUDA-aware MPI (direct graphics-memory messaging). The numerical model has been verified against analytical melting and freezing benchmarks. A literature-based AlSi12 screening study demonstrates heating, melting and subsequent solidification, with explicit material-property sensitivity and numerical-resolution checks. Material-specific experimental validation for the intended application remains a planned milestone.

Do not replace “numerically verified” with “experimentally validated material”.

Defined Illustration

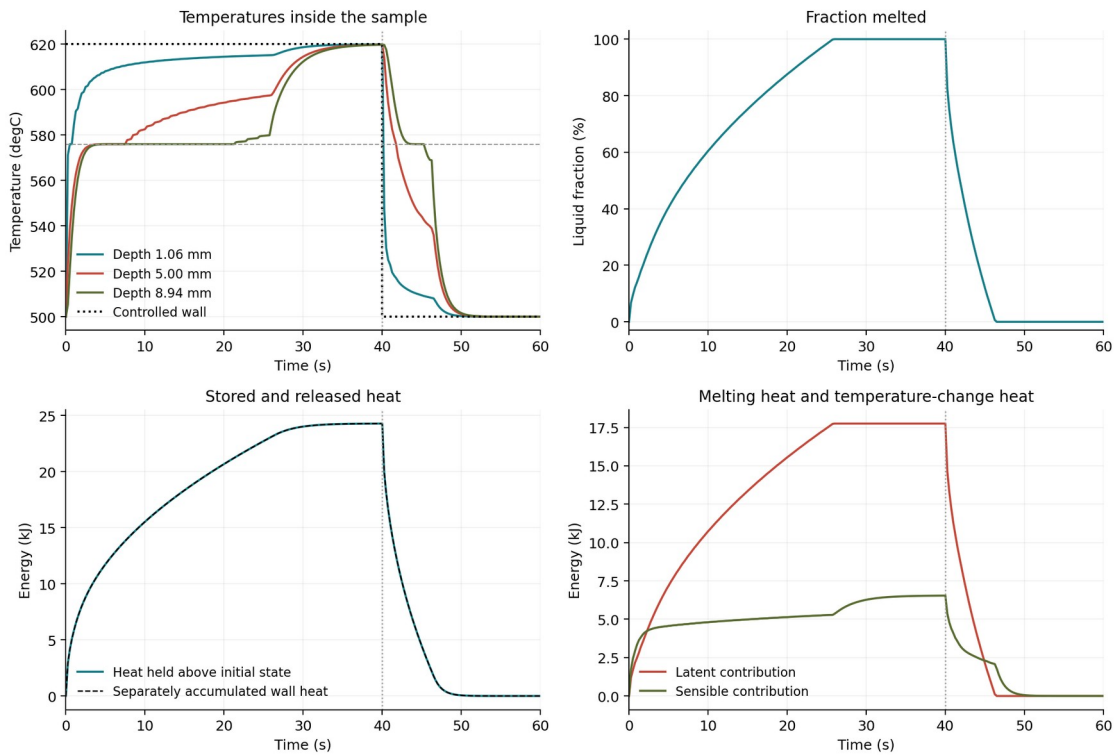
- Assumed dense sample: 40 x 30 x 10 mm, 31.704 g, initially 500 degC.
- One controlled wall: 620 degC for 40 s, then 500 degC for 20 s. Other walls insulated.
- Nominal grid: 5 x 3 x 33 cells, split over four graphics processors on node02.
- Adopted nominal latent heat: 560 kJ/kg; sharp transition at 576 degC.
- Constant phase-mean heat capacities: 1692.554 / 1769.109 J/(kg K), solid/liquid.
- Density stays fixed; no melt motion, container, contact loss, radiation, expansion or degradation.

Computed Results

- Heat held above the initial state at 40 s: **24.293 kJ**.
- Heat released over the next 20 s: **24.293 kJ**.
- Reaches 99 percent melted within **25.25-25.50 s**.
- Reaches 99 percent frozen within **6.00-6.25 s after cooling starts**.
- Residual heat above initial state at 60 s: 0.00268395 J.
- Nominal maximum numerical energy residual / equilibrium capacity: 1.317e-14.

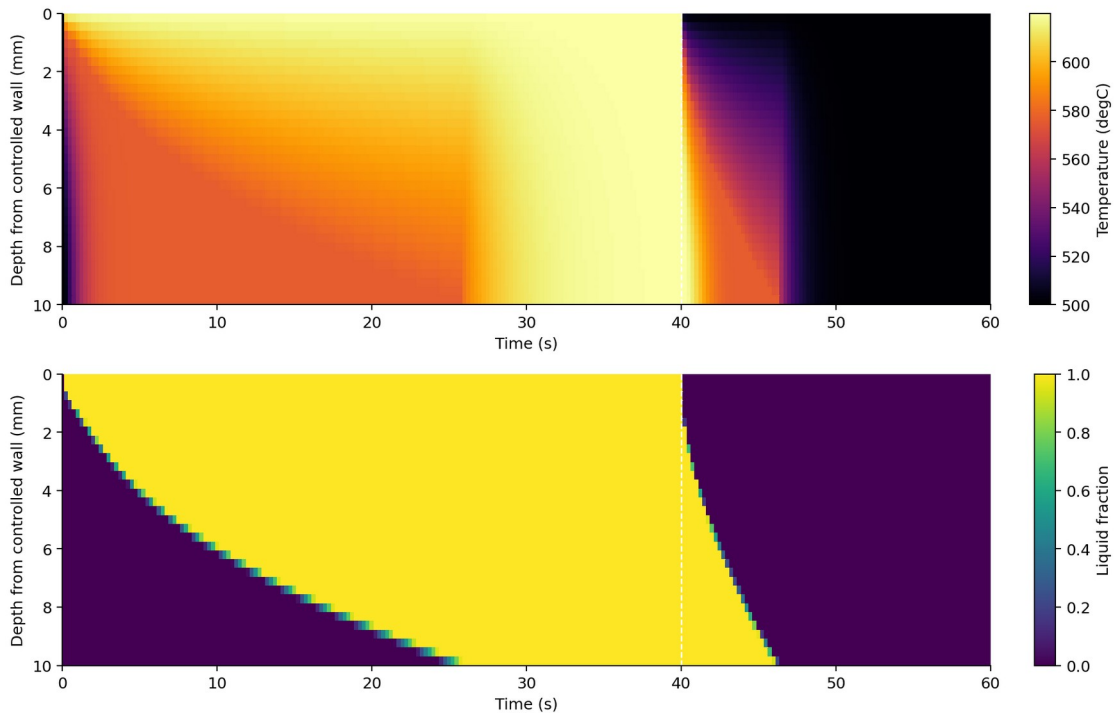
These are conditional simulation predictions. Near-complete heat recovery follows from the ideal insulated setup and is not an efficiency claim. Event intervals reflect 0.25-second output sampling, not experimental uncertainty.

MAT4EU | AISi12 screening: heating and freezing
Assumed 40 x 30 x 10 mm guarded sample; literature inputs; NOT experimental validation



Heating and freezing

MAT4EU | Temperature and phase through the thickness
Screening prediction, not measured data; cell samples without spatial interpolation



Depth and phase

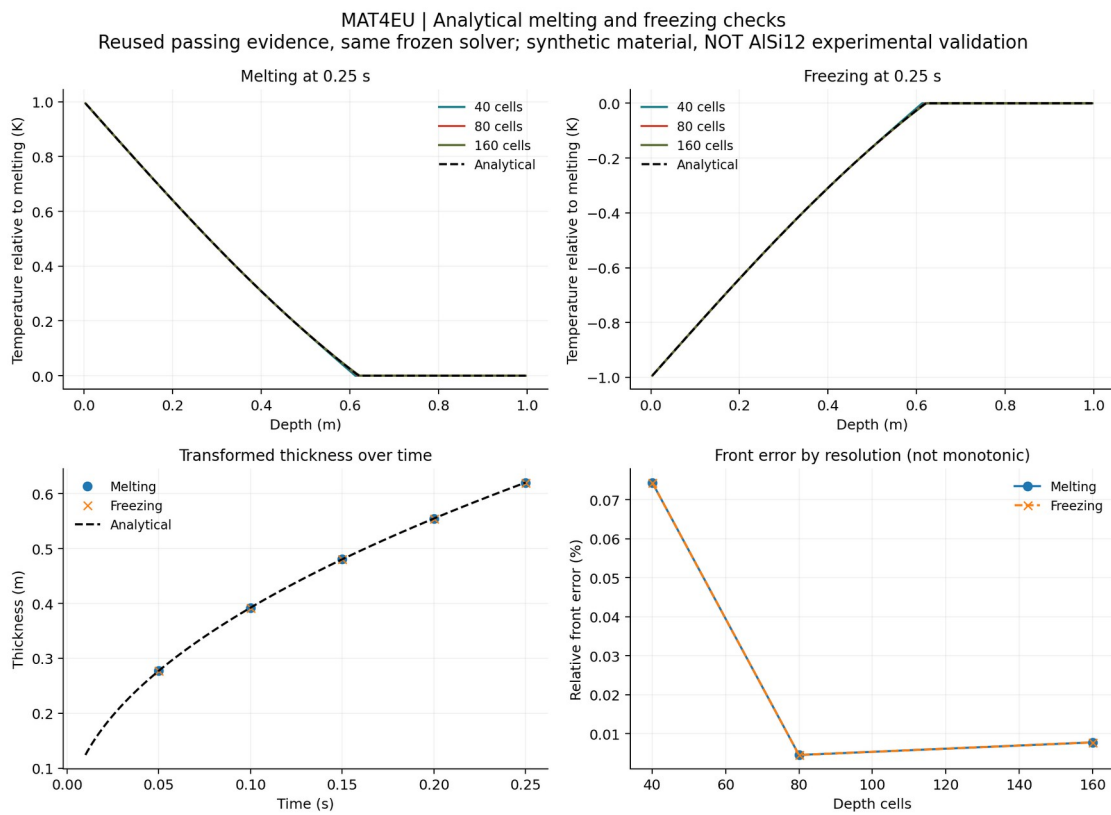
Numerical Evidence

219 of 220 declared numerical checks passed in the raw campaign (raw status: FAIL).

The 17-plane exploratory grid failed the predeclared centre-temperature target and is rejected. The originally selected 33-plane working grid passes its finer 65-plane and time-step comparisons. The separate baseline acceptance does not change the raw FAIL result or loosen any tolerance.

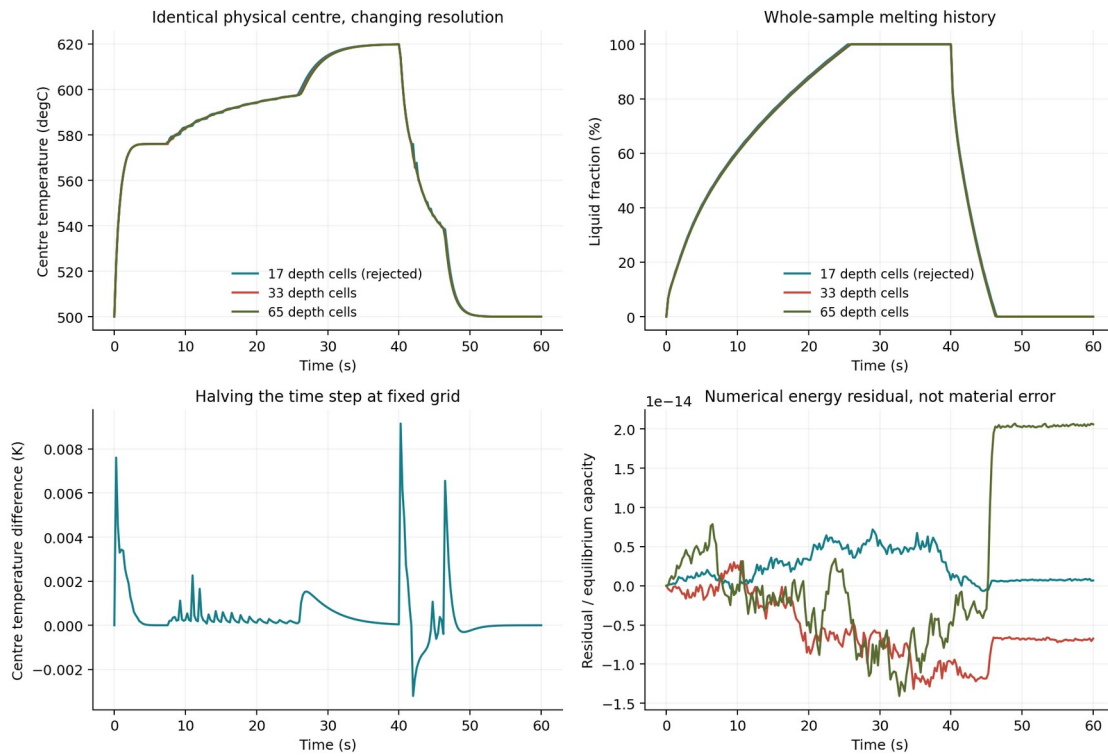
- Rejected coarse-grid check: nominal_n17_r4: resolution centre_temperature_k_max, observed 5.7487, limit 3.
- nominal_n33_r1: maximum final enthalpy difference 0 J/kg; complete probe histories exactly match: True.
- nominal_n33_r2: maximum final enthalpy difference 0 J/kg; complete probe histories exactly match: True.
- nominal_n17_r4: maximum liquid-fraction change 1.2193 percentage points; energy change 0.9429 percent of nominal capacity; centre-temperature change 5.7487 K.
- nominal_n65_r4: maximum liquid-fraction change 0.6547 percentage points; energy change 0.4406 percent of nominal capacity; centre-temperature change 1.4207 K.
- nominal_n33_half_dt_r4: maximum liquid-fraction change 0.0047 percentage points; energy change 0.0043 percent of nominal capacity; centre-temperature change 0.0092 K.

Previously completed mathematical suite: 434 checks passed across 31 successful cases, using the same source and binary. Finest analytical melting/freezing front error: 0.00773 percent. The resolution trend is not monotonic; no measured convergence order is claimed.



Analytical verification

MAT4EU | Resolution and conservation checks
Matched times and centre position; no interpolation, experimental tolerance or convergence-order claim



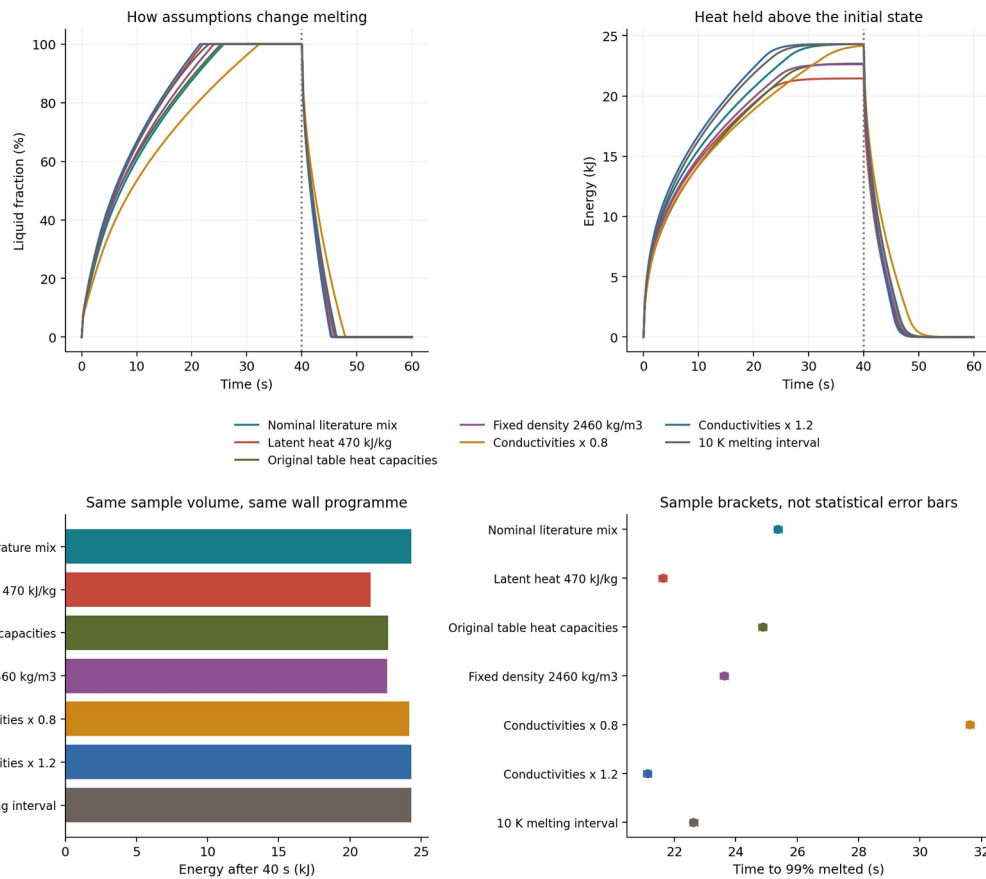
Resolution

Material Sensitivity

Each alternative changes one property choice. These alternatives are not a statistical confidence interval or measured supplier limits.

Alternative	Heat stored at 40 s (kJ)	99% melt bracket (s)
Nominal literature mix	24.293	25.25-25.50
Latent heat 470 kJ/kg	21.445	21.50-21.75
Original table heat capacities	22.679	24.75-25.00
Fixed density 2460 kg/m ³	22.624	23.50-23.75
Conductivities x 0.8	24.169	31.50-31.75
Conductivities x 1.2	24.300	21.00-21.25
10 K melting interval	24.298	22.50-22.75

MAT4EU | One-at-a-time property alternatives
Deterministic scenarios only; neither a confidence interval nor a supplier specification

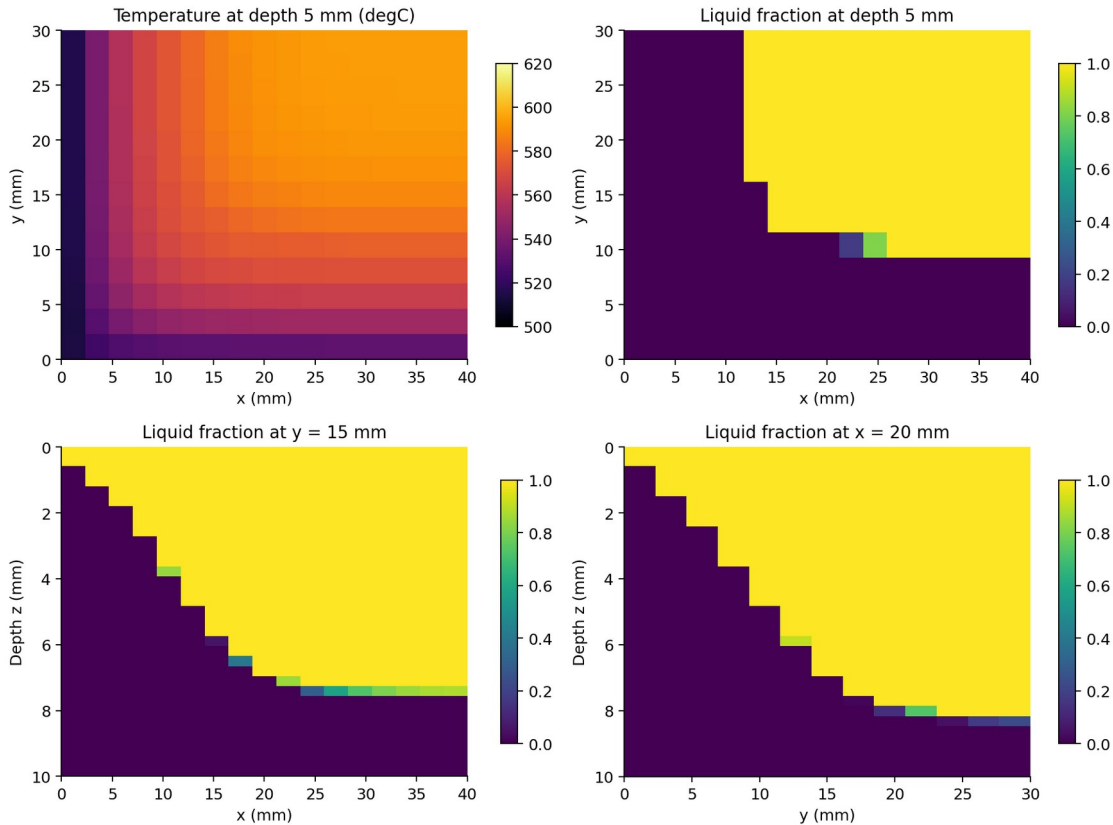


Sensitivity

Three-Dimensional Example

An auxiliary case applies three different controlled face temperatures. It produces nonuniform fields in all directions. It is not the guarded baseline and has no device-level or independent mesh-accuracy claim.

MAT4EU | Three controlled faces, at 20 s
Walls: $z=0$ at 620 degC, $x=0$ at 500 degC, $y=0$ at 520 degC; illustrative, not device validation



Three-dimensional fields

Readiness and Limits

Claim

Status

Conservative thermal phase-change calculation

Numerically verified within stated tests

GPU-to-GPU domain communication

Actual device-buffer probe and matching partitions

AlSi12 property choices

Literature-screening assumptions, not a batch certificate

material accuracy

Not experimentally established

Actual storage-unit charge/discharge time or efficiency

Not established

Melt flow, radiation, contact, shrinkage and cycling damage

Outside this result

Full communication-library memory/API checker

Not clean in earlier diagnostics; no clean-check claim

Faster or universally scalable execution

Not claimed by this campaign

The production source, binary and system libraries were not changed. Historical communication-library diagnostic issues remain documented; this numerical evidence does not erase them. The small sample does not require large graphics memory, and no graphics reset or interruption of unrelated jobs was needed.

Files and Reproduction

- `PROPERTY_AUDIT.md`: what each published property does and does not support.
- `METHODS_AND_VALIDATION_PLAN.md`: equations, assumptions and the next independent sample test.
- `case_definition.json`: conditions and predeclared numerical limits.

- `screening_claim.json`, `manifest.json`: run commands, checks, original paths and source/binary hashes.
- `baseline_qualification.json`: working-grid decision with every rejected coarse-grid check retained.
- `scenario_summary.csv`, `nominal_depth_history.csv`: numerical tables behind the main figures.
- `benchmark_evidence/`: selected original mathematical results plus their full campaign claim and manifest.
- `reproduce.sh`: rerun the unchanged solver and render a fresh report; requires the recorded node02 CUDA/MPI environment.

Scientific input sources: [Chaomurilige et al., 2023](#) and [Quick et al., 2023](#). See the property audit for the unverified upstream latent-heat reference and failed local PDF conversions.

Recommendation: submit the numerical evidence and labelled screening predictions; make independent sample validation the next milestone.