Bridging Manufacturing to Operation: A Validated Multi-Scale SOFC Stack Model for Digital Twin Deployment

Live demo
paper + poster

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≈ 26 mV
per-cell spread, invisible at the terminal

38 → 76 mV
worst cell, 0.5 → 1.0 A/cm²

8 / 12
experimental I–V within 50 mV RMSE

~16 cells
full per-cell, real-time (300 ms HIL · laptop)

Introduction

A **digital twin of the as-built SOFC stack assembly** must link two domains usually modelled in isolation — the mechanical state set at manufacture and the electrochemical performance in operation. Manufacturing tolerances (cell warp, interconnect flatness, preload) set per-cell voltage and lifetime, yet operators see only the **stack terminal voltage**; per-cell variability stays hidden.

Multi-scale model chain

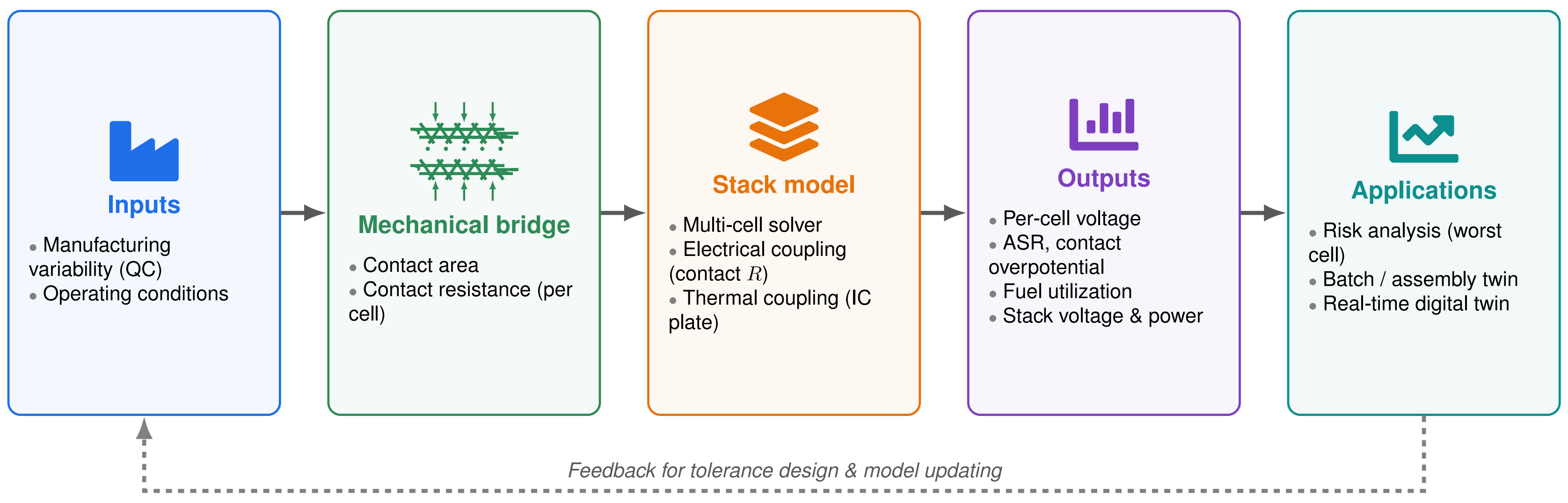

Fig. 1 — Manufacturing QC → mechanical bridge → stack solver → per-cell voltage.

Contribution

No prior SOFC-stack model couples first-principles cell physics, per-cell stack resolution, real-time HIL feasibility and a-priori QC dispersion in one end-to-end chain.

- 1D finite-volume cell solver (first-principles transport & thermo; calibrated kinetics)
- phenomenological mechanical→electrical contact closure
- multi-cell stack solver at HIL-relevant rates
- validation with **named physical causes**, not re-tuned

Cell-level solver

1D axial, N_z control volumes, seven gas species (H_2, H_2O, O_2, N_2, CO, CO_2, CH_4); convection–reaction with Butler–Volmer electrochemistry and internal reforming. Closures: NASA-Glenn 7-coefficient thermodynamics, symmetric Butler–Volmer (inverse-sinh), Hafsi binary-diffusion, Xu–Froment reforming (SMR / WGS).

$$Vcell = VNernst - \eta ohm - \eta act - \eta conc - Rcontact \cdot j$$

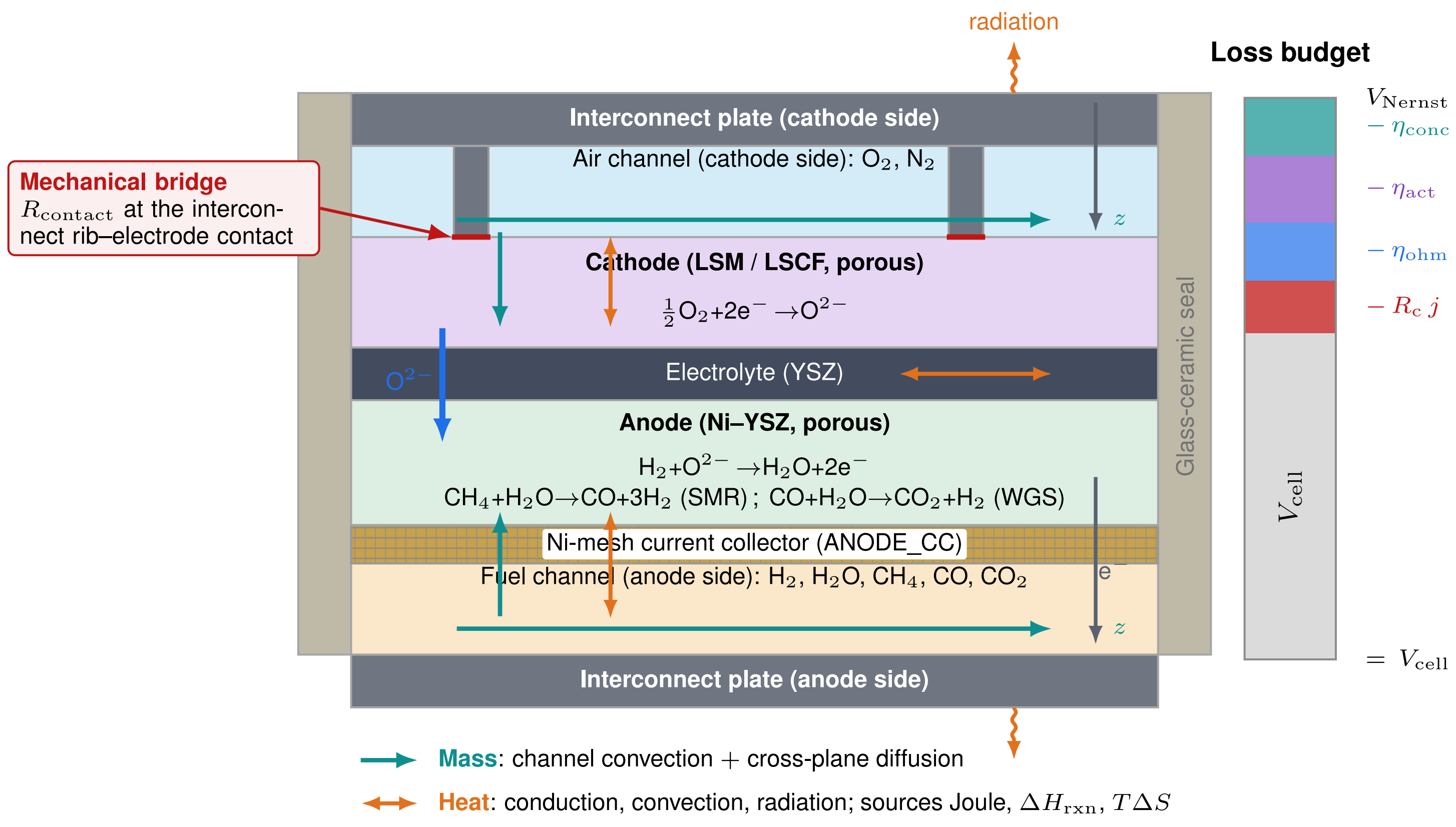

Fig. 2 — Modelled cell repeat unit and the per-cell voltage-loss budget.

Mechanical bridge

The mechanical→electrical bridge carries most stack-level uncertainty: contact area from a geometric thresholding (cell/interconnect/assembly variances in quadrature), then per-cell resistance via a **Holm constriction model** — calibrated vs FE sims (Klein), phenomenological.

Validation

- **8 of 12** steady-state I–V within a 50 mV RMSE band (vs published data)
- 4 documented xfails — each a named physical cause; not re-tuned
- Hafsi 2024: anode diffusivity from microstructure, not fitted
- **dynamic load-step response reproduced** vs Zaccaria 2016 (NETL HYPER): step direction + thermal τ

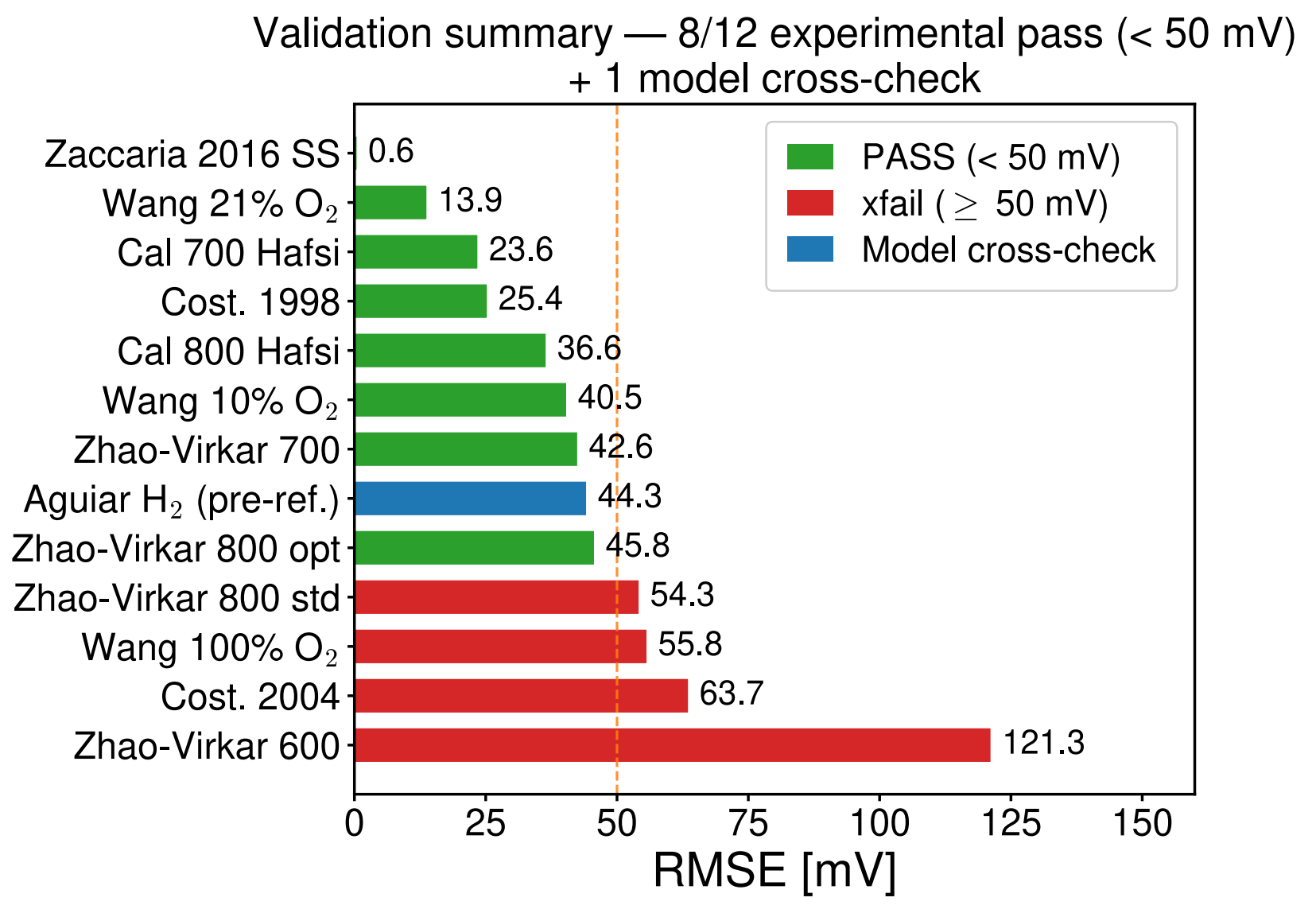

Fig. 3 — RMSE vs steady-state I–V; 8/12 < 50 mV (hardware pending).

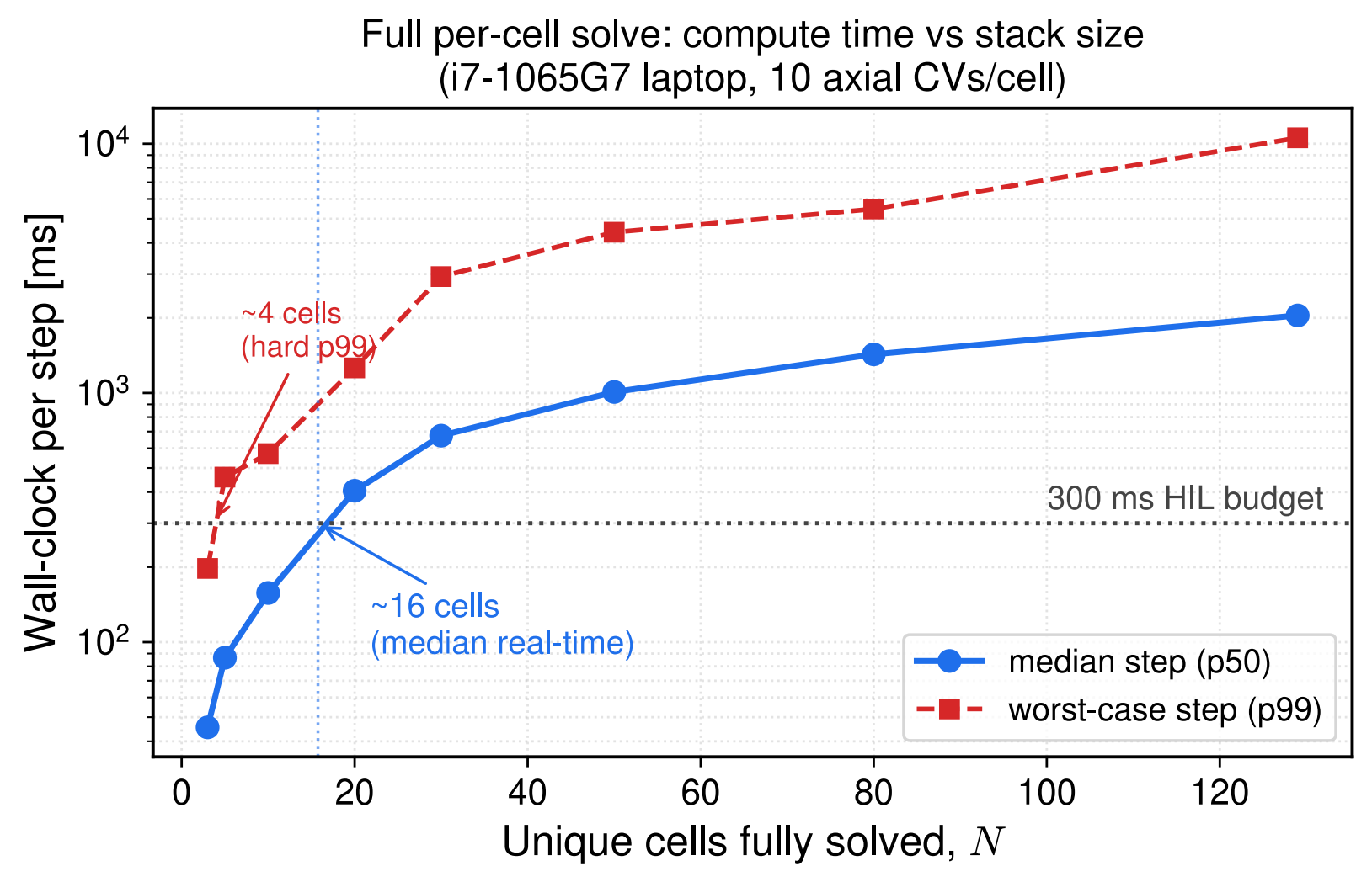

Fig. 4 — Full per-cell solve: real-time to **~16 cells** (median; worst-case p99 ~4).

Assembly twin: 30-cell batch

The per-cell spread comes from a production-grade QC dispersion run through the chain. It is **plate-dominated** and tracks the load: the 26 mV median (σ_{ASR} = 13 mΩ·cm² at 0.5 A/cm²) grows with current density. Largest levers: current density, then ASR dispersion σ_{ASR}; mean ASR is minor.

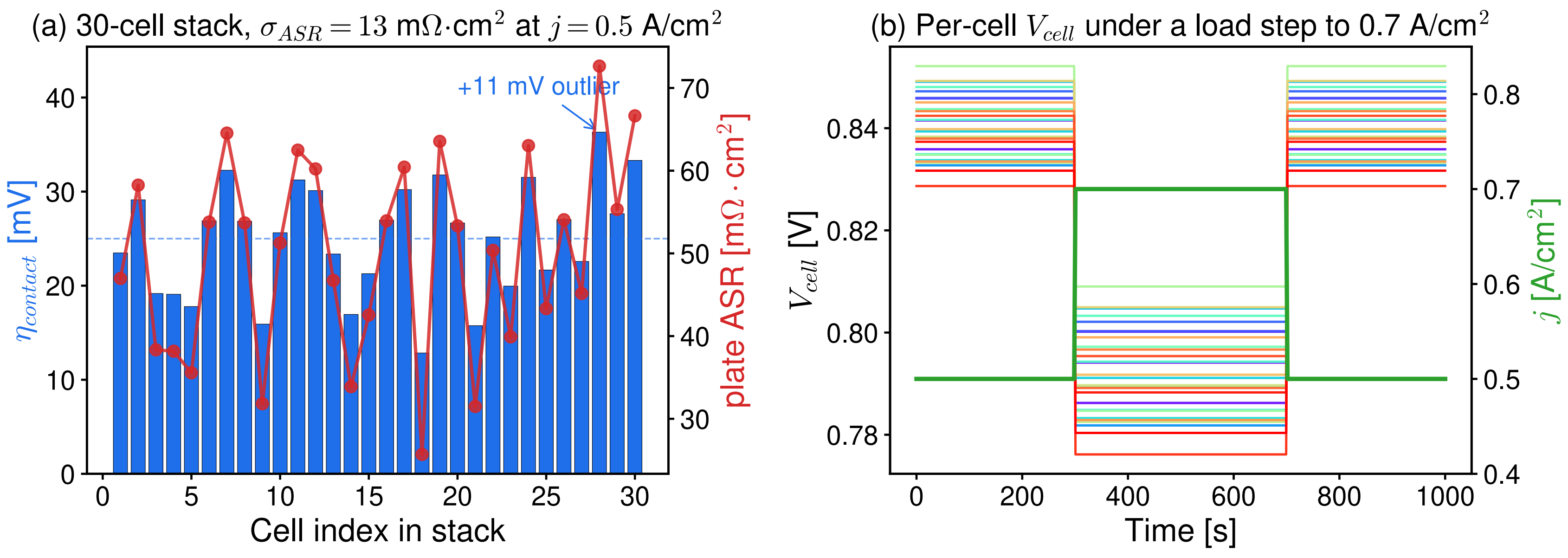

Fig. 5 — Per-cell overpotential + plate ASR; voltage under a load step.

Conclusions

One end-to-end chain from QC to per-cell voltage: 8/12 steady-state I–V within 50 mV (four named xfails) + dynamic load-step response reproduced. Full per-cell solve is real-time to **~16 cells** on a laptop (Fig. 4); the representative-cell + exact ASR mapping extends per-cell resolution to the full 129-cell stack.

Contact

Key refs: Hafsi et al., Int. J. Hydrogen Energy 95 (2024) 1126; Xu & Froment, AIChE J. 35 (1989) 88; Holm, Electric Contacts (1967); Klein, MSc thesis, TU Liberec (2026); Zaccaria et al., J. Power Sources 311 (2016) 175.

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