

Physics-informed neural networks for drift–diffusion simulation of silicon solar cells: a current-based formulation and a comparison with finite volumes

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1. Introduction

Drift–diffusion simulation with the Scharfetter–Gummel discretization [3] is the standard tool for solar-cell analysis. Physics-informed neural networks (PINNs) [1] offer a mesh-free alternative, in which a neural network is trained to minimize the residual of the governing equations, and they have recently been applied to p–n junctions and generic semiconductor devices [6, 7].

To our knowledge, no PINN has yet computed the current–voltage (J–V) characteristic of an illuminated solar cell, nor has one been compared on equal terms with a classical solver. This matters because 79% of studies reporting that machine learning outperforms a numerical method compare against a weak baseline [5].

2. Objectives

1. To determine what is required for a PINN to reproduce the J–V characteristic of a crystalline-silicon solar cell.
2. To assess, accounting for the total computational cost, whether a PINN is preferable to a finite-volume solver or to a data-driven surrogate in forward and parametric studies.

3. Physical model and reference

We consider a one-dimensional n⁺–p silicon cell of thickness 180 μm, with a Gaussian emitter (N_D = 10¹⁹ cm^{−3}, x_j = 0.5 μm) and a base with N_A = 10¹⁶ cm^{−3}. The steady-state drift–diffusion equations are

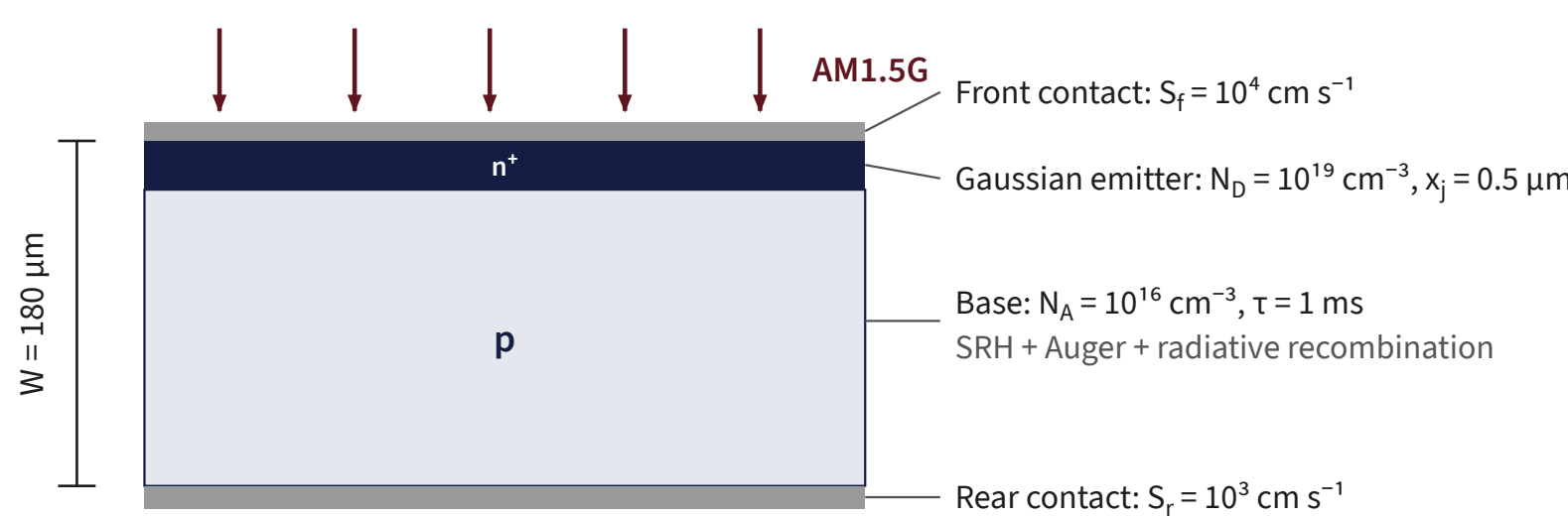


Figure 1. One-dimensional n⁺–p silicon cell studied (not to scale).

$$\begin{aligned} \varepsilon \psi'' &= -q(p - n + N), & (1) \\ J'_n &= q(U - G), & J'_p &= -q(U - G), & (2) \\ J_n &= -q\mu_n n \varphi'_n, & J_p &= -q\mu_p p \varphi'_p, & (3) \end{aligned}$$

with SRH ($\tau = 1$ ms), Auger and radiative recombination, Caughey–Thomas mobility, AM1.5G Beer–Lambert generation and surface recombination velocities $S_F = 10^4$ and $S_R = 10^3$ cm s^{−1}. The reference solution is computed with DEVSIM [2], a finite-volume code with Scharfetter–Gummel fluxes, on a 1077-node mesh.

Table 1. DEVSIM reference cell under AM1.5G and its verification.

Quantity	Value
J _{sc}	38.01 mA cm ^{−2}
V _{oc}	630.5 mV
Fill factor, FF	83.30%
Efficiency, η	19.96%
Max. deviation from Hovel's solution (12 cases)	0.091%
Discretization error in J _{sc} (2nd-order convergence)	0.007%

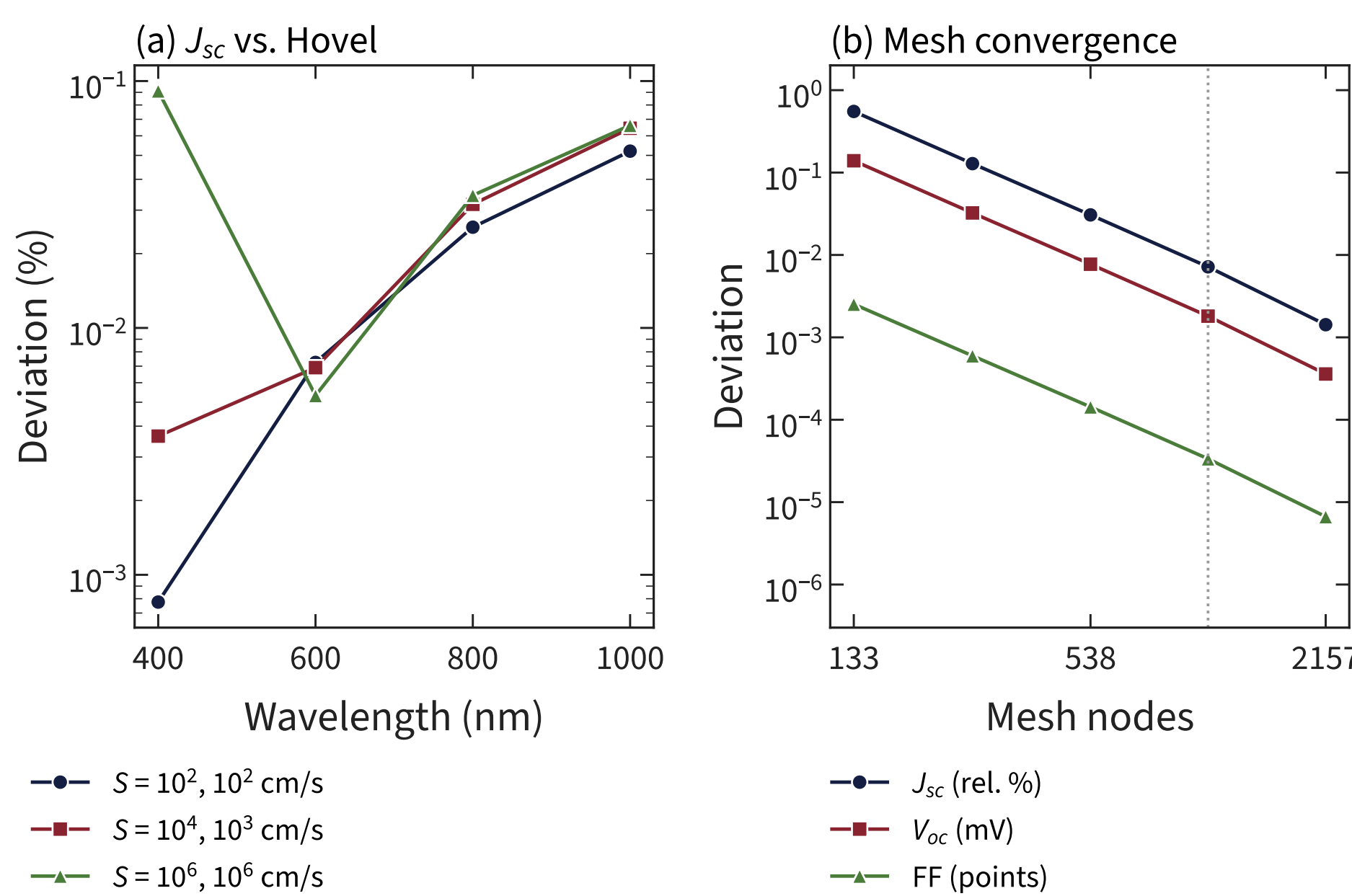


Figure 2. Verification of the DEVSIM reference. (a) Short-circuit current against Hovel's analytical solution under monochromatic light. (b) Second-order mesh convergence; the dotted line marks the 1077-node mesh used.

4. PINN formulation

4.1 Failure of the conventional formulation

The usual PINN outputs ψ , Φ_n and Φ_p and obtains the currents from Eq. (3). In the emitter, where $n \approx 10^{19}$ cm^{−3}, a current of 30 mA cm^{−2} requires

$$|\varphi'_n| = \frac{J}{q\mu_n n} \approx 2 \times 10^{-4} \text{ V cm}^{-1}, \quad (4)$$

that is, about 3×10^{-8} in scaled units. No trained network approached this flatness, and the resulting currents were about 10^8 times too large.

4.2 Current-based integral formulation

The network outputs the potential $u = \psi/V_t$ and the electron current. The Slotboom variables $\Phi_n = e^{-\Phi_n/V_t}$, $\Phi_p = e^{\Phi_p/V_t}$ satisfy

$$\Phi'_n = \frac{J_n e^{-u}}{q\mu_n V_t n_i}, \quad \Phi'_p = -\frac{J_p e^u}{q\mu_p V_t n_i}, \quad (5)$$

which are integrated with exponential fitting (u linear in each interval), as in the Scharfetter–Gummel scheme. In addition:

- the hole current is $J_p = J_{\text{tot}}(V) - J_n$, so that the total current is conserved by construction;
- $J_{\text{tot}}(V)$ and an additive constant in J_n are fixed in closed form by the ohmic or Robin contact conditions;
- the loss is $\mathcal{L} = 100\langle r_p^2 \rangle + \langle r_n^2 \rangle + w_g \langle r_g^2 \rangle$, minimized with Adam followed by L-BFGS.

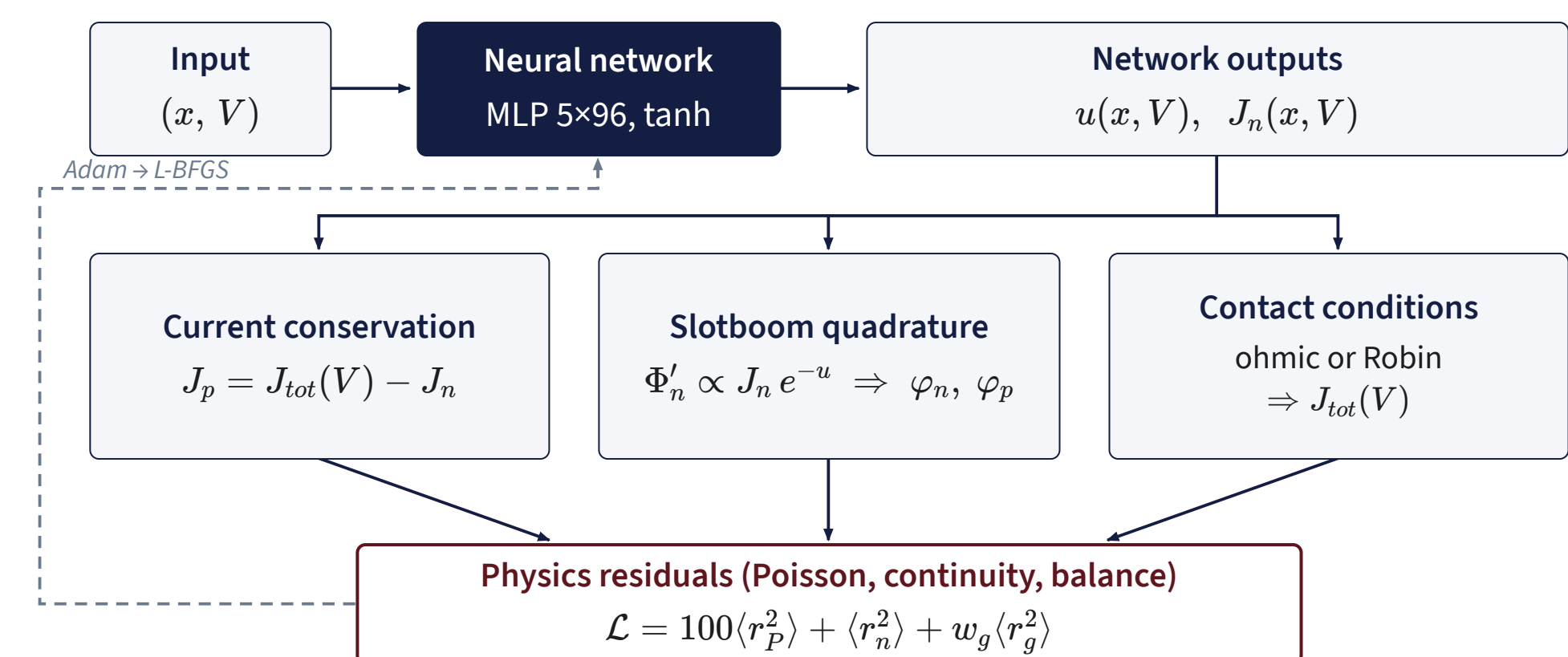


Figure 3. Current-based formulation. The quasi-Fermi levels are not network outputs but are reconstructed from the predicted current, so that the majority-carrier problem of Eq. (4) does not arise.

Table 2. Ablation of the formulation (short runs): relative error in J (dark) or η (light).

Formulation	Error	Cause
Pointwise, outputs ψ , Φ_n , Φ_p	$\sim 10^8 \times$	majority-carrier gradient
Integral, bounded ψ	$\times 0.34$	saturated tanh
Integral, quasi-neutral ψ	29%	loss imbalance
... + Poisson weight $\times 100$	3.1%	—
Light, independent J_n , J_p	η : $\sim 15\%$	$J_n + J_p$ not constant
Light, conserved current	η : $\sim 0.34\%$	—

5. Results

5.1 Equilibrium

A logarithmic mapping with a normalized residual reduces the potential error from 764 mV to 0.044 mV (Fig. 4). Variant D reached a low loss (6×10^{-4}) with an error of 0.9 V: a low loss did not imply a correct solution.

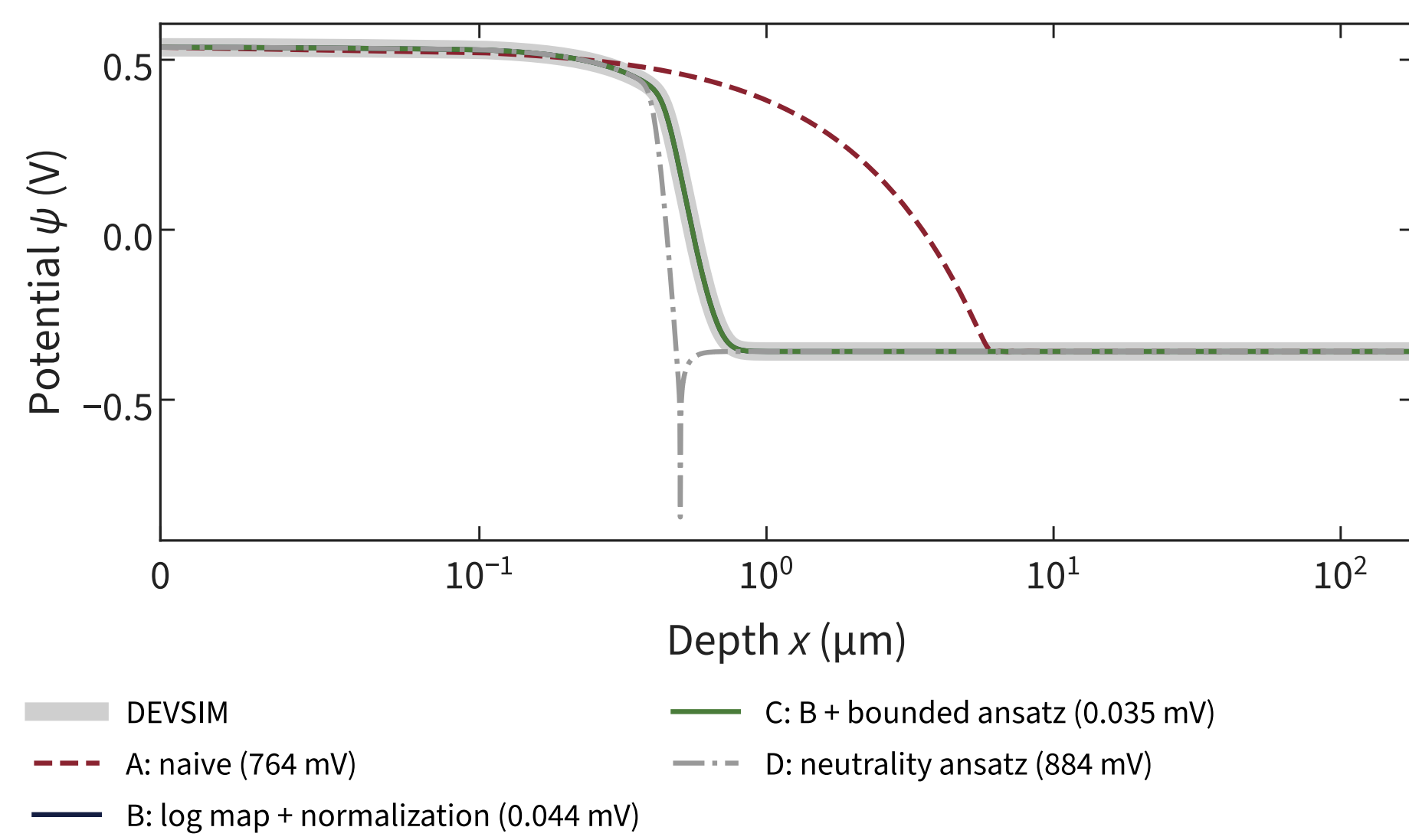


Figure 4. Equilibrium potential of four PINN variants and DEVSIM. In brackets, median over three seeds of the maximum error.

5.2 Illuminated cell, ohmic contacts

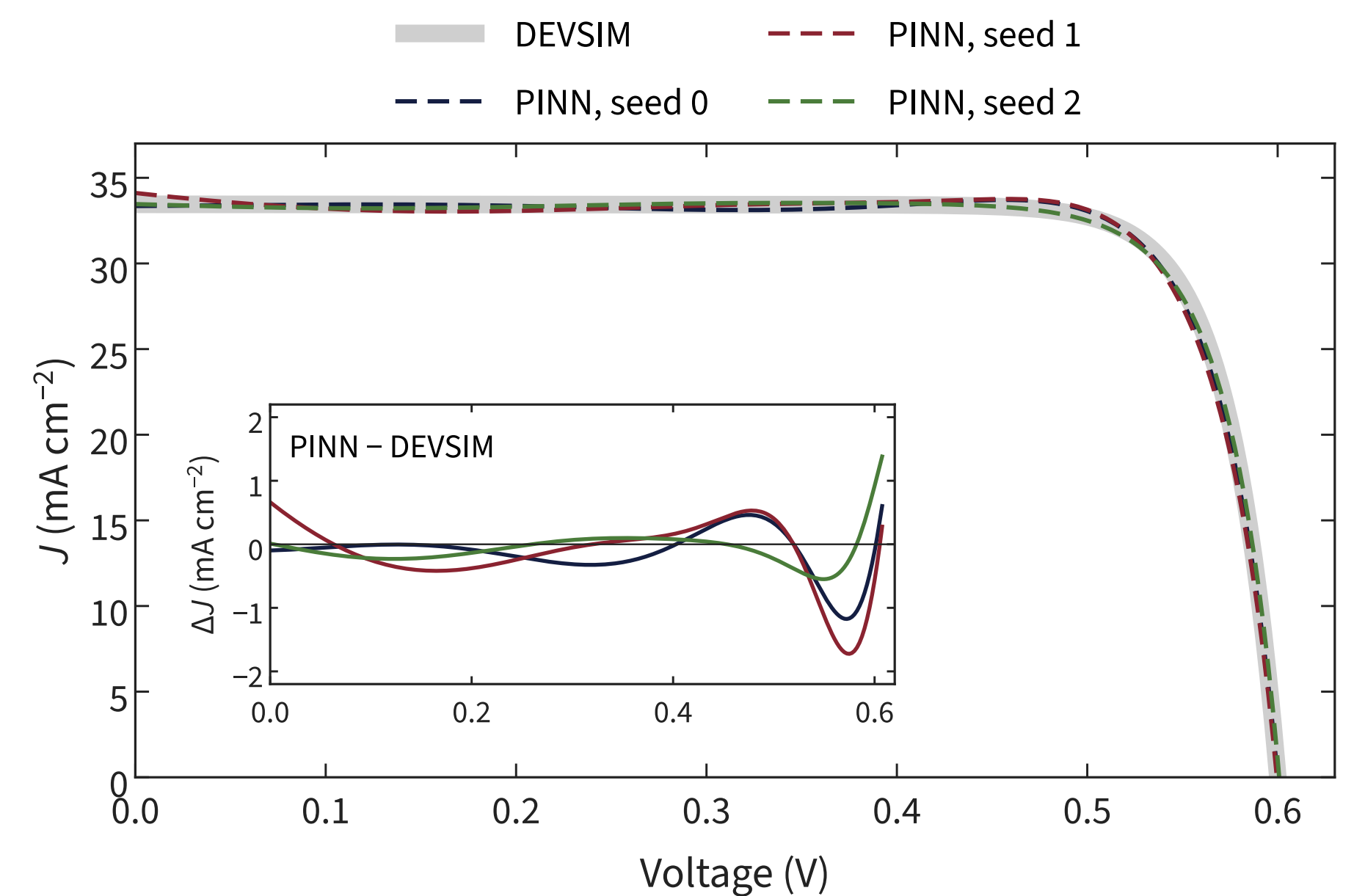


Figure 5. J–V characteristic under AM1.5G: DEVSIM and the PINN for three seeds. Inset: difference PINN – DEVSIM.

Table 3. Figures of merit, PINN relative to DEVSIM.

	DEVSIM	Seed 0	Seed 1	Seed 2	Median
J _{sc} (mA cm ^{−2})	33.452	−0.29%	+1.98%	+0.03%	+0.03%
V _{oc} (mV)	600.09	−0.08	−0.49	+0.72	−0.08
FF (%)	82.67	+0.41	−1.29	−1.11	−1.11
η (%)	16.589	+0.19%	+0.30%	−1.18%	+0.19%

5.3 Finite surface recombination

With Robin contacts the terminal current depends on the integral of the continuity residual. A global current-balance term reduced the efficiency error to $\sim 1.2\%$ (V_{oc} : ~ 0.2 mV), but increased the potential error in the junction from 10 to 64 mV (Fig. 6).

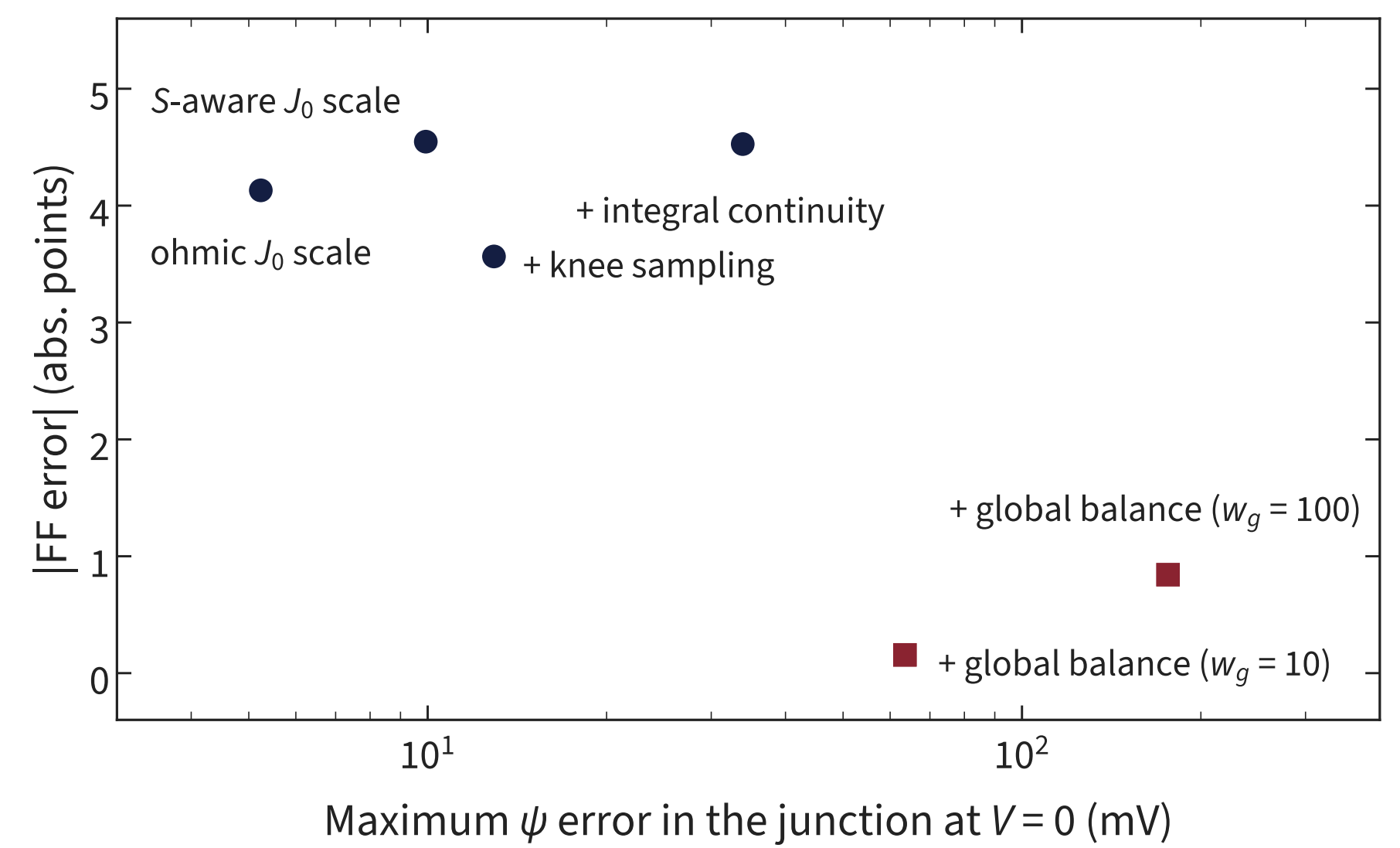


Figure 6. Trade-off between terminal accuracy (FF) and internal accuracy (ψ in the junction) for the design variants studied.

5.4 Computational cost and accuracy

All methods were run on the same computer and evaluated on test cells not used for fitting. The cost is the total wall-clock time: training for the PINN, and DEVSIM runs plus fitting for the surrogates. With two parameters, a spline fitted to 8×8 DEVSIM runs reached 0.007% in 9.4 min, against 1.5% for the PINN after 64 min. With five parameters, a neural network fitted to 64 DEVSIM runs reached 0.17% in about 2 min, against 4.1% for the PINN after 103 min.

6. Conclusions

1. A PINN reproduces the J–V characteristic of an illuminated silicon cell with an efficiency error of 0.19% (ohmic contacts) and 1.2% (finite surface recombination), provided the conventional formulation is abandoned.
2. The current must be a network output, the quasi-Fermi levels must be obtained from an exponentially fitted integral, and current conservation and contact conditions must be imposed by construction.
3. With the total cost taken into account, the PINN was not advantageous in the forward problem or in the studies with two and five parameters.
4. Inverse problems, two- and three-dimensional devices and long transients remain open settings for PINNs.

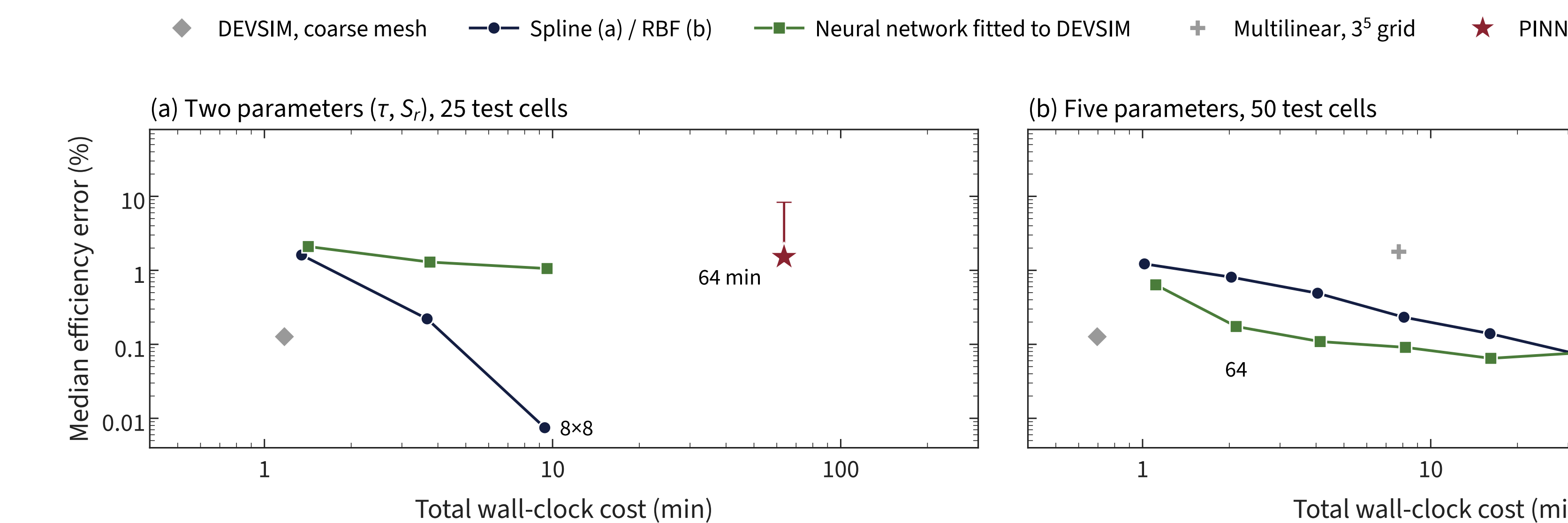


Figure 7. Median efficiency error against total cost with (a) two and (b) five varied parameters. Whiskers on the PINN show the maximum error (clipped at 50%). Lines join surrogates fitted to an increasing number of DEVSIM runs.