Supplementary Information for

Knowledge extraction and transfer in data-driven fracture mechanics

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ML solution to the 2D cantilever problem

1. Problem description

As shown in Fig. S1, a 2D notched cantilever, whose dimensions are $\{a, H, L_0, L_1\}$, is loaded at its free end by a line force, p. It is desired to determine the stress intensity factor at the crack, K_I, for a given p. This linear elastic fracture mechanics problem involves four independent dimensionless variables, *i.e.*,

$$\begin{cases} \underline{x}^{2\mathrm{D}} = (x_1, x_2, x_3) = \left(\frac{a}{H}, \frac{L_0}{H}, \frac{L_1}{H}\right) \\ y^{2\mathrm{D}} = \frac{K_I}{P(L_0 + L_1)a^{0.5}(H-a)^{-0.5}H^{-1.5}w^{-1}} \end{cases} . \tag{S1}$$

The ML solution, Γ_{2D}, should provide an accurate output of $y^{2\mathrm{D}}$ for an arbitrary input, $\underline{x}^{2\mathrm{D}}$, in a predefined parameter space, $\Lambda_{2\mathrm{D}} = [0.04, 0.8] \times [0.04, 0.4] \times [0.8, 5.0]$.

2. Data acquisition

The development of the ML solution is entirely data-driven. To provide a broad scope of the correlation between $y^{2\mathrm{D}}$ and $\underline{x}^{2\mathrm{D}}$, 2,541 training data points are selected from a uniform grid across the entire parameter space, $\Lambda_{2\mathrm{D}}$, with each input domain being discretized into $(20, 10, 10)$ intervals. The target value of $y^{2\mathrm{D}}$ at each point is acquired from two-dimensional finite element simulations in ABAQUS (1), as shown in Fig. S2. Domain *J*-integral (2–4) is used to evaluate the stress intensity factor, K_I, at the crack tip. An *encastré* boundary condition is applied to the fixed end of the cantilever and a displacement-controlled boundary condition to the free end. More than 5,000 elements (CPE8) are employed with refined mesh near the crack tip.

To collect sufficient data for model assessment, a series of datasets are built by refining the interval of the sampling grid, *i.e.*, $\left\{\chi_{2\mathrm{D}}^{(0)}, \chi_{2\mathrm{D}}^{(1)}, \chi_{2\mathrm{D}}^{(2)}, \ldots\right\}$. $\chi_{2\mathrm{D}}^{(0)}$ corresponds to a uniform grid with $(20, 10, 10)$ intervals in each dimension, and $\chi_{2\mathrm{D}}^{(n)}$ corresponds to the grid a $(20, 10, 10) \times 2^n$ intervals.

3. Model training

A simple fully connected NN ("3/64/64/1" with the "ReLU" activation function) is selected for this problem. The training of NNs is performed on the open-source platform TensorFlow r2.2 (5), with the "mean absolute percentage error" loss function and the Nadam algorithm. A two-step strategy is adopted, *i.e.*, 10,000 training iterations with a learning rate of 0.01 followed by another 10,000 iterations with a learning rate of 0.001. In this way, the trained NNs make accurate predictions on the training dataset. However, its performance outside the training data points is yet to be investigated.

4. Model assessment

To correctly assess the accuracy of the trained model, its performance is tested on a series of assessment datasets, *i.e.*, $\left\{\chi_{2\mathrm{D}}^{(0)}, \chi_{2\mathrm{D}}^{(1)}, \chi_{2\mathrm{D}}^{(2)}, \ldots\right\}$. Most of the trained models can be correctly assessed with $\chi_{2\mathrm{D}}^{(2)}$, *i.e.*, a convergent value of model accuracy is observed with 136,161 data points. Among these well-assessed models, one can choose the appropriate model as the ML solution according to their accuracy. Consequently, with 2,541 training data and 136,161 assessment data, a ML solution with less than 3.21% prediction error can be obtained.

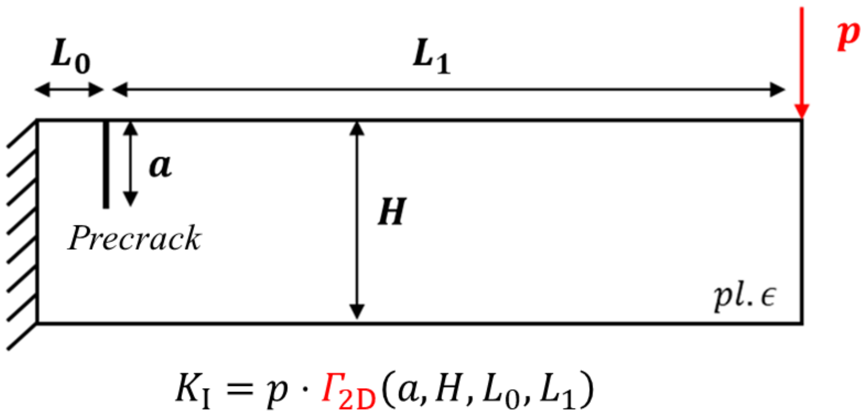

Fig. S1. ML solution to the 2D notched cantilever problem. A 2D notched cantilever, whose dimensions are $\{a, H, L_0, L_1\}$, is loaded at one end by a line force, p. The solution to this problem, Γ_{2D}, describes the stress intensity factor at the crack, K_I, for a given p.

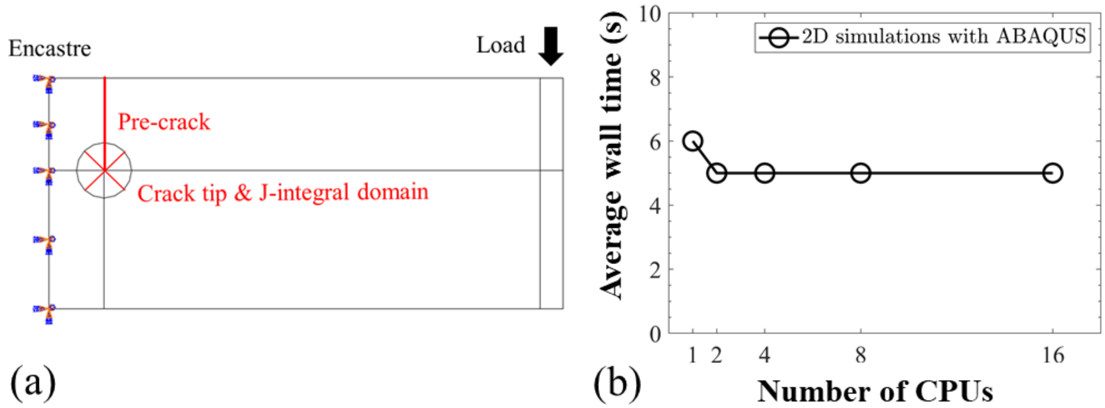

Fig. S2. Data acquisition from FEM simulations. (*a*) The domain J-integral method is used to evaluate the intensity factor at the crack tip. An *encastré* boundary condition is applied to the fixed end of the cantilever and a displacement-controlled boundary condition to the free end. (*b*) The computational cost of the two-dimensional simulation is low, and parallel computing cannot further reduce the time. The average wall time for each simulation is ~6 seconds when running on a single CPU with ABAQUS.

SI References

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