Statistical Physics of Design: Supplementary Materials

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S1. SUPPLEMENTARY METHODS

A. Evaluation of Outcomes and Variability

The importance of the partition function $\mathcal{Z}$ is in that it contains all information about statistical averages of design objectives. The average outcome for a design objective is given by

$$\langle \mathcal{O}_i \rangle = \sum_\sigma \mathcal{O}_i(\sigma) p_\sigma = \frac{1}{\mathcal{Z}} \sum_\sigma \mathcal{O}_i(\sigma) e^{-\sum_j \lambda_j \mathcal{O}_j(\sigma)} \tag{S1}$$

$$= -\frac{\partial}{\partial \lambda_i} \ln \mathcal{Z} \ . \tag{S2}$$

The variability in an outcome can be evaluated by further differentiation

$$\left\langle \mathcal{O}_i^2 \right\rangle_c = \left\langle \mathcal{O}_i^2 \right\rangle - \left\langle \mathcal{O}_i^2 \right\rangle = \left(-\frac{\partial}{\partial \lambda_i} \right)^2 \ln \mathcal{Z} \ . \tag{S3}$$

The variability in an outcome is directly related to the sensitivity of the design objective average to design pressures:

$$\left\langle \mathcal{O}_i^2 \right\rangle_c = -\frac{\partial}{\partial \lambda_i} \left\langle \mathcal{O}_i \right\rangle \ . \tag{S4}$$

B. Case 1: Computation Details

Two units at separated by distances $\Delta x, \Delta y$ along the two axes can be joined with multiple routings of the same Manhattan length $\Delta x + \Delta y$. Since the routing consists of a fixed number of vertical and horizontal steps which can be taken in any order, the number of possible routings is given by the binomial coefficient

$$n(\Delta x, \Delta y) = \binom{\Delta x + \Delta y}{\Delta x} = \frac{(\Delta x + \Delta y)!}{\Delta x! \Delta y!} \ . \tag{S5}$$

The number of paths $n(\Delta x, \Delta y)$ grows rapidly with path length, thus creating the entropic stress pushing the units apart. The partition function (Eq. 2 in main text) is a sum over all candidate designs. We separate that sum into summing over possible unit positions and possible paths. For two units this becomes

$$\mathcal{Z} = \sum_\sigma e^{-E_\sigma/T} = \sum_{x_1, y_1, x_2, y_2} e^{-E_\sigma/T} n_\sigma(\Delta x, \Delta y) \ . \tag{S6}$$

To understand the origin of T_{crit} more intuitively, we can use an approximation. If we assume large separations $\Delta x \sim \Delta y \ll 1$, Stirling's approximation for the binomial coefficient gives

$$\ln n(x,y) \approx x \ln\left(1 + \frac{y}{x}\right) + y \ln\left(1 + \frac{x}{y}\right) \approx (x+y) \ln 2 \tag{S7}$$

Substituting this into the partition function gives

$$\mathcal{Z} = \sum_{x_1, y_1} \sum_{\Delta x, \Delta y} \exp\left(\left(\ln 2 - \frac{C}{T} \right) (\Delta x + \Delta y) \right) , \tag{S8}$$

where the unit separation $\Delta x, \Delta y \in [0, L]$. Because the contributions that correspond to energy and entropy have the same form, depending on the sign of $(\ln 2 - C/T)$, this is either a descending or ascending finite geometric series. In either case it evaluates to a finite value that changes rapidly near $T = T_{\mathsf{crit}} = \frac{C}{\ln 2}$. The average cost and the cost variance/susceptibility are evaluated with straightforward derivatives with respect to $\lambda_1 = 1/T$.

C. Case 2: Computation Details

We consider two types of routings between the two units: through the bulkhead and around the bulkhead. Since they are mutually exclusive, the partition function can be computed as

$$\mathcal{Z} = \mathcal{Z}_{\mathsf{t}} e^{-\gamma} + \mathcal{Z}_{\mathsf{r}} \ , \tag{S9}$$

with the two component partition functions being

$$\mathcal{Z}_t = \sum_{\sigma \ \mathsf{through}} \exp(-E(\sigma)/T) \tag{S10}$$

$$\mathcal{Z}_r = \sum_{\sigma \ \mathsf{around}} \exp(-E(\sigma)/T) \ . \tag{S11}$$

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The fraction of bulkhead penetrations, $\langle B \rangle$, is a design objective conjugate to bulkhead penalty, thus it can be evaluated via a partial derivative

$$\langle B \rangle = -\frac{\partial}{\partial \gamma} \ln \mathcal{Z} = \frac{Z_t e^{-\gamma}}{Z_t e^{-\gamma} + Z_r} \ . \tag{S12}$$

Free energy landscapes $F(x, y)$ are computed via Eq. 8 of main text with the "design feature" $S(x, y)$ evaluated as follows, respectively for unit and routing free energies:

$$S_{\textsf{unit}}(x, y) = \begin{cases} 1, & \text{there is a unit at } (x, y) \\ 0, & \text{otherwise} \end{cases} \tag{S13}$$

$$S_{\textsf{route}}(x, y) = \begin{cases} 1, & \text{there is a routing through } (x, y) \\ 0, & \text{otherwise} \end{cases} \tag{S14}$$

The vertical node correlation is defined the usual way with averages taken in the sense of Eq. 7 of main text:

$$cor(y_1, y_2) = \frac{\langle y_1 y_2 \rangle_c}{\sqrt{\langle y_1^2 \rangle_c \langle y_2^2 \rangle_c}} \tag{S15}$$

S2. SUPPLEMENTARY RESULTS

For the inhomogeneous embedding (Case 2) unit positions explicitly couple to the geometric features of the embedding space, as shown in Fig. 4 (main text) for a system size of 20×20. SI Figs. S1, S2, and S3 show identical computations performed for a series of other system sizes. Fig. S1 depicts a system size of 20×40. Fig. S2 depicts a system size of 40×12. Fig. S3 depicts a system size of 20×20, with the bulkhead off-center.

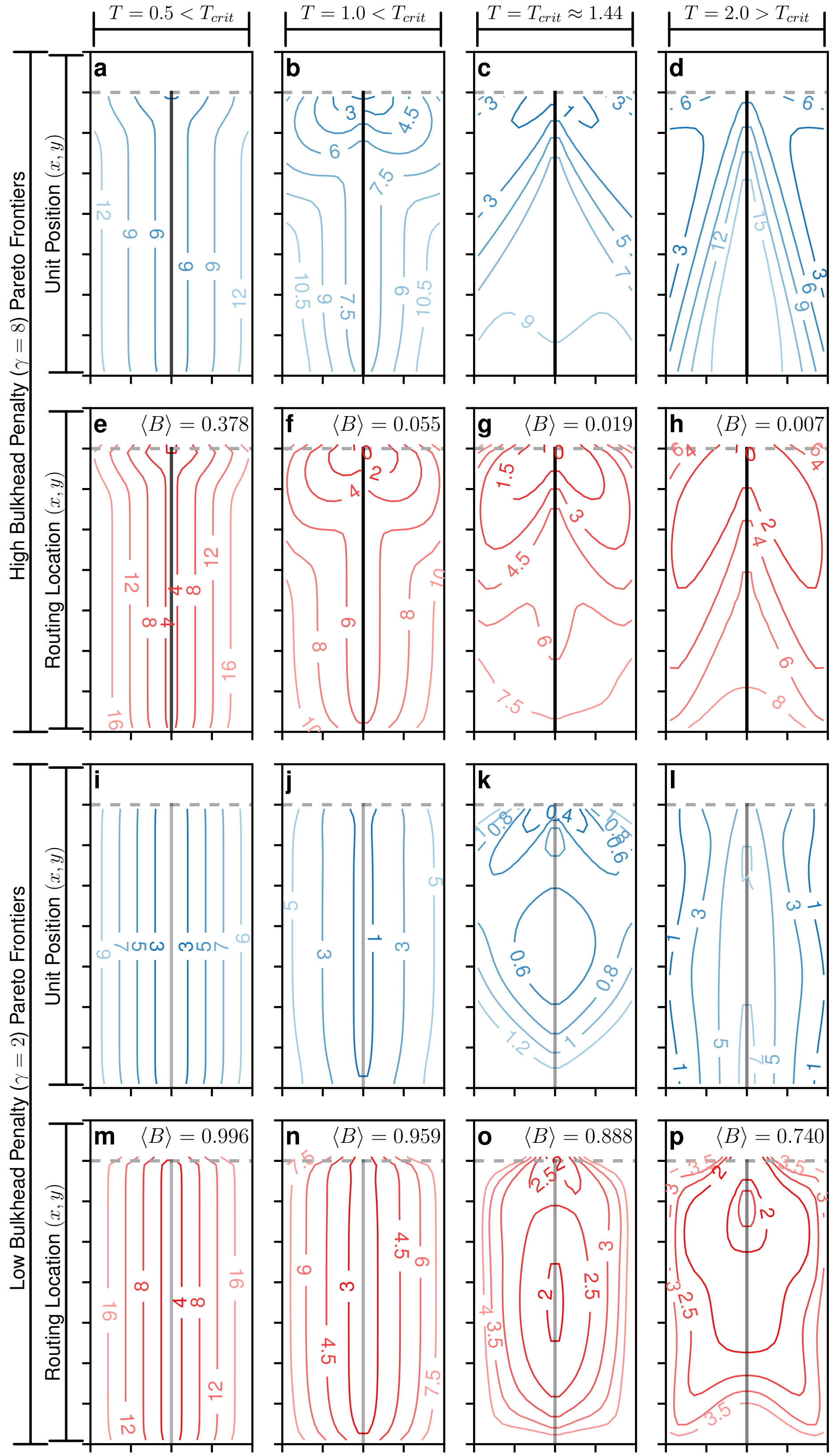

FIG. S1. Pareto frontiers (Landau free energy isosurfaces) for unit and routing locations for spatially inhomogeneous subsystem embeddings (Case 2). System size is 20×40 (width and height), bulkhead is positioned horizontally in the center and extends up to height $h = 35$. Normalization for free energies is identical to that of Fig. 4 of main text. Organization of rows and columns of (T, γ) parameters is also identical to that of Fig. 4 of main text.

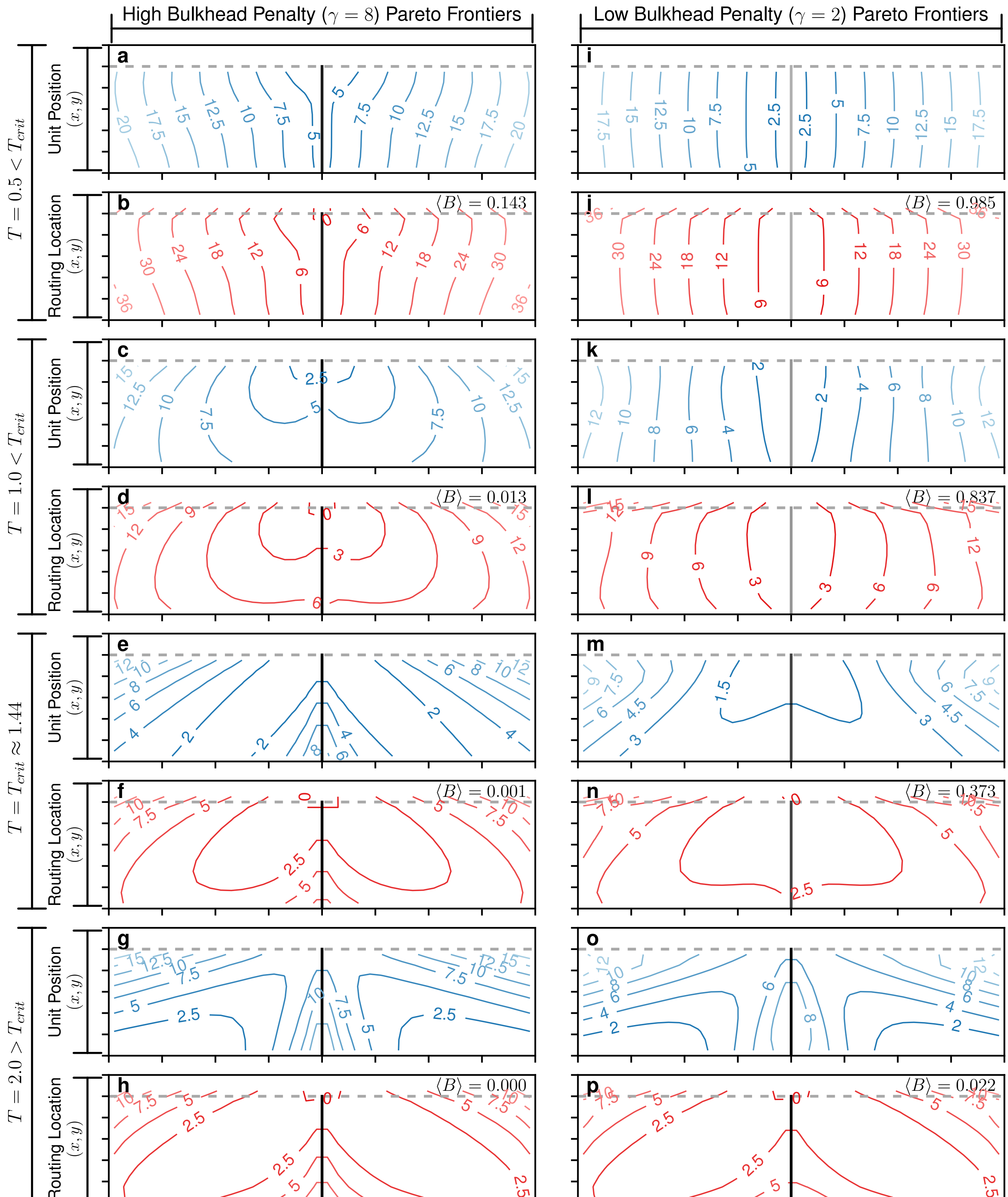

FIG. S2. Pareto frontiers (Landau free energy isosurfaces) for unit and routing locations for spatially inhomogeneous subsystem embeddings (Case 2). System size is 40×12 (width and height), bulkhead is positioned horizontally in the center and extends up to height $h = 10$. Normalization for free energies is identical to that of Fig. 4 of main text. First column corresponds to $\gamma = 8$, second to $\gamma = 2$. Four rows of graph pairs correspond to cost tolerances of $T = 0.5, 1.0, T_{\text{crit}}, 2.0$, respectively.

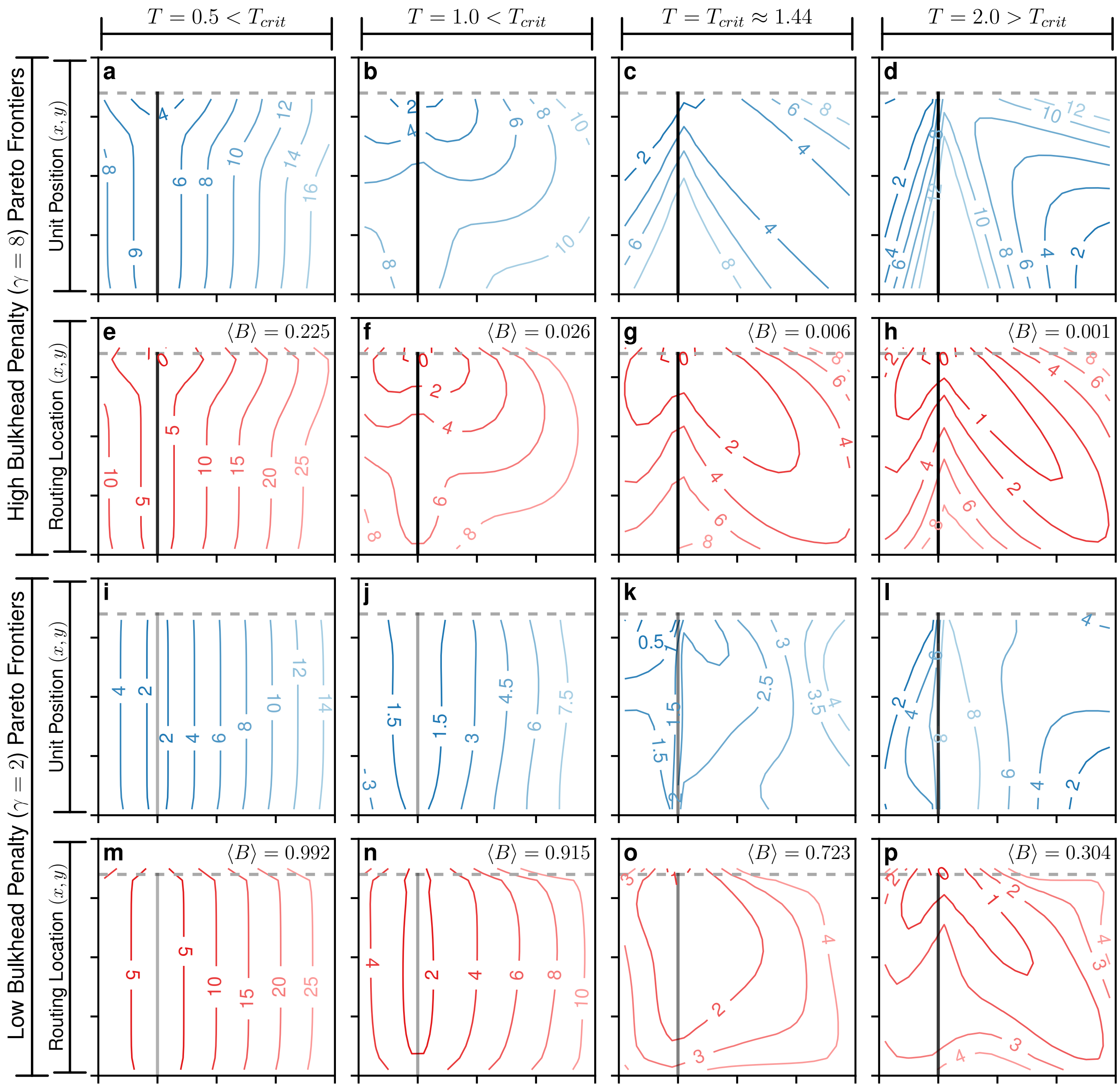

FIG. S3. Pareto frontiers (Landau free energy isosurfaces) for unit and routing locations for spatially inhomogeneous subsystem embeddings (Case 2). System size is identical to that in Fig. 4 of main text at 20×20 (width and height), however bulkhead is positioned horizontally off center at $x_{\mathrm{bh}} = 5$ and extends to the same height $h = 17$ as in Fig. 4 of main text. Normalization for free energies is identical to that of Fig. 4 of main text. Organization of rows and columns of (T, γ) parameters is also identical to that of Fig. 4 of main text.