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Industrial design process as scientific discovery

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Computational Approaches to Scientific Discovery
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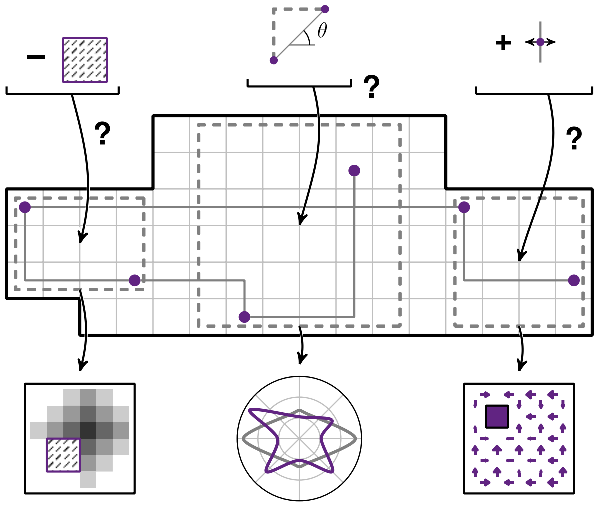

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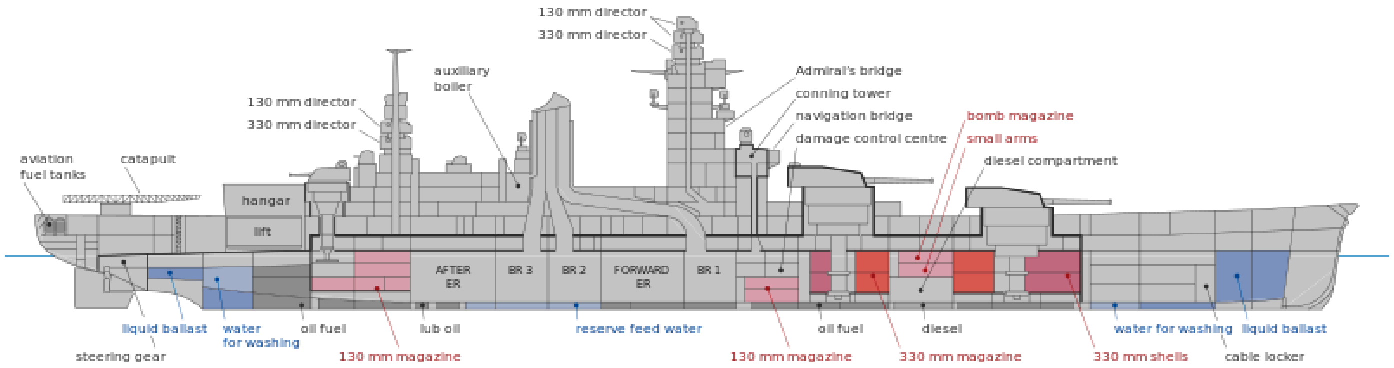
Design problems



Maxrossomachin for Wikipedia

Needs to be as cheap as possible.
Needs to float, even after being shot at.
Needs to support our best current-gen weapons, as well as next-gen and next-next gen.
Have redistributable power.
Have mission flexibility.
And be fixable when it breaks.
And ...
...
...

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Nouns, verbs, questions

- Design (noun): solution or plan for an object or system that fulfils the desired function.
- Design (verb): the process that sometimes somehow results in design (noun).

- What solution should we choose?
- Why is that solution preferable?

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Design as optimization

> The objective function is sometimes called a "cost" function since minimum cost often is taken to characterize the "best" design.

Principles of optimal design: modeling and computation,
PY Papalambros and DJ Wilde.
Cambridge University Press, 2000.

$$f(\alpha) = \sum_m \lambda_m \mathcal{O}_m(\alpha) \xrightarrow{\text{Optimization}} \alpha^* = \arg\min_\alpha f(\alpha)$$

Why would I want to take a *sub*optimal solution?

How do solutions change with choice of λ_m?
How many solutions of same cost are there?

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Design is not optimization: Wicked Problems

- Never completely defined
- Many stakeholders
- Can't tell when solved
- Can't have a prototype

CW Churchman, *Management Science* (1967)
HW Rittel and MM Webber, *Policy Sciences* (1973)
DJ Andrews, *Proc. Roy. Soc. A* (2012)
R Farrell and C Hooker, *Design studies* (2013)

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Operational definition of design

~ computation ~ information

Design is the act of generating knowledge
for decision-making through time.

~ ??? ~ non-equilibrium

CPF Shields, PhD Thesis, *University of Michigan* (2017)

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Maximal entropy statistical mechanics

How do you make the least informative random choice of design α?

Pick at random with p_α that maximizes Shannon entropy S.

$$S = -\sum_{\alpha} p_\alpha \ln p_\alpha - \sum_m \overbrace{\lambda_m}^{\text{Design pressure } m} \underbrace{\left(\sum_\alpha p_\alpha \overbrace{\mathcal{O}_m(\alpha)}^{\text{Objective } m \text{ in design } \alpha} - \langle \mathcal{O}_m \rangle \right)}_{\text{Design objectives } \langle \mathcal{O}_m \rangle \text{ are reached on average}} \to max$$

Boltzmann distribution in statistical physics:

$$p(\alpha) = \frac{1}{\mathcal{Z}} \exp\left(-\sum_m \lambda_m \mathcal{O}_m(\alpha) \right)$$

Maximum of $p(\alpha)$
is minimum of $f(\alpha) = \sum_m \lambda_m \mathcal{O}_m(\alpha)$

ET Jaynes, *Phys. Rev.* (1957)
AAK, CPF Shields, DJ Singer, G van Anders, *New J. Phys.* (2018)

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Q: Does solution entropy change anything?

How many solutions of cost $f(\alpha)$ are there?
How does entropy affect average solutions?
Is entropy / flexibility a virtue?

Cf. density of states in physics

AAK, CPF Shields, DJ Singer, G van Anders, *New J. Phys.* (2018)

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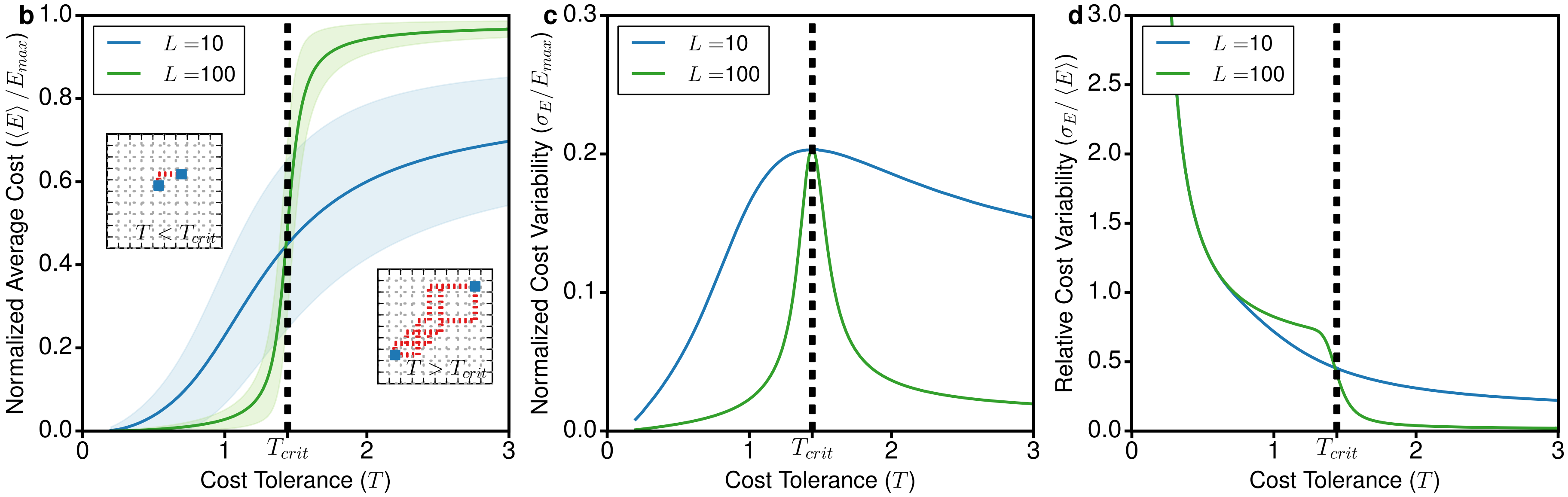
Entropy-driven phase transition



$$E_{max} = 2CL$$

$$T_{crit} = \frac{C}{\ln 2} \approx \boxed{1.44}\, C$$

AAK, CPF Shields, DJ Singer, G van Anders, *New J. Phys.* (2018)

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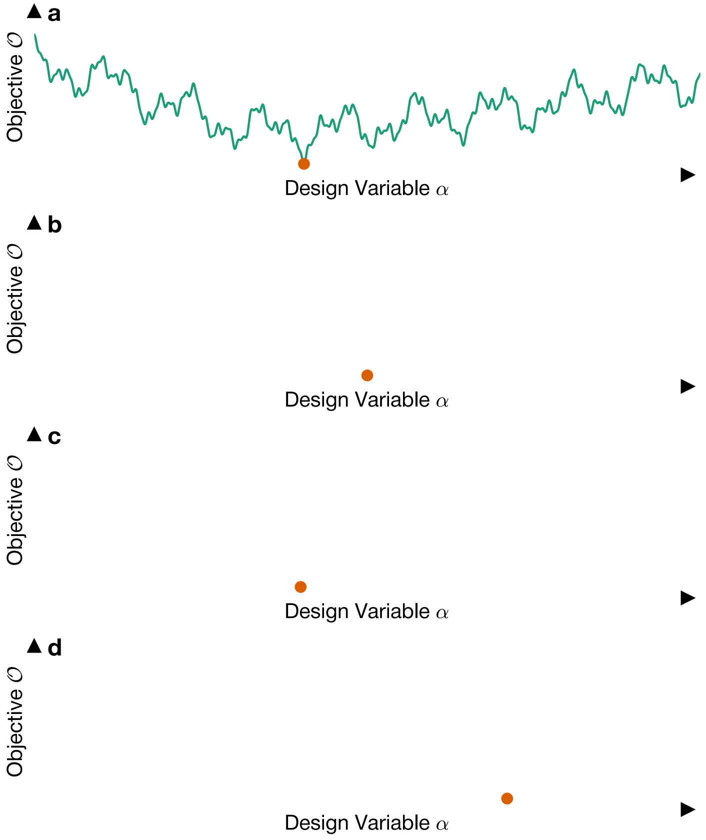
Q: Are solutions robust to problems?

Over-constrained / rough problem
→ hard to find the “best” solution

Under-constrained / flat problem
→ “best” solution is useless



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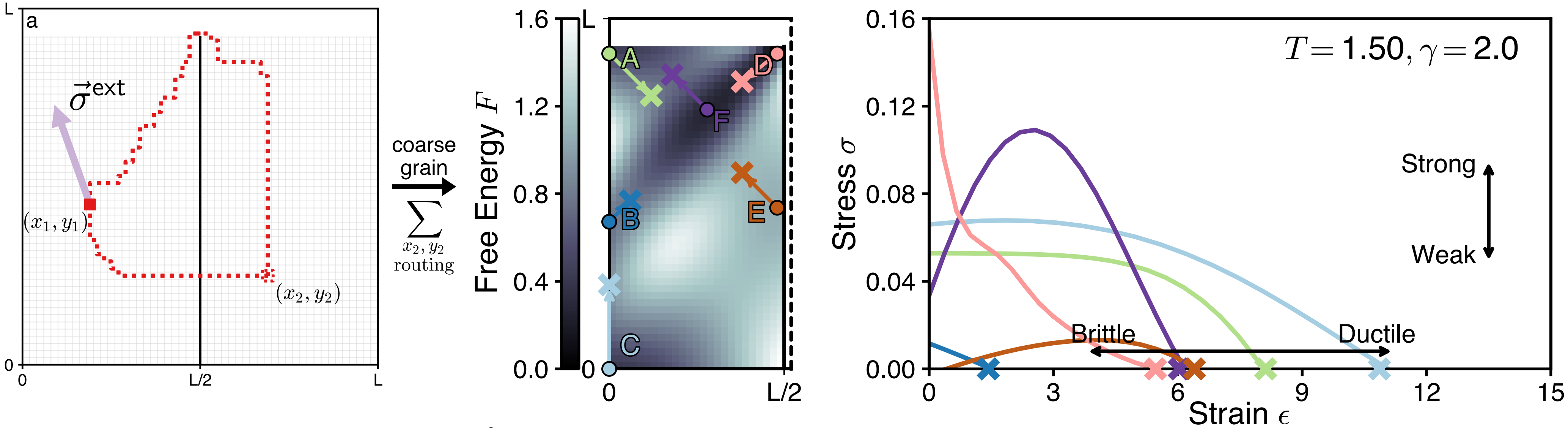
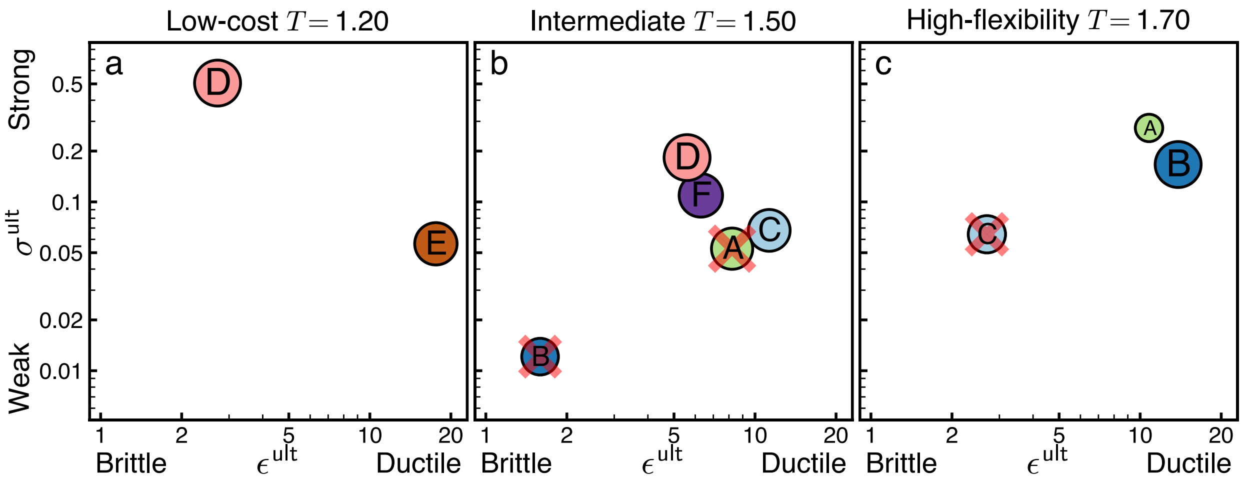
Two-factor robust design





AAK, A Kirkley, DJ Singer, G van Anders, *Sci. Rep.* (2020)

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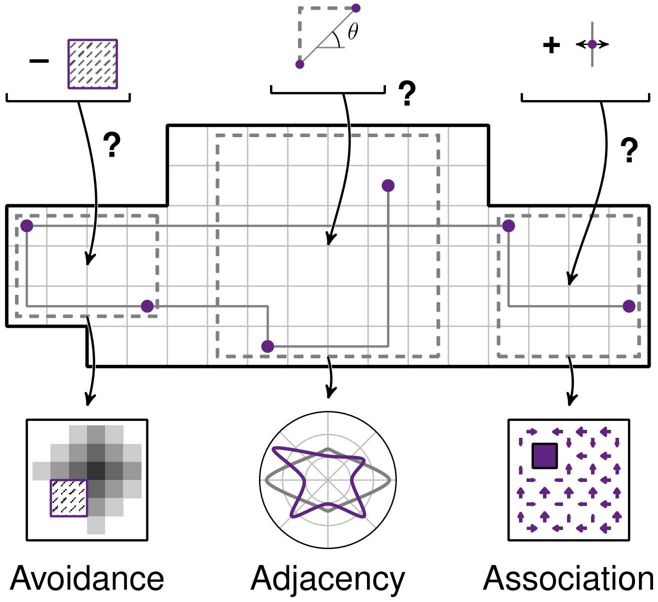
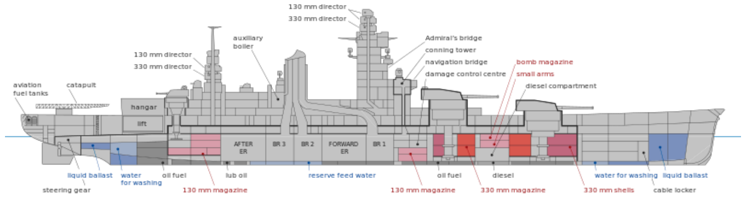
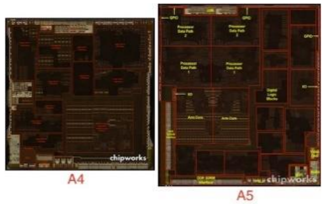
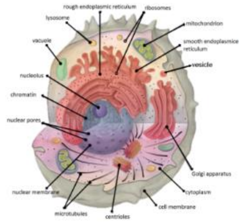
Q: What is the structure of design space?



Avoidance: Where do we pay high space premium?
Adjacency: How does indirect coupling emerge?
Association: How do early design decisions constrain design freedom?







Equipment in a warship?
Transistors on a chip?
Organelles in a cell?

Maxrossomachin for Wikipedia http://techztalk.com/ Koswac for Wikipedia

AAK, DJ Singer, G van Anders, *J. Phys. Complexity* (2021)

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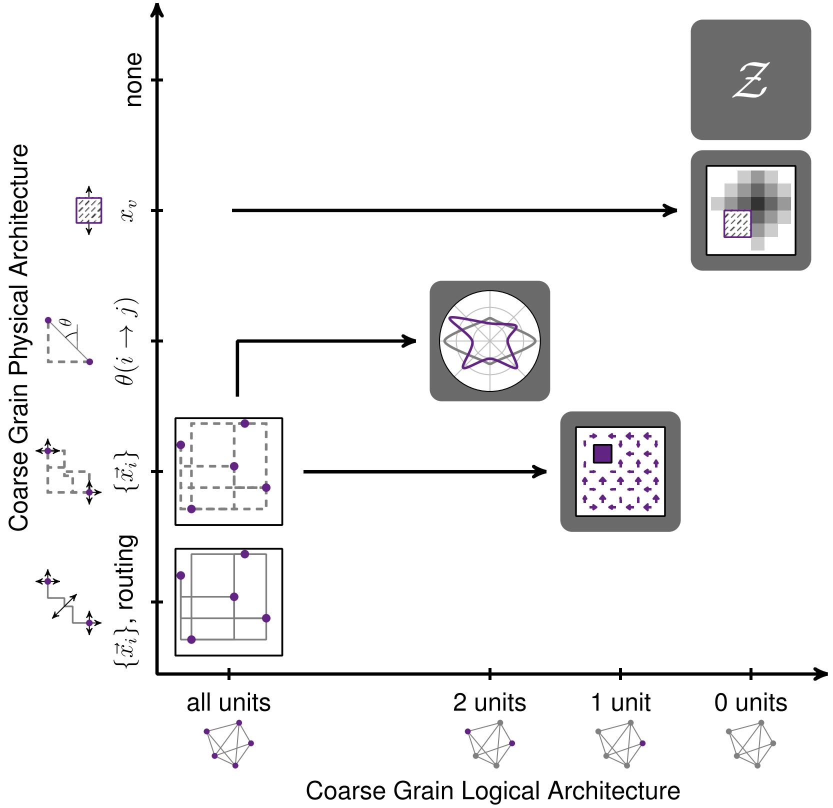
Two directions of coarse graining

- Arrangement patterns span *two dimensions* of architectural detail

- Arrangement patterns ~ physical phenomena:
    - Avoidance ~ symmetry breaking
    - Adjacency ~ emergent correlation
    - Association ~ emergent localization



AAK, DJ Singer, G van Anders, *J. Phys. Complexity* (2021)

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Q: How to make a posteriori value statements?

$\mathcal{O}_m(\alpha)$ is what objective we care about.
λ_m is how much we care about it.

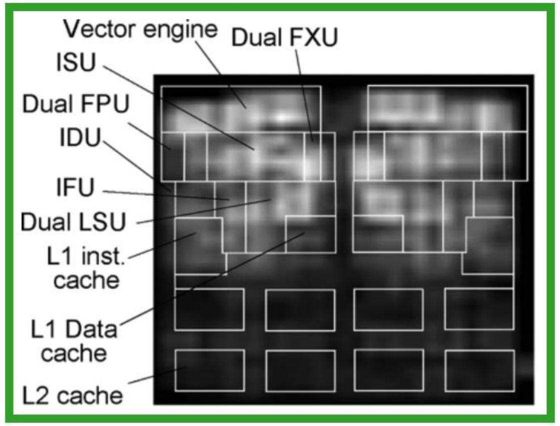
$$\{\lambda_m\} \xrightarrow{\text{Math}} \alpha^*, \{\langle \mathcal{O}_m \rangle\}$$

Choosing λ_m is a value statement.
Do we make an a priori or a posteriori choice?

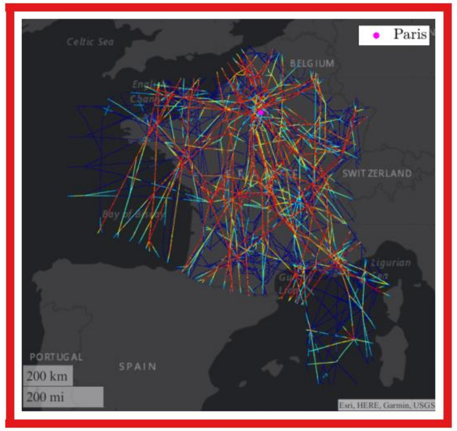
AAK, CPF Shields, DJ Singer, G van Anders, *New J. Phys.* (2018)

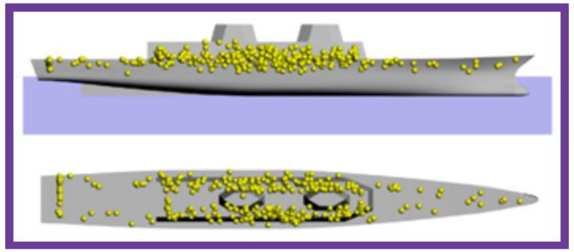
No Free Lunch for clustering vulnerabilities

Hot spots in microprocessors[1]

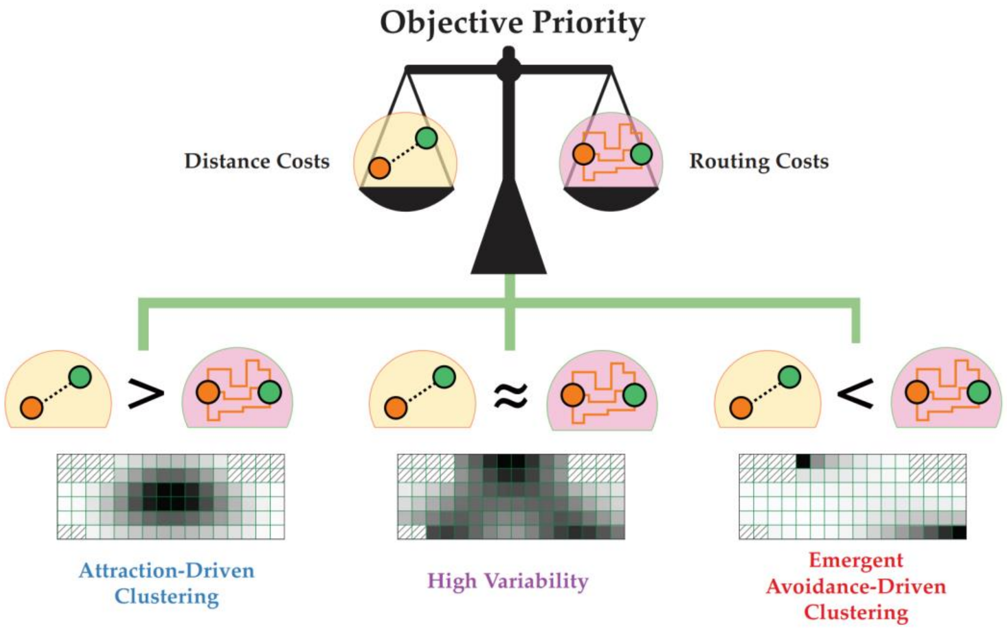


Airline congestion[2]





Weak points in warship design[3]



Slide by P Chitnelawong;
1. HF Hamann et al., *IEEE J. Solid-State Circuits* (2007)
2. J Lavandier et al., *Aerospace* (2021)
3. N Doerry, *Naval Eng. J.* (2007)

P Chitnelawong, **AAK**, et al., *in preparation* (2023)

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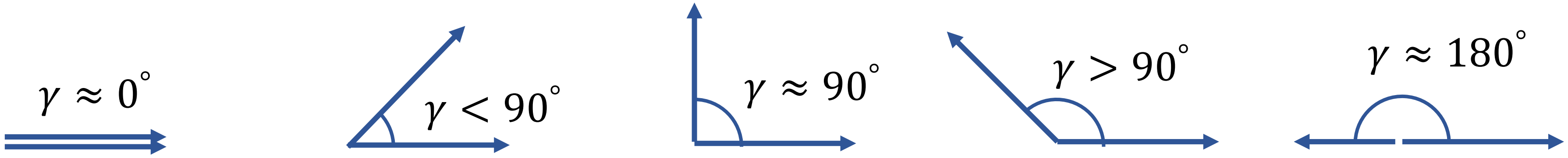
Q: Are the objectives compatible?

Road users in a transit system:

- Walking
- Biking
- Public transit
- Driving

Does helping one objective help another?



Objective angle idea from:
O Braganza, *R. Soc. Open Science* (2022)

aklishin.science

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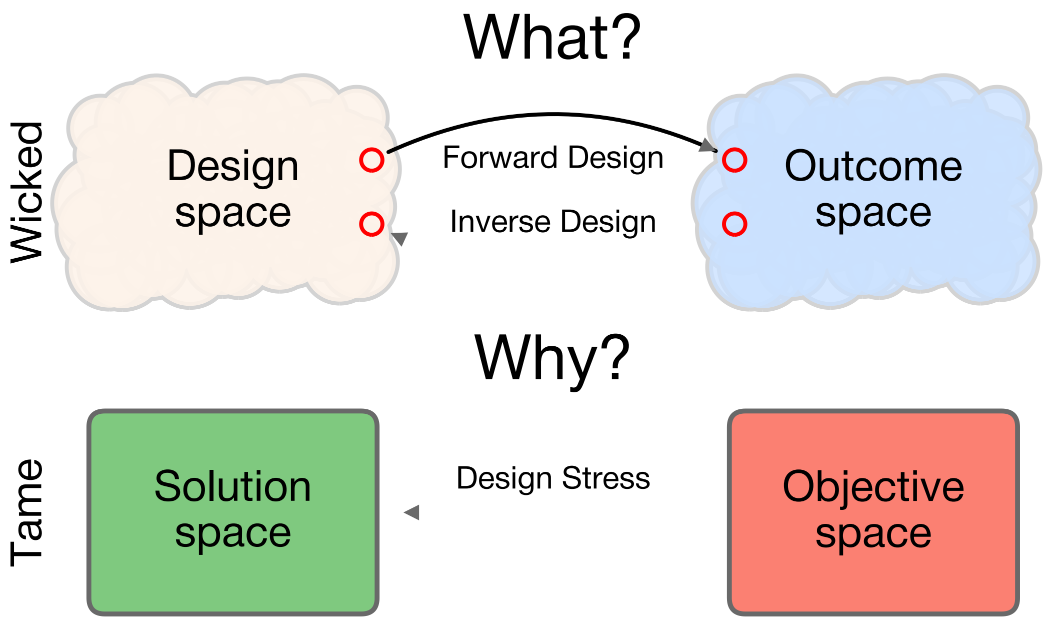
Inverse problems in design



Desired material properties → optimal synthesis pathway
Target flow structure → geometry and boundary conditions
Focal distance / aberration → optical lens system

Not just a one-off solution, but a design rule

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Outlook

- Real life design problems require an analysis frame broader than optimization
- We discover new design phenomena in an example naval engineering problem

- What is the "experiment" for these phenomena?
- What happens in a different problem space?
- What if the operational metaphor was not physics?

Acknowledgements

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- Colin PF Shields
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- Signac framework

signac.io

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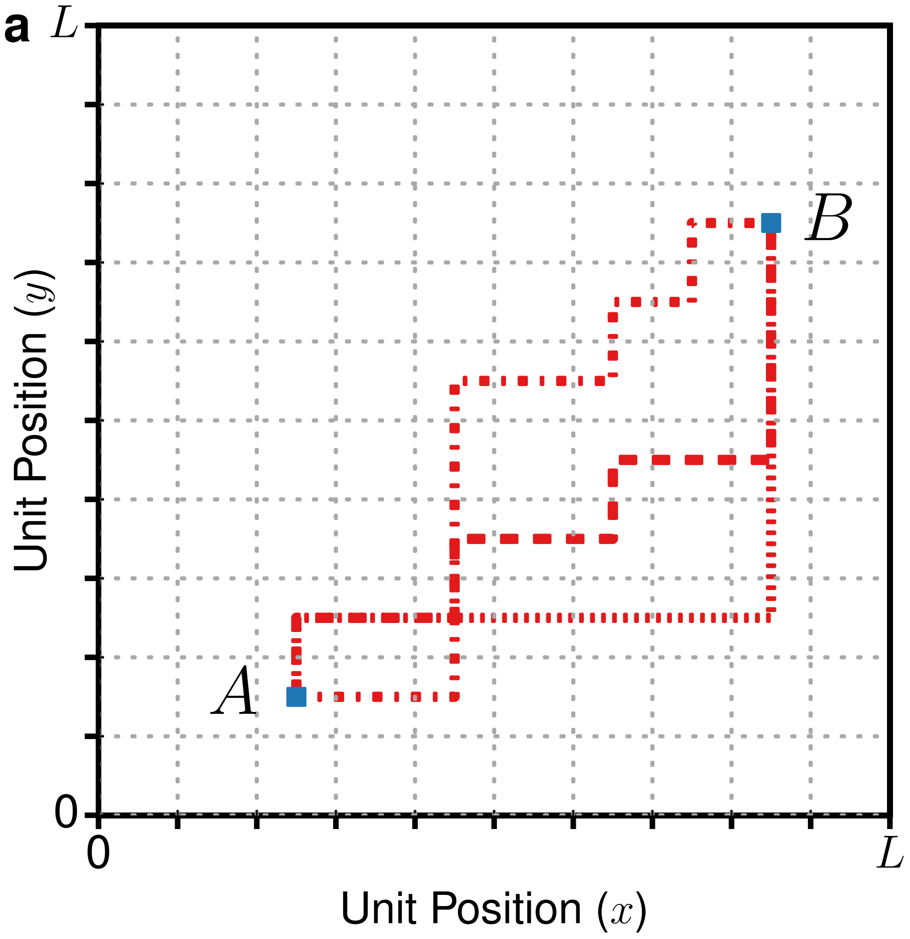
Cost vs entropy



Design objective: Cost

$$\mathcal{O}_1 = E = C(\Delta x + \Delta y)$$

Design pressure: Cost **T**olerance

$$\lambda_1 = \frac{1}{T}$$

Free energy

$$T \cdot F(\Delta x, \Delta y) \approx E - T \ln n(\Delta x, \Delta y)$$

AAK, CPF Shields, DJ Singer, G van Anders, *New J. Phys.* (2018)

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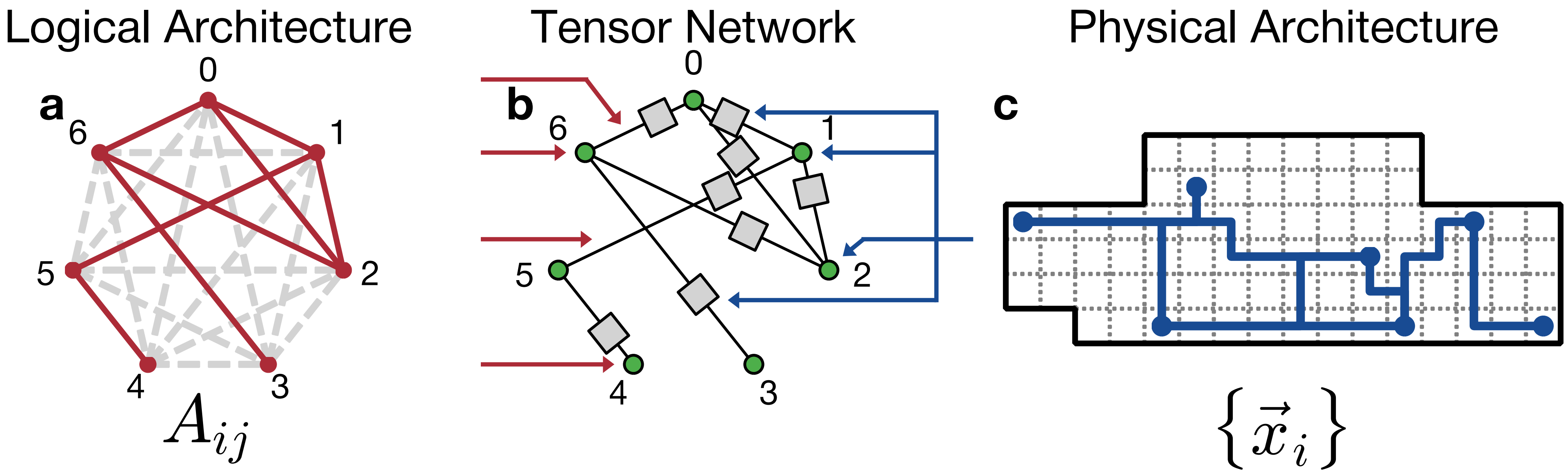
Tensor network as information structure



AAK, DJ Singer, G van Anders, *J. Phys. Complexity* (2021)

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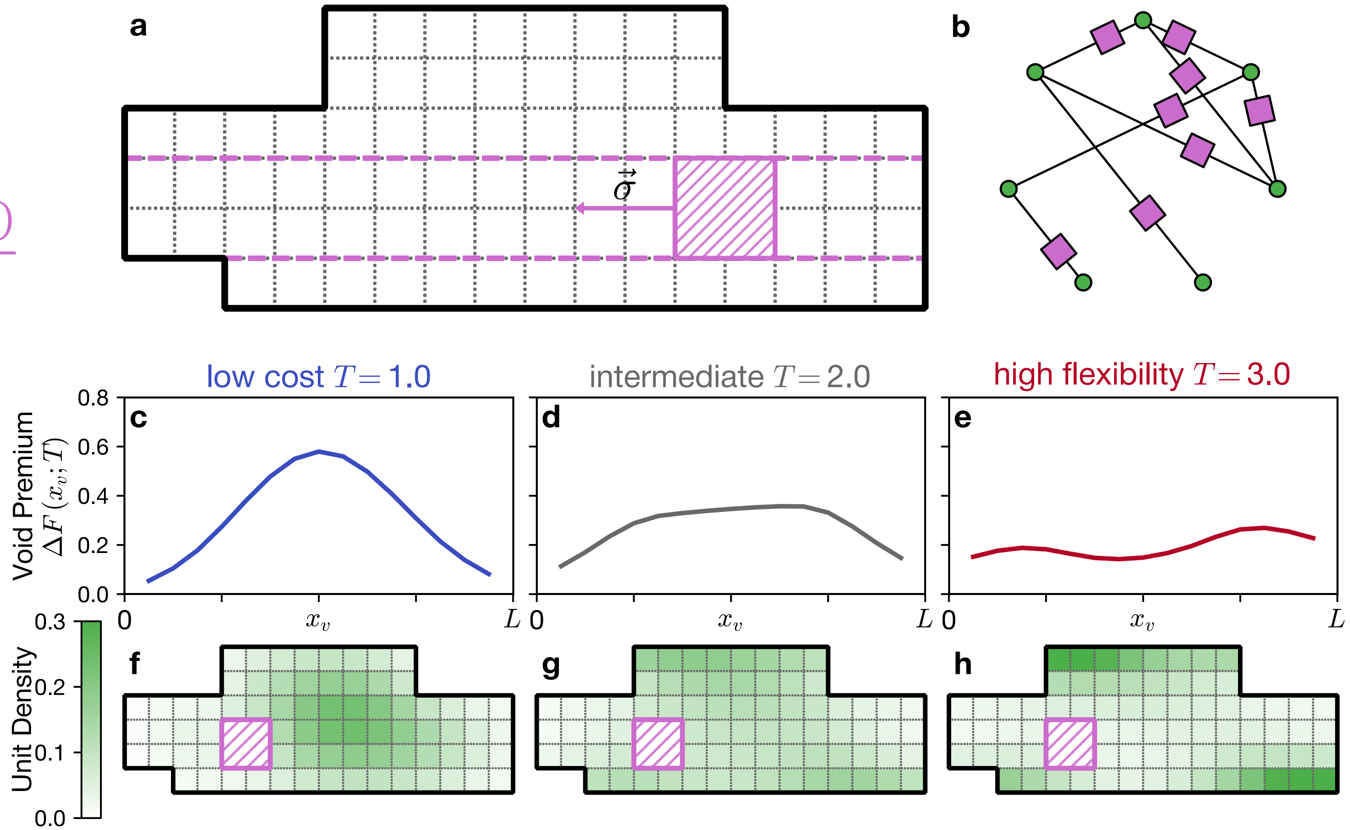
Avoidance: void premium

Void premium

$$\Delta F = -\ln \frac{\mathcal{Z}(x_v;T)}{\mathcal{Z}(T)}$$

Unit density

$$\rho(\vec{x}\,) \simeq \sum_i p_i(\vec{x})$$



AAK, DJ Singer, G van Anders, *J. Phys. Complexity* (2021)

Adjacency: bond diagrams

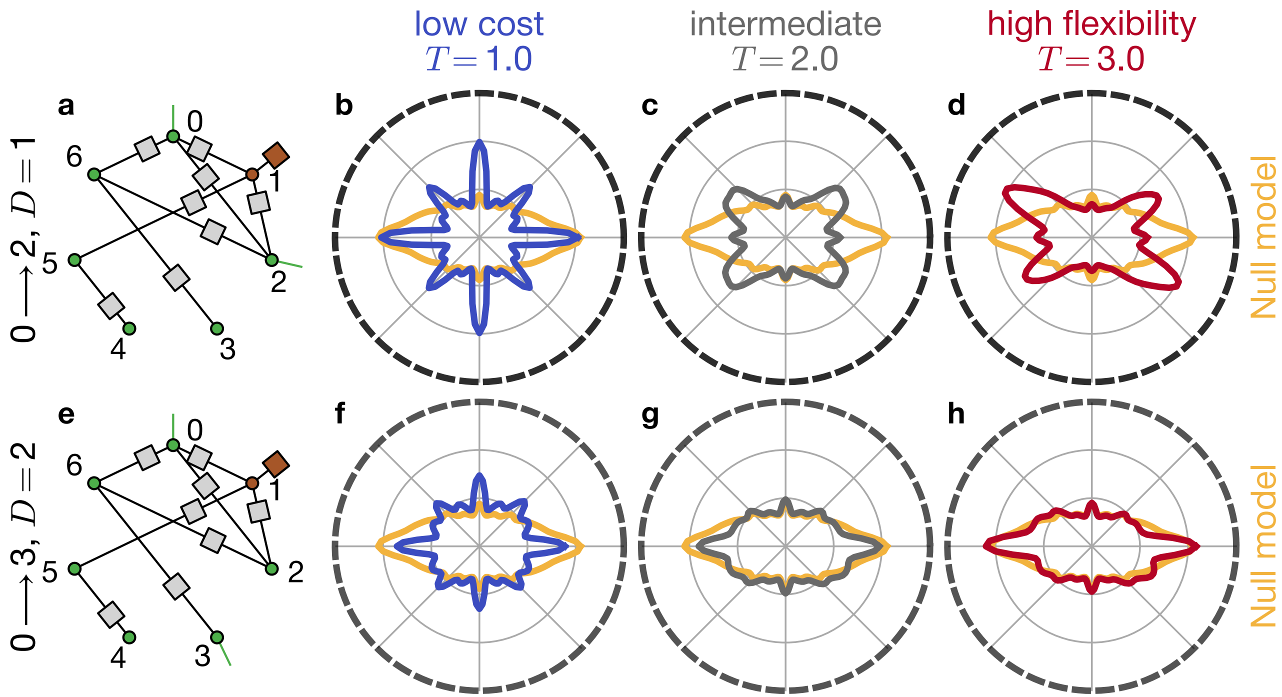
Bond diagram (with KDE smoothing)

$$p_{i\to j}(\theta) = \frac{1}{\mathcal{N}} \sum_k \sum_{\vec{x}_i \neq \vec{x}_j} p(\vec{x}_i, \vec{x}_j) e^{-\frac{1}{2}(hk)^2} \cos\left(k\left(\theta - \theta(\vec{x}_i, \vec{x}_j)\right)\right)$$

PJ Steinhardt, DR Nelson, M Ronchetti, *PRB* (1983)
J Roth, AR Denton, *PRE* (2000)

Null model

$$p(\vec{x}_i, \vec{x}_j) = const$$



AAK, DJ Singer, G van Anders, *J. Phys. Complexity* (2021)

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Association

Design freedom

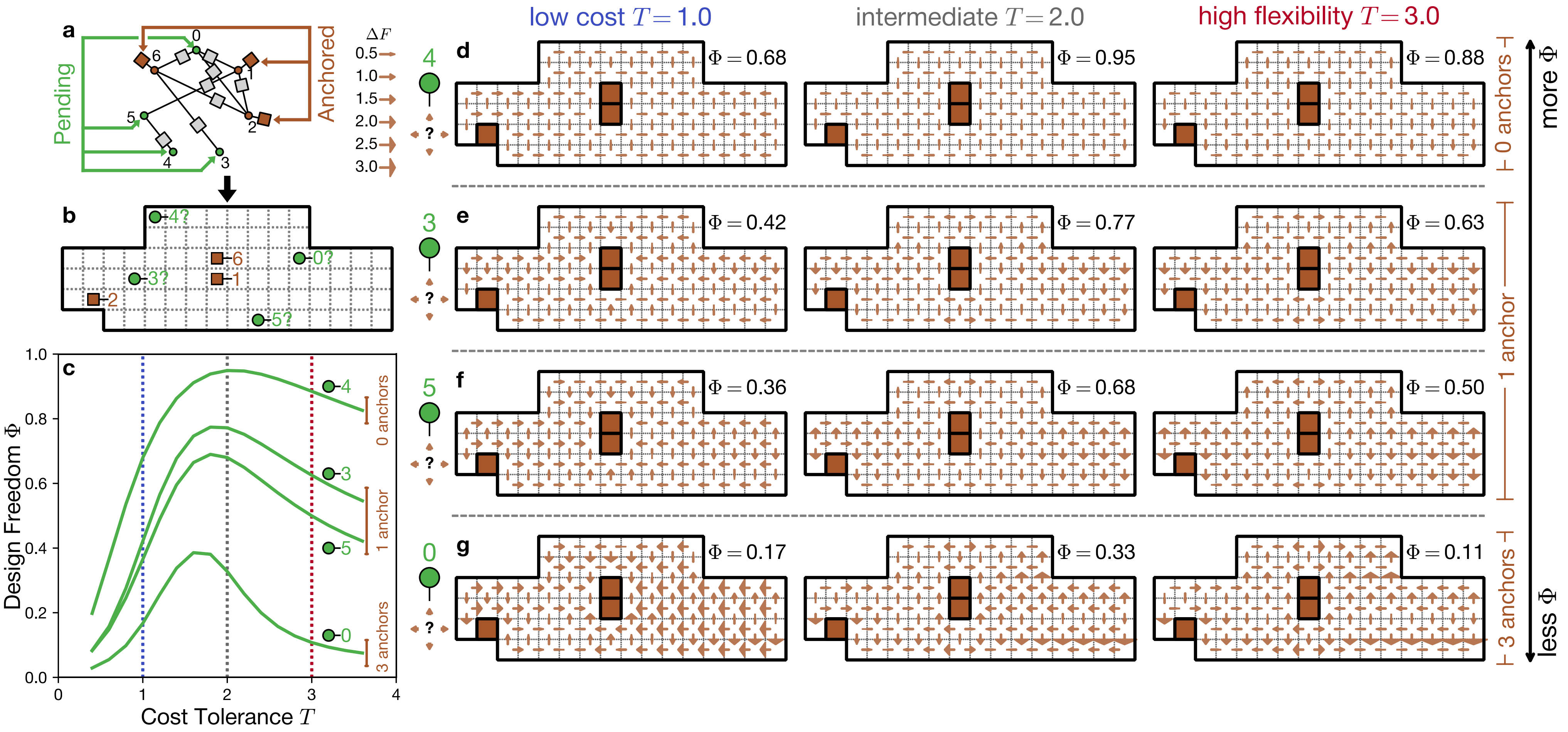
$$\Phi = \frac{1}{Y_0}\frac{\left(\sum_{\vec{x}} p(\vec{x})\right)^2}{\sum_{\vec{x}} p(\vec{x})^2}$$

Free energy

$$F(\vec{x}) = -\ln p(\vec{x})$$

Design stress

$$\Delta F = -\nabla F$$



DJ Thouless, *Physics Reports* (1974)

M Filoche, S Mayboroda, *PRL* (2009)

AAK, DJ Singer, G van Anders, *J. Phys. Complexity* (2021)

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Coarse-graining

- Introduce a design feature / order parameter $\vec{x}_\alpha$ s.t. $\alpha \to \vec{x}$ is surjective (compressing).

- Landau (effective) free energy:

$$e^{-F(\vec{x})} = \sum_\alpha \delta(\vec{x} - \vec{x}_\alpha) e^{-\sum_m \lambda_m \mathcal{O}_m(\alpha)}$$

- Defines effective landscapes on a smaller space.

Lectures on phase transitions and the renormalization group, N. Goldenfeld (1992)

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Systems Physics computations

Objective function with only 2-point couplings
(aka 2-body Hamiltonian) along a network

$$\lambda \mathcal{O}_{eff}(\{x\}) = \sum_{i<j} A_{ij} f(x_i, x_j; T)$$

T = cost tolerance
$T < 1.44$ attract
$T > 1.44$ repel

Partition function

$$\mathcal{Z} = \sum_{\{x_i\}} \prod_{ij:A_{ij}\neq 0} e^{-f(x_i,x_j;T)} = ???$$

Sum over **all** sites $\sim 10^{13}$ terms

One-unit marginal distribution

$$p(x_k) = \frac{1}{\mathcal{Z}} \sum_{\{x_{i\neq k}\}} \prod_{ij:A_{ij}\neq 0} e^{-f(x_i,x_j;T)} = ???$$

Sum over **all but one** sites

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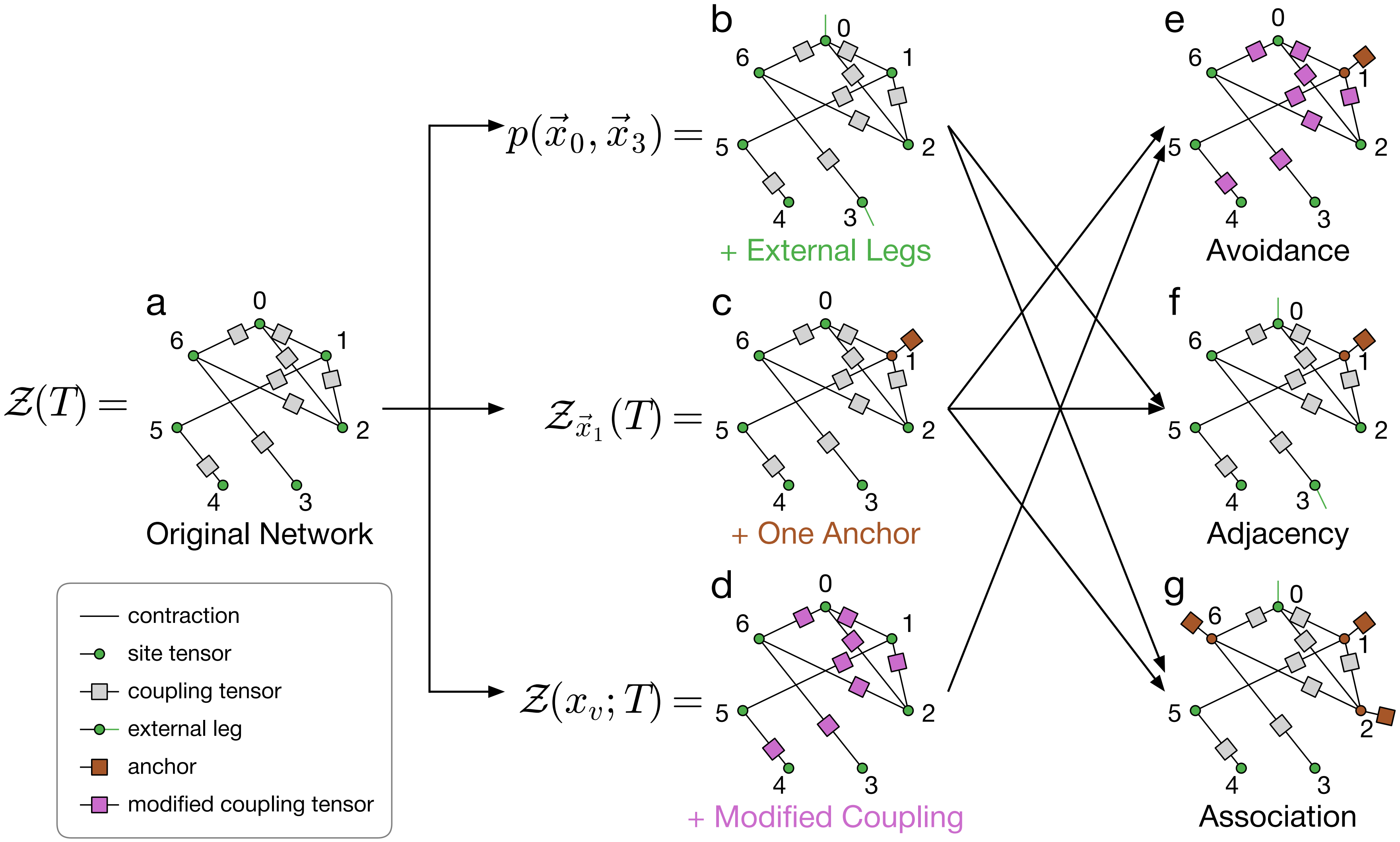
Tensor network query language



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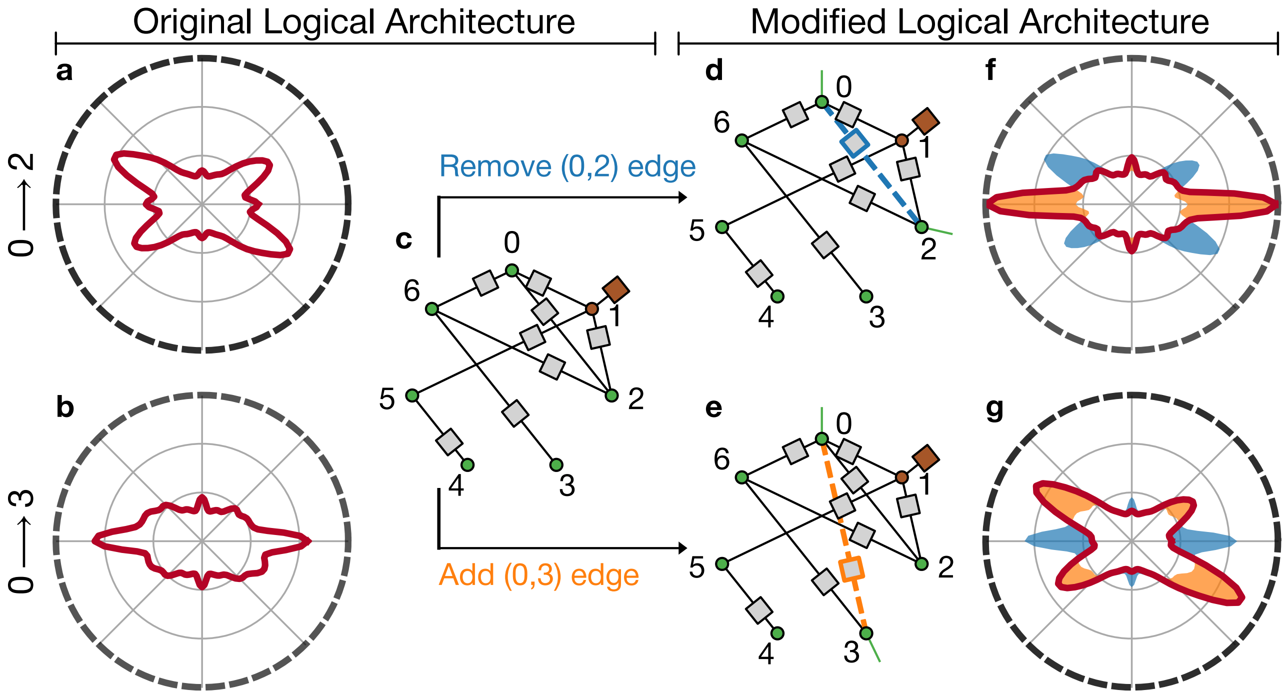
Adjacency: add and remove links



AAK, DJ Singer, G van Anders, *J. Phys. Complexity* (2021)