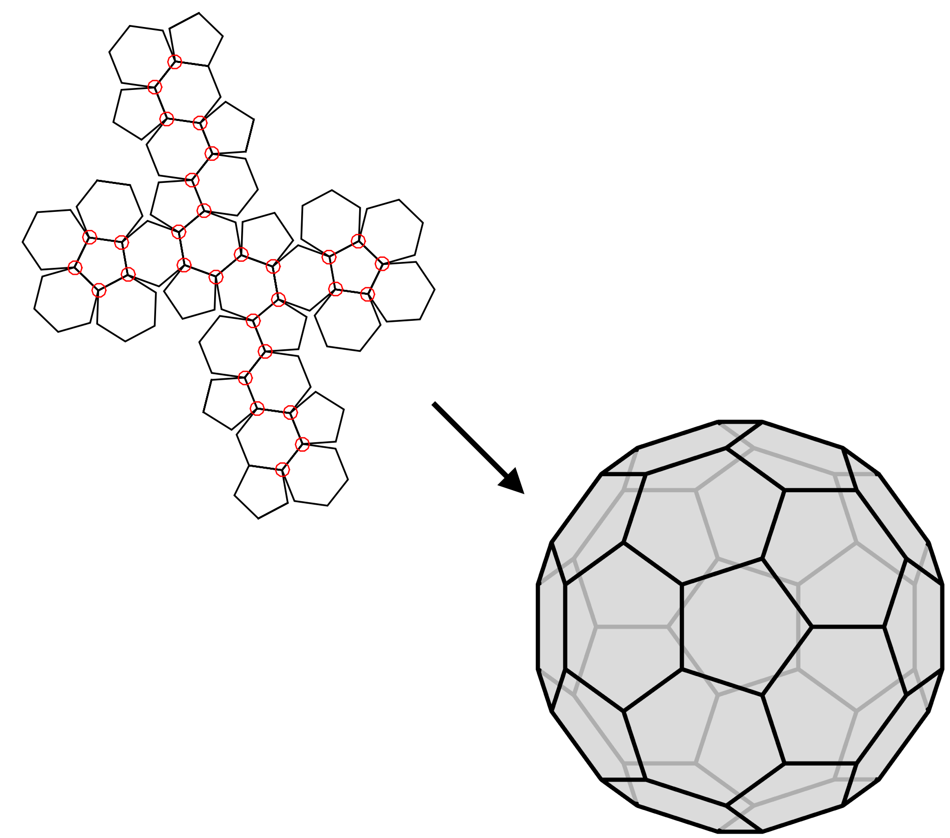
Kinetics of self-folding at the microscale



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with C. Dias, H. P. Melo (U. Lisboa)

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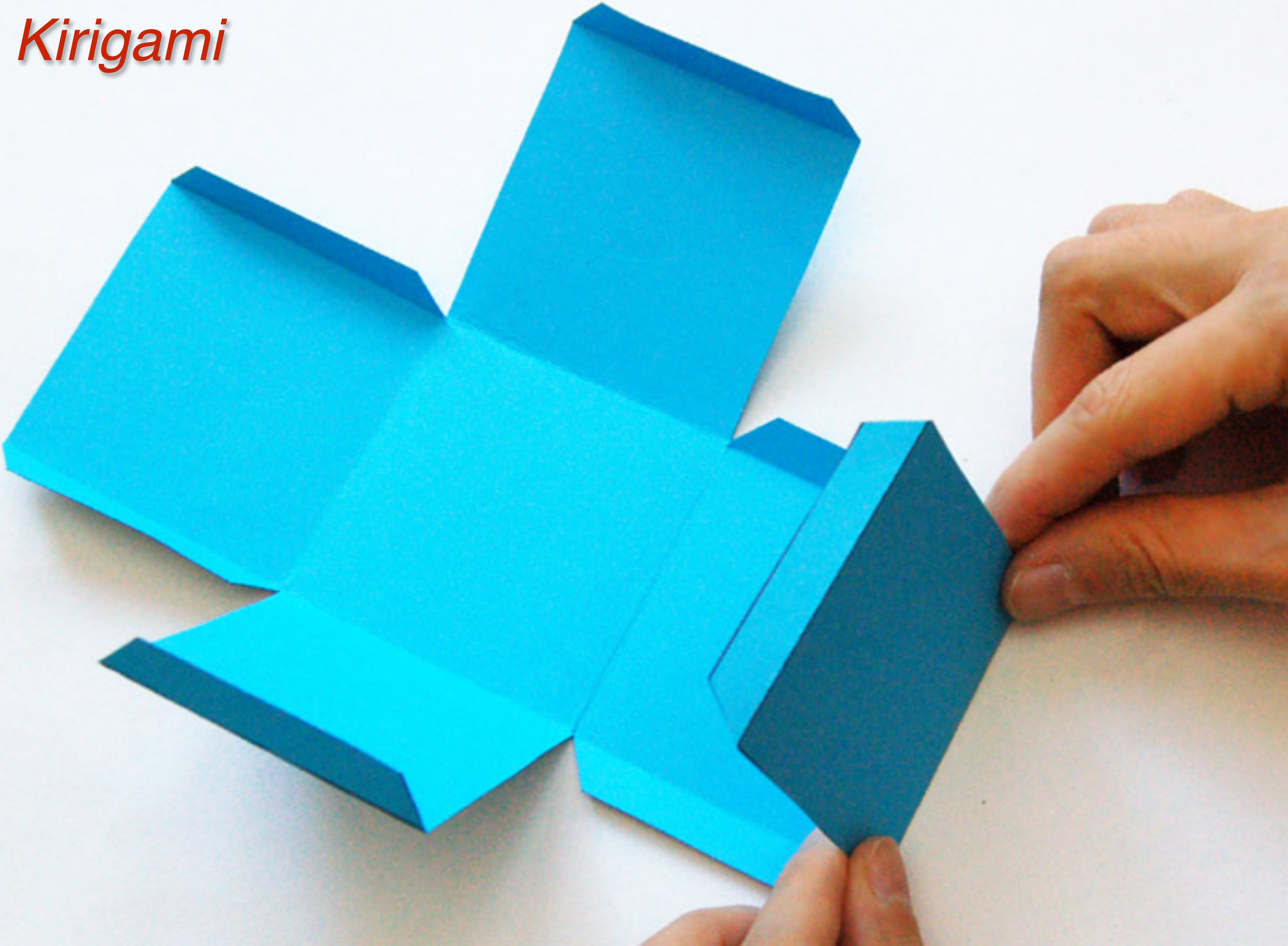
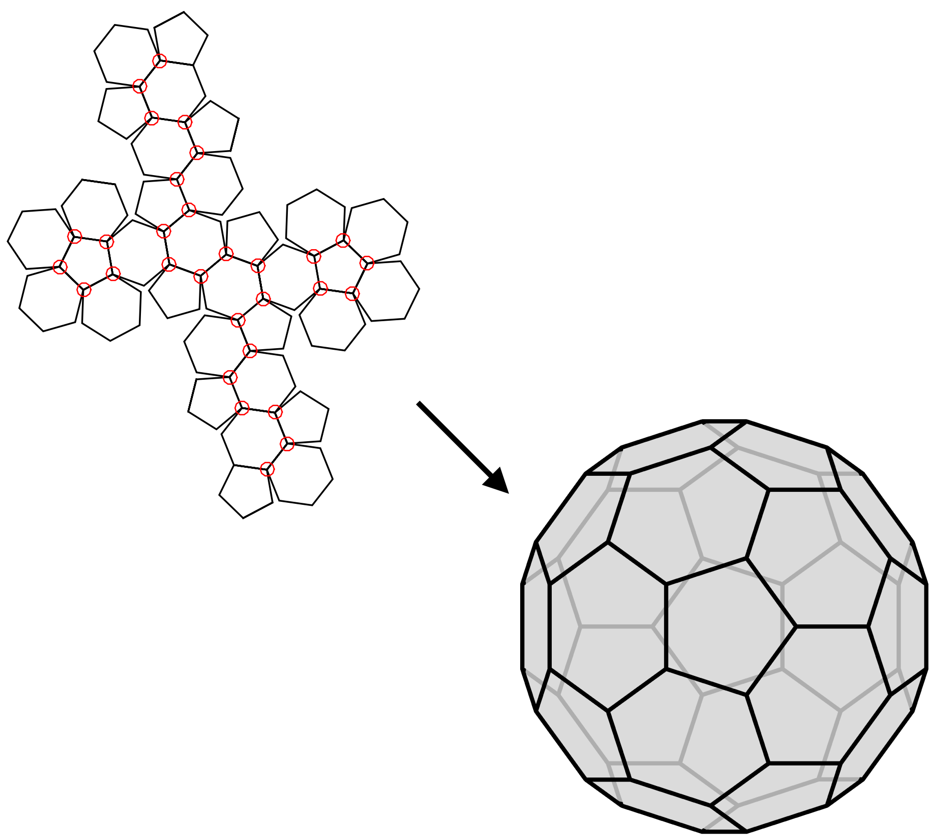
Origami

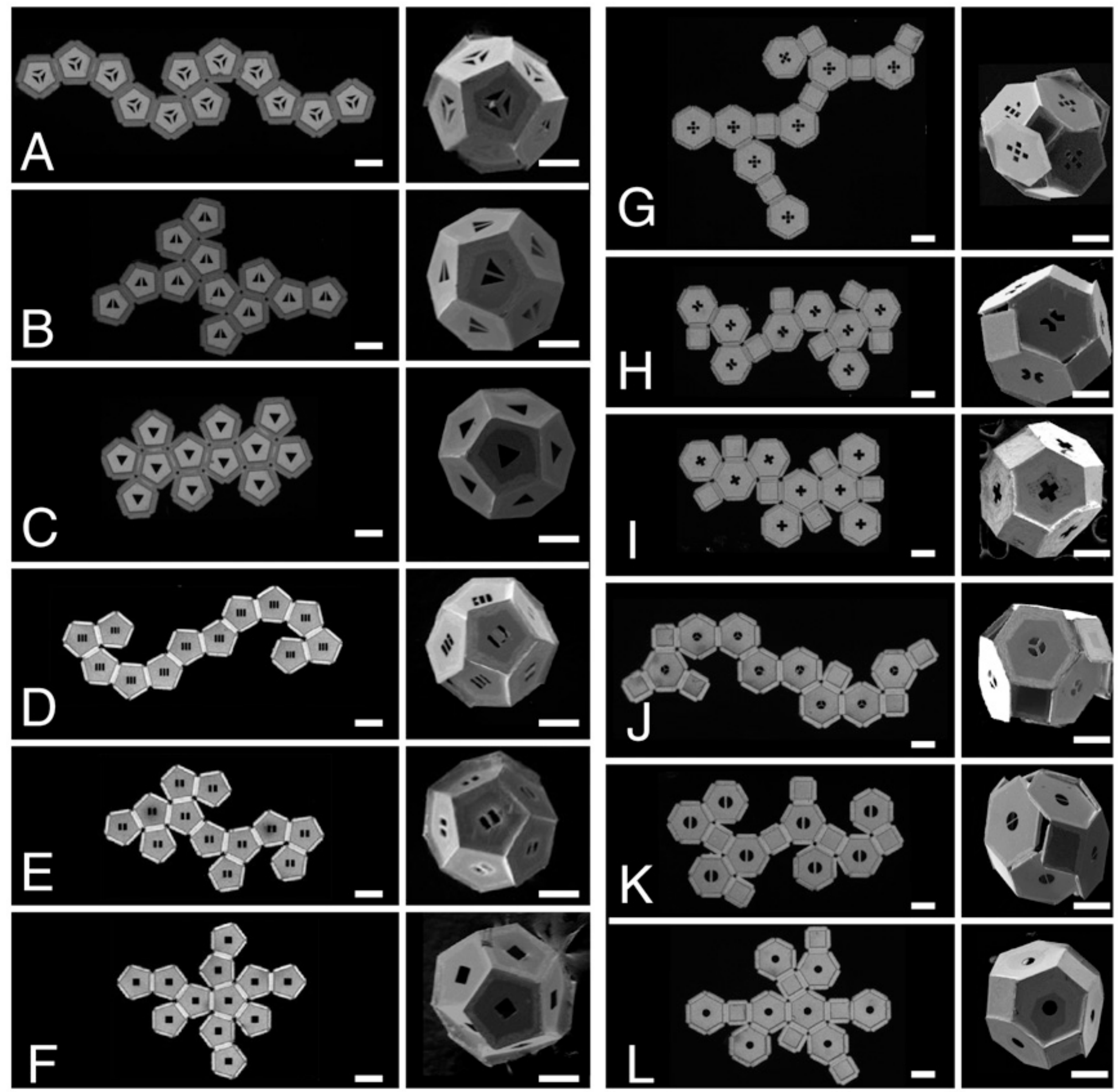

Ori to Kiri
Velpon
ALLESLIJM
COLLE TOUT

Kirigami



Kirigami @microscale





Mechanisms of folding at different scale

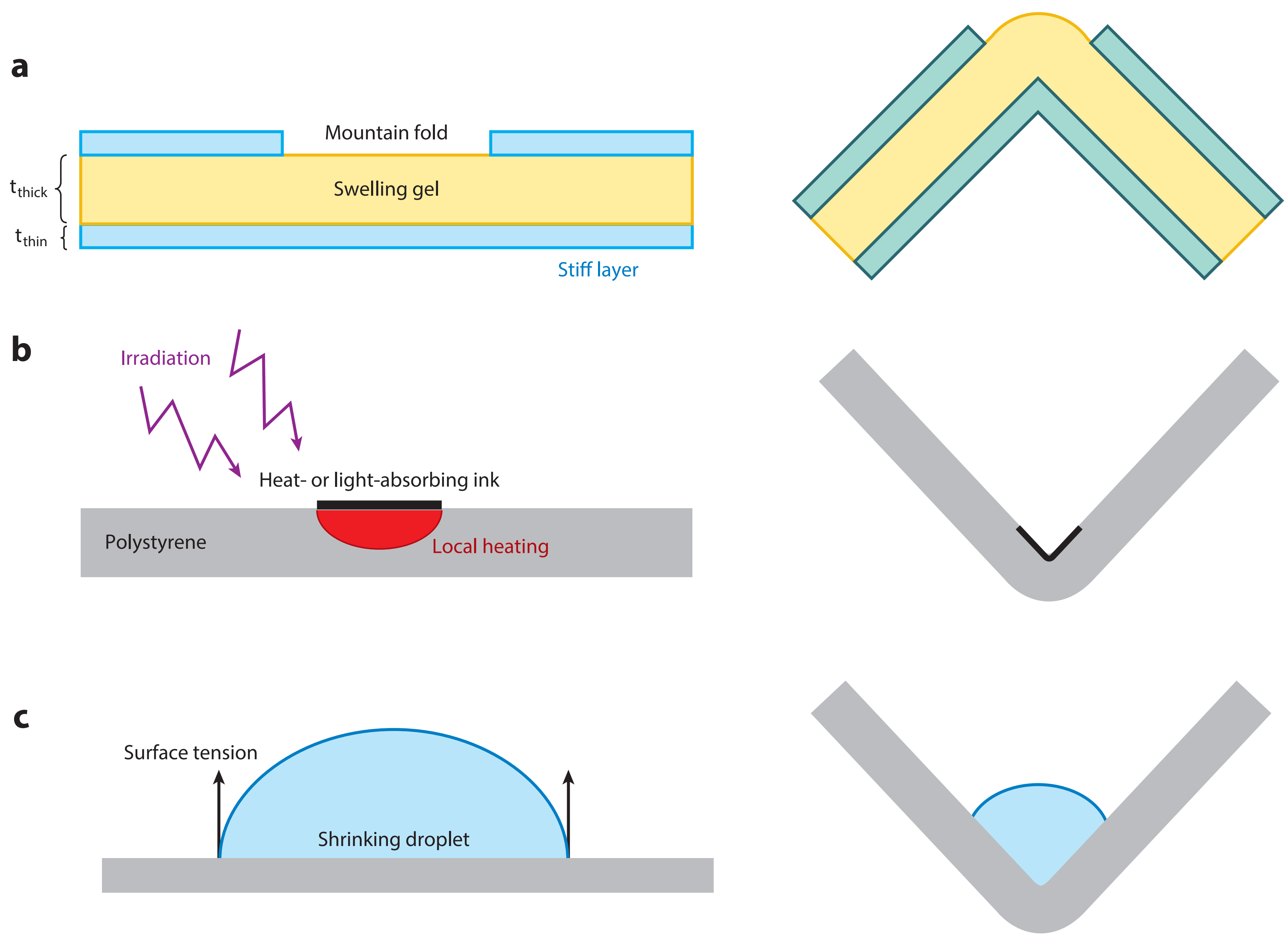
nm μm cm

http://www.ks.uiuc.edu/ Research/folding/

Science **359**, 1386 (2018)

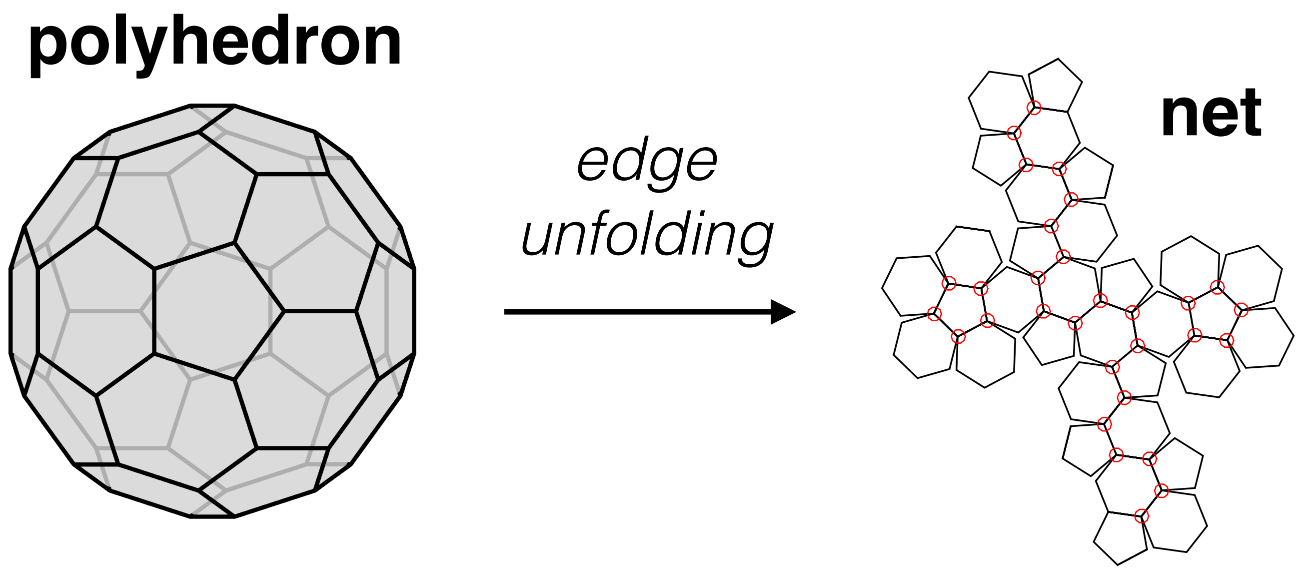
interactions are relevant	***excluded volume***	***stress relaxation***
minimum of the free energy	***kinetically trapped***	***unique folded state***

Technological challenge of self-folding



C. D. Santangelo. *Annu. Rev. Condens. Matter Phys.* **8**, 165 (2017)

Theoretical challenges of self-folding

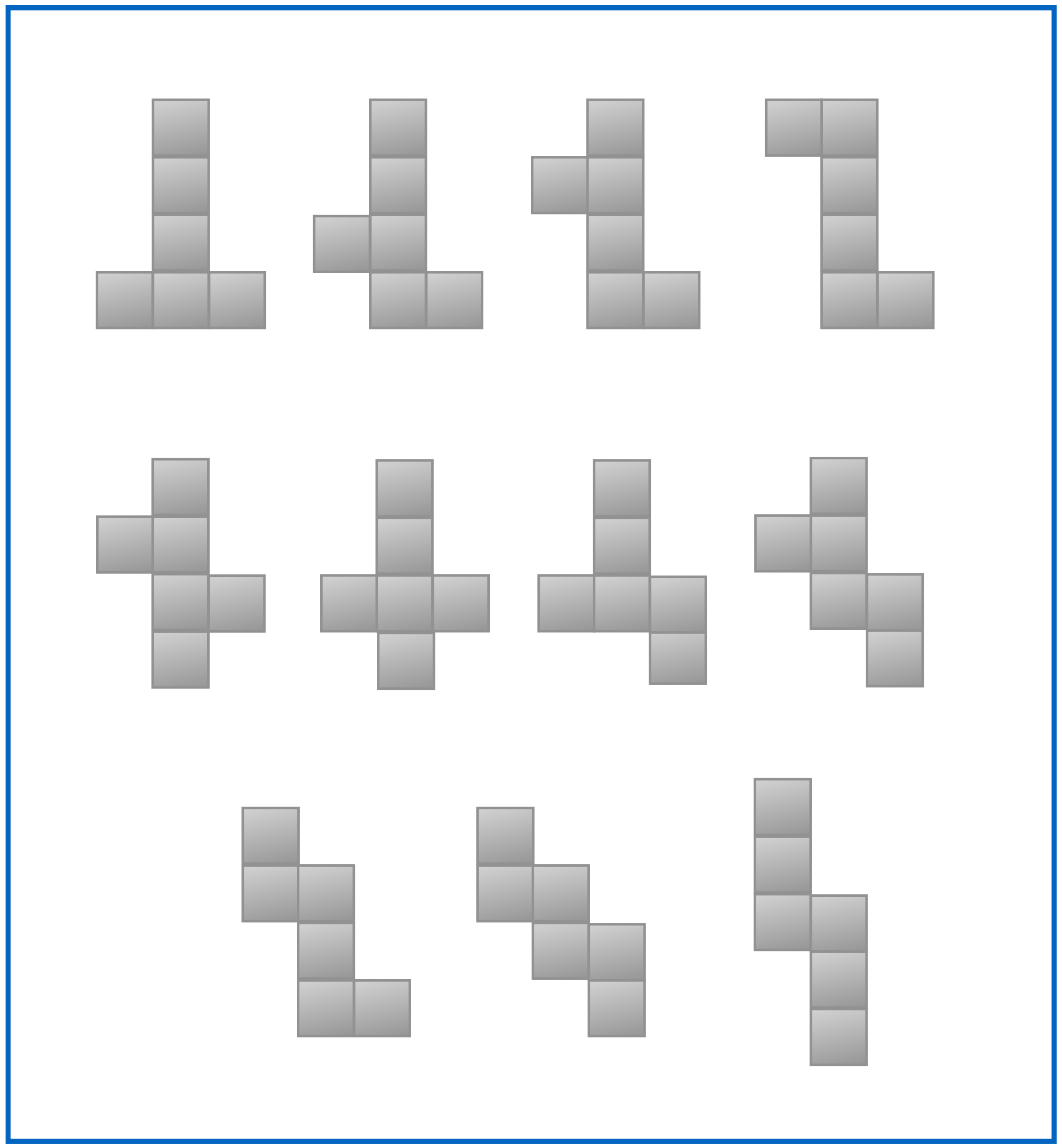


Does every convex polyhedron have a net?

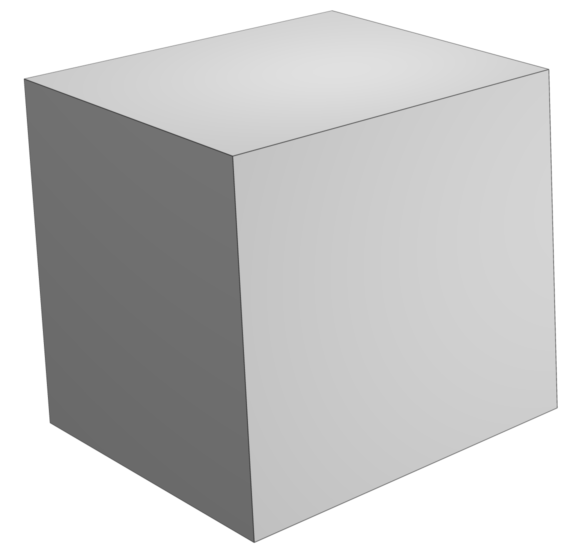
- single, simply **connected** piece;
- the unfolding is a **union of polyhedron faces**;
- the unfolding does **not self-overlap**.

E. D. Demaine, J. O'Rourke. *Geometric folding algorithms*. Cambridge University Press (2007)

Theoretical challenges to self-folding



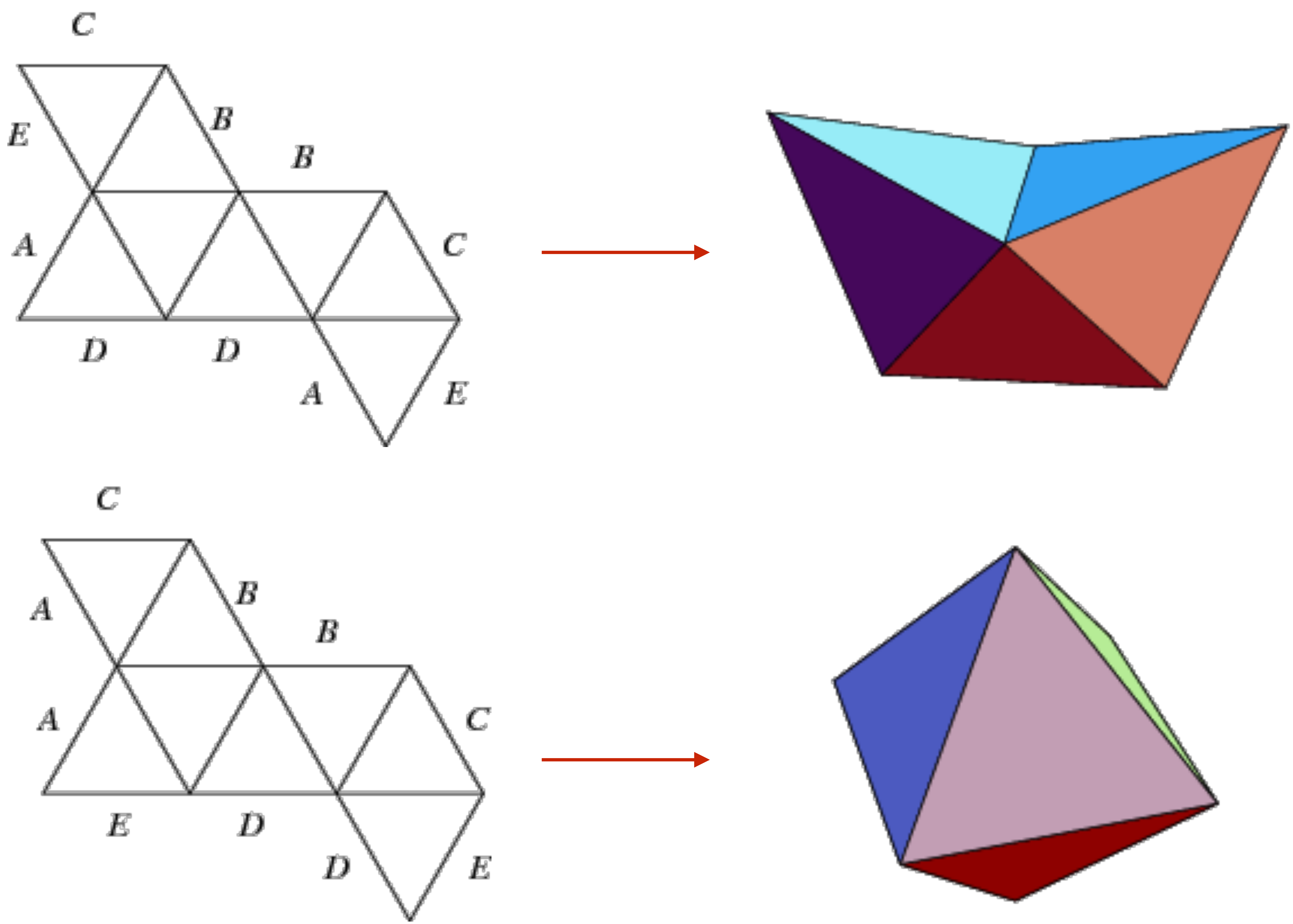
What is the optimal net for self-folding?



N ⟶ 1

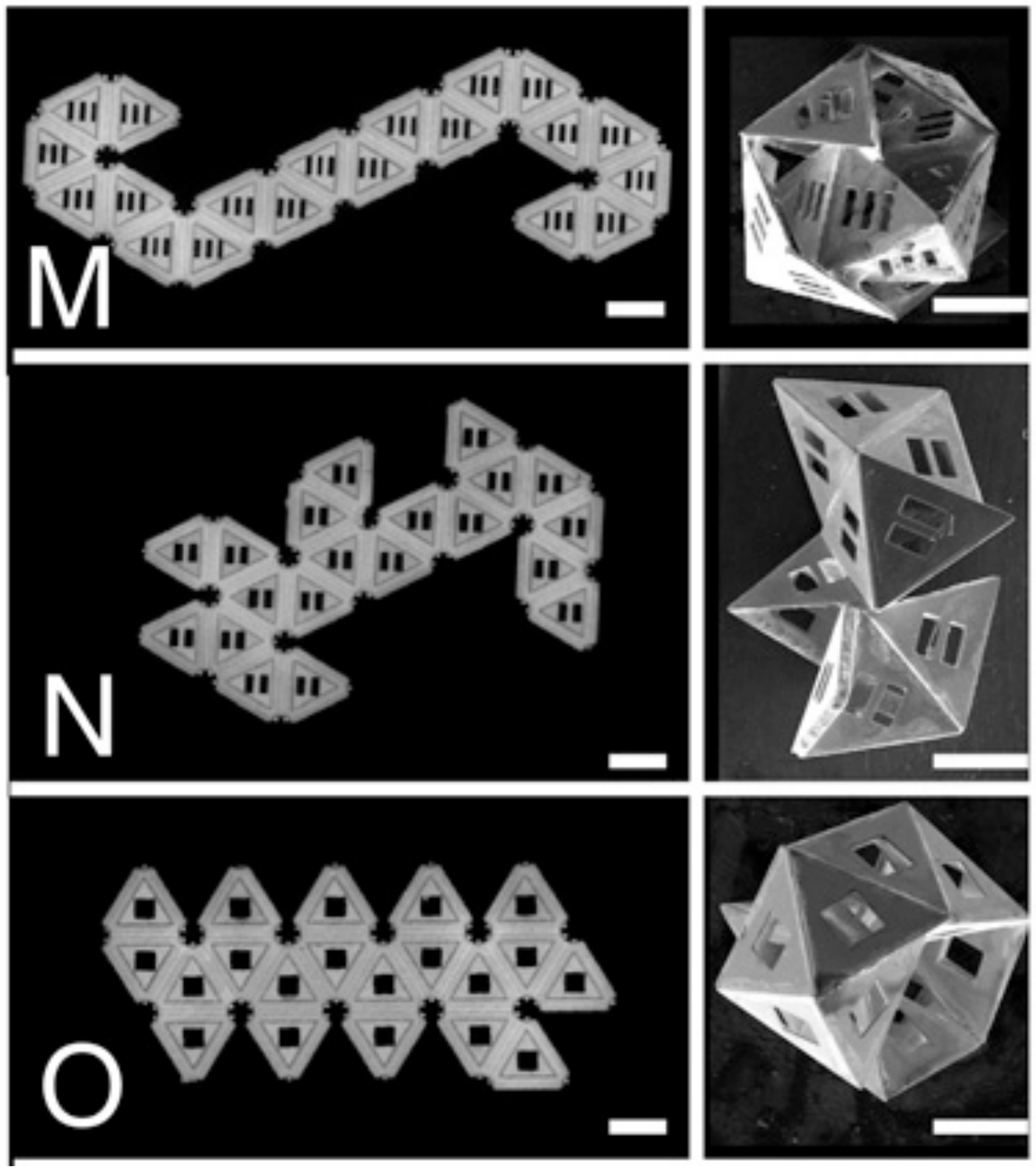
S. Pandey, M. Ewing, A. Kunas, N. Nguyen, D. H. Gracias, G. Menon. *PNAS* **108**, 19885 (2011)
N.A.M. Araújo, R. A. da Costa, S. N. Dorogovtsev, J. F. F. Mendes, *Physical Review Letters* **120**, 188001 (2018)

Theoretical challenges to self-folding



Weisstein, Eric W. "Boat." From MathWorld--A Wolfram Web Resource. http://mathworld.wolfram.com/Boat.html

Theoretical challenges to self-folding

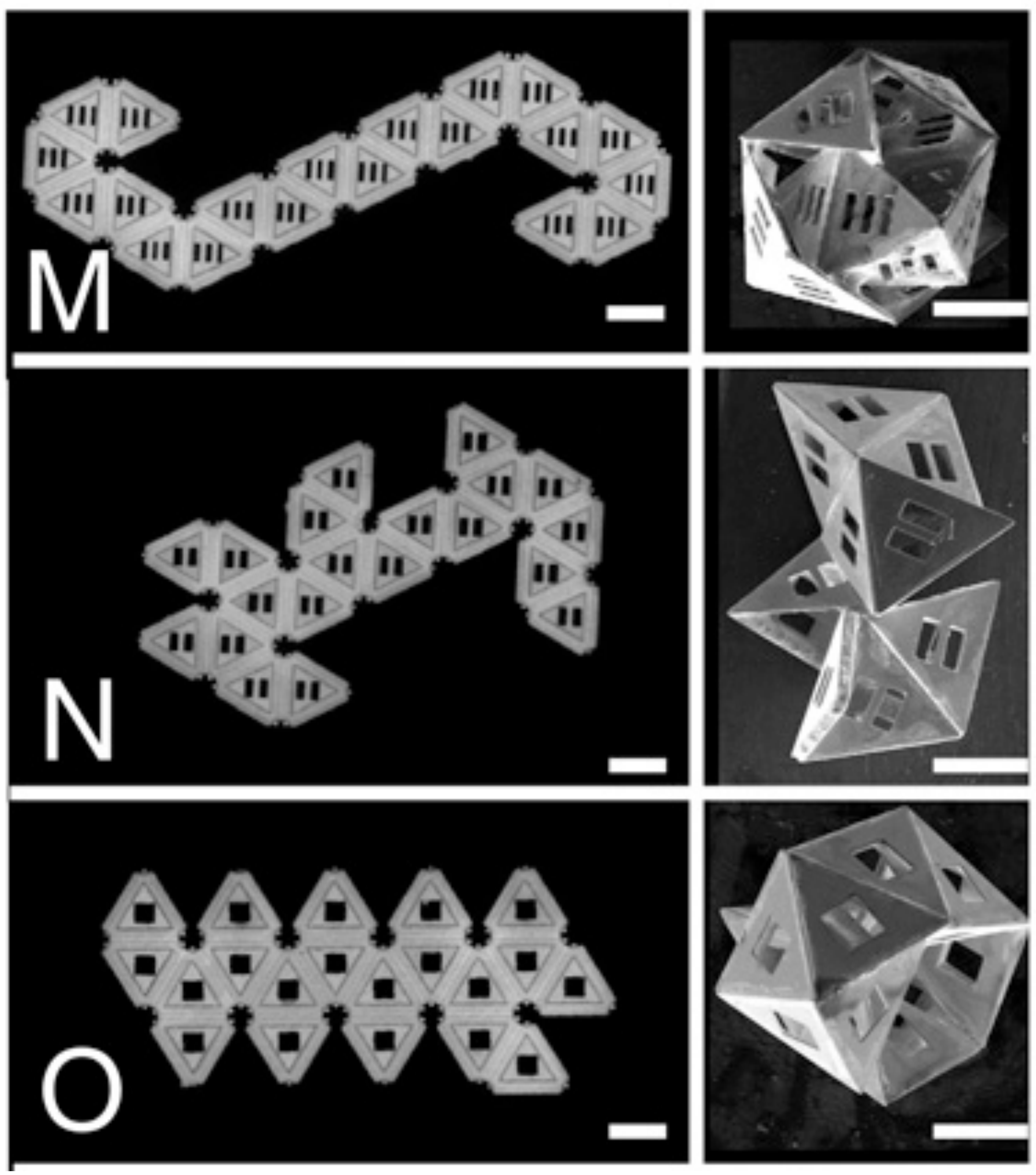


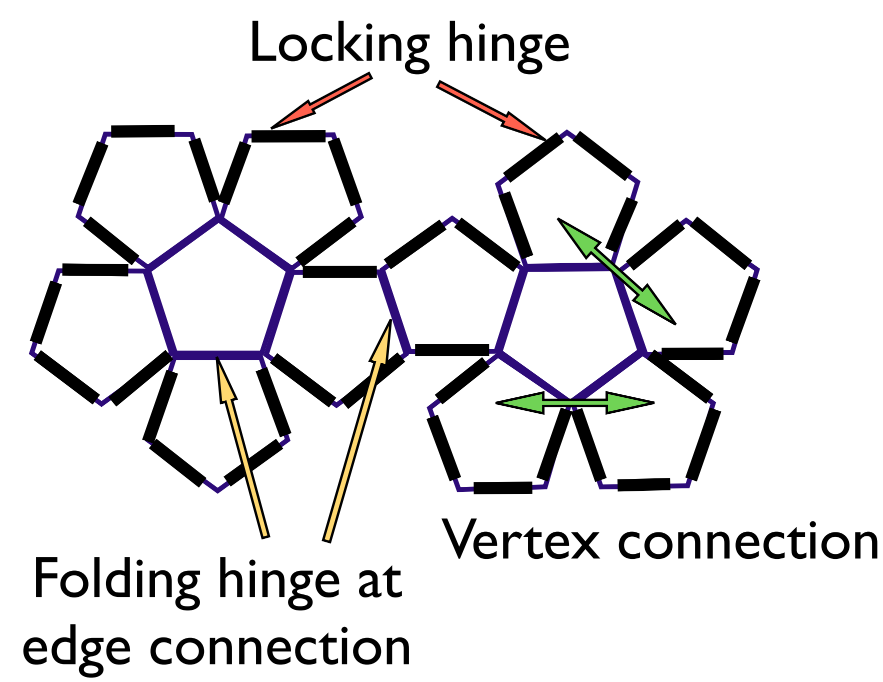
What are the kinetic pathways of folding?

N ⟶ M (?)

S. Pandey, M. Ewing, A. Kunas, N. Nguyen, D. H. Gracias, G. Menon. *PNAS* **108**, 19885 (2011)
P. M. Dodd, P. F. Damasceno, S. C. Glotzer, *PNAS* **115**, E6690 (2018)

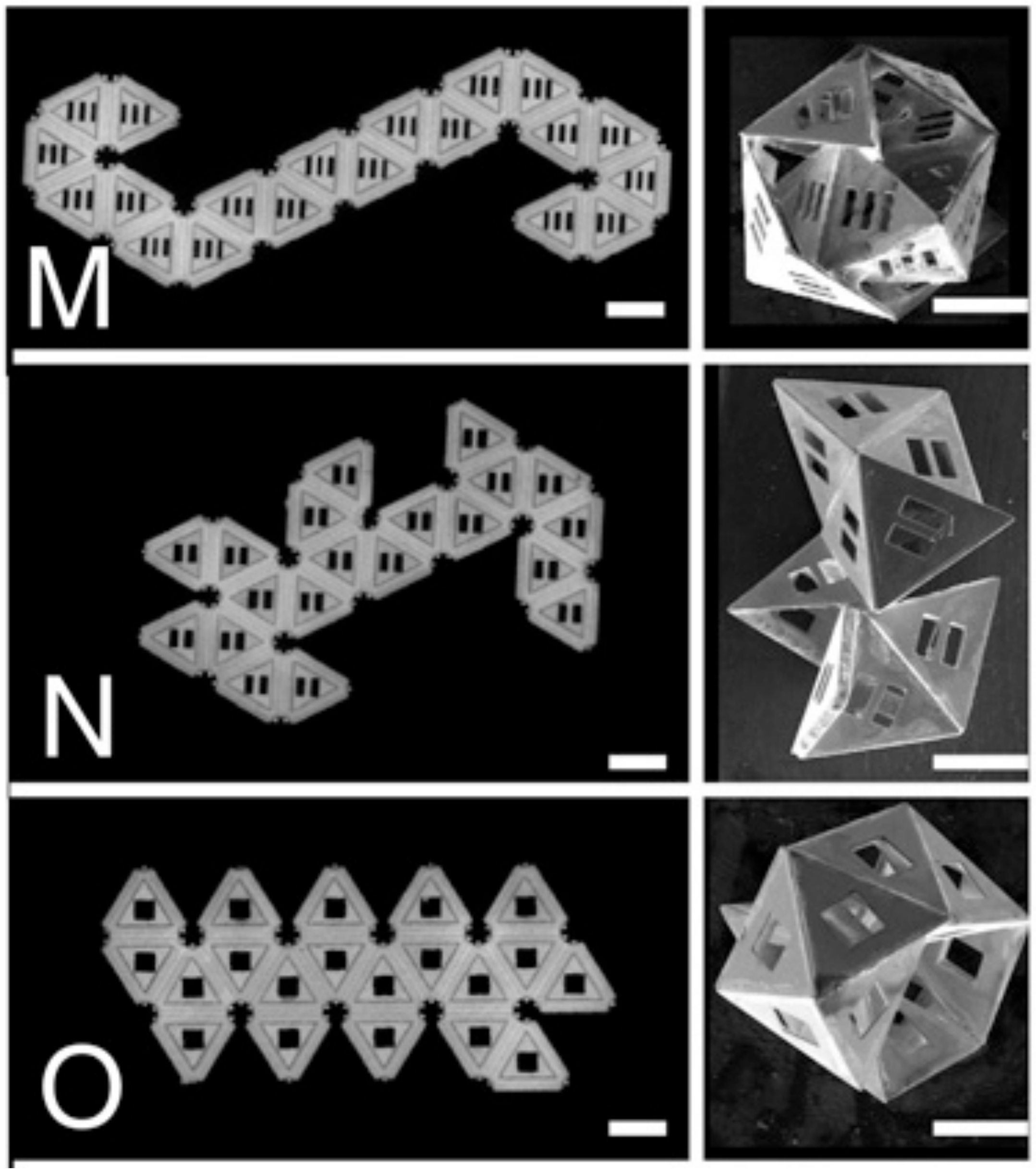
Experimental realization

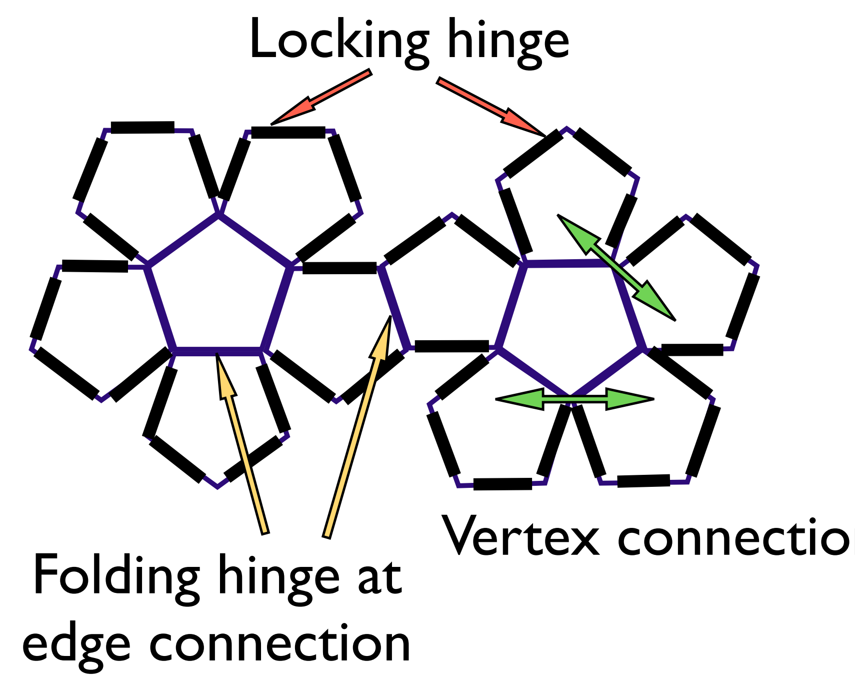




S. Pandey, M. Ewing, A. Kunas, N. Nguyen, D. H. Gracias, G. Menon. *PNAS* **108**, 19885 (2011)

Topological vs geometrical compactness





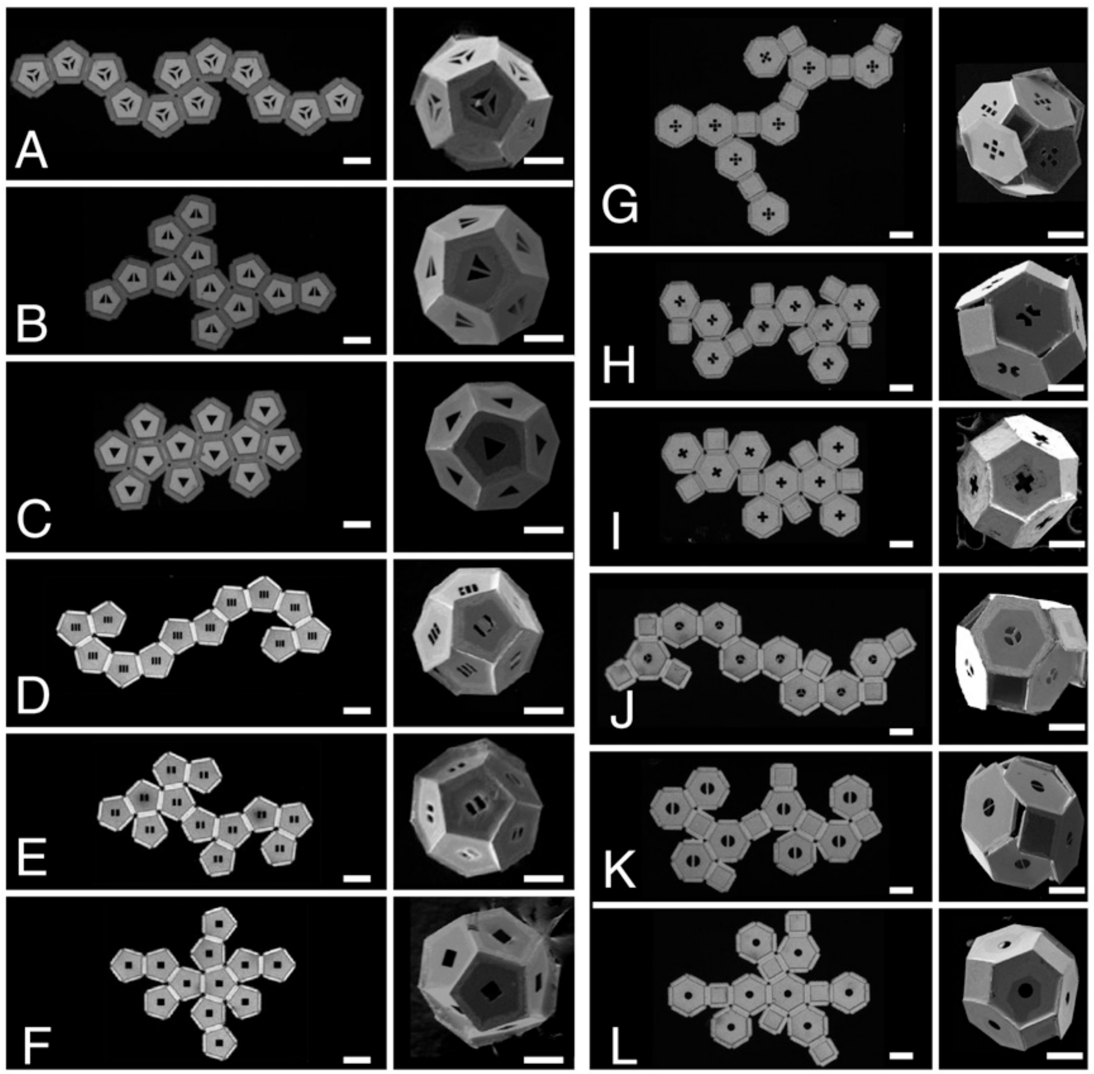
number of vertex connections (Vc)

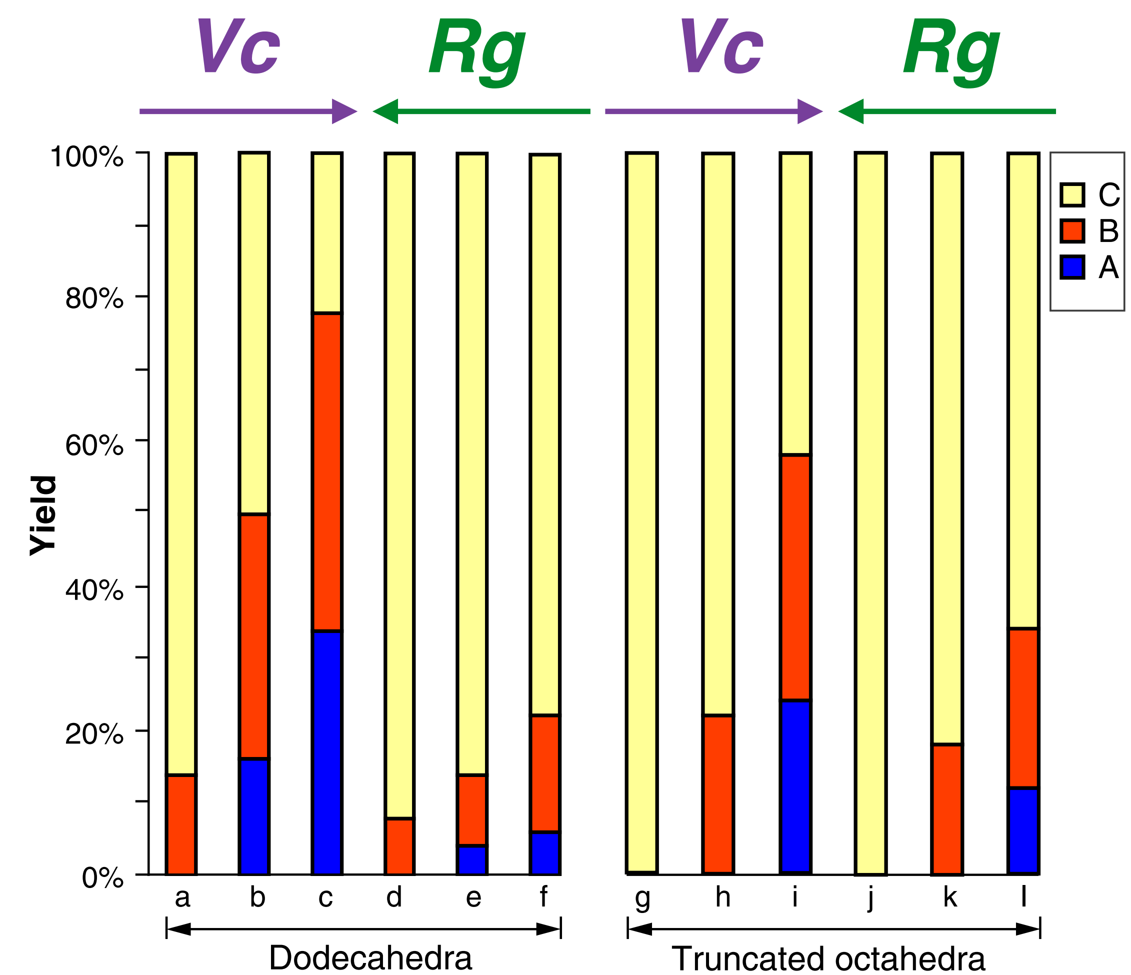
VS

radius of gyration (Rg)

S. Pandey, M. Ewing, A. Kunas, N. Nguyen, D. H. Gracias, G. Menon. *PNAS* **108**, 19885 (2011)

Topological vs geometrical compactness





C → defective

B → minor defects

A → defect free

number of vertex connections (Vc)

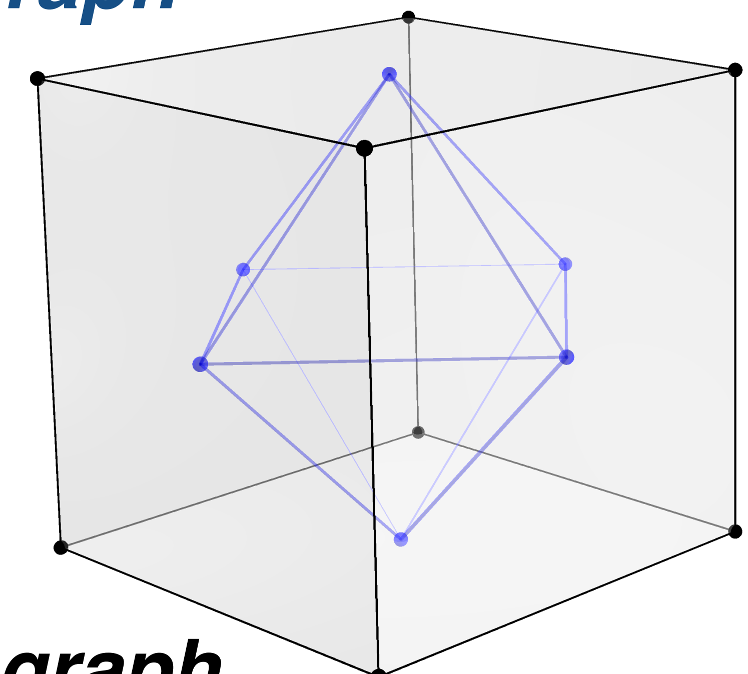
vs

radius of gyration (Rg)

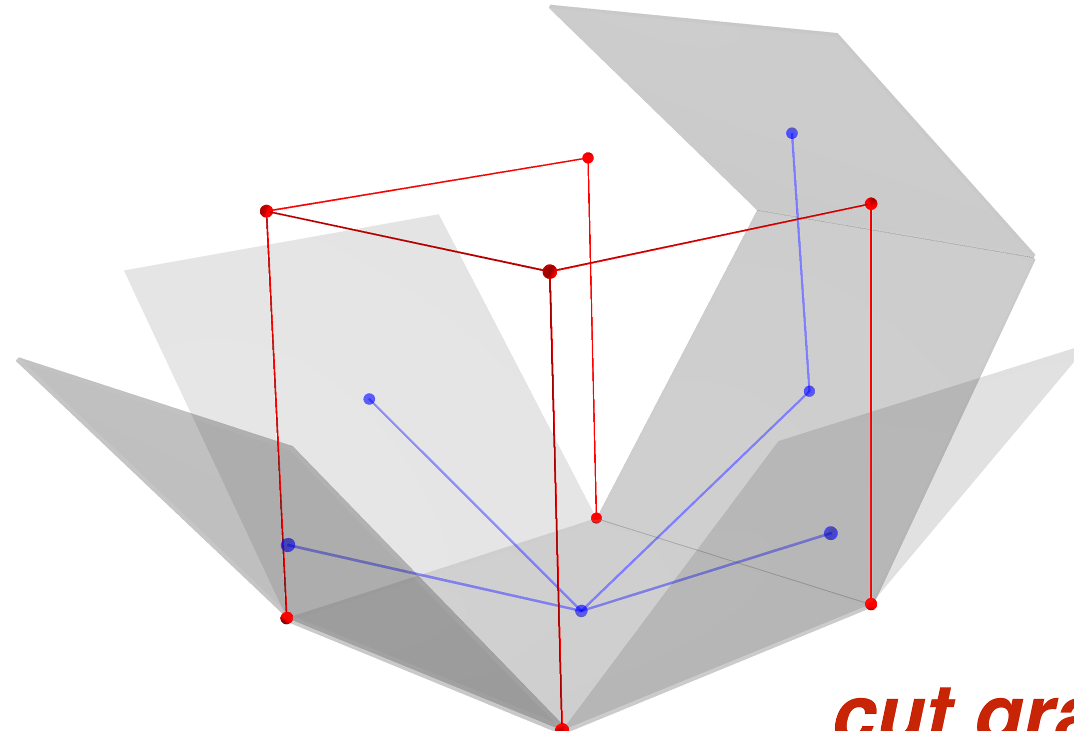
S. Pandey, M. Ewing, A. Kunas, N. Nguyen, D. H. Gracias, G. Menon. *PNAS* **108**, 19885 (2011)

Mapping into a graph

face graph

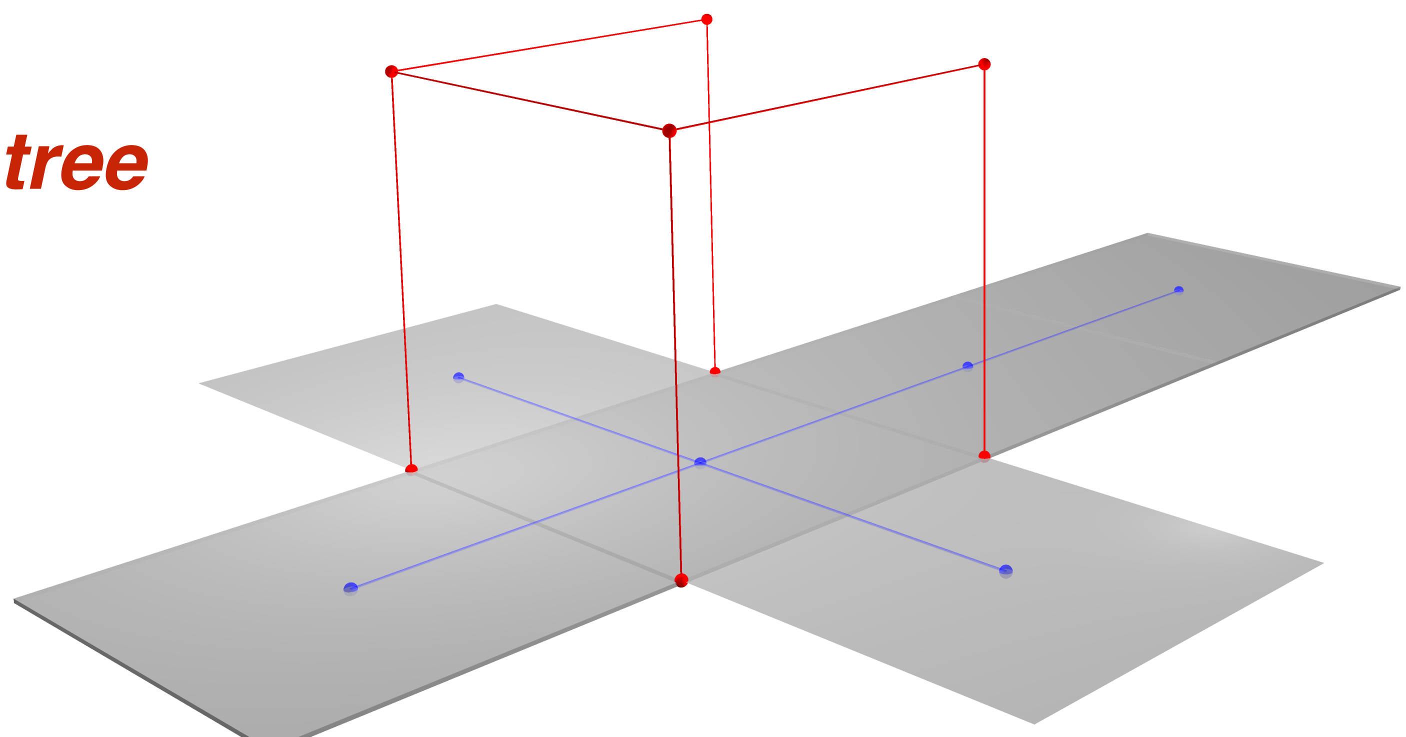


shell graph



cut graph

spanning tree



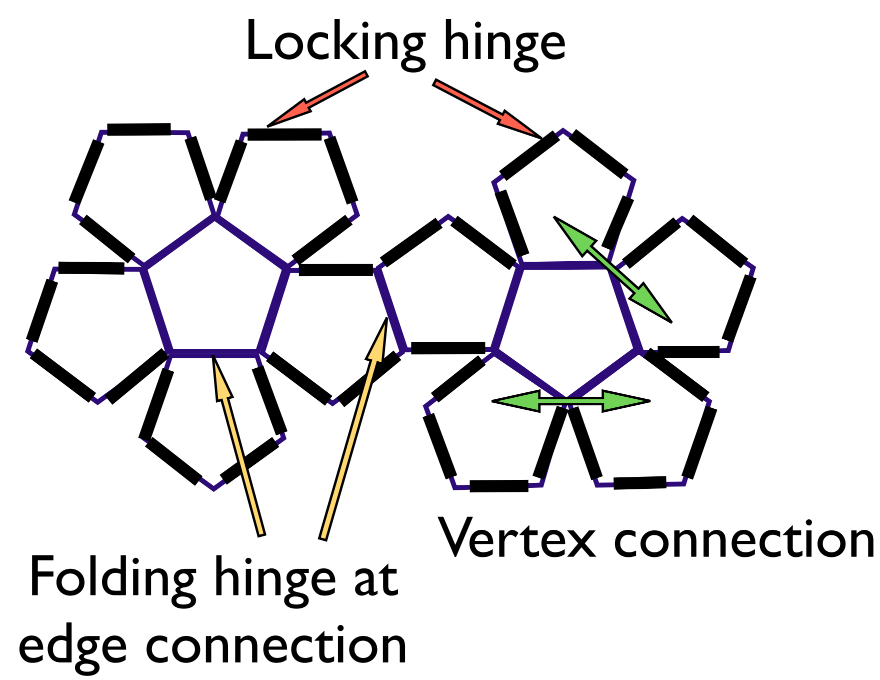
span all vertices

loopless

simply connected

N.A.M. Araújo, R. A. da Costa, S. N. Dorogovtsev, J. F. F. Mendes, *Physical Review Letters* **120**, 188001 (2018)

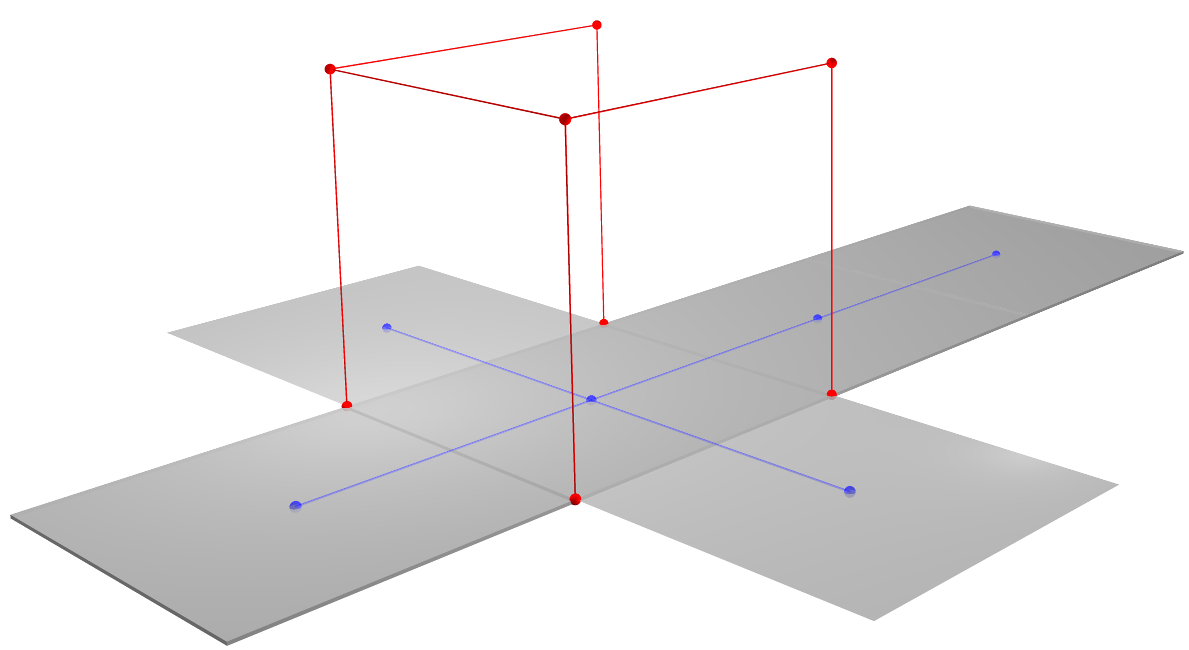
Vertex connections



vertex connections** are **leaves

↓

Maximum leaf spanning tree



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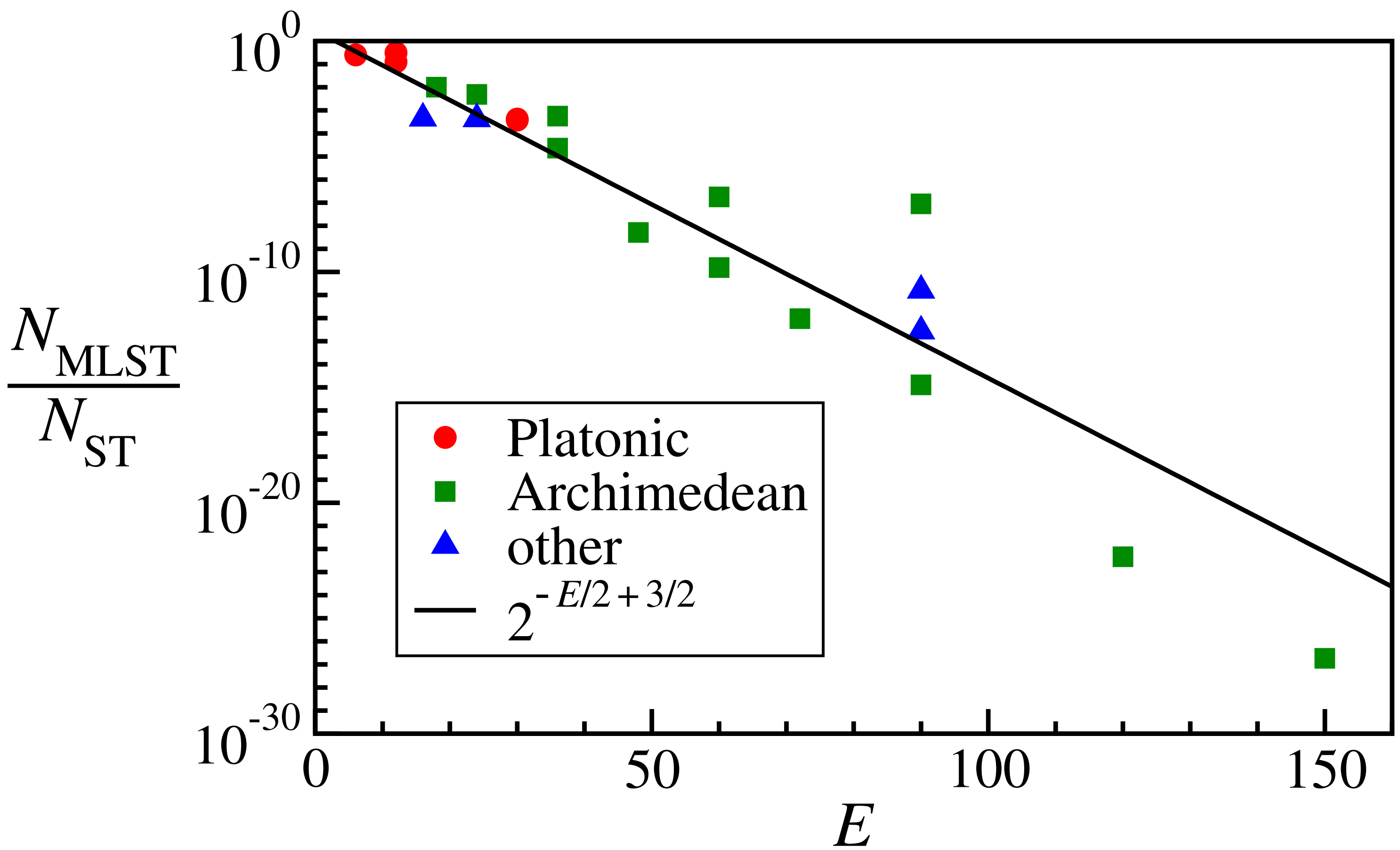
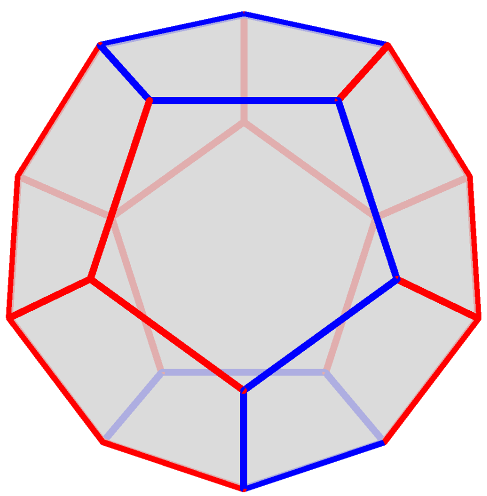
Fraction of optimal nets



dodecahedron

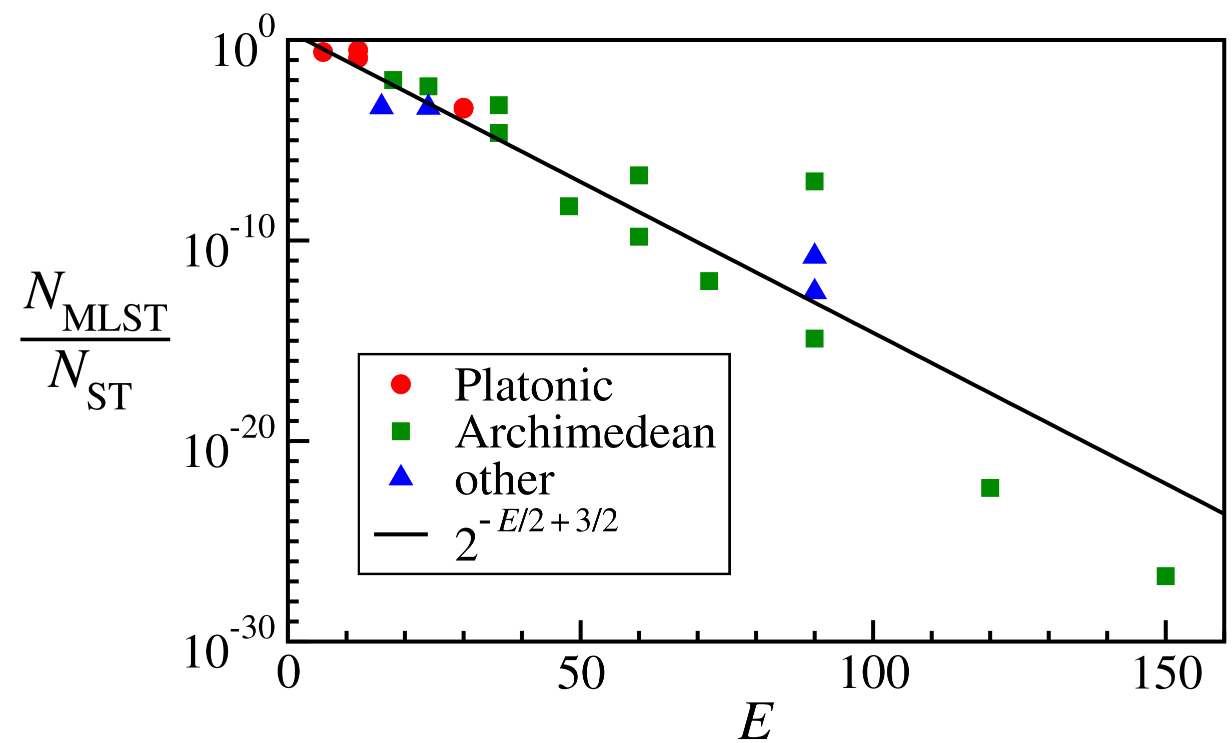


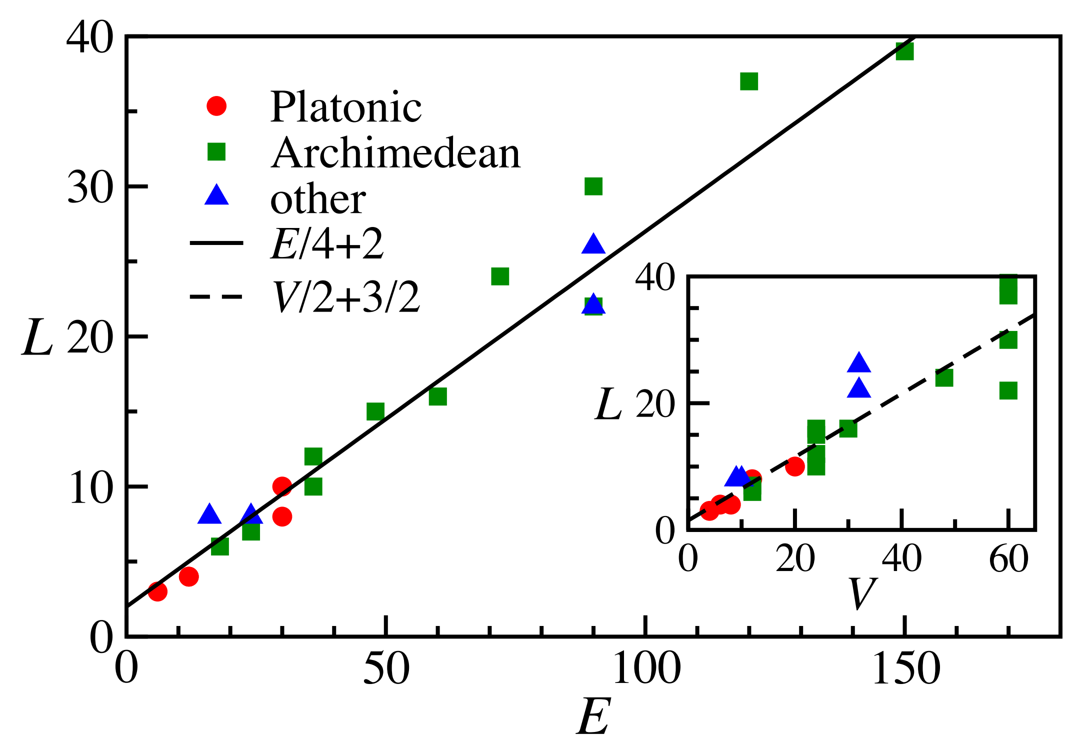
1980 MLSTs
+5 million STs
~0.04% (1/2500)

*The use of **random methods** is practically **impossible** for large shells.*

N.A.M. Araújo, R. A. da Costa, S. N. Dorogovtsev, J. F. F. Mendes, *Physical Review Letters* **120**, 188001 (2018)

Fraction of optimal nets (exponential decay)





upper bound:

$$N_{ST} = \binom{E}{V-1}$$

$$N_{MLST} = \binom{V}{L}$$

$$L \sim E/4 + 2$$

$$V \sim E/2 + 1$$

$$N_{MLST}/N_{ST} \sim 2^{-E/2+3/2}$$

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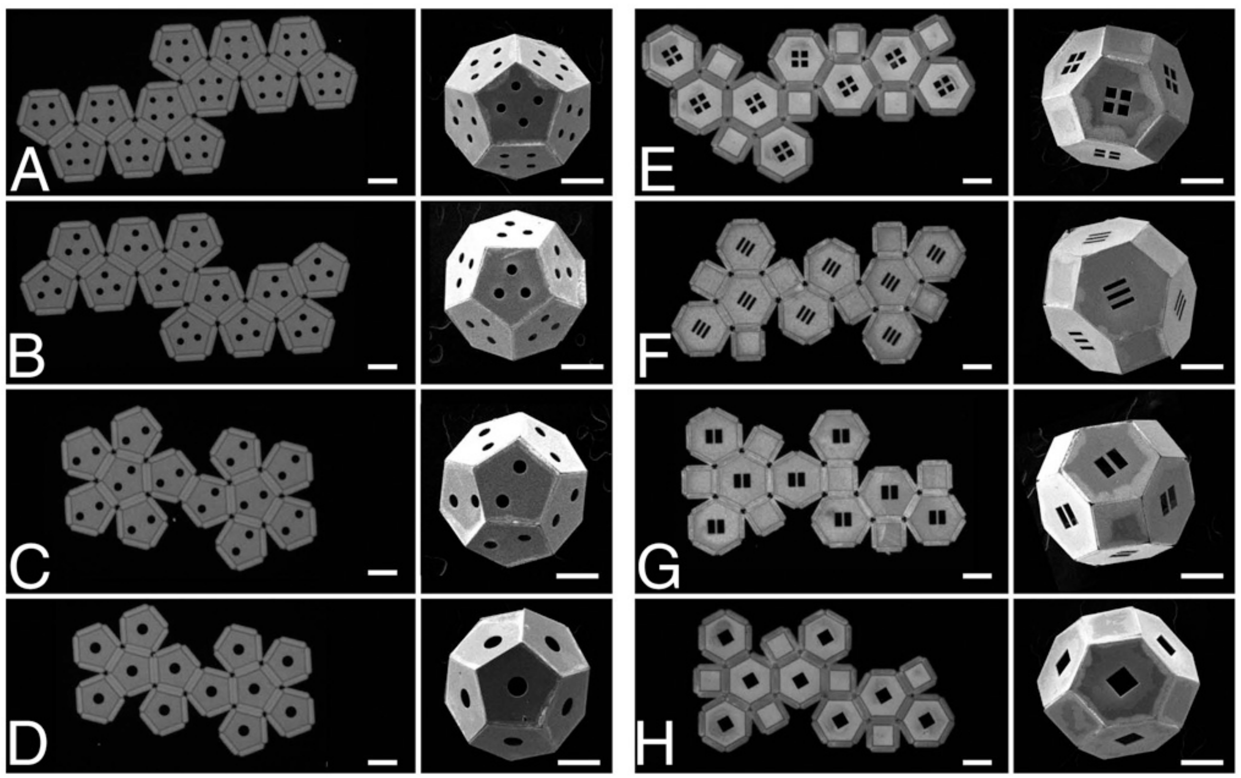
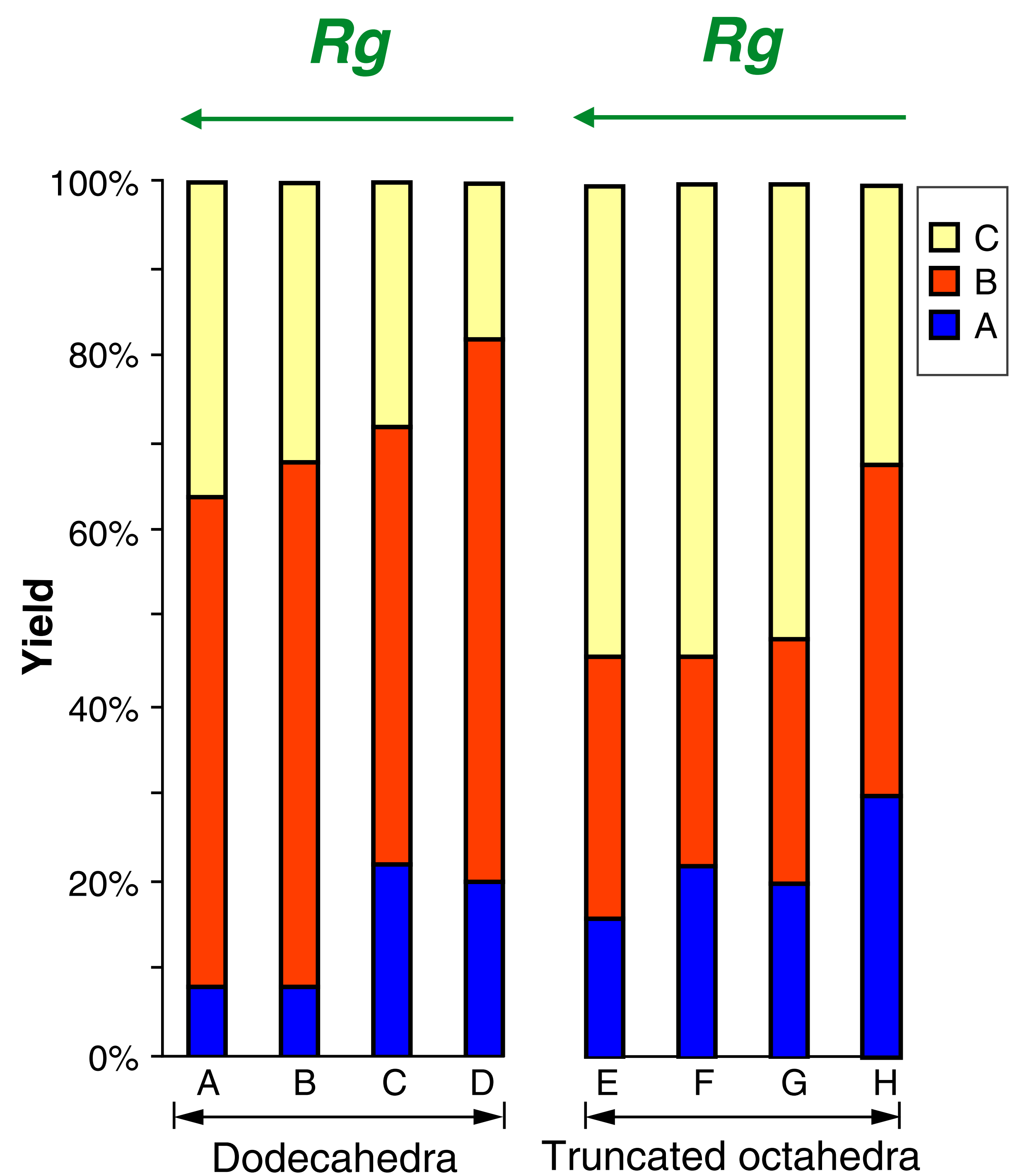
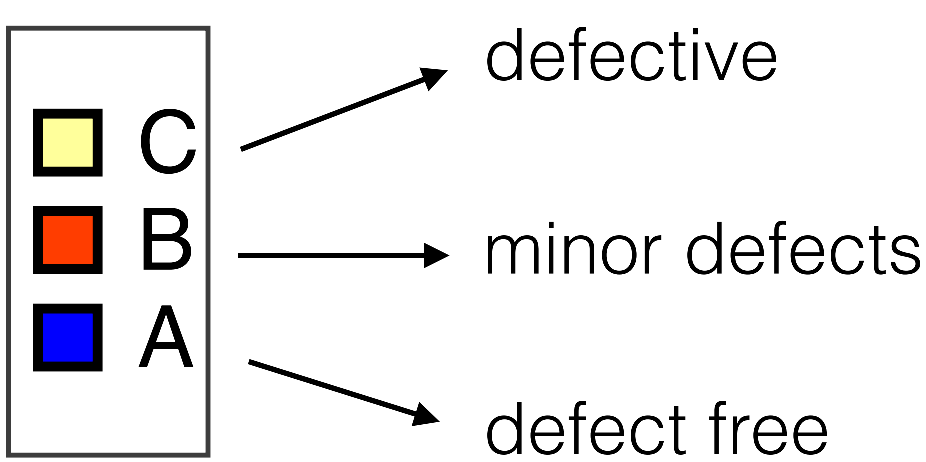
Second criterion (Radius of gyration?)







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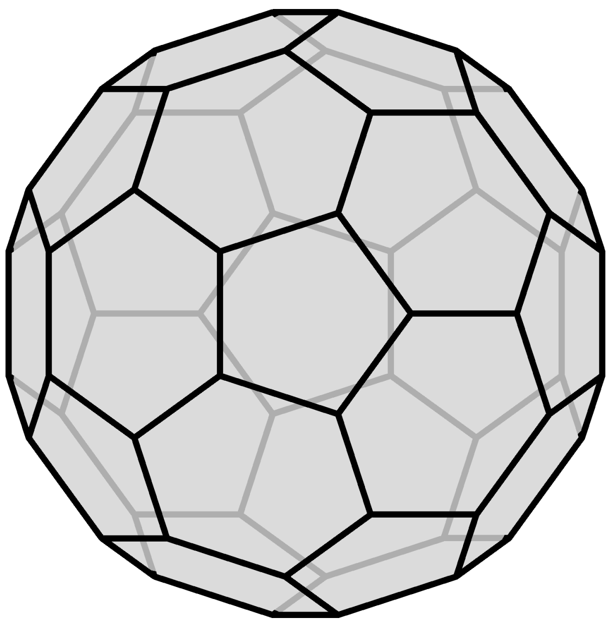
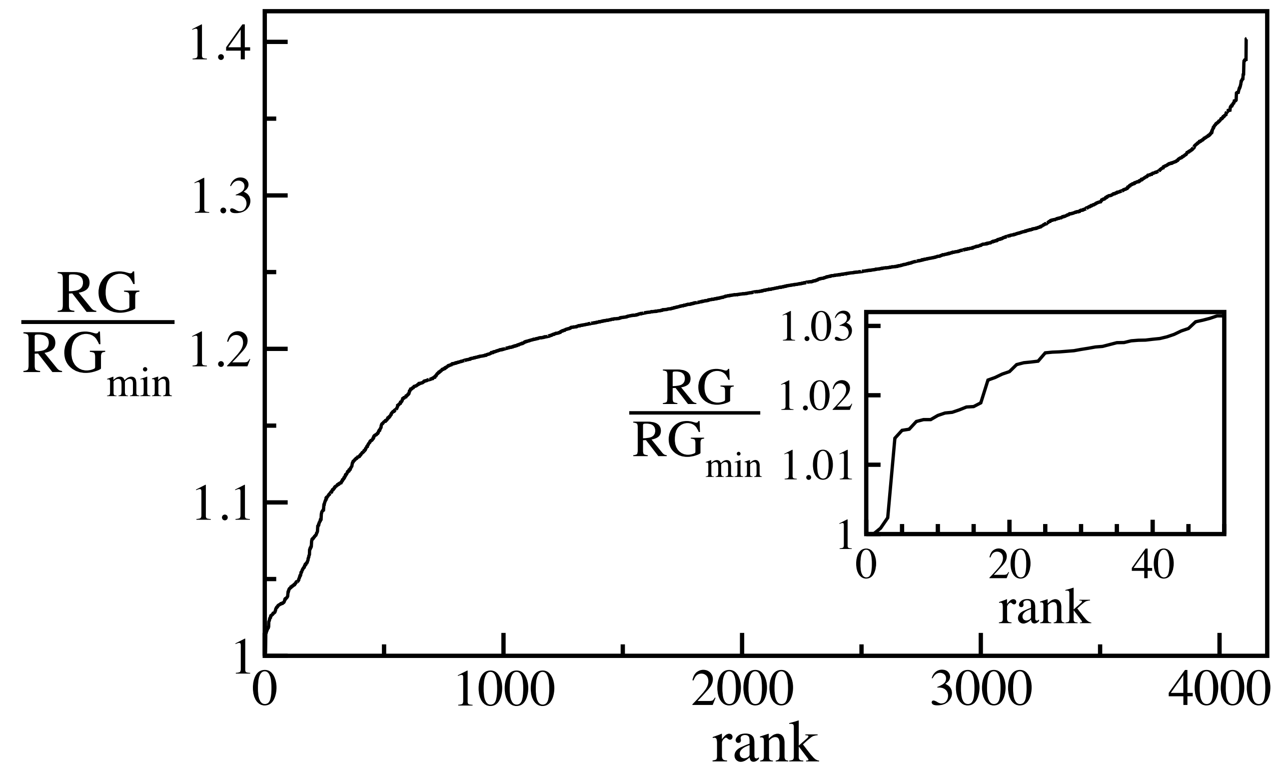
Second criterion (Radius of gyration?)

truncated icosahedron





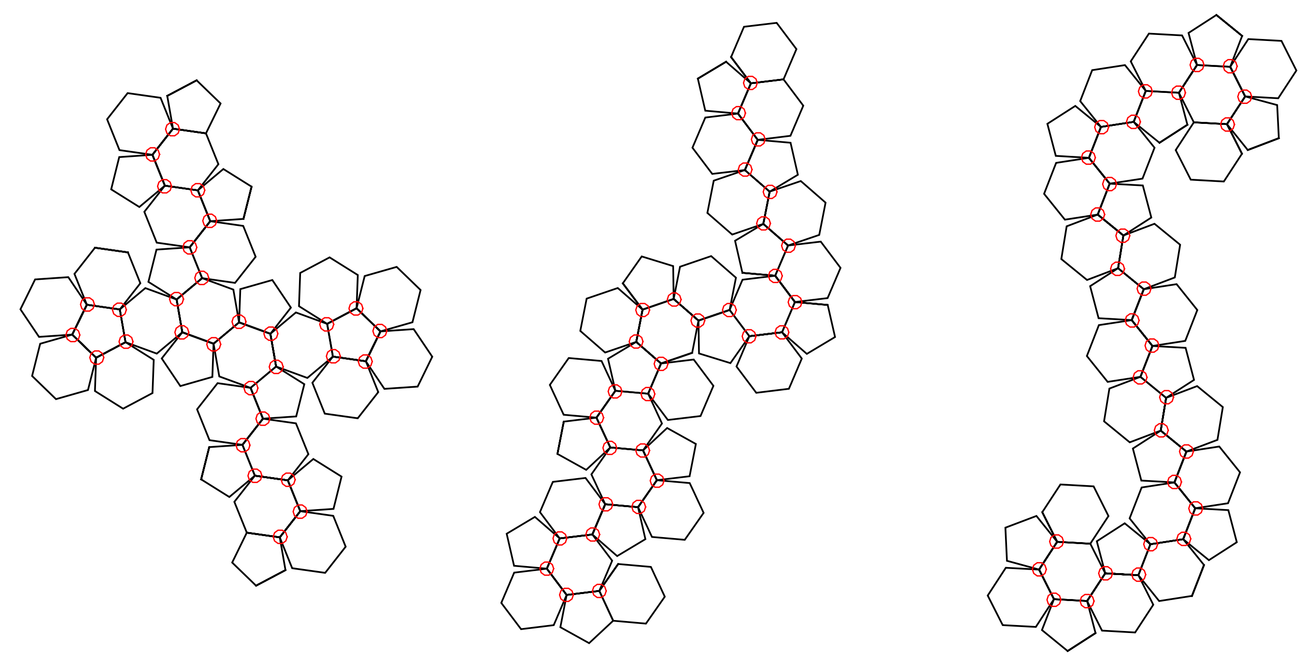
32 faces

60 vertices

90 edges

484 800 MLSTs

4114 nonisomorphic



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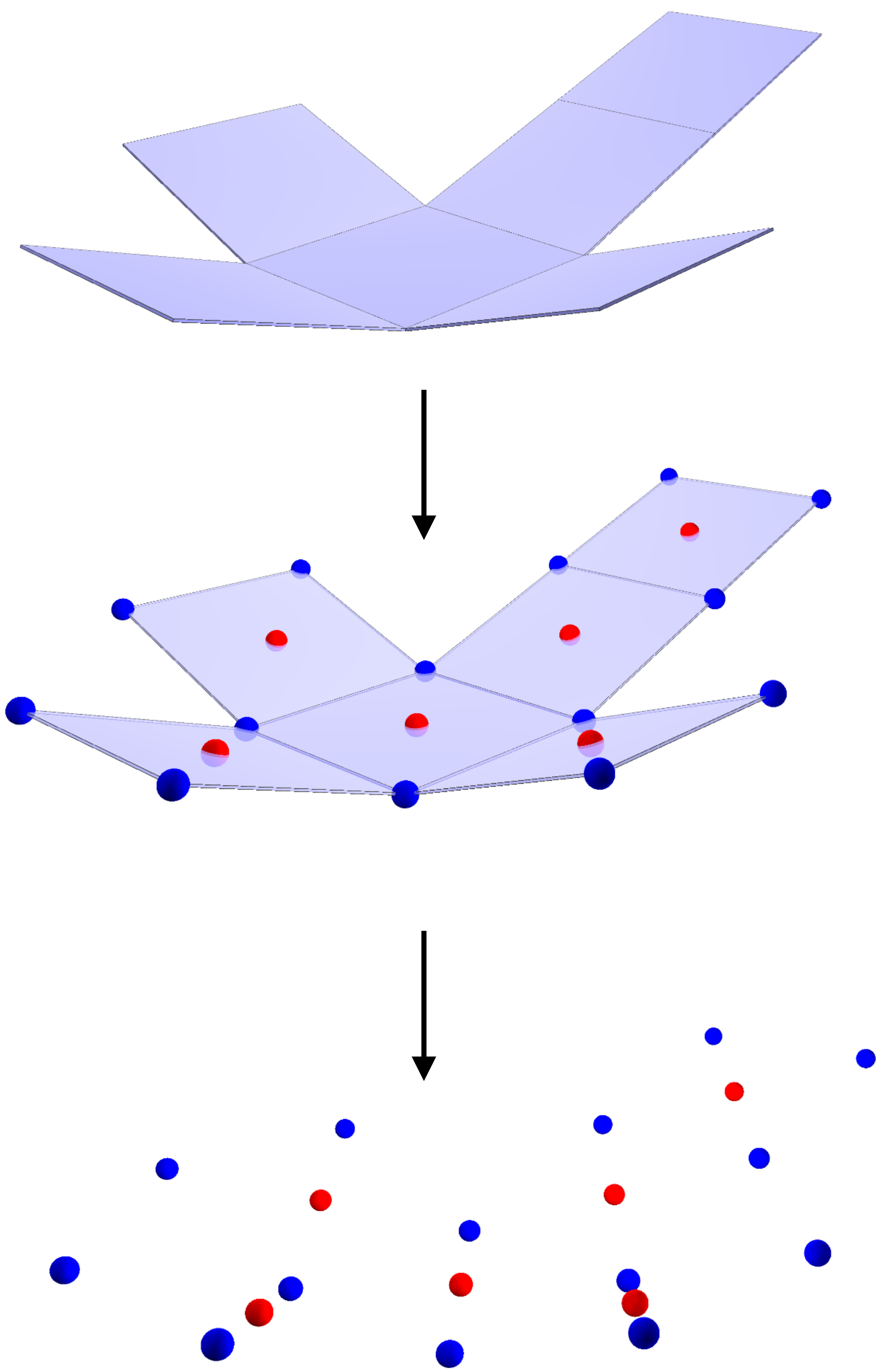
Numerical simulations



Yukawa type potential:

$$V_Y(r) = \frac{A}{k}\exp\left(-k\left[r-\left(R_i+R_j\right)\right]\right)$$

Inverse screening length

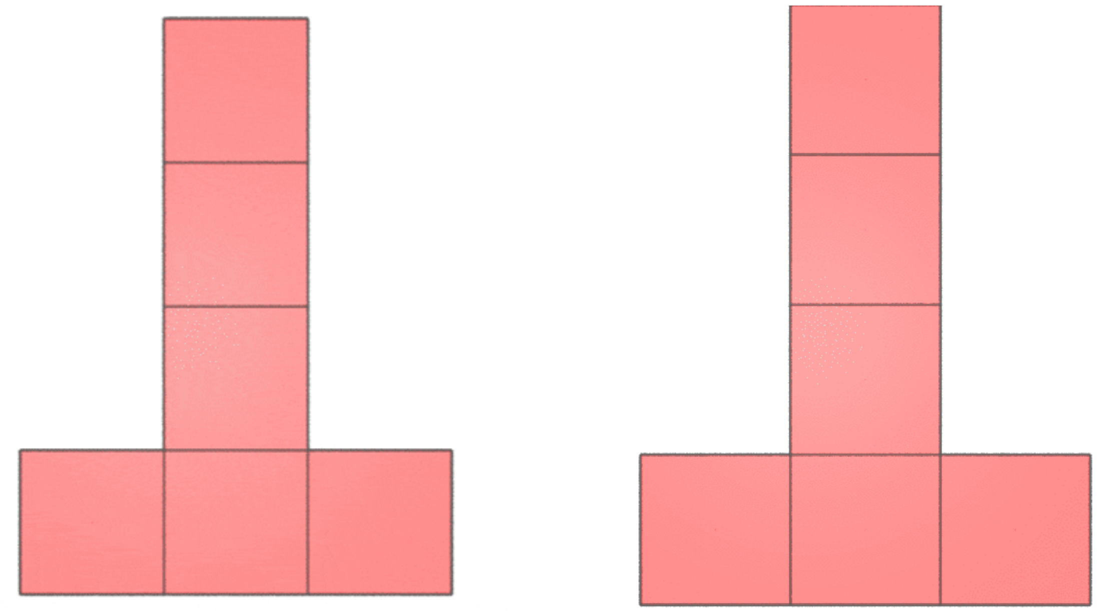
Gaussian potential

$$V_G\left(r_p\right) = -\epsilon\ \exp\left(-\sigma r_p^2\right)$$

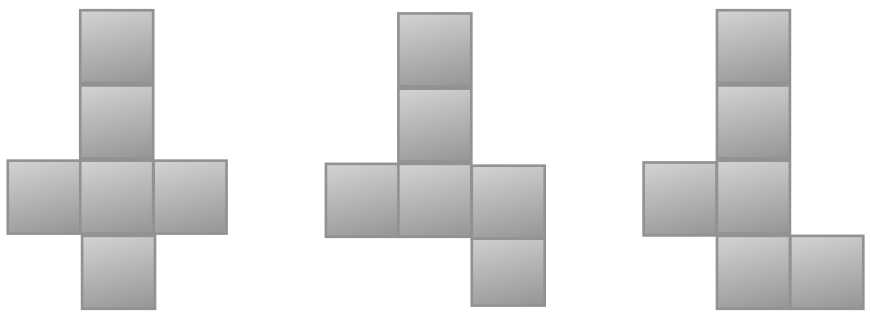
Energy well

Well width

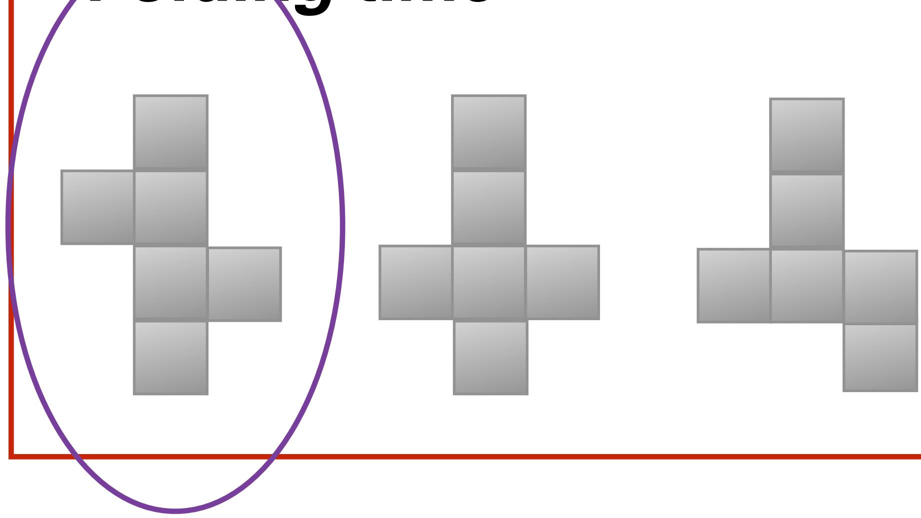
Optimal nets

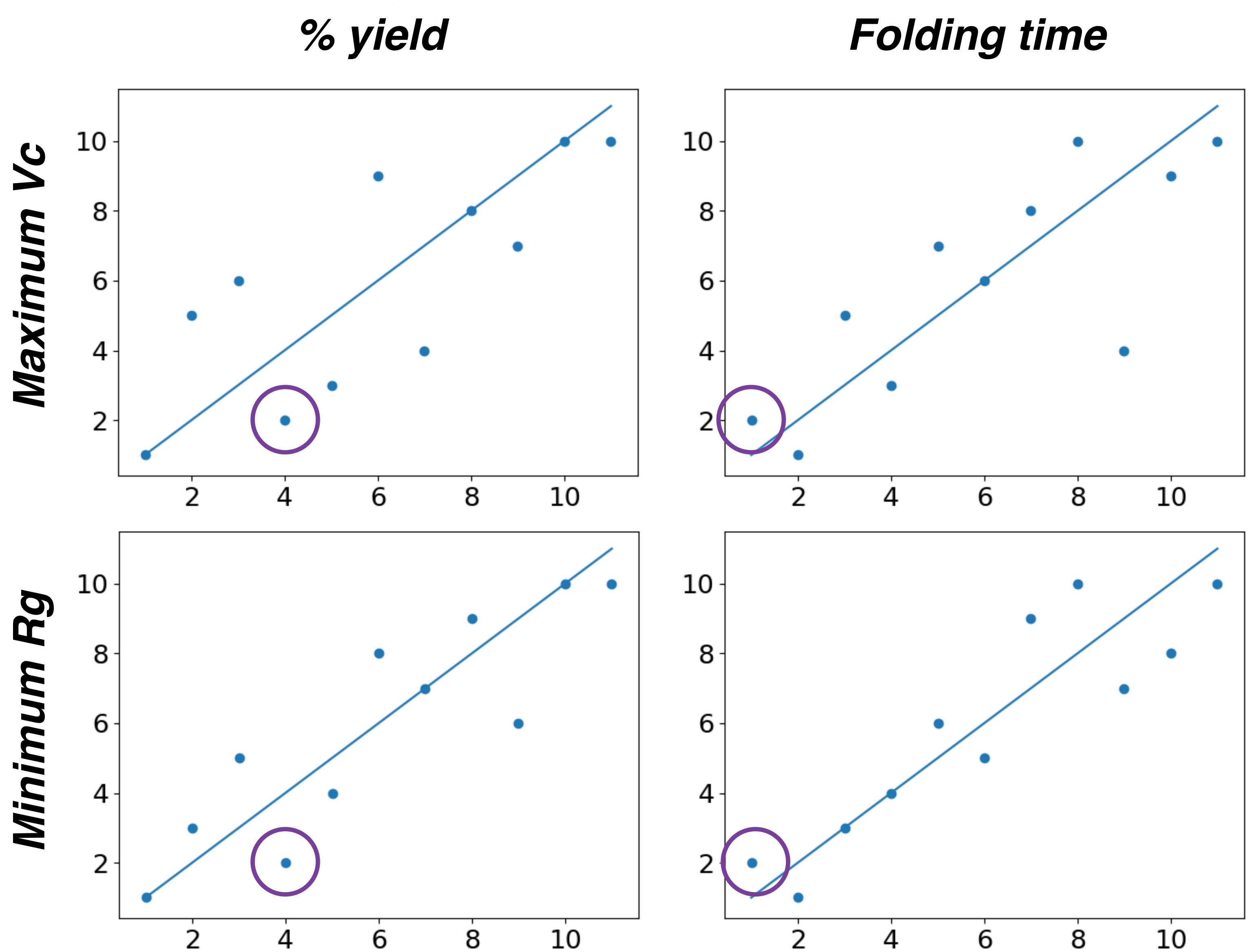


% yield

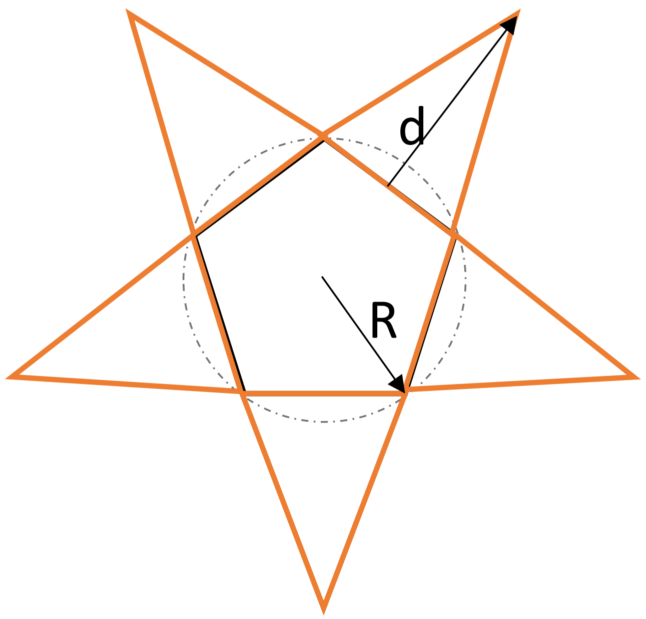


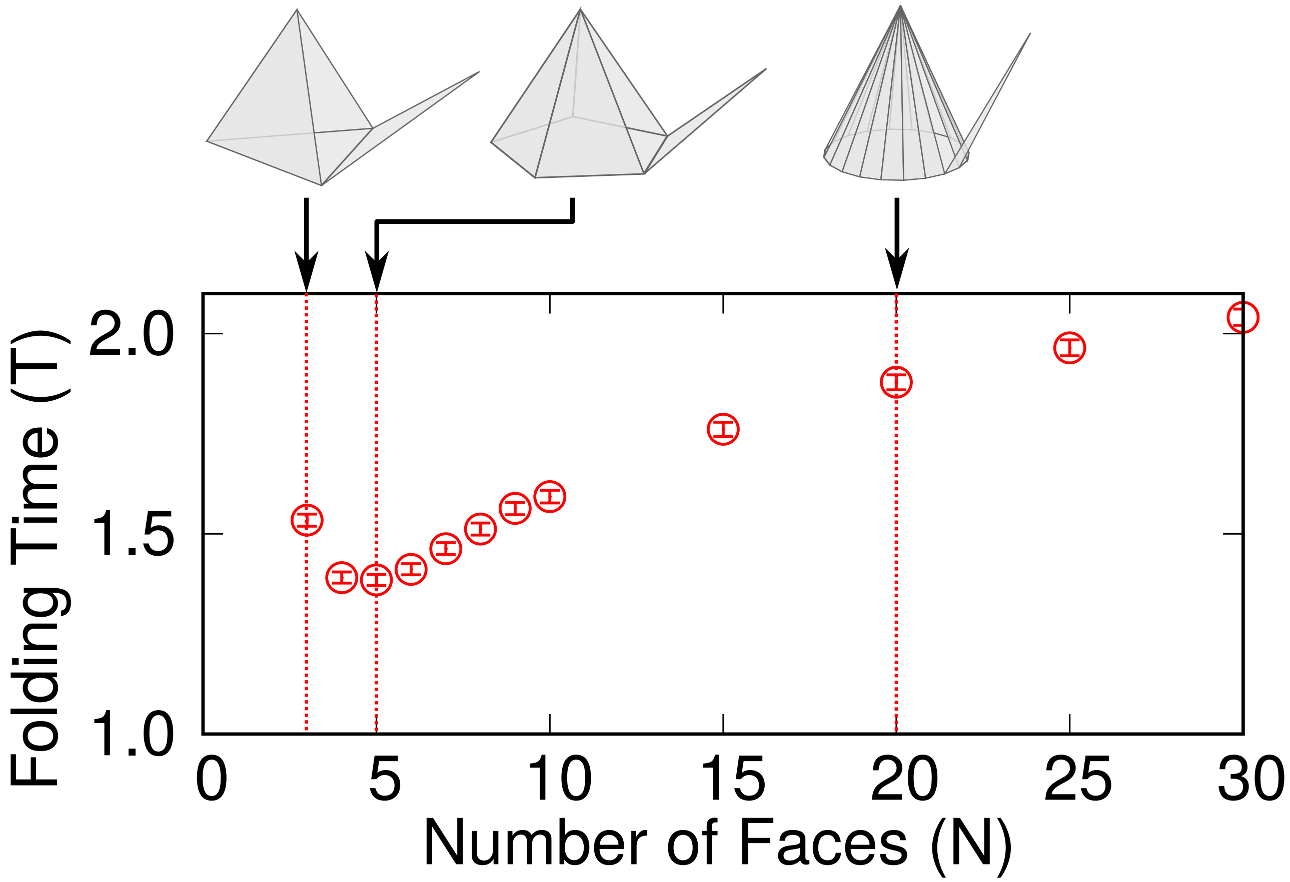
Folding time

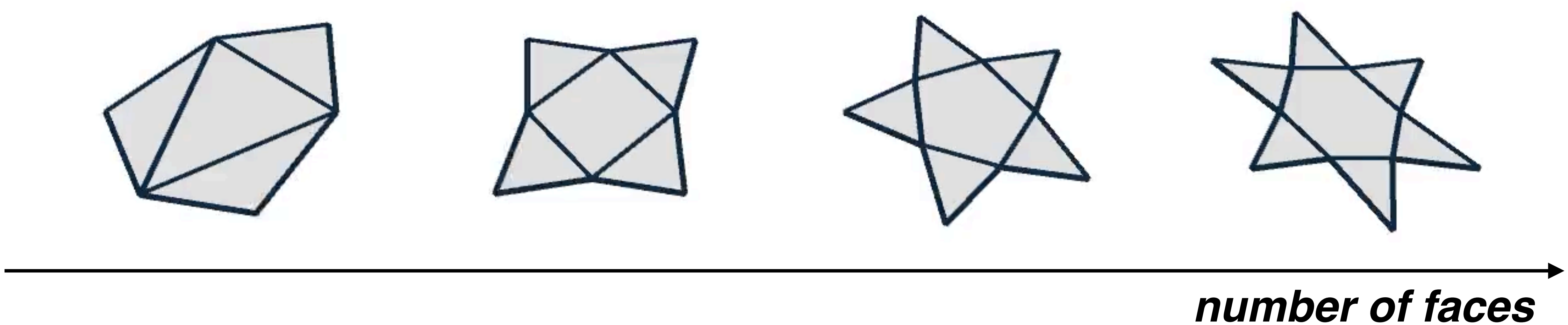




Folding time







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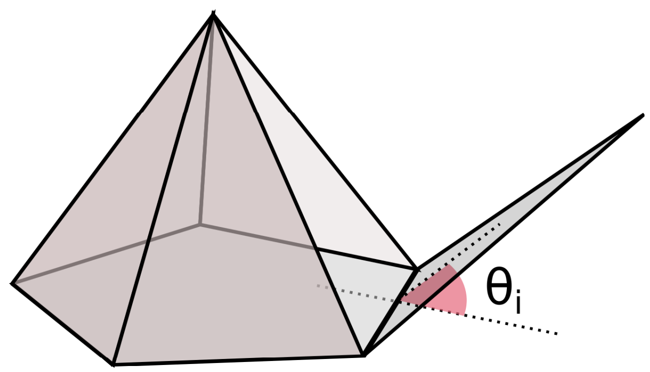
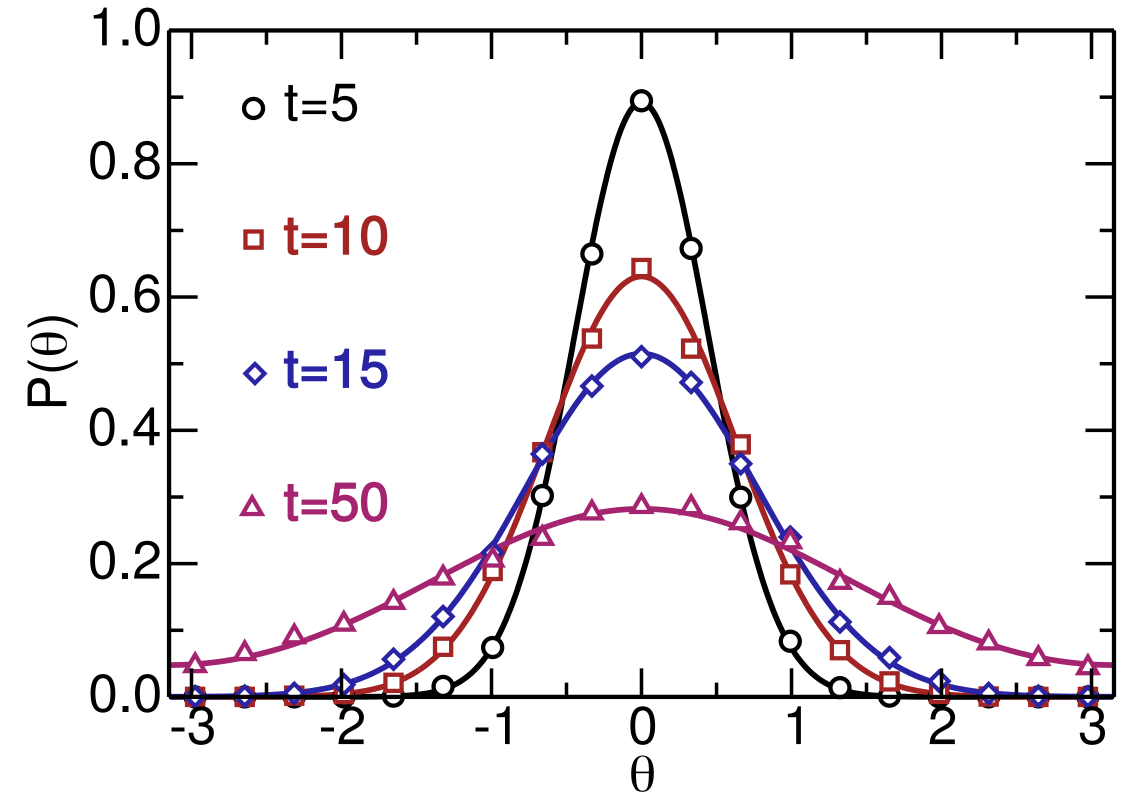
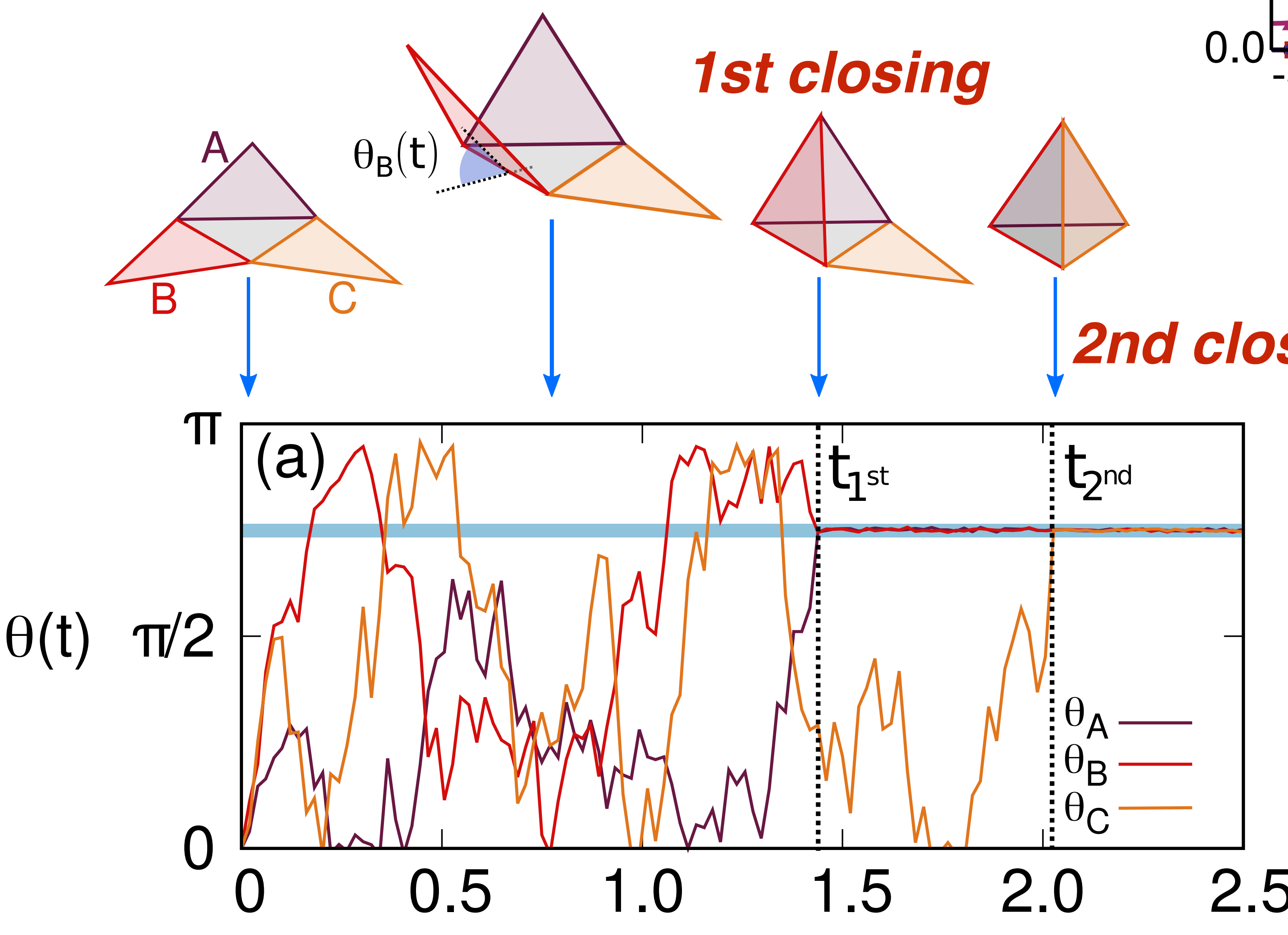
Trajectories of the panels

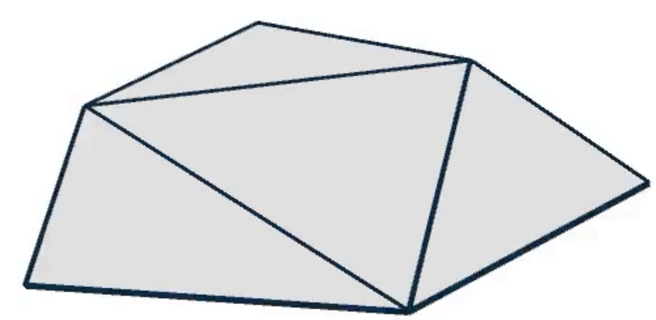




1st closing

2nd closing





Confined random walk

3 faces

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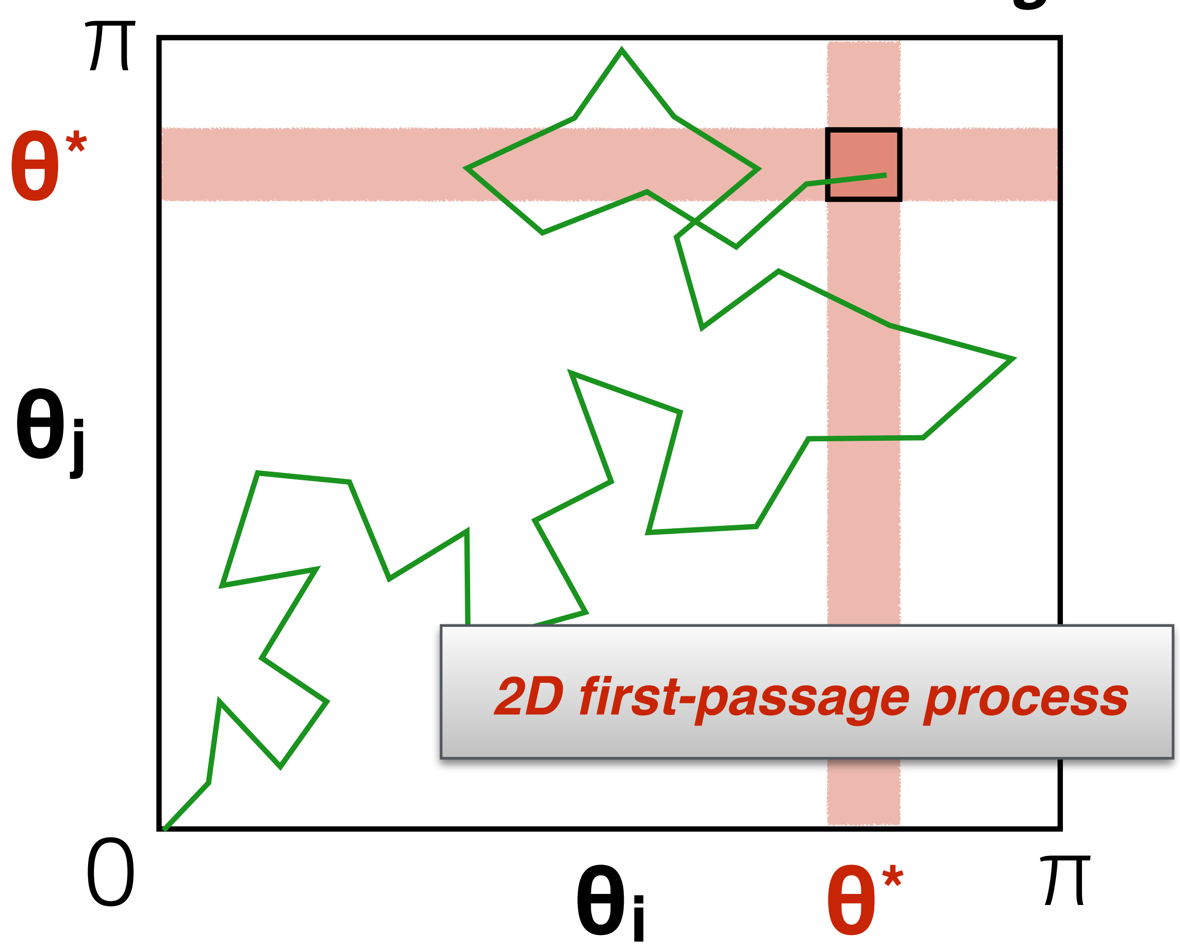
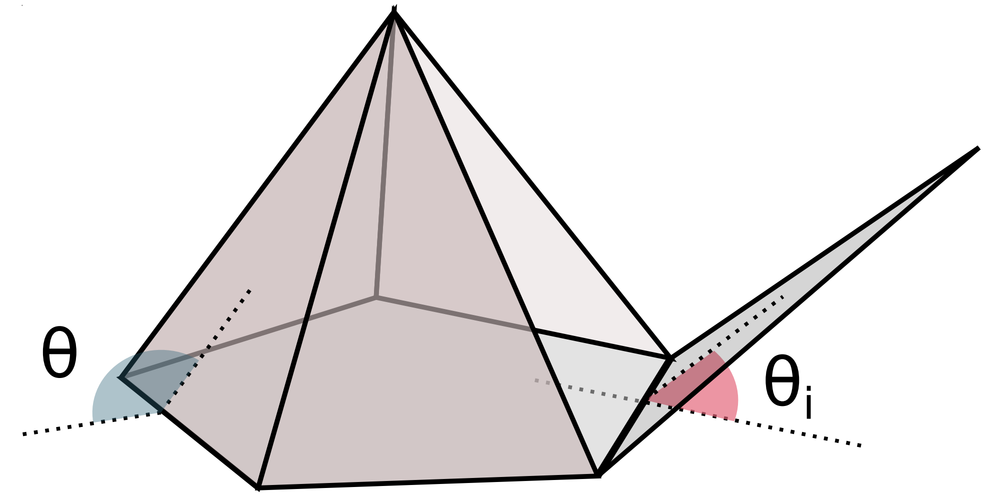
Closing events

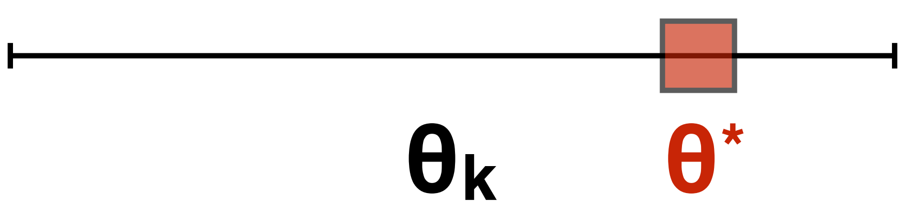
first closing





$$t_{\text{first}} \sim 1/\ln\left[N(N-1)/2\right]$$

other closings



1D first-passage process

$$t_{\text{folding}} \sim \tau \ln\left[N-2\right]$$

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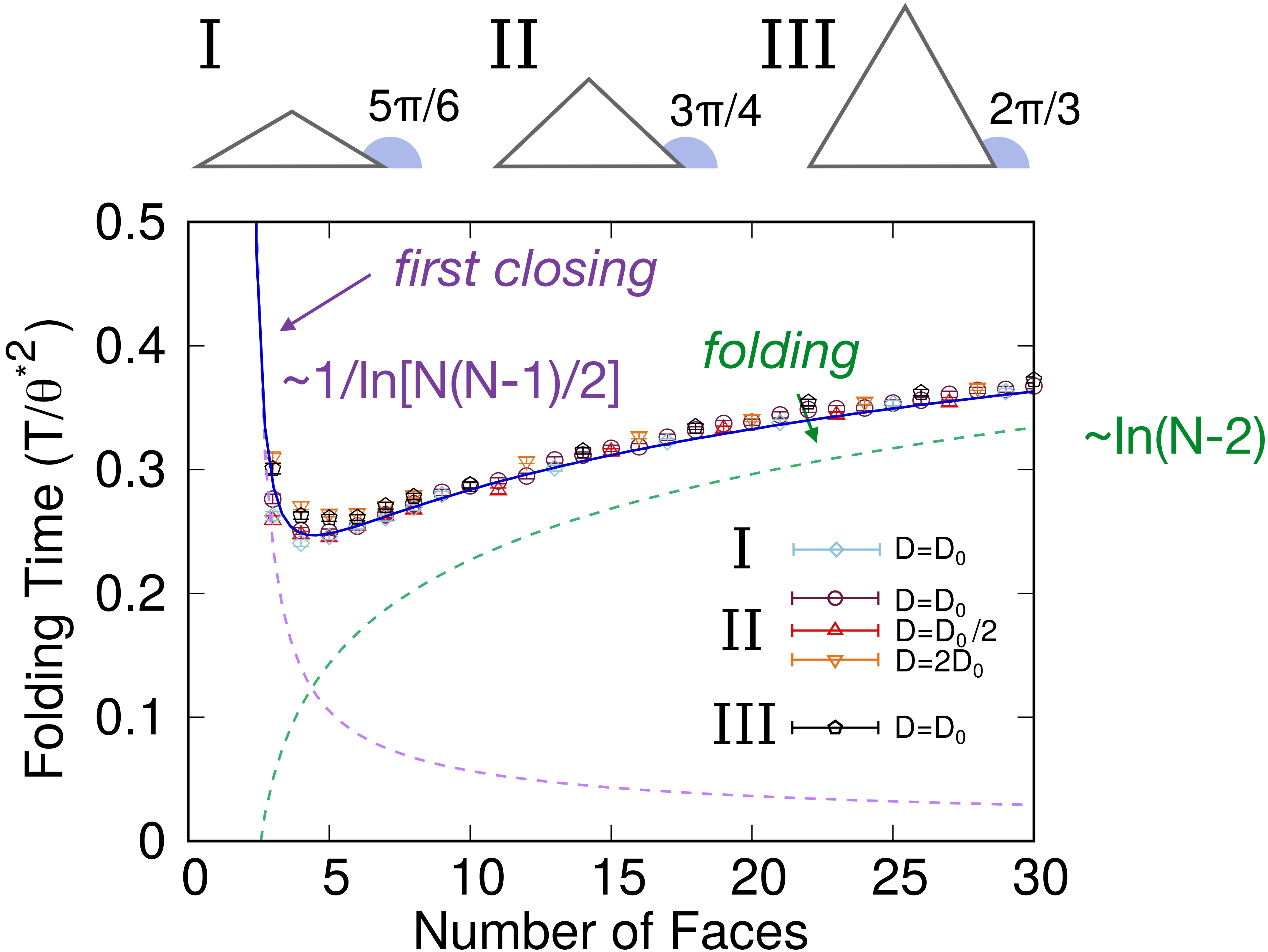
Two time scales



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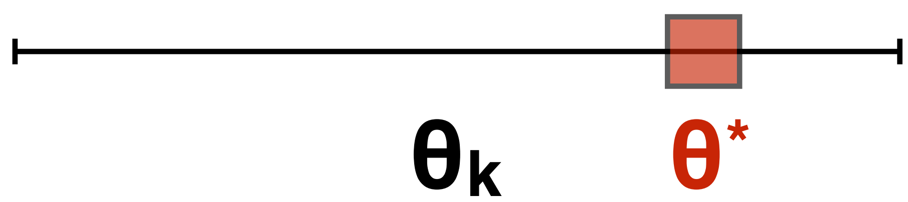
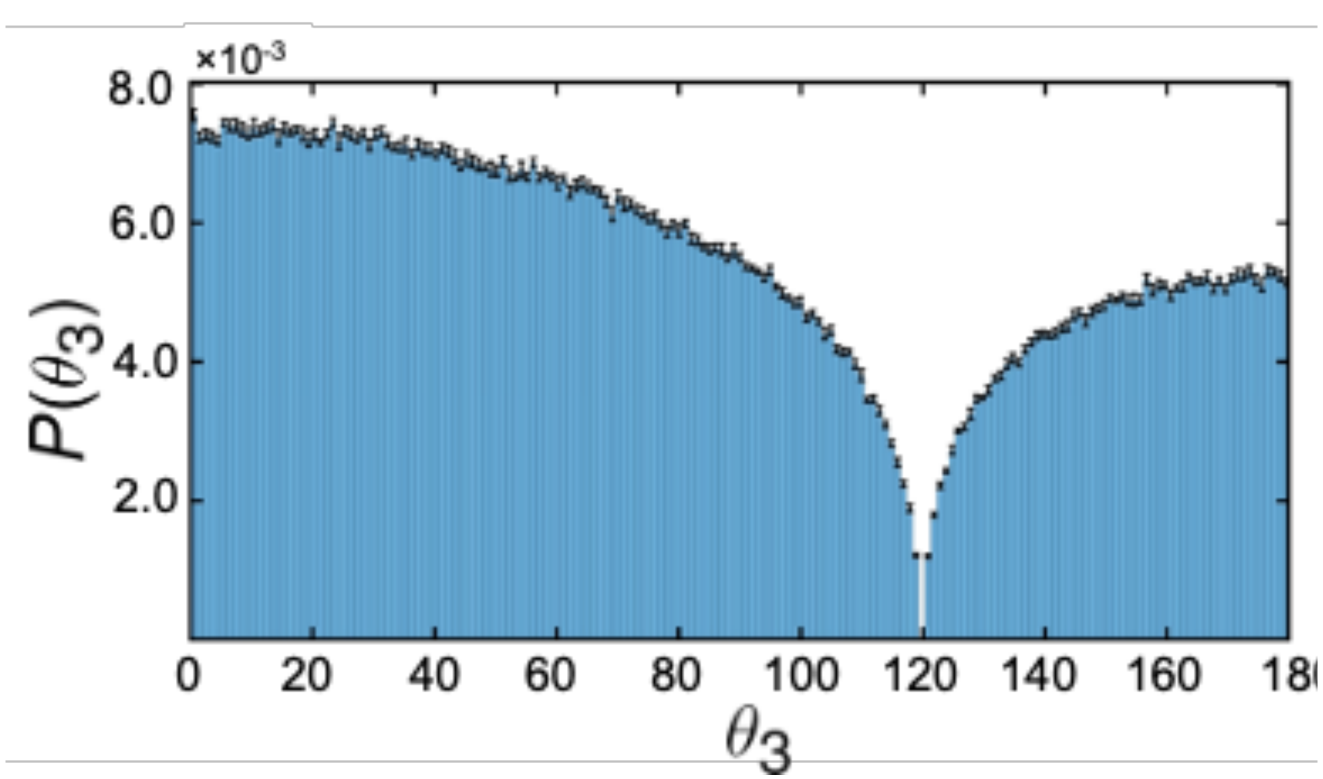
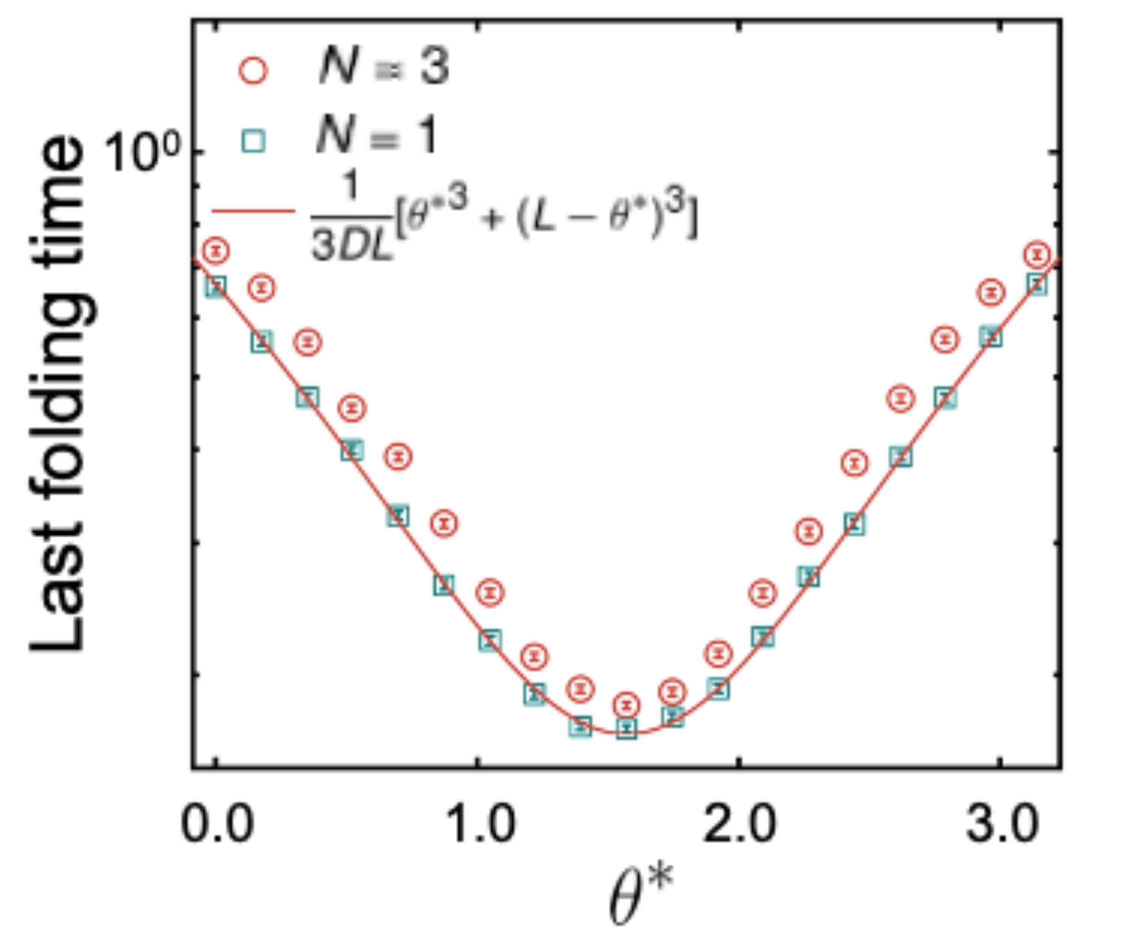
Food for thought: 3 faces



Where is the **third one**, when the first two close?





Final remarks

- ***Folding*** *at the microscale is a* ***N to M problem****;*
- *Finding the nets that maximize the* ***number of single vertex*** *connections corresponds to finding the* ***maximum leaf spanning tree*** *of the shell graph;*
- ***Our method*** *provides a* ***unique and optimal solution****;*
- *From the* ***complete list*** *of maximum leaf spanning trees it is possible to apply* ***other criteria****;*
- *The* ***optimal net*** *does* ***not have the lowest folding time****;*
- *The* ***folding time*** *is a* ***non-monotonic*** *function of the number of faces.*

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T. S. A. N. Simões, H. P. M. Melo, N. A. M. Araújo. *The European Physical Journal E* **44**, 46 (2021)

Financial support from the Portuguese Foundation for Science and Technology (FCT) under Contracts no. UIDB/00618/2020, UIDP/00618/2020, and PTDC/FIS-MAC/28146/2017 (LISBOA-01-0145-FEDER-028146).

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