3-PERIODIC MINIMAL SURFACES AND NETS: BRIEF SUMMARY NOTES, EXERCISES

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1. Surface topology

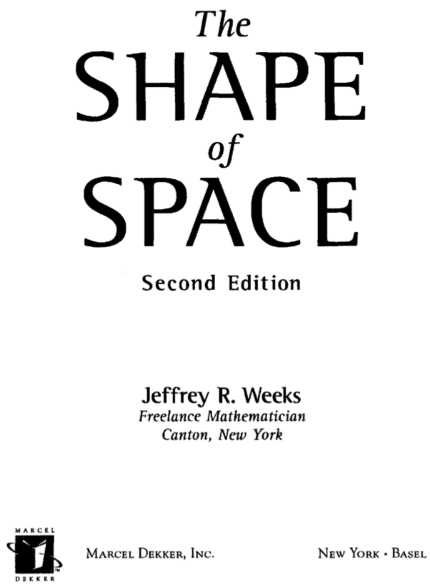
The
SHAPE
of
SPACE
Second Edition

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Figure 1. A recommended introduction to topology and surface geometry, by Jeffrey Weeks [14]

- **Euler-(Poincaré) characteristic, χ.**
The sum of the number of faces F, edges E and vertices V for conventional polyhedra is given by **Euler's Theorem**:

$$F - E + V := \chi$$

For usual (hole-free) polyhedra, $\chi = 2$, regardless of the polyhedron.
Clearly we can deform the faces and edges as much as we want, as long as we don't change our total count of vertices, edges and faces, and χ remains unchanged. This is therefore a topological measure.

Exercise 1: The buckminsterfullerene molecule, C_{60} , consists of pentagonal and hexagonal carbon rings, with each atom bonded to three neighbours. How many rings are there in each molecule?
(*Hint* "Rings" are faces, i.e. "F". And the number of edges, "E" can be calculated from the number of vertices, "V" and the valency / coordination number / degree of each vertex.)

Exercise 2: Determine the Euler characteristic, χ and genus of the deltahedron shown in Fig 2. See `http://www.ac-noumea.nc/maths/amc/polyhedr/Stewart_.htm` for a 3D animation (also `http://www.uwgb.edu/dutchs/symmetry/stewart.htm`) or – better – build the polyhedral model yourself.

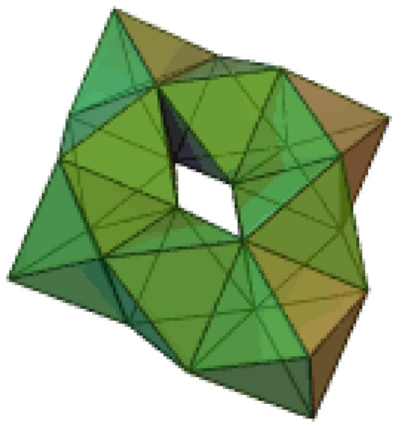


FIGURE 2. A toroidal triangular polyhedron(a *deltahedron*, from [12]).

Exercise 3: What are the genera (g) of the multiple-genus polyhedra in Fig. 3? Work out the value of χ for each from the number of faces, edges and vertices, using Euler's Theorem.

Exercise 4: Find cap&pants decompositions of the surfaces in Fig. 4 to establish topological equivalence.

Exercise 5: Compute the genus per conventional unit cell of some infinite (regular triangular) polyhedra (or "deltahedra") shown in Fig. 5. (Images from [1].) Many of these are well-known to crystal chemists. Determine the 3-periodic minimal surfaces that can be triangulated to form nets corresponding most closely to the patterns shown in the images.

(1) 3^7: This is a fascinating structure and is reported in [10] as the lowest density sphere packing known (thereby refuting a claim by David Hilbert [5]!). Vertices at

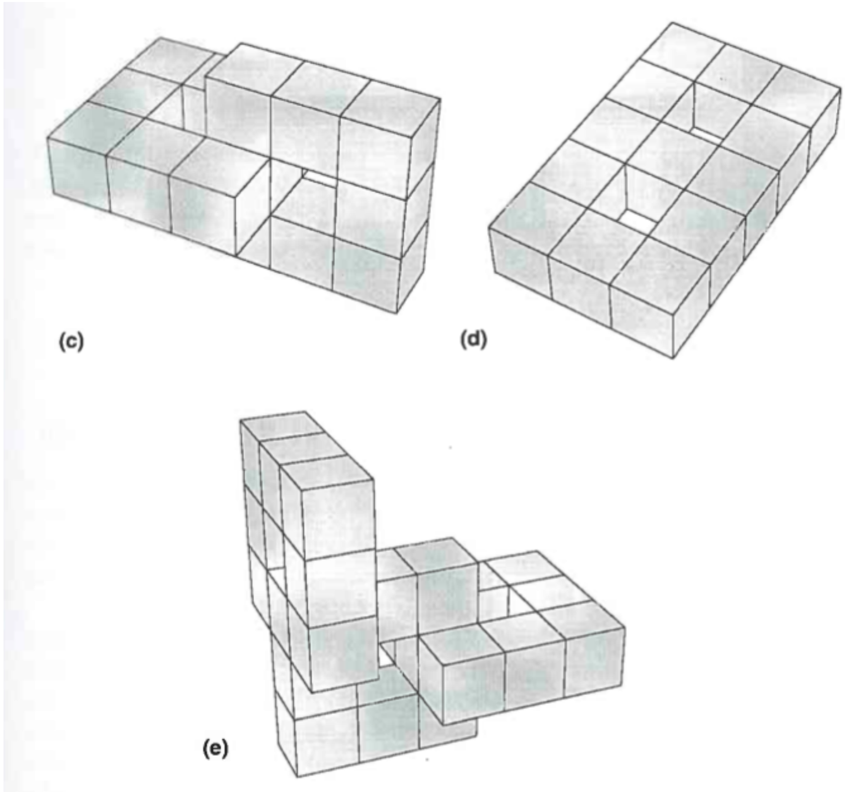


FIGURE 3. Some topologically non-trivial polyhedra, from [7].

$\{x, y, z\} = \{0.032, 0.125, 0.2755\}$ in $Fd\overline{3}$ (2nd origin setting 2nd origin setting in International Tables). (Lattice parameter $a = 5.376$ for spheres of unit diameter, see, [10], page 281).

(2) 3^8: the *pyrochlore* structure. Vertices at *48f* sites of the space group $Fd\overline{3}m$, $\{0.412, 0.125, 0.125\}$ and equivalents sites (2nd origin setting in International Tables). (Lattice parameter $a = 3.771$ for (almost equal) spheres of unit diameter (with small variations), see, [10], page 236).

(3) 3^8: partial structure of Zn atoms in the $NaZn_{13}$ structure. Vertices at $96i$ sites of the space group $Fm\overline{3}c$, $\{0, 0.176, 0.114\}$ and equivalent sites. (Lattice parameter $a = 4.570$ for spheres of unit diameter, see, [10], page 273).

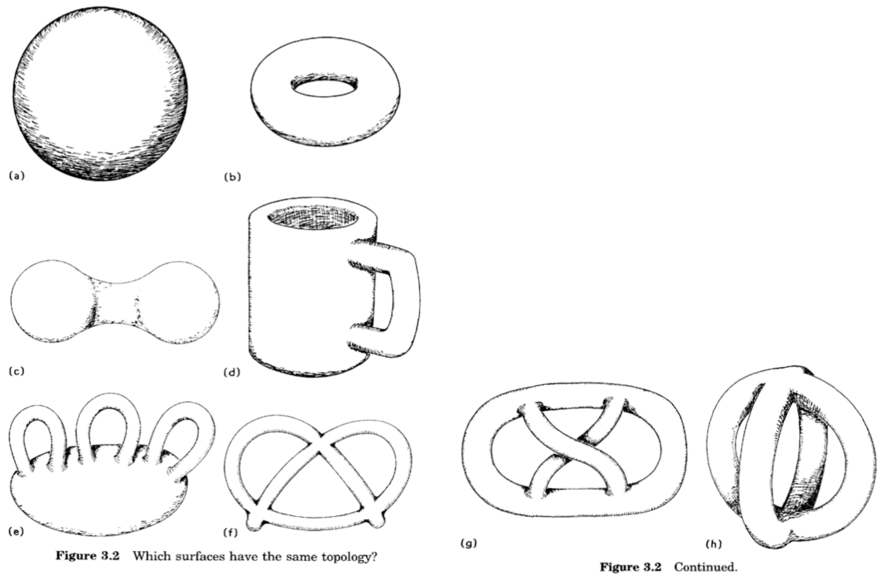
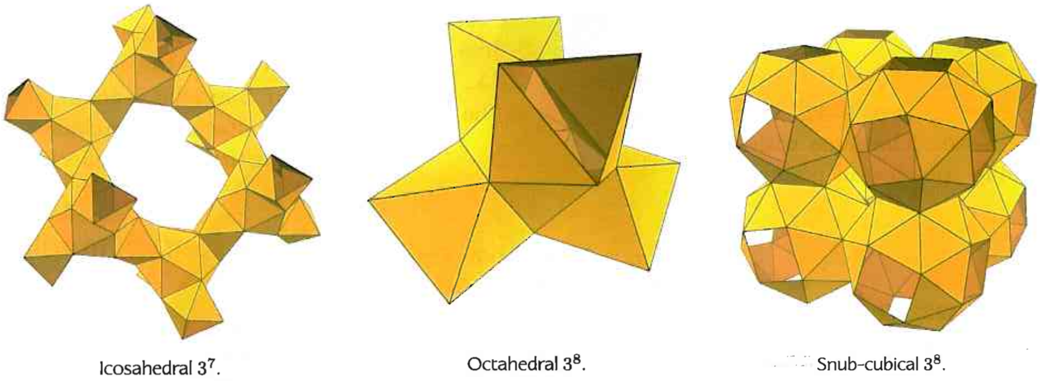


FIGURE 4. from [14]



(1) (2) (3)

FIGURE 5. Some infinite polyhedra composed of triangular faces only ('deltahedra').

2. 3-Periodic minimal surfaces (TPMS) and labyrinth graph pairs: bicontinuous structures

- Minimal surfaces: mean curvature $H = 0$

  The grandfather of TPMS were the great 19th century mathematicians, Bernhard Riemann and Hermann Amandus Schwarz. Their findings lay dormant, until Alan Schoen's remarkable studies in the 1960's, later described in a NASA Technical Note [11].

  A collection of minimal surfaces, sorted by periodicity and genus (per unit cell), can be viewed at Matthias' Webers site
  `http://www.indiana.edu/ minimal/archive/index.html`

  A gentle introduction to minimal surface theory is [6]; more rigorous crystallographic papers, with detailed analyses of non-cubic 3-periodic minimal surfaces are [3],[9] (and references therein). A text on TPMS for materials scientists is not yet available (we are working on one provisionally entitled *Superficial Geometry*); books by Hildebrandt *et. al* give an exhaustive mathematical survey of the broader area of minimal surfaces in general [2]; Karcher and Grosse-Brauckmann have analysed many of Schoen's TPMS to rigorously their existence, [8, 4]

  Useful approximations to TPMS are afforded by *nodal surfaces*, see [13].

Exercise 6: Model-building.

(1) Pack the white "saddle polyhedra" to construct

a space-filling pattern

Two distinct 3-periodic minimal surfaces. Name these surfaces.

(2) Construct a primitive and conventional unit cell of the gyroid surface using the curved triangular tiles. (There are just enough tiles to build a single conventional unit cell of the two-coloured pattern, or two primitive unit cells.) Determine the site symmetries at the tile vertices and the mid-point of the longest edges.

Exercises 7 (to explore at your leisure): Using *Surface Evolver* software.
(`http://www.susqu.edu/brakke/evolver/evolver.html`)

You need to download an install the *Surface Evolver* freeware to run these examples (see the url above for details). Input data files have been posted at
`https://files.me.com/sth4minsurf01/im2irw`

Starting out with Evolver examples

(1) open either the Windows (.bat) file `evolve dia-c-fstuck` or (Unix or Mac) open `d-fs-solo.fe` within *Evolver*.

- look at the starting surface and its bounding skew hexagon, which is the Petrie

polygon of a cube.
- evolve by typing `go5` into the command window, explore the result
- evolve again by typing `go5` into the command window
-look for straight lines in the surface; deduce the smallest linear polygonal boundary for $dia - c$ and the D surface

(2) open <u>either</u> the Windows (.bat) file `evolve dia-c` <u>or</u> (Unix or Mac) open `d-cells.tfe` within *Evolver*.

- explore the initial Voronoi partition:
-type `o`, retype `o` to toggle on and off the bounding cube
-type `f` to remove faces; thicken or thin edges by pointing cursor in graphics window and typing `+` or `-`
- move cursor back to command window; evolve by typing `g5` into the command window, explore the result
-type `g10` into the command window, explore the result
-type `go5` into the command window, explore the result
-Look for the network of straight lines in the D surface: fit the linear polygons of the previous example
-type `cstar` into the command window, explore the result (toggle on bounding box, if necessary)
-to rescale the image, move cursor to graphics window, type `z` and slide cursor horizontally with mouse button held down; type `r` to return to 3D rotate mode
-Look for the network of straight lines in the D surface: fit the linear polygons of the previous example

(3) open `evolve dia-c-plus-fstuck` (Windows)or within *Evolver*, open `d-cells-plus-fstuck.tf`
(Unix or Mac)
-check the structure by evolving as in previous examples.

(4) open `evolve pcu-c-fstuck` (Windows) or (Unix or Mac) within *Evolver*, open `p-fs-solo.fe`
-repeat operations done for `evolve dia-c-fstuck` example
-can you find any extra lines in the surface?
-can you see what determines the presence of a line in the minimal surface?
-fit smallest polygonal boundary into a cube; extend through the cube

(5) open `evolve pcu-c` (Windows) or (Unix or Mac) within *Evolver*, open `p-cells.tfe`
-repeat operations done for `evolve dia-c` example
-fit the `evolve pcu-c-fstuck` example into the P surface
-check result by exploring `evolve pcu-c-plus-fstuck` file

(6) open `evolve srs-c` (Windows) or (Unix or Mac), within *Evolver*, open `g-cells.tfe`
-evolve as per `evolve dia-c` example
-any straight lines?

Absolute basics of *Evolver* to get going:

COMMAND WINDOW ("Enter command:" prompt)

#to do a minor evolution:
`gN`
(where N is the number of iterations, typically between 10-50)

#to refine the mesh before evolving:
`r`

#commmands can be combined, separated by a semi-colon, e.g.
`r; g10; r; g20`

#to add a bounding box:
`o`

#if you are stuck with a "Graphics command:" prompt:
`ex`
to get back to the main command window

#to get out (to load a new file, or to quit):
`q`
as often as necessary

#special commands for periodic models that change number of unit cells (dia, pcu, srs, tfa, ths, tfc, hms, cds) :
(single cell) `clipped`
(multiple cells) `lat1` or `lat2` or `cstar`
(courtesy of Christophe Oguey: use sparingly to avoid huge processing overheads)

GRAPHICS WINDOW COMMANDS (type while cursor is in graphics window) (all options available on *Windows* with rightb-click mouse?)

#3D rotation mode (default)
`r`

#zoom mode
`z`

#spin mode
`c`

#3D rotation mode
r

#translate mode `t`

#to recentre image in graphics window `m`

#to view / hide (black) edges in Voronoi faces
toggle `e`

#to view / hide surface (leaving the only the labyrinth graph)
toggle `f`

#to thicken/thin edges
`+` or `-`

commands documented at `http://www.susqu.edu/brakke/evolver/htbml/evolver.htbm#doc`

References

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