Isometric Diamond Subgraphs

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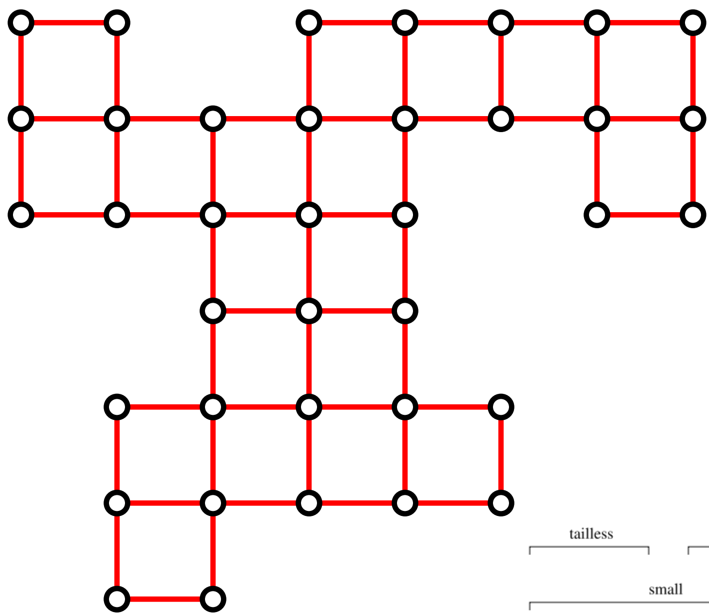
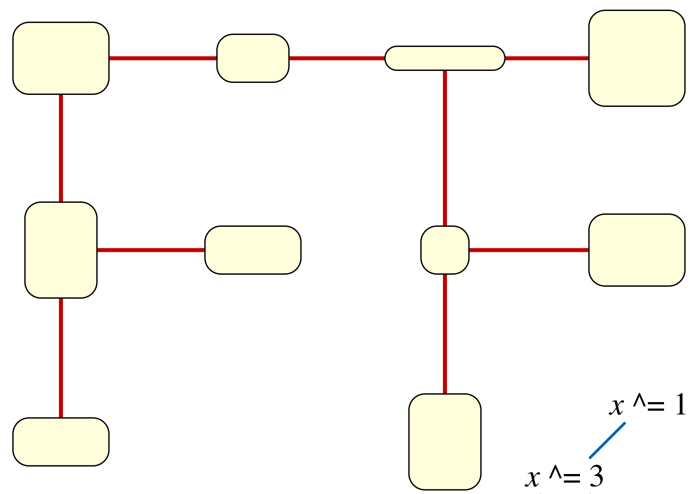
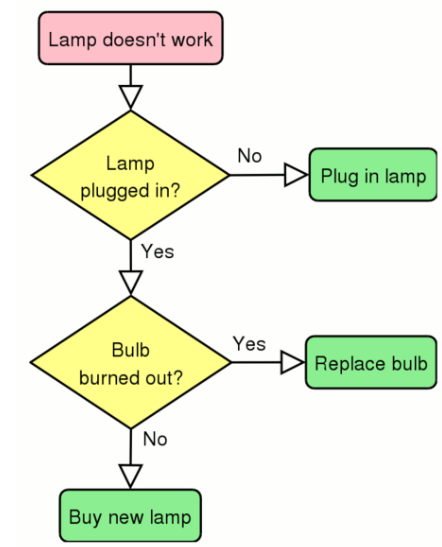
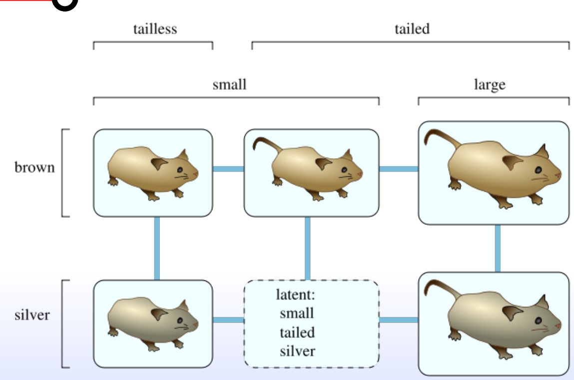
Starting point: graph drawing on an integer grid

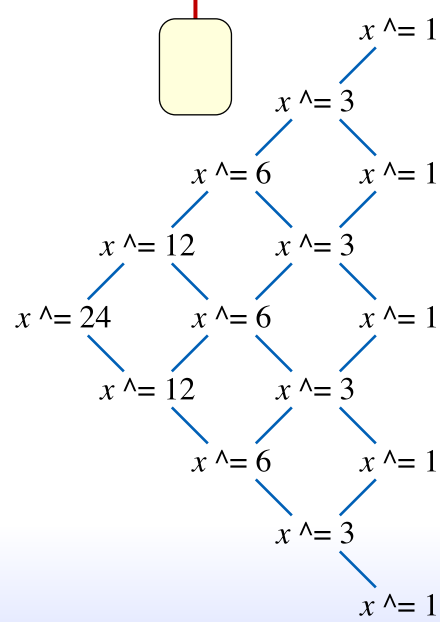
Vertex placement: points of two-dimensional integer lattice
Edges connect only adjacent lattice points











Integer grid drawings are high quality graph drawings

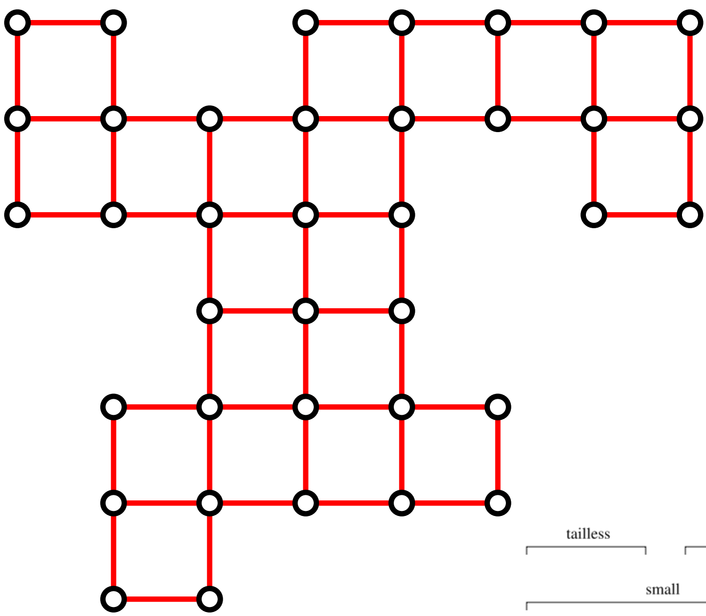
Uniform vertex spacing

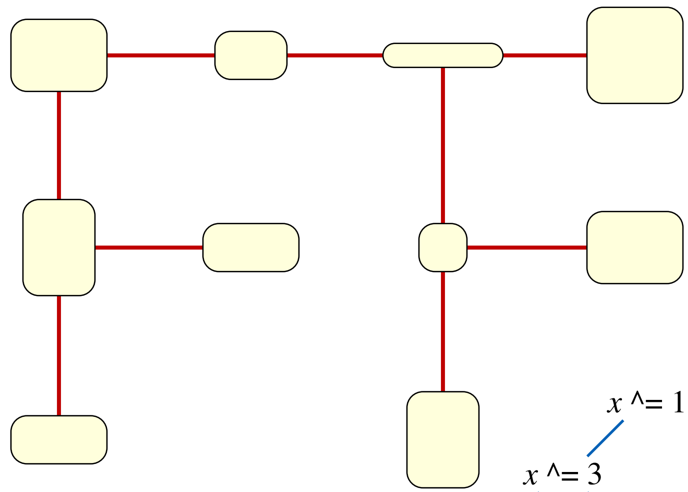
High angular resolution

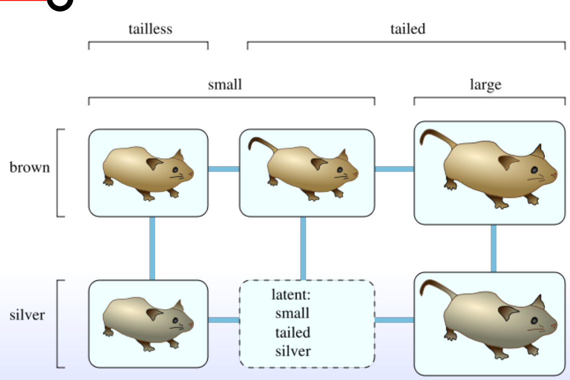
Few edge slopes

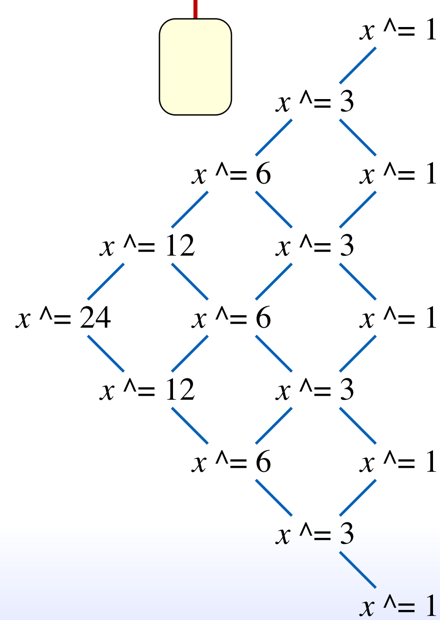
Low area

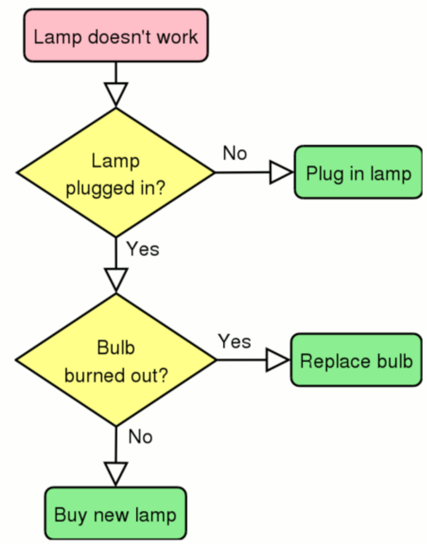
No crossings



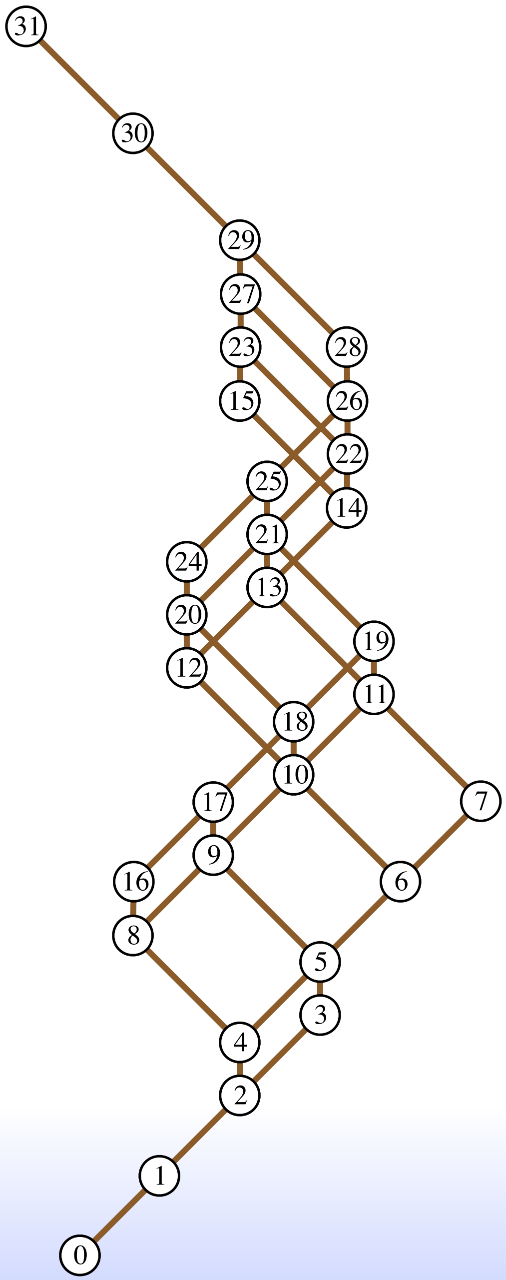




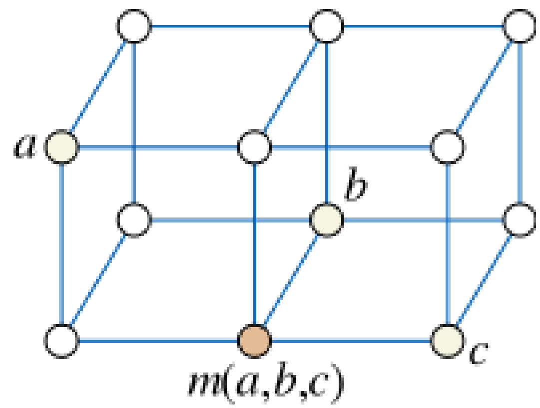


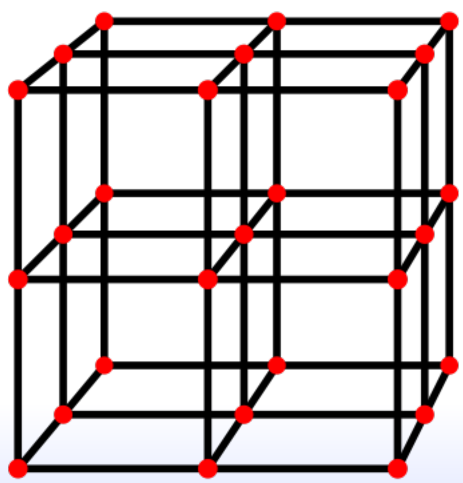


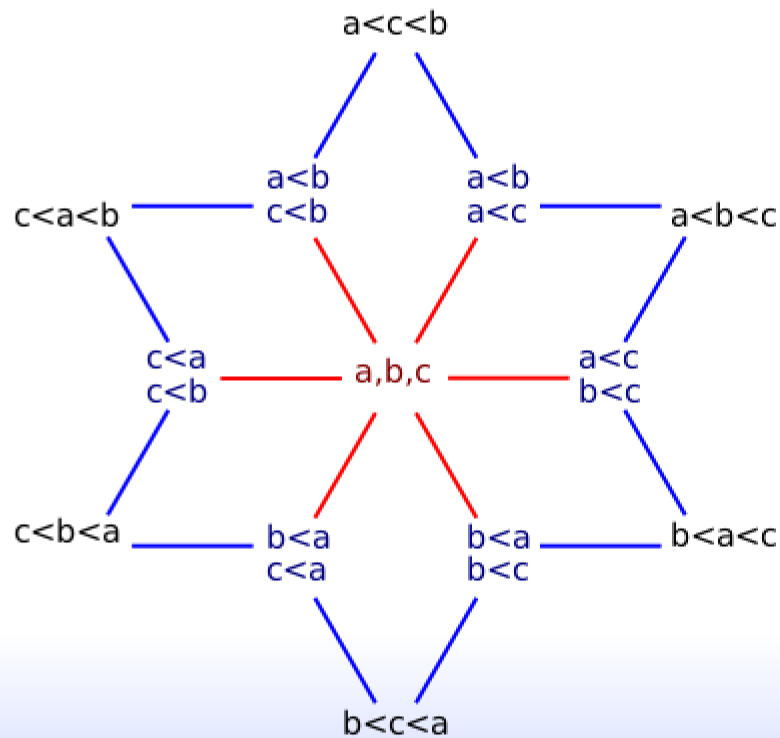
Other regular placements have similar quality guarantees



Three-dimensional grid drawing

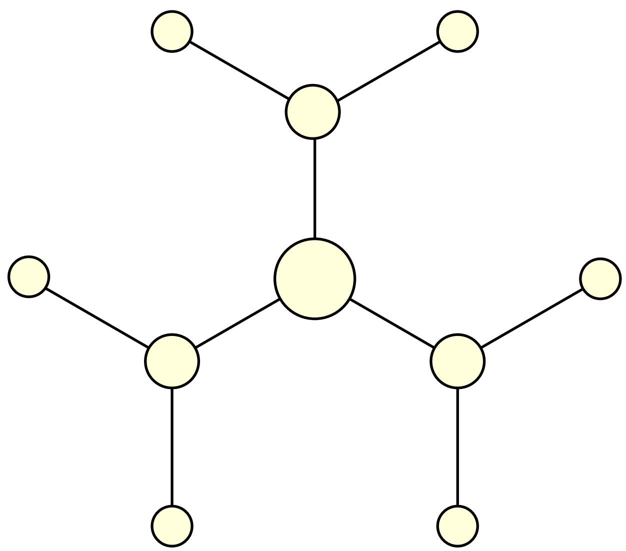


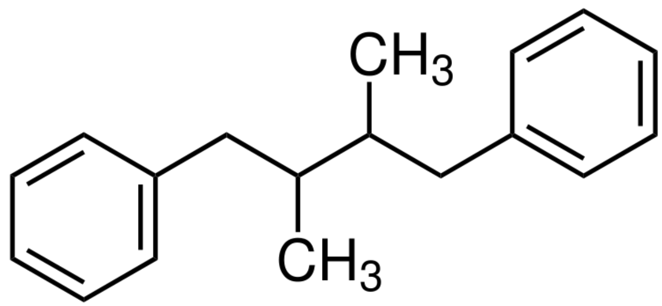


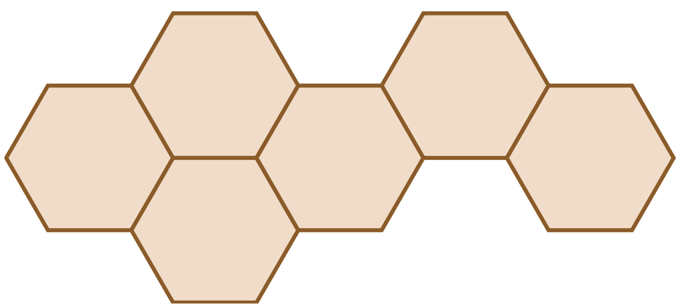


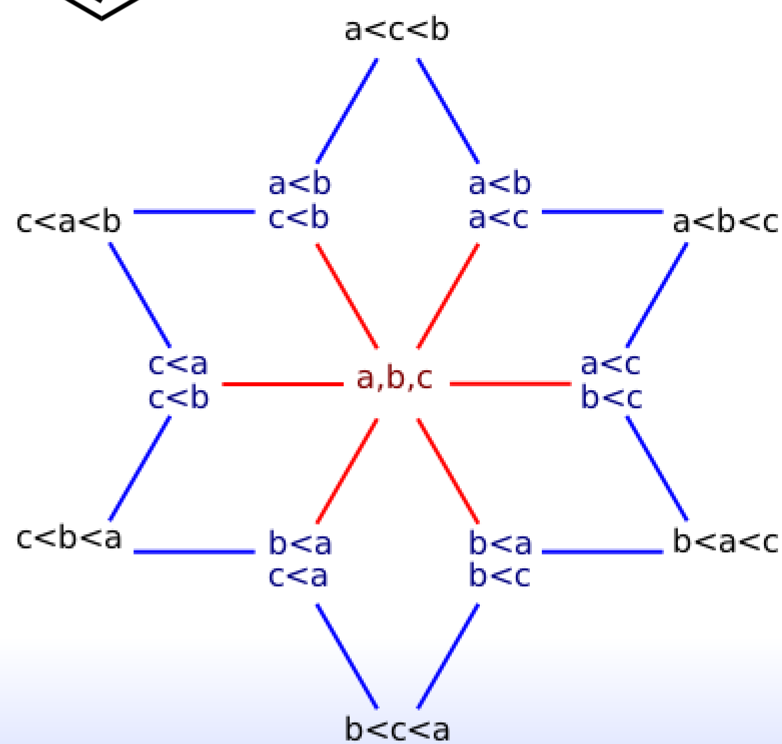
Other regular placements have similar quality guarantees

Drawing in the hexagonal and triangular tilings of the plane





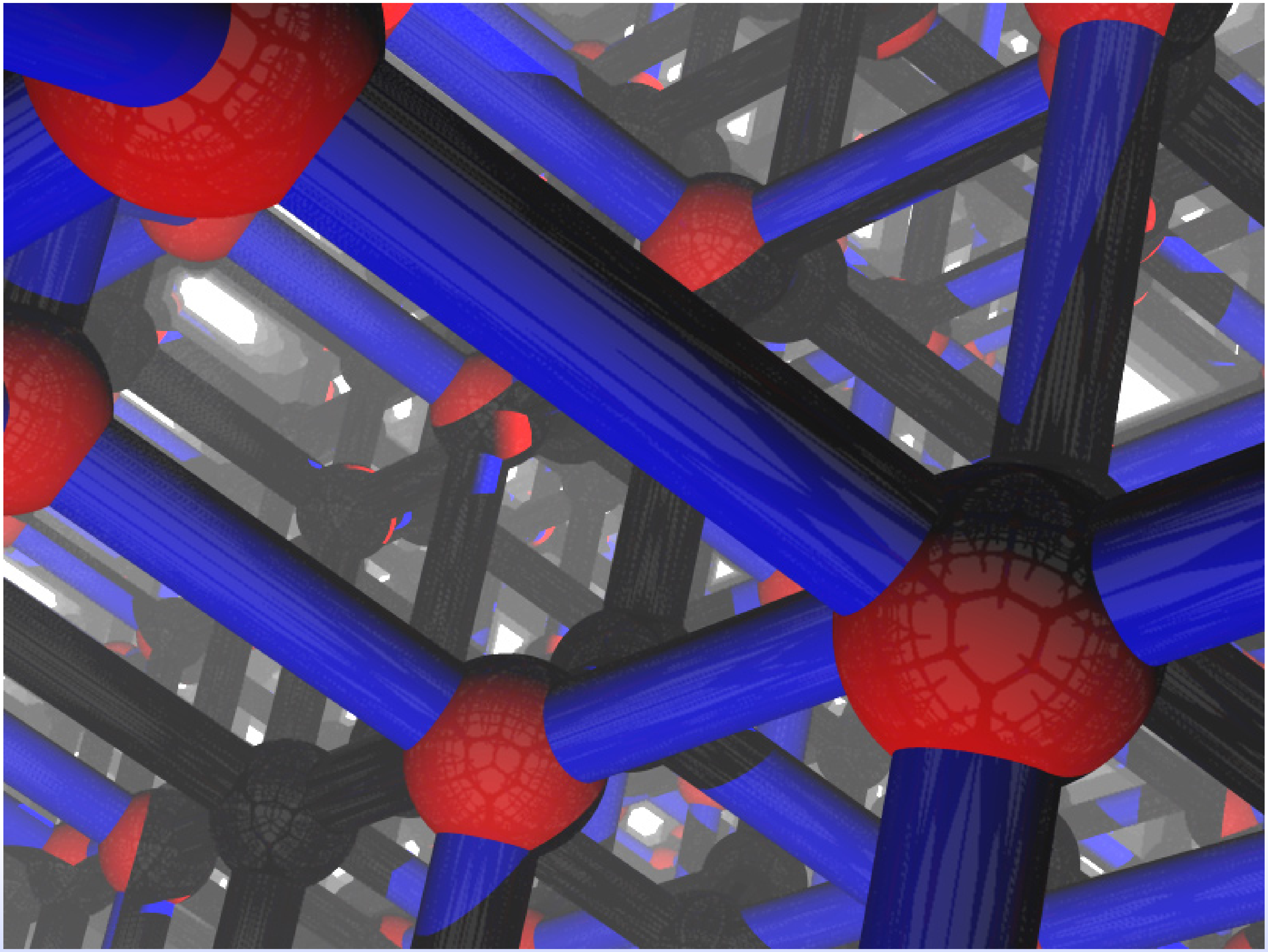




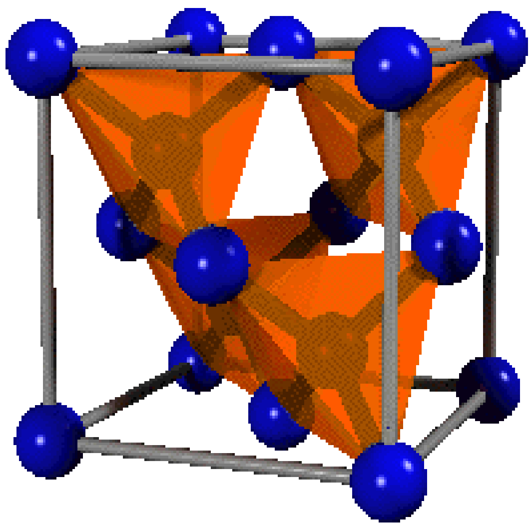
Molecular structure of lignane drawn using ChemDraw by Calvero, on Wikimedia commons as http://commons.wikimedia.org/wiki/Image:Lignane_acsv.svg, licensed PD

Other regular placements have similar quality guarantees

Drawing in the three-dimensional diamond lattice



What is the diamond lattice?



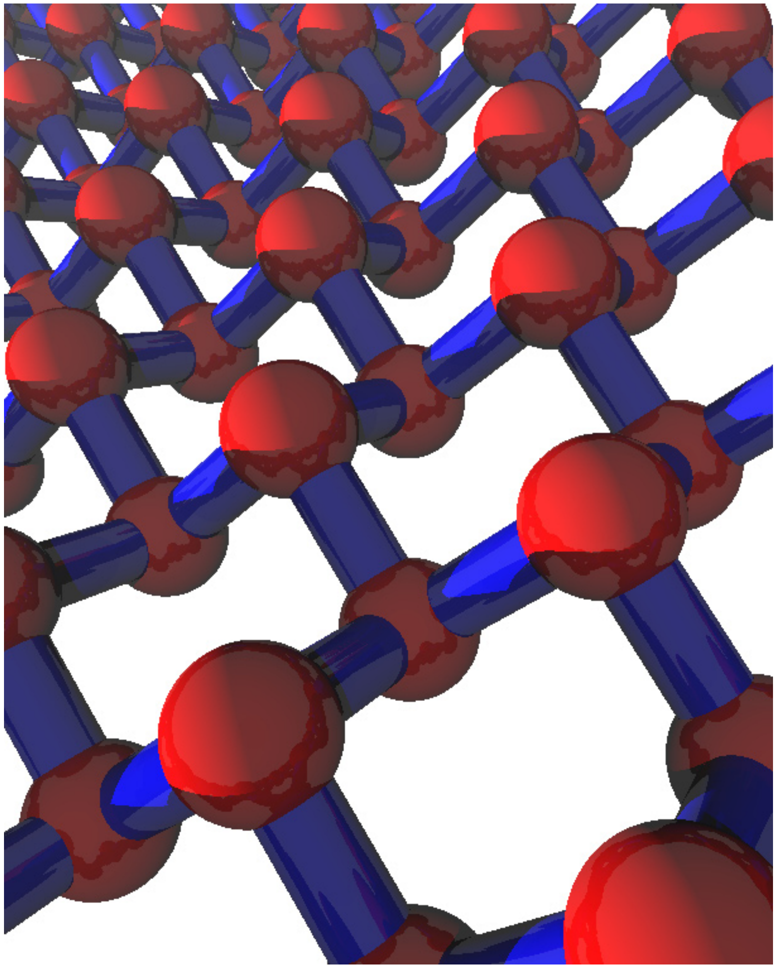
Mathematically, not a lattice
(discrete subgroup of a vector space)

The molecular structure of
the diamond crystal

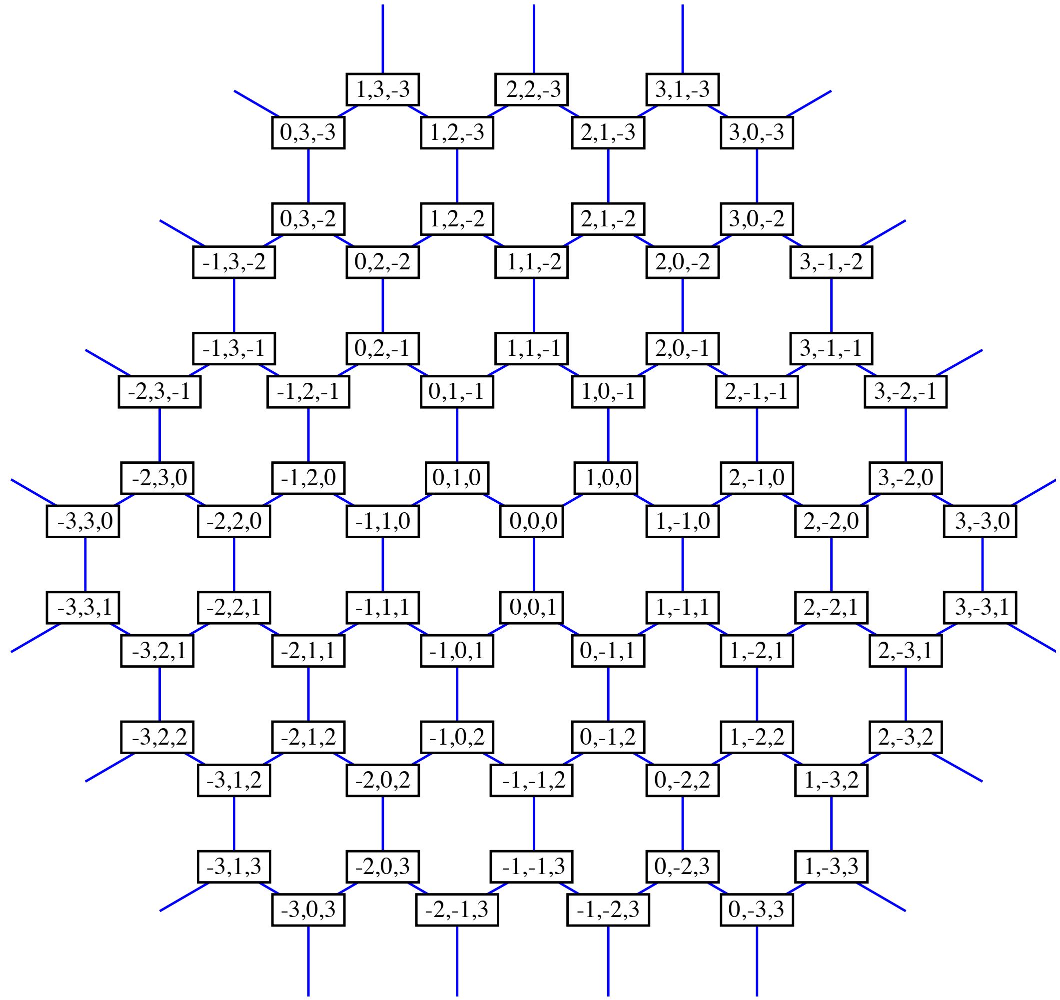
Repeating pattern of points in space
congruent to
(0,0,0) (0,2,2) (2,0,2) (2,2,0)
(1,1,1) (1,3,3) (3,1,3) (3,3,1)
modulo 4

For a simpler description, we need to go up one dimension:
Diamond comes from a 4d structure analogous to 3d structure of hexagonal tiling

Three-dimensional structure of hexagonal tiling



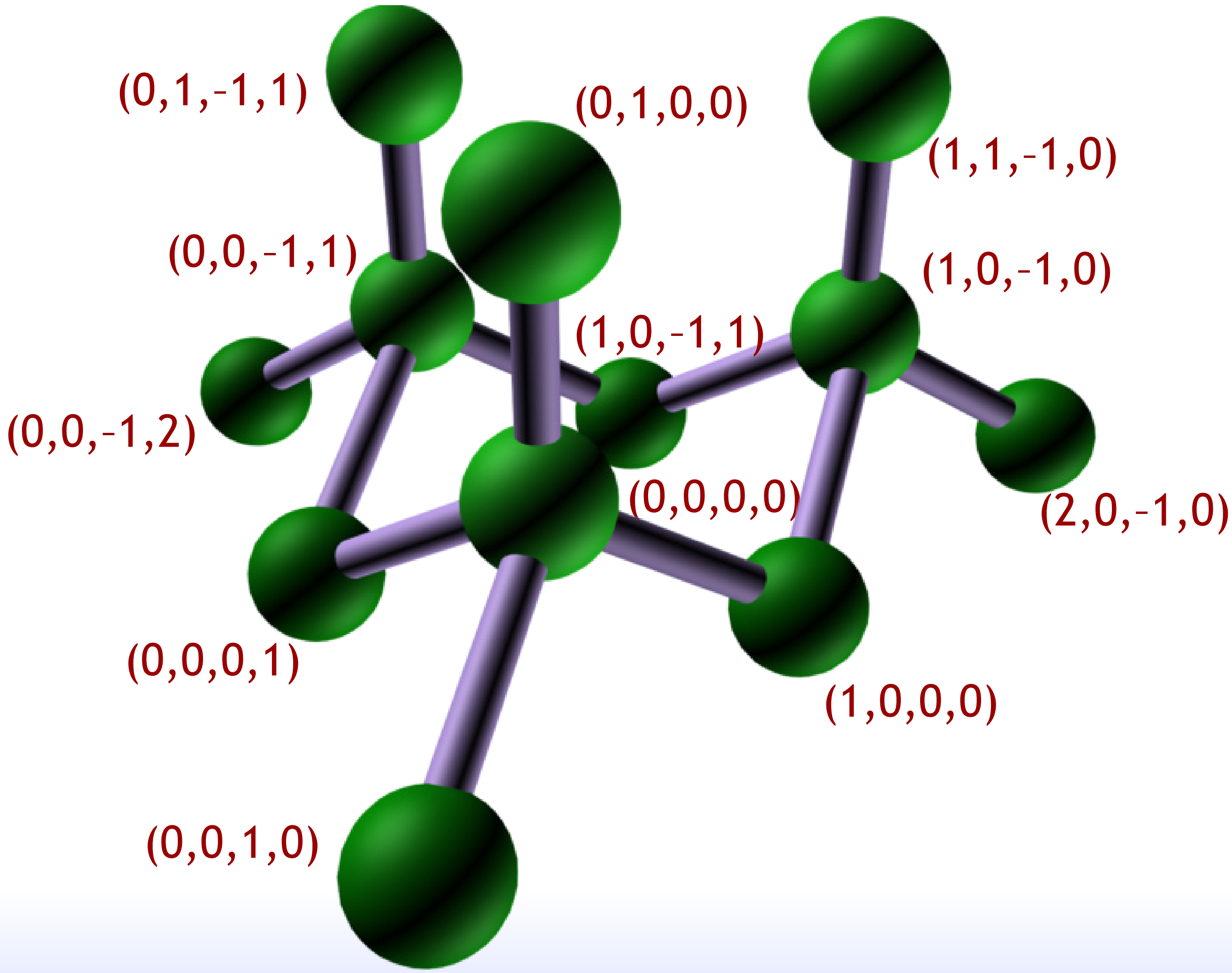
Integer points (x,y,z)
such that x+y+z=0 or x+y+z=1

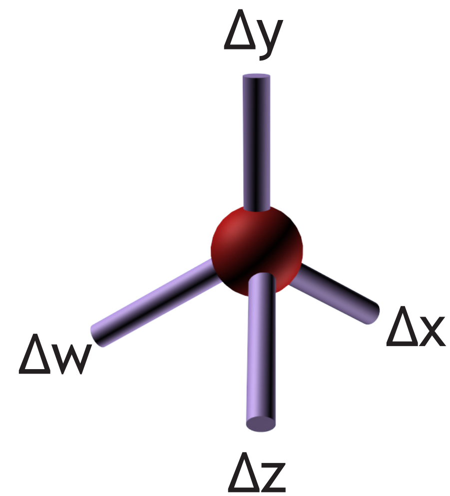


Projected onto a plane
perpendicular to the vector (1,1,1)

Four-dimensional structure of diamond lattice

Integer points (x,y,z,w) such that x+y+z+w=0 or x+y+z+w=1
Projected onto a 3d hyperplane perpendicular to the vector (1,1,1,1)

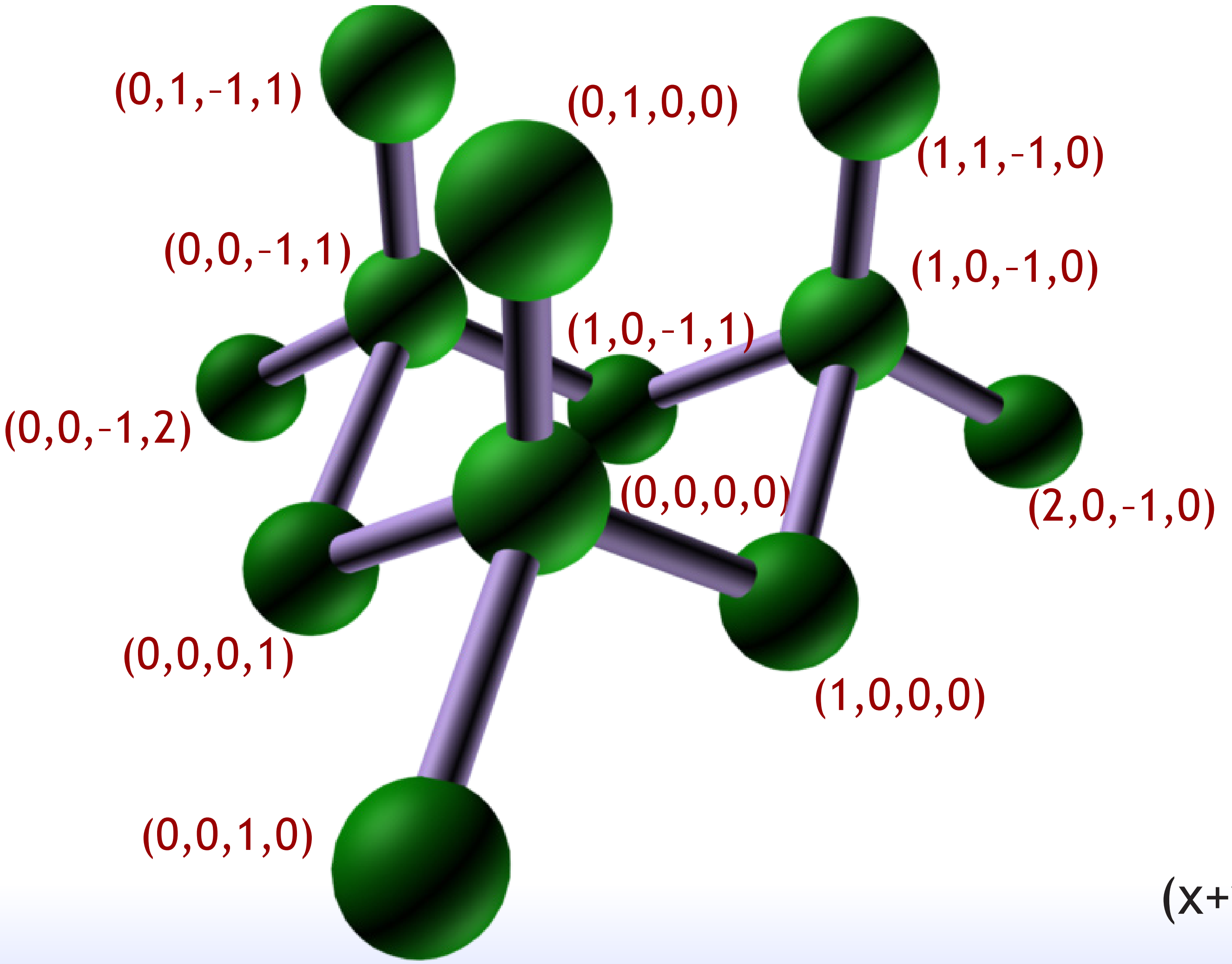




Orientation of 3d edge determines which 4d coordinate differs between neighbors

Four-dimensional structure of diamond lattice

Integer points (x,y,z,w) such that x+y+z+w=0 or x+y+z+w=1
Projected onto a 3d hyperplane perpendicular to the vector (1,1,1,1)



Projection details:

(x,y,z,w)

maps to

x(1,1,1) +
y(1,-1,-1) +
z(-1,-1,1) +
w(-1,1,-1)

=

(x+y-z-w, x-y-z+w, x-y+z-w)

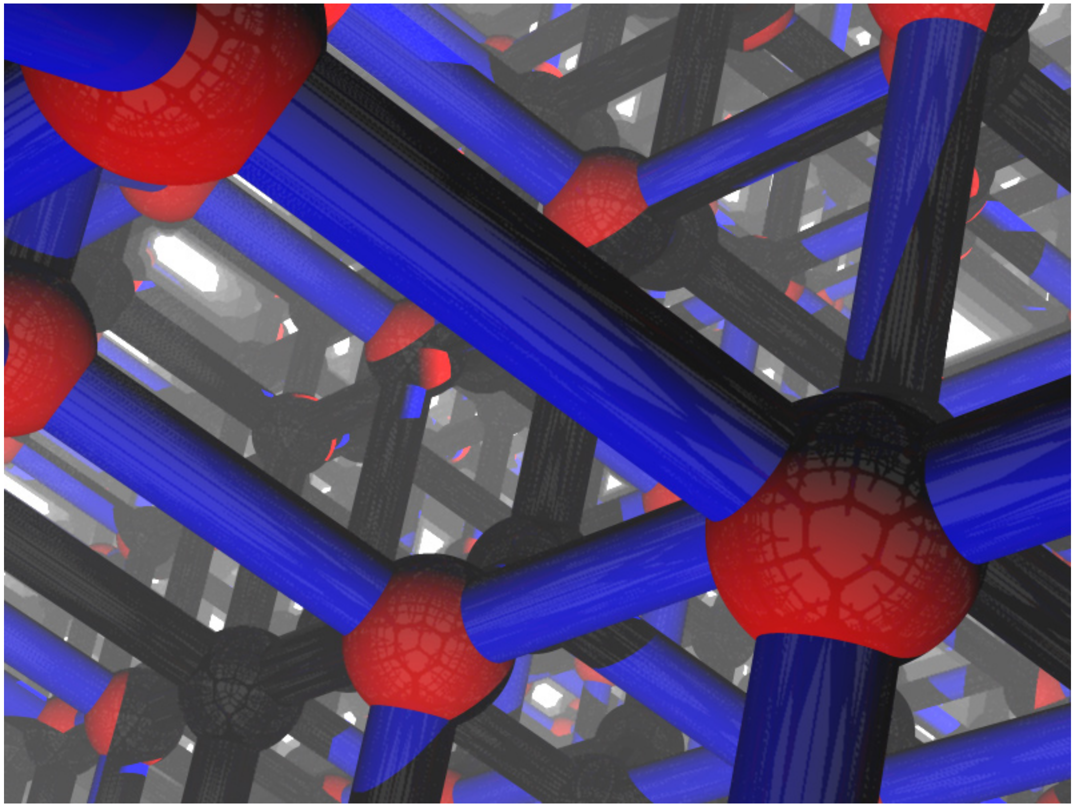
Graph drawing properties of the diamond lattice

Uniform vertex spacing

All edges have unit length

Optimal angular resolution
for degree-four graph in space

Symmetric:
every vertex, every edge,
and every vertex-edge incidence
looks like any other



So what's the problem?

Not every graph can be embedded in a grid, hexagonal tiling, or diamond tiling

Recognizing subgraphs of grids, or induced subgraphs of grids, is NP-complete

Grid subgraphs: Bhatt & Cosmodakis 1987 motivated by wirelength minimization in VLSI

Generalized to related problems using "Logic Engine" of Eades & Whitesides 1996

Same Logic Engine proof technique works just as well for hexagonal tiling and diamond tiling

A solution for grids: isometric embedding

For an isometric subgraph H of a graph G,
distance in H = distance of the same nodes in G

More restrictive notion than induced subgraphs

Isometric subgraphs of integer lattices = **partial cubes**
important class of graphs

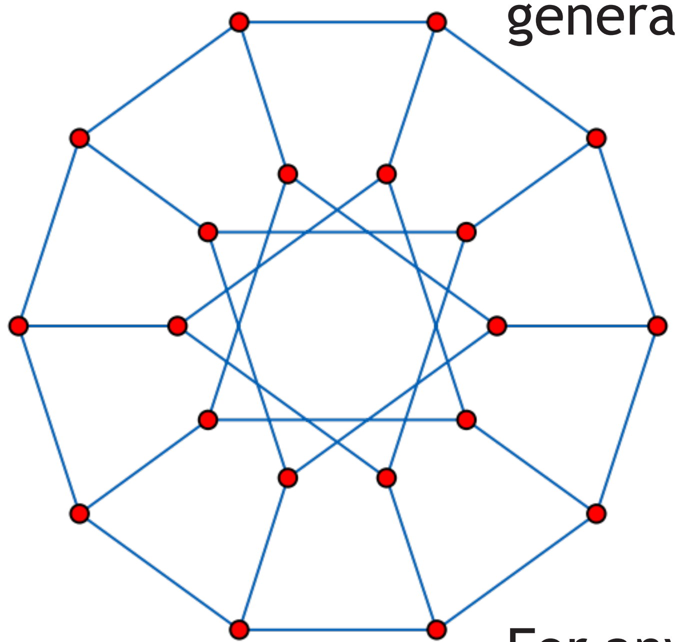
[e.g. see E., Falmagne, & Ovchinnikov, *Media Theory*]

For any (fixed or variable) dimension d
can test whether a given graph is an isometric subgraph
of the d-dimensional integer lattice in polynomial time

[E., GD 2004 and Eur. J. Comb. 2005]

New results

Define a class of d-dimensional (d+1)-regular graphs generalizing hexagonal tiling and diamond lattice



Example: The Desargues graph, a 3-regular 20-vertex graph used in chemistry to model variant physical structures of 5-ligand compounds, is an isometric subgraph of the 4d diamond graph (points with five integer coords summing to 0 or 1)

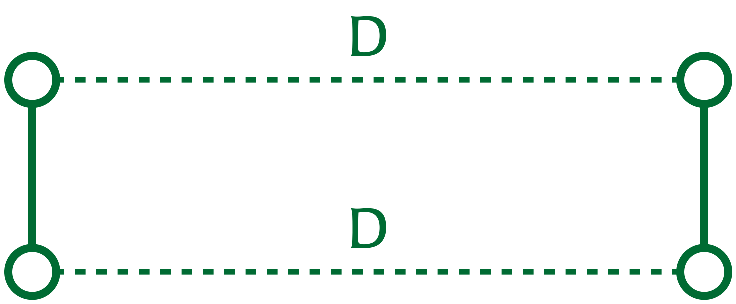
For any (fixed or variable) dimension d can test whether a given graph is an isometric subgraph of the d-dimensional diamond graph in polynomial time

In particular can find isometric graph drawings in the hexagonal tiling and diamond lattice

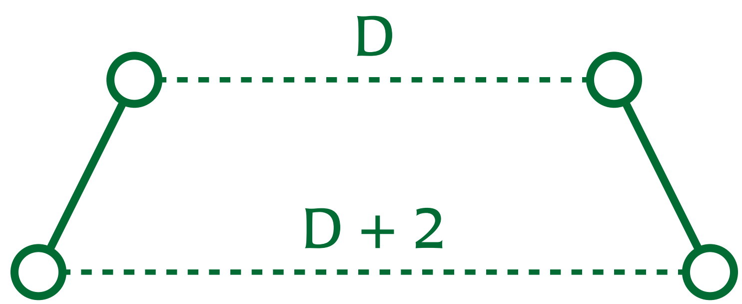
Main ideas of graph drawing algorithm (I)

Djokovic–Winkler relation, a binary relation on graph edges

$$(u,v) \sim (x,y) \;\text{ iff }\; d(u,x) + d(v,y) \neq d(u,y) + d(v,x)$$



related edges



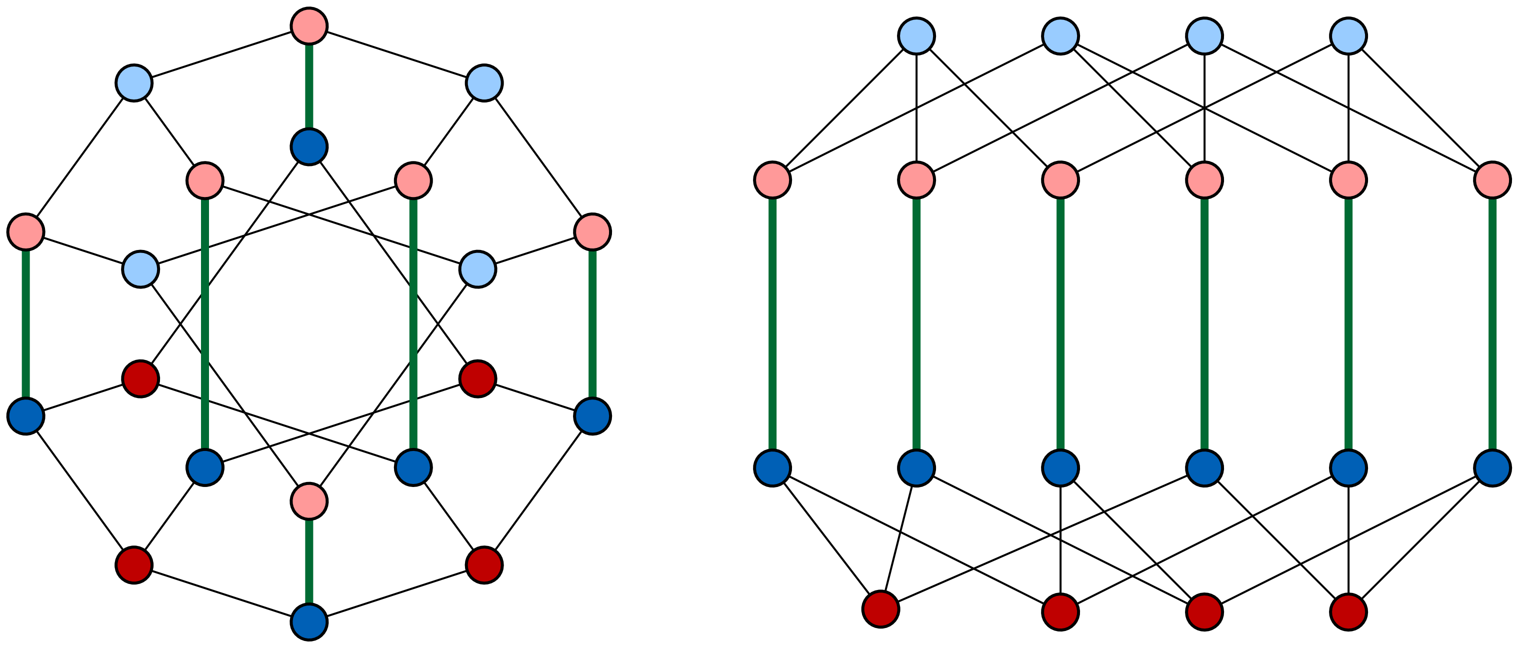
unrelated edges

A graph is a partial cube iff it is bipartite
and the Djokovic-Winkler relation is an equivalence relation

In this case, each equivalence class forms a cut that
splits the vertices of the graph in two connected subsets

Main ideas of graph drawing algorithm (II)

In a diamond graph of any dimension,
Djokovic–Winkler equivalence classes form cuts that are **coherent**:



Endpoints of cut edges on one side of the cut
all have the same color in a bipartition of the graph

Main ideas of graph drawing algorithm (III)

Coherence allows us to distinguish red and blue sides of each cut

Form partial order

cut X ≤ cut Y
iff
red side of cut X is a subset of red side of cut Y
iff
blue side of cut X is a superset of blue side of cut Y

Families of cuts that can be embedded as parallel to each other
in a diamond graph
= chains (totally ordered subsets) of the partial order

Main ideas of graph drawing algorithm (IV)

Minimum number of parallel edge classes of diamond embedding

=

Minimum number of chains needed to cover partial order

=

[Dilworth's theorem]

Maximum size of antichain (set of incomparable elements)
in the partial order

=

"Width" of the partial order

Algorithm outline

Test whether the graph is a partial cube
and compute its Djokovic equivalence classes
[E., SODA 2008]

Verify that all cuts are coherent

Construct partial order on cuts

Use bipartite graph matching techniques
to find the width of the partial order
and compute an optimal chain decomposition

width = 2 iff isometric hex tile subgraph
width = 3 iff isometric diamond subgraph

Construct embedding from chain decomposition

Conclusions

Efficient algorithms for nontrivial lattice embedding problems

Resulting graph drawings have high quality by many standard measures

Restricting attention to isometric embedding avoids NP-hardness difficulty

Interesting new subclass of partial cubes
worth further graph-theoretic investigation

4d structural description of diamond lattice
may be useful for other graph drawing problems in the same lattice