Triangulating the 3D Periodic Space

Manuel Caroli, Monique Teillaud
Contributions by Nico Kruithof

INSTITUT NATIONAL DE RECHERCHE EN INFORMATIQUE ET EN AUTOMATIQUE | INRIA
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TGDA – July 2009 – Paris

Outline

Outline

Applications

Flat torus

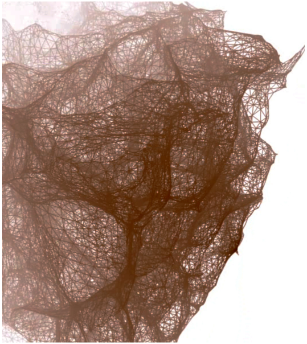
Triangulations

Covering Spaces

Algorithm

Extensions and Future work

Astronomy / Cosmic web



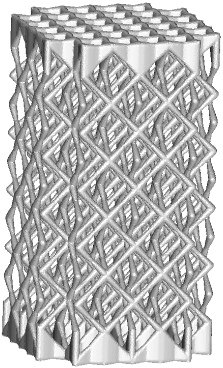
R. v. d. Weijgaert (Kapteyn Institute, Groningen)
G. Vegter (Groningen)

Associate Team “OrbiCG” (INRIA – Groningen)

http://www-sop.inria.fr/geometrica/collaborations/OrbiCG

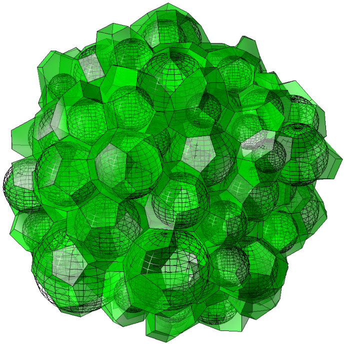
C. Dullemond, MPI for Astronomy (Heidelberg)

Material engineering / Bone scaffolding



M. Moesen (Leuven)

Mechanics of granular materials



N. P. Kruyt (Twente)

CGAL Workshop on Periodic Spaces

http://www.cgal.org/Events/PeriodicSpacesWorkshop

And more. . .

- Physics of condensed matter (V. Robins (Canberra))
- Structural biology
  (D. Weiss (Stanford), J. Bernauer (INRIA Sophia))
- Crystallography
- Fluid dynamics
- Modeling of foams
- Kelvin conjecture (R. Gabrielli (Bath))
- ...

Outline

The 2D Periodic Space $\mathbb{T}^2$

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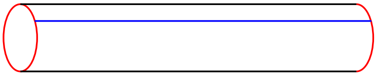
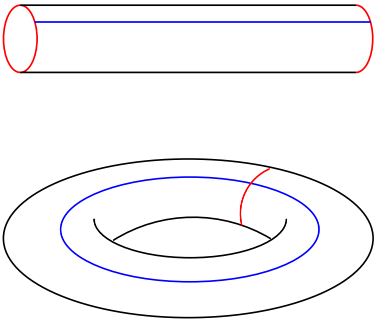


The 2D Periodic Space $\mathbb{T}^2$



Homeomorphic to the surface of a torus in 3D

The 3D Periodic Space $\mathbb{T}^3$

Flat torus:

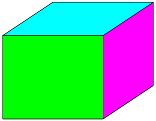
$$\mathbb{T}^3 = \mathbb{R}^3/\mathbb{Z}^3$$

$$\pi : \mathbb{R}^3 \to \mathbb{T}^3 \text{ quotient map}$$

$\mathbb{T}^3$ homeomorphic to the 3D hypersurface of a torus in 4D

original domain

$$\mathcal{D} = [0,1) \times [0,1) \times [0,1)$$

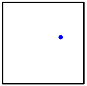


$\mathcal{D}$ contains exactly one representative for each element of $\mathbb{T}^3$

Mapping into $\mathbb{R}^3$

$$\varphi : \mathcal{D} \times \mathbb{Z}^3 \rightarrow \mathbb{R}^3$$
$$(p, \zeta) \mapsto p + \zeta$$
is bijective

ζ = offset of a periodic copy



Mapping into $\mathbb{R}^3$

$$\begin{array}{rcl} \varphi : \mathcal{D} \times \mathbb{Z}^3 & \to & \mathbb{R}^3 \\ (p, \zeta) & \mapsto & p + \zeta \end{array} \qquad \text{is bijective}$$

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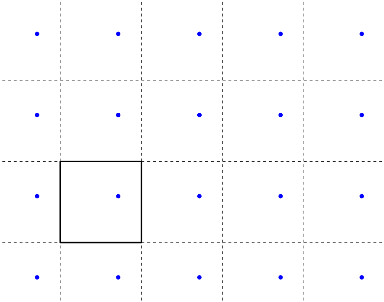
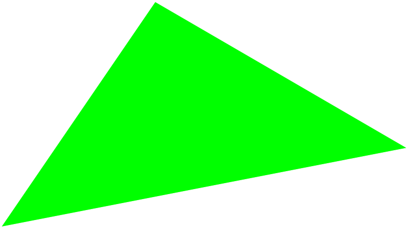


Outline

Definition

simplicial complex
= collection K of simplices such that:

- if $\sigma \in K$ and τ is a face of σ, then $\tau \in K$,
- if $\sigma_1, \sigma_2 \in K$ and $\sigma_1 \cap \sigma_2 \neq \emptyset$,
  then $\sigma_1 \cap \sigma_2$ is a face of both σ_1 and σ_2.
- (local finiteness)
  Every point in a simplex of K has a neighborhood that intersects at most finitely many simplices in K



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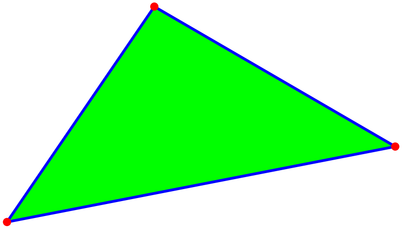

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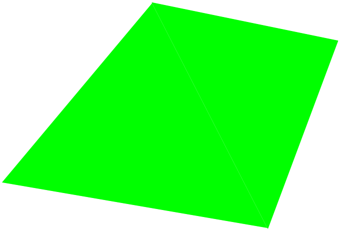

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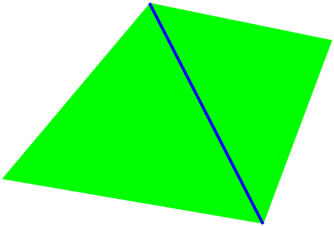

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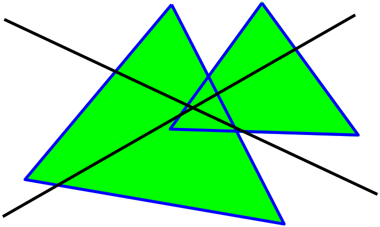


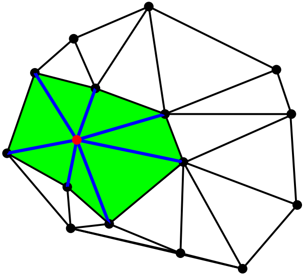
Definition

Star

Simplex σ, Simplicial complex K

Star of σ in K:

$$St(\sigma) = \{\tau \in K \mid \sigma \text{ face of } \tau\}$$



$St(v)$

$$|St(v)| := \bigcup_{\sigma \in St(v)} \sigma$$

Definition

Triangulation

$\mathbb{X}$ topological space, $\mathcal{S}$ set of points

simplicial complex K is a triangulation of $\mathcal{S}$ if

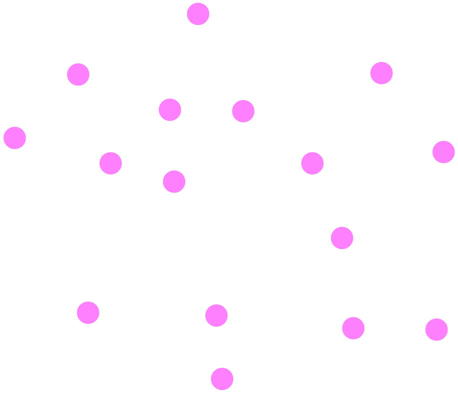
- each point in $\mathcal{S}$ is a vertex of K
- $\bigcup_{\sigma \in K} \sigma$ is homeomorphic to $\mathbb{X}$.

Delaunay Triangulation

The circumsphere of each tetrahedron does not contain any other point of $\mathcal{S}$.

Example

point set $\mathcal{S}$



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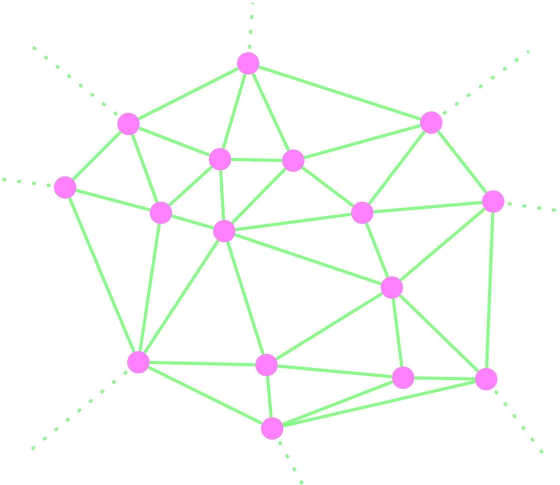
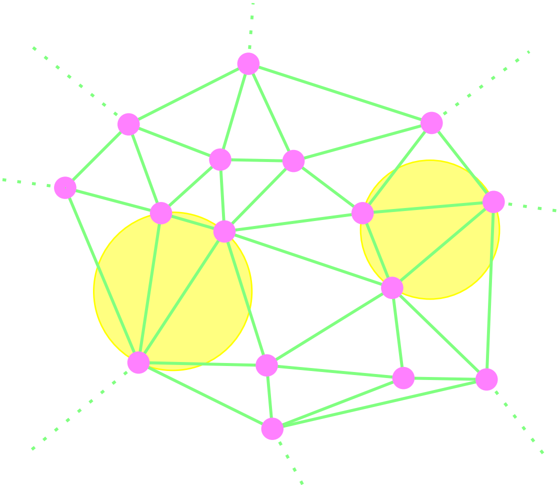


Example

Delaunay triangulation $\mathcal{T}$



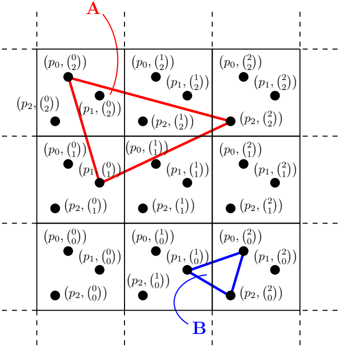
Simplex in $\mathbb{T}^3$?

k-simplex in $\mathbb{R}^3$: Convex hull of $k+1$ points

Simplex in $\mathbb{T}^3$?

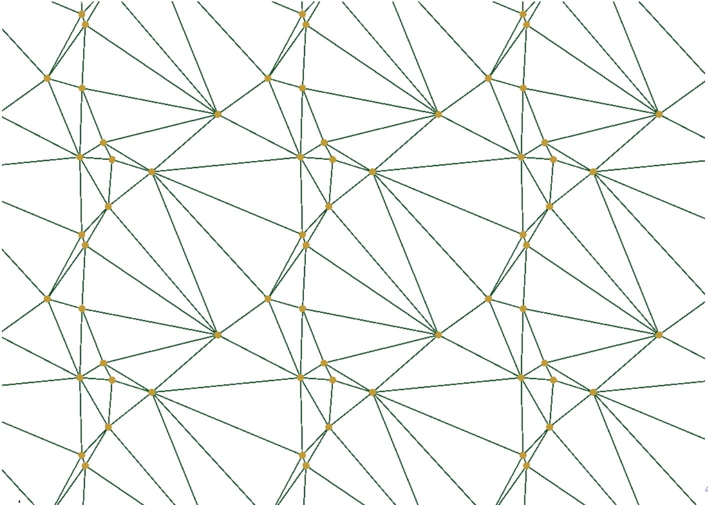
$\mathcal{P} = \{(p_i, \zeta_i) \in \mathcal{D} \times \mathbb{Z}^3, i = 1, \ldots, k+1\}, k \leq 3$
Ch($\mathcal{P}$) = convex hull of $\varphi(\mathcal{P}) = \{p_i + \zeta_i\}$

If $\pi|_{\mathrm{Ch}(\mathcal{P})}$ is a homeomorphism,
then $\pi(\mathrm{Ch}(\mathcal{P}))$ is a *k*-simplex in $\mathbb{T}^3$.



Delaunay triangulation in $\mathbb{T}^3$?

Idea:
Consider the image under π of an
infinite periodic Delaunay triangulation in $\mathbb{R}^3$



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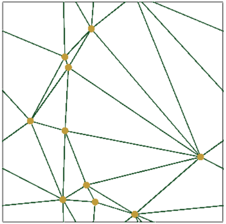


Delaunay triangulation in $\mathbb{T}^3$?

$\mathcal{S}$ finite point set in $\mathcal{D}$

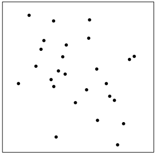
$DT_{\mathbb{T}}(\mathcal{S})$ Delaunay triangulation of $\pi(\mathcal{S})$ in $\mathbb{T}^3$

= projection under π

of the Delaunay triangulation $DT_{\mathbb{R}}(\mathcal{S}^{\varphi})$ of $\varphi(\mathcal{S} \times \mathbb{Z}^3)$ in $\mathbb{R}^3$

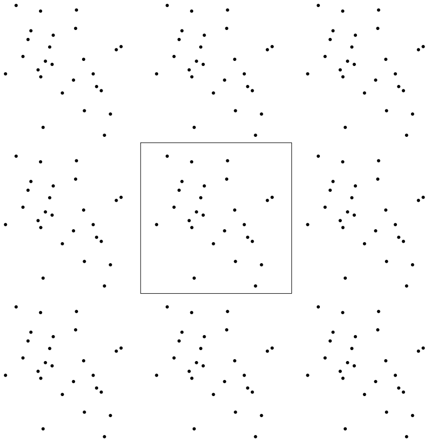
only if $\pi(DT_{\mathbb{R}}(\mathcal{S}^{\varphi}))$ is a simplicial complex

Delaunay triangulation of a periodic point set



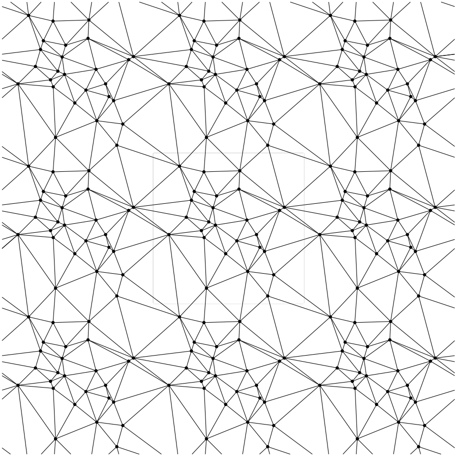
$\mathcal{S}$

Delaunay triangulation of a periodic point set



$$\varphi(\mathcal{S} \times \mathbb{Z})$$

Delaunay triangulation of a periodic point set



Why is $DT(\varphi(\mathcal{S} \times \mathbb{Z}))$ a triangulation?

Motivation for definition of $DT_{\mathbb{T}}(\mathcal{S})$

$$\bigcup_{\sigma \in DT_{\mathbb{T}}(\mathcal{S})} \sigma \text{ homeomorphic to } \mathbb{T}^3$$

Is $\pi(DT_{\mathbb{R}}(\mathcal{S}^{\varphi}))$ a simplicial complex ?

Theorem

If for all vertices v of $DT_{\mathbb{R}}(\mathcal{S}^{\varphi})$

$$\pi|_{|St(v)|} \text{ is a homeomorphism,}$$

then $\pi(DT_{\mathbb{R}}(\mathcal{S}^{\varphi}))$ is a simplicial complex.

Proof of the theorem

Theorem

If for all vertices v of $DT_{\mathbb{R}}(\mathcal{S}^{\varphi})$, $\pi|_{|St(v)|}$ *is a homeomorphism, then* $\pi(DT_{\mathbb{R}}(\mathcal{S}^{\varphi}))$ *is a simplicial complex.*

Proof sketch:

σ simplex in $DT_{\mathbb{R}}(\mathcal{S}^{\varphi})$

If $\pi|_{\sigma}$ homeomorphism $\Rightarrow$ simplices "match" under π

Degenerate cases solved by symbolic perturbation, invariant by translations [Devillers-Teillaud 03]

Proof of the theorem

Theorem

If for all vertices v of $DT_{\mathbb{R}}(\mathcal{S}^{\varphi})$, $\pi|_{|St(v)|}$ is a homeomorphism, then $\pi(DT_{\mathbb{R}}(\mathcal{S}^{\varphi}))$ is a simplicial complex.

Proof sketch:

1. simplices “match” under π

$\pi(DT_{\mathbb{R}}(\mathcal{S}^{\varphi}))$ is finite

follows from local finiteness of $DT_{\mathbb{R}}(\mathcal{S}^{\varphi})$ and 1.

Proof of the theorem

Theorem

If for all vertices v of $DT_{\mathbb{R}}(\mathcal{S}^{\varphi})$, $\pi|_{|St(v)|}$ is a homeomorphism, then $\pi(DT_{\mathbb{R}}(\mathcal{S}^{\varphi}))$ is a simplicial complex.

Proof sketch:

1. simplices "match" under π
2. $\pi(DT_{\mathbb{R}}(\mathcal{S}^{\varphi}))$ is finite

$\sigma_{\mathbb{R}}, \tau_{\mathbb{R}}$ simplices in $DT_{\mathbb{R}}(\mathcal{S}^{\varphi})$

π maintains the incidence relation, i.e.

$$\tau_{\mathbb{R}} \text{ face of } \sigma_{\mathbb{R}} \Rightarrow \pi(\tau_{\mathbb{R}}) \text{ face of } \pi(\sigma_{\mathbb{R}})$$

Proof of the theorem

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If for all vertices v of $DT_{\mathbb{R}}(\mathcal{S}^{\varphi})$, $\pi|_{|St(v)|}$ *is a homeomorphism, then* $\pi(DT_{\mathbb{R}}(\mathcal{S}^{\varphi}))$ *is a simplicial complex.*

Proof sketch:

1. simplices "match" under π
2. $\pi(DT_{\mathbb{R}}(\mathcal{S}^{\varphi}))$ is finite
3. $\pi(\tau_{\mathbb{R}})$ face of $\pi(\sigma_{\mathbb{R}})$

σ, τ simplices in $\pi(DT_{\mathbb{R}}(\mathcal{S}^{\varphi}))$

Lemma

$\sigma \cap \tau$ *consists of simplices in* $\pi(DT_{\mathbb{R}}(\mathcal{S}^{\varphi}))$

Proof using 1.

Proof of the theorem

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Theorem

If for all vertices v of $DT_{\mathbb{R}}(\mathcal{S}^{\varphi})$, $\pi|_{|St(v)|}$ is a homeomorphism, then $\pi(DT_{\mathbb{R}}(\mathcal{S}^{\varphi}))$ is a simplicial complex.

Proof sketch:

1. simplices "match" under π
2. $\pi(DT_{\mathbb{R}}(\mathcal{S}^{\varphi}))$ is finite
3. $\pi(\tau_{\mathbb{R}})$ face of $\pi(\sigma_{\mathbb{R}})$
4. $\sigma \cap \tau \subseteq \pi(DT_{\mathbb{R}}(\mathcal{S}^{\varphi}))$

σ, τ simplices in $\pi(DT_{\mathbb{R}}(\mathcal{S}^{\varphi}))$

Remains to show:

$\#(\sigma \cap \tau) = 1$

Use $\pi_{|St(v)|}$ is a homeomorphism

Proof of the theorem

Theorem

If for all vertices v of $DT_{\mathbb{R}}(\mathcal{S}^{\varphi})$, $\pi|_{|St(v)|}$ is a homeomorphism, then $\pi(DT_{\mathbb{R}}(\mathcal{S}^{\varphi}))$ is a simplicial complex.

Proof sketch:

1. simplices "match" under π
2. $\pi(DT_{\mathbb{R}}(\mathcal{S}^{\varphi}))$ is finite
3. $\pi(\tau_{\mathbb{R}})$ face of $\pi(\sigma_{\mathbb{R}})$
4. $\sigma \cap \tau \subseteq \pi(DT_{\mathbb{R}}(\mathcal{S}^{\varphi}))$
5. $\sigma \cap \tau \in \pi(DT_{\mathbb{R}}(\mathcal{S}^{\varphi}))$

Proof of the theorem

Theorem

If for all vertices v of $DT_{\mathbb{R}}(\mathcal{S}^{\varphi})$, $\pi|_{|St(v)|}$ is a homeomorphism, then $\pi(DT_{\mathbb{R}}(\mathcal{S}^{\varphi}))$ is a simplicial complex.

Proof sketch:

1. simplices "match" under π
2. $\pi(DT_{\mathbb{R}}(\mathcal{S}^{\varphi}))$ is finite — local finiteness
3. $\pi(\tau_{\mathbb{R}})$ face of $\pi(\sigma_{\mathbb{R}})$ — criterion 1
4. $\sigma \cap \tau \subseteq \pi(DT_{\mathbb{R}}(\mathcal{S}^{\varphi}))$
5. $\sigma \cap \tau \in \pi(DT_{\mathbb{R}}(\mathcal{S}^{\varphi}))$ — criterion 2

□

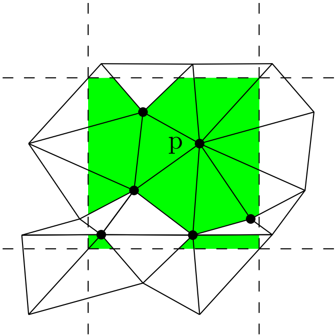
Another criterion

Theorem

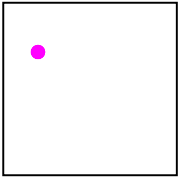
$\pi(DT_{\mathbb{R}}(\mathcal{S}^{\varphi}))$ is a simplicial complex

(if and) only if

no cycles of length 2 in its 1-skeleton

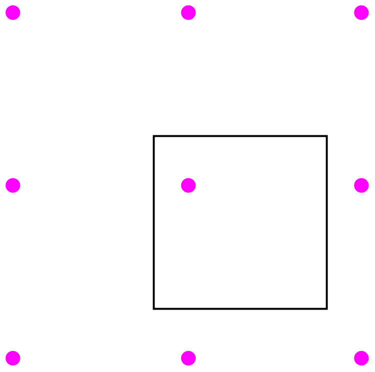


$\pi(DT_{\mathbb{R}}(\mathcal{S}^{\varphi}))$ is not always a simplicial complex



One point in $\mathbb{T}^2$

$\pi(DT_{\mathbb{R}}(\mathcal{S}^{\varphi}))$ is not always a simplicial complex



One point in $\mathbb{T}^2$

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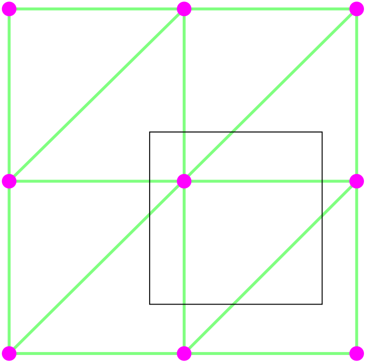

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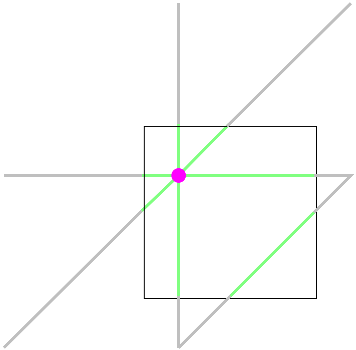
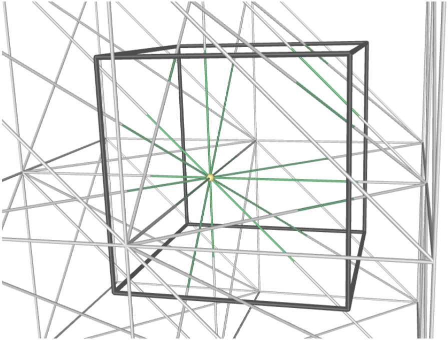


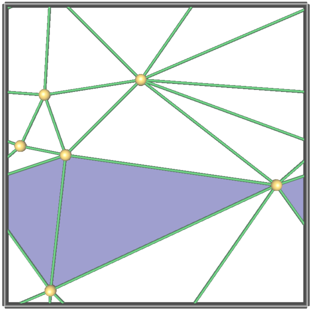
One point in $\mathbb{T}^2$: self-edges

$\pi(DT_{\mathbb{R}}(\mathcal{S}^{\varphi}))$ is not always a simplicial complex



One point in $\mathbb{T}^3$: self-edges

$\pi(DT_{\mathbb{R}}(\mathcal{S}^{\varphi}))$ is not always a simplicial complex



Cycle of length 2

Outline

Covering Space

$\mathbb{X}$ a topological space.

$\rho : \tilde{\mathbb{X}} \rightarrow \mathbb{X}$ is a covering map,
and $\tilde{\mathbb{X}}$ is a covering space of $\mathbb{X}$ if:

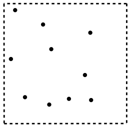
$\forall x \in \mathbb{X}$

- $\exists V_x$ open neighborhood of x
- $\exists$ a decomposition of $\rho^{-1}(V_x)$ as a family $\{U_{\alpha_x}\}$, $U_{\alpha_x} \subset \tilde{\mathbb{X}}$ pairwise disjoint

s.t. $\rho|_{U_{\alpha_x}}$ is a homeomorphism for each α_x.

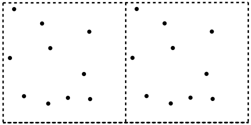
If $h = max_{x \in \mathbb{X}} |U_{\alpha_x}|$ is finite, then $\tilde{\mathbb{X}}$ = *h*-sheeted covering space.

Covering Space



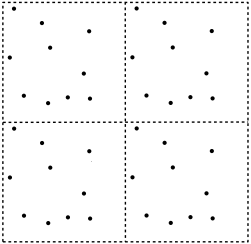
1-sheeted covering

Covering Space



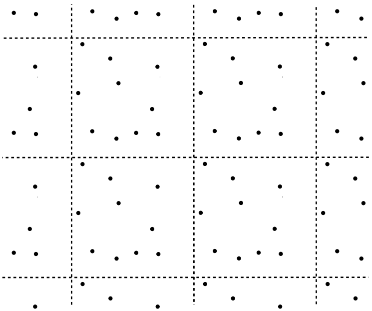
2-sheeted covering

Covering Space



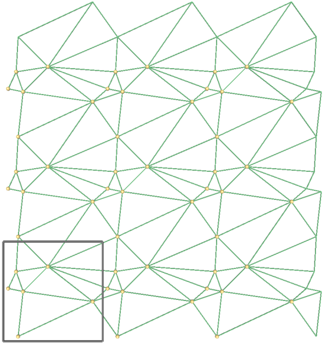
4-sheeted covering

Covering Space



∞-sheeted covering = $\mathbb{R}^2$ = *universal covering*

$\mathbb{T}^3_{27}$



$\mathbb{T}^3_{27}$ = 3^3-sheeted covering

$$\mathbb{T}^3_{27} = \mathbb{R}^3 / 3\mathbb{Z}^3$$

$$\pi_{27} : \mathbb{R}^3 \rightarrow \mathbb{T}^3_{27}$$

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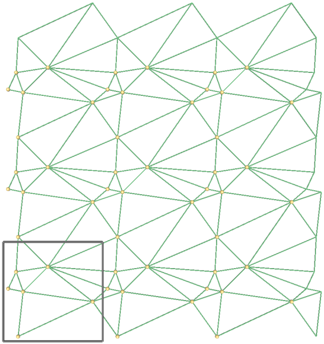
$\mathbb{T}^3_{27}$



$\mathbb{T}^3_{27}$ = 3^3-sheeted covering

$\mathbb{T}^3_{27} = \mathbb{R}^3 / 3\mathbb{Z}^3$

$\pi_{27} : \mathbb{R}^3 \rightarrow \mathbb{T}^3_{27}$

$\pi_{27}(DT_{\mathbb{R}}(\mathcal{S}^{\varphi}))$ is always a simplicial complex

Proof uses `[Dolbilin-Huson 97]`
but the simplicial complex is homeomorphic to $\mathbb{T}^3$

Outline

Incremental Algorithm

- Compute initially in $\mathbb{T}^3_{27}$

  27 copies of each point

- As soon as possible

  Compute in $\mathbb{T}^3$

Incremental Algorithm

- Compute initially in $\mathbb{T}^3_{27}$

27 copies of each point

- As soon as possible

Compute in $\mathbb{T}^3$

As soon as possible =

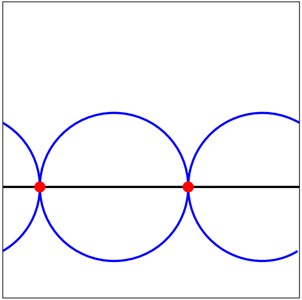
- not just when $\pi(DT_{\mathbb{R}}(\mathcal{S}^{\varphi}))$ is a simplicial complex
- but when $\pi(DT_{\mathbb{R}}(\mathcal{T}^{\varphi}))$ is guaranteed to be a simplicial complex for any $\mathcal{T} \supseteq \mathcal{S}$

Ball diameter criterion

Δ tetrahedron in $\pi(DT_{\mathbb{R}}(\mathcal{S}^{\varphi}))$

Circumsphere diameter of any $\Delta < \frac{1}{2}$

$\Rightarrow \pi(DT_{\mathbb{R}}(\mathcal{S}^{\varphi}))$ is a triangulation

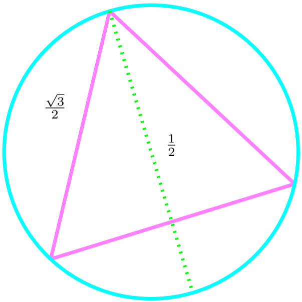


Edge length criterion

e edge in $\pi(DT_{\mathbb{R}}(\mathcal{S}^{\varphi}))$

Length of any $e < \frac{1}{\sqrt{6}}$

$\Rightarrow \pi(DT_{\mathbb{R}}(\mathcal{S}^{\varphi}))$ is a triangulation



Properties

- Structure always a Delaunay triangulation

  [Thompson 02] computes a “tessellation”
  not always a triangulation
  not always Delaunay

- No duplication of points if possible

  [Dolbilin-Huson 97] and others always 27 copies

Vertex removal works too

Theoretical Analysis

Randomized worst-case optimal $O(n^2)$
with adapted Delaunay hierarchy [Devillers 02]

Experimental Analysis

Optimizations

- Spatial sorting from CGAL [Delage]
- Optional insertion of dummy points to force 1-sheeted covering

- Data from research in cosmology
- Random points

1 million random points in 23 seconds

2.33 GHz Intel Core 2 Duo processor

Factor $\simeq$ 1.6 compared to Delaunay triangulation in $\mathbb{R}^3$ on large data sets in CGAL [Pion-Teillaud]

Outline

Extensions

- General cube: same
- Weighted Delaunay triangulation: adapted number of sheets
- Iso-cuboid: adapted number of sheets
- Non-orthogonal translations: similar

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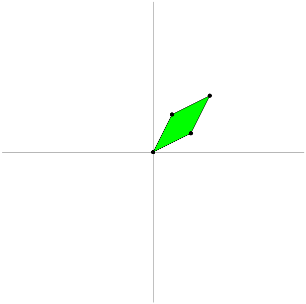

parallelogram: find shortest translation vectors

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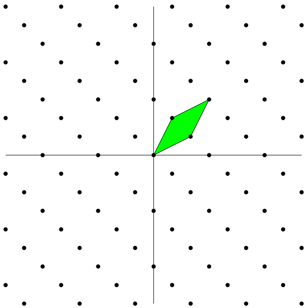

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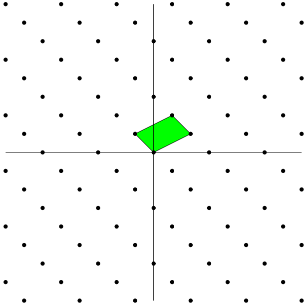

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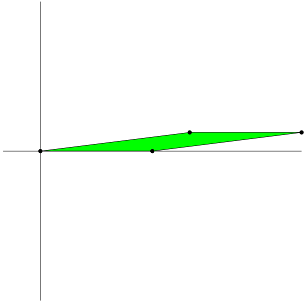

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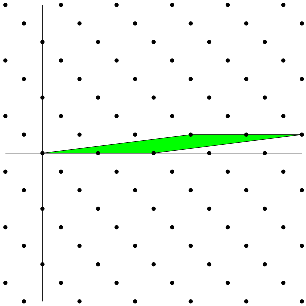

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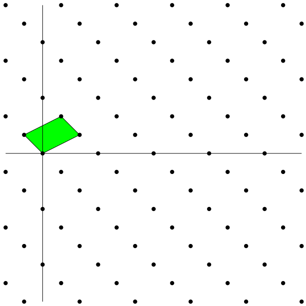

parallelogram: find shortest translation vectors

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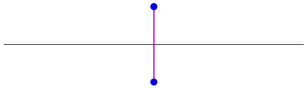
- Other groups?



reflection: always a self-edge

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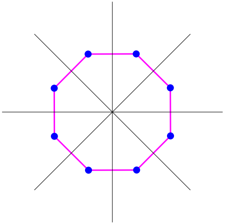

rotation: always self-edges

Future work

- Periodic meshes
- Periodic alpha shapes
- Applications
- Other orbifolds
  - of $\mathbb{R}^3$ (e.g. crystallographic space groups)
  - of the sphere
    projective plane [Aanjaneya–Teillaud 07]
  - of the hyperbolic space
  - general approach
  - Preliminary work with M. Aanjaneya

Demo

(to appear in CGAL 3.5)

Thank you!

Accepted for next release of CGAL

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