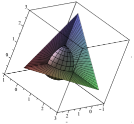
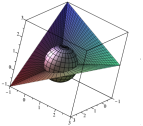
3D positive random walks and spherical triangles





Kilian Raschel

Joint with B. Bogosel, V. Perrollaz & A. Trotignon

CNRS

INSTITUT DENIS POISSON
ORLÉANS • TOURS
Mathématiques & Physique Théorique

Seminar “Computations and Proofs” — SpecFun
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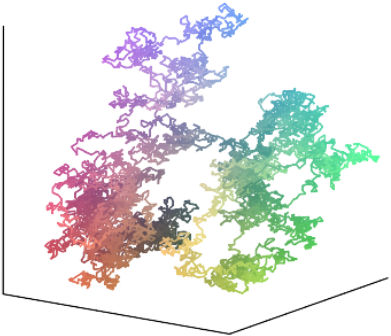
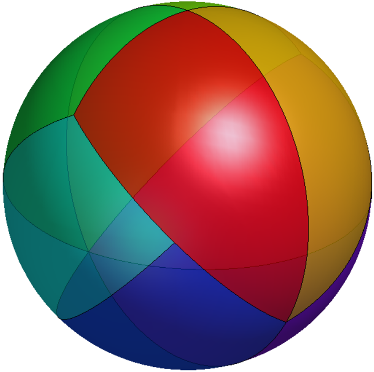
Inria

Special thanks to M. Bousquet-Mélou for some slides!

Main idea

Relate probabilistic/combinatorial properties of a given random walk to geometric properties of the associated spherical triangle

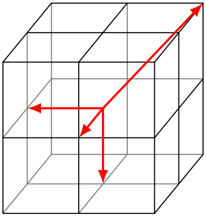




Presentation of the problem

Let $\mathcal{S} \subset \mathbb{Z}^3$ be a *finite set of steps* in 3D

Consider walks that start from the origin, take their steps in $\mathcal{S}$, and are *confined to the positive octant* $\mathbb{N}^3$



Questions

- Determine $o(n)$, the *number of such walks* that have length n
- or $o(i, j, k; n)$ the *number of walks* that have length n and end at position (i, j, k)
- or the associated 4-variable *generating function*:

$$O(x, y, z; t) = \sum_{i,j,k,n \geqslant 0} o(i, j, k; n) x^i y^j z^k t^n$$

- or the *nature* of this generating function

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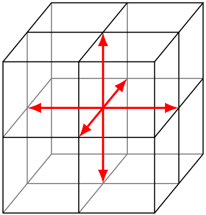

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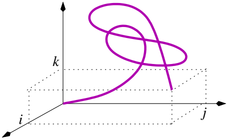

Courtesy of M. Bousquet-Mélou

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- or the *nature* of this generating function

A hierarchy of power series

The formal power series $A(t)$ is ...

- ... *rational* if it can be written, with $P(t)$ and $Q(t)$ polynomials

$$A(t) = \frac{P(t)}{Q(t)}$$

- ... *algebraic* if it satisfies a (non-trivial) polynomial equation

$$P(t, A(t)) = 0$$

- ... *D-finite* if it satisfies a (non-trivial) linear differential equation

$$P_k(t)A^{(k)}(t) + \cdots + P_0(t)A(t) = 0$$

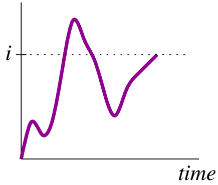
+ extension to several variables + closure properties

Lattice paths confined to convex cones

1D: walks confined to the $\geqslant 0$ half-line

The generating function $H(x;t)$ is *algebraic*

[Gessel 80], [Labelle-Yeh 90], [Bousquet-Mélou-Petkovšek 00], [Duchon 00], [Banderier-Flajolet 02]



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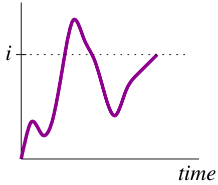
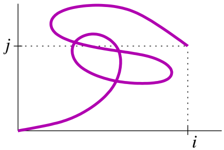


2D: walks confined to the $\geqslant 0$ quadrant

The generating function $Q(x, y; t)$ is sometimes algebraic, D-finite, non-D-finite

Complete classification for walks with small steps: $\mathcal{S} \subset \{\bar{1}, 0, 1\}^2$



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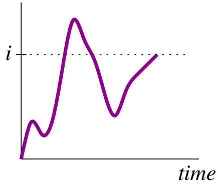

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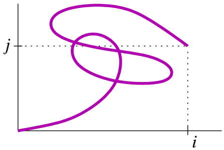


A rich literature

Bernardi, Bostan, Bousquet-Mélou, Chyzak, Cori, Denisov, Dulucq, Fayolle, Gessel, Gouyou-Beauchamps, Guy, Janse van Rensburg, Johnson, Kauers, Koutschan, Krattenthaler, Kurkova, Kreweras, Melczer, Mishna, Niederhausen, Petkovšek, Prellberg, R., Rechnitzer, Sagan, Salvy, Viennot, Wachtel, Wilf, Yeats, Zeilberger...

The number of interesting 3D distinct models

Rest of the talk: small step case

$\mathcal{S} \subset \{\bar{1}, 0, 1\}^3 \setminus \{(0,0,0)\}$ — only 2^{26} such problems!

Reduction of the number of models

Remove

- models in which *all steps are non-negative* (rational)
- models in which *one positivity condition implies the other two* ($\sim$ walks in a half-space $\Longrightarrow$ algebraic)
- models in which *one step is never used*

and declare *equivalent* models that only differ by a *permutation of the coordinates*

Proposition

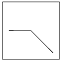
One is left with $11\,074\,225 \simeq 2^{23.4}$ distinct models [Bostan-Bousquet-Mélou-Kauers-Melczer 16]

The group of the walk in 2D

[Fayolle-Iasnogorodski-Malyshev 99], [Bousquet-Mélou-Mishna 10]

Take the example of the tandem queue

$\mathcal{S} = \{\mathsf{N}, \mathsf{W}, \mathsf{SE}\}$



Observation

The *jump polynomial* reads

$$S(x,y) = \overline{x} + y + x\overline{y}$$

$S(x,y)$ is *left unchanged* by the rational transformations

$$\Phi : (x,y) \mapsto (\overline{x}y, y) \quad \text{and} \quad \Psi : (x,y) \mapsto (x, x\overline{y})$$

They are involutions, and generate a finite group G:

$$\{(x,y), (\overline{x}y, y), (\overline{x}y, \overline{x}), (\overline{y}, \overline{x}), (\overline{y}, x\overline{y}), (x, x\overline{y})\}$$

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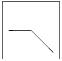

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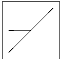
A general construction

The group is not always finite

$\mathcal{S} = \{\mathrm{S}, \mathrm{W}, \mathrm{SW}, \mathrm{NE}\}$



$$\Phi : (x,y) \mapsto (\overline{xy}(1+\bar{y}), y) \quad \text{and} \quad \Psi : (x,y) \mapsto (x, \overline{xy}(1+\bar{x}))$$

The group in 3D

An example

Take $\mathcal{S} = \{\bar{1}\bar{1}\bar{1}, \bar{1}\bar{1}1, \bar{1}10, 100\}$. The *jump polynomial* is

$$S(x, y, z) = \overline{xyz} + \overline{xy}z + \overline{x}y + x$$

The group G is generated by

- $[x, y, z] \xrightarrow{\Phi} [\overline{x}(y + \overline{y}z + \overline{yz}), y, z]$
- $[x, y, z] \xrightarrow{\Psi} [x, \overline{y}(z + \overline{z}), z]$
- $[x, y, z] \xrightarrow{\Lambda} [x, y, \overline{z}]$

It has order 8

The group in 3D

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Classification

$11\,074\,225 = 165\,962$ $(|G| < \infty)$ $+$ $10\,908\,263$ $(|G| = \infty)$
[Bostan-Bousquet-Mélou-Kauers-Melczer 16], [Kauers-Wang 17]

Relevance of the group size and a toolbox

A toolbox in the finite group case (2D and 3D)

- Write a functional equation for

$$O(x,y,z;t) = \sum_{i,j,k,n \geqslant 0} o(i,j,k;n) x^i y^j z^k t^n$$

- Determine if the group of the walk is finite
- If it is, form the orbit equation
- And *try* to extract the generating function $O(x,y,z;t)$

[Bousquet-Mélou-Mishna 10], [Bostan-Bousquet-Mélou-Kauers-Melczer 16], [Kauers-Wang 17], [Yatchak 17]

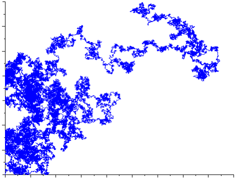
Infinite group case in 3D

- Apart from the functional equation, no result so far

Asymptotics of the excursion sequence

Standard Brownian motion in cones C

- Persistence probability $\mathbb{P}_x[\tau_C > t]$
- Local limit theorem $\mathbb{P}_x[\tau_C > t, B_t \in K]$



[DeBlassie 87], [Bañuelos-Smits 97]

(heat kernel estimates on manifolds)

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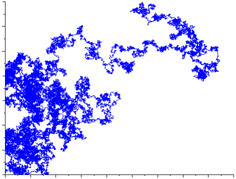


RW in cones $C \subset \mathbb{R}^D$: local limit theorem

$$o(i,j,k;n) \sim \varkappa \cdot V(i,j,k) \cdot \rho^n \cdot n^{-\alpha}$$

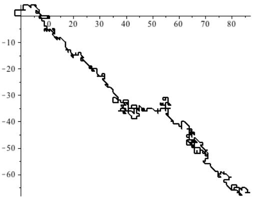
with $\alpha = \sqrt{\lambda_1 + (\frac{D}{2} - 1)^2} + 1$ and λ_1 is the smallest eigenvalue of the Dirichlet problem

$$\begin{cases} \Delta_{\mathbb{S}^{D-1}} m = -\lambda m & \text{in } C \cap \mathbb{S}^{D-1} \\ m = 0 & \text{in } \partial(C \cap \mathbb{S}^{D-1}) \end{cases}$$

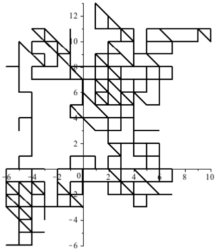
$C \cap \mathbb{S}^{D-1}$ section of the cone on the sphere [Denisov-Wachtel 15]

Critical exponents in 2D and wedges

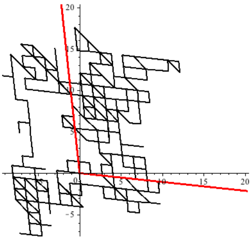
From the quarter plane to an arbitrary wedge



Initial model
(Quadrant)



Remove drift
(Quadrant)



Covariance identity
(Wedge opening β)

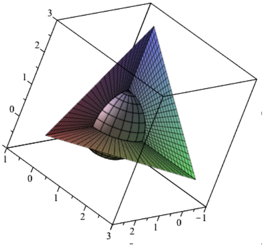
Critical exponent $\alpha = 1 + \frac{\pi}{\beta}$ [Denisov-Wachtel 15]

Consequences

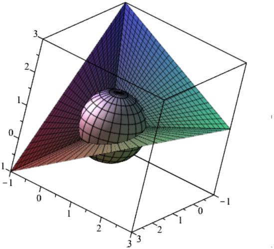
α rational iff group finite iff $Q(x, y; t)$ D-finite [Bostan-R-Salvy 14]

Critical exponents in 3D and spherical triangles

Transformation of $\mathbb{N}^3$ (drift $=0$ and covariance $=$ identity)

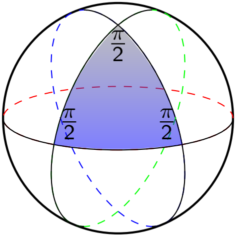


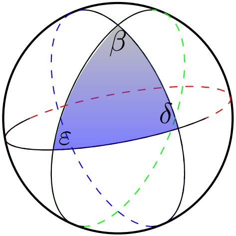
(Orthant $\mathbb{N}^3$)



(Cone $A\cdot\mathbb{N}^3$)

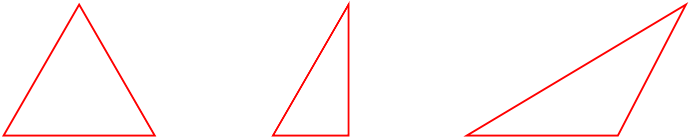
Spherical triangles arise as the sections $(A\cdot\mathbb{N}^3)\cap\mathbb{S}^2$





Dirichlet eigenvalues of spherical triangles 1/3

Warm-up: spectrum of flat triangles



(Equilateral)	(Half-equil.)	(Generic)
Spectrum known	known	unknown

Remarkable family of spherical triangles with known spectrum

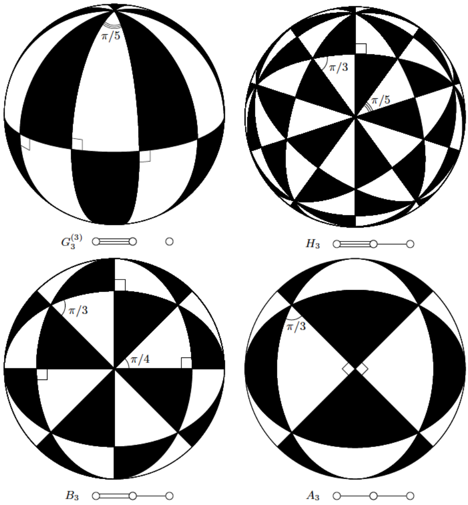
[Bérard 83] Consider triangles with angles

$$\left(\frac{\pi}{p}, \frac{\pi}{q}, \frac{\pi}{r}\right), \qquad p, q, r \in \mathbb{N} \setminus \{0, 1\}$$

Only possible triplets are

- $(2, 3, 3)$ tetrahedral group
- $(2, 3, 4)$ octahedral group
- $(2, 3, 5)$ icosahedral group
- $(2, 2, r)$ dihedral group or order $2r \geqslant 4$

Tilings of the sphere



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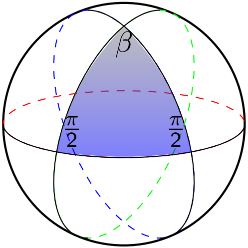
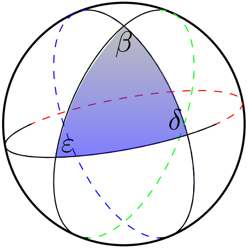
Dirichlet eigenvalues of spherical triangles

A (the?) non-trivial soluble case: birectangular triangles



- Dirichlet problem
$$\begin{cases} \Delta_{\mathbb{S}^2} m = -\lambda m & \text{in } \mathbb{S}^2 \cap C \\ m = 0 & \text{in } \partial(\mathbb{S}^2 \cap C) \end{cases}$$
- Smallest eigenvalue: $\lambda_1 = (\frac{\pi}{\beta}+1)(\frac{\pi}{\beta}+2)$
[Walden 74]
- SRW in 3D: $\beta = \frac{\pi}{2}$ and $\lambda_1 = 12$

Generic case



- No closed-form formula known
- Is there a miracle for Kreweras?
$(\beta = \delta = \varepsilon = \frac{2\pi}{3})$
Tetrahedral tiling of the sphere

Summary of the results

Relate combinatorial properties of a given model to geometric properties of the associated spherical triangle

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Other random processes and other cones

- Critical exponent for Brownian motion
- Eigenvalues of other cones (e.g., spherical cap)

Another view on the classification of the group G

Classification of infinite group models

Group	Number of models	Group	Number of models
$G_1 = \langle a, b, c \mid a^2, b^2, c^2 \rangle$	10,759,449	$G_7 = \langle a, b, c \mid a^2, b^2, c^2, (ab)^4 \rangle$	82
$G_2 = \langle a, b, c \mid a^2, b^2, c^2, (ab)^2 \rangle$	84,241	$G_8 = \langle a, b, c \mid a^2, b^2, c^2, (ab)^3, (bc)^3 \rangle$	30
$G_3 = \langle a, b, c \mid a^2, b^2, c^2, (ac)^2, (ab)^2 \rangle$	58,642	$G_9 = \langle a, b, c \mid a^2, b^2, c^2, acbacbcabc \rangle$	20
$G_4 = \langle a, b, c \mid a^2, b^2, c^2, (ac)^2, (ab)^3 \rangle$	1,483	$G_{10} = \langle a, b, c \mid a^2, b^2, c^2, (ab)^3, (cbca)^2 \rangle$	8
$G_5 = \langle a, b, c \mid a^2, b^2, c^2, (ab)^3 \rangle$	1,426	$G_{11} = \langle a, b, c \mid a^2, b^2, c^2, (ca)^3, (ab)^4, (babc)^2 \rangle$	8
$G_6 = \langle a, b, c \mid a^2, b^2, c^2, (ac)^2, (ab)^4 \rangle$	440	$G_{12} = \langle a, b, c \mid a^2, b^2, c^2, (ab)^4, (ac)^4 \rangle$	4

[Kauers-Wang 17]

Classification of finite group models

Group	Hadamard	Non-Hadamard OS $\neq 0$	Non-Hadamard OS $= 0$
$\mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_2$	1852	0	0
D_{12}	253	66	132
$\mathbb{Z}_2 \times D_8$	82	0	0
S_4	0	5	26
$\mathbb{Z}_2 \times S_4$	0	2	12

[Bacher-Kauers-Yatchak 16]

Interpretation on the reflection group

- A relation $(ab)^m = 1$ corresponds to an angle $\frac{n}{m}\pi$
- In particular, Hadamard models correspond to G_3

An interesting Hadamard structure

Definition: a decomposition of $S(x,y,z) = \sum_{(i,j,k)\in\mathcal{S}} x^i y^j z^k$

- Type $(1,2)$: $S(x,y,z) = U(x) + V(x)T(y,z)$
- Type $(2,1)$: $S(x,y,z) = U(x,y) + V(x,y)T(z)$

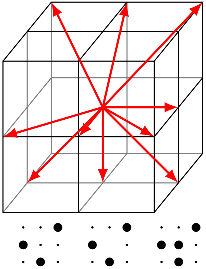
Extends the notion of *independent random walks*

An example

Take $S(x,y,z) = x + (1 + x + \overline{x})(yz + \overline{y} + \overline{z})$

The group has order 12

D-finite generating function by
[Bostan-Bousquet-Mélou-Kauers-Melczer 16]
[Bostan-Bousquet-Mélou-Melczer 18]



Generating function as Hadamard product $O = Q \odot H$

Hadamard models: exact computation of λ_1

Reminders

- Type $(1,2)$: $S(x,y,z) = U(x) + V(x)T(y,z)$
- Type $(2,1)$: $S(x,y,z) = U(x,y) + V(x,y)T(z)$
- Their spherical triangles are birectangular

Type $(1,2)$: a unified result

If the group associated to the step set T is infinite, the series $O(0,0,0;t)$ (and thus also $O(x,y,z;t)$) is non-D-finite

Hadamard models: exact computation of λ_1

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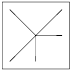
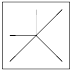
Type $(2,1)$: mixture of two 2D laws

Let $T'(z_0) = 0$. If the critical exponent of the *mixture* $U(x,y) + V(x,y)T(z_0)$ is not in $\mathbb{Q}$, $O(0,0,0;t)$ is non-D-finite

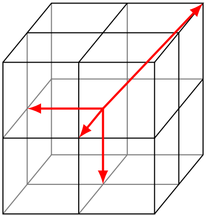
Example: any mixing of  and  is non-D-finite

Asymptotic counting of quadrant walks with inhomogeneities [D'Arco-Lacivita-Mustapha 16]

The very intriguing Kreweras 3D model

Finite group but non-D-finite? Estimation of λ_1

- [5.15,5.16] [Costabel 08]
- 5.159 [Ratzkin-Treibergs 09]
- 5.1606 [Balakrishna 13]
- 5.1589 [Bostan-R-Salvy 14]
- 5.1591452 [Bacher-Kauers-Yatchak 16]
- 5.159145642466 [Guttmann 17]
- 5.159145642466 [Bogosel-Perrollaz-R-Trotignon 18]



Some further aspects

No diff. equation of order r with polynomial coefficients of degree d for any r and d such that $(r+2)(d+1) < 2000$

Extends to finite group models with no Hadamard structure and zero orbit-sum

Other open problems

- Tutte's invariant approach for 3D models

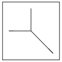
- Non-D-finiteness results beyond the Hadamard structure

- Express D-finite length generating functions in terms of hypergeometric series [Bostan-Chyzak-van Hoeij-Kauers-Pech 17]

- Closed-form expression for eigenvalues

Step-by-step construction and functional equation in 2D

Take the example of the tandem queue
$\mathcal{S} = \{\mathrm{N}, \mathrm{W}, \mathrm{SE}\}$



Generating function

$$Q(x, y; t) \equiv Q(x, y) = \sum_{i,j,n \geqslant 0} q(i, j; n) x^i y^j t^n$$

Step-by-step construction and functional equation in 2D

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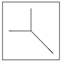

Generating function

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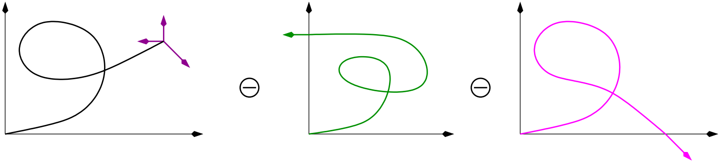
Functional equation

$$Q(x,y) = 1 + tyQ(x,y) + t\frac{Q(x,y) - Q(0,y)}{x} + tx\frac{Q(x,y) - Q(x,0)}{y}$$

A simple exclusion-inclusion proof

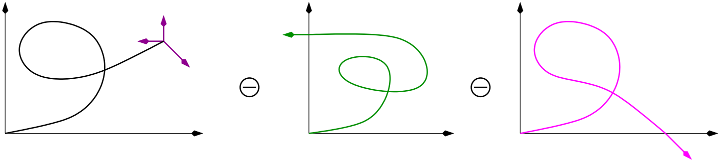


[Bousquet-Mélou-Mishna 10]

A kernel functional equation in 2D

A linear discrete partial differential equation

$$Q(x,y) = 1 + tyQ(x,y) + t\frac{Q(x,y) - Q(0,y)}{x} + tx\frac{Q(x,y) - Q(x,0)}{y}$$



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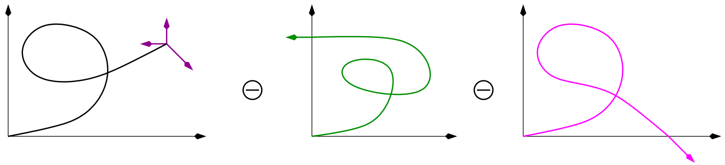

A kernel equation with catalytic variables

With $\overline{x} = 1/x$ and $\overline{y} = 1/y$,

$$\{1 - t(y + \overline{x} + x\overline{y})\}Q(x,y) = 1 - t\overline{x}Q(0,y) - tx\overline{y}Q(x,0)$$

or equivalently

$$\{(1 - t(y + \overline{x} + x\overline{y})\}xyQ(x,y) = xy - tyQ(0,y) - txQ(x,0)$$

We call $K(x,y) = 1 - t(y + \overline{x} + x\overline{y})$ the kernel of the equation

The kernel functional equation in 3D

An example

- Take $\mathcal{S} = \{\bar{1}\bar{1}\bar{1}, \bar{1}\bar{1}1, \bar{1}10, 100\}$. The functional equation reads

$$\begin{aligned} O(x,y,z) =& 1 + t(\overline{xyz} + \overline{xy}z + \bar{x}y + x)O(x,y,z) \\ & - t\bar{x}(y + \bar{y}z + \overline{yz})O(0,y,z) - t\overline{xy}(z+\bar{z})O(x,0,z) - t\overline{xyz}O(x,y,0) \\ & + t\overline{xy}(z+\bar{z})O(0,0,z) + t\overline{xyz}O(0,y,0) + t\overline{xyz}O(x,0,0) \\ & - t\overline{xyz}O(0,0,0) \end{aligned}$$

- Equivalently,

$$\begin{aligned} K(x,y,z)xyzO(x,y,z) &= xyz - tyz(y + \bar{y}z + \overline{yz})O(0,y,z) - tz(z+\bar{z})O(x,0,z) \\ & - tO(x,y,0) + tz(z+\bar{z})O(0,0,z) + tO(0,y,0) + tO(x,0,0) - tO(0,0,0), \end{aligned}$$

with kernel

$$K(x,y,z) = 1 - t(\overline{xyz} + \overline{xy}z + \bar{x}y + x)$$

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with kernel

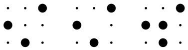
$$K(x,y,z) = 1 - t(\overline{xyz} + \overline{xy}z + \bar{x}y + x)$$

An idea of the complexity (even in D-finite cases)

Determine $O(x,y,z;t)$ up to a large order (in t) and try to guess if it is algebraic or D-finite (order $\simeq 50$ and degree $\simeq 3000$ is not unusual)

An example (continued)

$S(x,y,z) = x + (1 + x + \bar{x})(yz + \bar{y} + \bar{z})$



Construction of an octant walk of length n with steps in $\mathcal{S}$

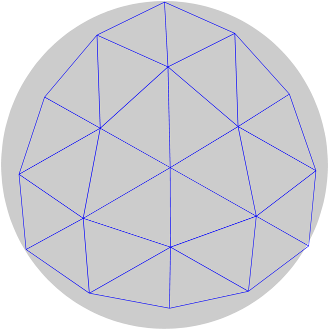
- Take a 1D walk $h = h_1 \dots h_n$ with steps in $\{\bar{1}, 0, 1, 1\}$ on the x-axis; say it has ℓ black steps
- Take a quadrant walk $q = q_1 \dots q_\ell$ with steps in $\{11, \bar{1}0, 0\bar{1}\}$ in the yz-plane
- In h, replace h_i by $(h_i, 0, 0)$ if h_i is red, by (h_i, q_j) if h_i is the jth black step of h

Hadamard product of generating functions $O = Q \odot H$

D-finiteness of $O(x,y,z;t)$ follows from the D-finiteness of the generating functions $H(x;t)$ and $Q(y,z;t)$ of the two projected walks

Computation of the Eigenvalue

1. Construct the mesh



(successive midpoint refinements)

Computation of the Eigenvalue

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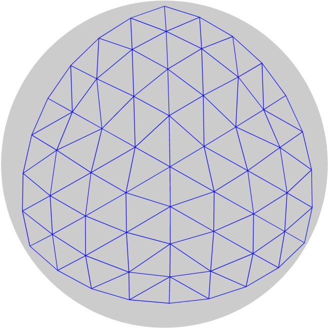

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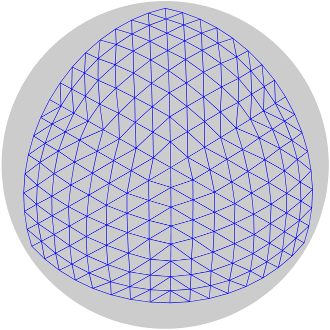

(successive midpoint refinements)

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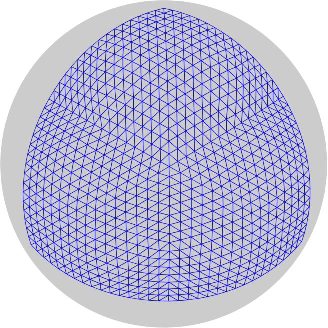

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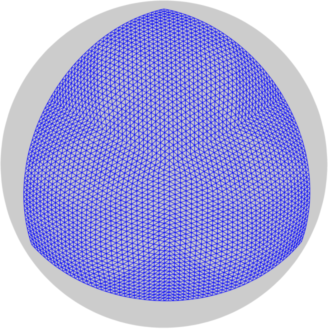


(successive midpoint refinements)

Computation of the Eigenvalue

2. Construct eigenvalue problem

- K, M matrices of rigidity and mass — Lagrange P1 finite elements
- Generalized eigenvalue problem (`eigs` in Matlab)

$$Ku = \lambda Mu$$

- Dirichlet boundary condition: penalize diagonal terms in K corresponding to the boundary

$$K \mapsto K + 1e16 \cdot \mathrm{diag}(\chi_{\partial T})$$

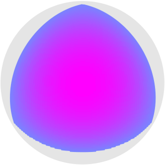
Examples of computation

1. Three right angles

	Approx	Exact
197377 points:	12.0001029159	12
787969 points:	12.0000257290	12
3148801 points:	12.0000064323	12
12589057 points:	12.0000016085	12

Examples of computation

2. Tetrahedral partition



	Approx
197377 points:	5.15918897549
787969 points:	5.15915647773
3148801 points:	5.15914835159
12589057 points:	5.15914632003

More precision

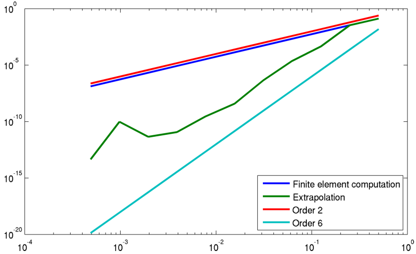
[The SIAM 100-Digit Challenge] — nice reference: accuracy in numerical computation

- Rather slow convergence
- Try to use convergence acceleration techniques
- Wynn's epsilon algorithm: recover the exact limit for the sum of n geometric sequences, given $2n + 1$ terms
- Increase the speed convergence by eliminating terms in the Taylor decomposition of the error

More accurate results

Compute λ_1 for discretizations corresponding to $h, h/2, h/2^2$, etc. Extrapolate this sequence...

1. Three right angles



Exact value:	12
Best using finite elements:	12.00000160856720
Using extrapolation:	11.99999999999946

More accurate results

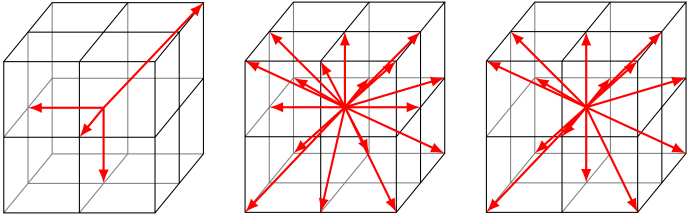
Compute λ_1 for discretizations corresponding to h, $h/2$, $h/2^2$, etc.
Extrapolate this sequence...

2. Three angles equal to $2\pi/3$

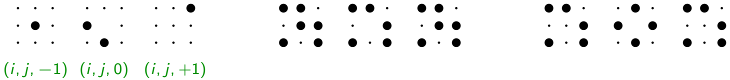
Best using finite elements:	**5.15914**63200323471
Using extrapolation:	**5.1591456424**704827

$\rightarrow$ coincides with best known estimates in the literature

Equivalent representations of 3D models



Kreweras 3D model, a $(1,2)$-type Hadamard model and a $(2,1)$-type Hadamard model. Cross-section views may be easier to read:



1D and 2D walks: from Kindergarden to PhD