# Groups and Symmetries in Numerical Linear Algebra Part 2b

## Mirrors and caleidoscopes

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# Chebyshev 101 (classical theory)

"*Chebyshev polynomials are everywhere dense in Numerical Analysis*" (G. Forsythe?)

## Definition

$$\begin{array}{rcl} \text{(1. kind)} & : & T_k(x) = \cos(k\theta) \\ \text{(2. kind)} & : & U_k(x) = \sin((k+1)\theta)/\sin(\theta) \\ \text{where} & & x = \cos(\theta). \end{array}$$

$$\begin{aligned} T_0(x) &= 1 \\ T_1(x) &= x \\ T_2(x) &= 2x^2 - 1 \\ T_3(x) &= 4x^3 - 3x \\ &\dots \end{aligned}$$

## 3-term recurrence

$$T_{k+1}(x) = 2xT_k(x) - T_{k-1}(x)$$

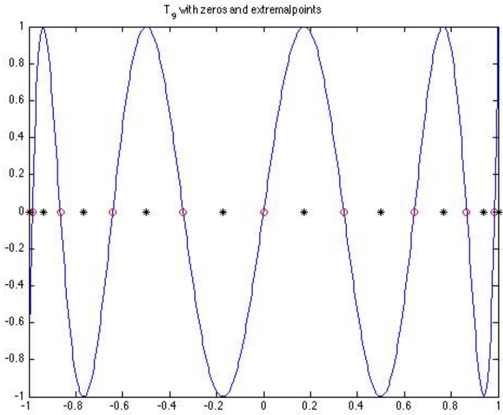
# Chebyshev 101 (classical theory)

## Orthogonality - continuous and discrete

$$\langle T_k, T_\ell \rangle_C = \int_{-1}^{1} \frac{T_k(x) T_\ell(x)}{\sqrt{1-x^2}} dx$$

$$\langle T_k, T_\ell \rangle_E = \frac{1}{N} \sum_{x_j \in \{*\}} T_k(x_j) T_\ell(x_j)$$

$$\langle T_k, T_\ell \rangle_Z = \frac{1}{N} {\sum_{x_j \in \{o\}}}' T_k(x_j) T_\ell(x_j)$$



# Chebyshev 101 (classical theory)

## Chebyshev interpolation

$$f(x) \approx \sum_{k=0}^{N} a(k) T_k(x) \quad \text{, interpolating in extremal points } \{*\}$$
$$a(k) = \langle T_k, f\rangle_E / \langle T_k, T_k\rangle_E .$$

**Note:**

- $\{f(x_j)\}_{x_j \in \{*\}} \leftrightarrow \{a_k\}_{k=0}^{N}$ in $\mathcal{O}(N \log N)$ flops via FCT.
- *Lebesgue constant* of Cheby-interpolation grows *logarithmically*

$$L_{\{*\}} = \mathcal{O}(\log N).$$

- *Exponentially fast convergence* for analytic $f(x)$.

# Chebyshev 101 (classical theory)

## Chebyshev interpolation

$$
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a(k) &= \langle T_k, f \rangle_E / \langle T_k, T_k \rangle_E .
\end{aligned}
$$

## Clenshaw-Curtis quadrature

$$
\int_{-1}^{1} f(x) dx \approx \sum_{k=0}^{N} a(k) \int_{-1}^{1} T_k(x) dx .
$$

# Chebyshev 101 (classical theory)

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## Pseudospectral derivation

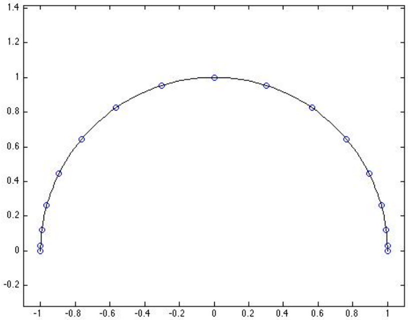
$$f'(x)dx \approx \sum_{k=0}^{N} a(k) T_k'(x)dx = \sum_{k=0}^{N} b(k) T_k(x)dx.$$

$\{a(k)\} \mapsto \{b(k)\}$ in $\mathcal{O}(N)$ flops by linear recursion.

# Example: Curve length

$$L[f] = \int_a^b ||f'(t)||dt$$

Pseudospectral derivation + Clenshaw-Curtis integration.
16 points on semicircle:




$>>$ ChebyL('semicircle',16)

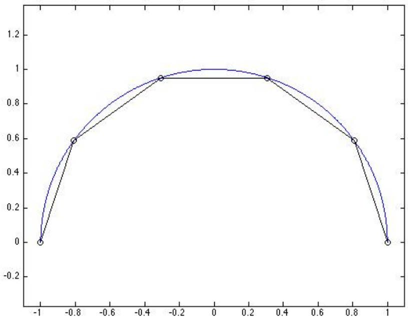
ans = 3.14159265358962**3**

error $= 1.7 \cdot 10^{-13}$

# Example: Curve length

$$L[f] = \int_a^b ||f'(t)||dt$$

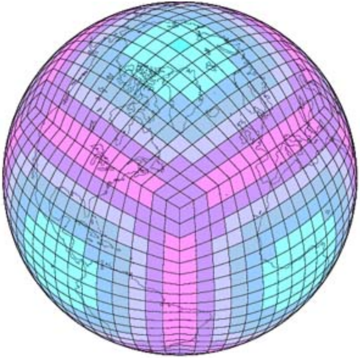
Archimedes: Inscribed 2N-gon:




$N = 16$ points:
error $= 0.006$

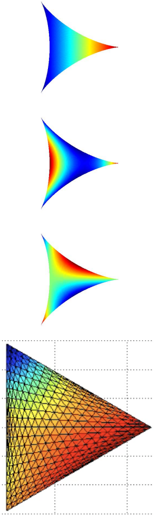
$N = 2 \cdot 10^6$ points:
error $= 3.2 \cdot 10^{-13}$

# Spectral– and spectral element methods

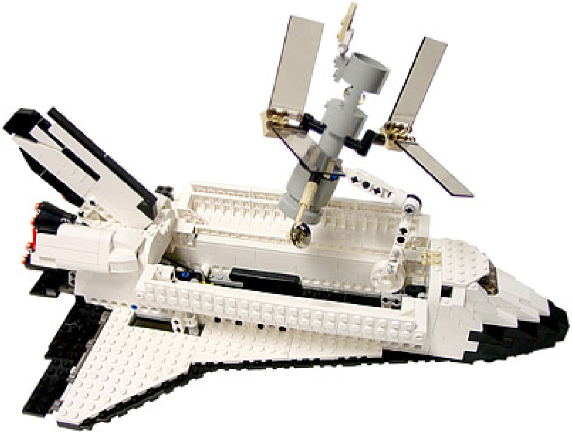


Current practice ↑. ↑ We want this.

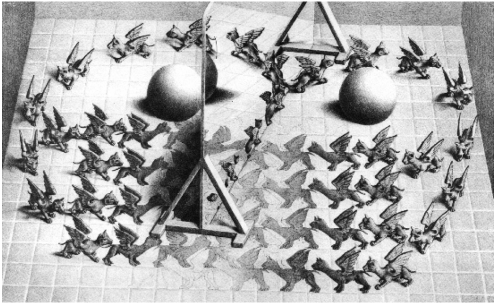
# Triangular 'lego bricks' in spectral elements



$\Rightarrow$



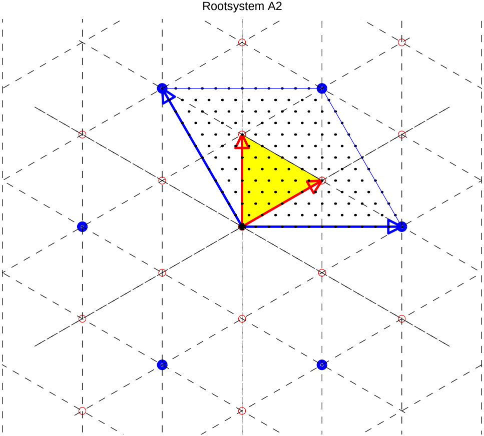
## MK 1989: "Symmetric FFTs, a general approach" (unpubl.)

### Laplace–Dirichlet eigenfunctions by anti-symmetrization:

$$\begin{aligned} \sigma &: \text{mirror}, \quad \Delta \circ \sigma = \sigma \circ \Delta \\ \Delta u &= \lambda u \\ u_a &= \frac{1}{2}(u - u \circ \sigma) \\ \Rightarrow \Delta u_a &= \lambda u_a, \quad u_a = 0 \quad \text{on mirror} \end{aligned}$$

# Example: $A_2$–Kaleidoscope



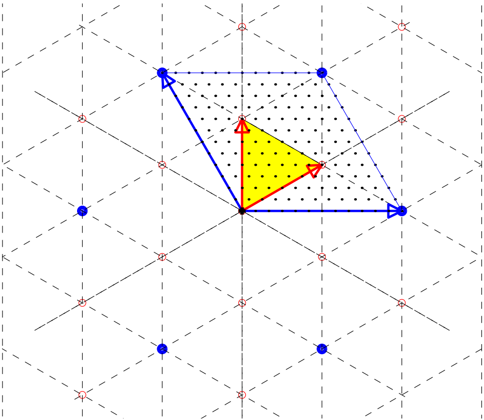

## Weyl group $A_2$

$$\sigma_i = I - 2\frac{\alpha_i \alpha_i^T}{\alpha_i^T \alpha_i}, \quad i = 1, 2$$
$$W = \langle \sigma_1, \sigma_2 \rangle$$

## Laplacian eigenfunctions:

$$u(\theta) = \exp(ik\theta) \Rightarrow \Delta u = \lambda u$$
$$u_s = \frac{1}{|W|} \sum_{g \in W} u \circ g$$
$$\Delta u_s = \lambda u_s \qquad \text{(Neumann)}$$

# Example: $A_2$–Kaleidoscope

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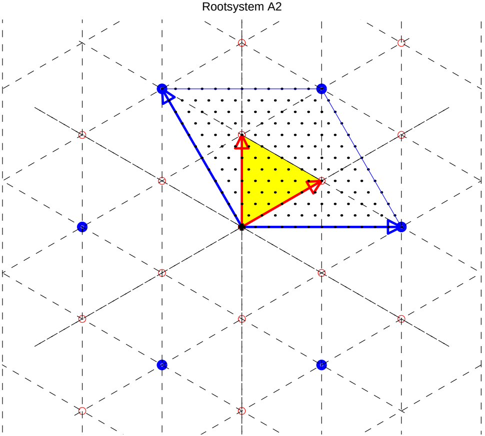
$$W = \langle \sigma_1, \sigma_2 \rangle$$

## Laplacian eigenfunctions:

$$u(\theta) = \exp(ik\theta) \Rightarrow \Delta u = \lambda u$$
$$u_a = \frac{1}{|W|} \sum_{g \in W} \det(g) u \circ g$$
$$\Delta u_a = \lambda u_a \qquad \text{(Dirichlet)}$$

# Example: $A_2$–Kaleidoscope




Properties of $u_a$ and $u_s$:

- Continuous and discrete orthogonality.
- Gaussian quadrature.
- Symmetric FFTs for interpolation, derivation, integration.
- Triangle based fast Poisson solvers.
- Sym. FFT have complicated data flow.
- Spectral convergence?

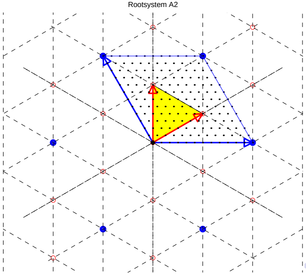
# Weyl groups

## How to define 'caleidoscopes' on general periodic domains?

### Definition

A root system is a subset of a euclidean space $\Phi = \{\alpha_i\} \subset E$ such that

1. $\Phi$ is finite, spans $E$ and does not contain 0.
2. If $\alpha \in \Phi$ then the only multiples of $\alpha$ in $\Phi$ are $\pm\alpha$.
3. If $\alpha \in \Phi$ then the reflection $\sigma_\alpha = I - 2\frac{\alpha\alpha^T}{\alpha^T\alpha}$ leaves $\Phi$ invariant.
4. If $\alpha, \beta \in \Phi$ then $2\frac{\alpha^T\beta}{\alpha^T\alpha} \in \mathbb{Z}$.



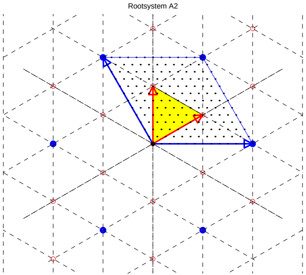
# Caleidoscopes (the Affine Weyl group)

## Definition

The group generated by the reflections $W = \langle \sigma_\alpha | \alpha \in \Phi \rangle$ is called the *Weyl group*.

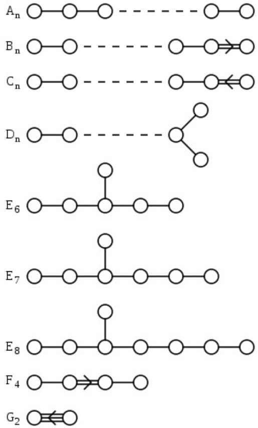
The set $\Lambda = \langle \theta \mapsto \theta + \alpha \mid \alpha \in \Phi \rangle$ is called the *Root lattice*.

The *affine Weyl group* $W' = \Lambda \rtimes W$ is the group generated by all these reflections and translations.



# Classification of Root systems

( Cartan–Weyl–Coxeter–Dynkin)



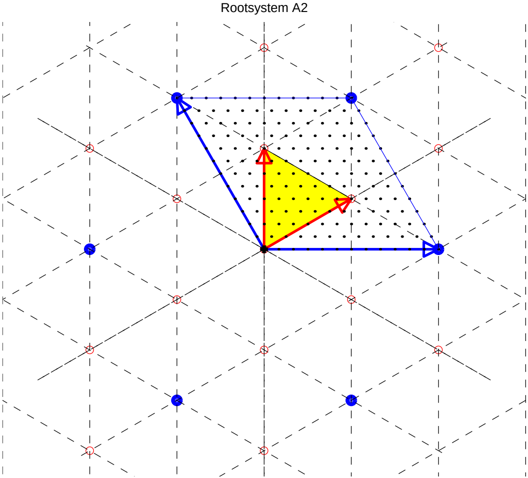

Dynkin diagram:

- Nodes = generating mirrors.
- Edges indicate mirror-angles

  no edge : $90^o$
  – one edge : $120^o$
  = two edges : $135^o$
  ≡ three edges : $150^o$

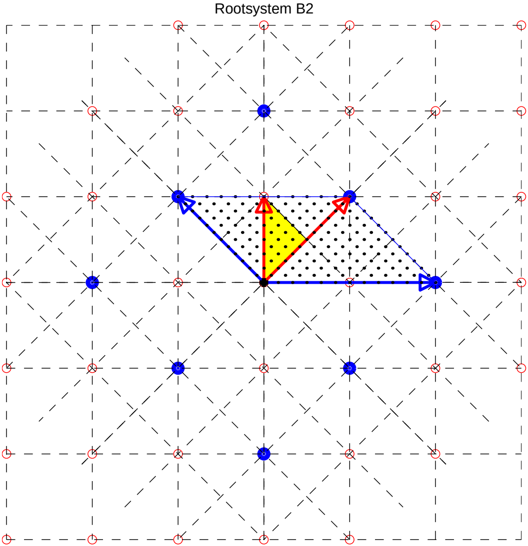
- Arrow separates *long* and *short* roots.

# Non-separable 2D cases: $A_2$, $B_2$ and $G_2$




- Blue dots: Roots.
- Blue arrows: Basis for root system.
- Red arrows: Fundamental dominant weights.
- Dotted lines: Mirrors in affine Weyl group.
- Yellow triangle: Fundamental domain of affine Weyl group.
- Red circles: Weights lattice.
- Black dots: Downscaled root lattice.

# Root system $B_2$:

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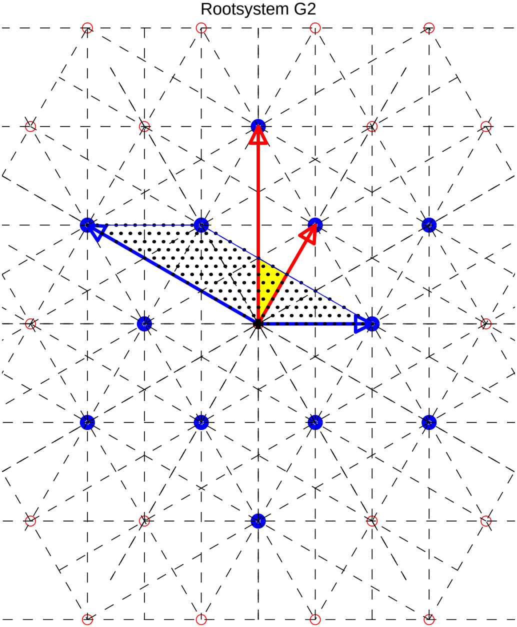
# Root system $G_2$:




- Blue dots: Roots.
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- Black dots: Downscaled root lattice.

# Multivariate Chebyshev polynomials

Let $\Phi$ be $d$-dimensional root system, $W$ Weyl group and $\Lambda$ root lattice.
Let $G = \mathbb{R}^d/\Lambda$ be the 'root-periodic' domain and $\widehat{G} = \Lambda^\perp$ the reciprocal lattice (Fourier space).

## Definition

Multivariate Chebyshev polynomials $T_k(x)$ are defined as follows for $\theta \in G$, $k \in \widehat{G}$:

$$T_k(x) = \frac{1}{|W|} \sum_{g \in W} e^{i(gk)^T \theta}$$

$$x_j(\theta) = \frac{1}{|W|} \sum_{g \in W} e^{i(g\lambda_j)^T \theta}, \qquad \lambda_j = (0, \ldots, 1, \ldots, 0)^T$$

# Multivariate Chebyshev polynomials

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\end{aligned}
$$

## Example: 1-D case

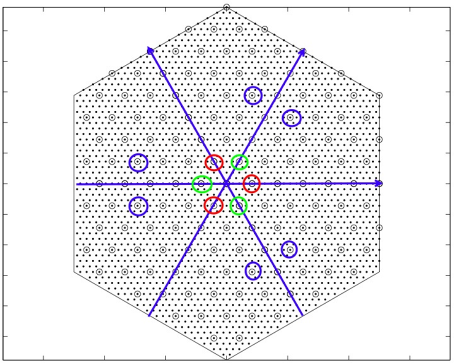
$$
\begin{aligned}
\Phi &= \{-\pi, \pi\}, \qquad W = \{-1, 1\} \\
T_k(x) &= \frac{1}{2}(e^{ik\theta} + e^{-ik\theta}) = \cos(k\theta) \\
x(\theta) &= \frac{1}{2}(e^{i\theta} + e^{-i\theta}) = \cos(\theta).
\end{aligned}
$$

# Multivariate Chebyshev polynomials

## Definition

$$T_k(x) = \frac{1}{|W|}\sum_{g\in W} e^{i(gk)^T\theta}, \qquad x_j(\theta) = \frac{1}{|W|}\sum_{g\in W} e^{i(g\lambda_j)^T\theta}$$

## Example: $A_2$ case

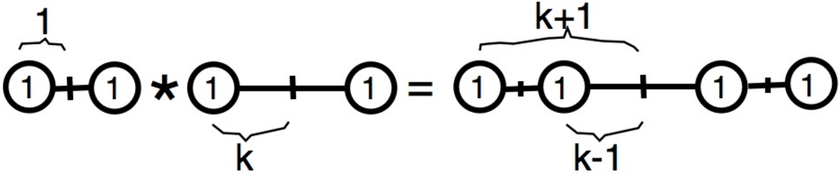


# Recurrence relations

$$T_0 = 1, \qquad T_{e_j} = x_j$$

$$T_\ell T_k = \frac{1}{|W|} \sum_{g \in W} T_{k+g^T \ell}.$$

Classical ($A_1$): $\quad xT_k(x) = \frac{1}{2}(T_{k-1}(x) + T_{k+1}(x))$



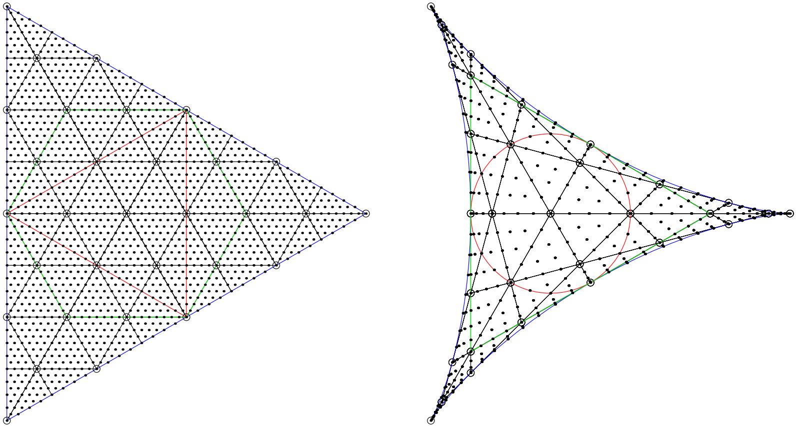
# Recurrence relations

$$T_0 = 1, \qquad T_{e_j} = x_j$$
$$T_\ell T_k = \frac{1}{|W|} \sum_{g \in W} T_{k+g^T \ell}.$$

## $A_2$ recurrence:

$$\begin{aligned} z &= x_1, \quad \overline{z} = x_2 \\ T_{-1,0} &= \overline{z}, \quad T_{0,0} = 1, \quad T_{1,0} = z \\ T_{n,0} &= 3zT_{n-1,0} - 3\overline{z}T_{n-2,0} + T_{n-3,0} \\ T_{n,m} &= (3T_{n,0}\overline{T_{m,0}} - T_{n-m,0})/2. \end{aligned}$$

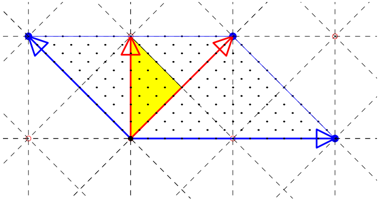
# The example: $A_2$

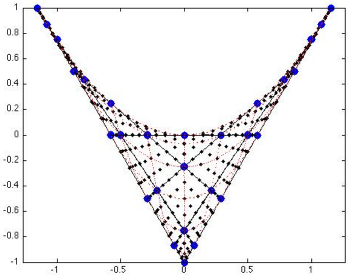


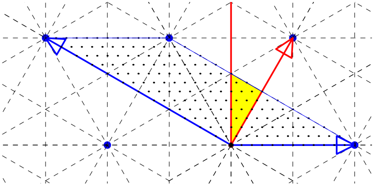
Fundamental domain of affine Weyl group mapped to Deltoid by $\theta \mapsto x$:

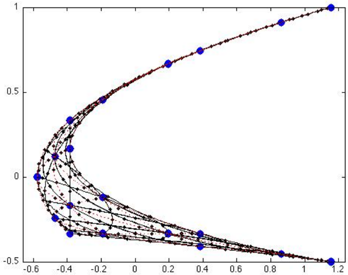
$$x_1 = \frac{1}{3}(\cos\theta_1 + \cos\theta_2 + \cos(\theta_1 - \theta_2)), x_2 = \frac{1}{3}(\sin\theta_1 - \sin\theta_2 - \sin(\theta_1 - \theta_2)).$$

# Domains for $B_2$ and $G_2$ Chebyshev polynomials

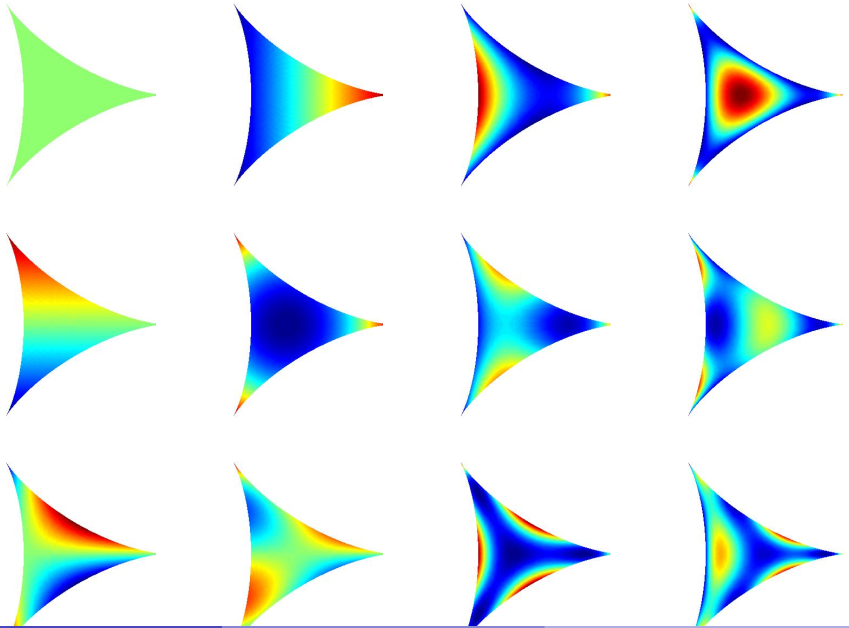




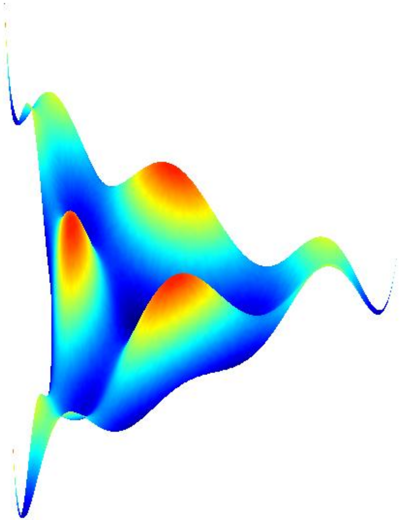





# A2 Chebyshev polynomials: 00r 10r 20r 30r | 10i 11r 21r 31r | 20i 21i 22r 32r



# A2 Chebyshev polynomial $T_{52}$, real part:



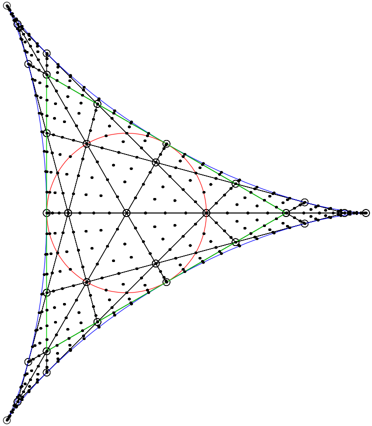
# Problem: Deltoid $\neq$ triangle

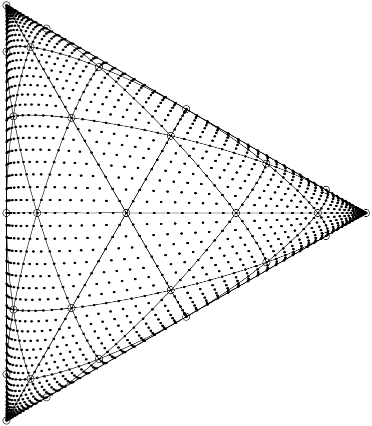
Possible solutions:

1. Straighten the deltoid to triangle.
2. Patch with overlap.
3. Work with (overdetermined) frame based on triangular trigonometric polynomials.

# Straightening the deltoid

We have constructed a coordinate map which straightens the deltoid to a triangle. The map has analytically computable jacobian. It is well behaved away from the corners, but has corner singularities due to the cusps of the deltoid. Interpolation points are given *analytically*.



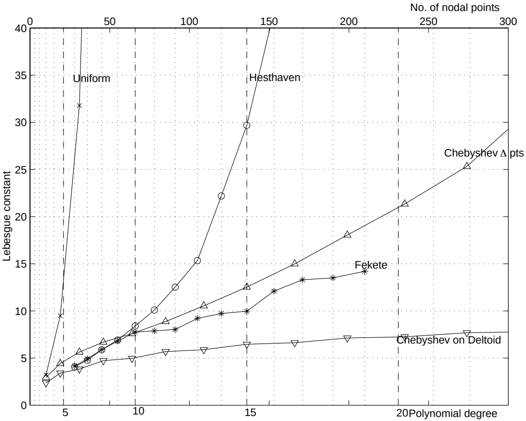


# Lebesgue constant in triangular interpolation

Lebesgue constant: $L = ||I||_\infty$, where $I$ is the (multivariate) interpolation operator in the given nodes. Slow growth of the Lebesgue constant is necessary for spectral convergence.
Define Lebesgue function:

$$\lambda(x) = \sum_{i \in \mathcal{I}} |\ell_i(x)|,$$

where $\ell_i(x)$ is Lagrangian cardinal polynominal at node $i$, then $L = ||\lambda(x)||_\infty$.




Bottom curve: Cheby-Lobatto points on Deltoid. All other curves: Interpolation points on triangle:

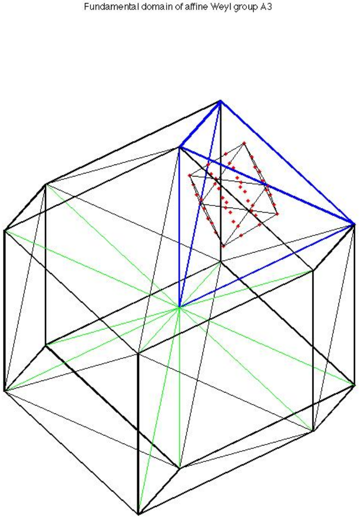
- Fekete points.
- Image of C–L points by straightening Deltoid to triangle.
- Hesthaven electrostatic points.
- Uniform meshpoints on triangle.

# $A_3$ polynomials

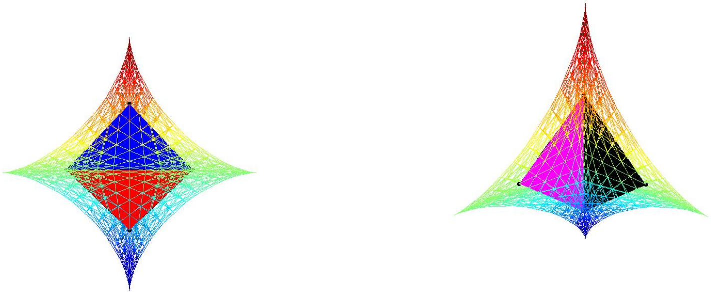
The root system $A_3$ (in 3D) is similar to the $A_2$ case:

- The Voronoi region of the root lattice is the *rhombic dodecahedron*.
- The fundamental domain of the affine Weyl group is a tetrahedron.
- Inside this tetrahedron sits a regular octahedron.
- Under the coordinate change $\theta \mapsto x$, the tetrahedron maps to a cusp-shaped domain, and the octahedron to a tetrahedron inside this.
- Restriction to faces: $A_3 \mapsto A_2$.
- Restriction to lines: $A_3 \mapsto A_1$.

# $A_3$ fundamental domains



# $A_3$ domain after change of variables



# Numerical algorithms

We have analytical formulas and algorithms for

- Integrating $T_k(x)$ over whole $x$-domain (deltoid etc.).
- Integrating $T_k(x)$ over inscribed triangle ($A_2$ case) and tetrahedron ($A_3$ case).
- Computing $\nabla T_k(x)$ by recursion in Fourier domain.

All algorithms are FFT based, cost $\mathcal{O}(N \log(N))$. Optimized symmetrized transforms exist.

# Dirichlet problem on L-shaped domain, decomposed into triangles