Topological Optimization Using the SIMP Method

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Outline

- Orthogonal Polynomials
- Chebyshev Polynomials
- Chebyshev Expansion
- Using Kernel Polynomials
- Application: Calculating the Density of States

Orthogonal Polynomials

Scalar product on $[a, b]$:

$$\langle f|g\rangle = \int_a^b w(x) f(x) g(x)\,\mathrm{d}x$$

Given a scalar product, we get a set of polynomials, p_n, which satisfy the orthogonality relation

$$\left\langle p_n|p_m\right\rangle = \delta_{n,m}\left\langle p_n|p_n\right\rangle .$$

This allows for an expansion of any given function $f(x)$ in terms of the $p_n(x)$:

$$f(x) = \sum_{n=0}^{\infty} \alpha_n p_n(x) \quad \text{with} \quad \alpha_n = \frac{\left\langle p_n|f\right\rangle}{\left\langle p_n|p_n\right\rangle}$$

Chebyshev Polynomials

I will focus on Chebyshev polynomials of the first kind, T_n:

Defined on interval $[-1, 1]$ with weight function $w(x) = \left(\pi\sqrt{1-x^2}\right)^{-1}$.

$$T_n = \cos\left(n \arccos(x)\right)$$

Recursively defined:

$$T_0(x) = 1, \quad T_{-1}(x) = T_1(x) = x,$$

$$T_{m+1}(x) = 2xT_m(x) - T_{m-1}(x).$$

The polynomials also follow the relation

$$2T_m(x)T_n(x) = T_{m+n}(x) + T_{m-n}(x).$$

Chebyshev Polynomials have some particular advantages which make them ideal for use in orthogonal polynomial expansions.

Chebyshev Expansion

The expansion of $f(x)$ in terms of Chebyshev polynomials

$$f(x) = \sum_{n=0}^{\infty} \frac{\langle f|T_n\rangle_1}{\langle T_n|T_n\rangle_1} T_n(x)$$

To make this a easier to compute, we rearrange:

$$f(x) = \frac{1}{\pi\sqrt{1-x^2}} \left[\mu_0 + 2\sum_{n=1}^{\infty} \mu_n T_n(x) \right], \quad \mu_n = \int_{-1}^{1} f(x) T_n(x) \, \mathrm{d}x.$$

However, calculating the moments μ_n can be quite computationally expensive.

Motivation for KPM: Gibbs Oscillations

In practice, we cannot compute an infinite series, so we need to truncate:

$$f(x) \approx \frac{1}{\pi\sqrt{1-x^2}} \left[\mu_0 + 2 \sum_{n=1}^{N-1} \mu_n T_n(x) \right]$$

Gibbs Oscillations:

Kernel Polynomials

To lessen the impact of the Gibbs Oscillations, we introduce a "damping function" in the form of a kernel polynomial, g_n:

$$f_{\mathsf{KPM}}(x) = \frac{1}{\pi\sqrt{1-x^2}}\left[g_0\mu_0 + 2\sum_{n=1}^{N-1} g_n\mu_n T_n(x)\right]$$

Application: Density of States Calculations

Density of States: How many energy states exist at a given energy E.

$$\rho(E) = \frac{1}{N} \sum_{k=0}^{N-1} \delta(E - E_k)$$

Scale E down to $[-1, 1]$:

$$E = aX + b$$

We can approximate $\rho(E)$ using KPM:

$$\rho(E) \approx \frac{1}{\pi\sqrt{1 - x^2}} \left[g_0\mu_0 + 2 \sum_{n=1}^{N-1} g_n \mu_n T_n(X) \right]$$

$$\mu_n \approx \frac{1}{N_r} \sum_r \langle r | T_n(X) | r \rangle$$

Disilicon Si_2 Density of States

Twisted Graphene Density of States

Topics of Further Exploration

- Effects of the number of random vectors (R) used in calculating the moments.
- Optimal resolution values (N) for various Hamiltonians.
- More in-depth comparisons of various kernels.

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Bibliography

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