A new faster FFT approach using a novel algebra of subspace collections to computing the fields in composites

Graeme W. Milton (Univ. Utah, USA)
Herve Moulinec (LMA, Marseille, France)
and Pierre Suquet (LMA, Marseille, France)

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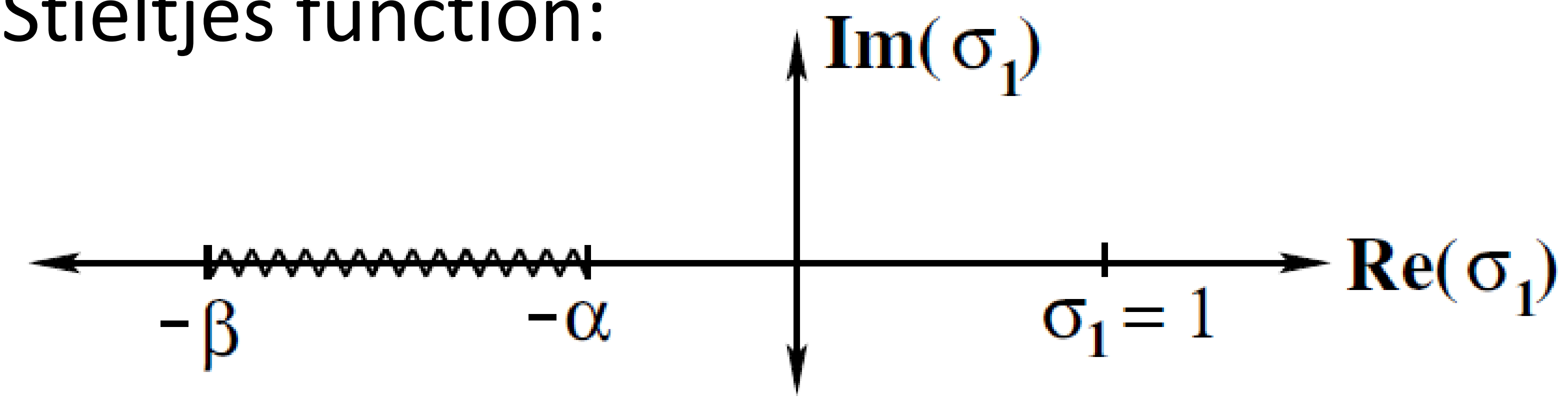
Accelerating some Fast Fourier Transform Methods in two-component composites

The effective conductivity σ_* is an analytic function of the component conductivities σ_1 and σ_2

With $\sigma_2 = 1, \; \sigma_*(\sigma_1)$ has the properties of a Stieltjes function:



Bergman 1978 (pioneer, but faulty arguments)
Milton 1981 (limit of resistor networks)
Golden and Papanicolaou 1983 (rigorous proof)

Original FFT approach of Moulinec and Suquet (1994,1998) based on the series expansion (Brown, Kroner, Willis…)

$$\boldsymbol{\sigma}_* = \sigma_0 \mathbf{I} + \sum_{j=0}^{\infty} \boldsymbol{\Gamma}_0[\boldsymbol{\sigma}(\mathbf{x}) - \sigma_0 \mathbf{I}][\boldsymbol{\Gamma}_1(\mathbf{I} - \boldsymbol{\sigma}/\sigma_0)]^j \boldsymbol{\Gamma}_0, \quad \mathbf{e} = \mathbf{e}_0 + \sum_{j=0}^{\infty} [\boldsymbol{\Gamma}_1(\mathbf{I} - \boldsymbol{\sigma}/\sigma_0)]^j \mathbf{e}_0,$$

$\boldsymbol{\Gamma}_0(\mathbf{k}) = \mathbf{I}$ if $\mathbf{k} = 0$, zero otherwise.
$\boldsymbol{\Gamma}_1(\mathbf{k}) = \mathbf{k}\mathbf{k}^T/(\mathbf{k} \cdot \mathbf{k})$ for $\mathbf{k} \neq 0$, $\boldsymbol{\Gamma}_1(\mathbf{0}) = 0$

Key point: the action of $\boldsymbol{\Gamma}_1$ is most easily evaluated in Fourier space, while the action of $\boldsymbol{\sigma}$ is most easily evalauated in real space. Therefore go back and forth between real and Fourier space, using FFTs, until the series converges.

With $\sigma_0 = (\sigma_1 + \sigma_2)/2$ and $\sigma_2 = 1$ one gets an expansion of the form

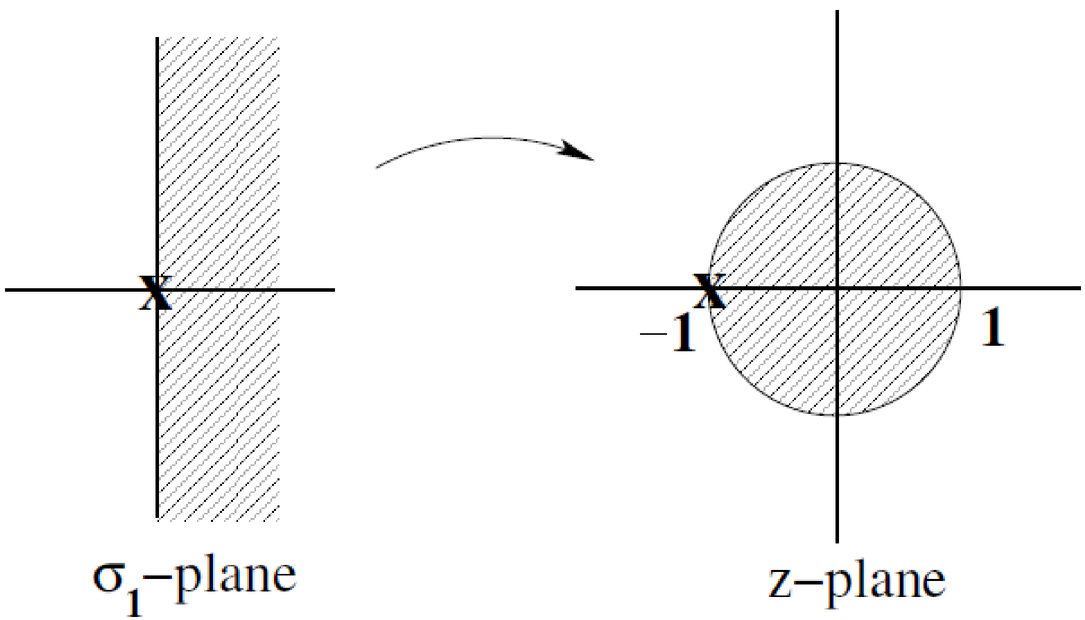
$$\sigma_*/\sigma_0 = 1 + \sum_{k=1}^{\infty} d_k \left(\frac{\sigma_1 - 1}{\sigma_1 + 1} \right), \qquad d_k = -\boldsymbol{\Gamma}_0[1 - 2\chi_1]\{\boldsymbol{\Gamma}_1[1 - 2\chi_1]\}^{k-1}\boldsymbol{\Gamma}_0$$

Complex analysis provides the theory for the convergence of such expansions. The convergence and asymptotic rate of converegence is dictated by the nearest singularity to the origin in the $(\sigma_1 - 1)/(\sigma_1 + 1)$-plane.

Numerical scheme of Moulinec and Suquet (1994)

$$\sigma_*/\sigma_0 = 1 + \sum_{k=1}^{\infty} d_k \left(\frac{\sigma_1 - 1}{\sigma_1 + 1} \right),$$

Let $z = (\sigma_1 - 1)/(\sigma_1 + 1)$

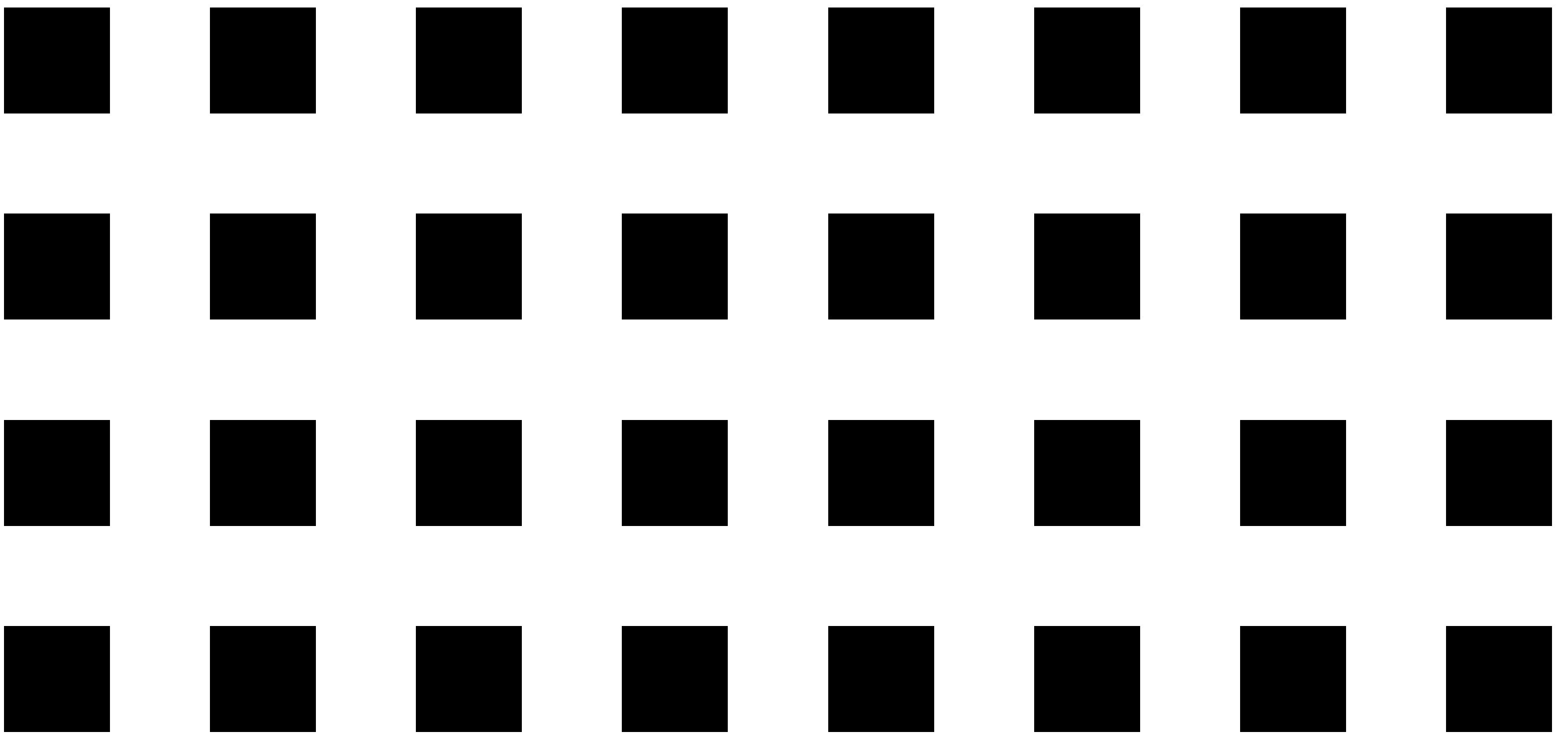


Taylor series converges in the unit disk in the z-plane, corresponding to the right-half plane in the σ_1 plane.

Expect better convergence if there is no singularity near the origin.

X marks position of singularity, assumed here near the origin $\sigma_1 = 0$.

Benchmark model example: a square array of squares at 25% volume fraction



Obnosov's exact formula

$$\sigma_* = \sqrt{(1+3\sigma_1)/(3+\sigma_1)}, \qquad \alpha = 1/3, \quad \beta = 3$$

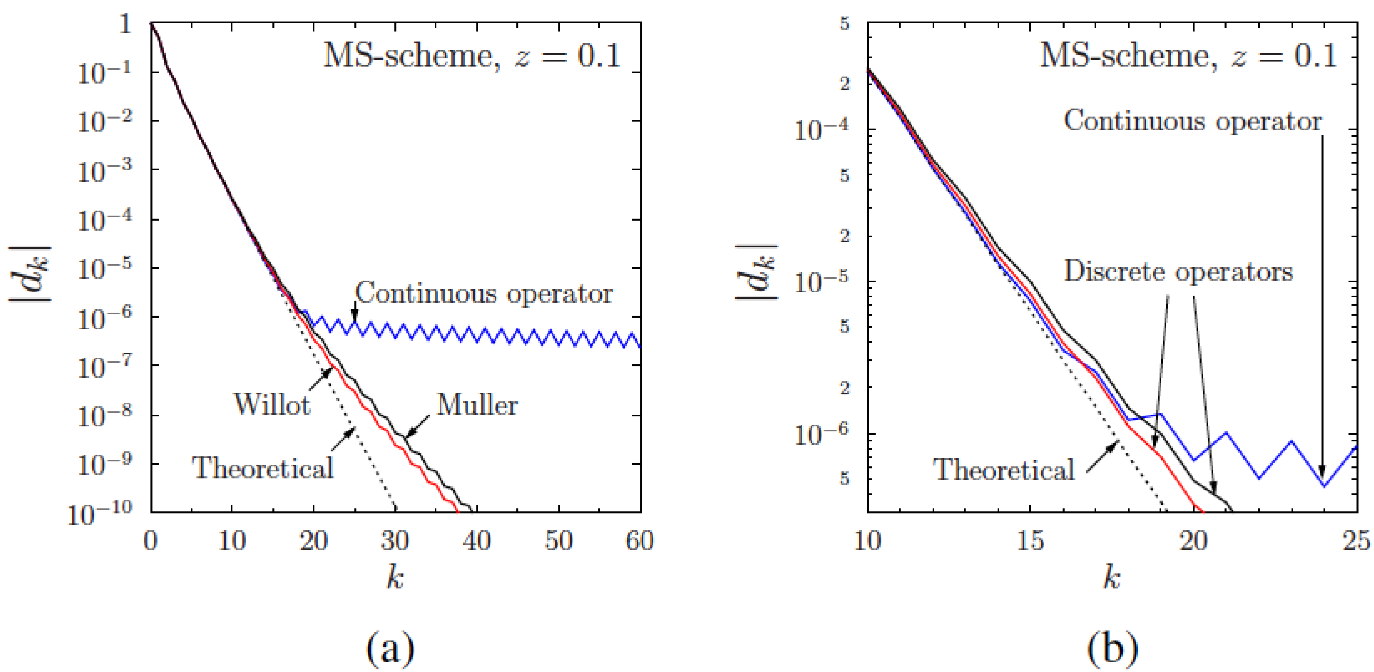
Remark: there is also an exact formula for the effective conductivity of a 4-phase checkerboard

$$\lambda_1^* = \sqrt{\frac{\sigma_1\sigma_2\sigma_3\sigma_4(1/\sigma_1 + 1/\sigma_2 + 1/\sigma_3 + 1/\sigma_4)(\sigma_1 + \sigma_4)(\sigma_2 + \sigma_3)}{(\sigma_1 + \sigma_2 + \sigma_3 + \sigma_4)(\sigma_1 + \sigma_2)(\sigma_3 + \sigma_4)}},$$

$$\lambda_2^* = \sqrt{\frac{\sigma_1\sigma_2\sigma_3\sigma_4(1/\sigma_1 + 1/\sigma_2 + 1/\sigma_3 + 1/\sigma_4)(\sigma_1 + \sigma_2)(\sigma_3 + \sigma_4)}{(\sigma_1 + \sigma_2 + \sigma_3 + \sigma_4)(\sigma_1 + \sigma_4)(\sigma_2 + \sigma_3)}}.$$

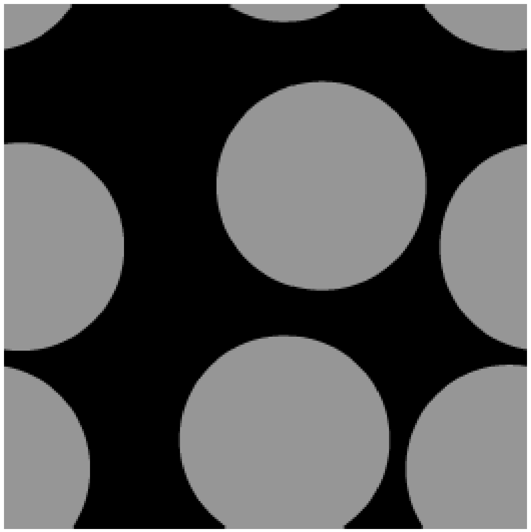
Conjectured by Mortola and Steffe (1985);
proved indendently and by different approaches by Craster and Obnosov (2001) and Milton (2001)

Series expansion coefficients:

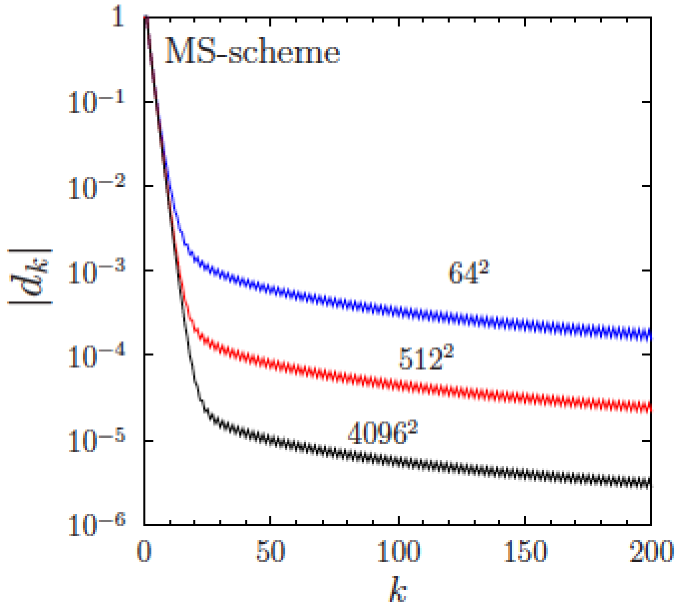


Obnosov's microstructure, discretization 512×512 pixels. MS scheme. Contrast $z = 0.1$. Coefficients d_k of the series (59) with different Green's operators: continuous operator (blue), Müller's operator [20] (black), Willot-Pellegrini operator [22] (red). (a): iterations 1 to 60. (b): close-up on iterations 10 to 25.

Or for a more realistic geometry:



(a)



(b)

(a) Microstructure: 4 circular inclusions, volume fraction 50%. (b) Coefficients d_k of the series (55) at different resolutions. MS scheme.

Upshot: it does not make sense too iterate too many times

“Improved” FFT approach of Eyre and Milton (1999) based on the series expansion

$$\boldsymbol{\sigma}_* = \sigma_0\mathbf{I} + \sum_{j=0}^{\infty} \boldsymbol{\Gamma}_0\mathbf{K}(\boldsymbol{\Upsilon}\mathbf{K})^j\boldsymbol{\Gamma}_0, \quad \mathbf{P} = \sum_{j=0}^{\infty} \mathbf{K}(\boldsymbol{\Upsilon}\mathbf{K})^j\mathbf{e}_0$$

$$\mathbf{K} = [\mathbf{I} + (\boldsymbol{\sigma} - \sigma_0\mathbf{I})\mathbf{M}]^{-1}(\boldsymbol{\sigma} - \sigma_0\mathbf{I}), \quad \boldsymbol{\Upsilon} = \mathbf{M} - (\boldsymbol{\Gamma}_1/\sigma_0)$$

$\mathbf{M}$ is an arbitrary constant tensor, now $\boldsymbol{\Upsilon}$ can have eigenvalues of both signs.

Key point: the action of $\boldsymbol{\Upsilon}$ is most easily evaluated in Fourier space, while the action of $\mathbf{K}$ is most easily evalauated in real space. Therefore go back and forth between real and Fourier space, using FFTs, until the series converges.

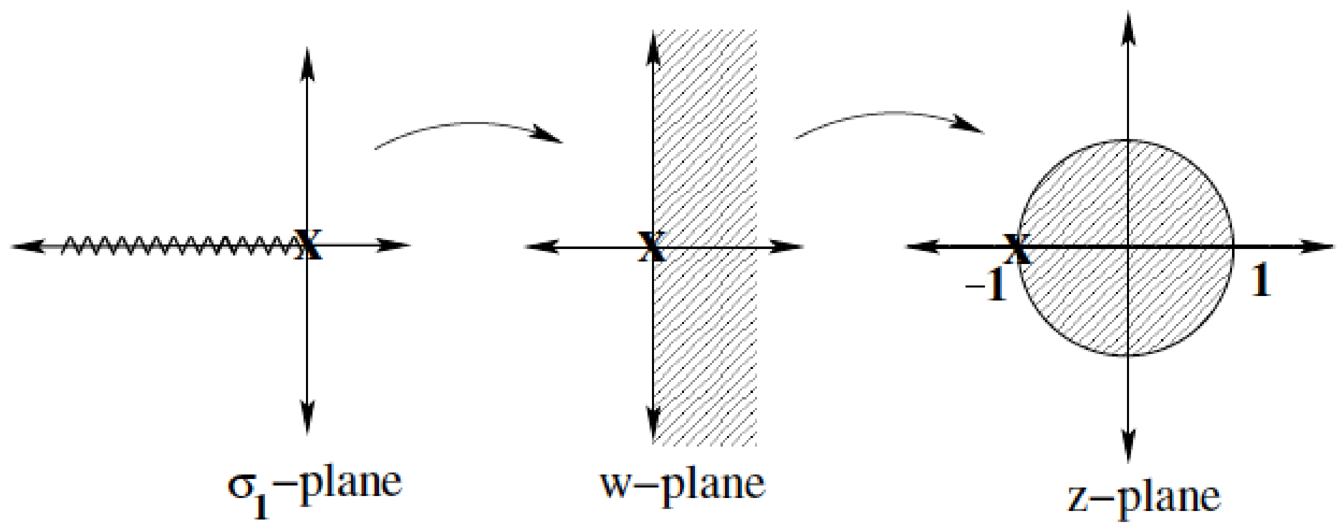
With $\sigma_0 = \sqrt{\sigma_1\sigma_2}$, $\sigma_2 = 1$ and $\mathbf{M} = \mathbf{I}/2\sigma_0$ one gets an expansion of the form

$$\sigma_*/\sqrt{\sigma_1} = 1 + \sum_{n=1}^{\infty} b_n \left(\frac{\sqrt{\sigma_1} - 1}{\sqrt{\sigma_1} + 1}\right)^n .$$

Complex analysis provides the theory for the convergence of such expansions. The convergence and asymptotic rate of converegence is dictated by the nearest singularity to the origin in the $(\sqrt{\sigma_1} - 1)/(\sqrt{\sigma_1} + 1)$-plane.

Quick explanation of the "enhanced" rate of convergence of the Eyre-Milton Scheme

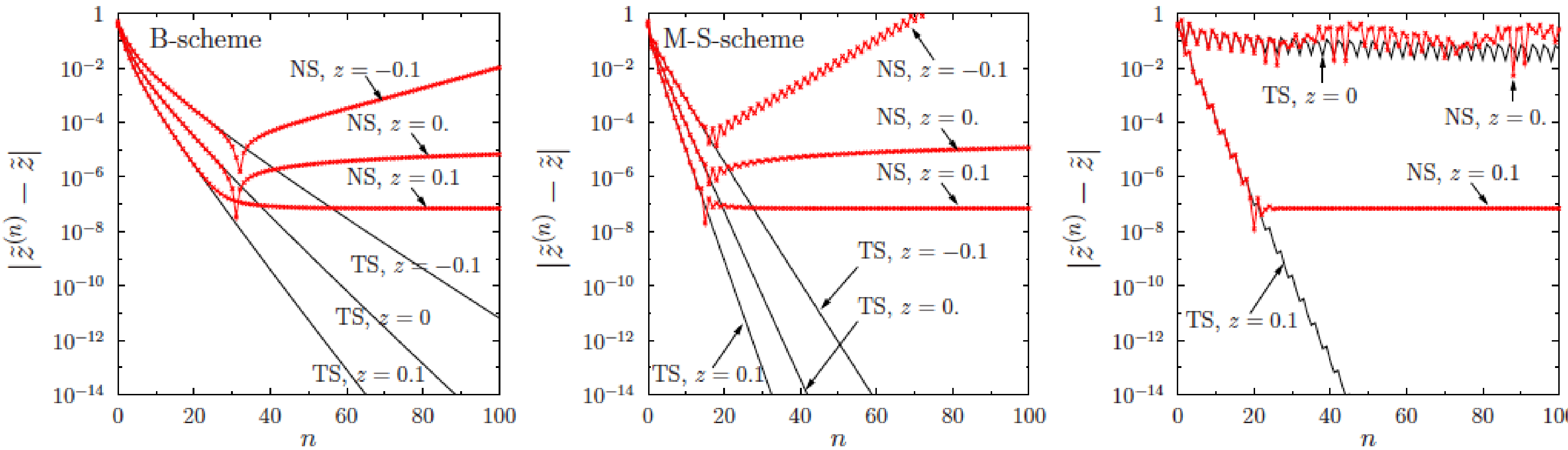
Let $w = \sqrt{\sigma_1}, \quad z = (w-1)/(w+1)$



If we want a series expansion which converges in the entire the σ_1-plane minus the negative real σ_1-axis, then we first make a square root transformation which maps the cut complex σ_1-plane to the right half of the w-plane, followed by a fractional linear transformation which takes it to the unit disk in the z-plane, and find an expansion in powers of z. The scheme of Eyre and Milton (1999) provides such an expansion.

Comparison of convergence for the Obnosov array of squares:

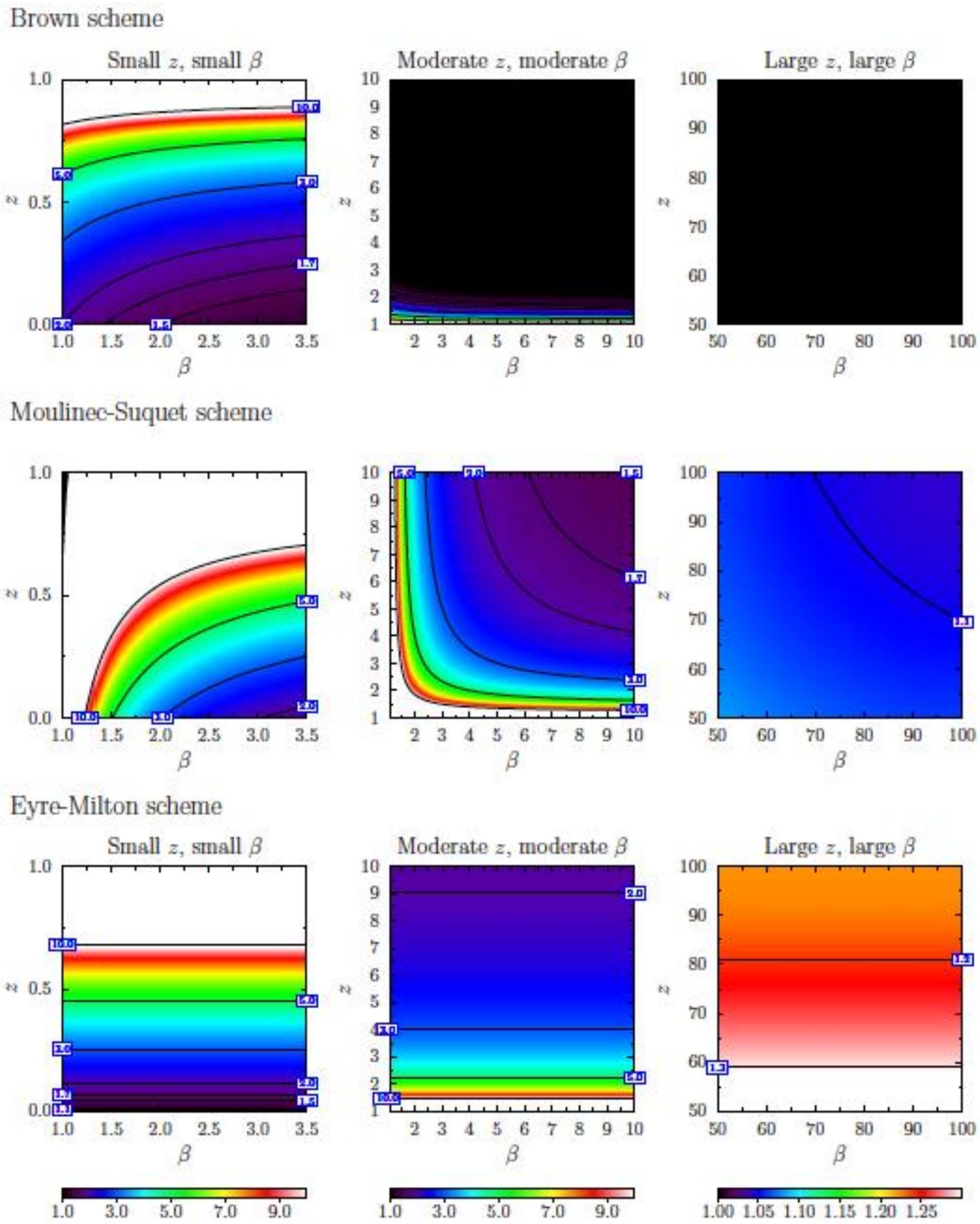
Here $\widetilde{z} = \sigma_* / \sigma_2$, and $z = \sigma_1 / \sigma_2$,
TS=Theoretical Scheme, NS=Numerical Scheme



(a) (b) (c)

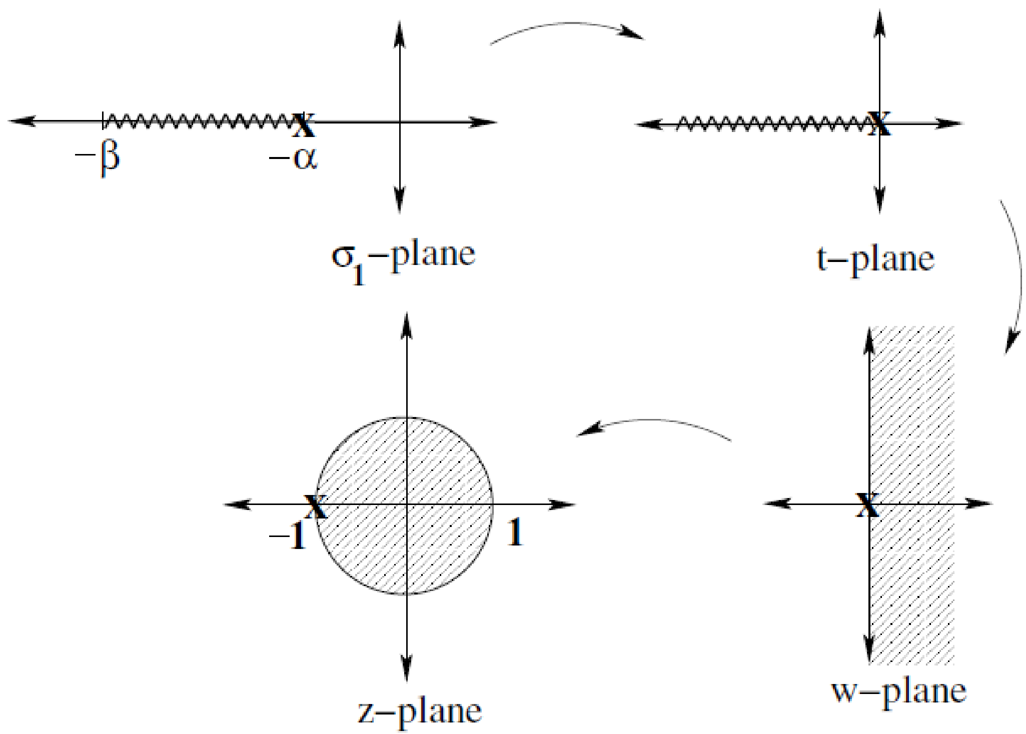
Obnosov problem. Comparison between the convergence of the theoretical series (TS) and the numerical series (NS) for different contrasts. (a) Reference medium: matrix (B-scheme). (b) Reference medium: arithmetic mean (MS-scheme). (c) Reference medium: geometric mean (EM-scheme). Discretization: 512×512 pixels.

None of the three schemes are entirely satisfactory



Snapshots of the rate of convergence for the 3 schemes in the plane (β, z). The brighter the color, the faster the rate of convergence.

If we know α, β then the ideal scheme should be:



$$t = \frac{(\sigma_1+\alpha)(1+\beta)}{(\sigma_1+\beta)(1+\alpha)} = 1 + \frac{(\sigma_1-1)(\beta-\alpha)}{(\sigma_1+\beta)(1+\alpha)}$$

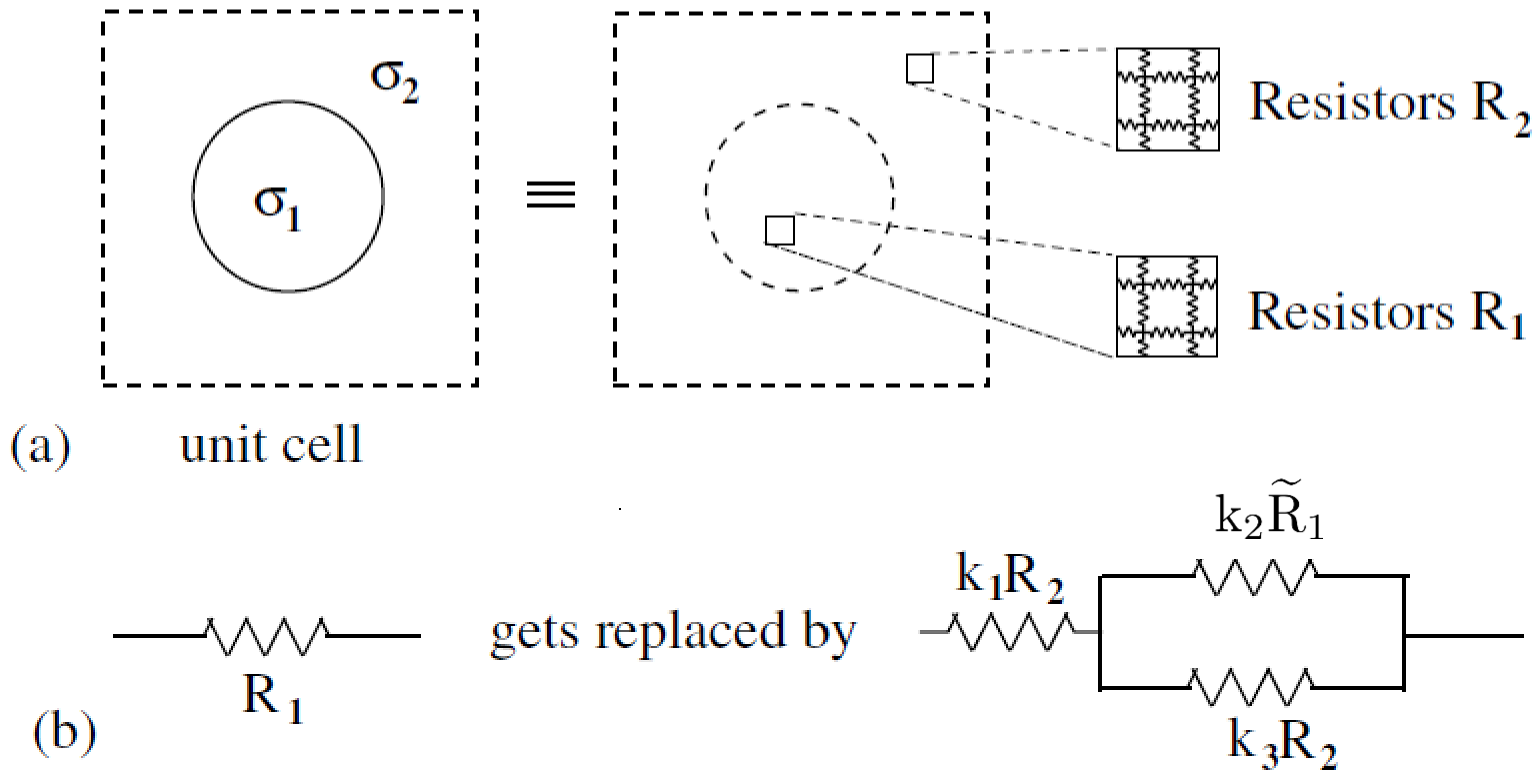
$$w = \sqrt{t}, \quad z = \frac{w-1}{w+1}$$

But we want to do this transformation at the level of the “subspace collection”, to recover the fields We need a new series expansion for the fields.

We need to find a FFT scheme that has an associated series expansion

$$\frac{\sigma_*}{\sqrt{[(\sigma_1+\alpha)(1+\beta)]/[(\sigma_1+\beta)(1+\alpha)]}} = 1 + \sum_{n=1}^{\infty} c_n \left(\frac{\sqrt{\frac{(\sigma_1+\alpha)(1+\beta)}{(\sigma_1+\beta)(1+\alpha)}} - 1}{\sqrt{\frac{(\sigma_1+\alpha)(1+\beta)}{(\sigma_1+\beta)(1+\alpha)}} + 1} \right)^n .$$

One idea: at a discrete level



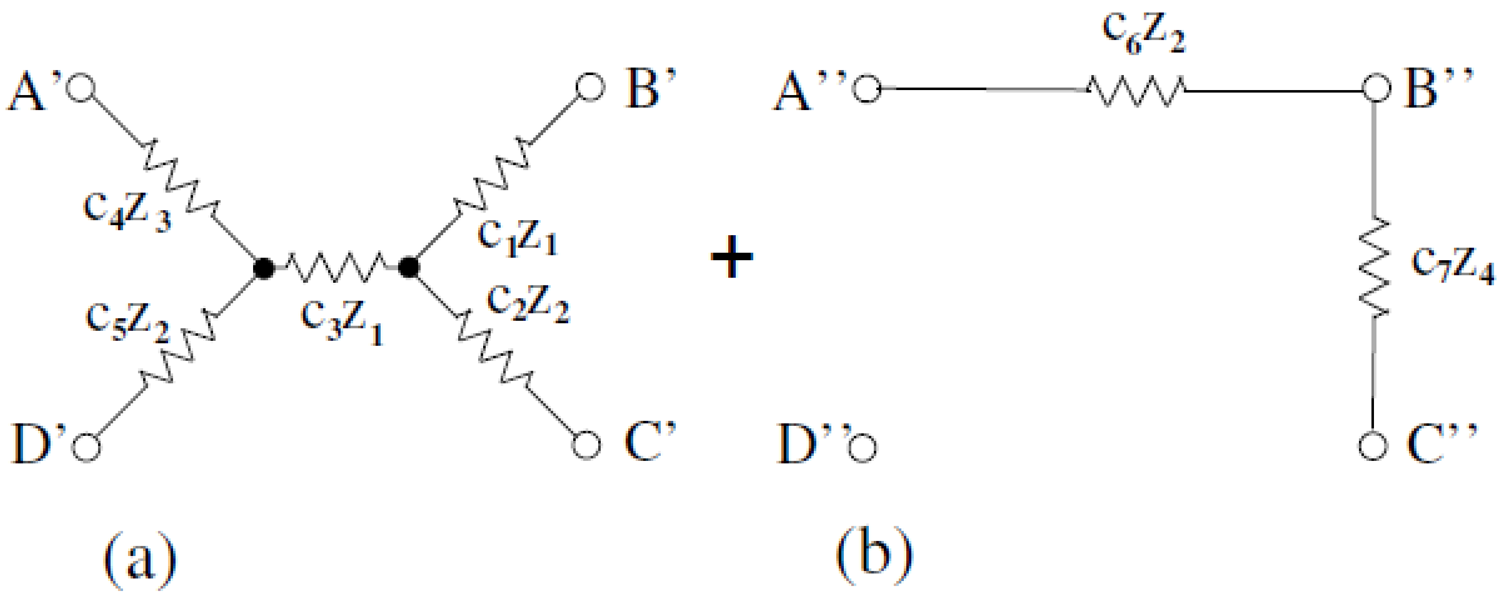
Locally, replace a 1-dimensional subspace by a 3-dimensional subspace

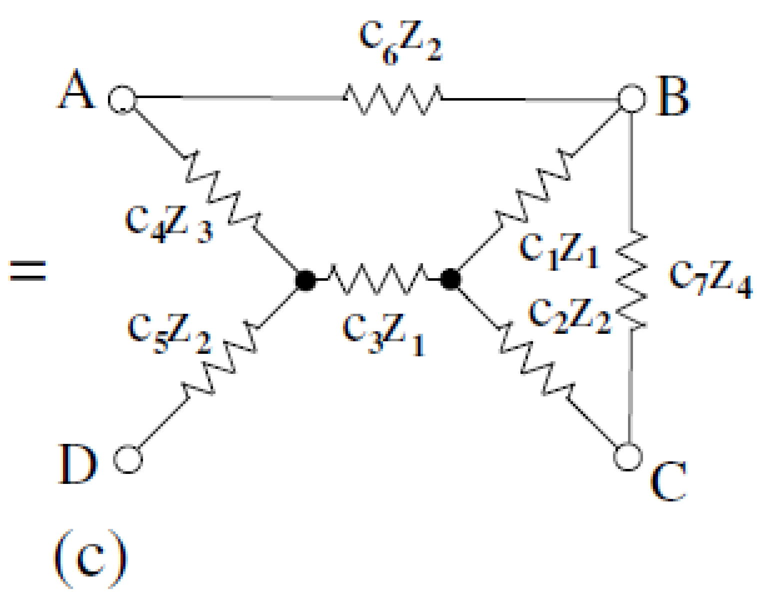
Problem: this substitution shortens the branch cut instead of lengthening it. Solution: Substitute “non-orthogonal subspace collections”

Non-orthogonal subspace collections allow one to generalize the concept of function to

Superfunctions!

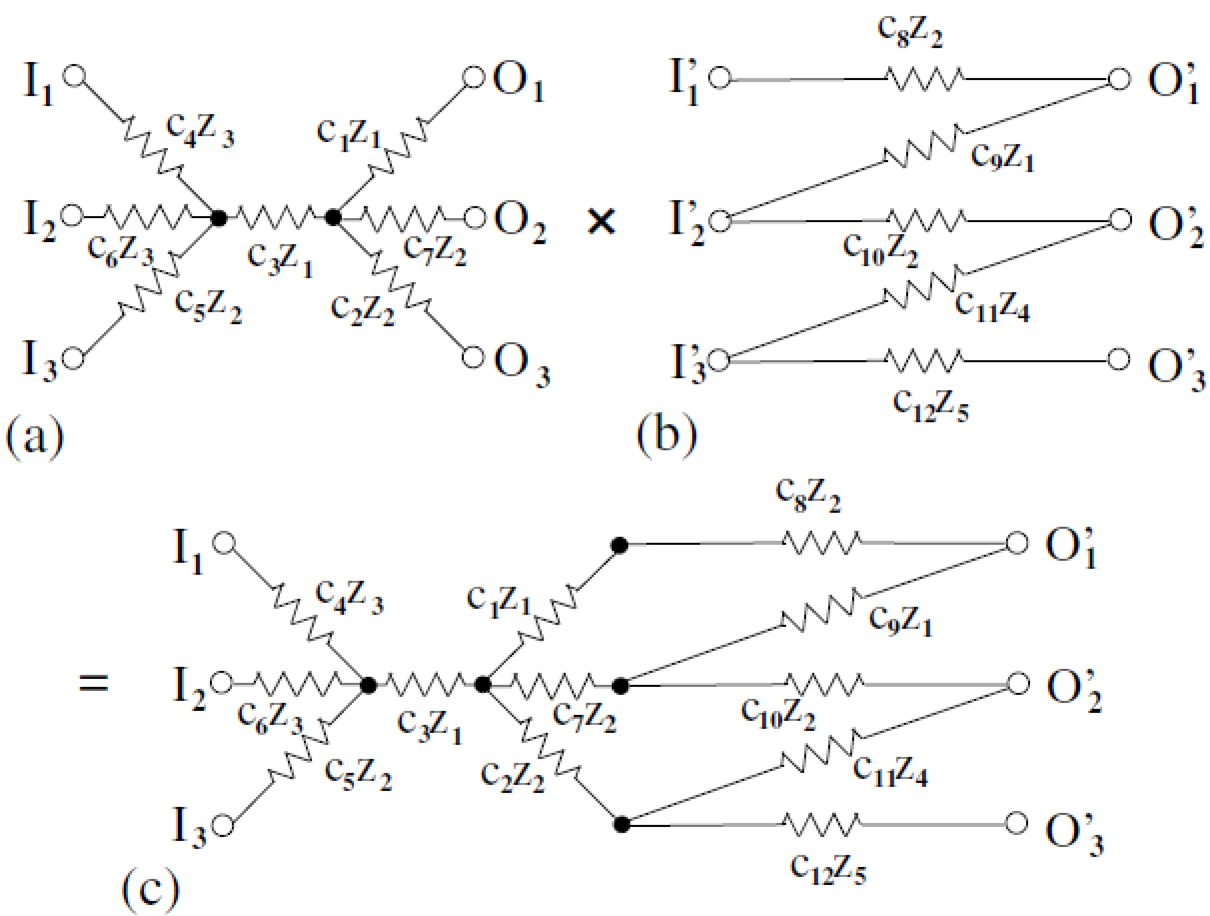
Adding resistor networks





With non-orthogonal subspace collections one can subtract "resistor networks"

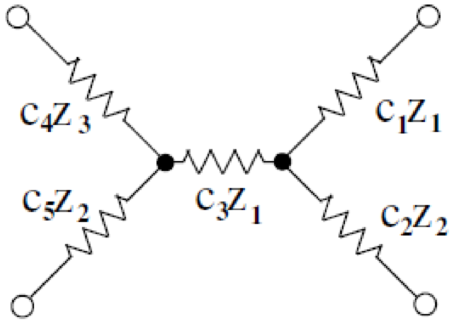
Multiplying resistor networks



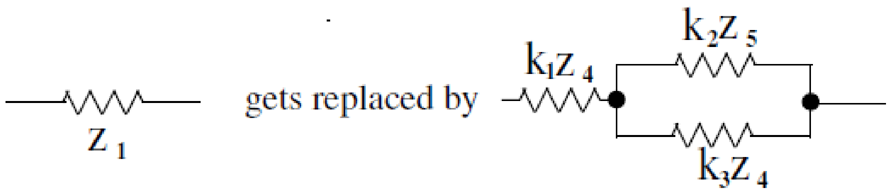
With non-orthogonal subspace collections one can divide "resistor networks".

Substitution of networks

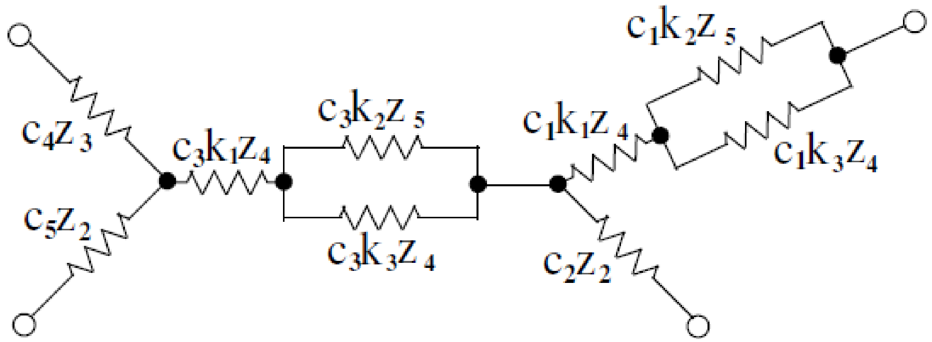
(a)



(b)



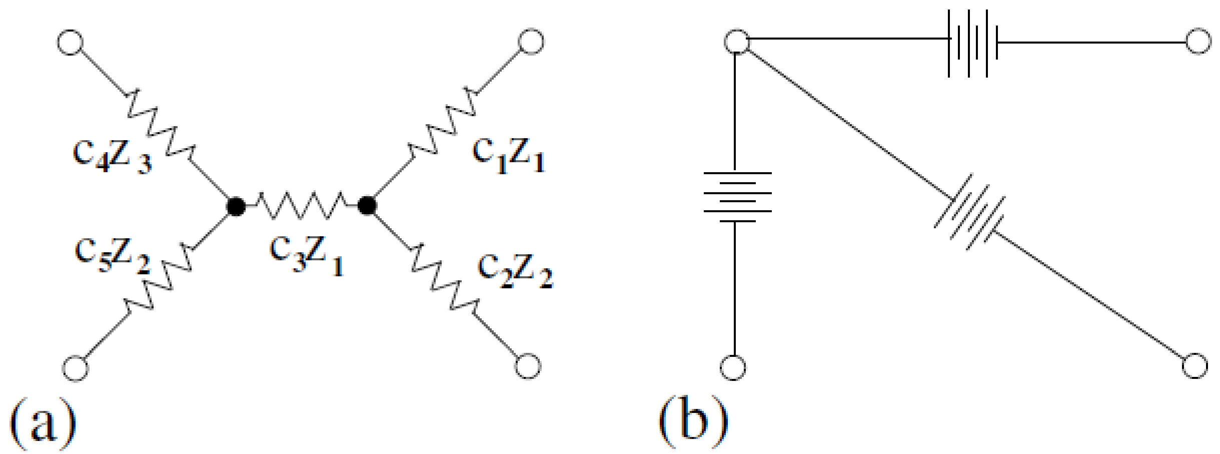
(c)



One is free to substitute a non-orthogonal subspace collection into an orthogonal one.

This is precisely what we will do.

We should consider a resistor network in conjunction with its batteries



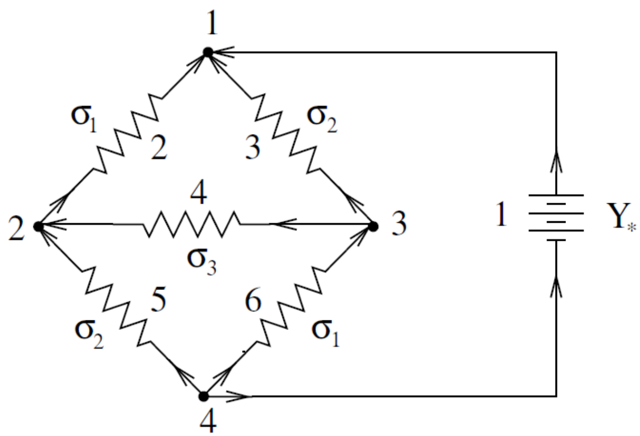
Space $\mathcal{H}$

Space $\mathcal{V}$

Combined Space

$$\mathcal{K} = \mathcal{H} \oplus \mathcal{V}$$

Incidence Matrices:



$$M = \begin{pmatrix} 1 & 0 & 0 & -1 \\ 1 & -1 & 0 & 0 \\ 1 & 0 & -1 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & 1 & 0 & -1 \\ 0 & 0 & 1 & -1 \end{pmatrix}.$$

$$\begin{aligned} M_{ij} &= +1 \text{ if the arrow of bond } i \text{ points towards node } j, \\ &= -1 \text{ if the arrow of bond } i \text{ points away from node } j, \\ &= 0 \text{ if bond } i \text{ and node } j \text{ are not connected.} \end{aligned}$$

Two natural subspaces:

$\mathcal{J}$ the null space of M^T (current vectors)

$\mathcal{E}$ the range of M (potential drops)

These are orthogonal spaces and $\mathcal{K} = \mathcal{E} \oplus \mathcal{J}$

Other spaces:

Divide the bonds in $\mathcal{H}$ into n groups (representing the different impedances).

Define $\mathcal{P}_i$ as the space of vectors $\mathbf{P}$ with elements P_j that are zero if bond j is not in group i.

The projection χ_i onto the space $\mathcal{P}_i$ is diagonal and has elements

$$\{\chi_i\}_{jk} = 1 \text{ if } j = k \text{ and bond } j \text{ is in group } i, \\ = 0 \text{ otherwise.}$$

Thus $\mathcal{K} = \mathcal{E} \oplus \mathcal{J} = \mathcal{V} \oplus \mathcal{P}_1 \oplus \mathcal{P}_2 \oplus \cdots \oplus \mathcal{P}_n,$

This is an orthogonal subspace collection Y(n)

Abstract Theory of Composites; the Z(2)-problem

Hilbert Space $\mathcal{H} = \mathcal{U} \oplus \mathcal{E} \oplus \mathcal{J} = \mathcal{P}_1 \oplus \mathcal{P}_2$

Operator $\mathbf{L} = \sigma_1\chi_1 + \sigma_2\chi_2, \ \chi_i \text{ projects on } \mathcal{P}_i$

Given $\mathbf{E}_0 \in \mathcal{U}$

Solve $\mathbf{J}_0 + \mathbf{J} = \mathbf{L}(\mathbf{E}_0 + \mathbf{E})$

With $\mathbf{J}_0 \in \mathcal{U}, \quad \mathbf{J} \in \mathcal{J}, \quad \mathbf{E} \in \mathcal{E},$

Then $\mathbf{J}_0 = \mathbf{L}_*\mathbf{E}_0$ defines $\mathbf{L}_* : \mathcal{U} \to \mathcal{U}$

and $\mathbf{L}_*$ is an analytic function of σ_1 and σ_2, $\mathbf{L}_*(\sigma_1, \sigma_2)$

Example: 2-Phase Conducting Composites

- $\mathcal{H}$ - Periodic fields that are square integrable over the unit cell
- $\mathcal{U}$ - Constant vector fields (the "applied fields")
- $\mathcal{E}$ - Gradients of periodic potentials
- $\mathcal{J}$ - Fields with zero divergence and zero average value
- $\mathcal{P}_i$ - Fields that are non-zero only in phase i
- $\mathbf{E}_0 + \mathbf{E}(\mathbf{x})$ - Total electric field
- $\mathbf{J}_0 + \mathbf{J}(\mathbf{x})$ - Total current field
- $\mathbf{L} = \boldsymbol{\sigma}(\mathbf{x})$ - Local conductivity
- $\mathbf{L}_* = \boldsymbol{\sigma}_*$ - Effective conductivity

Abstract Theory of Composites; the Y(2)-problem

Hilbert Space $\mathcal{K} = \mathcal{E} \oplus \mathcal{J} = \mathcal{V} \oplus \mathcal{H}, \quad \mathcal{H} = \mathcal{P}_1 \oplus \mathcal{P}_2$

Operator $\mathbf{L} = \sigma_1\chi_1 + \sigma_2\chi_2$, χ_i projects on $\mathcal{P}_i$

Given $\mathbf{E}_0 \in \mathcal{V}$

Solve $\mathbf{J}_1 = \mathbf{L}\mathbf{E}_1$

With $\mathbf{J}_1, \mathbf{E}_1 \in \mathcal{H}, \quad \mathbf{J}_0 + \mathbf{J}_1 \in \mathcal{J}, \quad \mathbf{E}_0 + \mathbf{E}_1 \in \mathcal{E}$

Then $\mathbf{J}_0 = -\mathbf{Y}_*\mathbf{E}_0$ defines $\mathbf{Y}_* : \mathcal{V} \to \mathcal{V}$

and $\mathbf{Y}_*$ is an analytic function of σ_1 and σ_2, $\mathbf{Y}_*(\sigma_1, \sigma_2)$

Y(n) subspace collection:

$$\mathcal{K} = \mathcal{E} \oplus \mathcal{J} = \mathcal{V} \oplus \mathcal{P}_1 \oplus \mathcal{P}_2 \oplus \cdots \oplus \mathcal{P}_n,$$

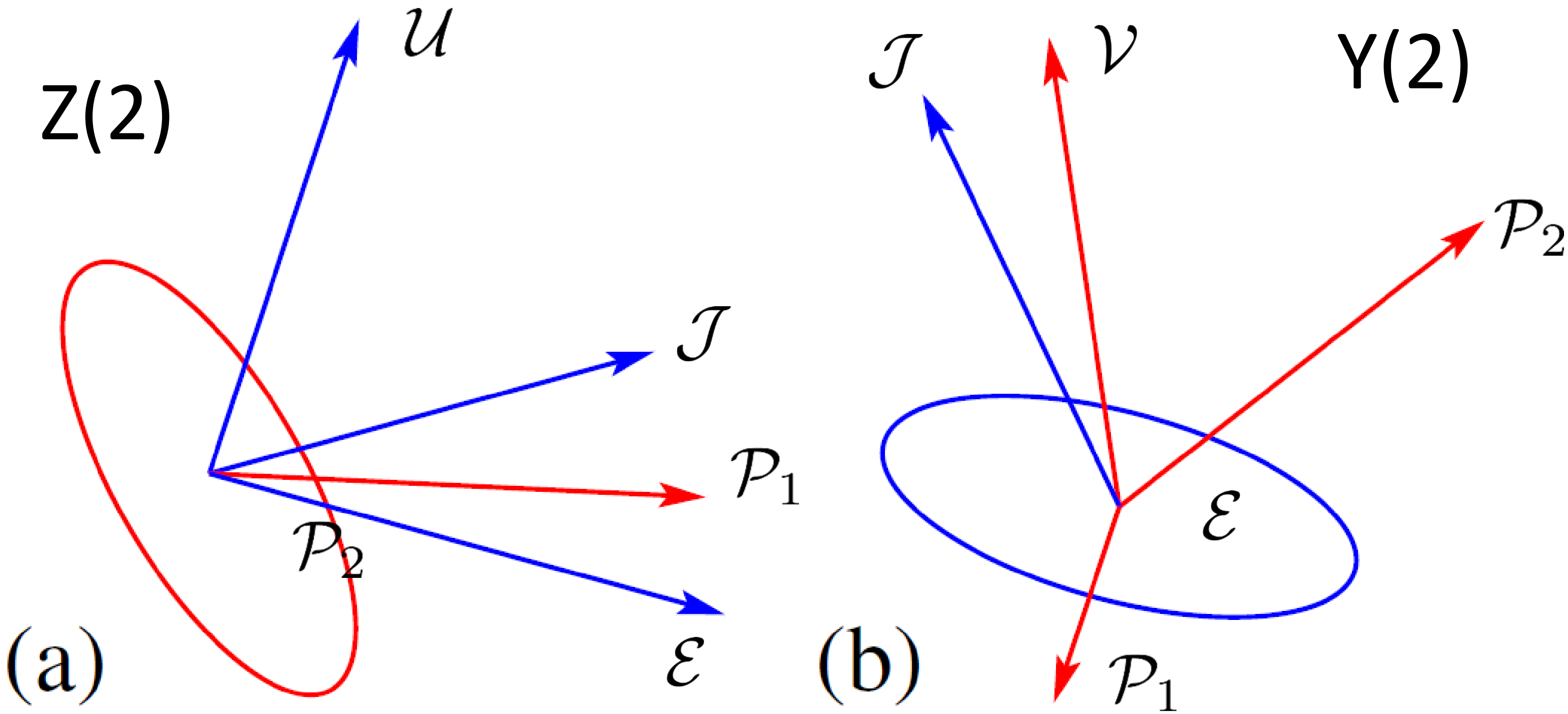
Z(n) subspace collection:

$$\mathcal{H} = \mathcal{U} \oplus \mathcal{E} \oplus \mathcal{J} = \mathcal{P}_1 \oplus \mathcal{P}_2 \oplus \cdots \oplus \mathcal{P}_n,$$

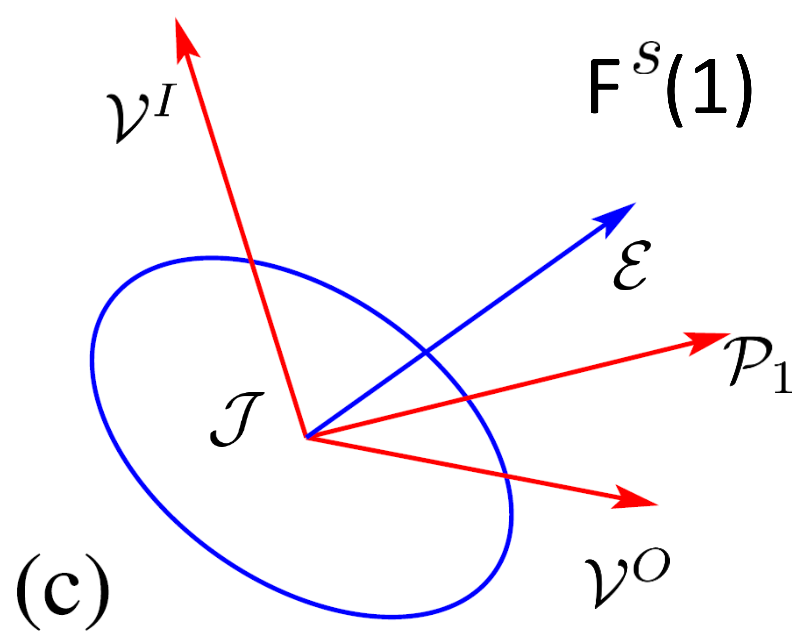
Superfunction F^{s}(n): Y(n) subspace collection with

$$\mathcal{V} = \mathcal{V}^I \oplus \mathcal{V}^O$$

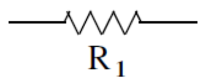
“Subspace collections” need not have orthogonal subspaces

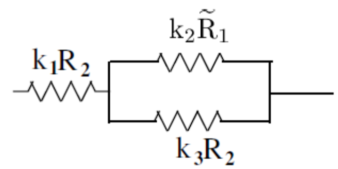


Key: Allow nonorthogonal "subspace collections". Then we have a whole algebra: can define "subtraction" and "division" of subspace collections.



The vector subspace collection that we substitute into the original subspace collection

Want an analog of replacing 

with 

using non-orthogonal subspaces

Now consider a 3−dimensional subspace collection $\mathcal{H}'$ consisting of 3 component vectors $\mathbf{P} = [P_1, P_2, P_3]^T$ with inner product

$$(\mathbf{P}, \widetilde{\mathbf{P}}) = \sum_{i=1}^{3} \overline{P}_i \widetilde{P}_i,$$

where the overline denotes complex conjugation. The projection $\chi' = p \otimes p$ projects onto the one dimensional space of fields proportional to the unit vector $\mathbf{p}$ where $\mathbf{p} = [p_1, p_2, p_3]^T$ and p_1, p_2, p_3 are given constants such that $p_1^2 + p_2^2 + p_3^2 = 1$. The p's could be complex but we *do not* mean $|p_1|^2 + |p_2|^2 + |p_3|^2 = 1$. Thus χ' is a projection but not an orthogonal projection when the p's are complex, as then $\chi' = p \otimes p$ is not Hermitian. We take the following:

$$\begin{aligned}
\mathcal{U}' &\text{ is the space of fields proportional to } (1, 0, 0)^T, \\
\mathcal{E}' &\text{ is the space of fields proportional to } (0, 1, 0)^T, \\
\mathcal{J}' &\text{ is the space of fields proportional to } (0, 0, 1)^T, \\
\mathcal{P}_1 &\text{ is the space of fields proportional to } (p_1, p_2, p_3)^T, \\
\mathcal{P}_2 &\text{ is the space of fields } (P_1, P_2, P_3)^T \\
&\text{such that } p_1 P_1 + p_2 P_2 + p_3 P_3 = 0.
\end{aligned}$$

The field equations become

$$\mathbf{J}' = [(t-\sigma_2)\chi' + \sigma_2]\mathbf{E}', \quad \mathbf{E}' \in \mathcal{U}' \oplus \mathcal{E}', \quad \mathbf{J}' \in \mathcal{U}' \oplus \mathcal{J}',$$

where the constant t will be chosen so the associated "effective modulus" is σ_1. That is

$$\mathbf{\Gamma}_0\mathbf{J}' = \sigma_1\mathbf{\Gamma}_0\mathbf{E}',$$

where $\mathbf{\Gamma}_0$ is the projection onto $\mathcal{U}$, so that

$$J_1' = \sigma_1 E_1'.$$

Without loss of generality we can choose $E_1' = 1$, $J_1' = \sigma_1$ so the field equations become

$$\begin{pmatrix} J_1' \\ 0 \\ J_3' \end{pmatrix} = (t-\sigma_2)\underbrace{\begin{pmatrix} p_1^2 & p_1p_2 & p_1p_3 \\ p_1p_2 & p_2^2 & p_2p_3 \\ p_1p_3 & p_2p_3 & p_3^2 \end{pmatrix}}_{\chi'}\begin{pmatrix} E_1' \\ E_2' \\ 0 \end{pmatrix} + \sigma_2\begin{pmatrix} E_1' \\ E_2' \\ 0 \end{pmatrix}.$$

From the middle equation we get

$$(t-\sigma_2)p_1p_2E_1' + [(t-\sigma_2)p_2^2 + \sigma_2]E_2' = 0,$$

which with $E_1' = 1$ gives

$$E_2' = \frac{(\sigma_2 - t)p_1p_2}{(t-\sigma_2)p_2^2 + \sigma_2}.$$

So we have

$$\begin{aligned}
\sigma_1 = J_1' &= p_1^2(t-\sigma_2)+\sigma_2-\frac{(\sigma_2-t)^2p_1^2p_2^2}{(t-\sigma_2)p_2^2+\sigma_2}\\
&= \sigma_2+\frac{p_1^2\sigma_2(t-\sigma_2)}{(t-\sigma_2)p_2^2+\sigma_2}\\
&= \sigma_2+\frac{p_1^2\sigma_2}{p_2^2+\sigma_2/(t-\sigma_2)},
\end{aligned}$$

which with $\sigma_2 = 1$ is satisfied with

$$t = 1+\frac{\sigma_1-1}{p_1^2-p_2^2(\sigma_1-1)} = 1+\frac{(\sigma_1-1)(\beta-\alpha)}{(\sigma_1+\beta)(1+\alpha)},$$

where

$$\begin{aligned}
\alpha &= -1-\frac{p_1^2}{p_2^2-1},\\
\beta &= -1-\frac{p_1^2}{p_2^2}.
\end{aligned}$$

The parameters p_1 and p_2 need to be complex.

The Hilbert space after the substitution

Now consider the Hilbert space $\mathcal{H}''$ consisting of all periodic fields of the form

$$\mathbf{P}''(\mathbf{x}) = \underbrace{\begin{pmatrix} 0 \\ \mathbf{S}(\mathbf{x}) \\ \mathbf{T}(\mathbf{x}) \end{pmatrix} \chi(\mathbf{x})}_{\in \mathcal{P}_1 \otimes (\mathcal{E}' \oplus \mathcal{J}')} + \underbrace{\begin{pmatrix} \mathbf{Q}(\mathbf{x}) \\ 0 \\ 0 \end{pmatrix}}_{\in \mathcal{H} \otimes \mathcal{U}'} = \begin{pmatrix} \mathbf{Q}(\mathbf{x}) \\ \chi(\mathbf{x})\mathbf{S}(\mathbf{x}) \\ \chi(\mathbf{x})\mathbf{T}(\mathbf{x}) \end{pmatrix}.$$

Fields in $\mathcal{U}''$ take the form

$$\mathbf{u}''(\mathbf{x}) = \begin{pmatrix} \mathbf{u}_0 \\ 0 \\ 0 \end{pmatrix} \in \mathcal{U} \otimes \mathcal{U}'.$$

Fields in $\mathcal{E}''$ take the form

$$\mathbf{E}''(\mathbf{x}) = \underbrace{\begin{pmatrix} 0 \\ \mathbf{S}(\mathbf{x}) \\ 0 \end{pmatrix} \chi(\mathbf{x})}_{\in \mathcal{P}_1 \otimes \mathcal{E}'} + \underbrace{\begin{pmatrix} \widetilde{\mathbf{E}}(\mathbf{x}) \\ 0 \\ 0 \end{pmatrix}}_{\in \mathcal{E} \otimes \mathcal{U}'} = \begin{pmatrix} \widetilde{\mathbf{E}}(\mathbf{x}) \\ \mathbf{S}(\mathbf{x})\chi(\mathbf{x}) \\ 0 \end{pmatrix},$$

where $\widetilde{\mathbf{E}}(\mathbf{x}) \in \mathcal{E}$. Fields in $\mathcal{J}''$ take the form

$$\mathbf{J}''(\mathbf{x}) = \underbrace{\begin{pmatrix} 0 \\ 0 \\ \mathbf{T}(\mathbf{x}) \end{pmatrix} \chi(\mathbf{x})}_{\in \mathcal{P}_1 \otimes \mathcal{J}'} + \underbrace{\begin{pmatrix} \widetilde{\mathbf{J}}(\mathbf{x}) \\ 0 \\ 0 \end{pmatrix}}_{\in \mathcal{J} \otimes \mathcal{U}'} = \begin{pmatrix} \widetilde{\mathbf{J}}(\mathbf{x}) \\ 0 \\ \mathbf{T}(\mathbf{x})\chi(\mathbf{x}) \end{pmatrix}, \qquad \text{where } \widetilde{\mathbf{J}}(\mathbf{x}) \in \mathcal{J}.$$

The space $\mathcal{P}_1'$ consists of all vectors of the form

$$c\begin{pmatrix} p_1 \\ p_2 \\ p_3 \end{pmatrix},$$

and $\mathcal{P}_1''$ consists of all fields $\mathbf{P}(\mathbf{x})$ of the form

$$\begin{pmatrix} p_1\mathbf{C}(\mathbf{x}) \\ p_2\mathbf{C}(\mathbf{x}) \\ p_3\mathbf{C}(\mathbf{x}) \end{pmatrix} \chi(\mathbf{x}) \in \mathcal{P}_1 \otimes \mathcal{P}_1'.$$

Also $\mathcal{P}_2'$ consists of all vectors of the form

$$c\begin{pmatrix} q_1 \\ q_2 \\ q_3 \end{pmatrix} \quad \text{where } \; p_1q_1 + p_2q_2 + p_3q_3 = 0,$$

and $\mathcal{P}_2''$ consists of all fields $\mathbf{P}(\mathbf{x})$ of the form

$$\underbrace{\begin{pmatrix}\mathbf{Q}_1(\mathbf{x})\\ \mathbf{Q}_2(\mathbf{x})\\ \mathbf{Q}_3(\mathbf{x})\end{pmatrix}\chi(\mathbf{x}) + (1-\chi(\mathbf{x}))\begin{pmatrix}\mathbf{R}(\mathbf{x})\\ 0\\ 0\end{pmatrix}}_{\in(\mathcal{P}_1\otimes\mathcal{P}_2'+\mathcal{P}_2\otimes\mathcal{U}')} \quad \text{where } p_1\mathbf{Q}_1(\mathbf{x}) + p_2\mathbf{Q}_2(\mathbf{x}) + p_3\mathbf{Q}_3(\mathbf{x}) = 0.$$

The inner product on $\mathcal{H}''$ is defined to be

$$(\mathbf{P},\widetilde{\mathbf{P}}) = \int_{\text{unit cell}} [\overline{\mathbf{S}(\mathbf{x})}\cdot\widetilde{\mathbf{S}}(\mathbf{x}) + \overline{\mathbf{T}(\mathbf{x})}\cdot\widetilde{\mathbf{T}}(\mathbf{x})]\chi(\mathbf{x}) + \overline{\mathbf{Q}(\mathbf{x})}\cdot\widetilde{\mathbf{Q}}(\mathbf{x}),$$

We define $\chi'' = (\mathbf{p}\otimes\mathbf{p})\chi$, i.e.,

$$\chi''\left\{\begin{pmatrix}0\\ \mathbf{S}(\mathbf{x})\\ \mathbf{T}(\mathbf{x})\end{pmatrix}\chi(\mathbf{x}) + \begin{pmatrix}\mathbf{Q}(\mathbf{x})\\ 0\\ 0\end{pmatrix}\right\} = \begin{pmatrix}p_1^2\mathbf{I} & p_1p_2\mathbf{I} & p_1p_3\mathbf{I}\\ p_1p_2\mathbf{I} & p_2^2\mathbf{I} & p_2p_3\mathbf{I}\\ p_1p_3\mathbf{I} & p_2p_3\mathbf{I} & p_3^2\mathbf{I}\end{pmatrix}\begin{pmatrix}\mathbf{Q}(\mathbf{x})\\ \mathbf{S}(\mathbf{x})\\ \mathbf{T}(\mathbf{x})\end{pmatrix}\chi(\mathbf{x}),$$

The field equations become

$$\mathbf{J}'' = [(t-\sigma_2)\chi'' + \sigma_2\mathbf{I}]\mathbf{E}'', \quad \mathbf{E}'' \in \mathcal{U}'' \oplus \mathcal{E}'', \quad \mathbf{J}'' \in \mathcal{U}'' \oplus \mathcal{J}''.$$

These are easy to solve given periodic solutions $\mathbf{J}(\mathbf{x})$ and $\mathbf{E}(\mathbf{x})$ to the equations in the Hilbert space $\mathcal{H}$, i.e.,

$$\mathbf{J} = [(\sigma_1-\sigma_2)\chi + \sigma_2]\mathbf{E}, \quad \nabla\cdot\mathbf{J} = 0, \quad \nabla\times\mathbf{E} = 0.$$

We take (with $E_1' = 1$)

$$\mathbf{E}'' = \begin{pmatrix} \mathbf{E}(\mathbf{x}) \\ E_2'\mathbf{E}(\mathbf{x})\chi(\mathbf{x}) \\ 0 \end{pmatrix}, \quad \mathbf{J}'' = \begin{pmatrix} \mathbf{J}(\mathbf{x}) \\ 0 \\ J_3'\mathbf{J}(\mathbf{x})/\sigma_1 \end{pmatrix}.$$

Note that we have $\mathbf{E}'' \in \mathcal{U}'' \oplus \mathcal{E}''$ and $\mathbf{J}'' \in \mathcal{U}'' \oplus \mathcal{J}''$. Also, with $\sigma_2 = 1$, we have

$$\begin{aligned}
((t-\sigma_2)\chi'' + \sigma_2)\mathbf{E}'' &= (\mathbf{p}\otimes\mathbf{p}(t-\sigma_2)+\sigma_2]) \begin{pmatrix} 1 \\ E_2'\mathbf{E}(\mathbf{x})\chi(\mathbf{x}) \\ 0 \end{pmatrix} \\
&\quad + \begin{pmatrix} \mathbf{E}(\mathbf{x})(1-\chi(\mathbf{x})) \\ 0 \\ 0 \end{pmatrix} \\
&= \begin{pmatrix} J_1'\mathbf{E}(\mathbf{x}) \\ 0 \\ J_3'\mathbf{E}(\mathbf{x}) \end{pmatrix}\chi(\mathbf{x}) + \begin{pmatrix} \mathbf{E}(\mathbf{x}) \\ 0 \\ 0 \end{pmatrix}(1-\chi(\mathbf{x})) \\
&= \begin{pmatrix} \mathbf{J}(\mathbf{x}) \\ 0 \\ J_3'\mathbf{E}(\mathbf{x}) \end{pmatrix}\chi(\mathbf{x}) + (1-\chi(\mathbf{x}))\begin{pmatrix} \mathbf{J}(\mathbf{x}) \\ 0 \\ 0 \end{pmatrix} = \mathbf{J}''.
\end{aligned}$$

Finally if $\mathbf{\Gamma}_0''$ is the projection onto $\mathcal{U}''$ we have

$$
\begin{aligned}
\mathbf{\Gamma}_0''\mathbf{E}'' &= \begin{pmatrix} \langle \mathbf{E} \rangle \\ 0 \\ 0 \end{pmatrix} \chi(\mathbf{x}) + \begin{pmatrix} \langle \mathbf{E} \\ 0 \\ 0 \end{pmatrix} \rangle (1 - \chi(\mathbf{x})), \\
\mathbf{\Gamma}_0''\mathbf{J}'' &= \begin{pmatrix} \langle \mathbf{J} \rangle \\ 0 \\ 0 \end{pmatrix} \chi(\mathbf{x}) + \begin{pmatrix} \langle \mathbf{J} \rangle \\ 0 \\ 0 \end{pmatrix} (1 - \chi(\mathbf{x})),
\end{aligned}
$$

and since $\langle \mathbf{J} \rangle = \sigma_* \langle \mathbf{E} \rangle$ we deduce that

$$\mathbf{\Gamma}_0''\mathbf{J}'' = \sigma_* \mathbf{\Gamma}_0''\mathbf{E}''.$$

UPSHOT: σ_* is still the effective tensor.

As expected, the Hilbert space substitution did not change it, but it does change the convergence rate of series expansions.

The operator χ'' is easily evaluated in real space. The operator $\mathbf{\Gamma}_1''$ which projects onto $\mathcal{E}''$ is easily evaluated in Fourier space since

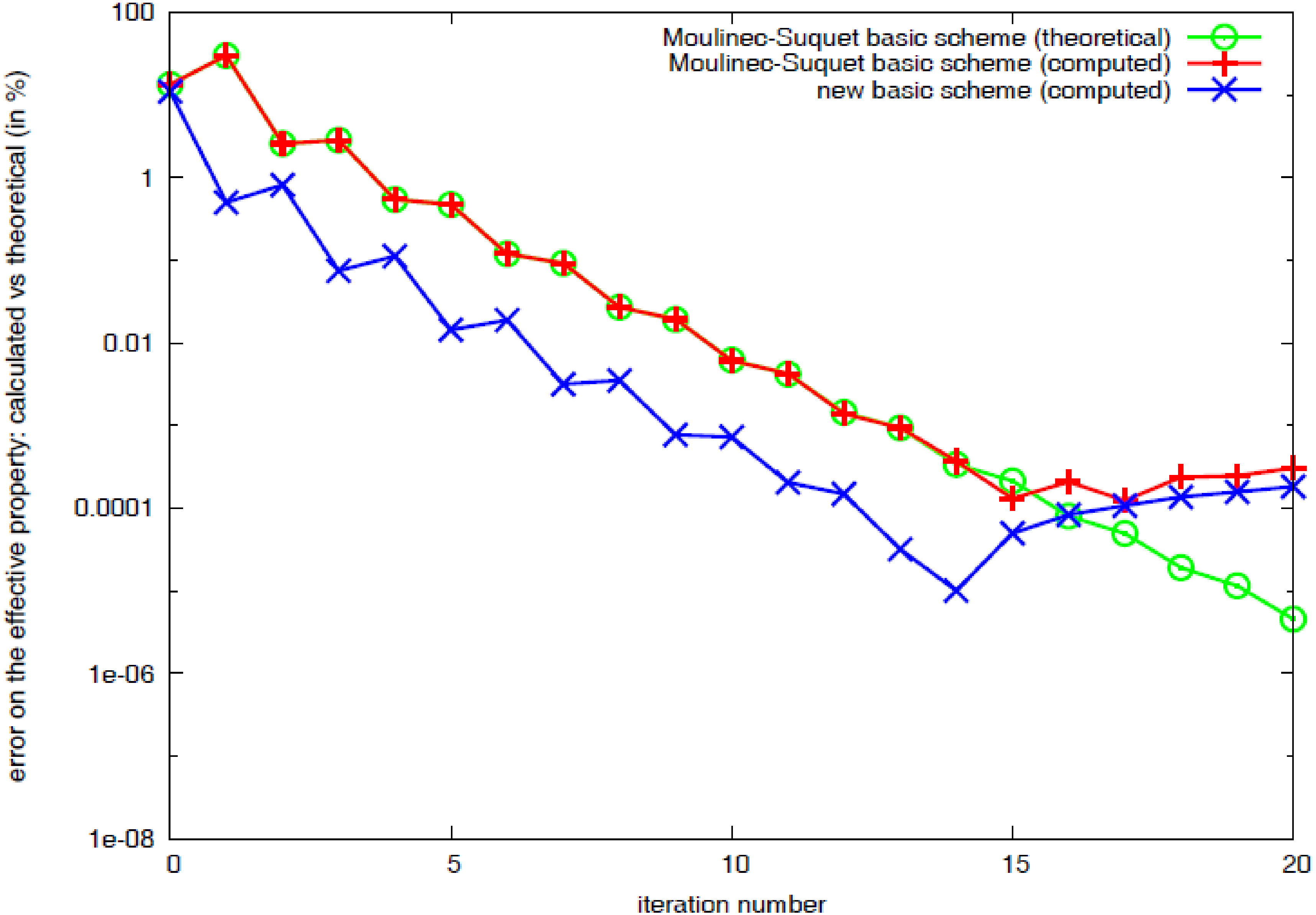
$$\mathbf{\Gamma}_1'' \begin{pmatrix} \mathbf{Q}(\mathbf{x}) \\ \chi(\mathbf{x})\mathbf{S}(\mathbf{x}) \\ \chi(\mathbf{x})\mathbf{T}(\mathbf{x}) \end{pmatrix} = \begin{pmatrix} \mathbf{\Gamma}_1\mathbf{Q}(\mathbf{x}) \\ \chi(\mathbf{x})\mathbf{S}(\mathbf{x}) \\ 0 \end{pmatrix}, \tag{8.46}$$

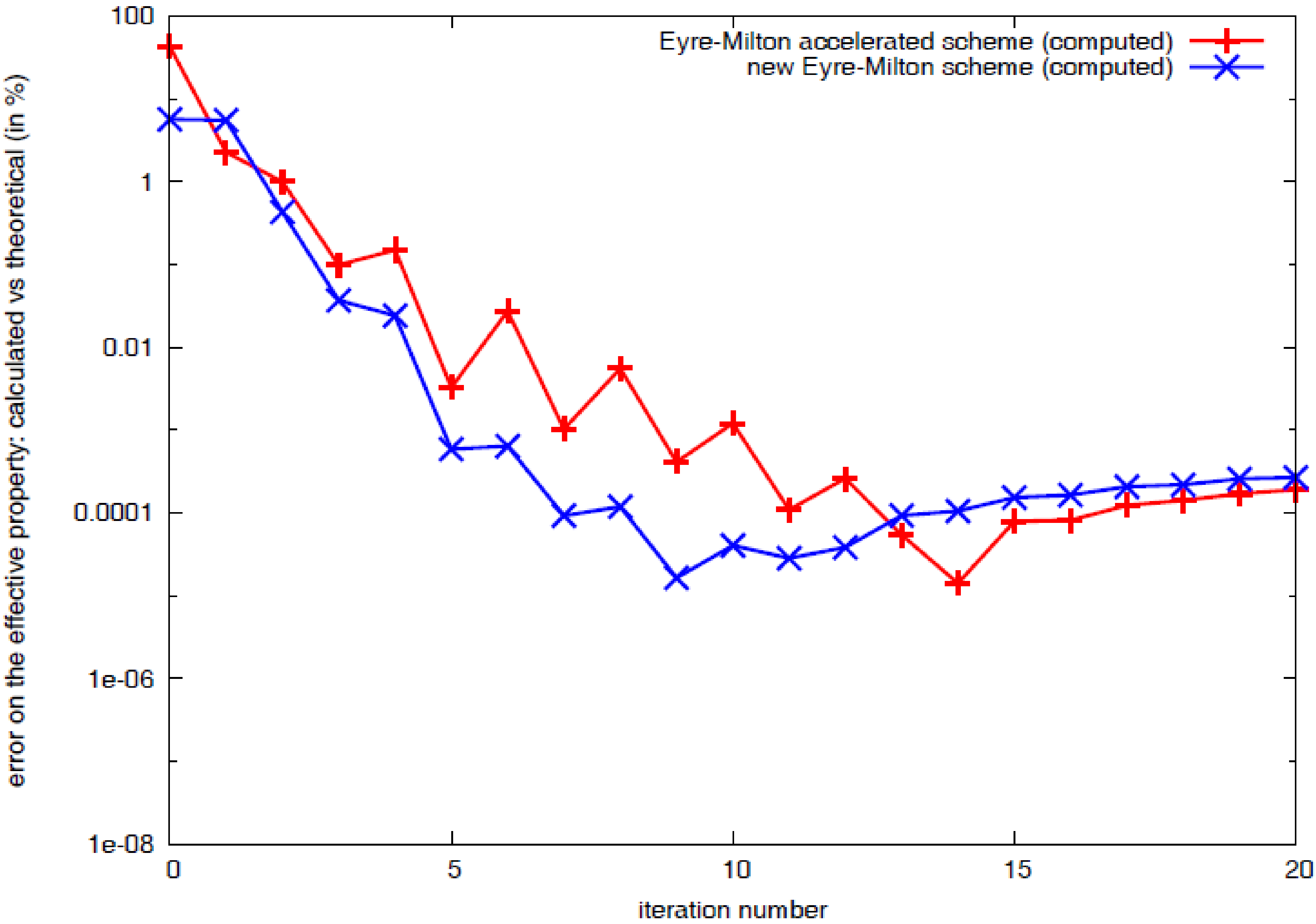
where in Fourier space

$$\mathbf{\Gamma}_1\widehat{\mathbf{Q}}(\mathbf{k}) = \begin{cases} \frac{\mathbf{k}\otimes\mathbf{k}\widehat{\mathbf{Q}}(\mathbf{k})}{|\mathbf{k}|^2}, & \mathbf{k}\neq 0, \\ 0, & \mathbf{k}=0. \end{cases} \tag{8.47}$$

Hence the Fast Fourier Transform methods of Moulinec and Suquet and of Milton and Eyre can be diectly applied in the Hilbert soace $\mathcal{H}$".

Does the idea work? YES!





Eyre-Milton accelerated scheme (computed)
new Eyre-Milton scheme (computed)
error on the effective property: calculated vs theoretical (in %)
iteration number
100
1
0.01
0.0001
1e-06
1e-08
0
5
10
15
20

Remark: The analysis relied heavily on knowledge of the parameters α and β that are associated with the spectrum of the operator $\mathbf{\Gamma}_1\boldsymbol{\chi}_1\mathbf{\Gamma}_1$. For periodic arrays of disks or spheres, bounds on the spectrum have been obtained by Bruno (1991). For more general geometries, and for elasticity and other problems, a new approach to getting bounds on the spectrum can be found here:

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A new route to finding bounds on the generalized spectrum of many physical operators

Graeme W. Milton[a)]
Department of Mathematics, University of Utah, Salt Lake City, Utah 84112, USA

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Also available on ArXiv: arXiv:1803.03726 [math-ph]

Thank you!

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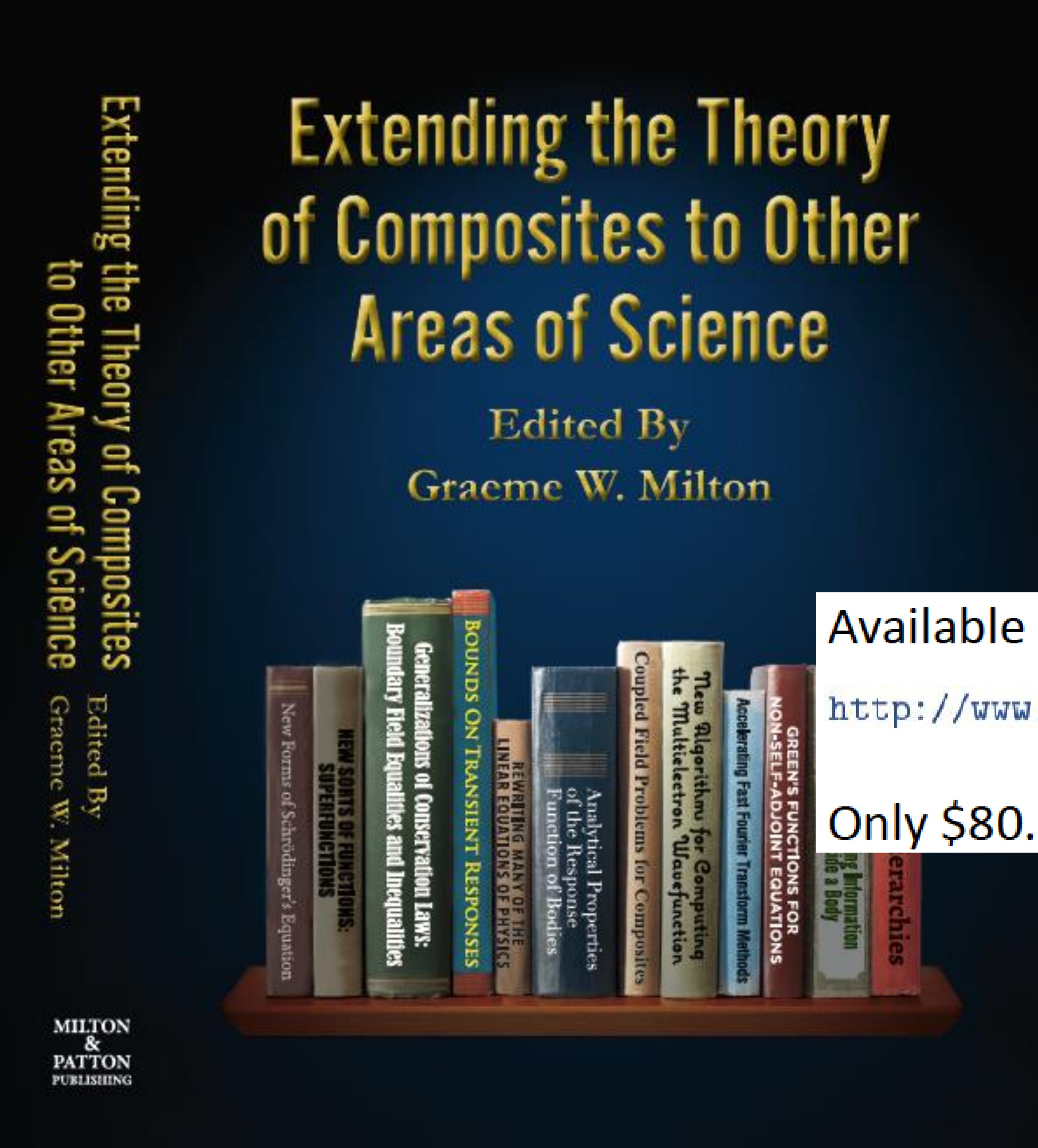

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