Homogenisation methods by solving the Lippmann-Schwinger equation and related numerical tools: state of the art

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Outline

Motivation

full-field numerical method for (periodic) homogenization

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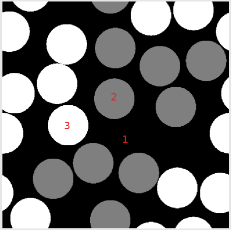
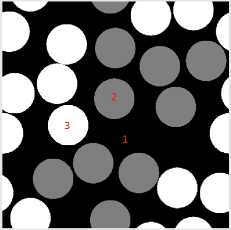
full-field numerical method for (periodic) homogenization



Motivation

full-field numerical method for (periodic) homogenization



+

- property material 1
- property material 2
- property material 3

⇒

Motivation

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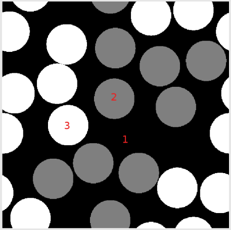

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$\Rightarrow$

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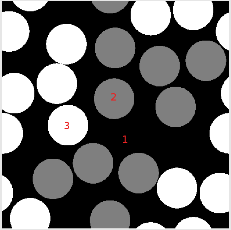

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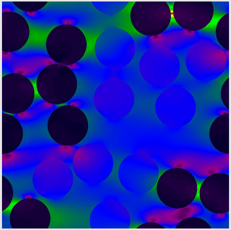
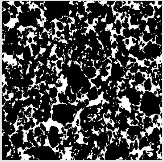


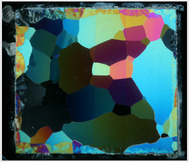
Motivation

→ numerical simulations of the response of heterogenous materials under mechanical loading

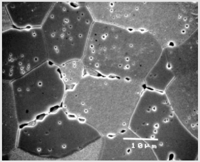
- taking into account the complexity of the microstructure



Fe-Ag alloy (LMS)



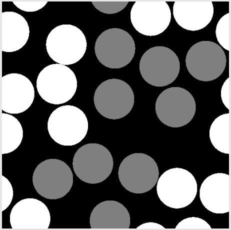
columnar ice (LGGE)



UO2 (IRSN)

- efficient method : high number of degrees of freedom
- ease of use : use directly an image of the microstructure (no mesh)

Problem to be solved



- microstructure : described by an image
- constitutive relations of the phases :
  $\boldsymbol{\sigma}(\boldsymbol{x}) = \boldsymbol{c}(\boldsymbol{x}) : \varepsilon(\boldsymbol{x})$
- boundary conditions :
  periodicity $+$ prescribed macroscopic strain

What is searched :

- homogenized behavior

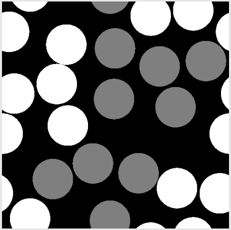
$$\langle \boldsymbol{\sigma} \rangle = \boldsymbol{c}^{\text{hom}} : \langle \varepsilon \rangle \quad ?$$

(where $\langle . \rangle$: spatial average)

- local fields

$$\boldsymbol{\sigma}(\boldsymbol{x})? \;\; \varepsilon(\boldsymbol{x})? \;\; ...$$

Problem to be solved



- microstructure : described by an image
- constitutive relations of the phases :
  $\boldsymbol{\sigma}(\boldsymbol{x}) = f(\boldsymbol{x}, \varepsilon(\boldsymbol{x}), ...)$
- boundary conditions :
  periodicity + prescribed macroscopic strain (or stress or others)

What is searched :

- homogenized behavior

$$\langle \boldsymbol{\sigma} \rangle = f^{\text{hom}}(\langle \varepsilon \rangle, ...) \quad ?$$

(where $\langle . \rangle$: spatial average)

- local fields

$$\boldsymbol{\sigma}(\boldsymbol{x})? \quad \varepsilon(\boldsymbol{x})? \quad ...$$

Lippmann Schwinger equation

Heterogeneous linear elastic problem :

Set of equations

$$
\begin{array}{ll}
\boldsymbol{\sigma}(\boldsymbol{x}) = c(\boldsymbol{x}) : \varepsilon(\boldsymbol{x}) \, , \; \forall \boldsymbol{x} \in \Omega & \text{(constitutive relations)} \, , \\
\mathrm{div} \boldsymbol{\sigma} = 0 & \text{(equilibrium)} \, , \\
\varepsilon(\boldsymbol{x}) = \frac{1}{2} \big(\nabla \boldsymbol{u}(\boldsymbol{x}) + \nabla^T \boldsymbol{u}(\boldsymbol{x}) \big) & \text{(compatibility)} \, , \\
< \varepsilon > = \overline{\varepsilon} \quad \text{and} \quad \varepsilon(\boldsymbol{x}) \text{ periodic on } \Omega & \text{(boundary conditions)}
\end{array}
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$$

$\Updownarrow$

Lippmann-Schwinger equation

$$
\left(\mathbf{I} + \boldsymbol{\Gamma}^0 \delta \boldsymbol{c}\right)\boldsymbol{\varepsilon} = \bar{\boldsymbol{\varepsilon}} \qquad (\text{ with } \delta \boldsymbol{c} = \boldsymbol{c} - \boldsymbol{c}^{\mathbf{0}} \ )
$$

Preliminary problem : prestressed homogeneous elastic material

prestressed homogeneous elastic material :

$\boldsymbol{\sigma}(\boldsymbol{x}) = \boldsymbol{c}^0 : \varepsilon(\boldsymbol{x}) \; + \; \boldsymbol{\tau}(\boldsymbol{x}) \;\; , \;\; < \varepsilon >= \bar{\varepsilon}$

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in real space

$\varepsilon(\boldsymbol{x}) = -\big(\Gamma^0 * \boldsymbol{\tau}\big)(\boldsymbol{x}) \ \ + \bar{\varepsilon}$

Γ^0 : Green operator associated to $\boldsymbol{c}^0$

$*$: convolution operator

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in Fourier space

$$\hat{\varepsilon}(\boldsymbol{\xi}) = -\hat{\boldsymbol{\Gamma}}^0(\boldsymbol{\xi}) : \hat{\boldsymbol{\tau}}(\boldsymbol{\xi}) \quad \forall \boldsymbol{\xi} \neq \boldsymbol{0} \ , \ \hat{\varepsilon}(\boldsymbol{0}) = \bar{\varepsilon}$$

$\boldsymbol{\xi}$: angular frequency

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$\boldsymbol{\xi}$: angular frequency

when $\boldsymbol{c}^0$ is isotropic :

$$\hat{\Gamma}^0_{ijkh}(\boldsymbol{\xi}) = \frac{1}{4\mu^0|\boldsymbol{\xi}|^2}(\delta_{ki}\xi_h\xi_j + \delta_{hi}\xi_k\xi_j + \delta_{kj}\xi_h\xi_i + \delta_{hj}\xi_k\xi_i) - \frac{\lambda^0 + \mu^0}{\mu^0(\lambda^0 + 2\mu^0)} \frac{\xi_i\xi_j\xi_k\xi_h}{|\boldsymbol{\xi}|^4}$$

Lippmann-Schwinger equation

Back to the **heterogeneous** linear elastic problem :

$$\boldsymbol{\sigma}(\boldsymbol{x}) = \boldsymbol{c}(\boldsymbol{x}) : \varepsilon(\boldsymbol{x})$$

Lippmann-Schwinger equation

Back to the **heterogeneous** linear elastic problem :

a homogeneous reference medium $\boldsymbol{c}^0$ is introduced

$$\boldsymbol{\sigma}(\boldsymbol{x}) = \boldsymbol{c}(\boldsymbol{x}) : \varepsilon(\boldsymbol{x}) \quad \Longleftrightarrow \quad \boldsymbol{\sigma}(\boldsymbol{x}) = \boldsymbol{c}^0 : \varepsilon(\boldsymbol{x}) \; + \; \boldsymbol{\delta c}(\boldsymbol{x}) : \varepsilon(\boldsymbol{x})$$

$$\textit{with} : \boldsymbol{\delta c}(\boldsymbol{x}) = \boldsymbol{c}(\boldsymbol{x}) - \boldsymbol{c}^0$$

Lippmann-Schwinger equation

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$$\textit{with} : \delta\boldsymbol{c}(\boldsymbol{x}) = \boldsymbol{c}(\boldsymbol{x}) - \boldsymbol{c}^0$$

Solution of the preliminary problem $\rightarrow$

Lippmann-Schwinger equation

$$\varepsilon = -\boldsymbol{\Gamma}^0 * (\delta\boldsymbol{c} : \varepsilon) \; + \bar{\varepsilon} \qquad (\textit{with } \delta\boldsymbol{c} = \boldsymbol{c} - \boldsymbol{c}^0 \,)$$

Lippmann-Schwinger equation

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Lippmann, Schwinger equation (1950) : scattering in quantum mechanics
Dederichs, Zeller (1972) : LSE for micromechanics
Ekkehart Kröner (1972-1977)

Lippmann-Schwinger equation

Lippmann-Schwinger equation - strain formulation

$$\varepsilon = -\mathbf{\Gamma}^0 * (\delta \boldsymbol{c} : \varepsilon) \quad + \bar{\varepsilon} \qquad\qquad (\textit{with } \delta \boldsymbol{c} = \boldsymbol{c} - \boldsymbol{c}^0 \ )$$

$$\left(\mathbf{I} \ + \mathbf{\Gamma}^0 \delta \boldsymbol{c}\right)\varepsilon = \bar{\varepsilon}$$

Lippmann-Schwinger equation

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$$\left(\mathbf{I} \; + \mathbf{\Gamma}^0 \delta \boldsymbol{c}\right)\varepsilon = \bar{\varepsilon}$$

Lippmann-Schwinger equation - stress formulation

$$\boldsymbol{\sigma} = -\mathbf{\Delta}^0 * (\delta \boldsymbol{s} : \boldsymbol{\sigma}) \;\; + \mathbf{\Sigma} \qquad\qquad (\textit{with } \delta \boldsymbol{s} = \boldsymbol{s} - \boldsymbol{s}^0 = \boldsymbol{c}^{-1} - {\boldsymbol{c}^0}^{-1} \;)$$

$$\left(\mathbf{I} \; + \mathbf{\Delta}^0 \delta \boldsymbol{s}\right)\boldsymbol{\sigma} = \mathbf{\Sigma}$$

$\mathbf{\Delta}^0$ has a simple formulation in Fourier space

Lippmann-Schwinger equation

Lippmann-Schwinger equation - strain formulation

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$\mathbf{\Delta}^0$ has a simple formulation in Fourier space

$$< . > + \mathbf{\Gamma}^0 \boldsymbol{c}^{\mathbf{0}} \; + \; \boldsymbol{c}^{\mathbf{0}^{-1}} \mathbf{\Delta}^0 \;\; = \mathbf{I} \qquad (\textit{strain})$$

$$< . > + \boldsymbol{c}^{\mathbf{0}} \mathbf{\Gamma}^0 \; + \; \mathbf{\Delta}^0 \boldsymbol{c}^{\mathbf{0}^{-1}} \;\; = \mathbf{I} \qquad (\textit{stress})$$

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COURSE HELD AT THE DEPARTMENT
OF GENERAL MECHANICS
OCTOBER 1971

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SPRINGER-VERLAG WIEN GMBH

an elastic tensor $\bar{\underline{c}}$ can be used if the grain number tends to infinity. (Question to the reader: Why does this statement need an additional consideration?)

b) Effective compliances

If the Lippmann-Schwinger equation for the strain (5.20.5) is multiplied by $\underline{c}^0$ and the quantities $\underline{\sigma}^0 = \underline{c}^0\underline{\varepsilon}^0$, $\underline{s}^0 = (\underline{c}^0)^{-1}$, $\delta\underline{s} = \underline{s} - \underline{s}^0$ are introduced one easily obtains the Lippmann-Schwinger equation for the stress

(5.20.8) $$\underline{\sigma} = \underline{\sigma}^0 - \underline{\Delta}\,\delta\underline{s}\,\underline{\sigma}$$

where

(5.20.9) $$\underline{\Delta} = \underline{c}^0 - \underline{c}^0\underline{\Gamma}\,\underline{c}^0$$

We put $\underline{s}^0 = \bar{\underline{s}}$, then $\delta\underline{s} = \underline{s}'$, and after performing the prime operation on eq. (5.20.8) we obtain

(5.20.10) $$\underline{\sigma}' = -\underline{\Delta}\,P\,\underline{s}'\underline{\sigma} = -\underline{\Delta}\,\underline{s}'\underline{\sigma} - \underline{\Delta}\,P\,\underline{s}'\underline{\sigma}'$$

where

(5.20.11) $$\underline{\Delta} = \bar{\underline{s}}^{-1} - \bar{\underline{s}}^{-1}\underline{\Gamma}\,\bar{\underline{s}}^{-1}$$

and $\underline{\Gamma}$ is calculated with $\bar{\underline{s}}^{-1}$ rather than with $\bar{\underline{c}}$. We now can write down the two rigorous equations

(5.20.12) $$\underline{C} = \bar{\underline{c}} - \overline{\underline{c}'\underline{\Gamma}P\underline{c}'} + \overline{\underline{c}'\underline{\Gamma}P\underline{c}'\underline{\Gamma}P\underline{c}'} - \overline{\underline{c}'\underline{\Gamma}P\underline{c}'\underline{\Gamma}P\underline{c}'\underline{\Gamma}P\underline{c}'} + \dots$$

Fixed-point scheme

$$\varepsilon \quad (\boldsymbol{x}) = -\boldsymbol{\Gamma}^0 * \left(\delta \boldsymbol{c}(\boldsymbol{x}) : \varepsilon\,(\boldsymbol{x})\right) \quad + \bar{\varepsilon}$$

Fixed-point scheme

Fixed-point iteration method (aka “basic scheme”)

$$\varepsilon^{i+1}(\boldsymbol{x}) = -\boldsymbol{\Gamma}^0 * \big(\delta \boldsymbol{c}(\boldsymbol{x}) : \varepsilon^{i}(\boldsymbol{x})\big) \quad + \bar{\varepsilon}$$

H. Moulinec, P. Suquet (1994)

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Iterative fixed-point scheme applied to a linear elastic problem

$$\boldsymbol{\sigma}^{i}(\boldsymbol{x}) = \boldsymbol{c}(\boldsymbol{x}) : \varepsilon^{i}(\boldsymbol{x})$$

$$\hat{\varepsilon}^{i+1}(\boldsymbol{\xi}) = \hat{\varepsilon}^{i}(\boldsymbol{\xi}) - \hat{\boldsymbol{\Gamma}}^0(\boldsymbol{\xi}) : \hat{\boldsymbol{\sigma}}^{i}(\boldsymbol{\xi}) \quad \forall \boldsymbol{\xi} \neq \mathbf{0}, \qquad \hat{\varepsilon}^{i+1}(\mathbf{0}) = \bar{\varepsilon}$$

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Iterative fixed-point scheme applied to a non-linear behaviour

$$\boldsymbol{\sigma}^{i}(\boldsymbol{x}) = \boldsymbol{f}(\boldsymbol{x}\ ,\ \varepsilon^{i}(\boldsymbol{x})\ ,\ ...)$$

$$\hat{\varepsilon}^{i+1}(\boldsymbol{\xi}) = \hat{\varepsilon}^{i}(\boldsymbol{\xi}) - \hat{\boldsymbol{\Gamma}}^0(\boldsymbol{\xi}) : \hat{\boldsymbol{\sigma}}^{i}(\boldsymbol{\xi}) \quad \forall \boldsymbol{\xi} \neq \boldsymbol{0}, \qquad \hat{\varepsilon}^{i+1}(\boldsymbol{0}) = \bar{\varepsilon}$$

H. Moulinec, P. Suquet (1994)

Liouville-Neumann series

expansion in Liouville-Neumann series of $\left(\boldsymbol{I} + \Gamma^0 \delta \boldsymbol{c}\right) \varepsilon = \bar{\varepsilon}$

$$\varepsilon = \sum_{j=0}^{\infty} \left(-\Gamma^0 \delta \boldsymbol{c}\right)^j \bar{\varepsilon} \qquad \text{(strain field)}$$

$$\boldsymbol{c}^{eff} = \boldsymbol{c}^0 + \sum_{j=0}^{\infty} \left\langle \delta \boldsymbol{c} \left(-\Gamma^0 \delta \boldsymbol{c}\right)^j \right\rangle \qquad \text{(effective properties)}$$

E. Kröner (1972)
Moulinec, Suquet, Milton (2018)

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The series truncated to the k-th term = fixed point iteration scheme

$$\varepsilon^{(k)} = \sum_{j=0}^{k} \left(-\boldsymbol{\Gamma}^0 \delta \boldsymbol{c}\right)^j \bar{\varepsilon} \qquad \Leftrightarrow \qquad \varepsilon^{(k+1)} = -\boldsymbol{\Gamma}^0 \delta \boldsymbol{c} \varepsilon^{(k)} + \bar{\varepsilon}$$

E. Kröner (1972)
Moulinec, Suquet, Milton (2018)

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$$\varepsilon^{(k)}=\sum_{j=0}^{k}\left(-\Gamma^0\delta\boldsymbol{c}\right)^j\bar{\varepsilon} \quad\Leftrightarrow\quad \varepsilon^{(k+1)}=-\Gamma^0\delta\boldsymbol{c}\varepsilon^{(k)}+\bar{\varepsilon}$$

Fixed point scheme with $c^0=\frac{c^1+c^2}{2}$ (conductivity)

$$\boldsymbol{c}^{\boldsymbol{eff}}=\boldsymbol{c}^0+\boldsymbol{c}^0\sum_{j=0}^{\infty}\left\langle\chi'(\boldsymbol{x})\Big(-\Gamma^0\boldsymbol{c}^0\chi'(\boldsymbol{x})\Big)^j\right\rangle t^{j+1} \quad,\quad \chi'=\begin{cases}1 & \text{in } 1\\ -1 & \text{in } 2\end{cases} \quad,\quad t=\left(\frac{c^1-c^2}{c^1+c^2}\right)$$

E. Kröner (1972)
Moulinec, Suquet, Milton (2018)

Properties of operators Γ^0 and Δ^0

$\boldsymbol{\Gamma}^0 \boldsymbol{\sigma} = \mathbf{0} \quad \Leftrightarrow \quad \boldsymbol{\sigma}$ is in equilibrium (i.e. $\mathrm{div}(\boldsymbol{\sigma}) = \mathbf{0}$)

$\boldsymbol{\Gamma}^0 \boldsymbol{c}^{\mathbf{0}}$ projector on the space of compatible fields with null average

Corollary

$\boldsymbol{\Gamma}^0 \boldsymbol{c}^{\mathbf{0}} \varepsilon = \varepsilon - < \varepsilon > \quad \Leftrightarrow \quad \varepsilon$ is compatible

$\boldsymbol{\Delta}^0 \varepsilon = \mathbf{0} \quad \Leftrightarrow \quad \varepsilon$ is compatible

${\boldsymbol{c}^{\mathbf{0}}}^{-1} \boldsymbol{\Delta}^0$projector on the space of equilibrated fields with null average

$< . >, \boldsymbol{\Gamma}^{\mathbf{0}}$ and $\boldsymbol{\Delta}^0$ are orthogonal : $\boldsymbol{\Gamma}^{\mathbf{0}} \, \boldsymbol{\Delta}^0 = \boldsymbol{\Delta}^0 \, \boldsymbol{\Gamma}^{\mathbf{0}} = \mathbf{0}$

Generalized Helmholtz decomposition

Lippmann-Schwinger equation

$$\left(\mathbf{I} \ + \boldsymbol{\Gamma}^0 \delta \boldsymbol{c}\right) \varepsilon = \bar{\varepsilon}$$

can be re-written as

$$\underbrace{< \varepsilon > - \bar{\varepsilon}}_{\text{macro conditions}} + \underbrace{\boldsymbol{c}^{0^{-1}} \boldsymbol{\Delta}^0 \varepsilon}_{\text{compatibility}} + \underbrace{\boldsymbol{\Gamma}^0 (\boldsymbol{c} \varepsilon)}_{\text{equilibrium}} = \mathbf{0}$$

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Lippmann-Schwinger equation

$$\big(\mathbf{I} + \mathbf{\Gamma}^0 \delta \boldsymbol{c}\big)\varepsilon = \bar{\varepsilon}$$

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based on a generalized Helmholtz decomposition
G.W. Milton (2002)

$$\mathcal{H} = \mathcal{U} \oplus \mathcal{E} \oplus \mathcal{J}$$

with :

$\mathcal{U}$: space of uniform fields

$\mathcal{E}$: space of compatible fields with zero mean

$\mathcal{J}$: space of divergence free fields with zero mean

$$\mathbf{I} = < . > + \mathbf{\Gamma}^0 \boldsymbol{c}^{\mathbf{0}} + \boldsymbol{c}^{\mathbf{0}^{-1}} \mathbf{\Delta}^0 \qquad (\textit{strain})$$

Energetic variational principle

Energetic functional

$$\mathcal{J} : \mathcal{E} \to \mathbb{R}, \quad \mathcal{J}(\boldsymbol{e}^*) = \frac{1}{2}\left\langle \boldsymbol{c}(\bar{\varepsilon} + \boldsymbol{e}^*) : (\bar{\varepsilon} + \boldsymbol{e}^*)\right\rangle$$

Minimization principle

$$\frac{1}{2}\boldsymbol{c}^{\boldsymbol{eff}}\bar{\varepsilon} : \bar{\varepsilon} \;=\; \min_{\boldsymbol{e}^* \in \mathcal{E}} \mathcal{J}(\boldsymbol{e}^*)$$

Energetic variational principle

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Minimization principle

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Energetic scalar product

$$\left(\boldsymbol{\eta}, \tilde{\boldsymbol{\eta}}\right) = \left\langle \boldsymbol{c}^{\boldsymbol{0}}\boldsymbol{\eta}(\boldsymbol{x}) : \tilde{\boldsymbol{\eta}}(\boldsymbol{x})\right\rangle$$

Energetic variational principle

Energetic functional

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Minimization principle

$$\frac{1}{2}\boldsymbol{c}^{\boldsymbol{eff}}\bar{\varepsilon} : \bar{\varepsilon} \;=\; \min_{\boldsymbol{e}^* \in \mathcal{E}} \mathcal{J}(\boldsymbol{e}^*)$$

Energetic scalar product

$$(\eta, \tilde{\eta}) = \left\langle \boldsymbol{c}^{\boldsymbol{0}} \eta(\boldsymbol{x}) : \tilde{\eta}(\boldsymbol{x})\right\rangle$$

Minimization of $\mathcal{J}$

$$\boldsymbol{\nabla}\mathcal{J}(\boldsymbol{e}^*) = \boldsymbol{\Gamma}^{\boldsymbol{0}}\boldsymbol{c}\big(\bar{\varepsilon} + \boldsymbol{e}^*\big)$$

Energetic variational principle

Energetic functional

$$\mathcal{J} : \mathcal{E} \to \mathbb{R}, \quad \mathcal{J}(\boldsymbol{e}^*) = \frac{1}{2}\left\langle \boldsymbol{c}(\bar{\varepsilon} + \boldsymbol{e}^*) : (\bar{\varepsilon} + \boldsymbol{e}^*)\right\rangle$$

Minimization principle

$$\frac{1}{2}\boldsymbol{c}^{\boldsymbol{eff}}\bar{\varepsilon} : \bar{\varepsilon} \;=\; \min_{\boldsymbol{e}^* \in \mathcal{E}} \mathcal{J}(\boldsymbol{e}^*)$$

Energetic scalar product

$$(\boldsymbol{\eta}, \tilde{\boldsymbol{\eta}}) = \left\langle \boldsymbol{c}^{\mathbf{0}}\boldsymbol{\eta}(\boldsymbol{x}) : \tilde{\boldsymbol{\eta}}(\boldsymbol{x})\right\rangle$$

Minimization of $\mathcal{J}$

$$\boldsymbol{\nabla}\mathcal{J}(\boldsymbol{e}^*) = \boldsymbol{\Gamma}^{\mathbf{0}}\boldsymbol{c}\left(\bar{\varepsilon} + \boldsymbol{e}^*\right)$$

$\boldsymbol{\nabla}\mathcal{J}(\boldsymbol{e}^*) = 0$ (optimality condition) $\Leftrightarrow$ $\boldsymbol{\varepsilon} = \bar{\varepsilon} - \boldsymbol{\Gamma}^{\mathbf{0}}\boldsymbol{\delta c \varepsilon}$ (Lippmann-Schwinger equation)

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(optimality condition) — (Lippmann-Schwinger equation)

- fixed point scheme $=$ fixed step gradient descent method
- $\rightarrow$ use of efficient gradient-descent methods

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Kabel, Böhlke, Schneider (2014)
Bellis, Suquet (2018)

Lippmann-Schwinger equation : formulation in u^*

fluctuating part of u : $u(\boldsymbol{x}) = u^*(\boldsymbol{x}) + \bar{\varepsilon}.\boldsymbol{x}$, u^* periodic , $< u^* >= 0$

solve : $div\big(\boldsymbol{c}(\boldsymbol{\nabla} u^* + \bar{\varepsilon})\big) = \boldsymbol{0}$

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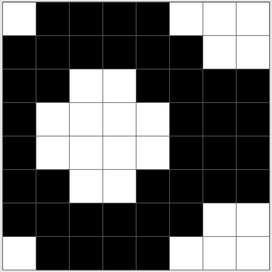
Ladecký, Pultarová, Zeman (2020)
Bellis, Moulinec (2025 ?)

(Periodic) digital images

- elementary volume
  $\Omega = [0, L_1[\times[0, L_2[$,
- discretisation in
  $n_1 \times n_2 = 8 \times 8$ pixels



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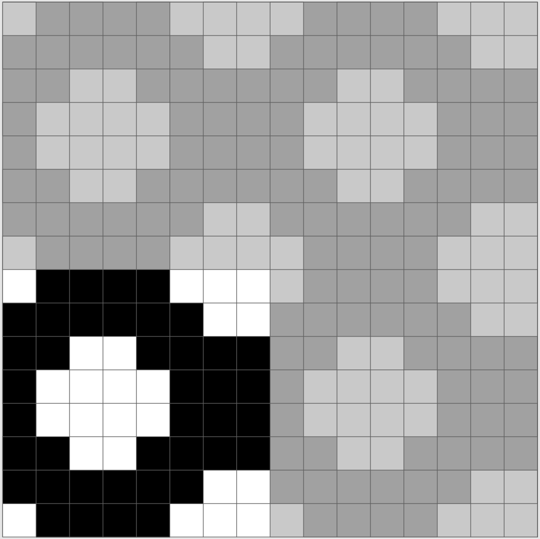

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  - sampling step :
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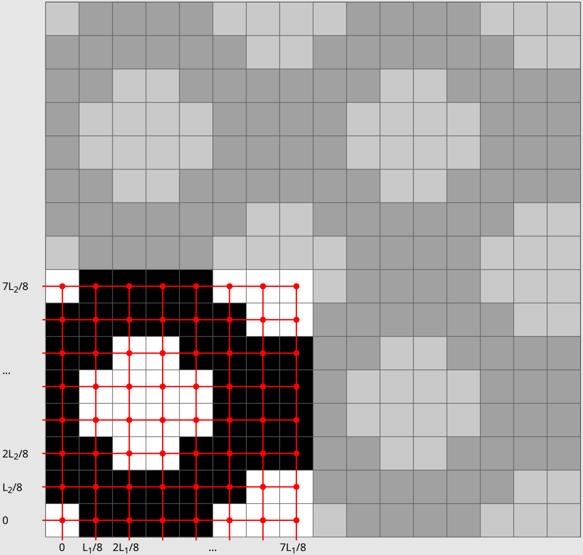
A. Bijaoui (1984)



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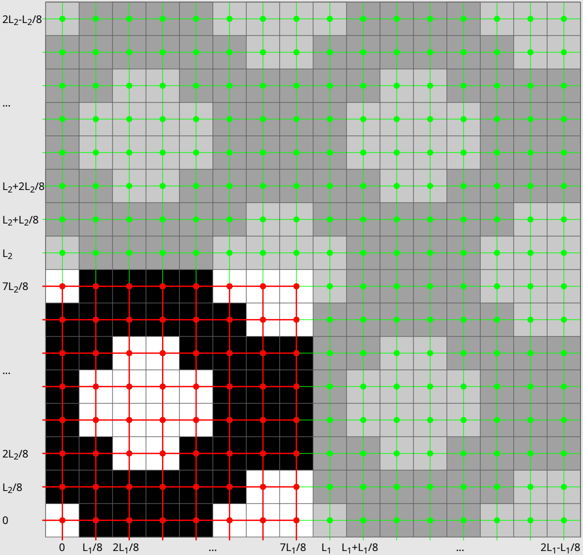

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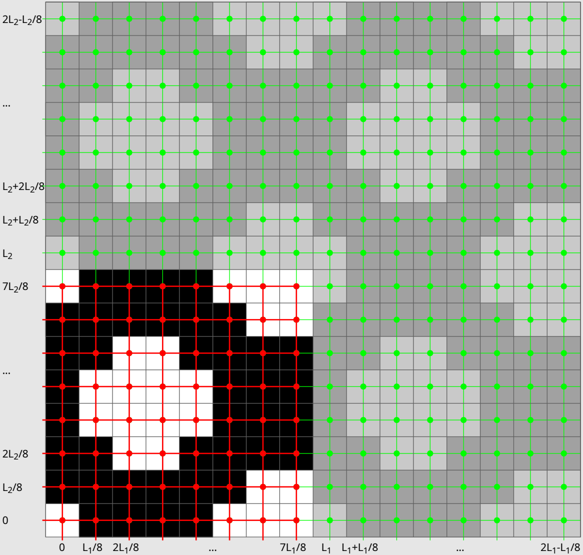
- Ω does not need to be rectangular
  in a space of dimension d :
  $\boldsymbol{L_k}$ with $k = 1, \ldots, d$
  $\boldsymbol{x} = \boldsymbol{s} + \sum_{k=1}^{d} (i_k - 1)\boldsymbol{L_k}$

  FFT-based methods work in that case

  A. Bijaoui (1984)



Fourier Transform - Definition

Fourier transform

$$\hat{f}(\nu) \stackrel{\text{def}}{=} \int f(x) e^{-\mathrm{i}2\pi\nu x} dx \qquad \text{(with spatial frequency } \nu\text{)}$$

$$\hat{f}(\xi) \stackrel{\text{def}}{=} \int f(x) e^{-\mathrm{i}\xi x} dx \qquad \text{(with angular spatial frequency } \xi = 2\pi\nu\text{)}$$

Inverse Fourier transform

$$f(x) = \int \hat{f}(\nu) e^{+\mathrm{i}2\pi\nu x} d\nu$$

$$f(x) = \int \hat{f}(\nu) e^{+\mathrm{i}\xi x} d\xi$$

Fourier Transform - Properties

3D Fourier transform

$$\hat{f}(\boldsymbol{\xi}) \stackrel{\text{def}}{=} \int f(\boldsymbol{x}) e^{-\mathrm{i}\boldsymbol{\xi}.\boldsymbol{x}} \boldsymbol{dx} \qquad \text{(with } \boldsymbol{x} = (x_1, x_2, x_3) \text{ and } \boldsymbol{\xi} = (\xi_1, \xi_2, \xi_3) \text{)}$$

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$$\hat{f}(\xi_1, \xi_2, \xi_3) = \int\int\int f(x_1, x_2, x_3) e^{-\mathrm{i}(\xi_1 x_1 + \xi_2 x_2 + \xi_3 x_3)} dx_1 dx_2 dx_3$$

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(successive 1D Fourier transforms on all directions)

Fourier Transform - Properties

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(successive 1D Fourier transforms on all directions)

Fourier transform of a multi-component field (vector, tensor, ...)

$$\boldsymbol{f} = \big(f_i(\boldsymbol{x})\big)_{i=1,\dots,n}$$

$$\hat{\boldsymbol{f}}(\boldsymbol{\xi}) = \big(\hat{f}_i(\boldsymbol{\xi})\big)_{i=1,\dots,n}$$

Fourier Transform - Properties

Convolution

$$f * g\,(x) \overset{\text{def}}{=} \int f(t)g(x-t)dt$$

Fourier transform of a convolution product and of a product

$$\mathcal{F}\left[f * g\right] = \mathcal{F}\left[f\right].\mathcal{F}\left[g\right]$$

$$\mathcal{F}\left[f.g\right] = \mathcal{F}\left[f\right] * \mathcal{F}\left[g\right]$$

Fourier transform of a derivative

$$\widehat{\frac{df}{dx}}(\nu) = 2i\pi\nu\,\hat{f}(\nu) \quad \text{(frequency } \nu\text{)}$$

$$\widehat{\frac{df}{dx}}(\xi) = i\xi\,\hat{f}(\xi) \quad \text{(angular frequency } \xi = 2\pi\nu\text{)}$$

Fourier Transform - Dirac comb

Dirac delta function

$$f * \delta = f$$

Dirac comb

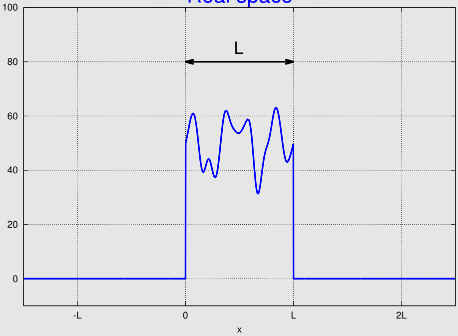
$$\text{Ш}_L(x) \stackrel{\text{def}}{=} \sum_{k=-\infty}^{+\infty} \delta(x - kL)$$

Fourier transform of a Dirac comb

$$\widehat{\text{Ш}}_L(\nu) = \frac{1}{L} \text{Ш}_{\frac{1}{L}}(\nu)$$

FT - DFT - FFT

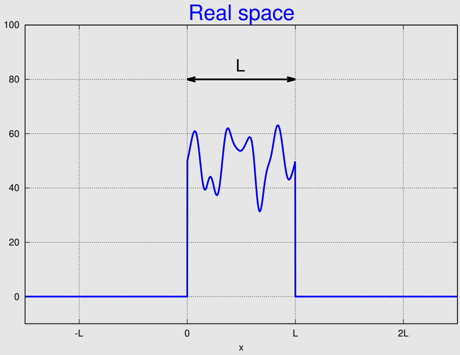
Real space

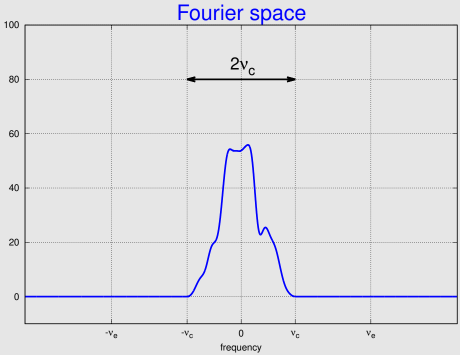


Fourier space

1. $f(x) = 0 \;\; \forall x < 0 \; or \; x > L$

FT - DFT - FFT

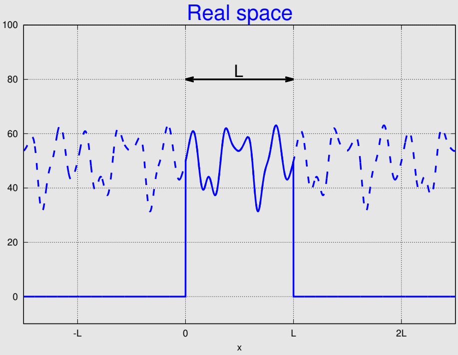


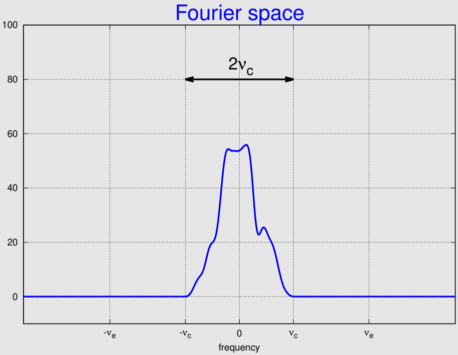


1. $f(x) = 0 \;\; \forall x < 0 \textit{ or } x > L$

1. (H) : $\hat{f}(\nu) = 0 \;\; \forall |\nu| > \nu_c$ (cutoff)

FT - DFT - FFT





1. $f(x) = 0 \ \ \forall x < 0 \textit{ or } x > L$
2. periodization (in real space)
   i.e. convolution : $f' = f * \text{III}_L$

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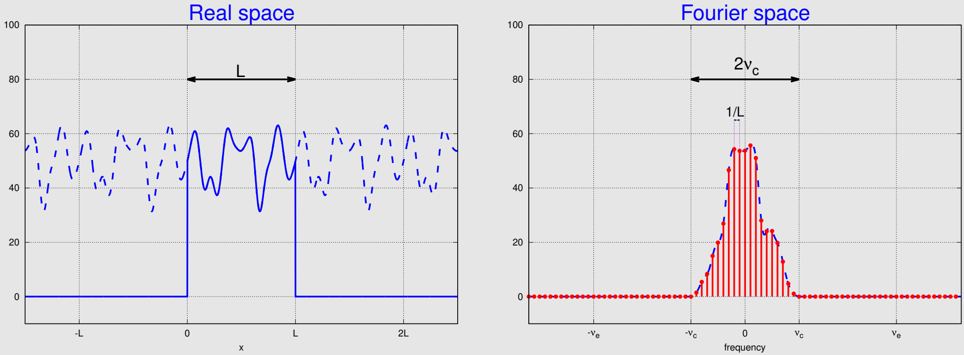

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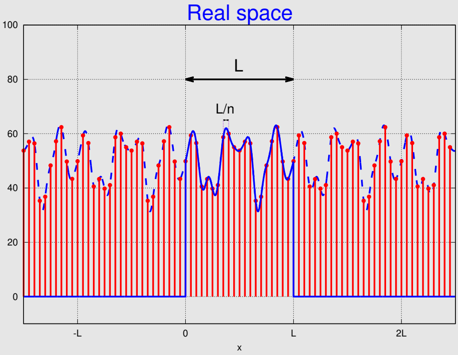

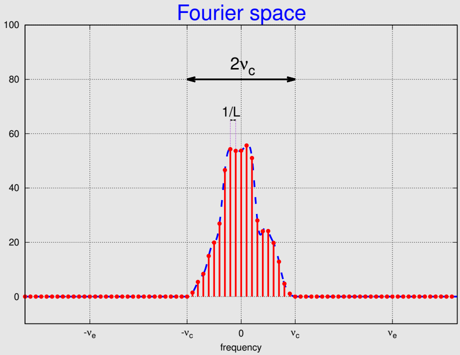

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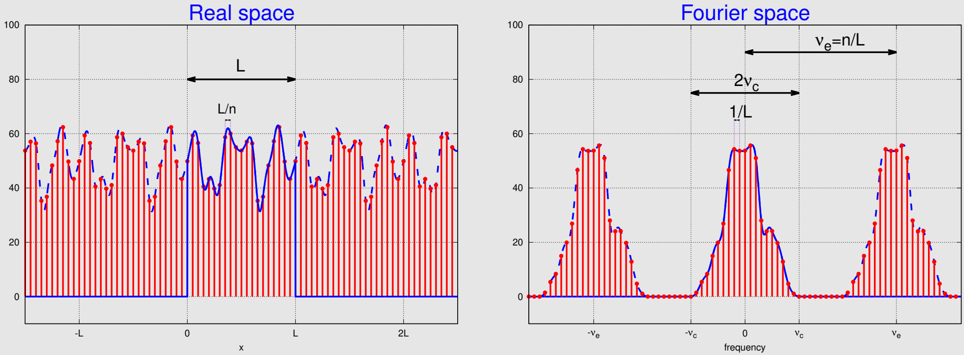

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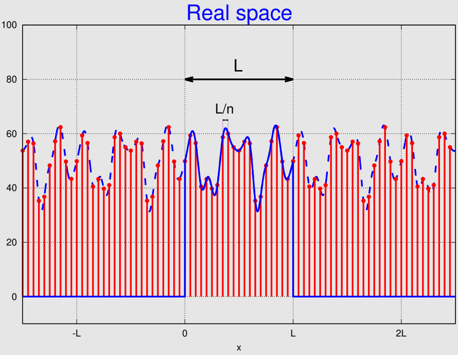
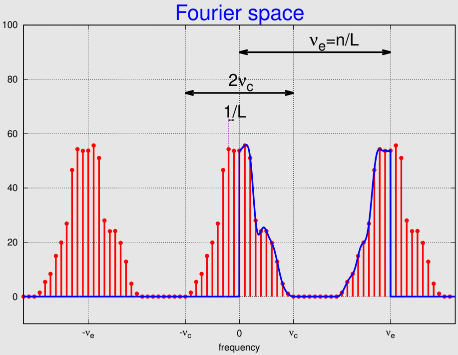
FT - DFT - FFT





1. $f(x) = 0 \ \ \forall x < 0 \ or \ x > L$
2. periodization (in real space)
   i.e. convolution : $f' = f * III_L$
3. discretization (in real space)
   i.e. product : $f'' = f'.III_{L/n}$

   n discrete values in a period L
   ($\delta = L/n$)

1. (H) : $\hat{f}(\nu) = 0 \ \ \forall|\nu| > \nu_c$ (cutoff)
2. discretization (in Fourier space)
   i.e. $\hat{f}' = \hat{f}.III_{1/L}$
3. periodization (in Fourier space)
   i.e. $\hat{f}'' = \hat{f}' * III_{\nu_e = n/L}$

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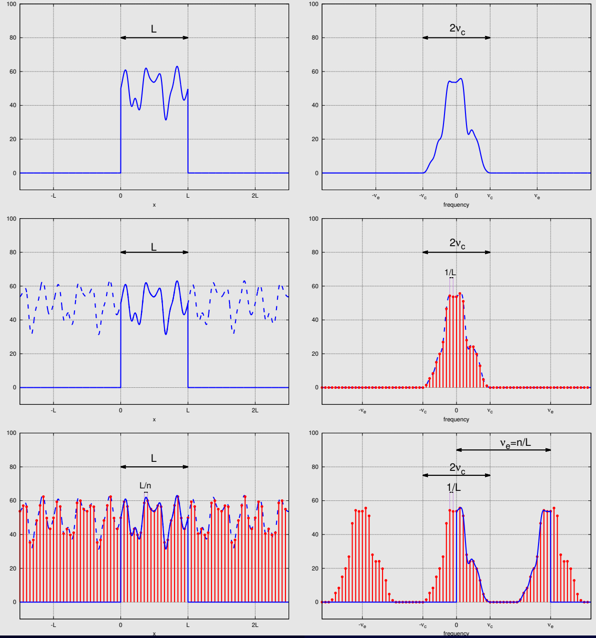
FT - DFT - FFT



Fourier Transform

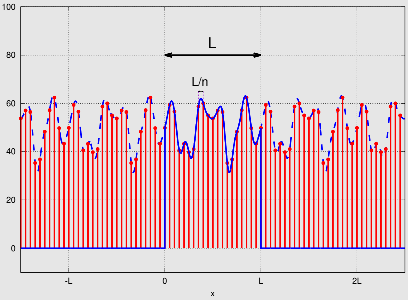
Fourier Series

Discrete Fourier Transform

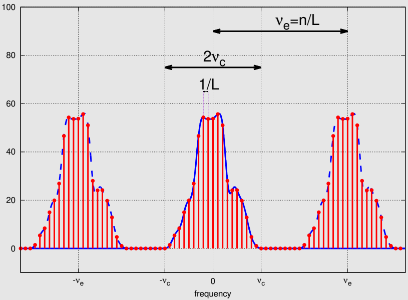
fast algorithm : FFT
(Fast (discrete) Fourier Transform)
performance in $n \log n \quad (\neq n^2)$

Aliasing

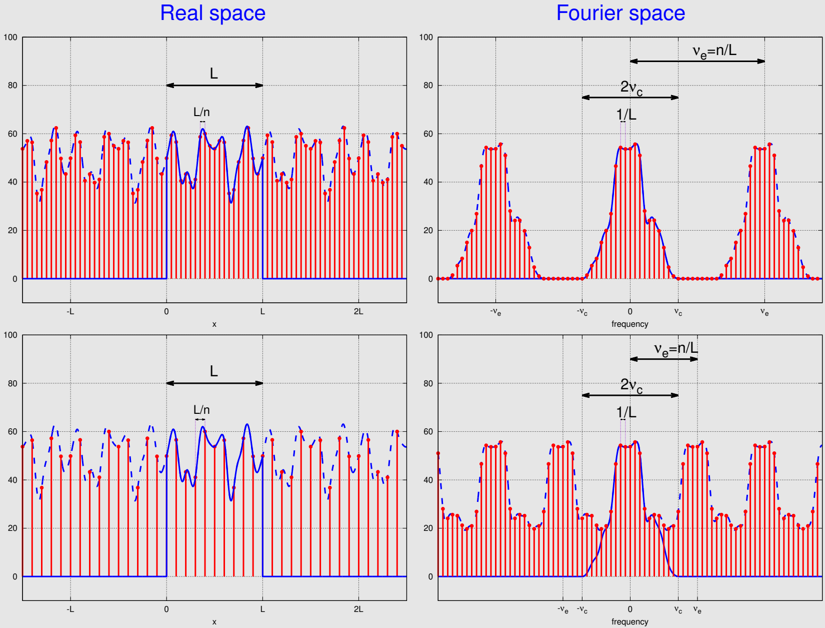
Real space



Fourier space

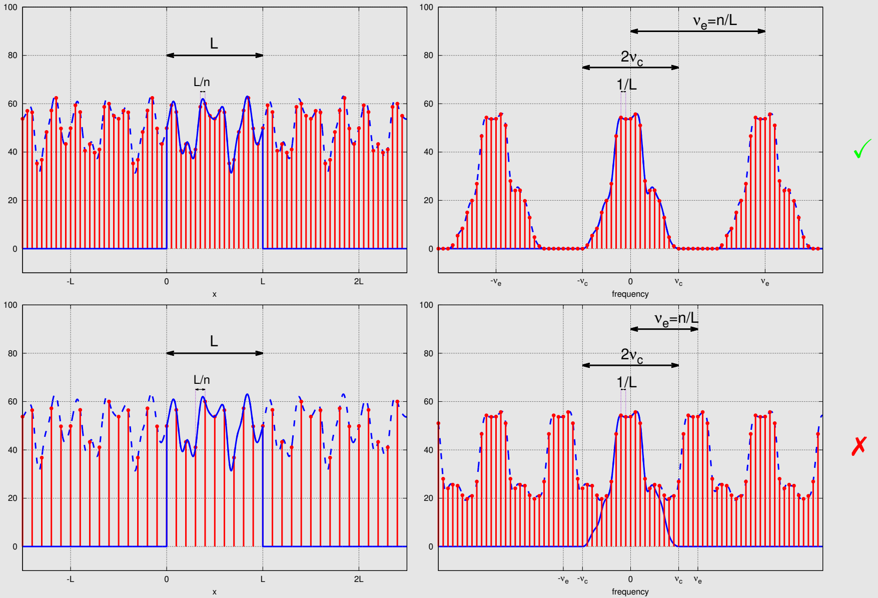


Aliasing


Real space
Fourier space
L
L/n
x
-L
0
2L
ν_e=n/L
$2\nu_c$
1/L
$-\nu_e$
$-\nu_c$
ν_c
ν_e
frequency
100
80
60
40
20
0

Aliasing

Real space | Fourier space



Precautions required for the use of FFT (specially in the case of periodic homogenization)

case of periodic homogenization

1. the function is supposed to be **periodic**

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2. satisfy the conditions of Shannon theorem

$$\nu_e (= n/L) > 2\nu_c$$

- "under-sampling" : $\nu_e < 2\nu_c \Rightarrow$ "aliasing"
- cutoff frequency ν_c : generally unknow
- cutoff frequency ν_c can be very high or may not exist !

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In particular when material properties vary abruptly with position (example : two-phase composite).

Contributions to the initial method

Non exhaustive list of contributions

- non-linear behaviour [Moulinec, Suquet (1994)]
- boundary conditions
  - prescribed macroscopic stress, prescribed direction of macroscopic stress
  - Dirichlet, Neuman conditions [Gélébart (2024) - Risthaus, Schneider (2024) - Morin, Paux (2024)]
- iterative scheme
  - "polarization-based" scheme [Eyre-Milton (1999) - Michel, Moulinec, Suquet (2000) - Monchiet, Bonnet (2012)]
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- modified Green operator [Müller (1999) - Willot (2015)]
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- porous materials, fractures, ... [To, Bonnet (2020)]
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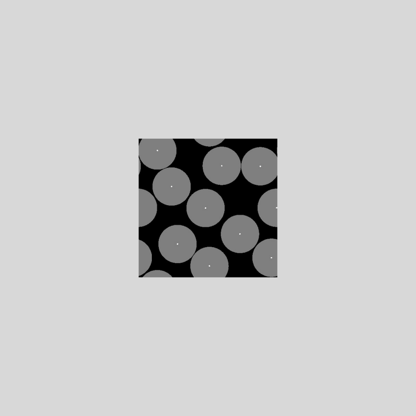
Review articles

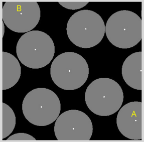
- Schneider, Acta Mech (2021)
- Lucarini, Upadhyay, Segurado, Modelling Simul. Mater. Sci. Eng. (2022)

Distance in a periodic media



10 discs - f=60%

Distance in a periodic media



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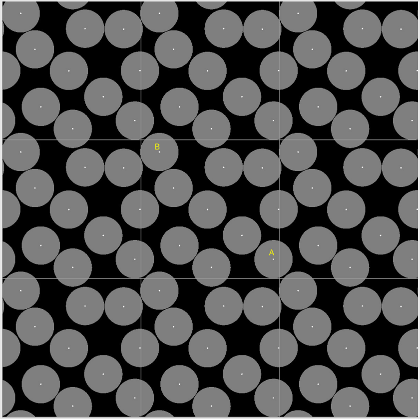

10 discs - f=60% - periodized 3 $\times$ 3

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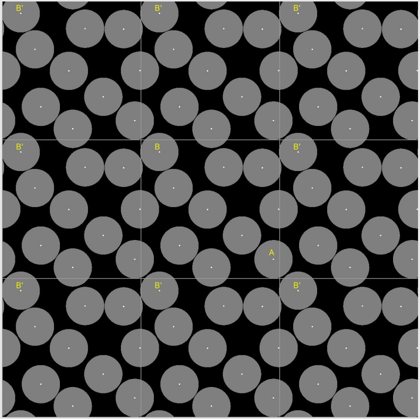

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$$d_{periodic}(A,B) = \min_{B'=3\times 3 \ periodized \ B} \left(d(A,B') \right)$$

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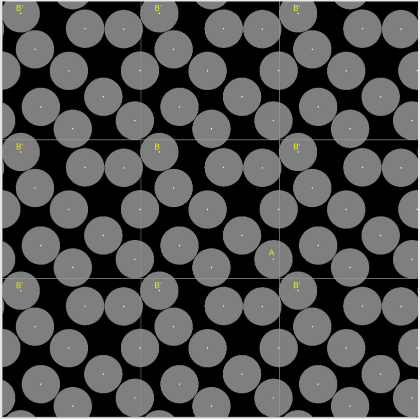

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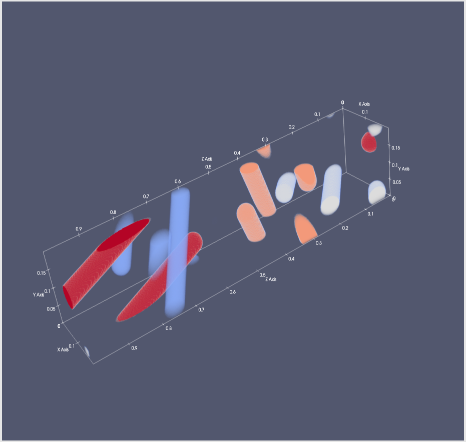
Distance in a periodic media

- $\Omega = 0.2 \times 0.2 \times 1$
- 4 fibres : L=0.42 D=0.053 L/D=8 - volume fraction f=10%



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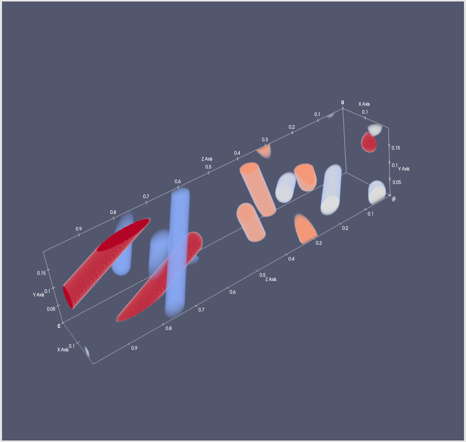

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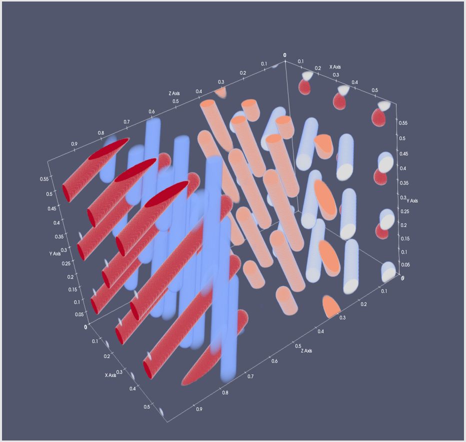

periodized microstructure $3 \times 3 \times 1$

“L-periodic distance”

distance in a periodic media of periods $(\boldsymbol{L}_i)_{i=1,\dots,n}$ in a n-dimensional space

$$d_L(\boldsymbol{x}, \boldsymbol{y}) = \min_{\boldsymbol{k} \in \mathbb{Z}^n} \left(d_E \big(\boldsymbol{x}, \boldsymbol{y} + \sum_{i=1}^{n} k_i \boldsymbol{L}_i \big) \right)$$

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when $\boldsymbol{L}_i = L_i \boldsymbol{e}_i$ with $(\boldsymbol{e}_i)$ orthogonal unit vector
(i.e. Ω is a rectangular parellelepiped)

$$d_L(\boldsymbol{x},\boldsymbol{y}) = \sqrt{\sum_{i=1}^{n} \left(y_i - x_i - \mathrm{N}\left(\frac{y_i - x_i}{L_i}\right) L_i \right)^2}$$

with $N(.)$: nearest integer function

Moulinec (2022)

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$$d_L^2(\boldsymbol{x},\boldsymbol{y}) = \sum_{i=1}^{n}\left(y_i - x_i - \mathrm{N}\left(\frac{y_i-x_i}{L_i}\right)L_i\right)^2$$

Moulinec (2022)

Dirichlet-Voronoï tessellations

Descartes (1644)

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Lejeune Dirichlet (1850)

John Snow (1855)

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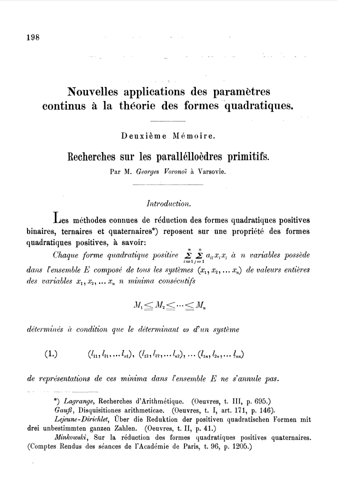

198

Nouvelles applications des paramètres continus à la théorie des formes quadratiques.

Deuxième Mémoire.

Recherches sur les paralléloèdres primitifs.

Par M. *Georges Voronoï* à Varsovie.

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Les méthodes connues de réduction des formes quadratiques positives binaires, ternaires et quaternaires*) reposent sur une propriété des formes quadratiques positives, à savoir:

Chaque forme quadratique positive $\sum_{i=1}^{n}\sum_{j=1}^{n} a_{ij}x_ix_j$ *à n variables possède dans l'ensemble E composé de tous les systèmes* $(x_1, x_2, \dots x_n)$ *de valeurs entières des variables* $x_1, x_2, \dots x_n$ *n minima consécutifs*

$$M_1 \leqq M_2 \leqq \cdots \leqq M_n$$

déterminés à condition que le déterminant ω *d'un système*

$$(1.)\qquad (l_{11}, l_{21}, \dots l_{n1}),\ (l_{12}, l_{22}, \dots l_{n2}), \dots (l_{1n}, l_{2n}, \dots l_{nn})$$

de représentations de ces minima dans l'ensemble E ne s'annule pas.

*) *Lagrange*, Recherches d'Arithmétique. (Oeuvres, t. III, p. 695.)
Gauß, Disquisitiones arithmeticae. (Oeuvres, t. I, art. 171, p. 146).
Lejeune-Dirichlet, Über die Reduktion der positiven quadratischen Formen mit drei unbestimmten ganzen Zahlen. (Oeuvres, t. II, p. 41.)
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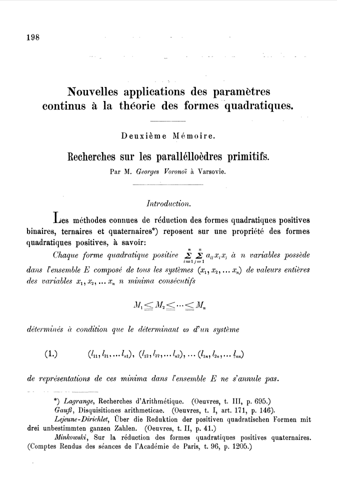
Dirichlet-Voronoï tessellations



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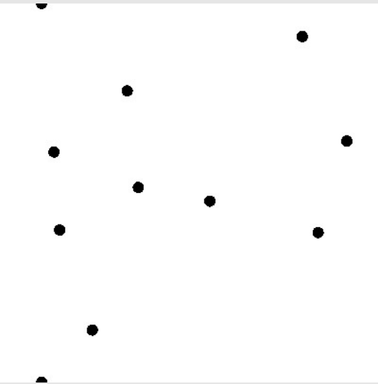
Voronoï (1908)

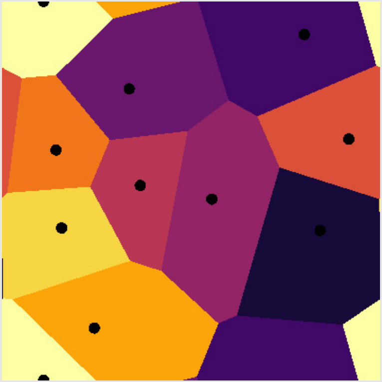
Aurenhammer (1991)
Okabe, Boots, Sugihara, Chiu (1992,2000)

Dirichlet-Voronoï tessellations



- set of n "seeds" ($\boldsymbol{x_s}$)

Dirichlet-Voronoï tessellations



- set of n “seeds” $(\boldsymbol{x_s})$
- cell C_s = set of points closer to $\boldsymbol{x_s}$ than to any other seed

$$\boldsymbol{x} \in C_s \Leftrightarrow d(\boldsymbol{x}, \boldsymbol{x_s}) \leq d(\boldsymbol{x}, \boldsymbol{x'_s}) \, \forall s' \neq s$$

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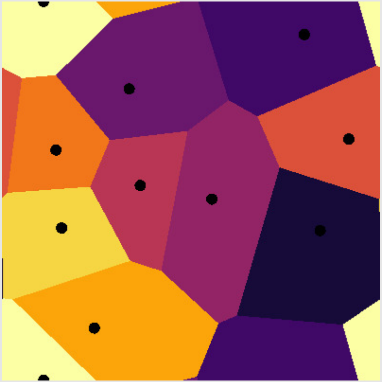

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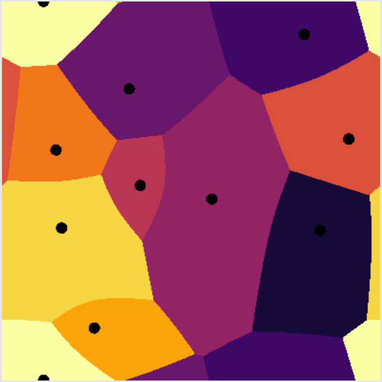
cells = convex polygons

Johnson-Mehl tessellations



crystal growth simulation

- set of n “seeds” $(\boldsymbol{x_s}, t_s)$

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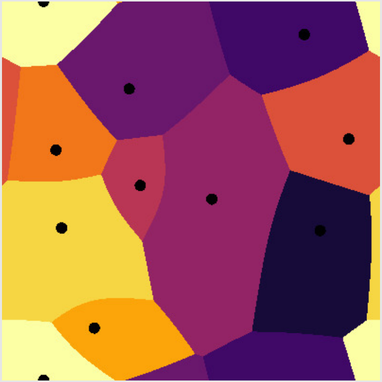

crystal growth simulation

- set of n “seeds” $(\boldsymbol{x_s}, t_s)$
- cell C_s = set of points reached by growth of crystal s before any other seed

$$\boldsymbol{x} \in C_s \Leftrightarrow \quad d(\boldsymbol{x}, \boldsymbol{x_s}) + Gt_s \leq d(\boldsymbol{x}, \boldsymbol{x'_s}) + Gt_{s'} \quad \forall s' \neq s$$

G = radial growth rate

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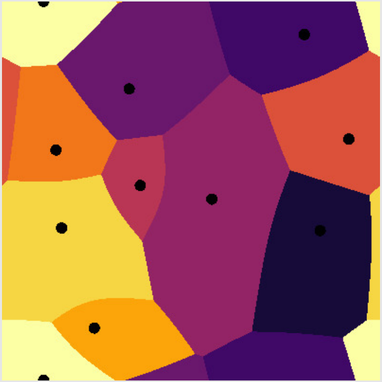

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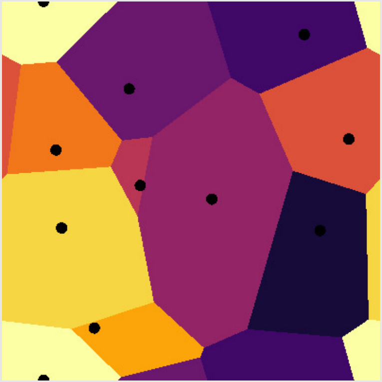
cells $\neq$ polygons
cells : non convex

Laguerre tessellations



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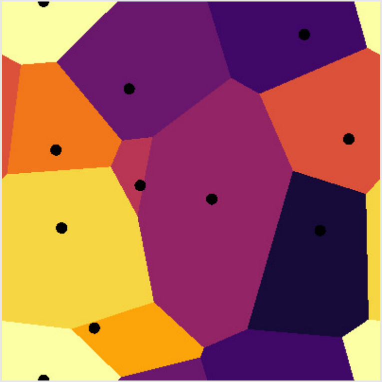

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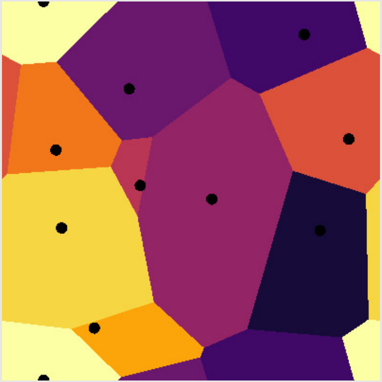

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higher cell size distribution than Voronoï

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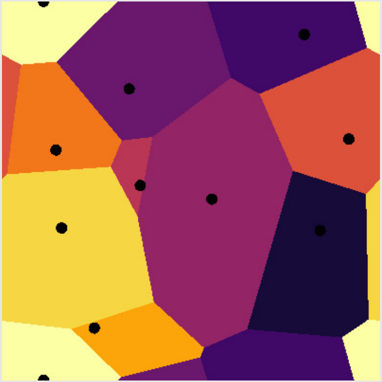

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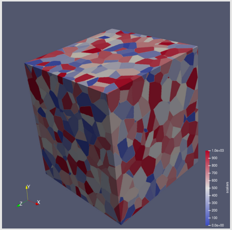
Laguerre tessellation = cross-section of a Voronoï tessellation in a n+1-dimensional space

Crystal-like microstructure

Voronoi tessellation - 100 grains

Laguerre tessellation

Johnson-Mehl tessellation

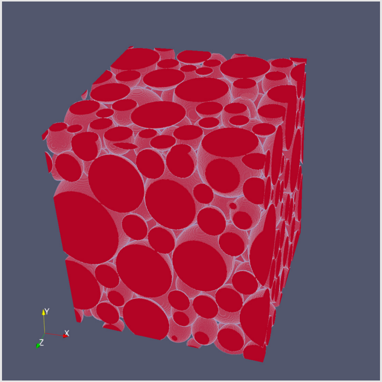


Voronoi tessellation - 1000 grains

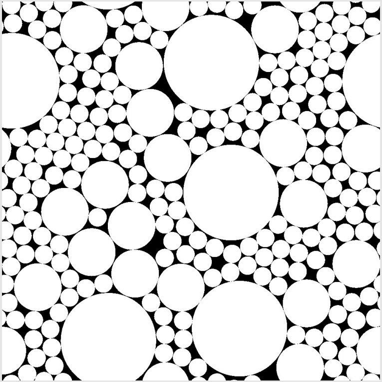
Codes :

- Voro++ Lawrence Berkeley Laboratory - Rycroft (2005)
- neper - R. Quey (2021)
- tsl in CraFT package - Moulinec (2022)

Hard sphere distribution



polydisperse spheres (5+20+200) - volume fraction=70%



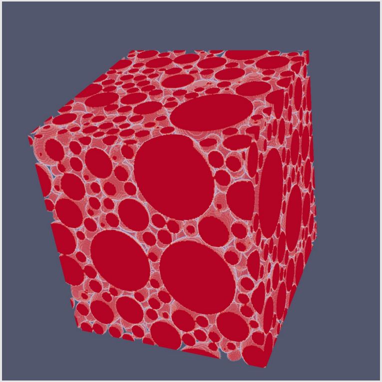
polydisperse discs (5+20+500) - volume fraction=87%

empilement compact (monodisperse)

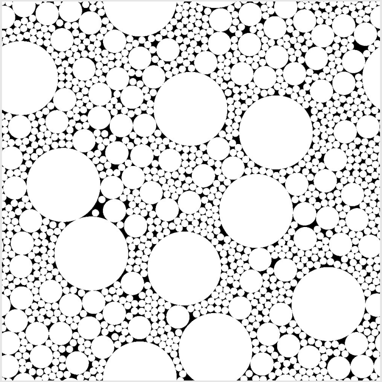
- 3D : max volume fraction $\simeq$ 74.0%
- 2D : max volume fraction $\simeq$ 90.7%

R. Valmalette

Hard sphere distribution



polydisperse spheres (10+100+1000) - volume fraction=71%



polydisperse discs (10+100+1000) - volume fraction=89%

Hard sphere distribution

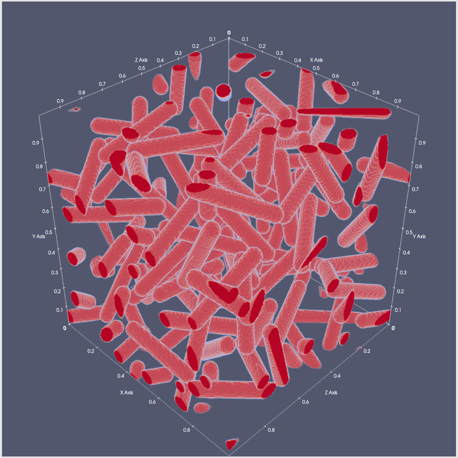
Algorithms :

- Random Sequential Addition : low efficiency
- Metropolis algorithm
- Molecular dynamics algorithms

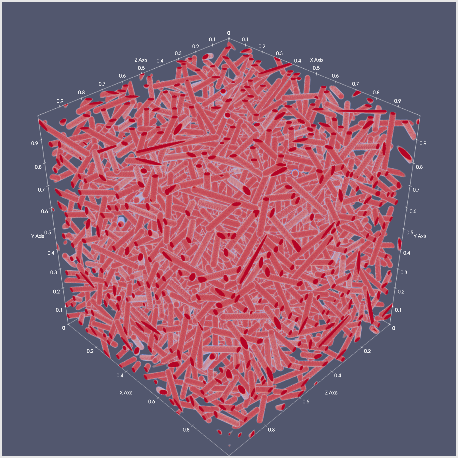
  ...

Codes ...

Fibre distribution

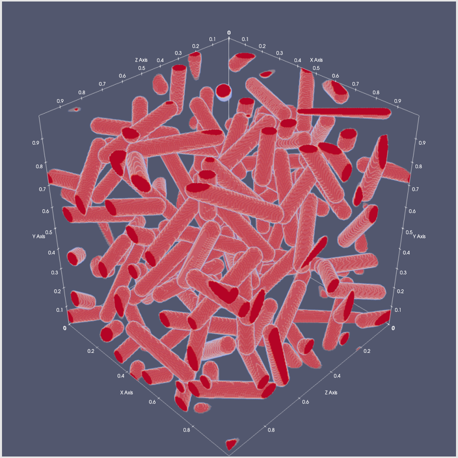


100 fibers - L/D=6 - f=10% (RSA algo)



1000 fibers - L/D=11 - f=10% (RSA algo)

Fibre distribution



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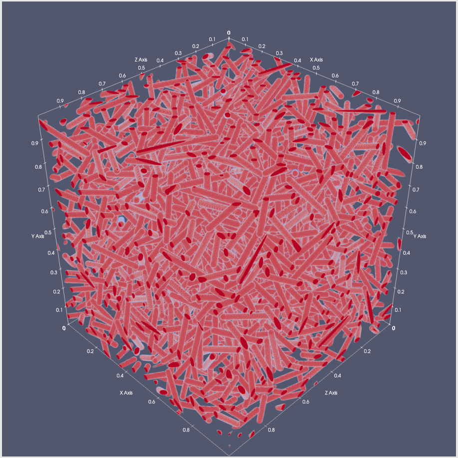

1000 fibers - L/D=11 - f=10% (RSA algo)

A nice trick :

- fibre = cylindre + hemisphere ends
- distance between 2 fibres = distance between 2 segments (-D)

Codes

FFT-based homogenization codes

code	author	institute	location
Amitex-FFTP	Lionel Gélébart	CEA Saclay	Gif sur Yvette, France
CraFT	Hervé Moulinec	LMA CNRS	Marseille, France
DAMASK	Martin Diehl	Max-Planck-Institut für Eisenforschung	Düsseldorf, Germany
FFTHomPy	Jaroslav Vondřejc	Technische Universität Braunschweig	Braunschweig, Germany
GeoDict		Math2Market GmbH	Kaiserslautern, Germany
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Microstructure generation tools

- Neper (Romain Quey, CNRS Mines Saint Étienne)
- Mérope (Marc Josien, CEA)
- Damask (Max Planck)
- CraFT (LMA)

...

Conclusion

- FFT-based homogenization method $\leftarrow$ micromechanics + Image Processing

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Thank you for your attention

Γ^0 Green operator

Case of the conductivity problem :

$$\boldsymbol{\sigma} = c^0 \boldsymbol{\varepsilon} + \boldsymbol{\tau}$$

($\boldsymbol{\sigma}$: current density, $\boldsymbol{\varepsilon}$: electric field, c^0 : conductivity)

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$$\boldsymbol{\Gamma^0} = \frac{1}{c^0} \frac{\boldsymbol{\xi} \otimes \boldsymbol{\xi}}{|\boldsymbol{\xi}|^2}$$