

# FDM solved by Fast Fourier transforms (FFT)

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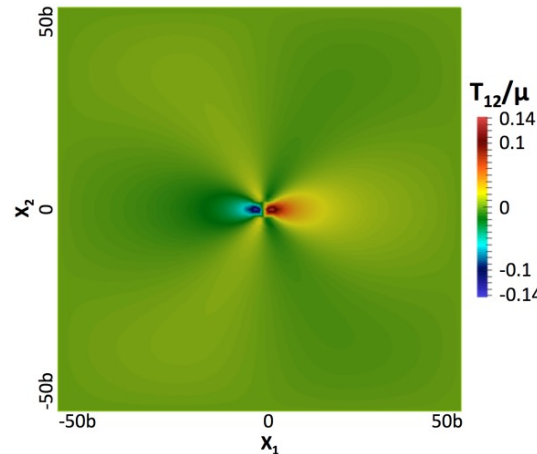


# Motivations

## Field Dislocation Mechanics(FDM)

(Kröner 1958; Mura 1963; Acharya 2001, 2003, Roy-Acharya 2005, 2006, Sandfeld et al 2010, ...)

Shear stress generated by an edge dislocation  
in isotropic elasticity (FEM)



**Problem :** implementation with 3D finite elements is CPU time consuming  
(Roy et Acharya 2005)



**Need a fast method to compute the mechanical fields of dislocations**



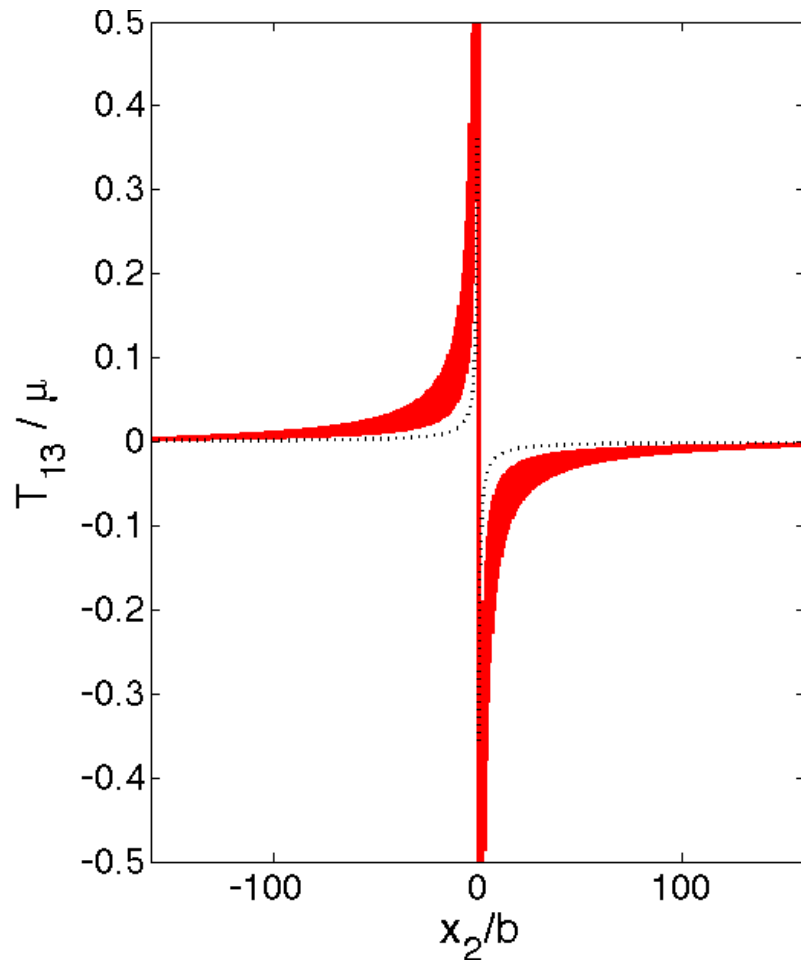
**Fast Fourier Transform (FFT)**

(Moulinec-Suquet, 1994; Muller, 1996; Lebensohn et al. , 2001, 2012;  
Brenner et al. 2014, Berbenni et al. 2014)

# Advantage of intrinsic DFT versus FFT

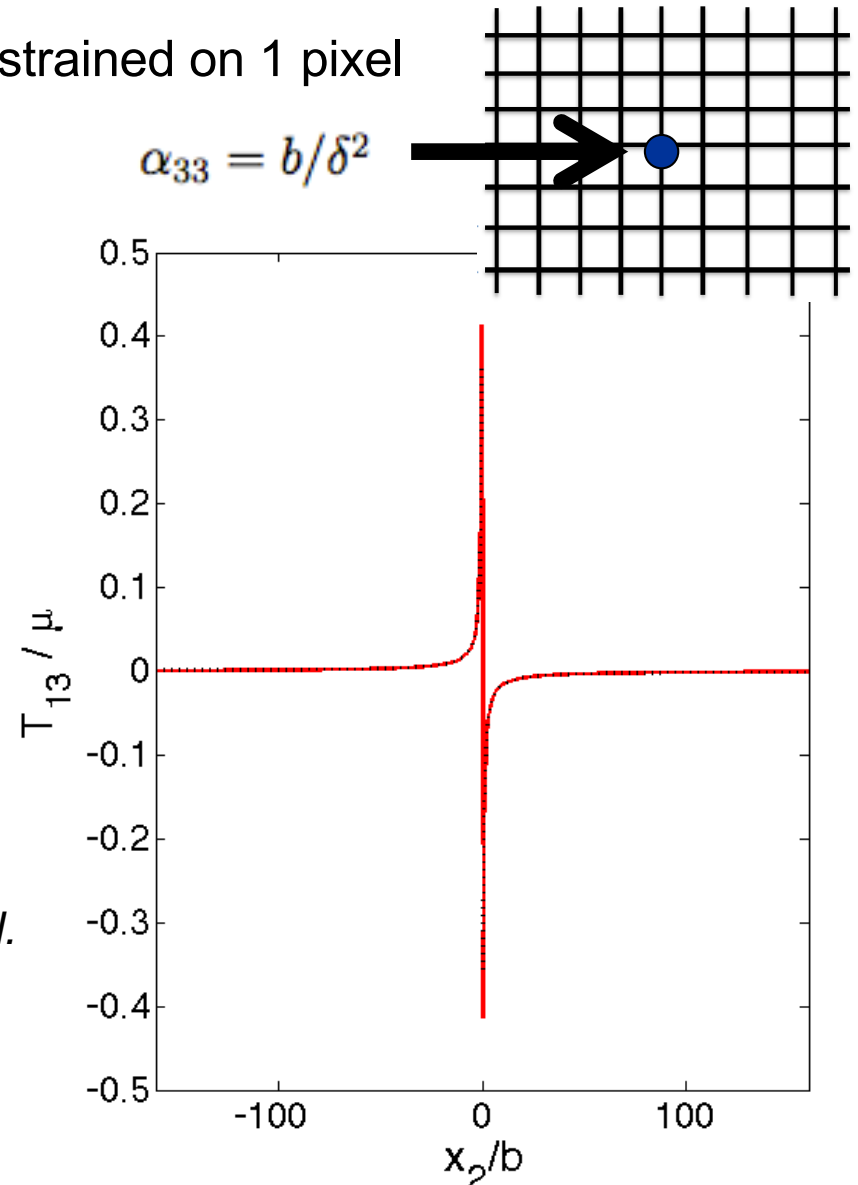
1024×1024 pixels  
(450b×450b)

Screw dislocation constrained on 1 pixel



FFT approx. of continuous FT

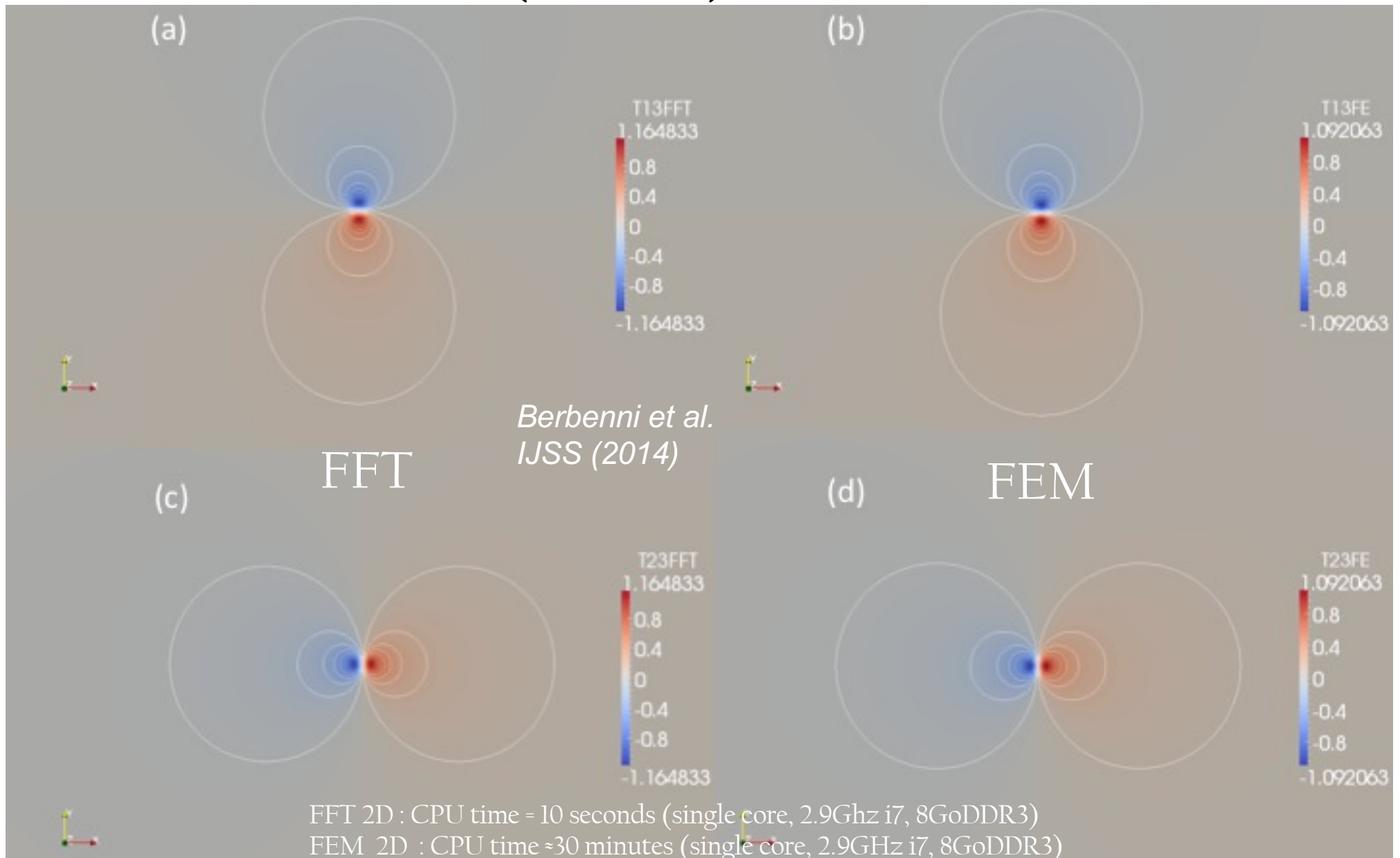
*Berbenni et al.  
IJSS (2014)*



FFT exact with DFT (present)

# Preliminary results in homogeneous isotropic elasticity

## FFT / FEM (stresses): screw dislocation



*Berbenni et al.  
IJSS (2014)*

FFT 2D : CPU time = 10 seconds (single core, 2.9Ghz i7, 8GoDDR3)

FEM 2D : CPU time ≈ 30 minutes (single core, 2.9GHz i7, 8GoDDR3)

# Outline

- ❑ Field Dislocation Mechanics equations
- ❑ Dislocation transport equation solved by FFT
- ❑ Elasto-static approach for FDM in the context of heterogeneous elasticity and spectral approach (FFT) with applications
- ❑ Summary and perspectives

# Field Dislocation Mechanics theory equations

- Lattice incompatibility (Nye tensor)

$$\begin{cases} \boldsymbol{\alpha} = \mathbf{curl}(\mathbf{U}_e) \\ \mathbf{div} \boldsymbol{\alpha} = \mathbf{0} \end{cases}$$

*Kröner 1958; Nye 1953; Indenbom 1965*

- Stress equilibrium (without body force)

$$\mathbf{div} \mathbf{T} = \mathbf{0}$$

$$\mathbf{T} = \mathbf{C} : \{\mathbf{U}_e\} = \mathbf{C} : \boldsymbol{\varepsilon}^e$$

*Mura, Phil Mag. 1963, PRSL 1964; Acharya 2001, 2003, ...*

- Dislocation density transport equation:

$$\dot{\boldsymbol{\alpha}} = -\mathbf{curl} (\boldsymbol{\alpha} \times \mathbf{V}) \quad \text{with} \quad \mathbf{V} = \mathbf{f}(\boldsymbol{\alpha}, \mathbf{T})$$

*Mura, Phil Mag. 1963, PRSL 1964; Acharya 2001, 2003..*

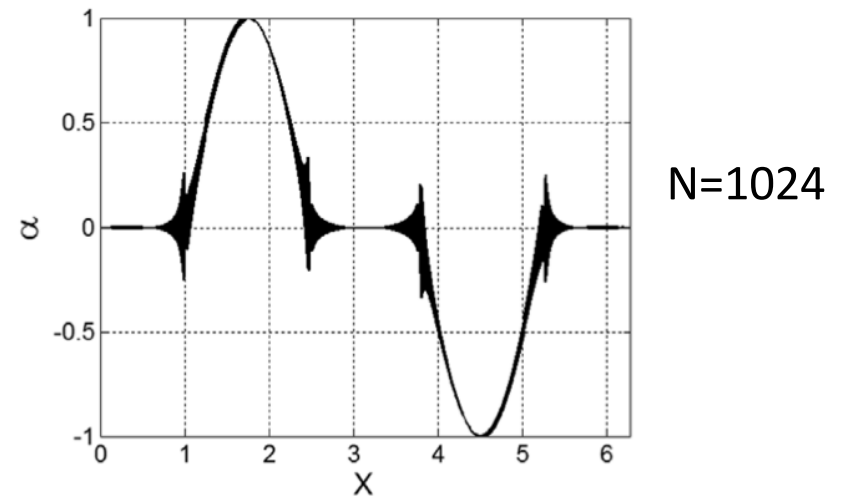
# FFT-solver for dislocation density transport equation

$$\dot{\alpha} = -\mathbf{curl} (\alpha \times \mathbf{V}) \quad \Rightarrow \quad \alpha_{ij}^{t+\Delta t} = \alpha_{ij}^t - \Delta t \left[ \left( \alpha_{ij} v_k \right)^t - \left( \alpha_{ik} v_j \right)^t \right]_{,k}$$

- FE-GLS approach (Galerkin Least square method, see *Varadhan et al., MSMSE 2006*)
- Spectral approach (FFT):

$$\tilde{\alpha}_{ij}^{t+\Delta t} = \left\{ \tilde{\alpha}_{ij}^t - \Delta t i \xi_k \left[ \left( \widetilde{\alpha_{ij} v_k} \right)^t - \left( \widetilde{\alpha_{ik} v_j} \right)^t \right] \right\}$$

Instabilities due to the PDE hyperbolic character  
and due to Gibbs oscillations inherent to classic  
spectral approach



*Djaka et al. MSMSE 2015*

- Filtered spectral approach

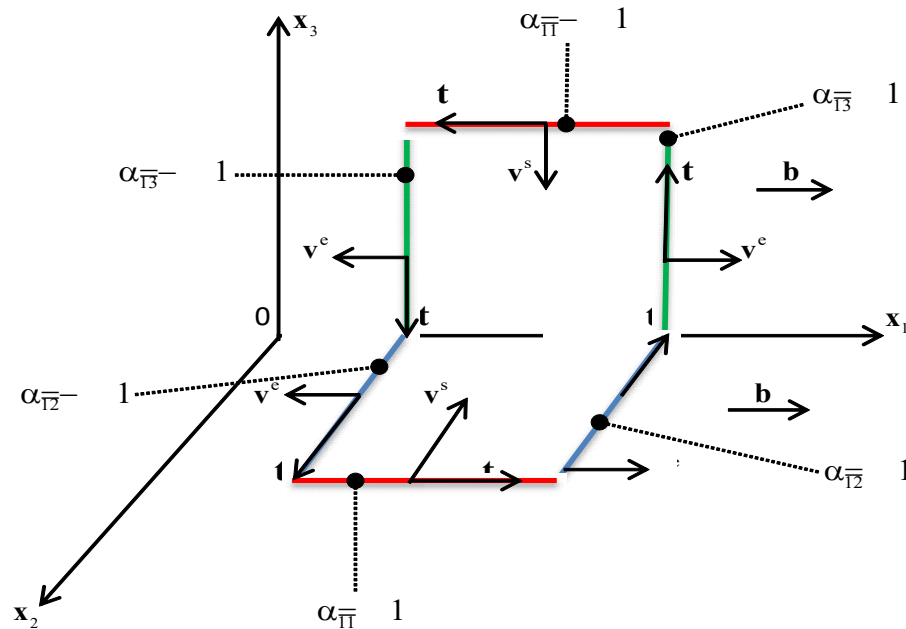
$$\tilde{\alpha}_{ij}^{t+\Delta t} = \sigma(\eta) \left\{ \tilde{\alpha}_{ij}^t - \Delta t i \xi_k \left[ \left( \widetilde{\alpha_{ij} v_k} \right)^t - \left( \widetilde{\alpha_{ik} v_j} \right)^t \right] \right\}$$

Exponential filter  $\sigma(\eta) = \exp(-\beta(\eta)^{2p})$   
(see *Gottlieb-Hesthaven, Spectral methods  
for hyperbolic problems 2001*)

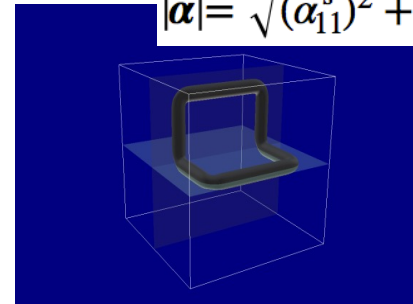
$\left\{ \begin{array}{l} \beta = -\log \varepsilon_M : \text{smoothing parameter} \\ \varepsilon_M : \text{small value} \\ \eta : \text{discrete frequencies} \\ 2p : \text{filter order} \end{array} \right.$

$$\sigma\left(\frac{k_1}{N_1}, \frac{k_2}{N_2}, \frac{k_3}{N_3}\right) = \exp\left(-\beta\left(\left(\frac{k_1}{N_1}\right)^{2p} + \left(\frac{k_2}{N_2}\right)^{2p} + \left(\frac{k_3}{N_3}\right)^{2p}\right)\right)$$

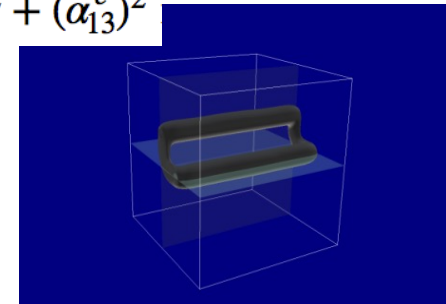
# Application to 3D polygonal dislocation loop shrinkage (constar velocities)



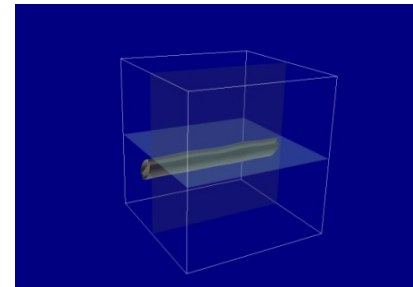
$$|\alpha| = \sqrt{(\alpha_{11}^s)^2 + (\alpha_{12}^e)^2 + (\alpha_{13}^e)^2}$$



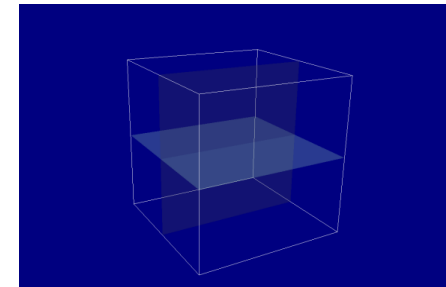
a:  $t = 0$  s



b:  $t = 4.9087 \times 10^{-10}$  s



c:  $t = 2.4543 \times 10^{-9}$  s



d:  $t = 3.6815 \times 10^{-9}$  s

| $N_{\text{tot}}$ | CPU time (s) |        |
|------------------|--------------|--------|
|                  | FFT          | FE-GLS |
| $32^3$           | 0.032        | 20.110 |
| $64^3$           | 0.081        | 164.82 |
| $128^3$          | 0.590        | 1354.3 |
| $256^3$          | 5.310        | /      |
| $512^3$          | 56.00        | /      |

Unit cell voxel number  $128 \times 128 \times 128$   
 Smoothing parameter  $\epsilon_M = 0.2$   
 Courant number  $c = 0.25$   
 Constant velocity  $v_0 = 5 \times 10^8 \text{ s}^{-1}$   
 Simulation 3D priodic domain:  $2\pi \times 2\pi \times 2\pi$   
 Filter order:  $2p=2$  ( $p=1$ )

Single core, 2.3Ghz i7, 16Go DDR3

Djaka et al. MSMSE 2015

# Static field dislocation mechanics in heterogeneous elasticity (stress equilibrium)

- Stokes-Helmholtz decomposition (*Acharya 2001*)

$$\mathbf{U}_e = \mathbf{U}_e^\perp + \mathbf{U}_e^\parallel = \mathbf{curl} \, \boldsymbol{\chi} + \mathbf{grad} \, \mathbf{w}$$

$$\boldsymbol{\alpha} = \mathbf{curl}(\mathbf{U}_e) \Rightarrow \begin{cases} \boldsymbol{\alpha} = \mathbf{curl}(\mathbf{U}_e^\perp) \\ \mathbf{div} \mathbf{U}_e^\perp = 0 & \text{in } \mathbf{V} \\ \mathbf{U}_e^\perp \cdot \mathbf{n} = 0 & \text{on } \partial \mathbf{V} \end{cases} \Rightarrow \begin{cases} \mathbf{div} \mathbf{grad} \, \mathbf{U}_e^\perp = \Delta \mathbf{U}_e^\perp = -\mathbf{curl} \, \boldsymbol{\alpha} \\ \mathbf{U}_e^\perp \cdot \mathbf{n} = 0 & \text{on } \partial \mathbf{V} \end{cases}$$

- Poisson's equation

1

- Stress equilibrium and new polarization stress

$$\mathbf{T}_{ij,j} = 0 \Rightarrow \mathbf{C}_{ijkl}^0 \mathbf{w}_{k,lj} + \boldsymbol{\tau}_{ij,j} = 0 \quad \text{with} \quad \begin{cases} \boldsymbol{\tau}_{ij} = \mathbf{T}_{ij}^\perp + \delta \mathbf{C}_{ijkl} \mathbf{w}_{k,l} \\ \mathbf{T}_{ij}^\perp = \mathbf{C}_{ijkl} \mathbf{U}_{kl}^{e,\perp} \end{cases}$$

- Lippman-Schwinger equation with incompatibilities

$$\boldsymbol{\varepsilon}_{ij}^{e,\parallel}(\mathbf{x}) = \mathbf{E}_{ij} - \int_V \Gamma_{ijkl}^0(\mathbf{x} - \mathbf{x}') \boldsymbol{\tau}_{kl}(\mathbf{x}') dV' \quad \text{with} \quad \begin{cases} \boldsymbol{\varepsilon}^{e,\parallel} = (\mathbf{grad} \, \mathbf{w})^{\text{sym}} \\ \Gamma_{ijkl}^0 = -\frac{1}{2}(\mathbf{G}_{ik,jl} + \mathbf{G}_{jk,il}) \\ \mathbf{E} = \langle \boldsymbol{\varepsilon}^{e,\parallel} \rangle \end{cases}$$

2

# Elasto-static field equations in heterogeneous elasticity solved by a spectral approach

- Incompatible field:

$$1 \quad \begin{cases} \mathbf{div grad} \mathbf{U}_e^\perp = \Delta \mathbf{U}_e^\perp = -\mathbf{curl} \, \boldsymbol{\alpha} \\ \mathbf{U}_e^\perp \cdot \mathbf{n} = 0 \quad \text{sur } \partial \mathbf{V} \end{cases} \quad \begin{matrix} \mathbf{F} \\ \mathbf{T} \Rightarrow \end{matrix} \quad \boxed{\begin{cases} \tilde{\mathbf{U}}_{ij}^{e,\perp}(\underline{\xi}) = \frac{i}{\xi^2} \xi_k \left( \mathbf{e}_{jkl} \tilde{\alpha}_{il}(\underline{\xi}) \right) & \forall \underline{\xi} \neq \mathbf{0} \\ \tilde{\mathbf{U}}_{ij}^{e,\perp}(\mathbf{0}) = \mathbf{0} \end{cases}}$$

(Brenner et al. 2014, Berbenni et al. 2014)

- Lippman-Schwinger-type equation with incompatibilities:

$$2 \quad \boldsymbol{\varepsilon}_{ij}^{e,\parallel}(\mathbf{x}) = \mathbf{E}_{ij} - \int_{\mathbf{V}} \Gamma_{ijkl}^0(\mathbf{x} - \mathbf{x}') \boldsymbol{\tau}_{kl}(\mathbf{x}') dV' \quad \xRightarrow{\text{FT}} \quad \boxed{\begin{cases} \tilde{\boldsymbol{\varepsilon}}^{e,\parallel}(\underline{\xi}) = \mathbf{E} - \tilde{\Gamma}^0(\underline{\xi}) : \tilde{\boldsymbol{\tau}}(\underline{\xi}) & \forall \underline{\xi} \neq \mathbf{0} \\ \tilde{\boldsymbol{\varepsilon}}^{e,\parallel}(\mathbf{0}) = \mathbf{E} \end{cases}}$$

with  $\tilde{\Gamma}_{ijkl}^0(\underline{\xi}) = \frac{1}{2} \left( \tilde{G}_{ik}(\underline{\xi}) \xi_l \xi_j + \tilde{G}_{jk}(\underline{\xi}) \xi_l \xi_i \right)$  and  $\begin{cases} \tilde{G}_{ik}(\underline{\xi}) = \left( \xi_j C_{ijkl}^0 \xi_l \right)^{-1} & \forall \underline{\xi} \neq \mathbf{0} \\ \tilde{G}_{ik}(\mathbf{0}) = \mathbf{0} \end{cases}$  (Mura 1987)

- Periodic boundary conditions

# Discrete Fourier Transforms: discretization and differentiation

- Discrete Fourier grid

See: Moulinec et Suquet (1994, 1998), Lebensohn (2001)

$$m_j = \left( \left( -\frac{N_j}{2} + 1 \right), \left( -\frac{N_j}{2} + 2 \right), \dots, -1, 0, 1, \dots, \left( \frac{N_j}{2} - 1 \right), \left( \frac{N_j}{2} \right) \right) \quad \text{even } N_j \quad \text{with } j = 1 \rightarrow 3$$

- Calculation methods of 1st derivatives in the Fourier space:

- Discrete approx. of continuous Fourier vectors (CFT)

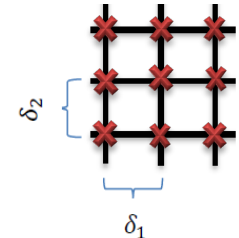
$$\frac{\partial}{\partial x_j} \Leftrightarrow i\xi_j = \frac{i2\pi}{T_j} m_j \quad \text{Moulinec et Suquet (1994, 1998)}$$

→ { Poisson : P  
Lippmann-Schwinger: BS

- Approximation based on centered 9pixel-based finite differences together with DFT : « centered » (C)

→ Poisson: P<sub>C</sub>

$$\frac{\partial}{\partial x_j} \Leftrightarrow i\xi_j^C = \frac{i}{\delta_j} \sin\left(\frac{2\pi m_j}{N_j}\right) \quad \text{Müller (1996), Dreyer-Muller (1999), Berbenni et al. (2014)}$$

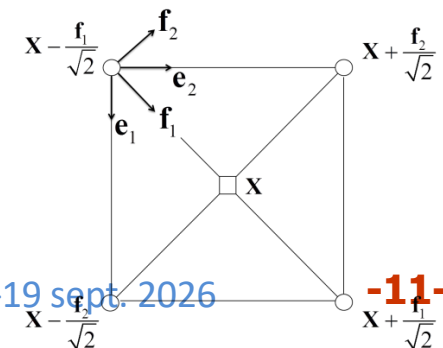


- Approximation based on rotated centered finite differences together with DFT : « rotated » (R)

→ Lippmann-Schwinger: BS<sub>R</sub>

$$\frac{\partial}{\partial x_j} \Leftrightarrow i\xi_j^R = \frac{i}{4} \tan\left(\frac{1}{2}\left(\frac{2\pi m_j}{N_j}\right)\right) \times \left(1 + \exp\left(i\frac{2\pi m_1}{N_1}\right)\right) \times \left(1 + \exp\left(i\frac{2\pi m_2}{N_2}\right)\right) \times \left(1 + \exp\left(i\frac{2\pi m_3}{N_3}\right)\right)$$

Willot (2015)



P-BS, P<sub>C</sub>-BS, P<sub>C</sub>-BS<sub>R</sub>

# Different iterative schemes to solve Lippmann-Schwinger by FFT

$$\begin{cases} \tilde{\varepsilon}^{e,||}(\underline{\xi}) = \mathbf{E} - \tilde{\Gamma}^0(\underline{\xi}) : \tilde{\tau}(\underline{\xi}) & \forall \underline{\xi} \neq \mathbf{0} \\ \tilde{\varepsilon}^{e,||}(\mathbf{0}) = \mathbf{E} \end{cases}$$

↓  
Different  
resolution  
schemes with  
FFT:

- Basic scheme (*Moulinec-Suquet 1994,1998*)
- Accelerated scheme (*Eyre-Milton 1999*)
- Augmented Lagrangian scheme (*Michel et al. 2001*)
- Conjugate gradient (not dependent on the choice of  $C^0$ ,  
(*Brisard et al. 2010, Zeman et al. 2010, Gélébart et al. 2013*))

Basic scheme here used (Convergence is dependent on the choice of the reference medium  $C^0$ )

# Basic scheme with incompatibilities

$$\tilde{\varepsilon}^{e,\parallel}(\underline{\xi}) = \mathbf{E} - \tilde{\Gamma}^0(\underline{\xi}) : \tilde{\mathbf{T}}^\perp - \tilde{\Gamma}^0(\underline{\xi}) : \widetilde{\delta \mathbf{C} : \varepsilon^{e,\parallel}}$$

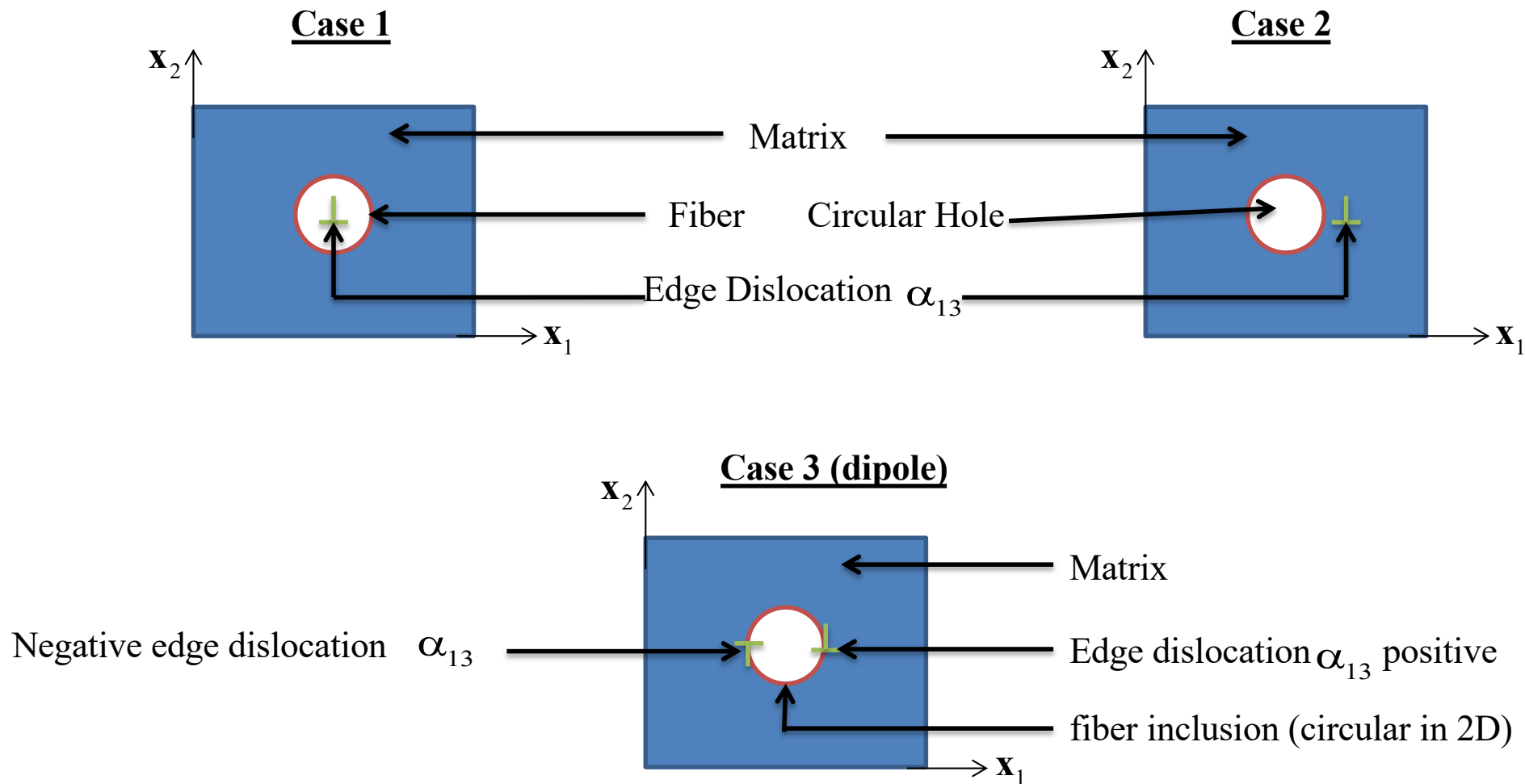
## A. Poisson (P) procedure and Initialization

- 1:  $\hat{\alpha} \leftarrow \text{FFT}(\alpha)$
- 2: Solve Poisson-type equation
 
$$\begin{cases} \hat{U}_{ij}^{e,\perp}(\underline{\xi}) = \frac{i}{\xi^2} \xi_k (e_{jkl} \hat{\alpha}_{il}(\underline{\xi})) & \forall \underline{\xi} \neq \mathbf{0} \\ \hat{U}_{ij}^{e,\perp}(\mathbf{0}) = \mathbf{0} \end{cases}$$
- 3:  $\mathbf{U}^{e,\perp} \leftarrow \text{FFT}^{-1}(\hat{U}^{e,\perp})$
- 4:  $\varepsilon^{e,\perp} \leftarrow \mathbf{U}_e^{\perp, \text{sym}}$
- 5:  $\mathbf{T}^\perp \leftarrow \mathbf{C} : \varepsilon^{e,\perp}$
- 6:  $\hat{\mathbf{T}}^\perp \leftarrow \text{FFT}(\mathbf{T}^\perp)$
- 7:  $\hat{\varepsilon}_0^{e,\perp} \leftarrow \hat{\Gamma}^0 : \hat{\mathbf{T}}^\perp$
- 8:  $\varepsilon_0^{e,\perp} \leftarrow \text{FFT}^{-1}(\hat{\varepsilon}_0^{e,\perp})$

## B. Global Basic Scheme (BS) Procedure

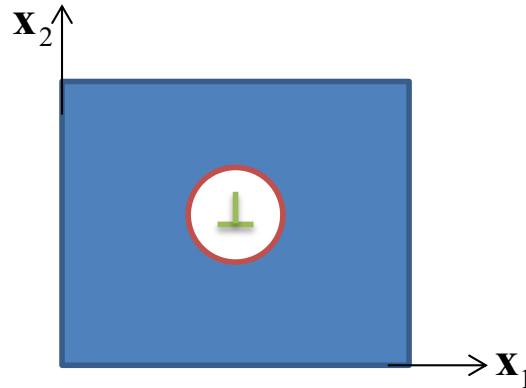
- 10:  $\varepsilon_0^{e,\parallel} \leftarrow \mathbf{E}$ ,  $\mathbf{T}_0 \leftarrow \mathbf{C} : (\varepsilon_0^{e,\parallel} + \varepsilon_0^{e,\perp})$
- 11: *For* n=0 to max\_iter *do*
- 12:  $\hat{\mathbf{T}}_n = \text{FFT}(\mathbf{T}_n)$
- 13: *If*  $e_n = \frac{\left( \langle \|\underline{\xi} \hat{\mathbf{T}}_n(\underline{\xi})\|^2 \rangle \right)^{\frac{1}{2}}}{\|\hat{\mathbf{T}}_n(\mathbf{0})\|} \leq \varepsilon$  *then*
- 14: *break*
- 15: *End if*
- 16:  $\hat{\mathbf{t}}_n(\underline{\xi}) \leftarrow \hat{\mathbf{T}}_n(\underline{\xi}) - \left( \mathbf{C}^0 : \varepsilon_n^{e,\parallel}(\underline{\xi}) \right)$
- 17:  $\hat{\varepsilon}_{n+1}^{e,\parallel}(\underline{\xi}) \leftarrow -\hat{\Gamma}^0(\underline{\xi}) : \hat{\mathbf{t}}_n(\underline{\xi}) \quad \forall \underline{\xi} \neq \mathbf{0}$   
 $\hat{\varepsilon}_{n+1}^{e,\parallel}(\mathbf{0}) \leftarrow \mathbf{E}$
- 18:  $\varepsilon_{n+1}^{e,\parallel}(\mathbf{x}) \leftarrow \text{FFT}^{-1}(\hat{\varepsilon}_{n+1}^{e,\parallel}(\underline{\xi}))$
- 19:  $\mathbf{T}_{n+1}(\mathbf{x}) \leftarrow \mathbf{C}(\mathbf{x}) : (\varepsilon_{n+1}^{e,\parallel}(\mathbf{x}) + \varepsilon_0^{e,\perp}(\mathbf{x}))$
- 20: *End For*

# Simple studied configurations to validate the FFT approach (2D configurations)



# Validations: comparisons with analytical solution

## Case 1 $\mu_I/\mu_M = 0.1$



No imposed loading

### Simulation data

Dislocation density  $\alpha_{13}(\mathbf{x}) = b / \delta^2$

Mesh:  $2048 \times 2048$  pixels

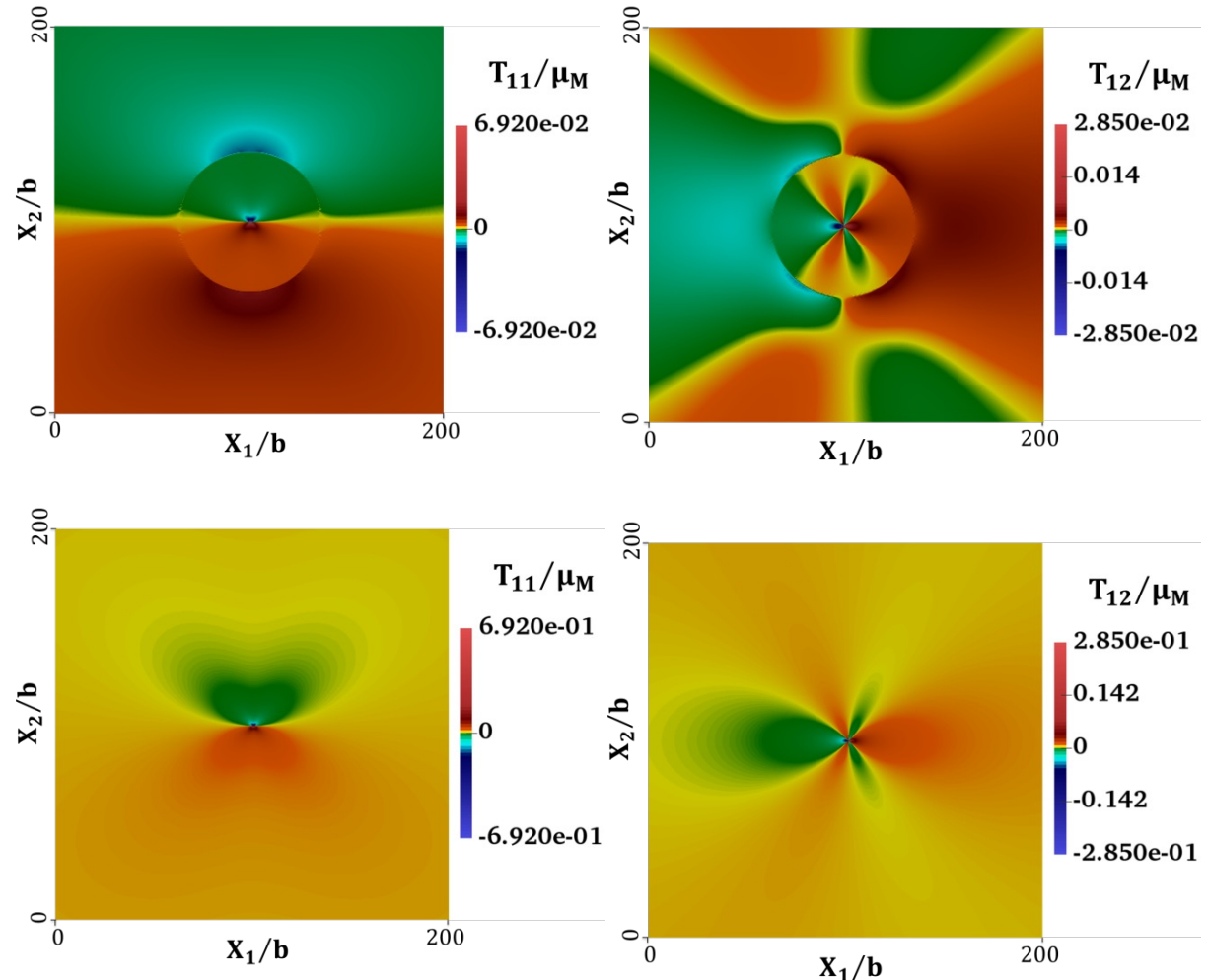
Pixel size:  $\delta_1 = \delta_2 = \delta \simeq 0.44b$

Fiber radius:  $R = 80\delta$

Convergence criterion:  $\varepsilon = 10^{-6}$

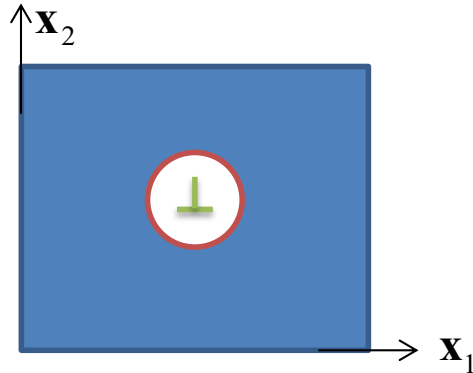
Burgers vector:  $b = 4.05 \times 10^{-4} \mu\text{m}$

Elastic constants:  $\begin{cases} \mu_I = 2.3001 \times 10^3 \text{ MPa} \\ \nu_I = \nu_M = 0.3647 \end{cases}$



# Validations: comparisons with analytical solution

## Case 1 $\mu_I/\mu_M = 0.1$



No imposed loading

### Simulation data

Dislocation density:  $\alpha_{13}(\mathbf{x}) = b / \delta^2$

Burgers vector magnitude:  $b = 4.05 \times 10^{-4} \mu\text{m}$

Unit cell size:  $2048 \times 2048$  pixels

Pixel size:  $\delta_1 = \delta_2 = \delta \approx 0.44b$

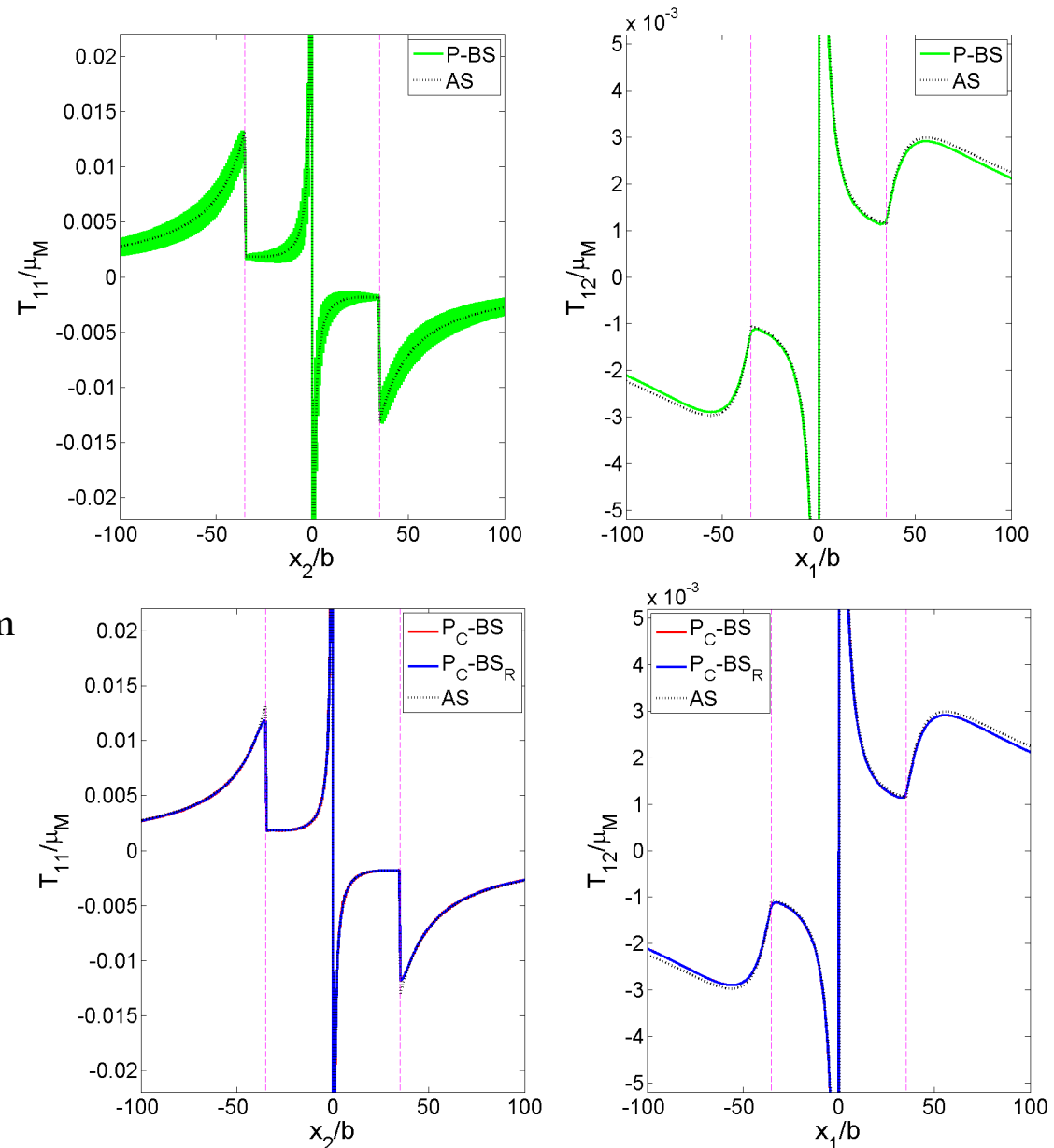
Fiber radius:  $R = 80\delta$

Elasticity:  $\begin{cases} \mu_I = 2.3001 \times 10^3 \text{ MPa} \\ \nu_I = \nu_M = 0.3647 \end{cases}$

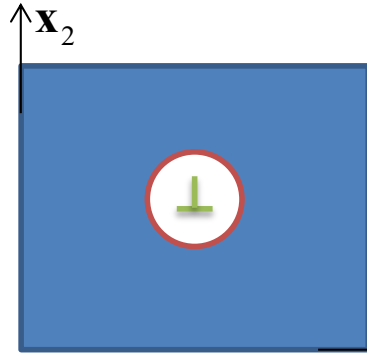
Convergence criterion:  $\varepsilon = 10^{-6}$

### Analytical solutions

Dundurs et Sendeckyj (JMPS 1965)



# Effect of spatial resolution (pixel size)



**Case 1**  $\mu_I/\mu_M = 0.1$

Elasticity:  $\begin{cases} \mu_I = 2.3001 \times 10^3 \text{ MPa} \\ \nu_I = \nu_M = 0.3647 \end{cases}$

Unit cell size:

900b×900b

No imposed loading

Pixel size (varying):

$$\delta_1 = \delta_2 = \delta$$

$$\approx 0.44b / 0.88b / 1.76b$$

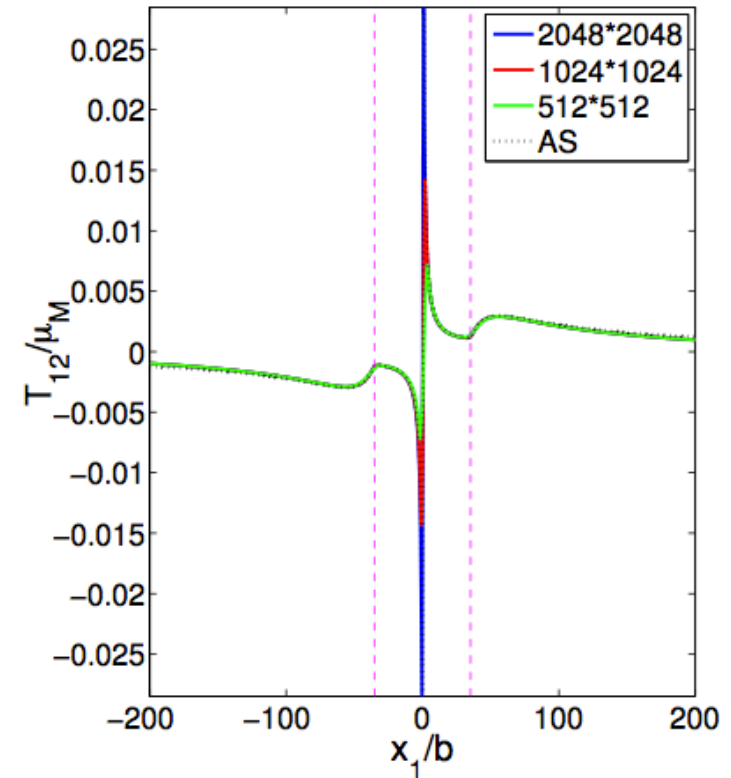
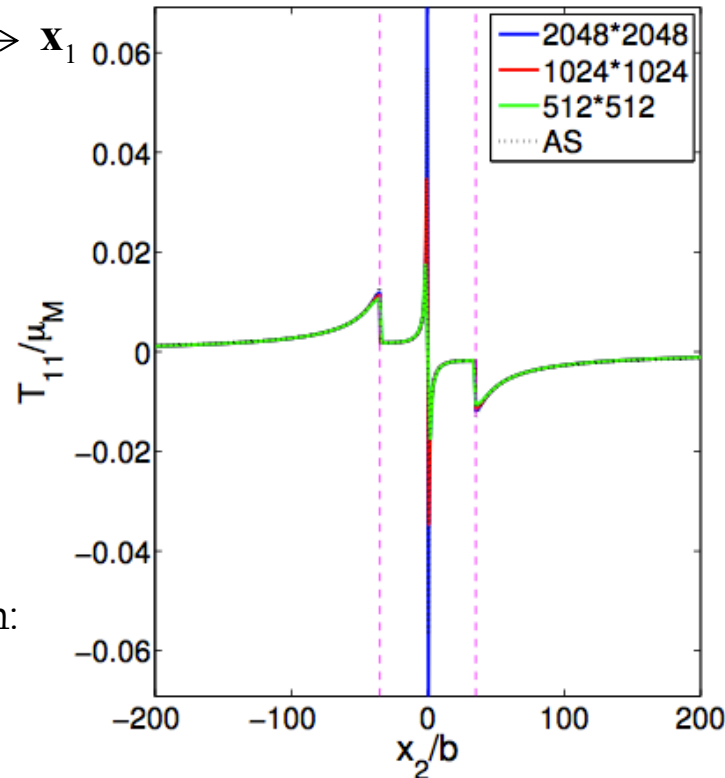
Fiber radius:

$$R = 36b$$

$$b = 4.05 \times 10^{-4} \mu\text{m}$$

Convergence criterion:

$$\varepsilon = 10^{-6}$$

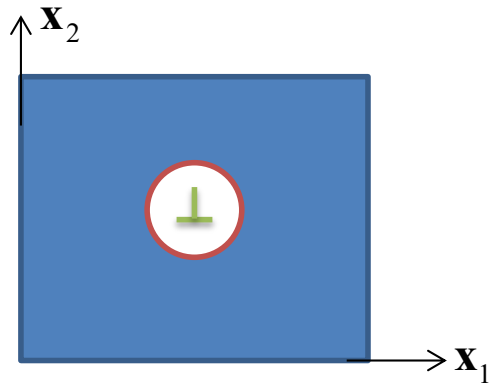


## ▪ Analytical solutions

*Dundurs et Sendeckyj (JMPS 1965)*

# Validations: comparisons with analytical solution

## Case 1 $\mu_I/\mu_M = 0.01$



No imposed loading

### Simulation data

Dislocation density:  $\alpha_{13}(\mathbf{x}) = b / \delta^2$

Burgers vector magnitude:  $b = 4.05 \times 10^{-4} \mu\text{m}$

Unit cell size:  $2048 \times 2048$  pixels

Pixel size:  $\delta_1 = \delta_2 = \delta \approx 0.44b$

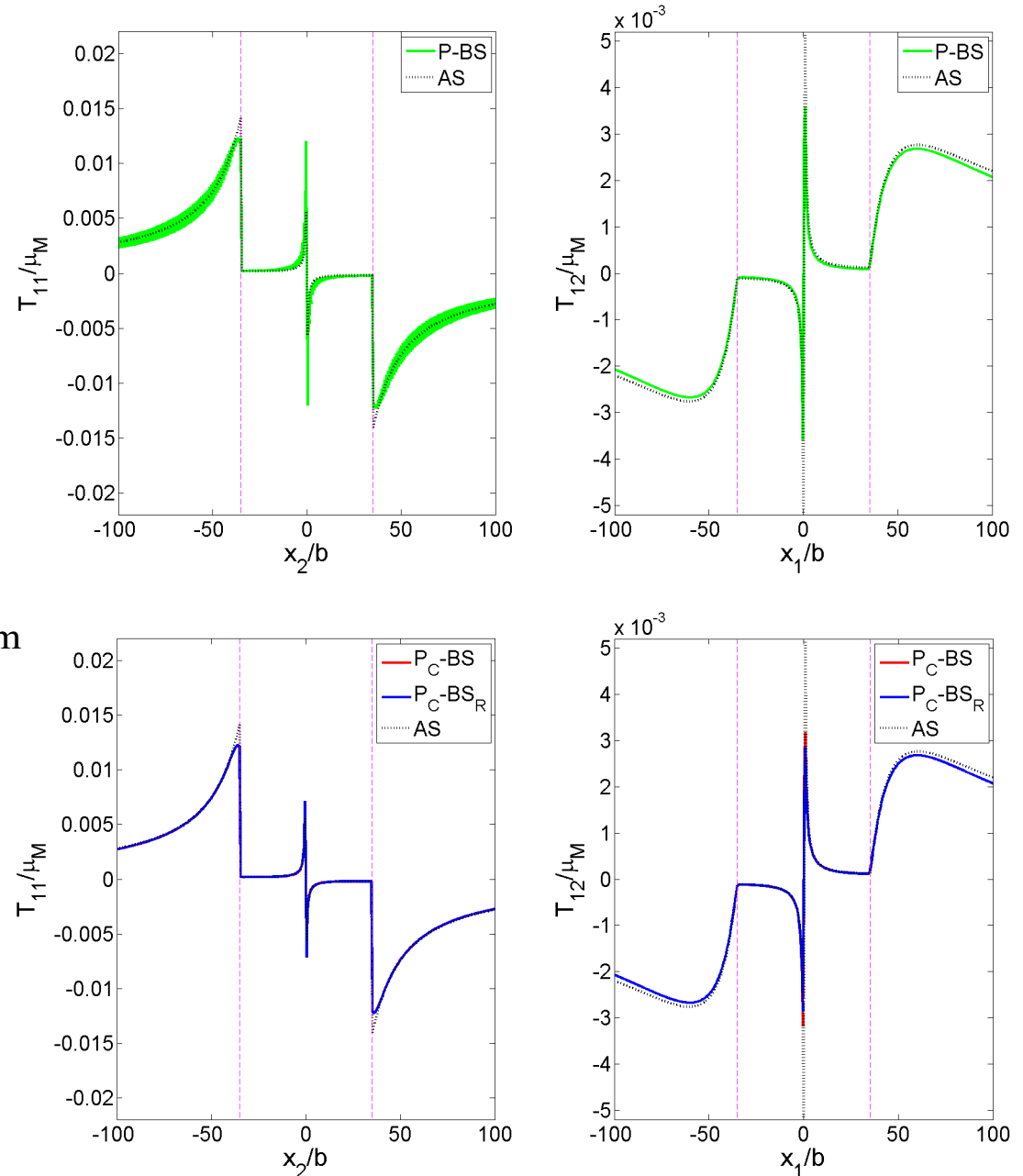
Fiber radius:  $R = 80\delta$

Elasticity:  $\begin{cases} \mu_I = 2.3001 \times 10^3 \text{ MPa} \\ \nu_I = \nu_M = 0.3647 \end{cases}$

Convergence criterion:  $\varepsilon = 10^{-6}$

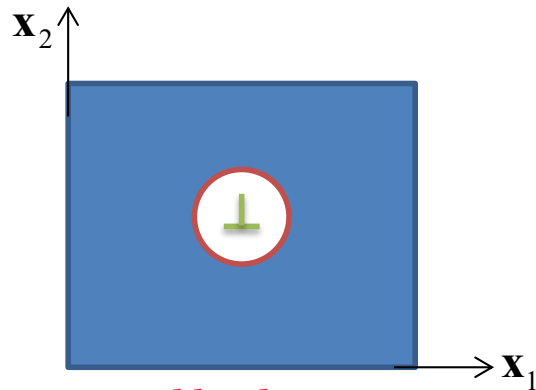
### Analytical solutions

Dundurs et Sendeckyj (JMPS, 1965)



# Validations: Comparisons with analytical solution

## Case 1 $\mu_I/\mu_M = 10$



No imposed loading

### Simulation data

Dislocation density:  $\alpha_{13}(\mathbf{x}) = b / \delta^2$

Burgers vector :  $b = 4.05 \times 10^{-4} \mu\text{m}$

Unit cell size:  $2048 \times 2048$  pixels

Pixel size:  $\delta_1 = \delta_2 = \delta \approx 0.44b$

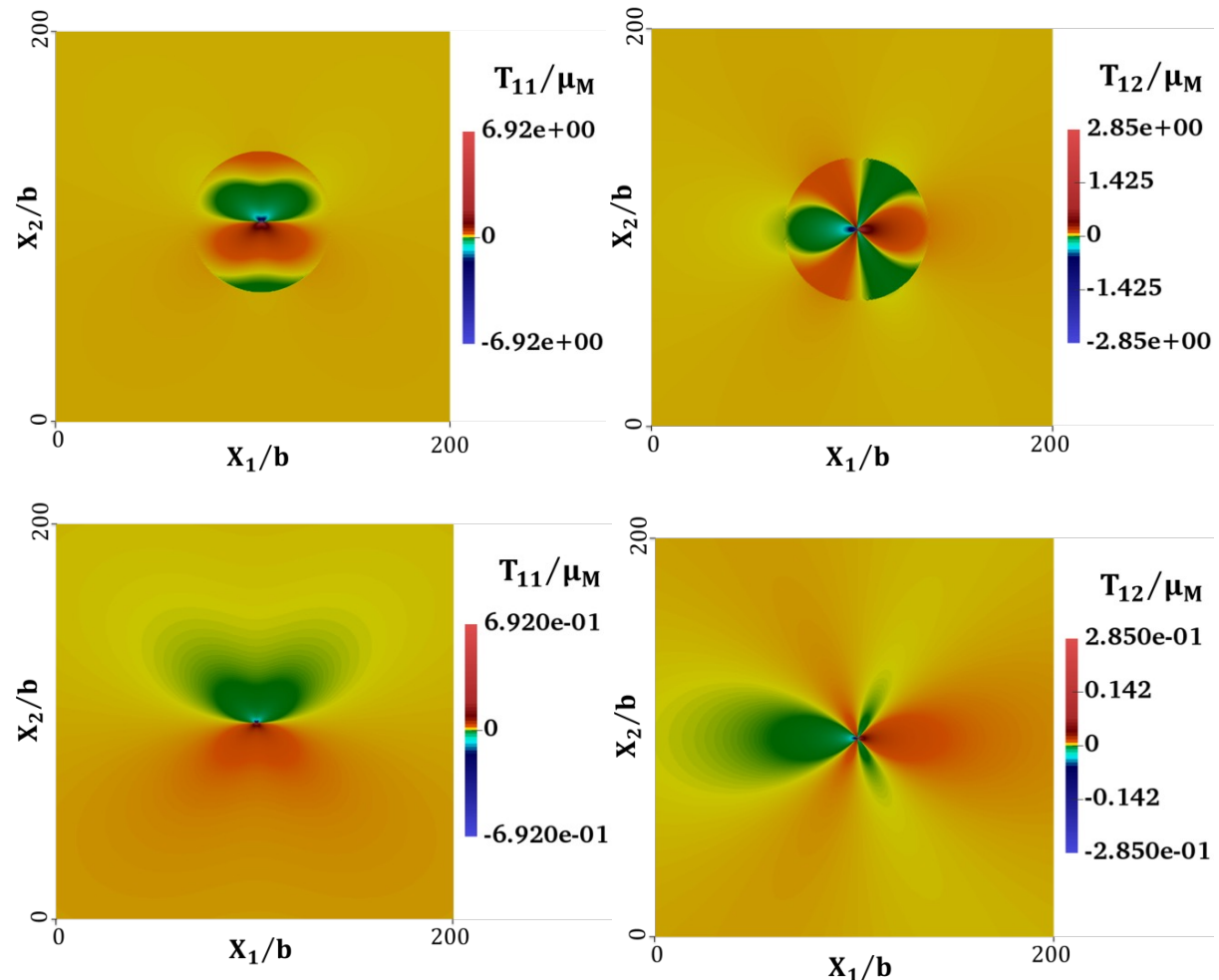
Fiber radius:  $R = 80\delta$

Elasticity:  $\begin{cases} \mu_I = 2.3001 \times 10^3 \text{ MPa} \\ \nu_I = \nu_M = 0.3647 \end{cases}$

Convergence criterion:  $\varepsilon = 10^{-6}$

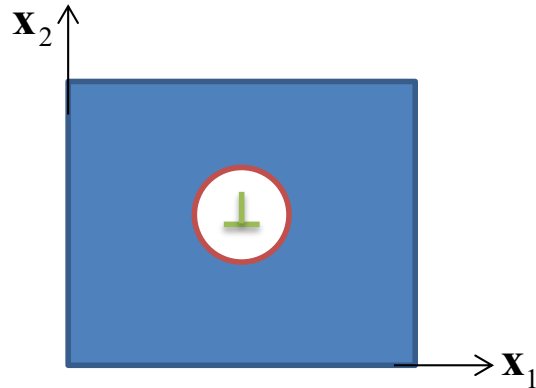
### Analytical solutions

*Dundurs et Sendeckyj (JMPS, 1965)*



# Validations: comparisons with analytical solution

## Case 1 $\mu_I/\mu_M = 10$



No imposed loading

### Simulation data

Dislocation density:  $\alpha_{13}(\mathbf{x}) = b / \delta^2$

Burgers vector:  $b = 4.05 \times 10^{-4} \mu\text{m}$

Unit cell size:  $2048 \times 2048$  pixels

Pixel size:  $\delta_1 = \delta_2 = \delta \simeq 0.44b$

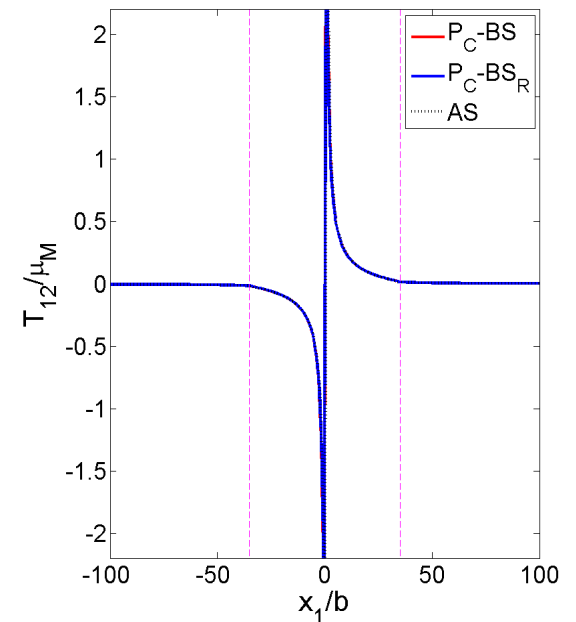
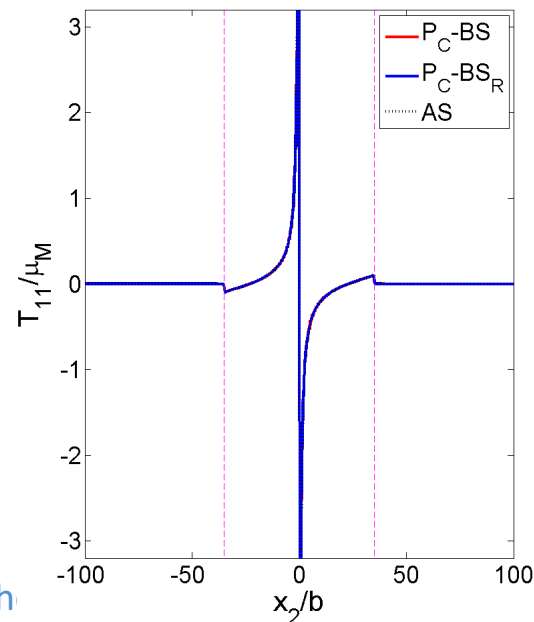
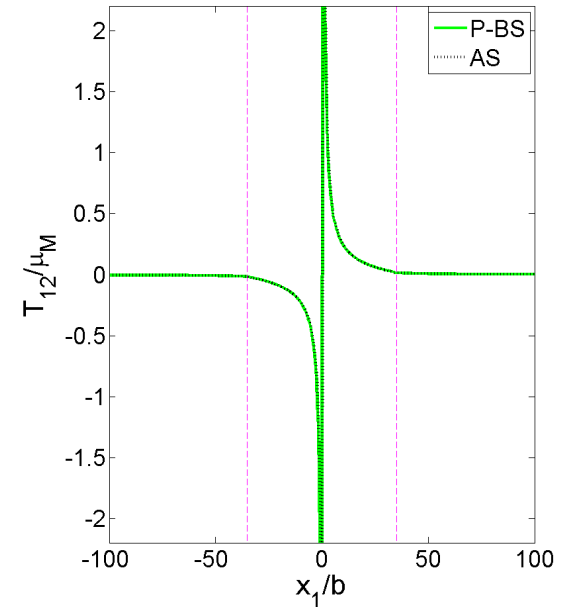
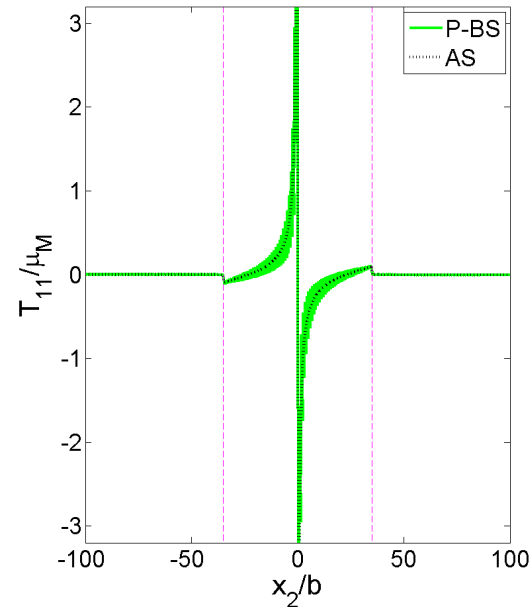
Fiber radius:  $R = 80\delta$

Elasticity:  $\begin{cases} \mu_I = 2.3001 \times 10^3 \text{ MPa} \\ \nu_I = \nu_M = 0.3647 \end{cases}$

Convergence criterion:  $\varepsilon = 10^{-6}$

### Analytical solutions

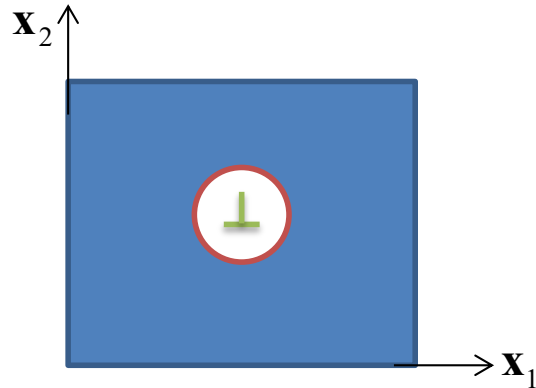
*Dundurs et Sendeckyj (JMPS 1965)*



# Validations: comparisons with analytical solution

## Case 1

$$\mu_I/\mu_M = 100$$



No imposed loading

### Simulation data

Dislocation density:  $\alpha_{13}(\mathbf{x}) = b / \delta^2$

Burgers vector magnitude:  $b = 4.05 \times 10^{-4} \mu\text{m}$

Unit cell size:  $2048 \times 2048$  pixels

Pixel size:  $\delta_1 = \delta_2 = \delta \approx 0.44b$

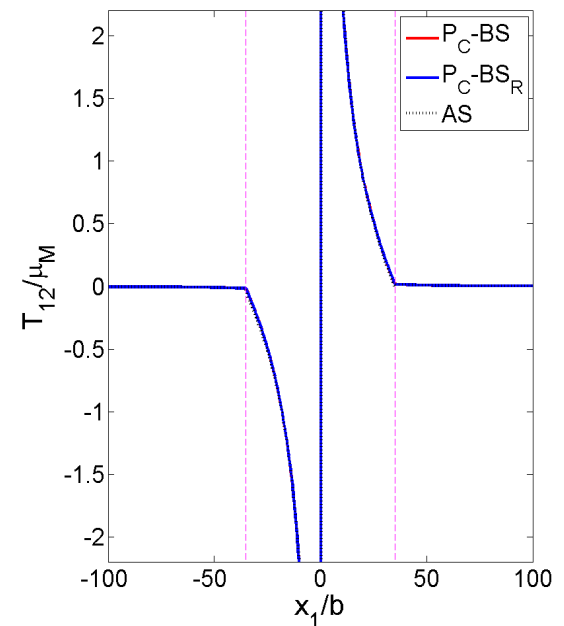
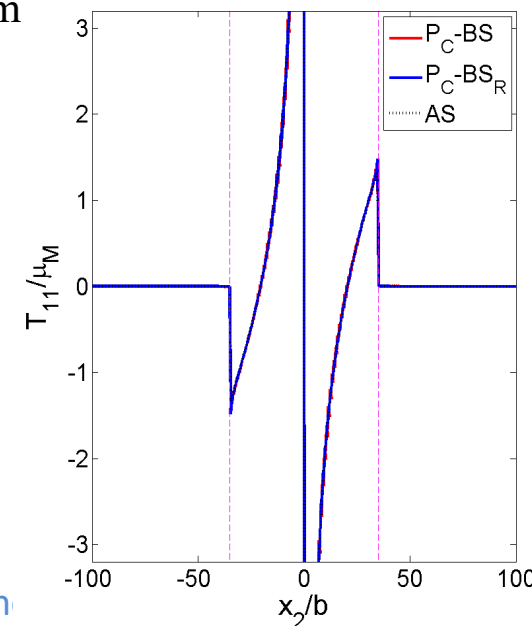
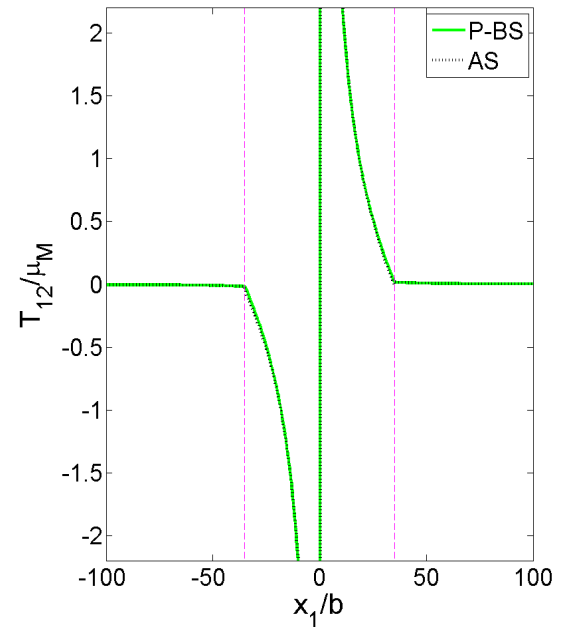
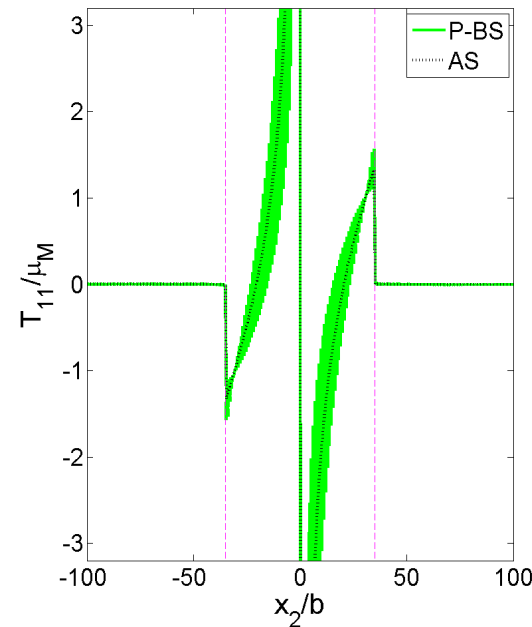
Fiber radius:  $R = 80\delta$

Elasticity:  $\begin{cases} \mu_I = 2.3001 \times 10^3 \text{ MPa} \\ \nu_I = \nu_M = 0.3647 \end{cases}$

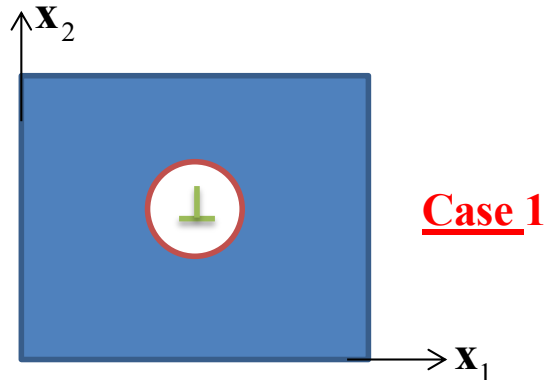
Convergence criterion:  $\varepsilon = 10^{-6}$

### Analytical solutions

*Dundurs et Sendeckyj (JMPS, 1965)*



# Validations: comparisons with analytical solution



**P-BS** : Strong Gibbs oscillations  
(unaccurate...)

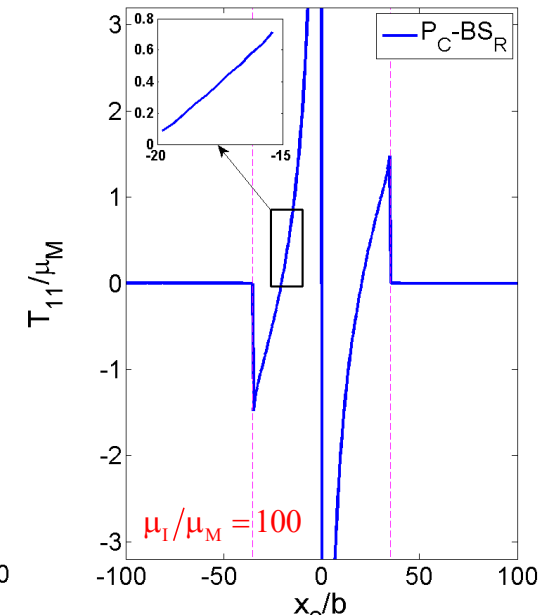
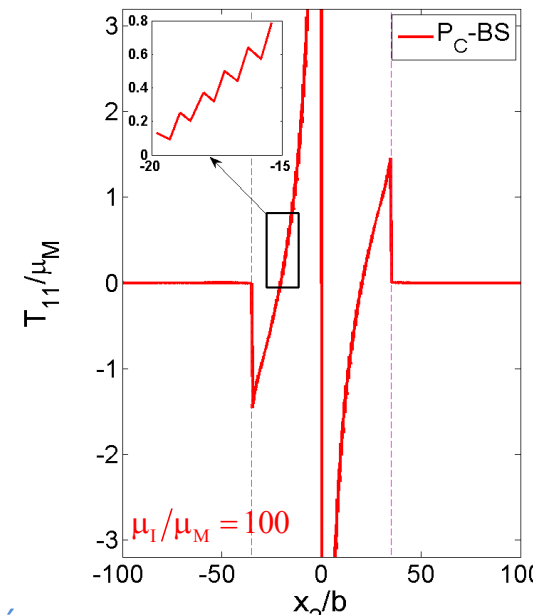
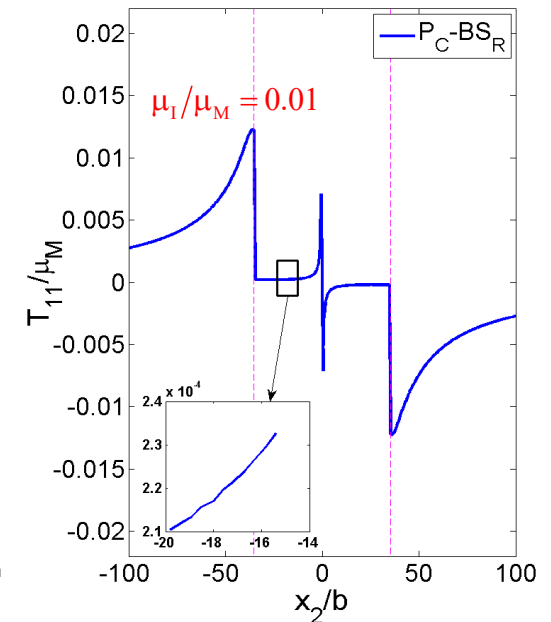
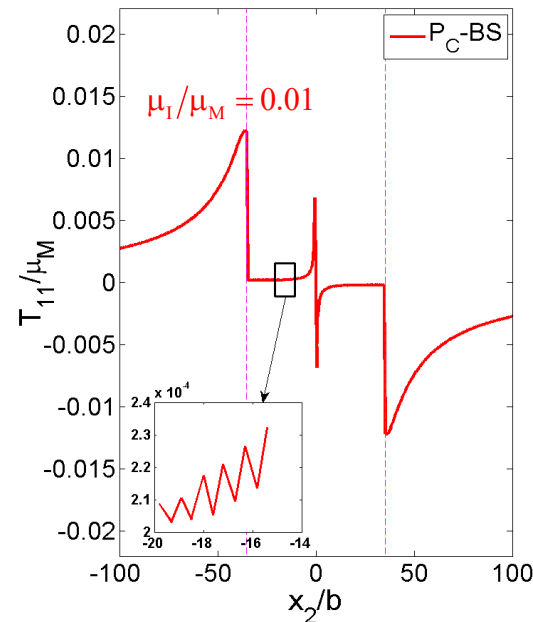
**P<sub>C</sub>-BS** : Stable solution (accurate, very  
litle oscillations)

**P<sub>C</sub>-BS<sub>R</sub>** : Stable solution (very  
accurate)

$\varepsilon = 10^{-6}$

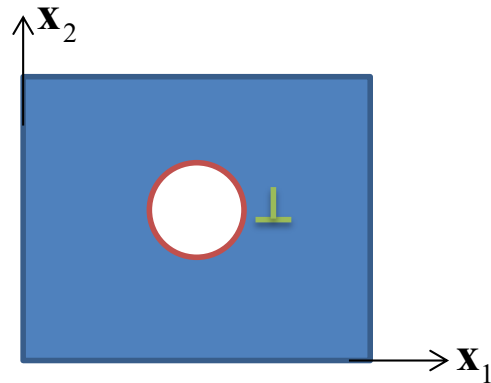
| Mechanical contrast | $10^{-2}$ | $10^{-1}$ | 1 | $10^1$ | $10^2$ |
|---------------------|-----------|-----------|---|--------|--------|
| Iterations          | 465       | 155       | 1 | 242    | 903    |

2048×2048



# Validations: Comparisons with analytical solution

## Case 2 : edge dislocation interaction with circular hole



No imposed loading

### Simulation data

Dislocation density:  $\alpha_{13}(\mathbf{x}) = b / \delta^2$

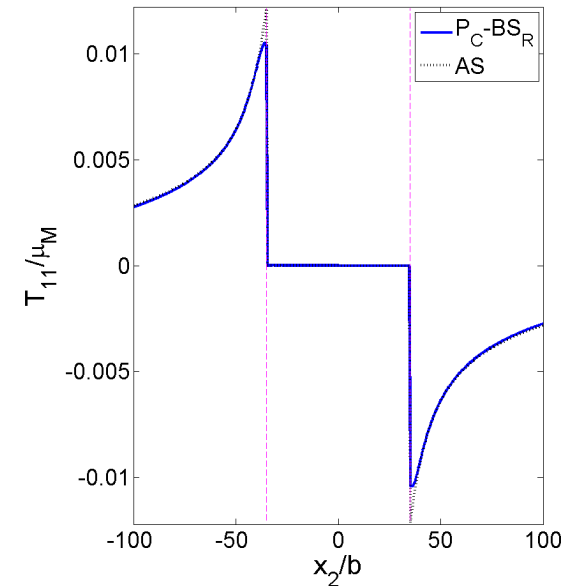
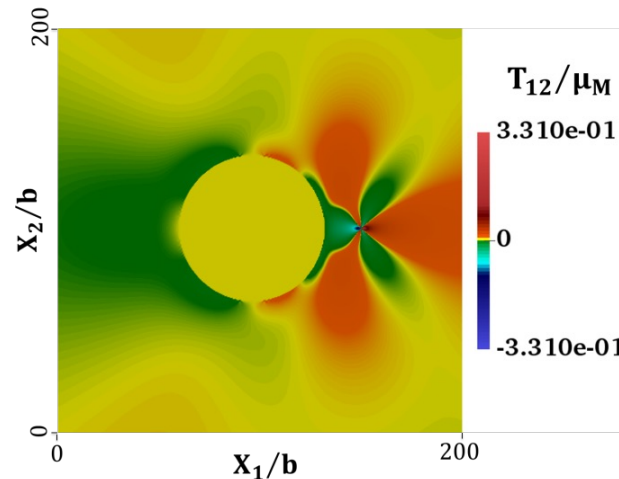
Burgers vector magnitude:  $b = 4.05 \times 10^{-4} \mu\text{m}$

Unit cell size:  $2048 \times 2048$  pixels

Pixel size:  $\delta_1 = \delta_2 = \delta \simeq 0.44b$

Fiber radius:  $R = 80\delta$

Elasticity:  $\begin{cases} \mu_1 = 2.3001 \times 10^3 \text{ MPa} \\ \nu_1 = \nu_M = 0.3647 \end{cases}$



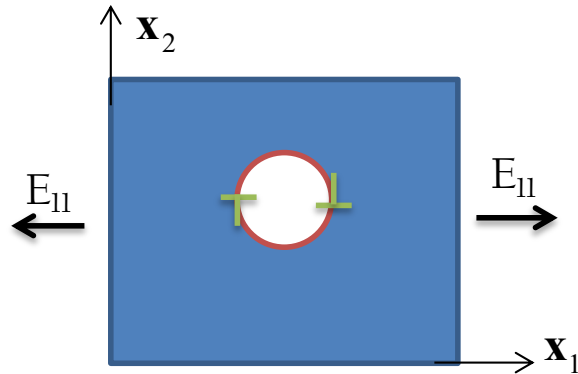
|                     |                   |
|---------------------|-------------------|
| Mechanical contrast | $10^{-10}$ (hole) |
| Iteration number    | 102               |

Stress equilibrium convergence criterion:  $\varepsilon = 10^{-6}$

Analytical solutions: Lubarda, Asaro (Mech. Solids Mater, Cambridge 2006), Dundurs and Mura (JMPS 1964)

# Edge dislocation dipoles constrained at the fiber/matrix interface in a composite under tensile loading

**Case 3**  $\mu_I/\mu_M = 0.1$



Imposed tensile loading:  $E_{11} = 1\%$

## Simulation data

Dislocation density:  $\alpha_{13}(\mathbf{x}) = b / \delta^2$

Burgers vector magnitude:  $b = 4.05 \times 10^{-4} \mu\text{m}$

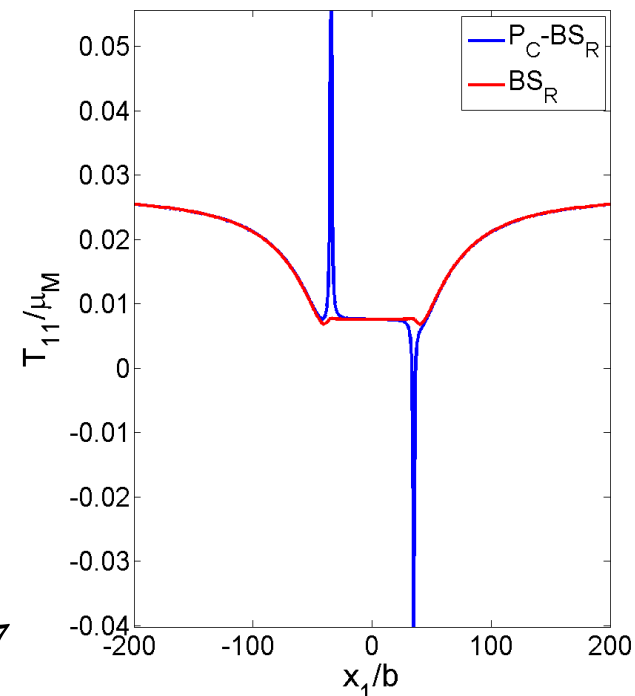
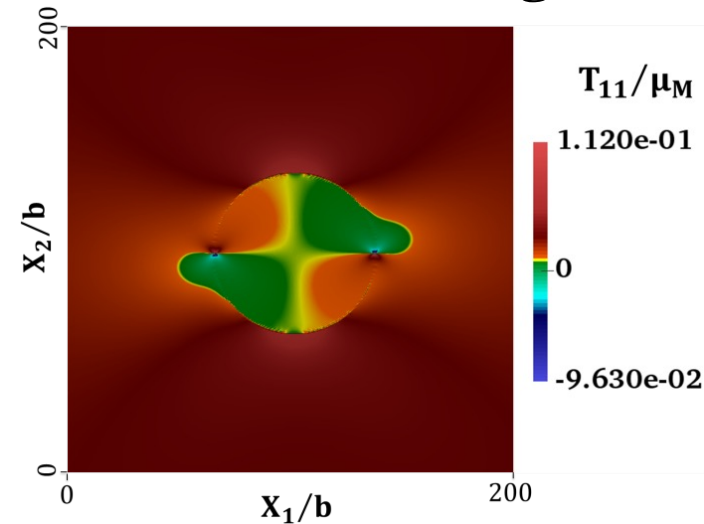
Unit cell size:  $2048 \times 2048$  pixels

Pixel size:  $\delta_1 = \delta_2 = \delta \approx 0.44b$

Fiber radius:  $R = 80\delta$

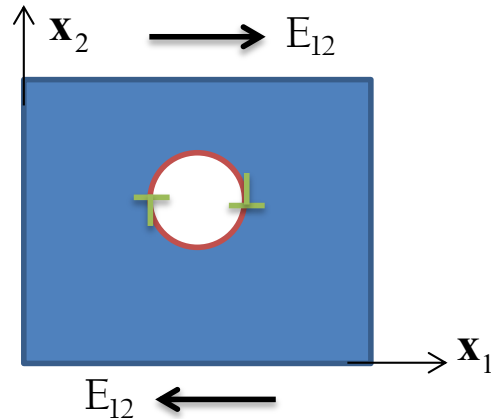
Elasticity:  $\begin{cases} \mu_I = 2.3001 \times 10^3 \text{ MPa} \\ \nu_I = \nu_M = 0.3647 \end{cases}$

Convergence criterion:  $\varepsilon = 10^{-8}$  Iterations: 77



# Edge dislocation dipoles constrained at the fiber/matrix interface in a composite under shear loading

**Case 3**  $\mu_I/\mu_M = 0.1$



Imposed shear loading:  $E_{12} = 1\%$

## Simulation data

Dislocation density:  $\alpha_{13}(\mathbf{x}) = b / \delta^2$

Burgers vector magnitude:  $b = 4.05 \times 10^{-4} \mu\text{m}$

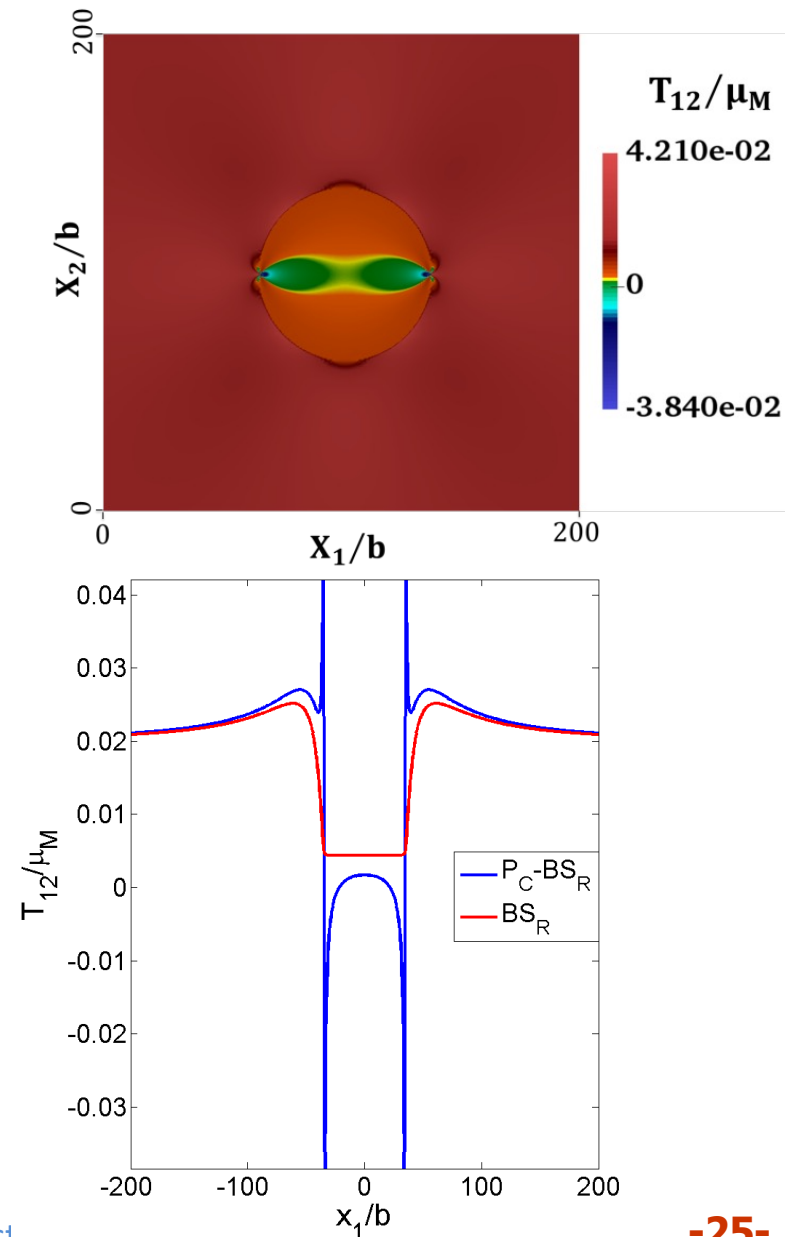
Unit cell size:  $2048 \times 2048$  pixels

Pixel size:  $\delta_1 = \delta_2 = \delta \approx 0.44b$

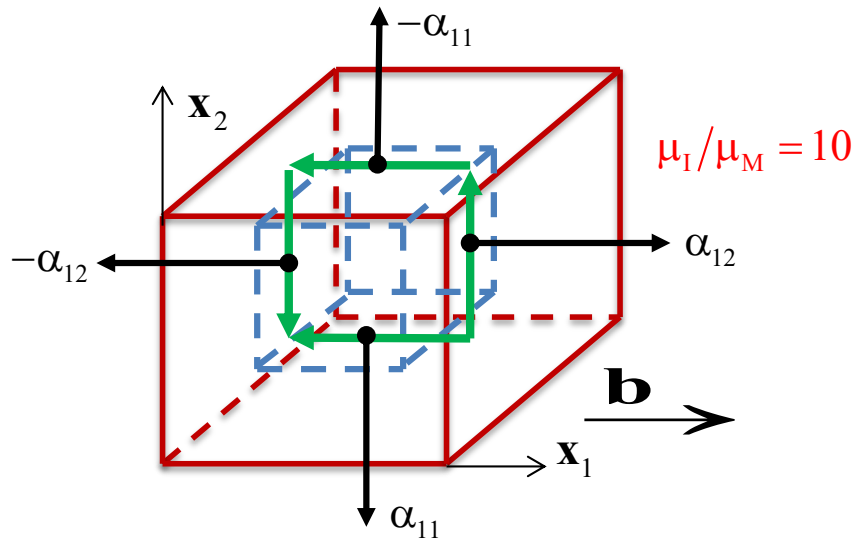
Fiber radius:  $R = 80\delta$

Elasticity:  $\begin{cases} \mu_I = 2.3001 \times 10^3 \text{ MPa} \\ \nu_I = \nu_M = 0.3647 \end{cases}$

Convergence criterion:  $\epsilon = 10^{-8}$  Iterations: 36



# Application to a cubic inhomogeneity encircled by a square dislocation loop



No imposed loading

Dislocation density:  $\alpha_{11}(\mathbf{x}) = b / \delta^2$   
 $\alpha_{12}(\mathbf{x}) = b / \delta^2$

Burgers vector:  $b = 4.05 \times 10^{-4} \mu\text{m}$

Unit cell:  $128 \times 128 \times 128$  voxels

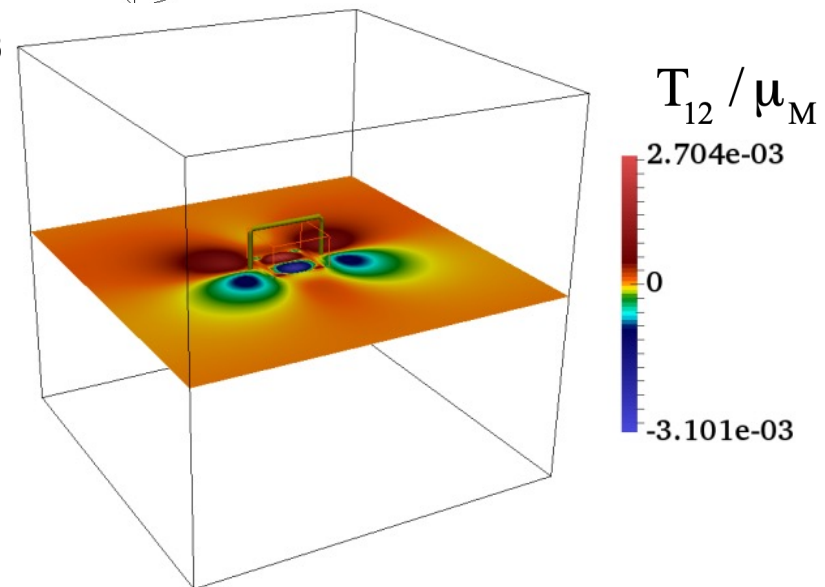
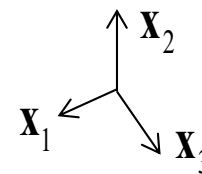
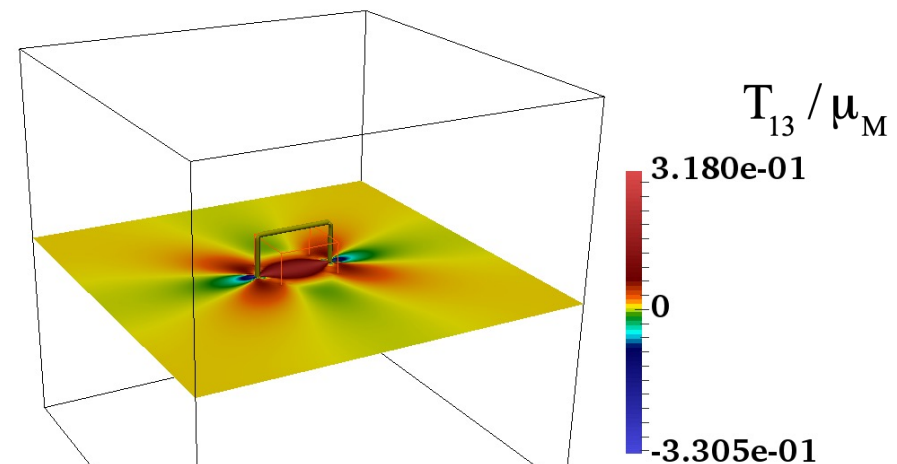
Pixel size:  $\delta_1 = \delta_2 = \delta \approx 0.44b$

Cubic inclusion size:  $c = 10\delta$

Convergence criterion:

$$\varepsilon = 10^{-6}$$

Elasticity:  $\begin{cases} \mu_I = 2.3001 \times 10^3 \text{ MPa} \\ \nu_I = \nu_M = 0.3647 \end{cases}$



Single core, 3.5Ghz i7, 8Go

Iterations: 52

# Elastic fields of climb dislocation loops distributions in periodic composites with cubic-shaped inclusions

## Parameters:

Elastic constants:

$$\begin{cases} \mu_M = 124.2 \times 10^3 \text{ MPa} \\ \nu_M = \nu_I = 0.3 \end{cases}$$

Burgers vector:

$$b = 4.05 \times 10^{-4} \mu\text{m}$$

Dislocation densities:

$$\alpha_{31} = \pm b / \delta^2 \quad \alpha_{32} = \pm b / \delta^2$$

Cubic inclusion size:

$$8 \pm 3 \cdot 10^{-9} \text{ m}$$

Mesh:

$128 \times 128 \times 128$  voxels

Voxel size:

$$\delta \approx 10^{-9} \text{ m}$$

Reference medium:

$$\mu_0 = 0.505(\mu_M + \mu_I)$$

Convergence criterion:

$$\varepsilon = 10^{-6}$$

Imposed overall stress:  $\bar{T}_{33} = 1 \text{ MPa}$

