UNIVERSITEIT GENT

FACULTEIT INGENIEURSWETENSCHAPPEN

Electromagnetic Modeling of Photonic Metamaterials

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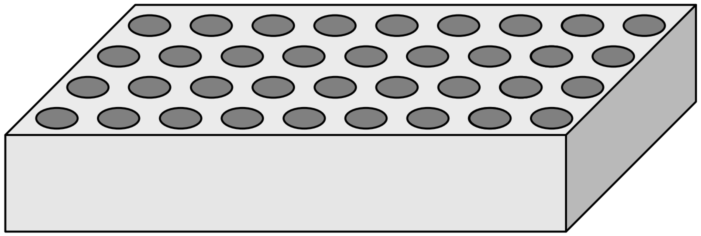
(Thanks to Davy Pissoort)

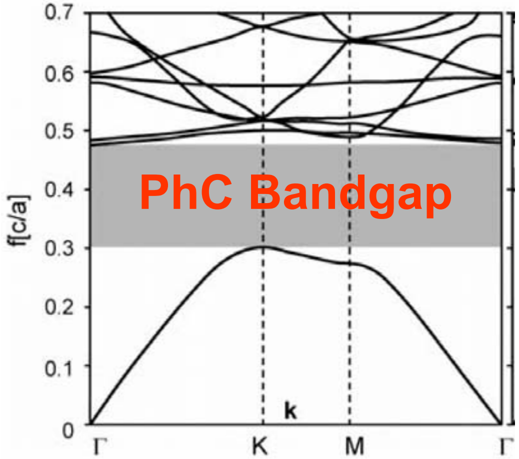
Outline

- **Introduction**
- **Field equivalence theorem**
- **Multiple scattering technique (MST)**
  - Free space Green function MST
  - PhC Green functions MST
- **Fast multipole method (MLFMA)**
- **Extensions**
- **Conclusions**

2D PhC Devices

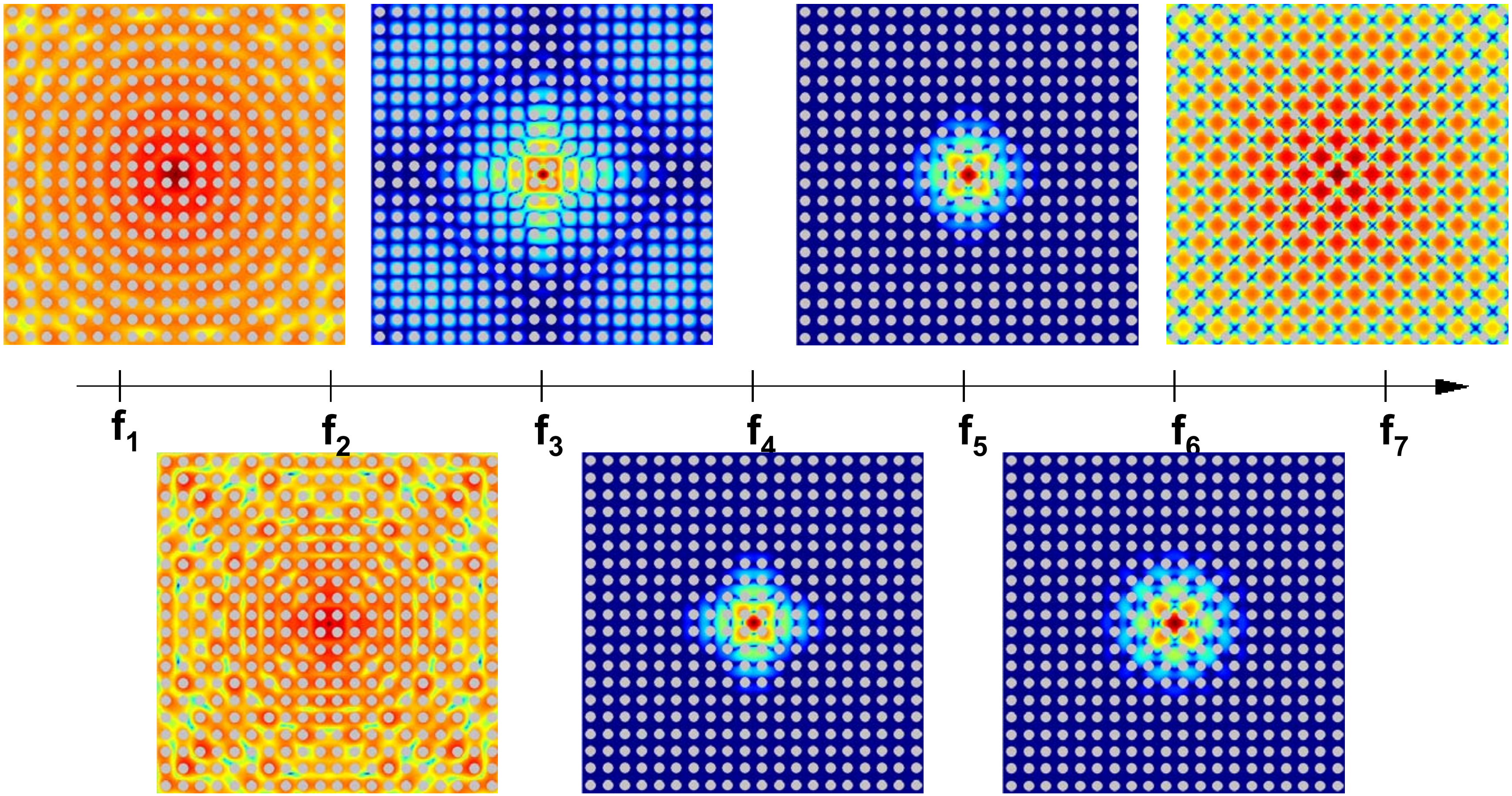
- **Set of parallel homogeneous dielectric cylinders residing on a periodic lattice in a homogeneous background medium**

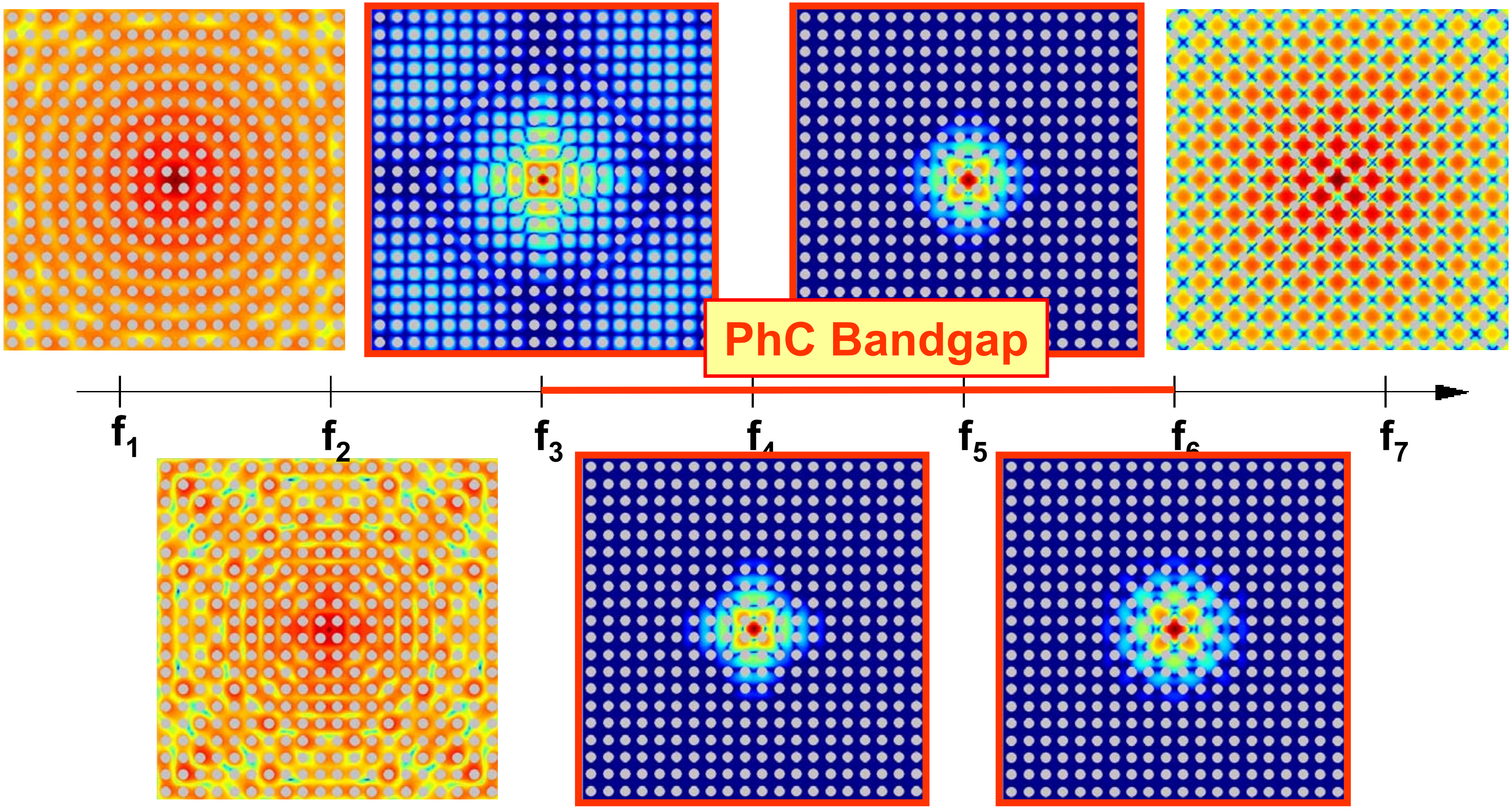




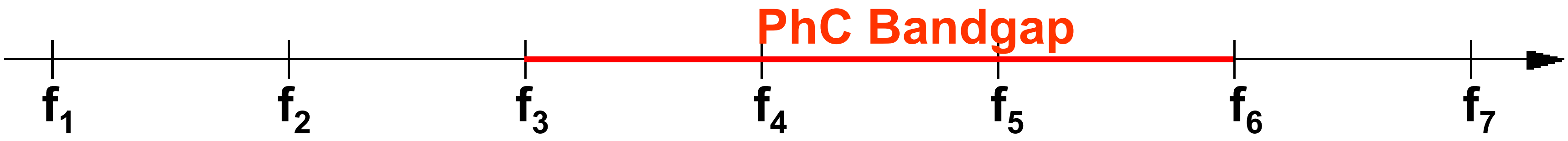
- **Periodicity → Photonic Band Gaps in which fields cannot propagate in given directions**
- **By removing/adding cylinders from/to otherwise perfect PhC, PhC devices capable of supporting localized modes result**
- **Creation of low-loss waveguides with sharp bends, multiplexers, filters, superprisms,…**

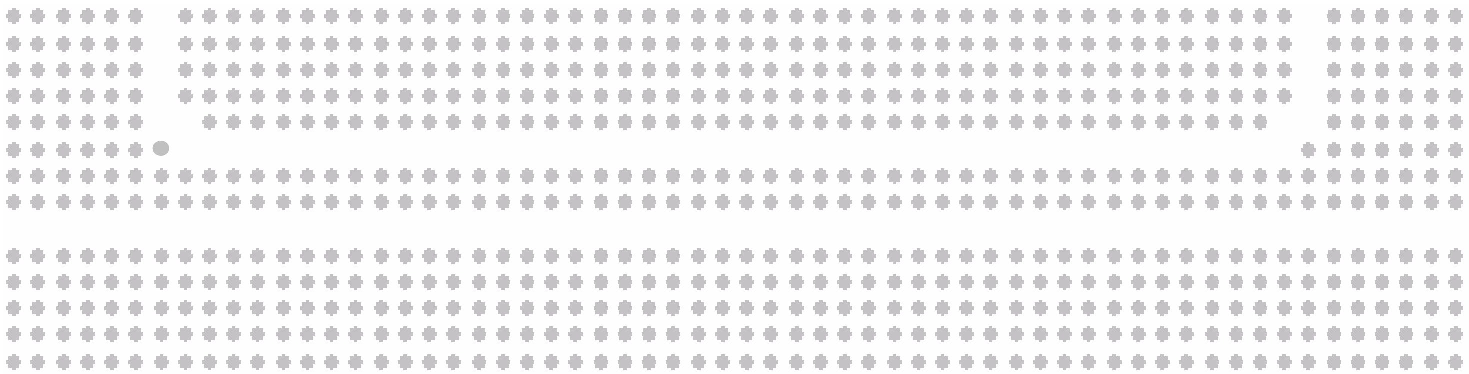
PhC Bandgap



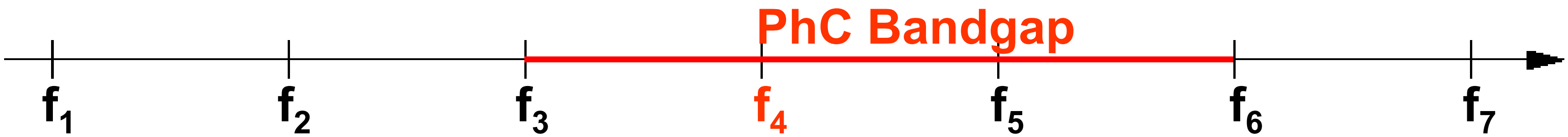

PhC Bandgap
f1
f2
f3
f4
f5
f6
f7

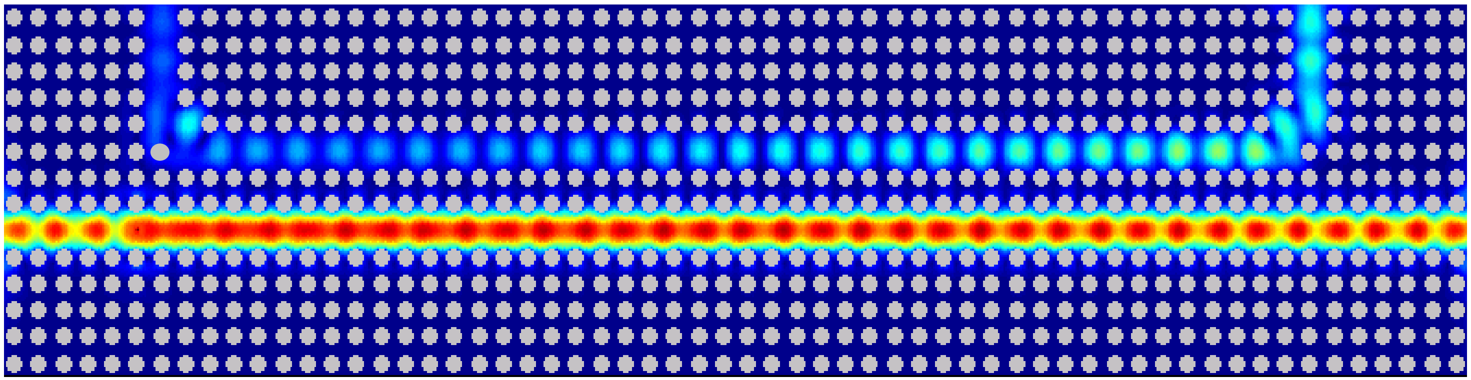
Multiplexer



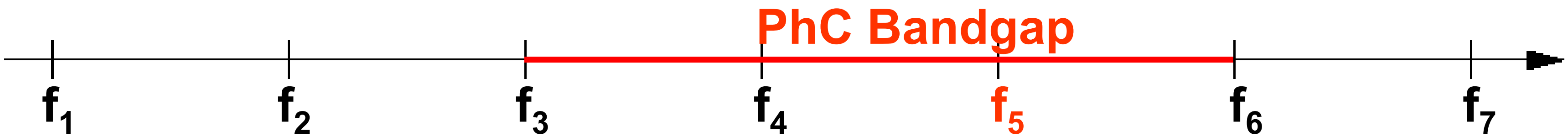


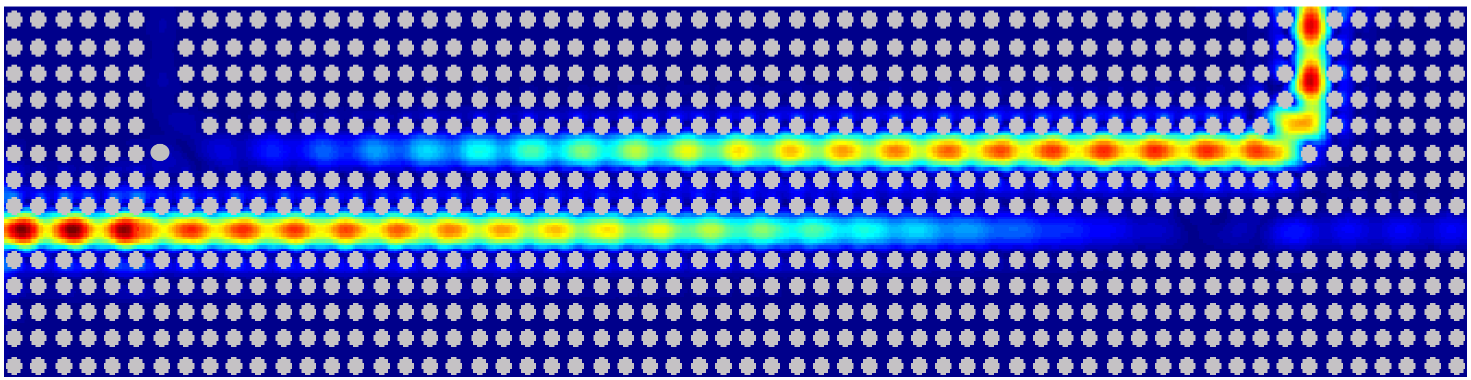
Multiplexer



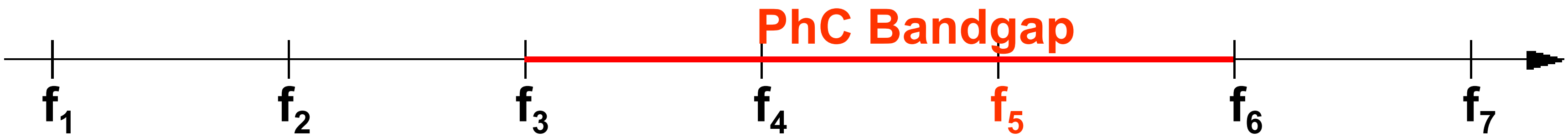


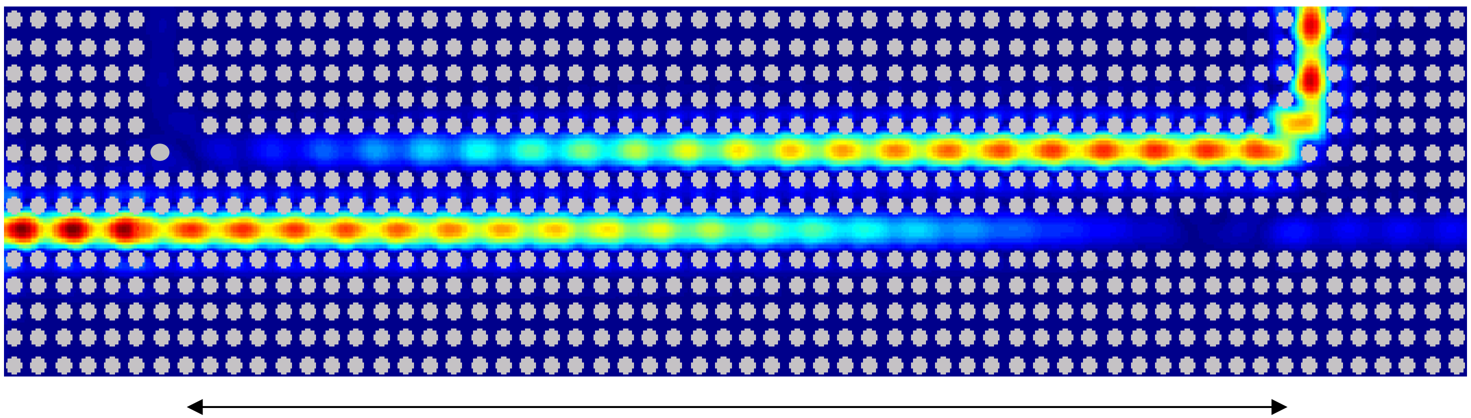
Multiplexer





Multiplexer





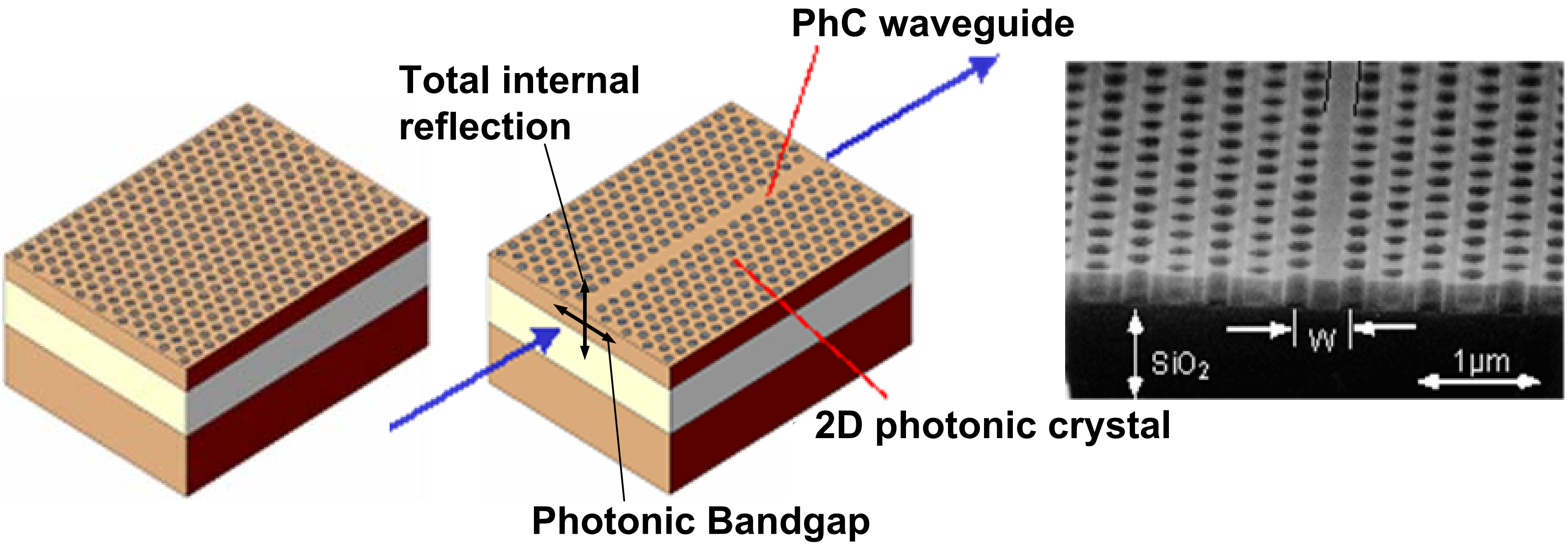
Length: 50 up to 3000 cylinders

Total: 1000 up to 40000 cylinders

⇒need for fast, efficient, and accurate modeling tools!

PhC Slab Devices

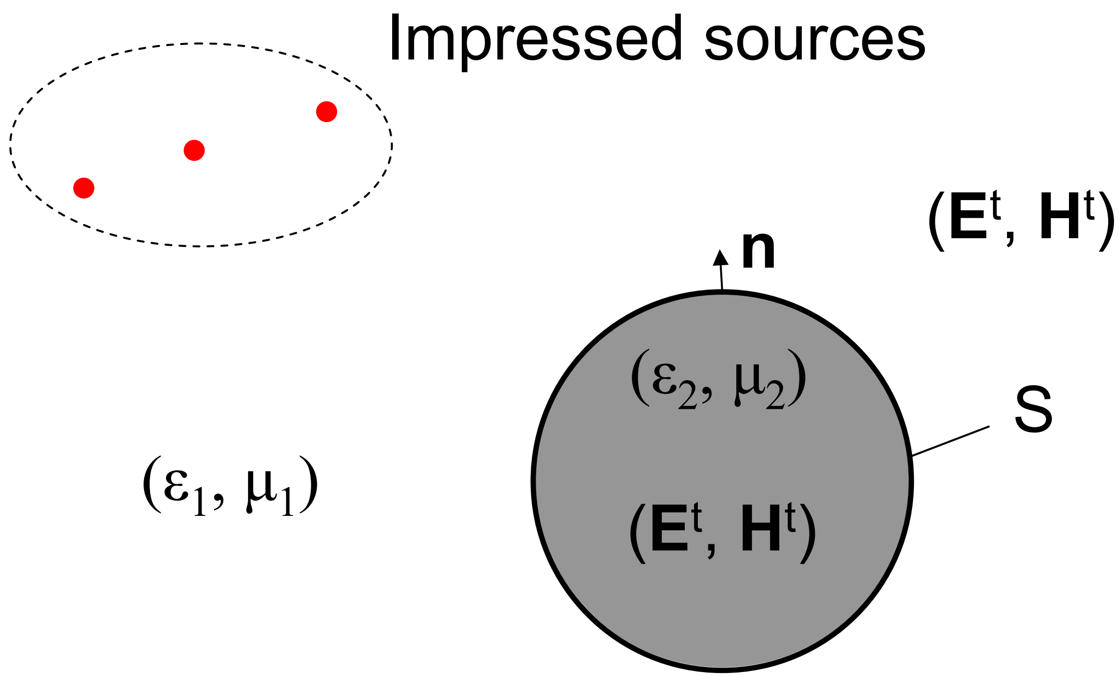
- Ideal 2D PhCs extend infinitelly in third direction, which cannot be realized in practice
- PhC Slabs: combination of a 2D PhC and a slab waveguide



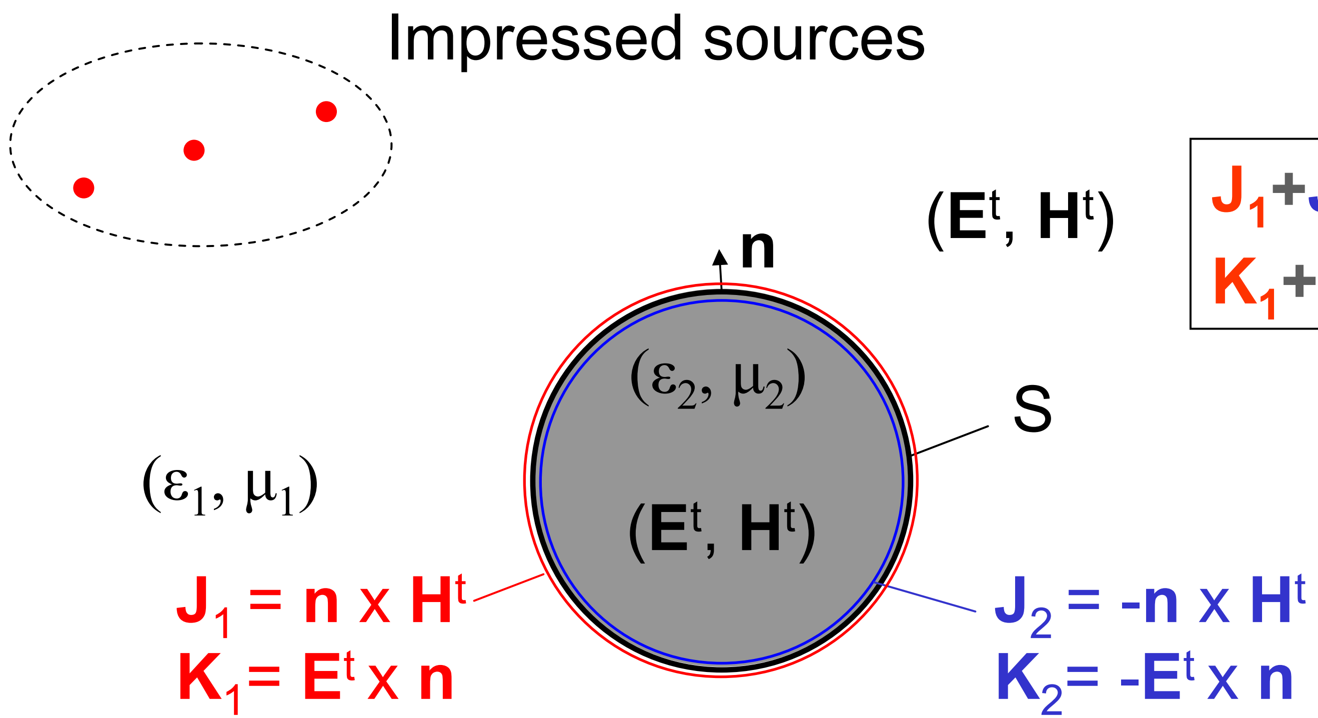
- Some layered media: 2D approximation is sufficient
- Other layered media: full 3D solution required!

Modeling Tools

- **FDTD:**
  - ☺ Wideband characterization via single simulation
  - ☹ Small spatial cells and time steps required
  - ☹ Phase dispersion
- **Eigenmode expansion**:
  - ☺ Attractive for regular structures
  - ☹ Unwieldy when many different sections and/or curved structures
- **Multiple Scattering Technique (MST):**
  - ☺ Exploits cylinders' circular nature (Bessel/Hankel functions): high accuracy with only a few unknowns per cylinder
  - ☹ Solution of dense linear system of equations



How to find $(\mathbf{E}^t, \mathbf{H}^t)$?

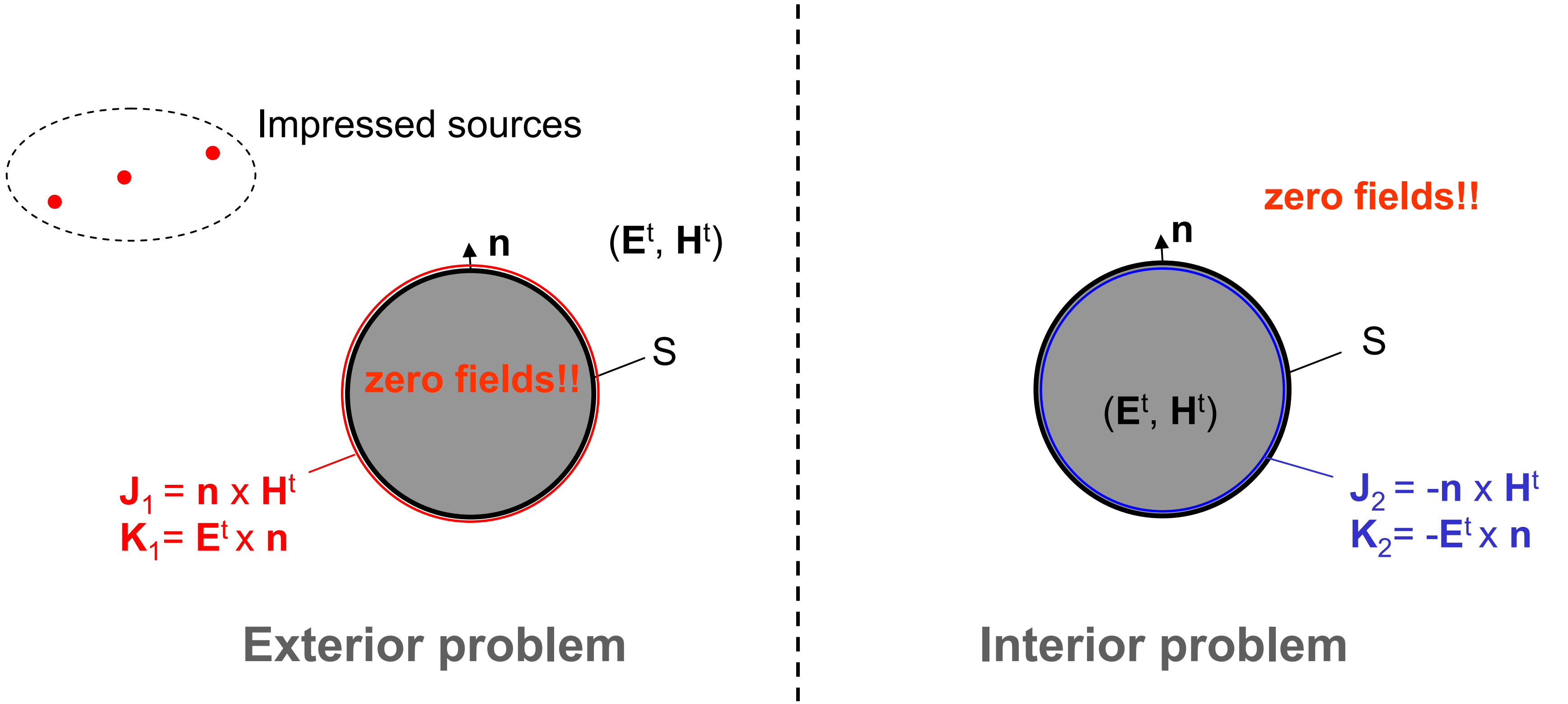


$J_1 + J_2 = 0$

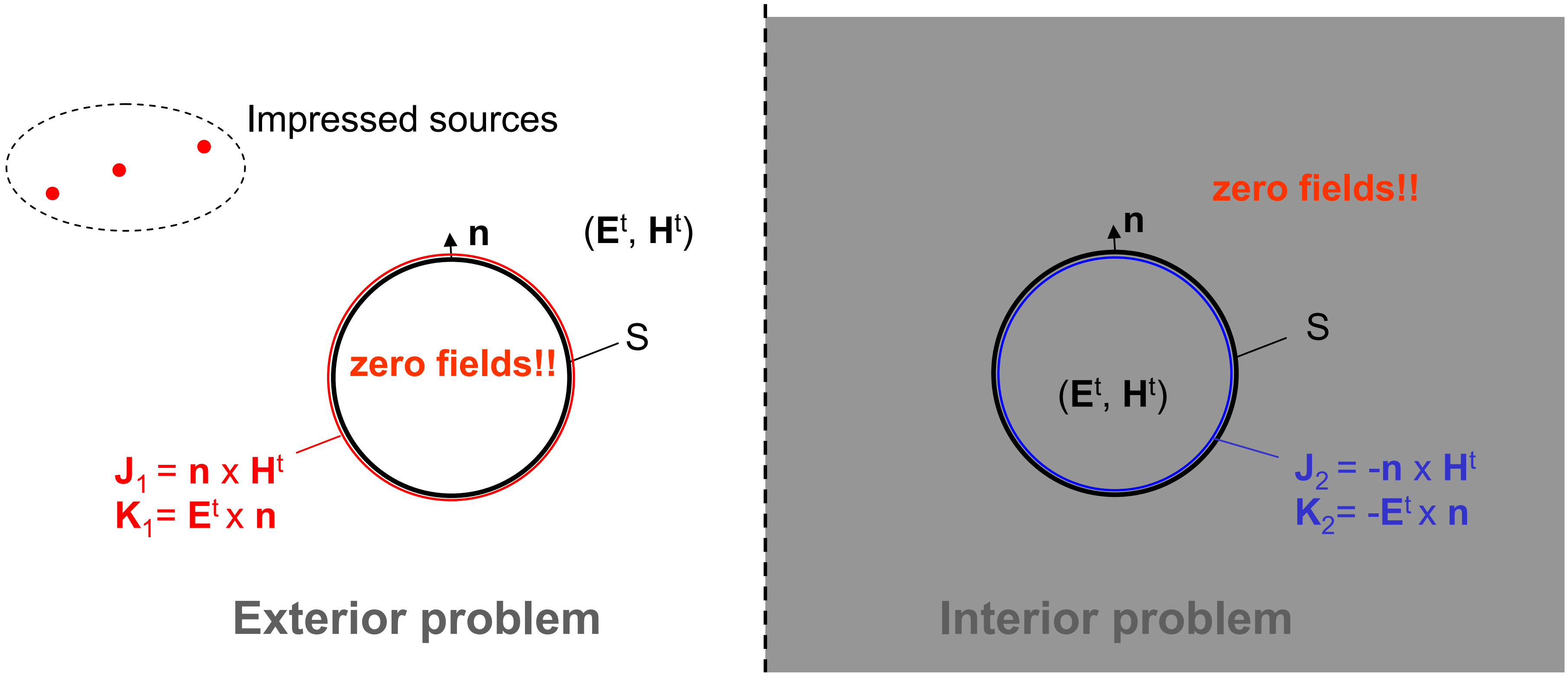
$K_1 + K_2 = 0$

Step 1: Introduce two sets of equivalent currents on S

Field Equivalence Theorem

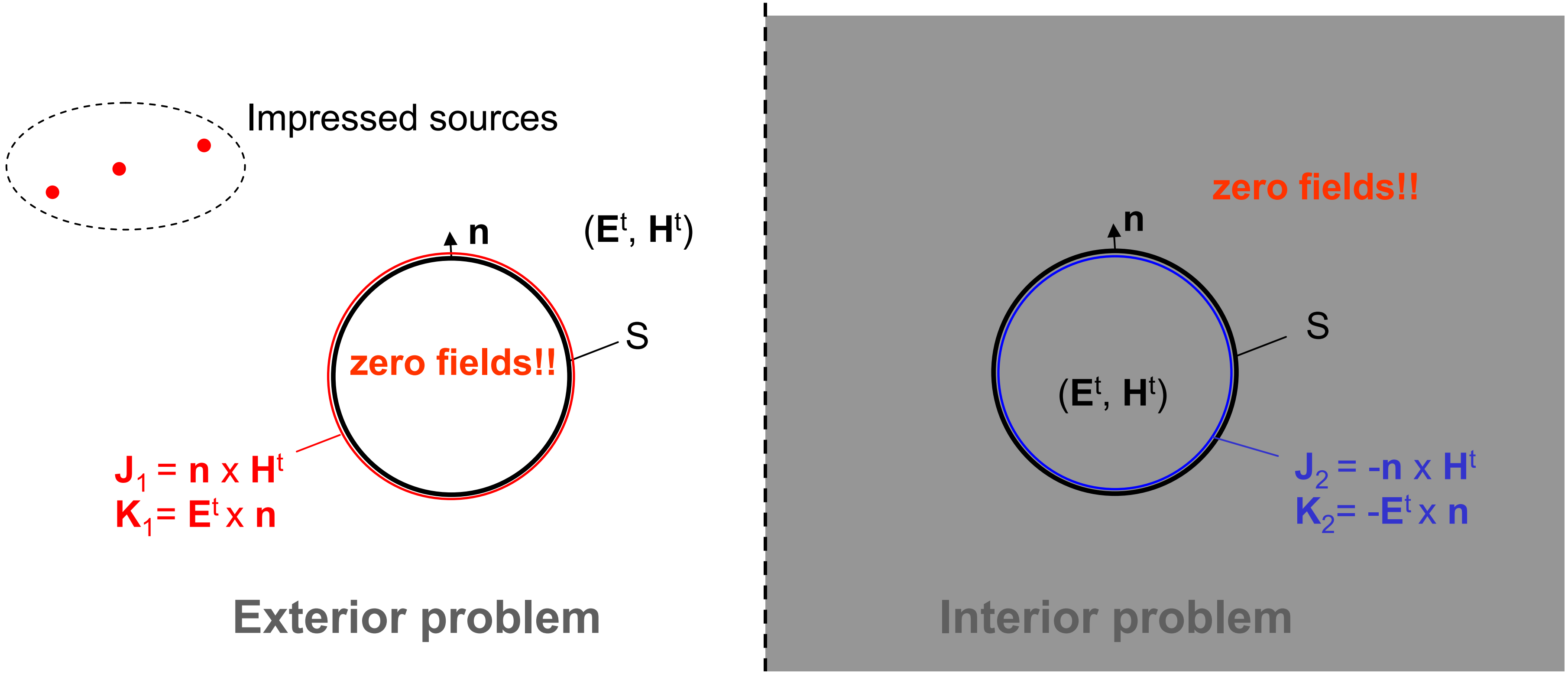


Observation: Original problem falls apart into an exterior and an interior problem



Step 2: Simplify exterior and interior problem

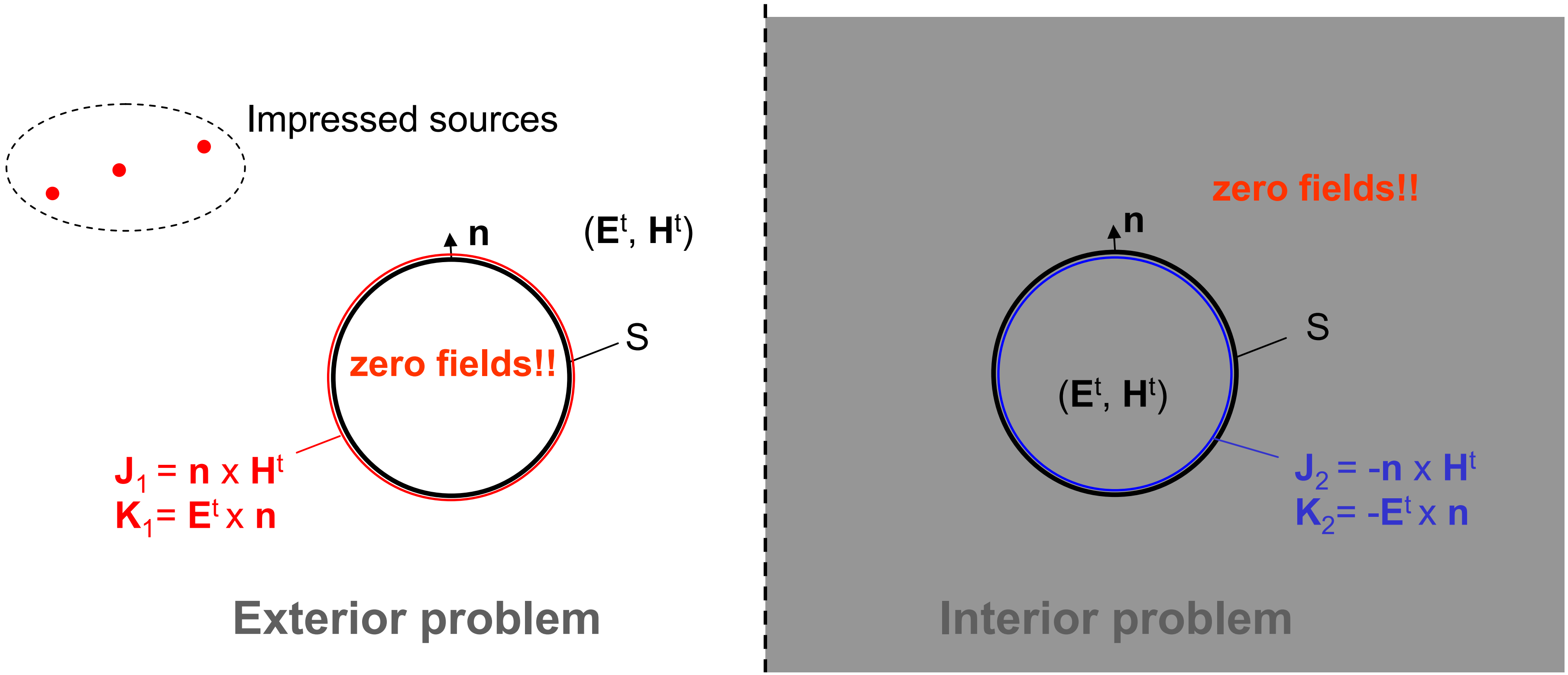
Field Equivalence Theorem



Step 3: Expand unknown currents

Step 4: Solve exterior and interior problem

Field Equivalence Theorem



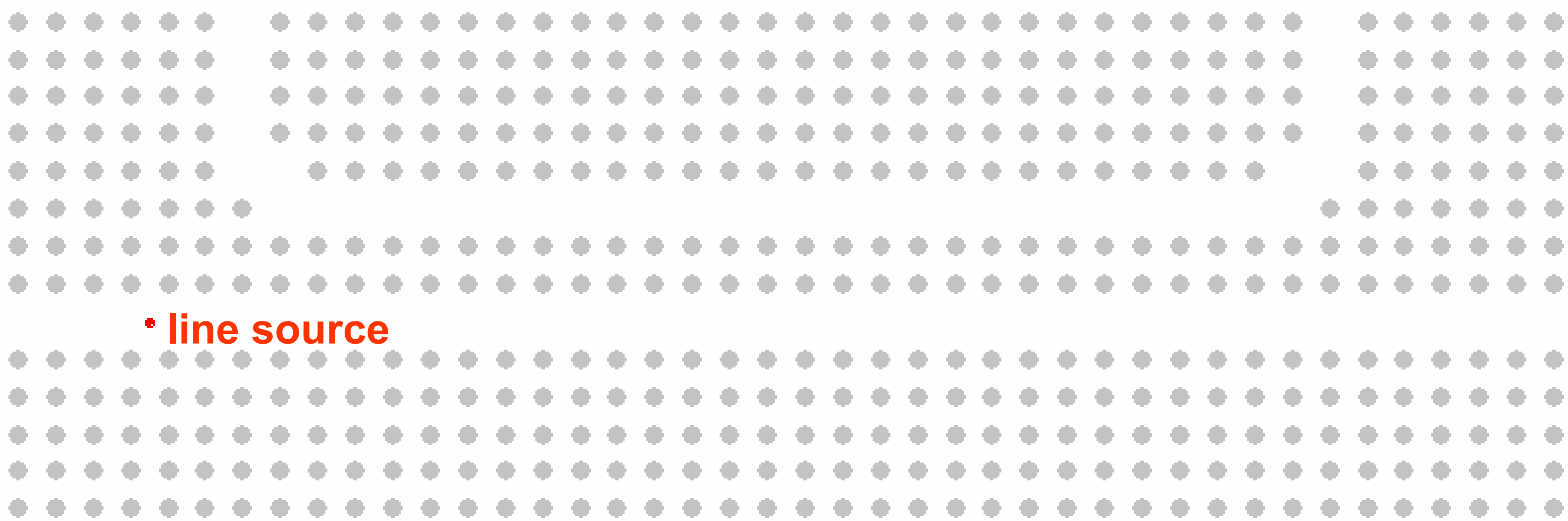
$$E^{inc}+E_1(J_1,K_1)=0 \text{ on } S^-$$

$$E_2(J_2,K_2)=0 \text{ on } S^+$$

Fields in medium (ε_1, μ_1)

Fields in medium (ε_2, μ_2)

Free Space GF MST

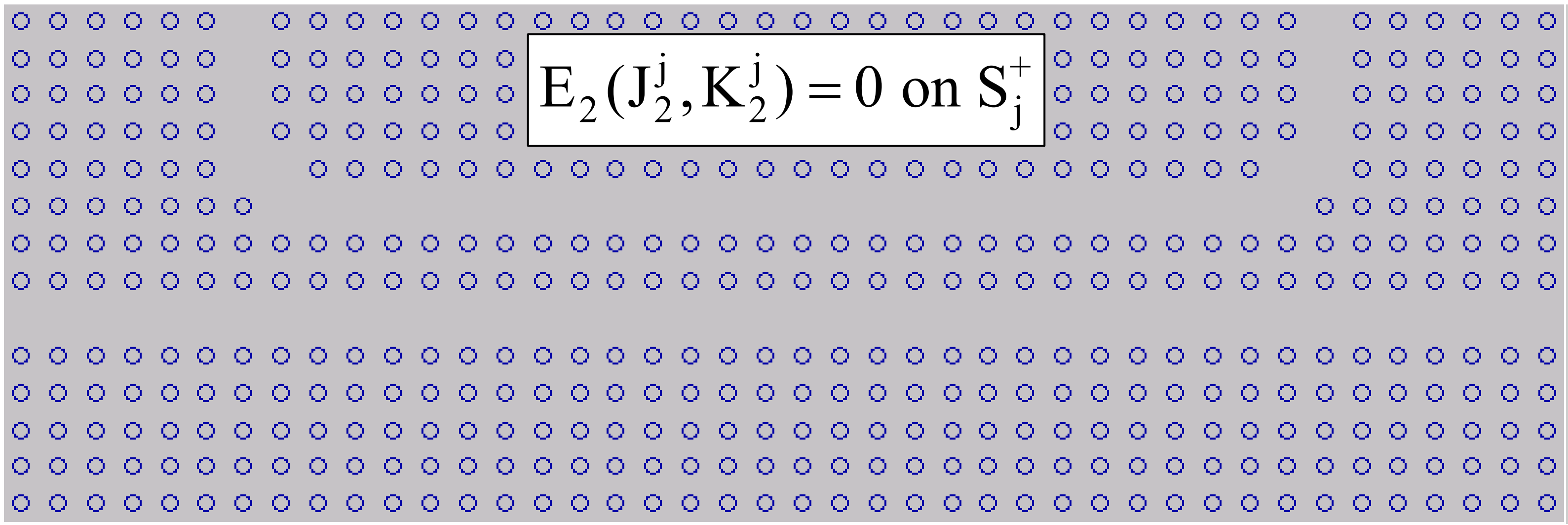


- N_c **cylinders placed in a homogeneous background medium**
- **TM-polarization: electric field is parallel to the cylinders**

Free Space GF MST

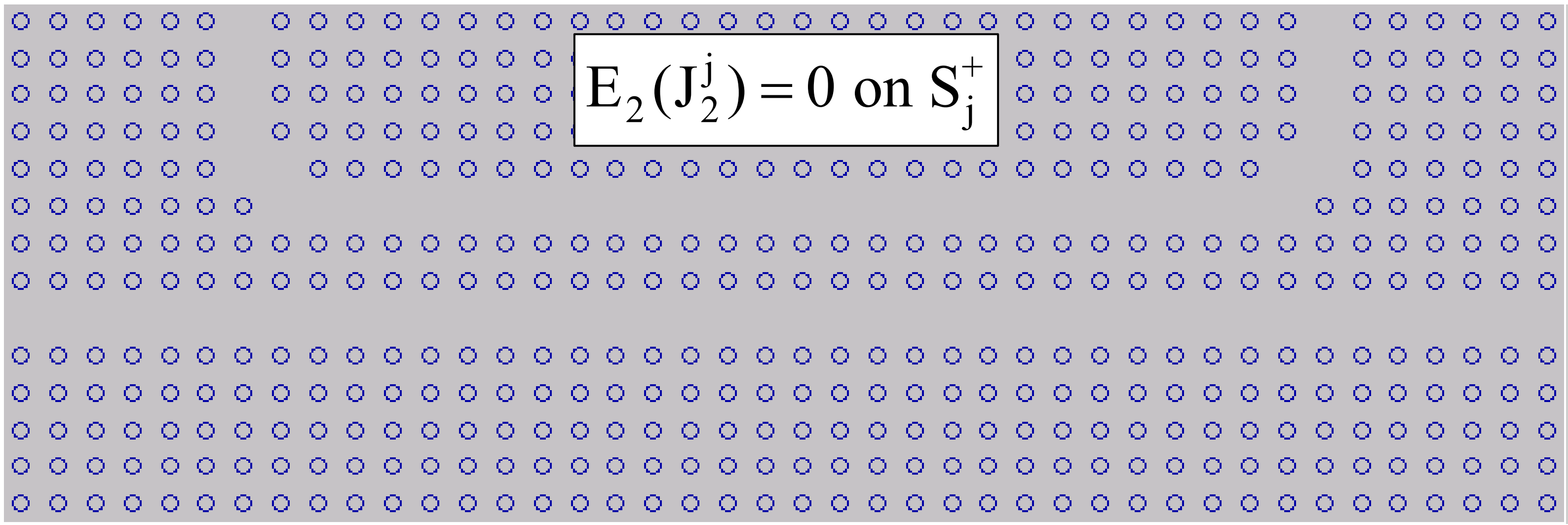
- **Step 1: Introduce two sets of equivalent currents on the surfaces of all N_c cylinders**
- **Step 2: Simplify exterior and interior problem**
  - Exterior problem: homogeneous medium (ε_1, μ_1)
  - Interior problem: homogeneous medium (ε_2, μ_2)
- **Step 3: Expand unknown currents in angular Fourier series**
- **Step 4: Solve exterior and interior problem**

Interior Problem



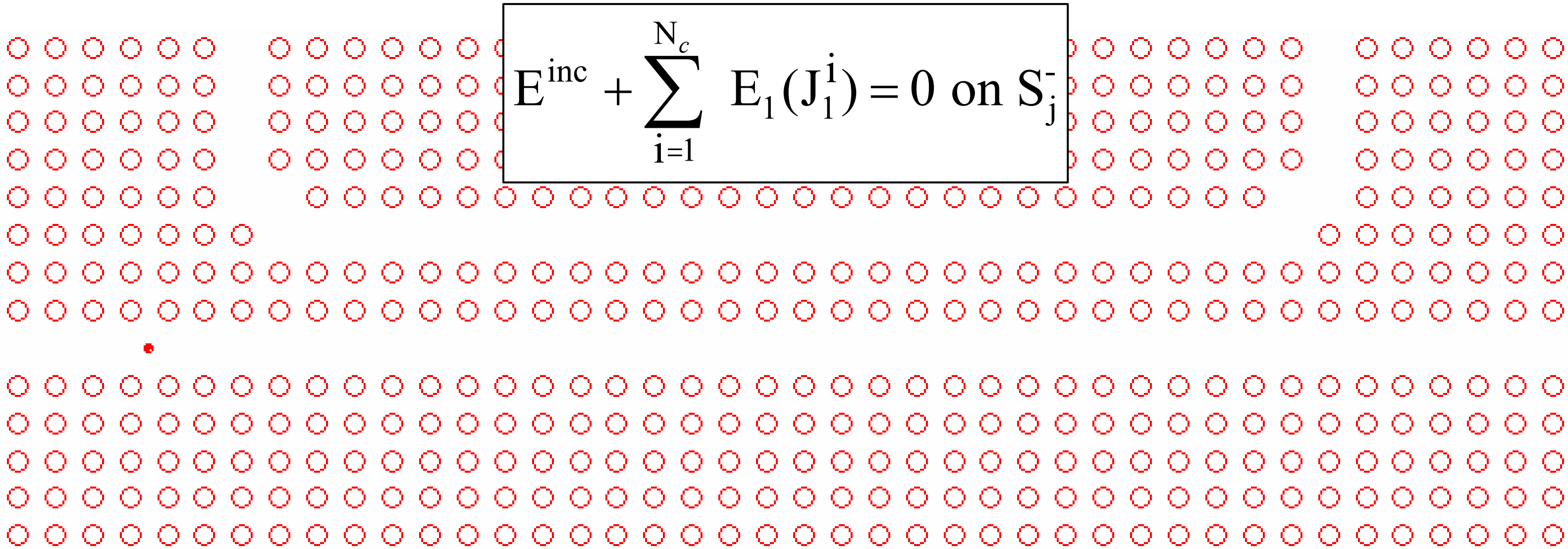
- Equations are decoupled for all cylinders
- Allows to eliminate all magnetic currents in favor of their electric counterparts
- All fields are calculated in the homogeneous medium **(ε_2, μ_2)**

Interior Problem



- **Equations are decoupled for all cylinders**
- **Allows to eliminate all magnetic currents in favor of their electric counterparts**
- **All fields are calculated in the homogeneous medium (ε_2, μ_2)**

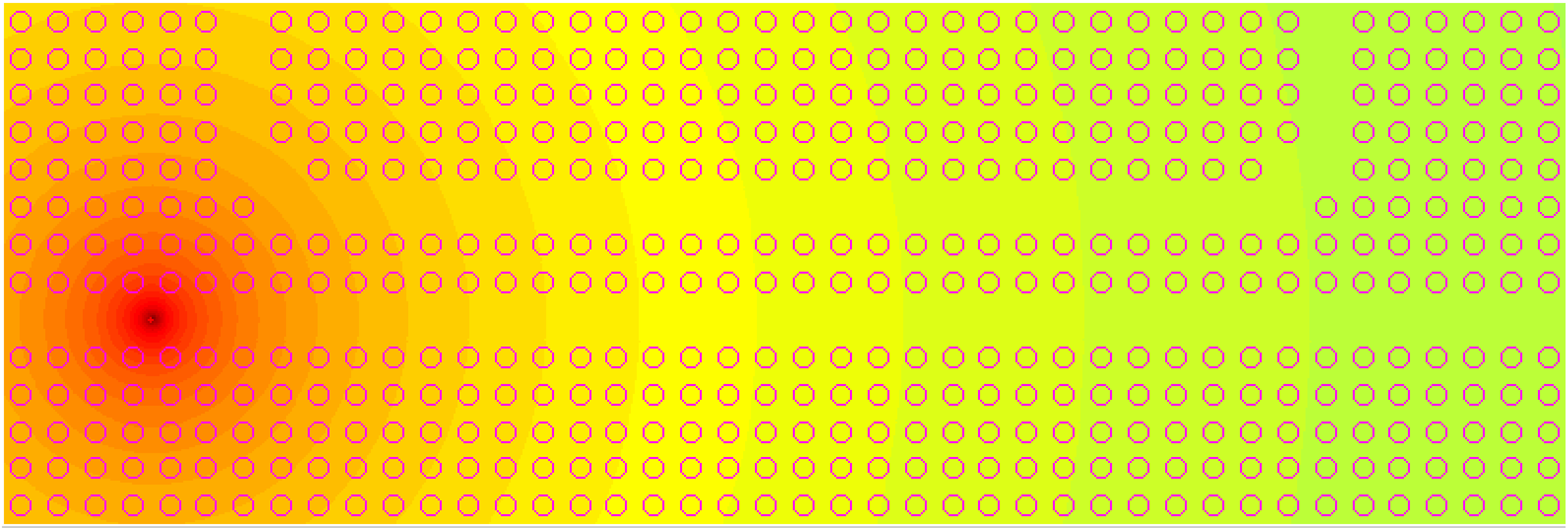
Exterior Problem



$$E^{inc} + \sum_{i=1}^{N_c} E_1(J_1^i) = 0 \text{ on } S_j^-$$

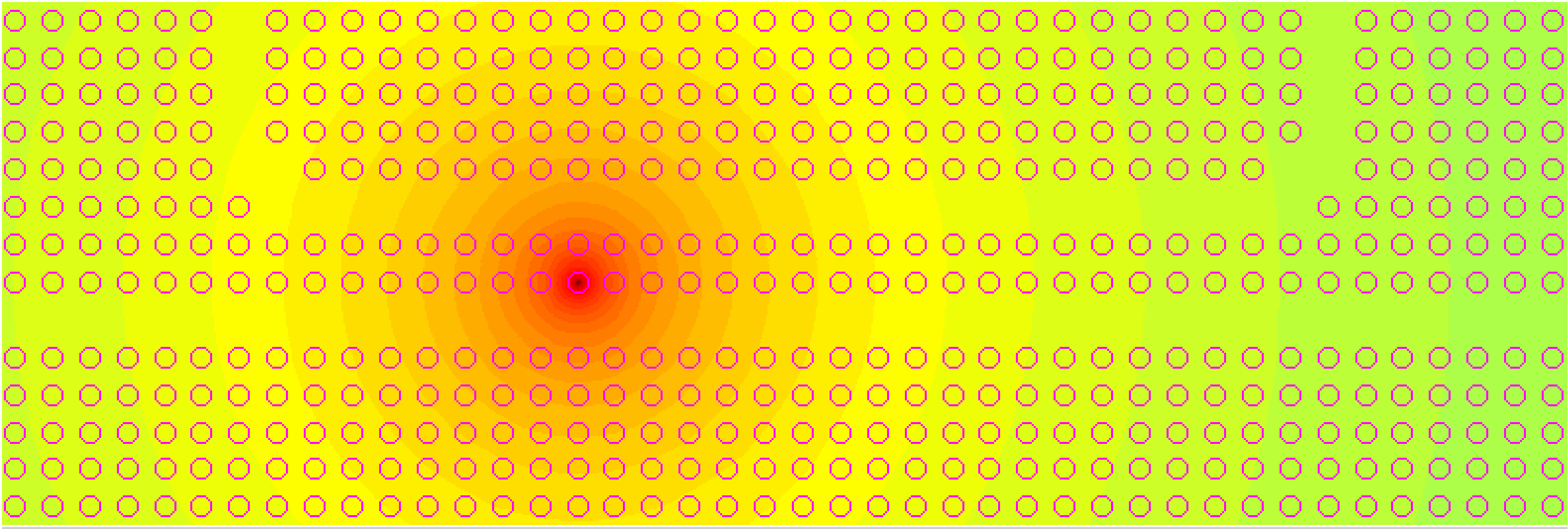
- **Equations on all cylinders are coupled**
- **All fields are calculated in the homogeneous medium (ε_1, μ_1)**

Incident Field



- Incident field E^{inc} decays very slowly
- All cylinders feel incident field

Scattered Field



- Scattered field $E_1(J_1)$ also decays very slowly
- All cylinders feel scattered field of all other cylinders

Dense Linear System

$$\begin{bmatrix} E^{\mathrm{i}}_1 \\ E^{\mathrm{i}}_2 \\ \vdots \\ E^{\mathrm{i}}_{N-1} \\ E^{\mathrm{i}}_N \end{bmatrix} = \begin{bmatrix} Z_{11} - \mathcal{Z}_1 & Z_{12} & \cdots & Z_{1,N-1} & Z_{1N} \\ Z_{21} & Z_{22} - \mathcal{Z}_2 & \cdots & Z_{2,N-1} & Z_{2N} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ Z_{N-1,1} & Z_{N-1,2} & \cdots & Z_{N-1,N-1} - \mathcal{Z}_{N-1} & Z_{N-1,N} \\ Z_{N1} & Z_{N2} & \cdots & Z_{N,N-1} & Z_{NN} - \mathcal{Z}_N \end{bmatrix} \begin{bmatrix} J_1 \\ J_2 \\ \vdots \\ J_{N-1} \\ J_N \end{bmatrix}$$

- E^{i}_i = incident field measured on cylinder *i*
- Z_{ij} = field radiated by unit current on cylinder *j* measured on cylinder *i*
- Both fields decay very slowly!

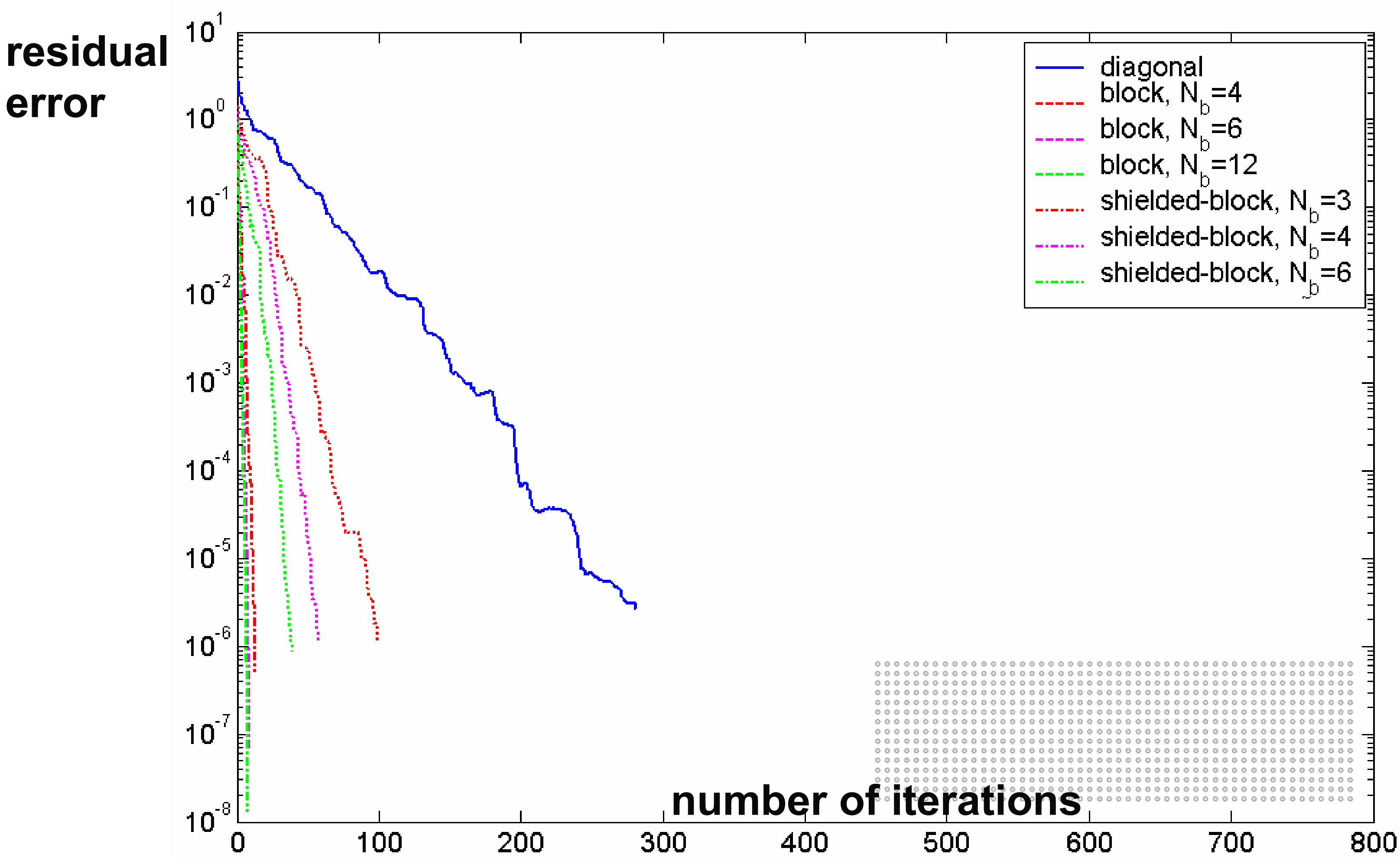
→ **All numbers are important!**

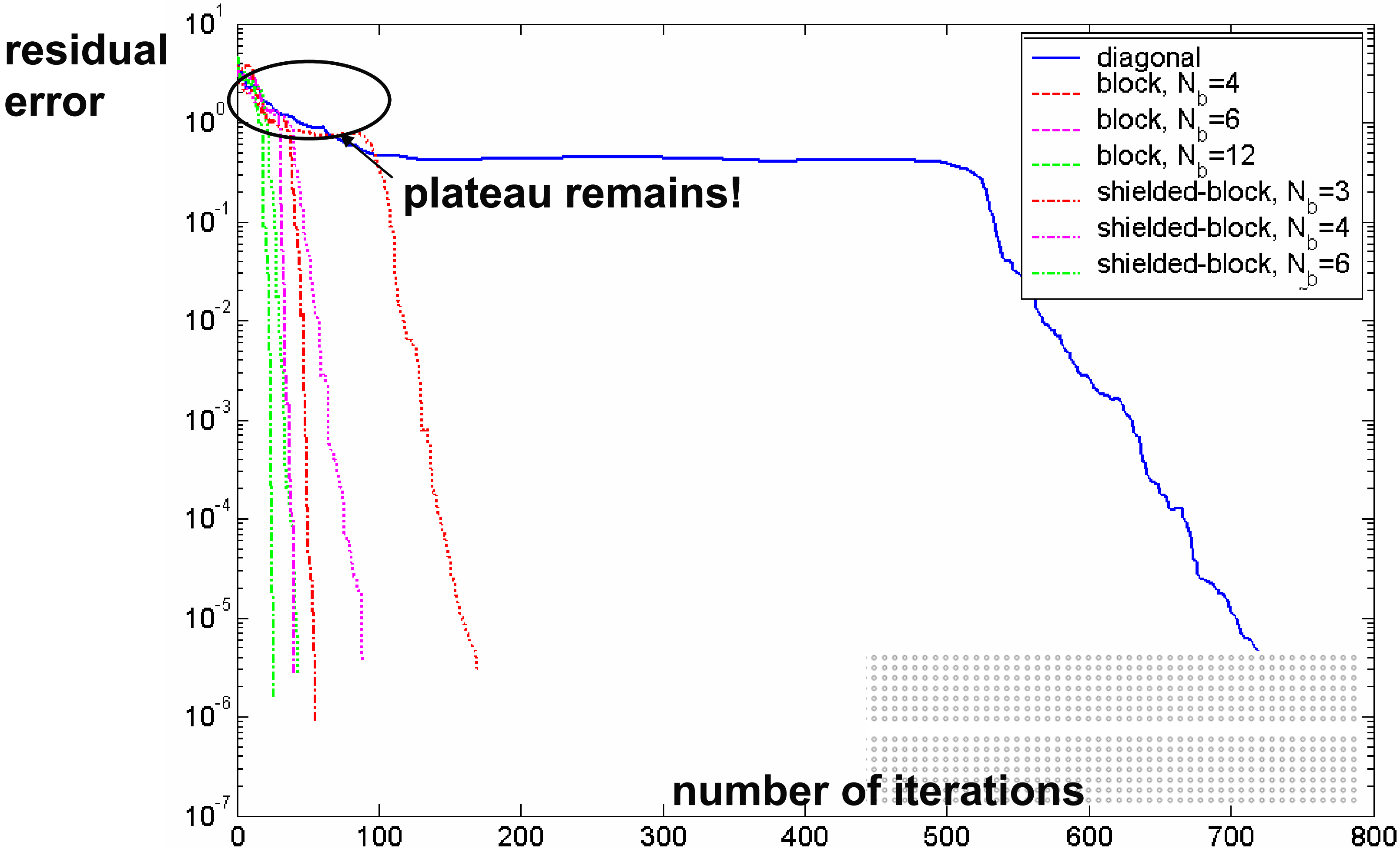
→ **Dense linear system of equations!**

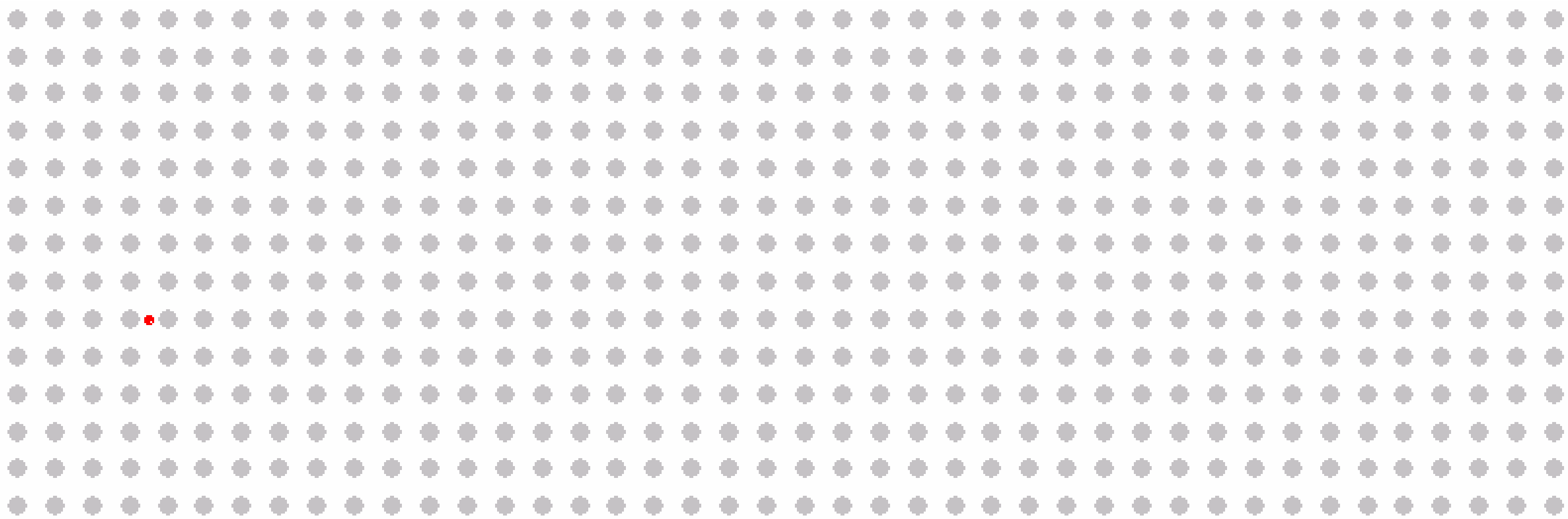
Computational Complexity

- **Dense** linear system of equations!
- Number of unknowns ~ N_c
- Direct solver (LU decomposition): $O(N_c^3)$
- Iterative solver: $O(N_c^2)$
- Fast multiplication schemes (FFT, MLFMA,...): $O(N_c \log N_c)$
- Number of iterations can be very high → preconditioning is a must!
- Different convergence behavior for defect-less PhC and PhC waveguide!

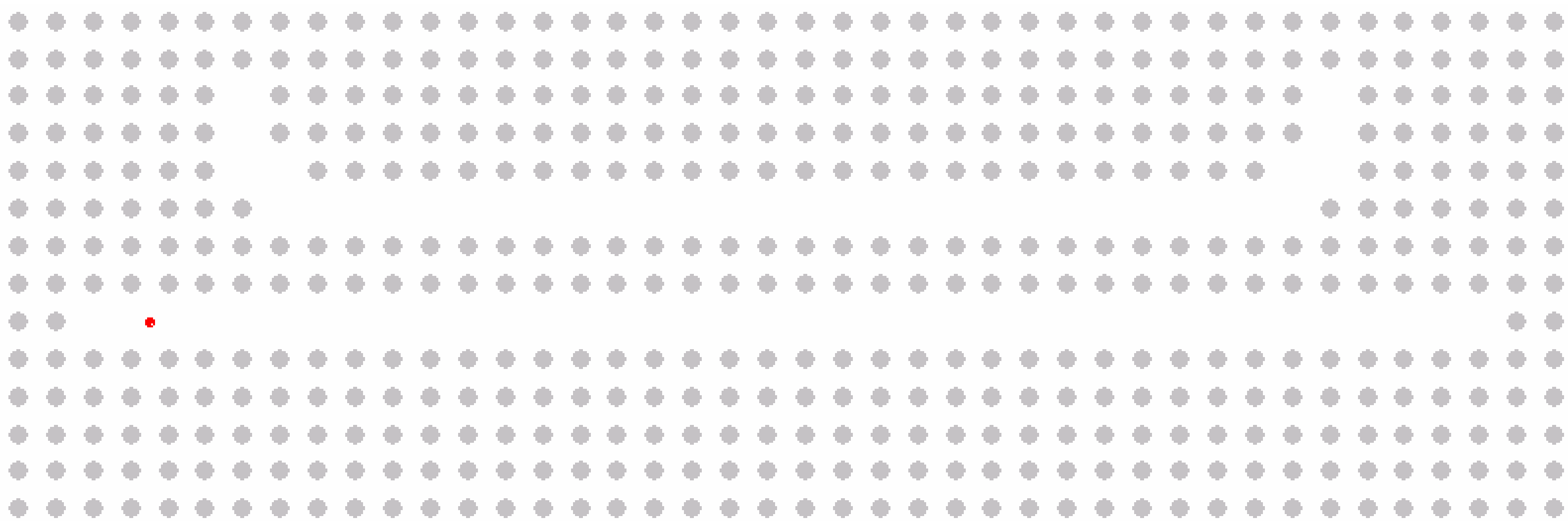
Defect-less PhC




residual error
plateau remains!
number of iterations
diagonal
block, N_b=4
block, N_b=6
block, N_b=12
shielded-block, N_b=3
shielded-block, N_b=4
shielded-block, N_b=6
10^1
10^0
10^-1
10^-2
10^-3
10^-4
10^-5
10^-6
10^-7
0
100
200
300
400
500
600
700
800



- **Start from infinite, defect-less PhC**

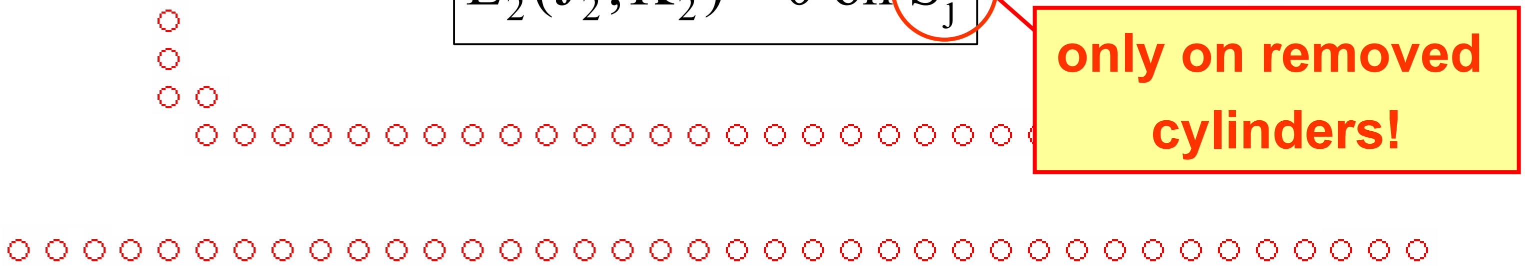


- Start from infinite, defect-less PhC
- Obtain PhC device by **removing** N_r cylinders

- **Step 1: Introduce two sets of equivalent currents only on the surfaces of the N_r removed cylinders**
- **Step 2: Simplify exterior and interior problem**
  - Exterior problem: infinite, defect-less PhC!
  - Interior problem: homogeneous medium (ε_1, μ_1)
- **Step 3: Expand unknown currents in angular Fourier series**
- **Step 4: Solve exterior and interior problem**

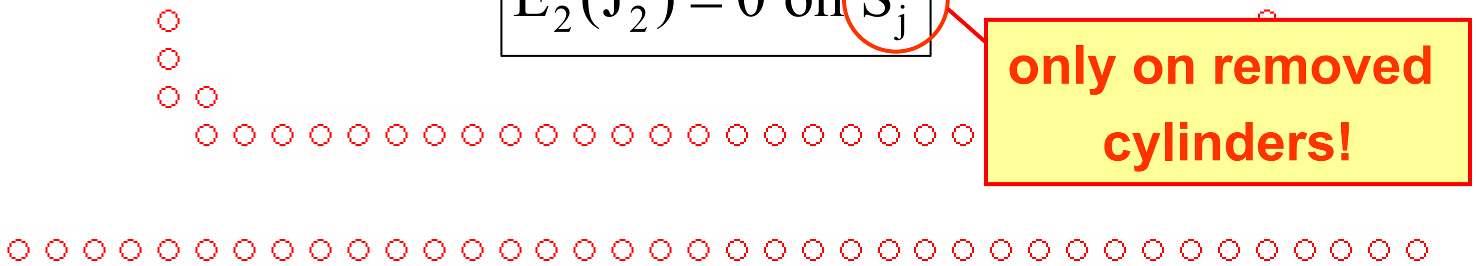
Interior Problem

$$E_2(J_2^j, K_2^j) = 0 \text{ on } S_j^+$$



- Equations are decoupled for all cylinders
- Allows to eliminate all magnetic currents in favor of their electric counterparts
- All fields are calculated in the homogeneous medium (ε_1, μ_1)

Interior Problem

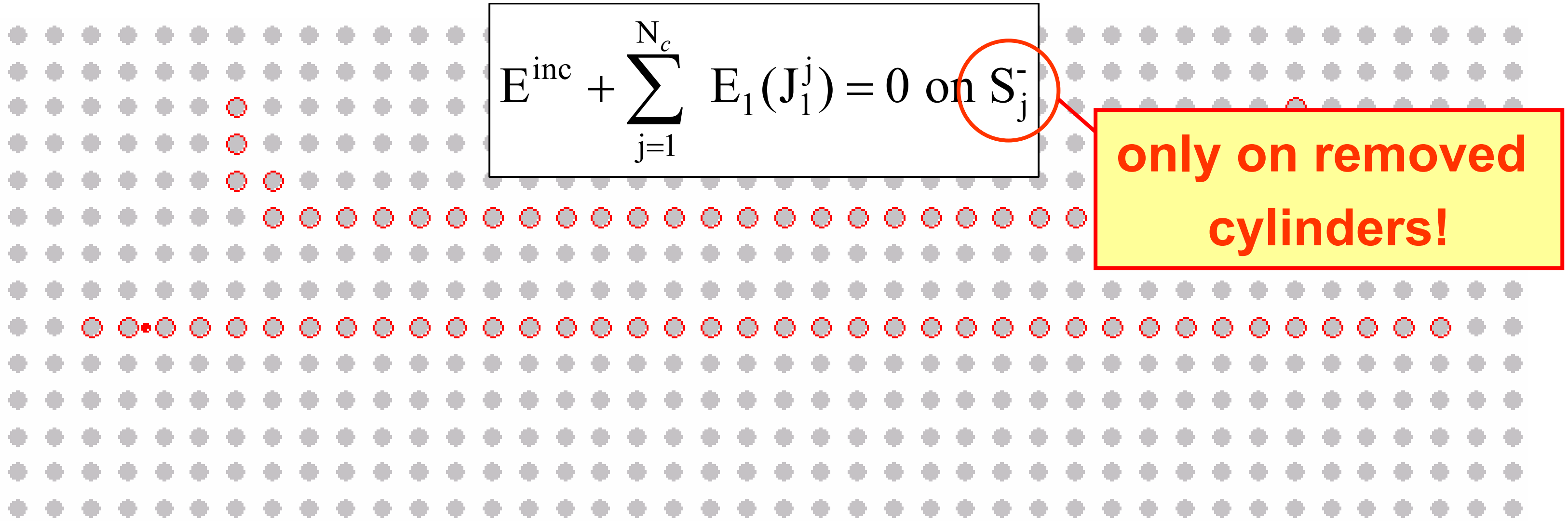


$$E_2(J_2^j) = 0 \text{ on } S_j^+$$

- **Equations are decoupled for all cylinders**
- **Allows to eliminate all magnetic currents in favor of their electric counterparts**
- **All fields are calculated in the homogeneous medium (ε_1, μ_1)**

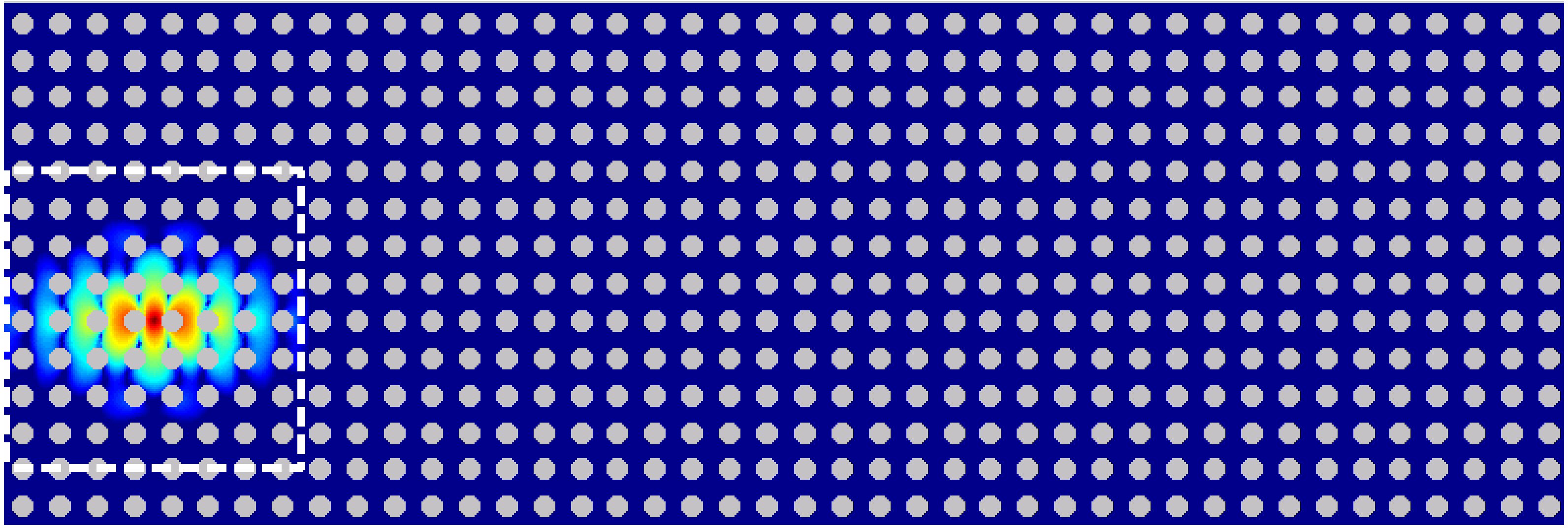
Exterior Problem

$$E^{inc} + \sum_{j=1}^{N_c} E_1(J_1^j) = 0 \text{ on } S_j^-$$

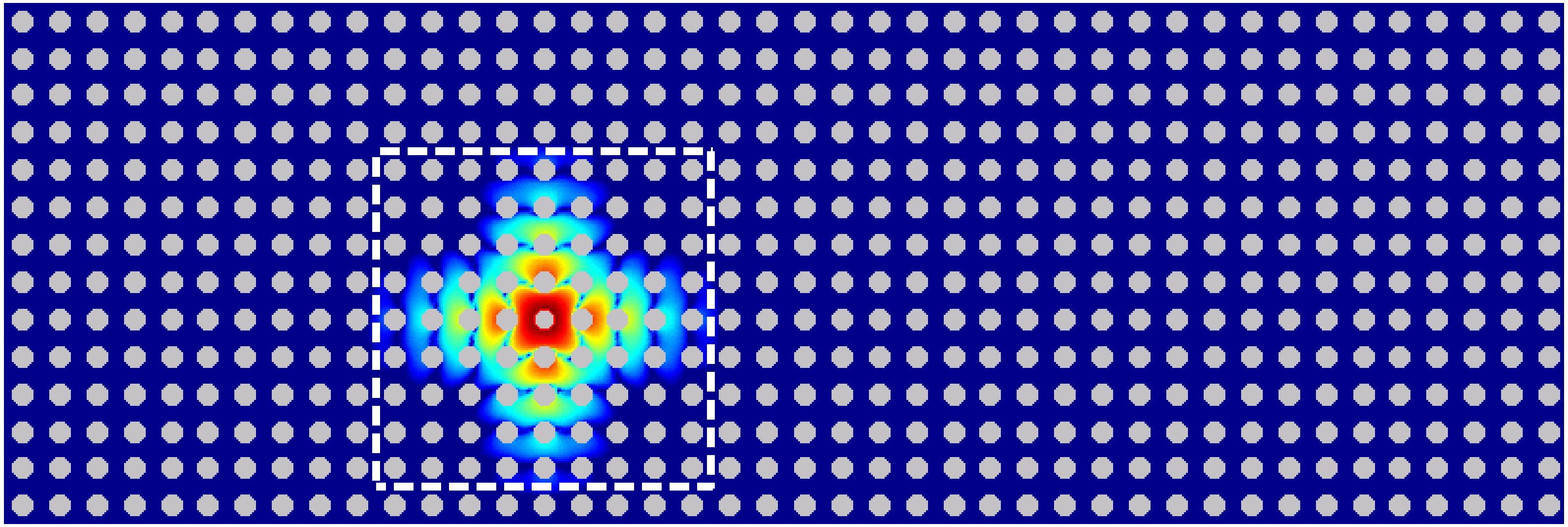


- **Equations on all cylinders are coupled**
- **All fields are calculated in the infinite, defect-less PhC**

Incident Field



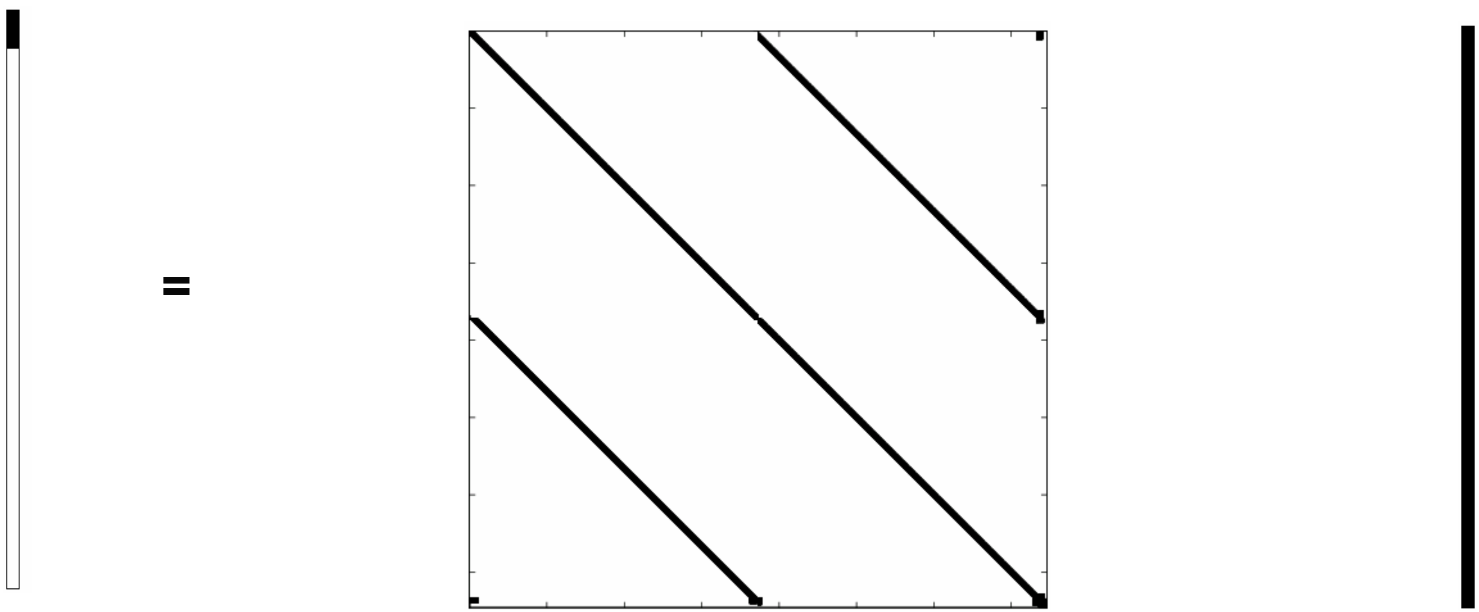
- **Incident field E^{inc} = field caused by source in the infinite, defect-less PhC**
- **For frequencies in the bandgap, the incident field decays exponentially with distance!**
- **Only the removed cylinders in the direct neighbor-hood of the source feel the incident field!**



- Scattered field $E_1(J_1)$ also decays exponentially with distance
- Every removed cylinder only interacts with removed cylinders in its direct neighbor-hood!

Sparse Linear System

$$
\begin{bmatrix} E^{\mathrm{i}}_1 \\ E^{\mathrm{i}}_2 \\ \vdots \\ E^{\mathrm{i}}_{N-1} \\ E^{\mathrm{i}}_N \end{bmatrix}
=
\begin{bmatrix}
Z_{11}-\mathcal{Z}_1 & Z_{12} & \dots & Z_{1,N-1} & Z_{1N} \\
Z_{21} & Z_{22}-\mathcal{Z}_2 & \dots & Z_{2,N-1} & Z_{2N} \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
Z_{N-1,1} & Z_{N-1,2} & \dots & Z_{N-1,N-1}-\mathcal{Z}_{N-1} & Z_{N-1,N} \\
Z_{N1} & Z_{N2} & \dots & Z_{N,N-1} & Z_{NN}-\mathcal{Z}_N
\end{bmatrix}
\begin{bmatrix} J_1 \\ J_2 \\ \vdots \\ J_{N-1} \\ J_N \end{bmatrix}
$$



Sparse Linear System

$$
\begin{bmatrix} E^{\mathrm{i}}_1 \\ E^{\mathrm{i}}_2 \\ \vdots \\ E^{\mathrm{i}}_{N-1} \\ E^{\mathrm{i}}_N \end{bmatrix}
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\begin{bmatrix}
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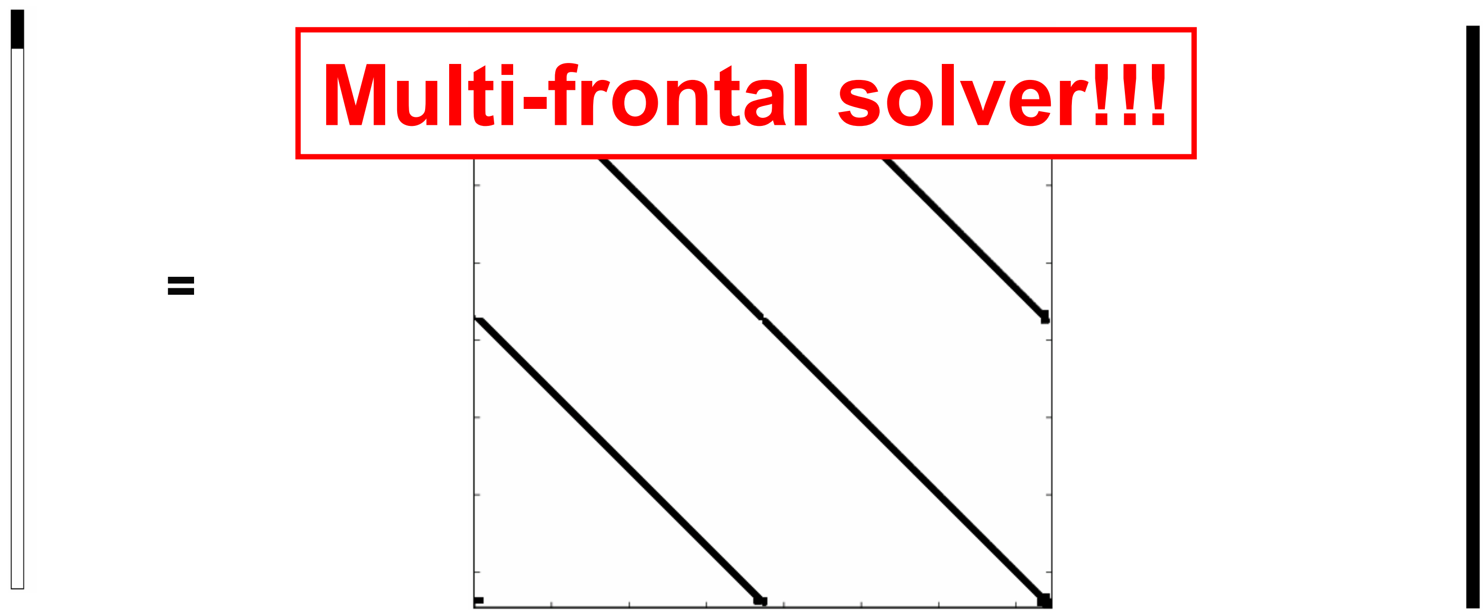
Z_{21} & Z_{22}-\mathcal{Z}_2 & \dots & Z_{2,N-1} & Z_{2N} \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
Z_{N-1,1} & Z_{N-1,2} & \dots & Z_{N-1,N-1}-\mathcal{Z}_{N-1} & Z_{N-1,N} \\
Z_{N1} & Z_{N2} & \dots & Z_{N,N-1} & Z_{NN}-\mathcal{Z}_N
\end{bmatrix}
\begin{bmatrix} J_1 \\ J_2 \\ \vdots \\ J_{N-1} \\ J_N \end{bmatrix}
$$

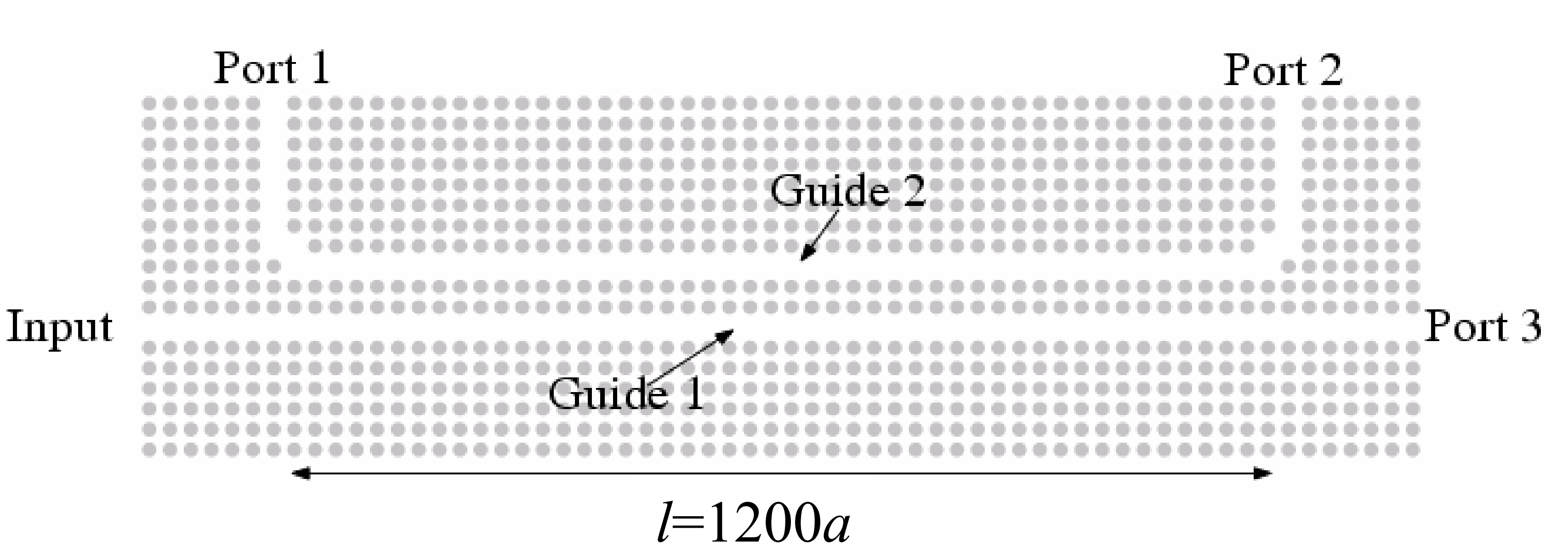
Multi-frontal solver!!!



PhC Green Function

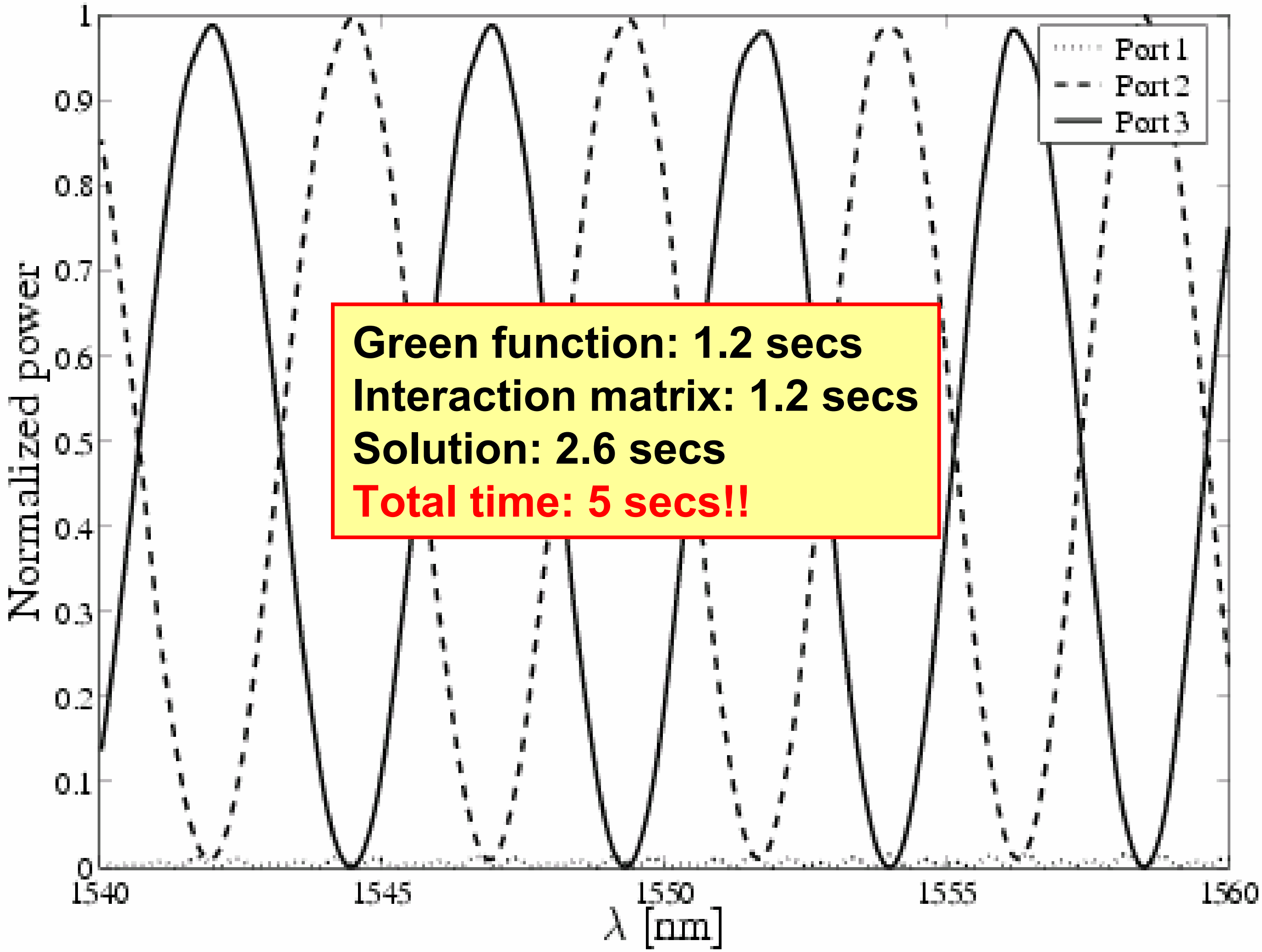
- Z_{ij} : field radiated by unit current on cylinder *j* and measured on cylinder *i*
- This quantity only depends on the relative position of cylinders *i* and *j*
- This "PhC Green function" is not known analytically
- However, it can be calculated very rapidly with the free-space GF MST, by using an iterative, preconditioned, and FFT-accelerated scheme!

Examples: EC Coupler



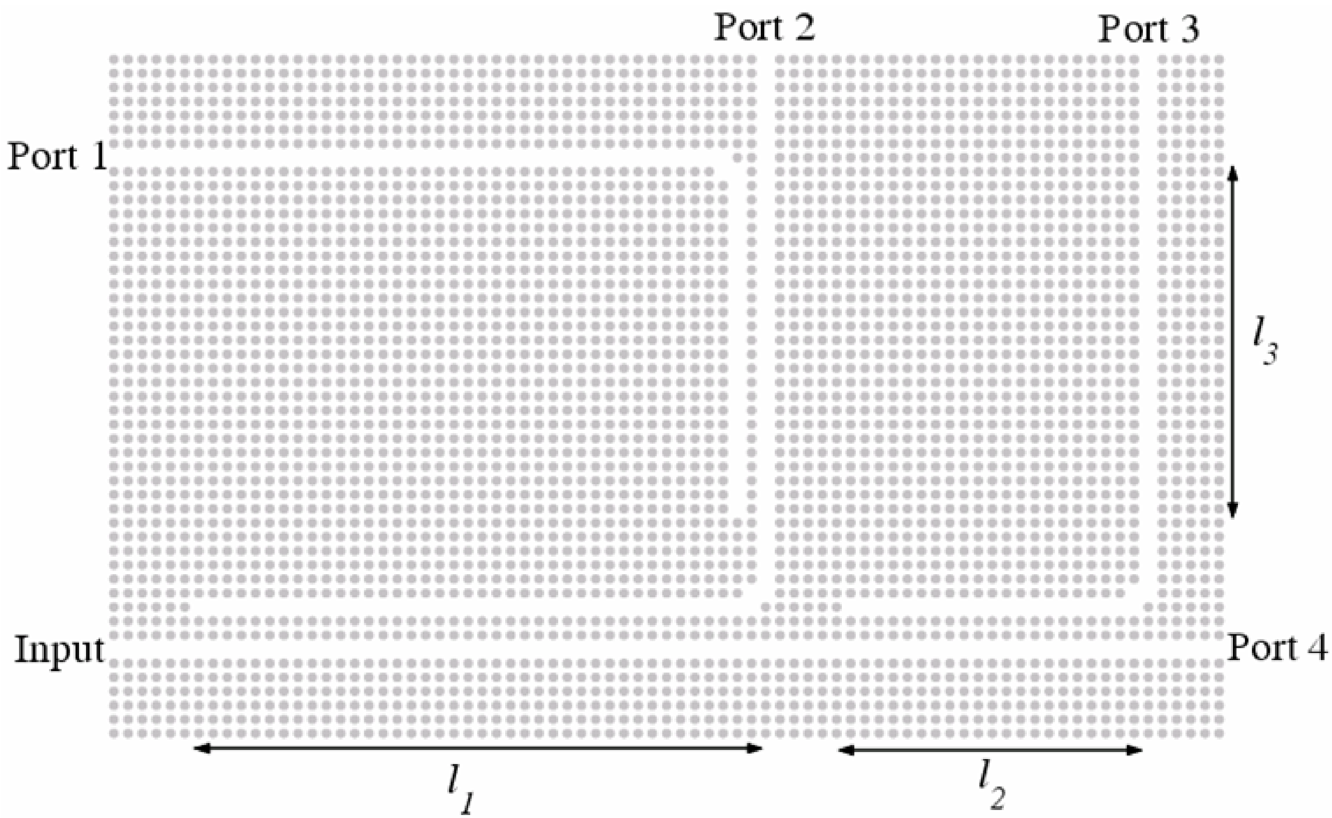
Total number of unknowns = 7465 << 47262 needed in the free-space GF MST

S. Boscolo, M. Midrio, and C.G. Someda, "Coupling and decoupling of electromagnetic waves in 2D photonic crystal waveguides," ***IEEE J. Quantum Electron*****, Jan. 2002**



Green function: 1.2 secs
Interaction matrix: 1.2 secs
Solution: 2.6 secs
Total time: 5 secs!!

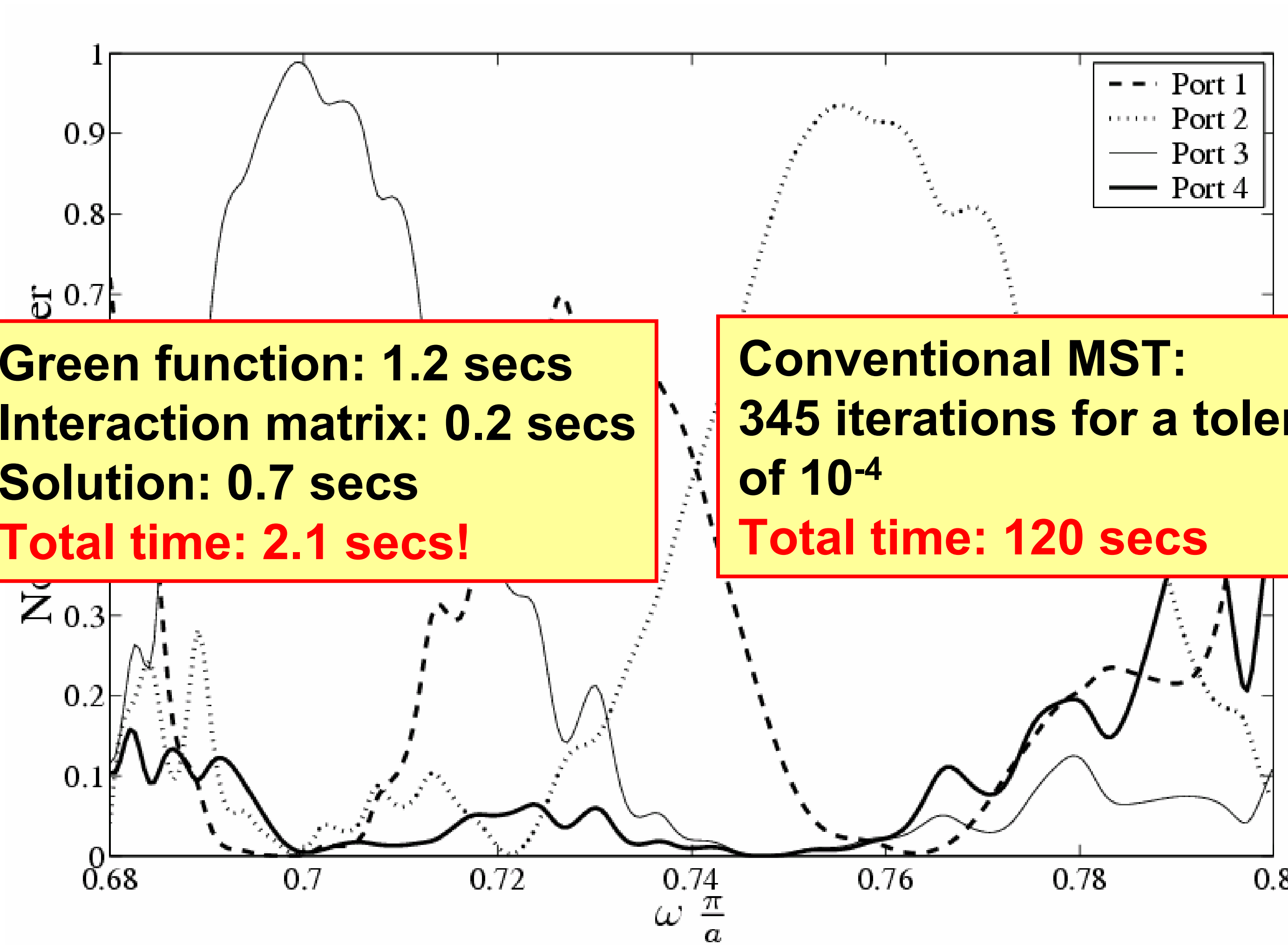
Example: Mux-Demux



Total number of unknowns = 1066 < 4638 needed in free-space GF MST

M. Koshiba, "Wavelength division multiplexing and demultiplexing with photonic crystal waveguide couplers," *J. Lightw. Technol.*, Dec. 2001

Example Mux-Demux



Green function: 1.2 secs
Interaction matrix: 0.2 secs
Solution: 0.7 secs
Total time: 2.1 secs!

Conventional MST:
345 iterations for a tolerance of 10^{-4}
Total time: 120 secs

Free Space vs PhC GF MST

Free Space GF MST

- Equivalent currents on surfaces of all physical cylinders
- Expands currents in angular Fourier series
- Free Space Green function
- Dense linear system
- Suitable for all frequencies
- Also applicable to non-periodic arrangements, e.g. random media

PhC GF MST

- Equivalent currents on surfaces of fictitious removed cylinders
- Expands currents in angular Fourier series
- Photonic Crystal Green function
- Sparse linear system
- Suitable only in bandgap
- Restricted to periodic arrangements (a few displaced cylinders are acceptable)

- **Remember:**

$$\begin{bmatrix} E^{\mathrm{i}}_1 \\ E^{\mathrm{i}}_2 \\ \vdots \\ E^{\mathrm{i}}_{N-1} \\ E^{\mathrm{i}}_N \end{bmatrix} = \begin{bmatrix} Z_{11} - \mathcal{Z}_1 & Z_{12} & \dots & Z_{1,N-1} & Z_{1N} \\ Z_{21} & Z_{22} - \mathcal{Z}_2 & \dots & Z_{2,N-1} & Z_{2N} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ Z_{N-1,1} & Z_{N-1,2} & \dots & Z_{N-1,N-1} - \mathcal{Z}_{N-1} & Z_{N-1,N} \\ Z_{N1} & Z_{N2} & \dots & Z_{N,N-1} & Z_{NN} - \mathcal{Z}_N \end{bmatrix} \begin{bmatrix} J_1 \\ J_2 \\ \vdots \\ J_{N-1} \\ J_N \end{bmatrix}$$

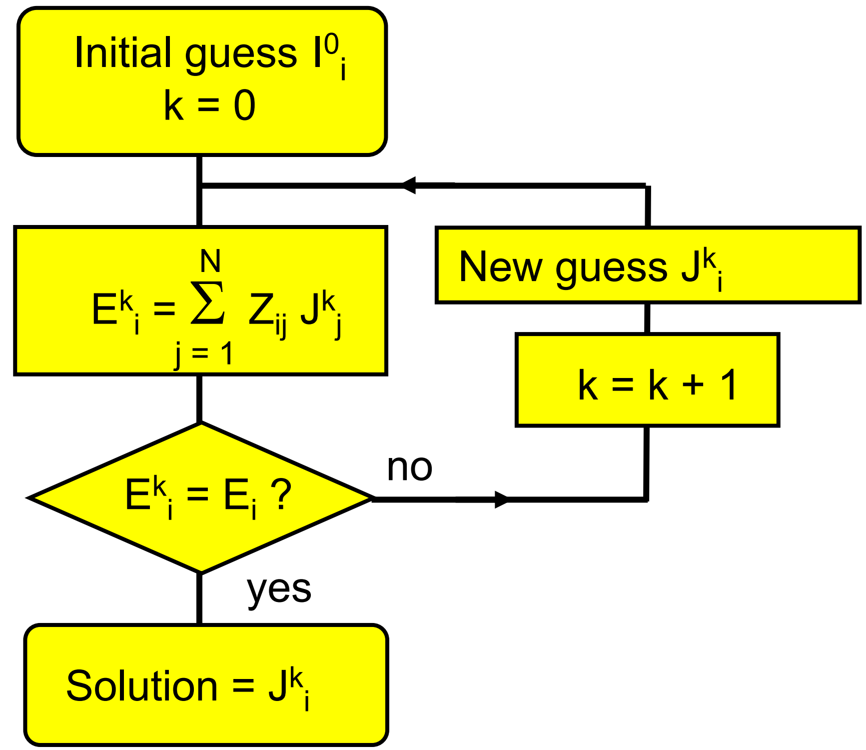
- E^{i}_i **= incident field measured on cylinder *i***
- Z_{ij} **= field radiated by unit current on cylinder *j* measured on cylinder *i***

Fast Multipole Method

$$E_i = \sum_{j=1}^{N} Z_{ij} J_j$$ Linear system of *N* equations with *N* unknowns

Gaussian elimination of LU decomposition: $O(N^3)$ computations

Iterative solution of system:

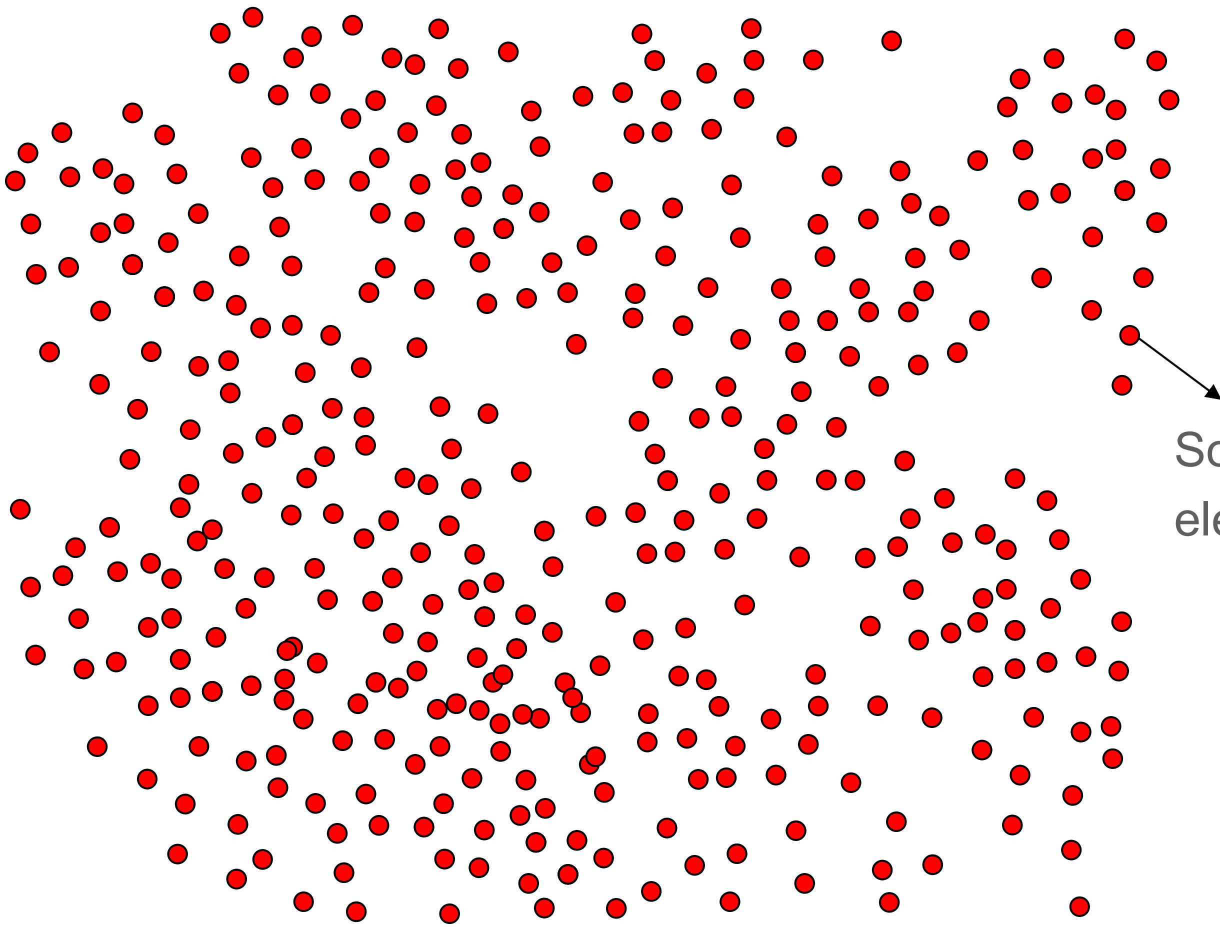


$O(N^2)$ computations ←

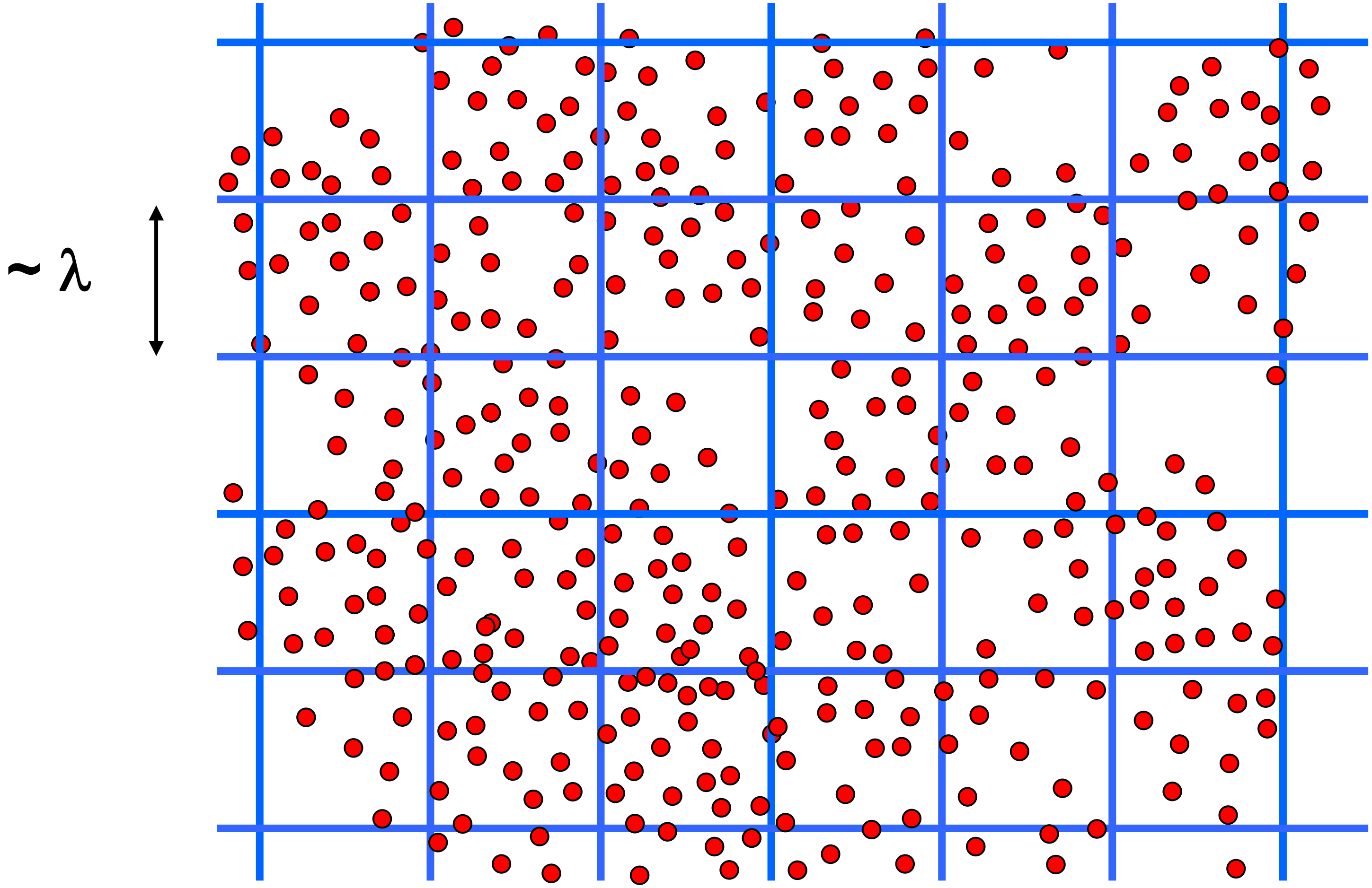
= fields generated by currents on *N* cylinders at the *N* cylinders

= $O(N \log N)$ computations through MLFMA !!

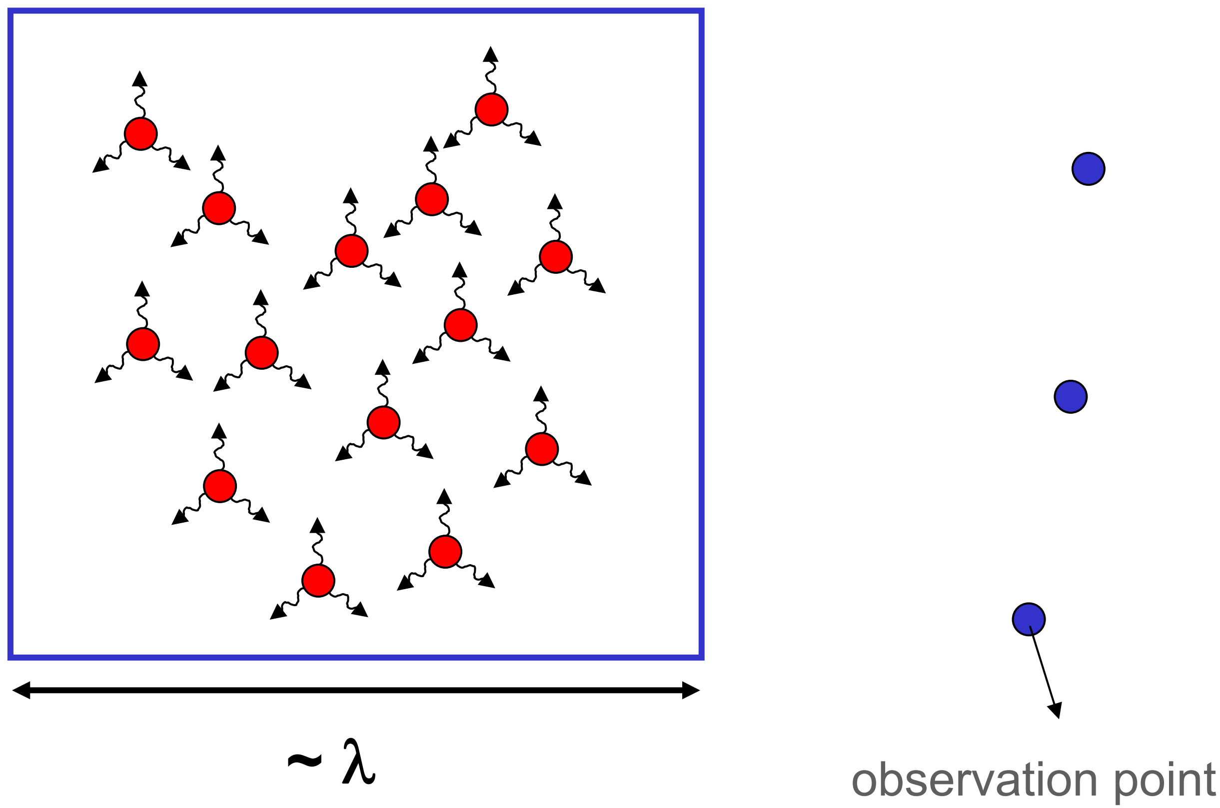
Calculate field generated by *N* cylinders at each of the cylinders: O(N^2) computations



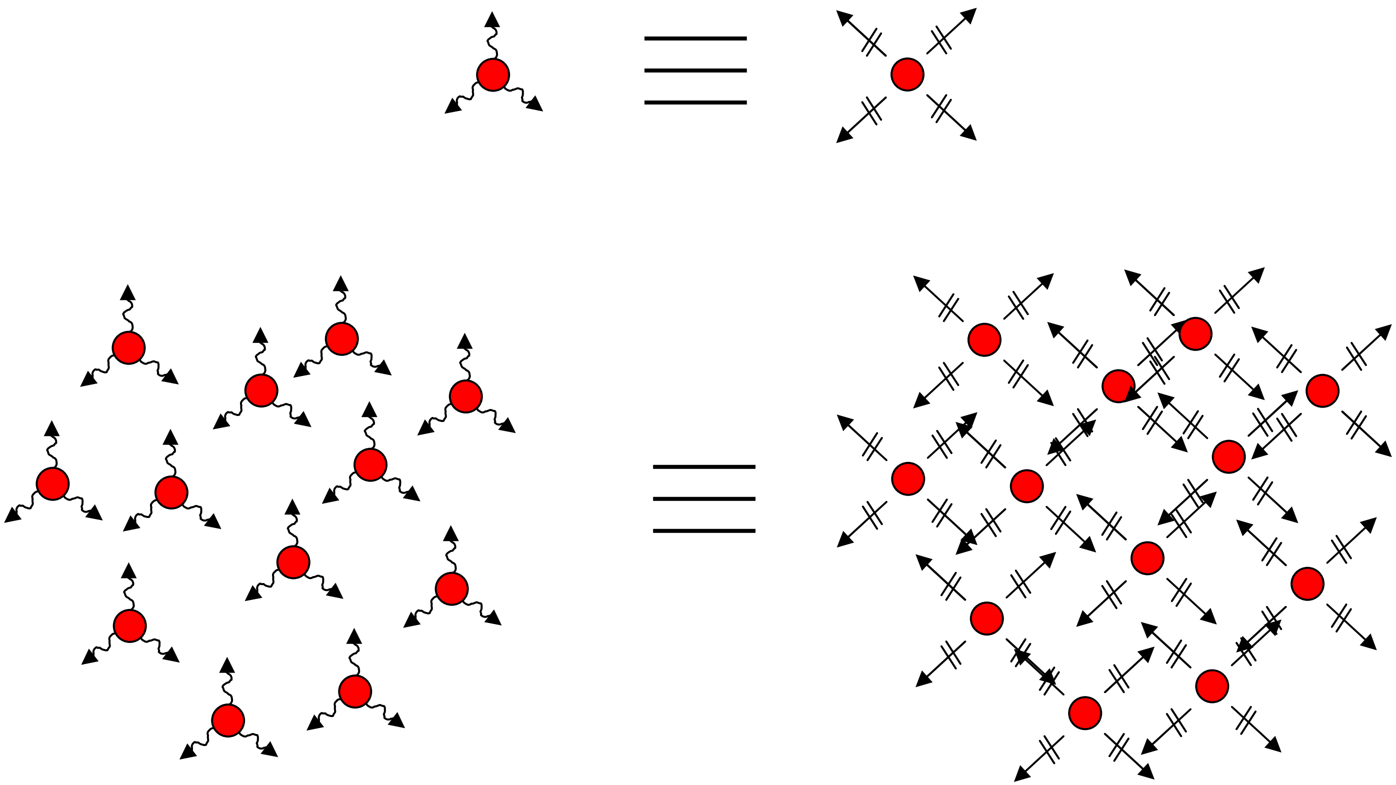
Divide the cylinders in groups

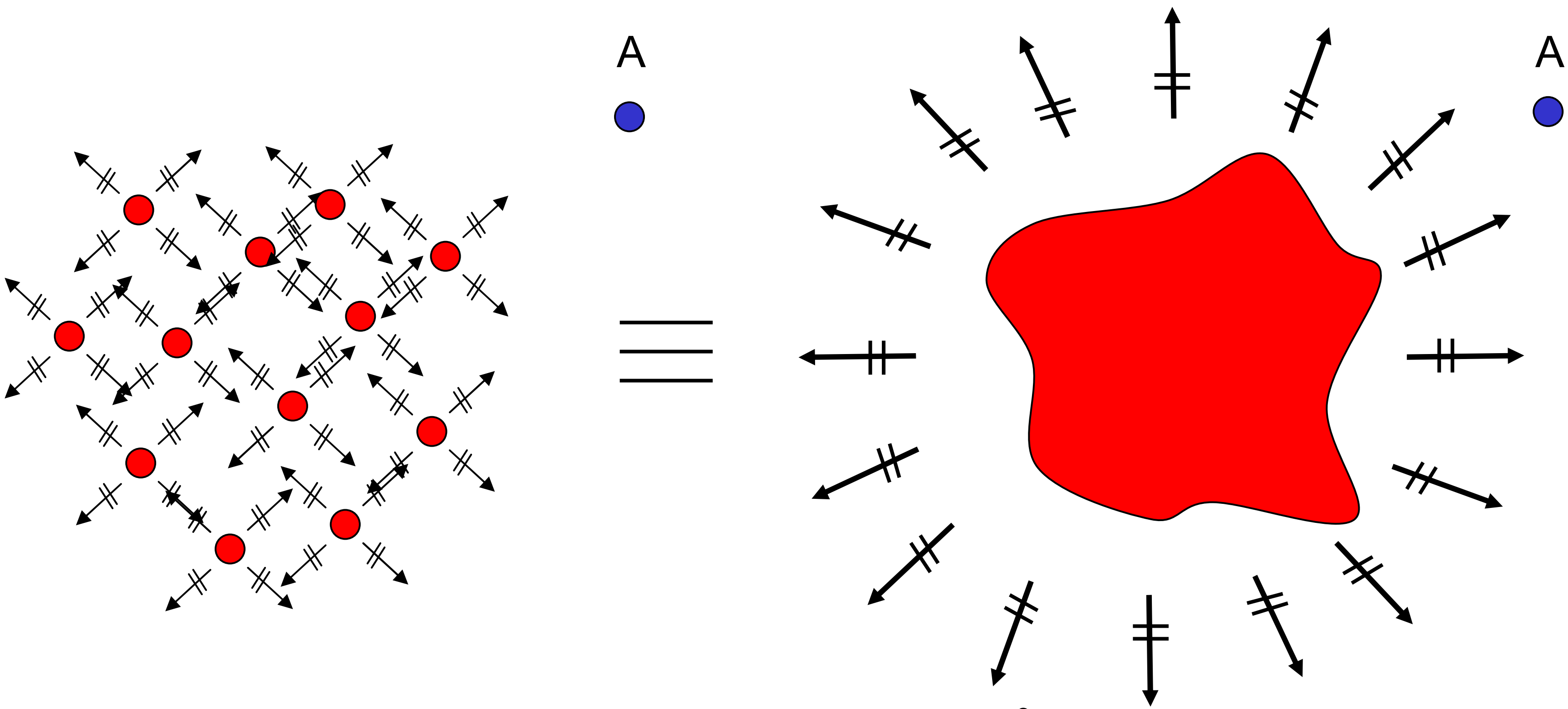


Fields from one group in a number of observation cylinders sufficiently far from the group



Expansion of field of each cylinder in propagating plane waves:



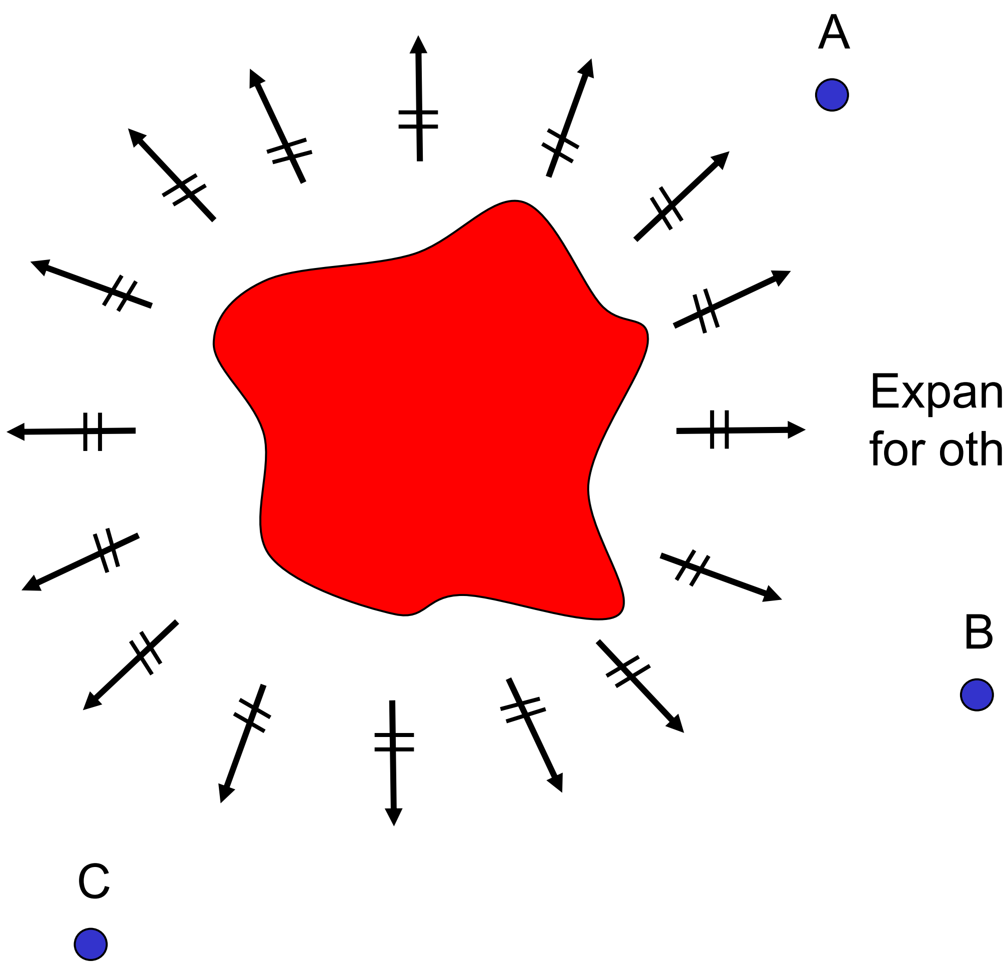


O(n) cylinders

Field in A: O(n) calculations

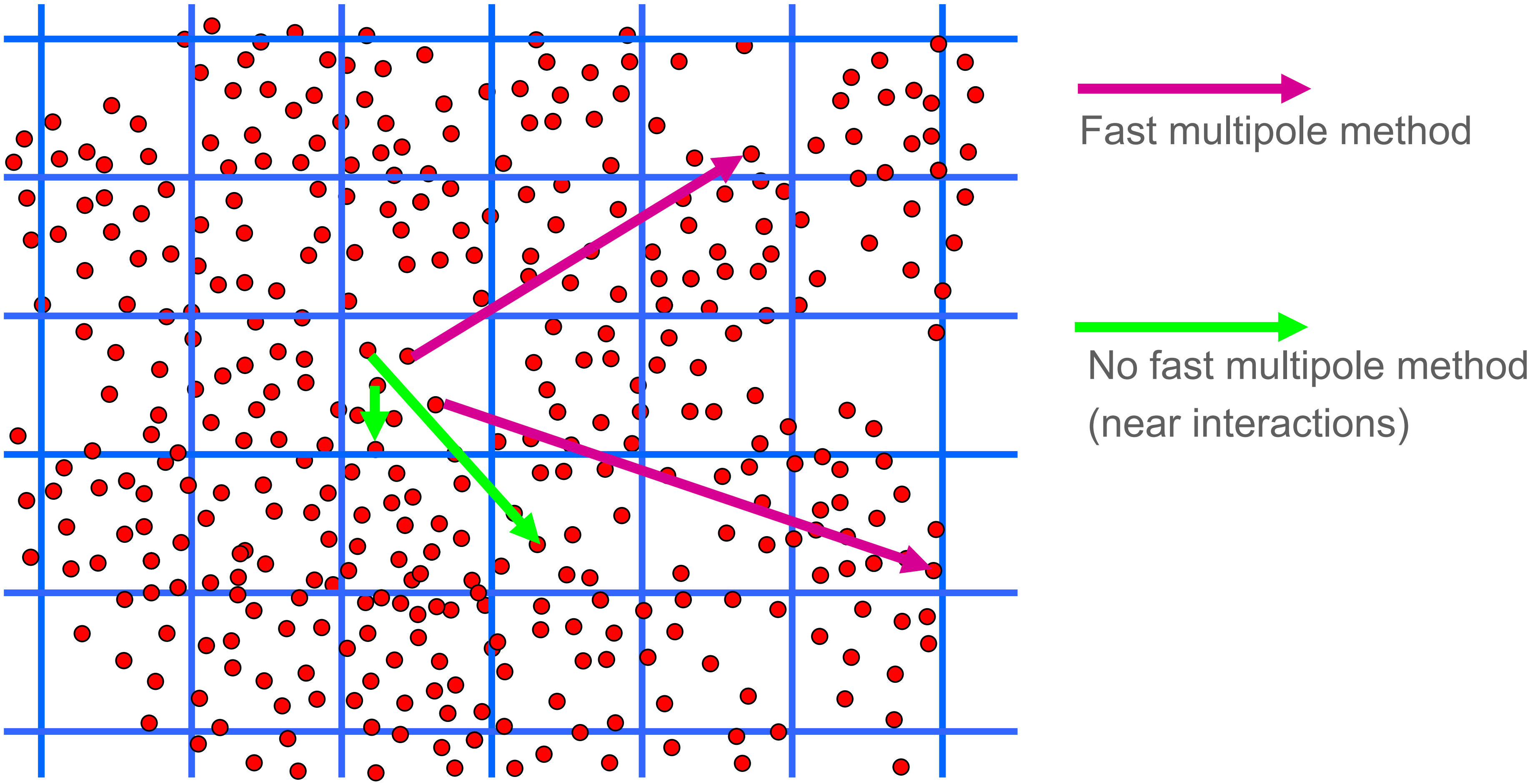
O($\sqrt[3]{n^2}$) plane waves

Field in A: O($\sqrt[3]{n^2}$) calculations



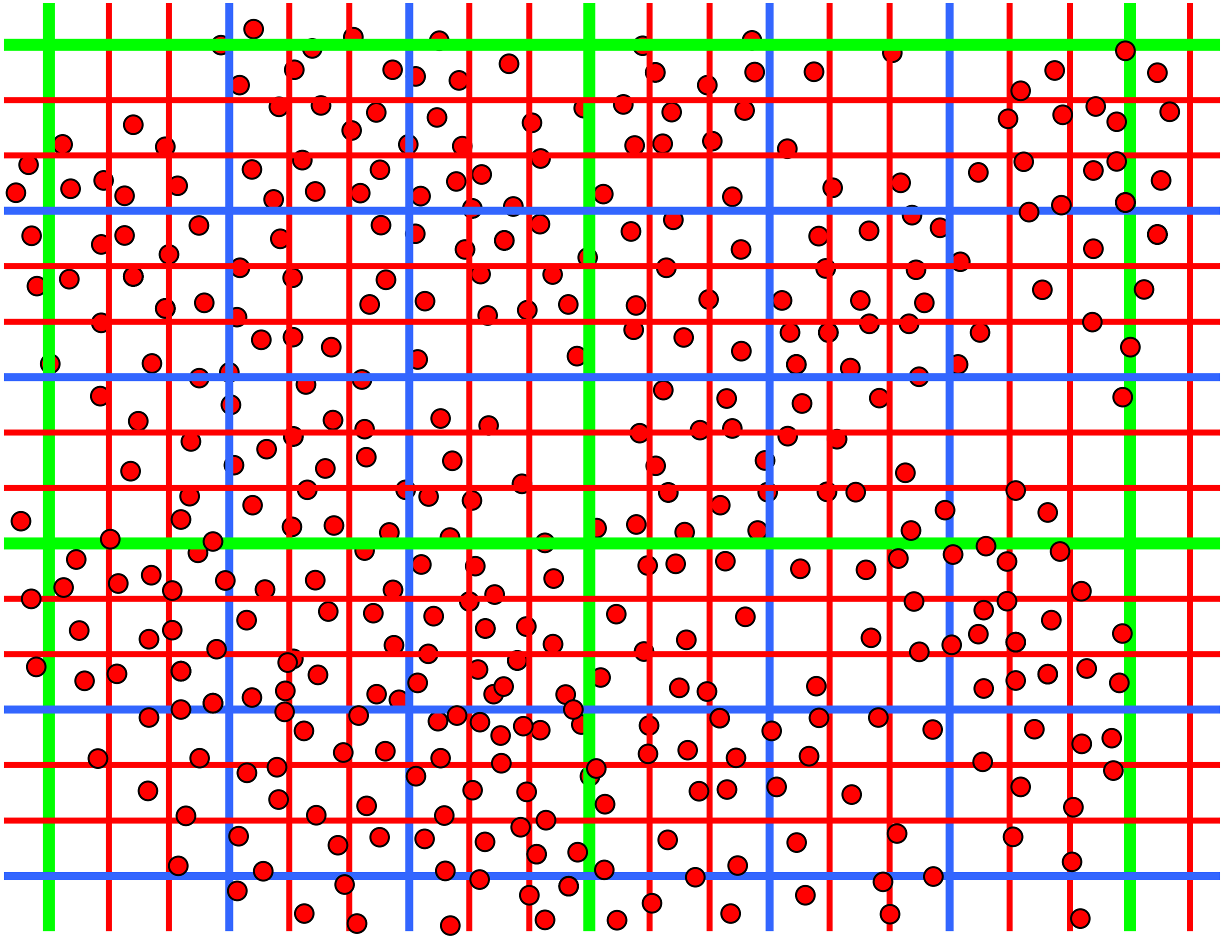
Expansion in plane waves reusable
for other observation cylinders A, B, C,... !

Fast Multipole Method



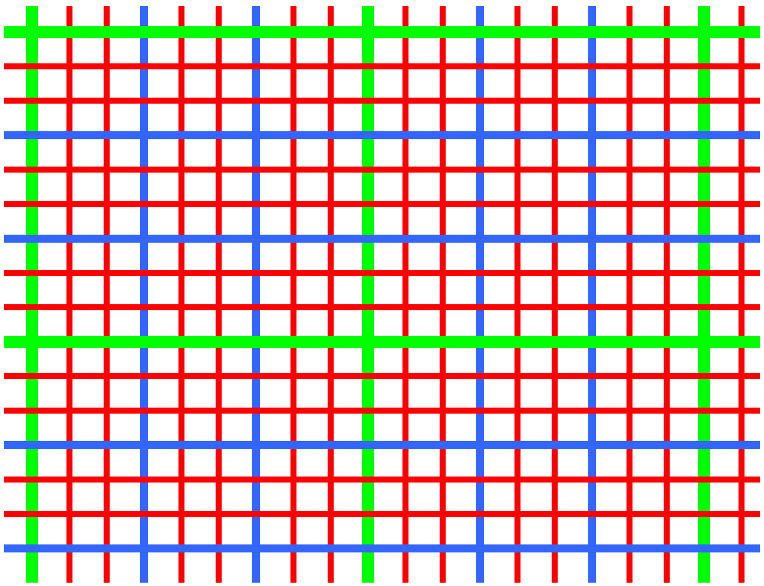
Fast Multipole Method

Groups hierarchically grouped in larger groups = MLFMA

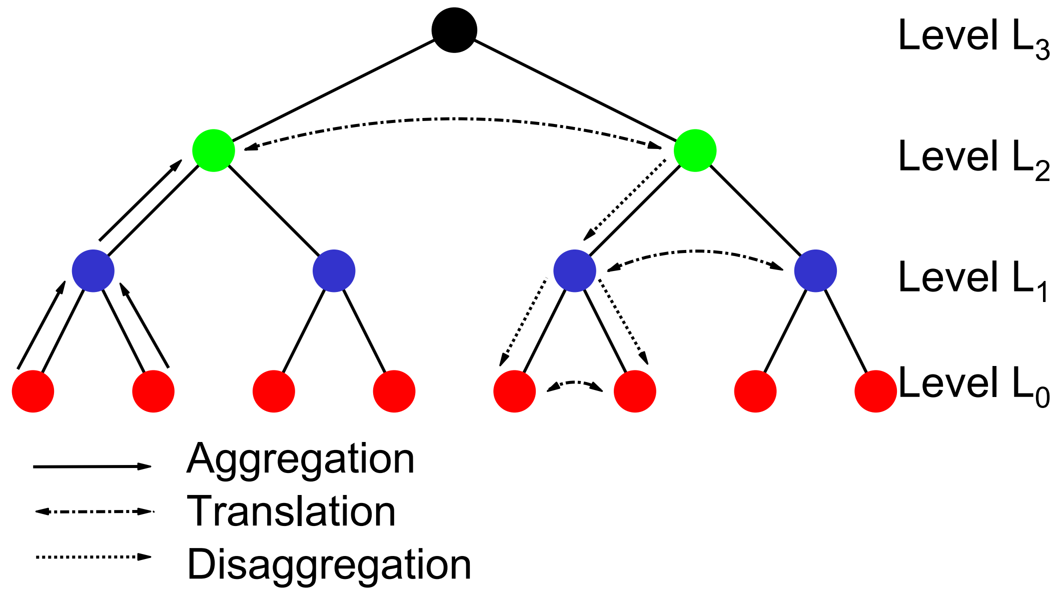


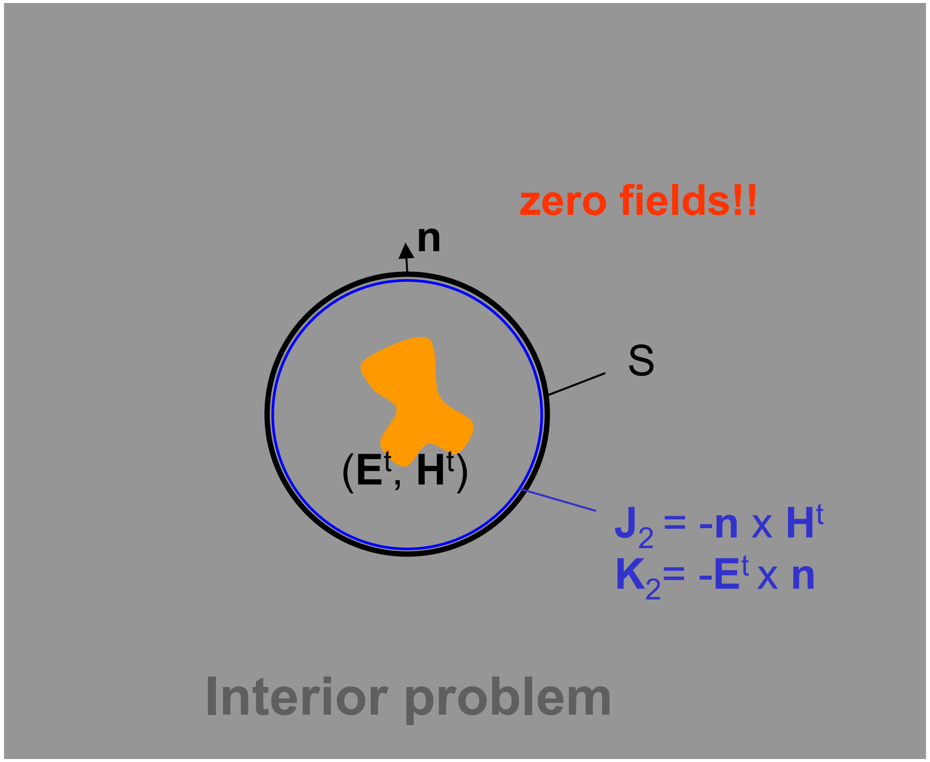
O(N Log N) computations !!

Fast Multipole Method



Tree structure





Non circular cylinders:

Define equivalent sources on a surrounding circular cylinder

Solve scattering problem with boundary condition:

$$\mathbf{E}_2(\mathbf{J}_2,\mathbf{K}_2)=0 \text{ on } S^+$$

Can be done with Integral Equation (MoM) or Finite Elements

Allows to eliminate all magnetic currents in favor of their electric counterparts

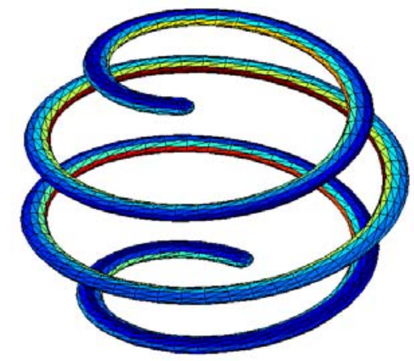
Other solution: do not use MST but entire Integral Equation solution with MLFMA

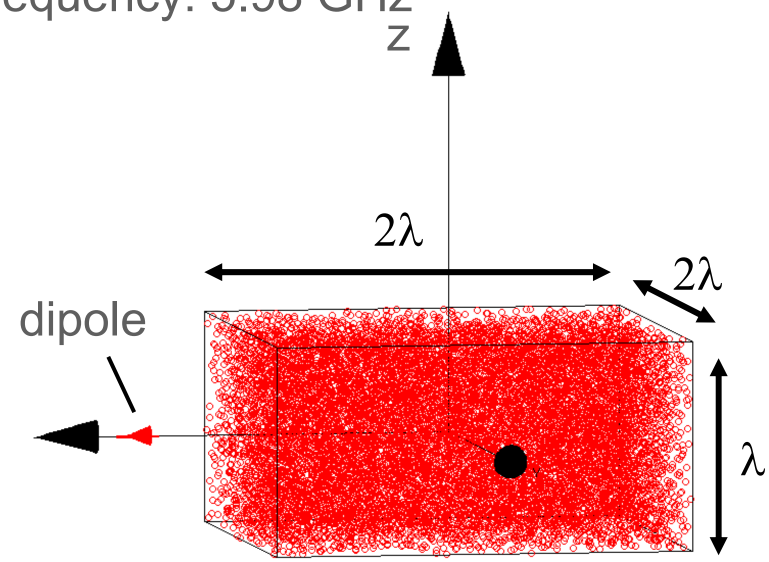
Extensions

- **Three dimensional problems:**
  - Suitable for metamaterials
  - MST is called T-matrix method
  - Expansion in vector spherical harmonics in stead of Fourier series

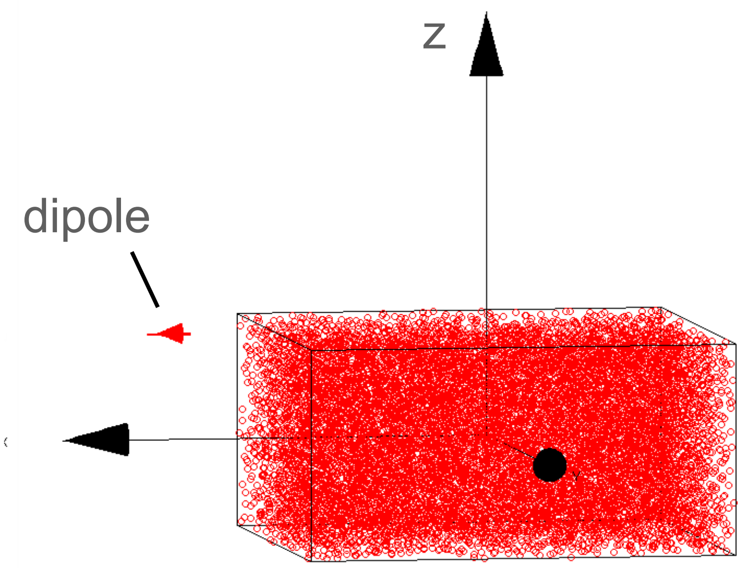
Chiral Metamaterial

- Rectangular block of random chiral wire inclusions
- Number of inclusions: 11580
- Simulated with T-matrix method accelerated by MLFMA
- Number of spherical harmonics per inclusion: 30
- Total number of unknowns T-matrix: 347400
- Density of inclusions: 0.023 inclusions per mm^3
- Frequency: 5.98 GHz





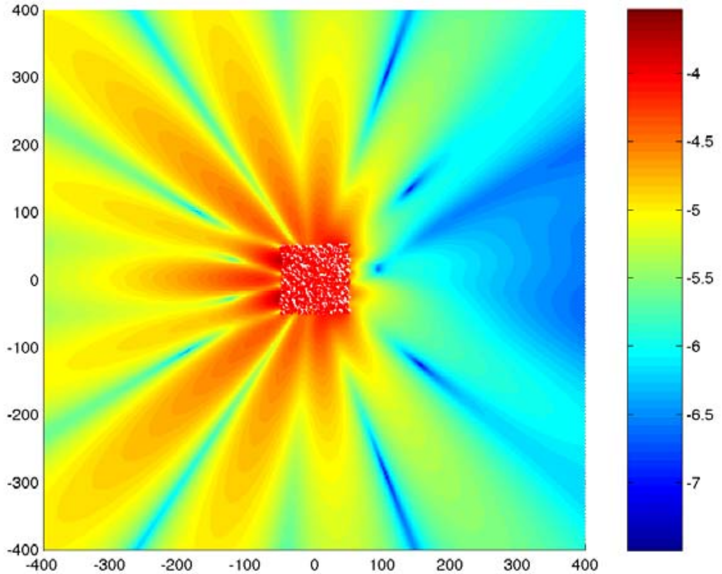
symmetric configuration



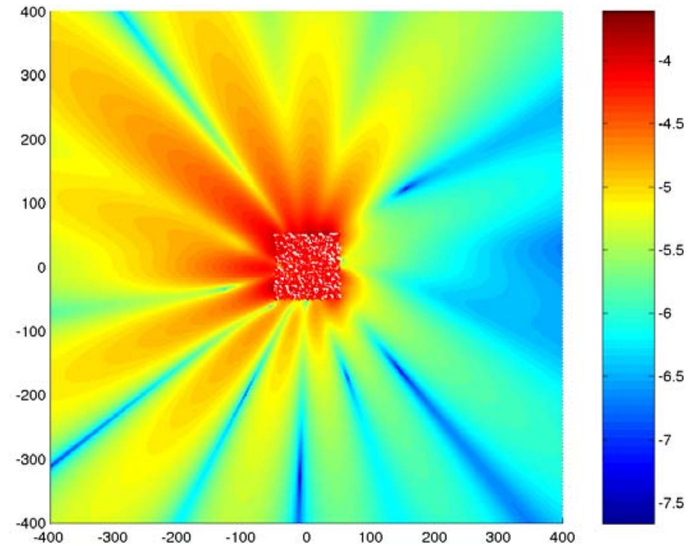
asymmetric configuration

Chiral Metamaterial

Field in *xy* plane



Symmetric configuration



Asymmetric configuration

Conclusions

- Advanced EM simulation tools are currently capable to simulate very large and complex photonic crystals, metamaterials and other structures.
- Open source software:
  openfmm.intec.ugent.be
- Further information:
  femke.olyslager@intec.ugent.be