Stochastic Maxwell Equations in Photonic Crystal Modeling and Simulations

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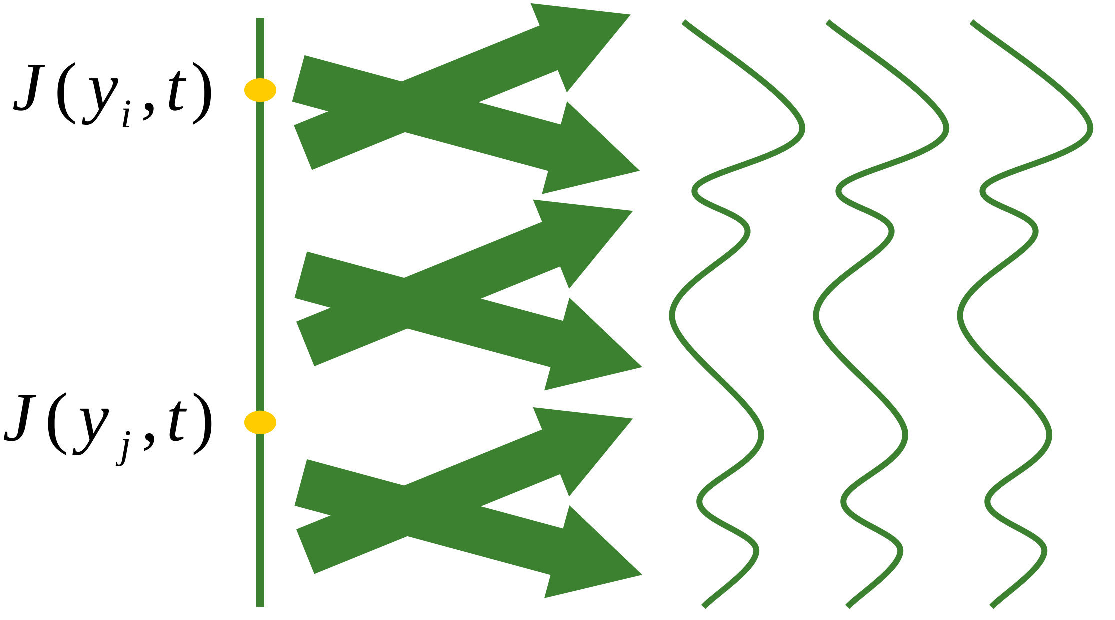
Outline

- Introduction & Motivation
- Direct Method
- A Stochastic Model
- Wiener Chaos Expansions (WCE)
- Numerical Method based on WCE
- Simulation results
- Conclusion

Introduction & Motivation

- Stochastic PDE’s :
  - Fluid Dynamics
  - Engineering
  - Material Sciences
  - Biology
  - Finance…
- Solutions are no longer deterministic.
- Main interest: statistical properties, such as mean, variance.
- Multi-scale structures.

Introduction & Motivation



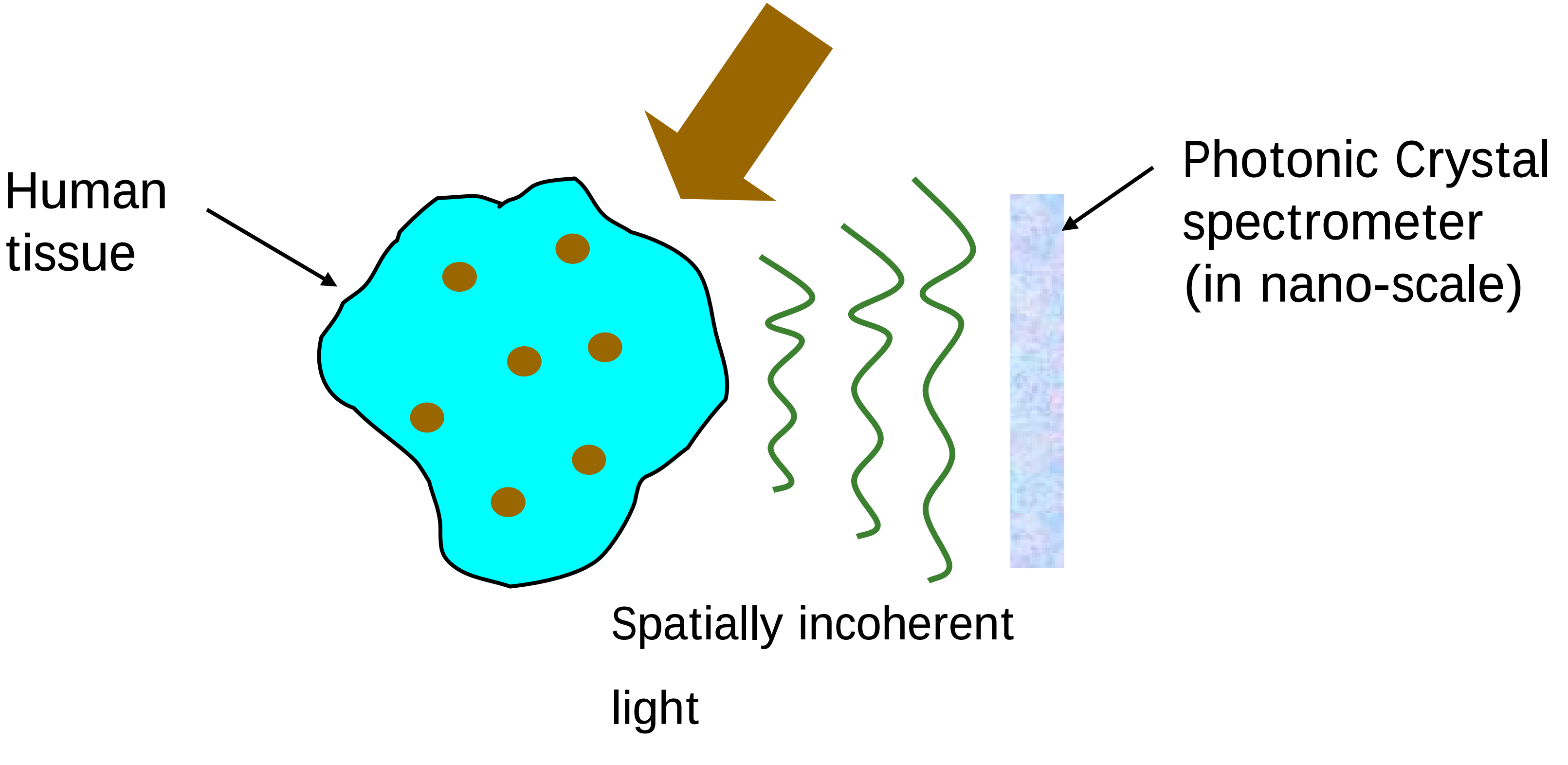
Spatially incoherent source: $\langle J^*(y_i, t) J(y_j, t) \rangle = \delta(y_i - y_j, t)$

Such as diffuse light in optics.

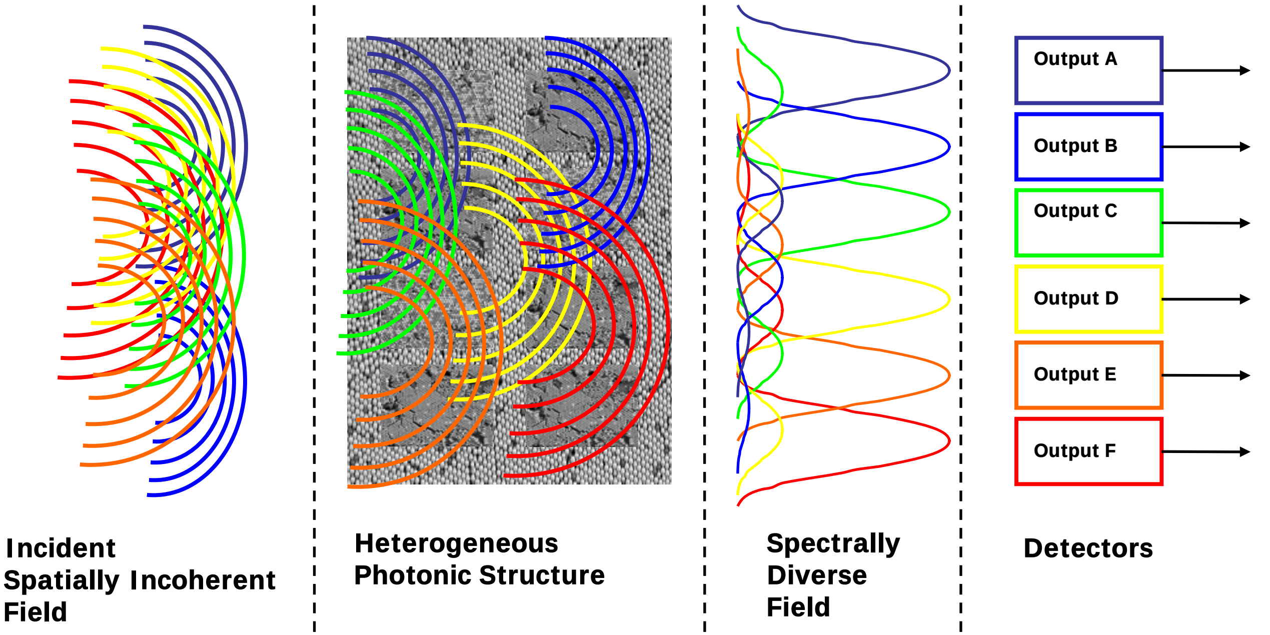
Introduction & Motivation

- Applications in sensing

Raman spectroscopy for bio and environmental sensing



Photonic Crystal Spectrometer

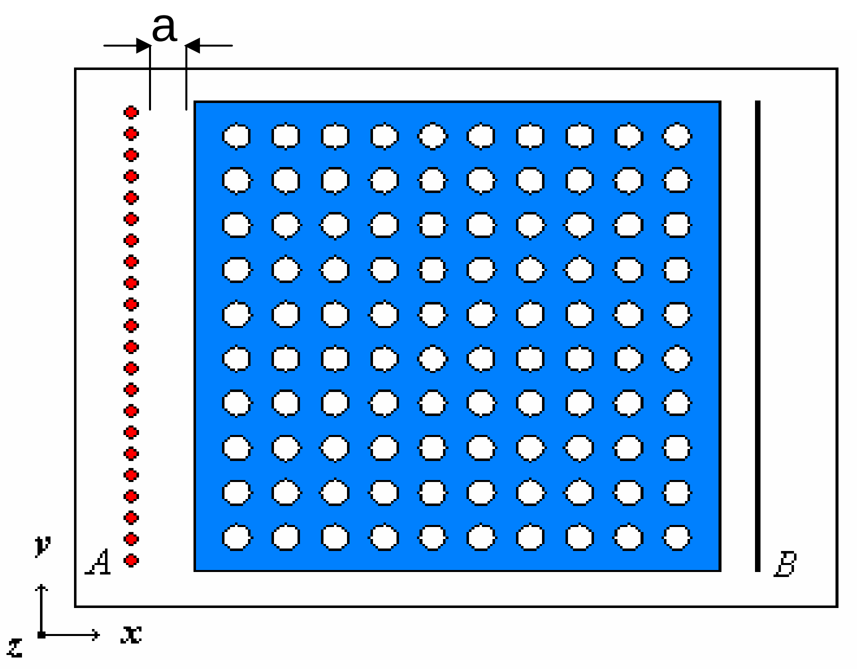


Multiplex multimodal spectrometer

Introduction & Motivation

Input Source (incoherent) at A

$$J(y,t)$$



Output at B (electric field intensity)

$$E^2(y,t)$$

- Photonic Crystal (designed) as the medium
- goal: model the incoherent source and simulate output
- First step in the design of Photonic Crystal spectrometers

  Optimal design of the shapes of Photonic Crystals for largest band gap (Kao-Osher-Yablonovitch, 05)
- Wave propagation is governed by Maxwell equations

Maxwell Equation

- Maxwell equations:

$$\nabla \times \mathbf{E}(\mathbf{r},t) = -\mu \frac{\partial \mathbf{H}(\mathbf{r},t)}{\partial t}$$

$$\nabla \times \mathbf{H}(\mathbf{r},t) = \varepsilon(\mathbf{r}) \frac{\partial \mathbf{E}(\mathbf{r},t)}{\partial t} + \mathbf{J}(\mathbf{r},t)$$

$$\nabla \cdot \mathbf{E} = 0$$

$$\nabla \cdot \mathbf{H} = 0$$

$\mathrm{E}(\mathrm{r},t)$ electric field

$\mathrm{H}(\mathrm{r},t)$ magnetic field

$\mathrm{J}(\mathrm{r},t)$ Input incoherent source

Helmholtz wave equation:

$$\nabla \times \nabla \times \mathbf{E}(\mathbf{r},t) = -\mu\varepsilon(\mathbf{r}) \frac{\partial^2 \mathbf{E}(\mathbf{r},t)}{\partial t^2} - \mu \frac{\partial \mathbf{J}(\mathbf{r},t)}{\partial t}$$

Helmholtz wave equation

- z-invariant structure implies
  - two sets of decoupled equations
  - Transverse Magnetic (TM) (E_z,H_x,H_y)
  - Transverse Electric (TE) (H_z,E_x,E_y)
  - 3D space structure reduces to 2D
  - Helmholtz TM wave equation:

$$(E(x,y,t))_{xx} + (E(x,y,t))_{yy} - \mu\varepsilon(x,y)(E(x,y,t))_{tt} = \mu(J(x,y,t))_{t}$$

PDE's are linear.

Direct Method for PC Spectrometer

- Incoherent property implies the direct (brute-force) method.

- Input nonzero point source $J^p(y_i, t)$ at y_i, and

  $J^p(y_j, t) = 0, (j \neq i).$

- Compute output electric field at B $E_i^p(y, t)$

- Total electric intensity at B: $E^2(x_B, y, t) = \sum_i (E_i^p(x_B, y, t))^2.$

- Why point source? Non-point sources, such as plane waves, lead to coherent outputs. $(\sum_i E_i^p)^2 = \sum_i (E_i^p)^2 + \sum_{i,j} E_i^p E_j^p$

- Pro: correct physics (linear equations + incoherent outputs).

- Con: very inefficient.

A Stochastic Model

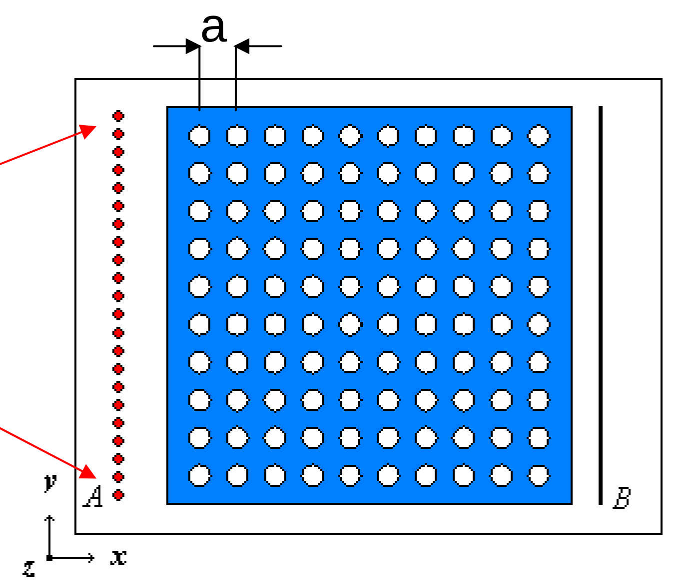
$$(E(x,y,t))_{xx} + (E(x,y,t))_{yy} - \mu\varepsilon(x,y)(E(x,y,t))_{tt} = \mu(J(x,y,t))_t$$

- Spatially incoherent source

$$J_z(x_A, y, t) = X(y)V(t)$$

?

$$V(t) = \sin(\omega(t-t_0))\exp\left(-\left(\frac{t-t_0}{T}\right)^2\right)$$



10ax10a Photonic Crystal as the simulation medium

- Stochastic model

$$X(y) = dW(y), \qquad W(y)$$ Brownian Motion.

- More general: $J_t(x,y,t) = f(x,y,t)dW(x,y,t),$

Stochastic Helmholtz Wave Equations

$$(E(x,y,t))_{xx} + (E(x,y,t))_{yy} - \mu\varepsilon(x,y)(E(x,y,t))_{tt} = \mu(J(x,y,t))_t$$

- Current density is a stochastic source.
- Solution for electric field is random.
- Monte Carlo simulation is slow, and hard to recover the incoherent properties
- Our strategy: WCE.

Monte Carlo

- **Not many computational methods available.**
- **Traditional methods, Monte Carlo (MC) simulations**,
  - Solve the equations realization by realization.
  - Each realization, the equations become deterministic and solved by classical methods.
  - The solutions are treated as samples to extract statistical properties.

Monte Carlo

- **MC can be very expensive:**
  - Has slow convergence, governed by law of large numbers $O(\frac{1}{\sqrt{n}})$, and the convergence is not monotone.(n is the number of MC realizations)

  - Need to resolve the fine scales in each realization to obtain the small scale effects on large scales, while only large scale statistics are of interests, such as long time and large scale behaviors.

  - Hard to estimate errors

  - Must involve random number generators, which need to be carefully chosen.

Wiener Chaos Expansions

- **Goal:** Design efficient numerical methods.
- Separate the deterministic properties from randomness.
- Has better control on the errors.
- Avoid random number generators, all computations are deterministic.

Wiener Chaos Expansions

- Functions $u(t, x, dW)$ depends on Brownian motion W.

- W contains infinitely many independent Gaussian random variables, is time and/or spatial dependent.

•WCE: decompose $u(t, x, dW)$ by orthogonal polynomials, similar to a spectral method, but for random variables.

Wiener Chaos Expansions

- $m_i(s)$ any orthonormal basis of $L^2(0,Y)$, such as harmonic functions in our computations.
- Define $\xi_i = \int_0^Y m_i(s)\,dW_s$, which are independent Gaussian.

- Let $\xi = (\xi_1, \xi_2, \cdots)$, construct Wick's products

$$T_\alpha(\xi) = \prod_{i=1}^{\infty} H_{\alpha_i}(\xi_i).$$

α is a multi-index, $H_{\alpha_i}(\xi_i)$ Hermite polynomials.

Wiener Chaos Expansions

•**Cameron-Martin(1947)**: any $u(t,x,dW)$ can be decomposed as

$$u(t,x,dW)=\sum_{\alpha} u_{\alpha}(t,x)T_{a}(\xi),$$

where

$$u_{\alpha}(t,x)=E(u(t,x,\xi)T_{\alpha}(\xi)).$$

Wiener Chaos Expansions

- Statistics can be reconstructed from Wiener Chaos coefficients
  - mean $Eu(t,x) = u_0(t,x),$
  - variance

$$E(u^2)(t,x) = \sum_{\alpha} \left| u_\alpha \right|^2$$

  - Higher order moments can be computed too.

Wiener Chaos Expansions

Properties of Wick's products:

$$E(T_0(\xi)) = 1,$$

$$E(T_\alpha(\xi)) = 0, \alpha \neq 0$$

$$E(T_\alpha T_\beta) = \begin{cases} 0 & \alpha \neq \beta \\ 1 & \alpha = \beta \end{cases}$$

Wiener Chaos Expansions

- Wiener Chaos expansions have been used in

•Nonlinear filtering, Zakai equation (Lototsky, Mikulevicius & Rozovskii, 97)

•Stochastic media problems (Matthies & Bucher, 99)

•Theoretical study of Stochastic Navier-Stokes equations (Mikulevicius & Rozovskii, 02)

Hermite Polynomial Expansions

- A long history of using Hermite polynomials in PDE's containing Gaussian random variables.
- Random flows: Orszag & Bissonnette (67), Crow & Canavan (70), Chorin (71,74), Maltz & Hitzl (79),
- Stochastic finite element: Ghanem, et al (91,99, …).
- Spectral polynomial chaos expansions: Karniadakis, Su and collaborators (a collection of papers), and …
- WCE for problems in fluid: Hou, Rozovskii, Luo, Zhou (04)

WCE for stochastic Helmholtz equation

- Expand the source and electric field:

$$J(y,t,dW) = \sum J_i(y,t)T_i(\xi)$$

$$E(x,y,t,dW) = \sum E_i(x,y,t)T_i(\xi)$$

- Take advantage of $dW(y) = \sum_{i=1}^{\infty} \xi_i m_i(y)$

$$J(y,t,dW) = \sum V(t)m_i(y)\xi_i$$

Only Gaussian (linear)

- Equation is linear, so electric field has expansion

$$E(x,y,t,dW) = \sum E_i(x,y,t)\xi_i$$

WCE for stochastic Helmholtz equation

- The stochastic equation is converted into a collection (decoupled) of deterministic Helmholtz equations

$$(E_i(x,y,t))_{xx} + (E_i(x,y,t))_{yy} - \mu\varepsilon(x,y)(E_i(x,y,t))_{tt} = \mu(V(t))_t m_i(y)$$

- Standard numerical methods, such as finite difference time domain (FDTD) in our simulation, can be applied.

WCE for stochastic Helmholtz equation

- WCE coefficients $E_i(x, y, t)$ are coherent!

- The electric field intensity at output is computed by

$$E^2(y,t) = \sum_i (E_i^p(y,t))^2 = \sum_i E_i^2(y,t).$$

WCE for stochastic Helmholtz equation

- The electric fields from point sources $E_i^p(x,y,t)$ can be recovered by

$$E_i^p(x,y,t) = \sum_j m_j(y_i) E_j(x,y,t)$$

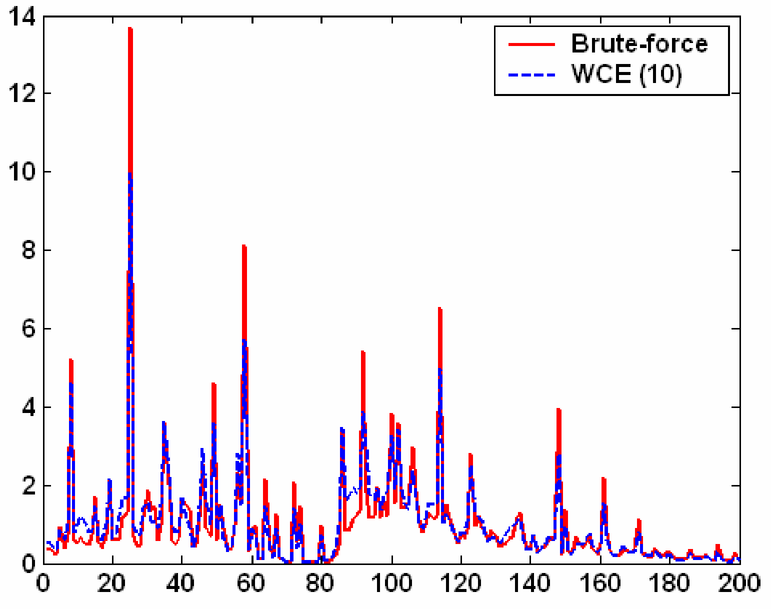
- Other moments can be computed by point source solutions in the standard ways.
- Under relative general conditions, WCE coefficients decay quickly,

$$\|E_i\| \le O\left(\frac{1}{i^r}\right),$$

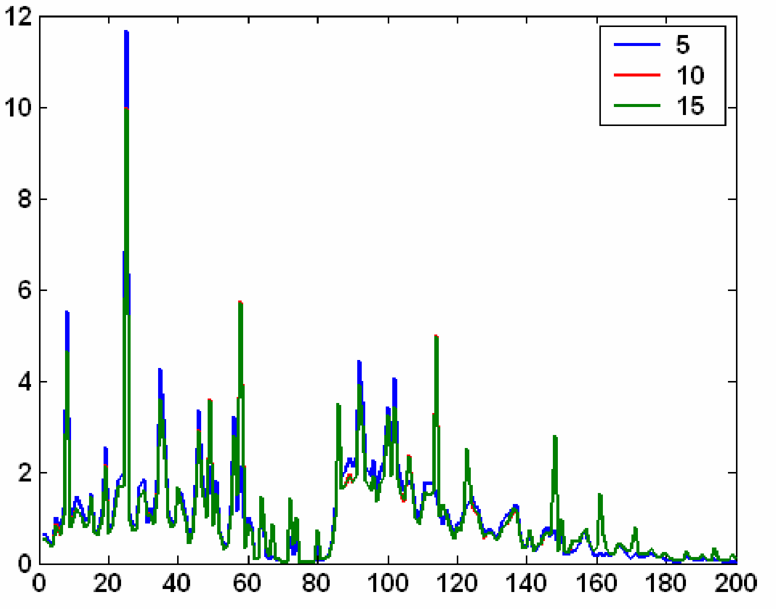
r Related to the smoothness of the solutions.

Simulation of a spatially incoherent source

Comparison of the direct method (brute-force) simulation and the WCE method



Convergence of the WCE method

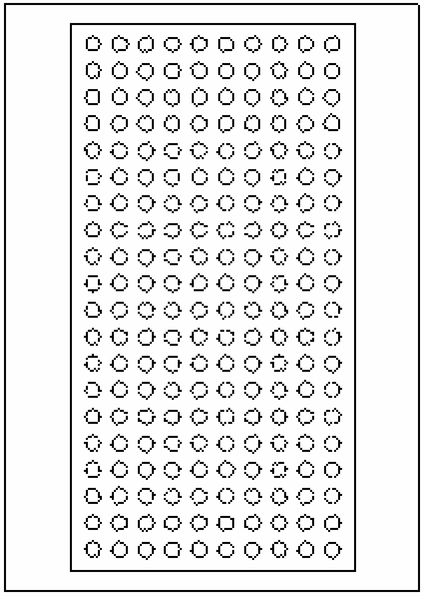


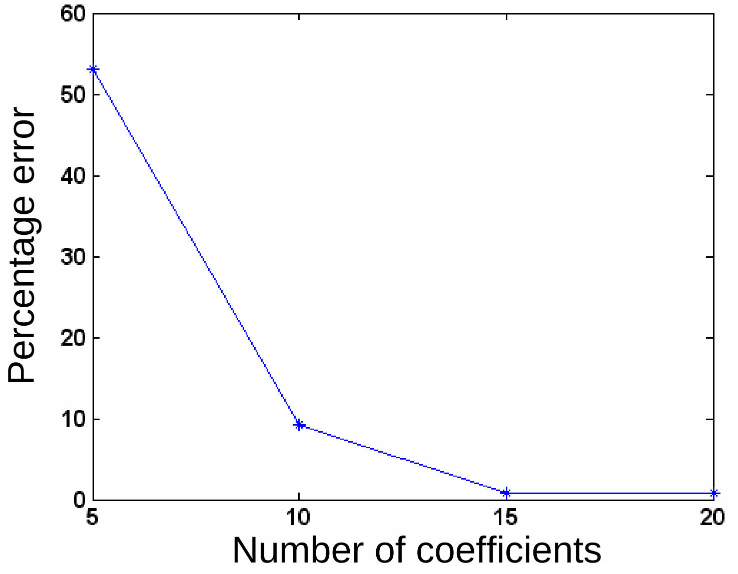
Extremely fast convergence for 10ax10a example

Simulation of a spatially incoherent source (3)

For a 20ax10a example (doubled sized)

20ax10a





For 15 coefficients the gain in simulation time is 32, i.e., 32 times faster simulation

Less than 1% error and more than one order of magnitude faster simulation,
Over 2 order of magnitude faster simulations for practical photonic crystals.

Conclusion

- Proposed a stochastic model for incoherent source

- Design a fast numerical method based on WCE to simulate the incoherent source for photonic crystals.

- The method can be coupled with other fast Maxwell equations solvers.

- More than 2 order of magnitude faster simulations can be achieved for practical structures.

- The model and method are general and can be applied to other types of stochastic problems involving incoherent sources.