Coupling Interface Method for Interface Problems

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Outline

- Introduction of Interface problems
- Coupling Interface Method for elliptic interface problems
- Coupling Interface Method for wave-guide modes of surface plasmon
- Concluding Remarks

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- Introduction of interface problems
- Coupling Interface Method for elliptic interface problem
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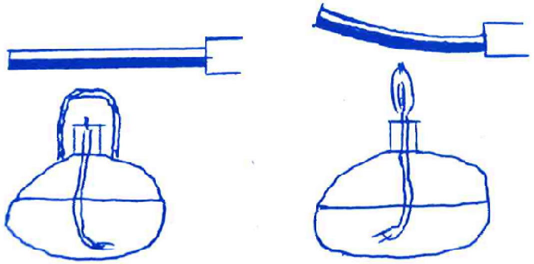
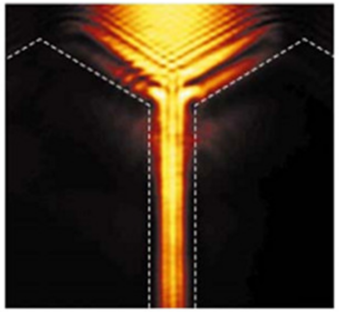
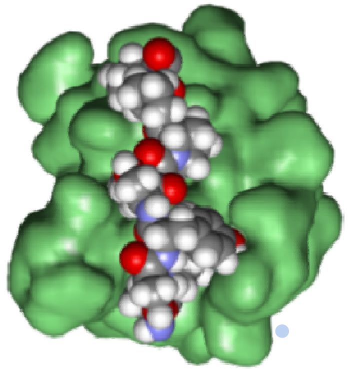
Interface Problems

- Interface problems appears in many fields such as fluid dynamics, solid mechanics, electrodynamics, material sciences, biochemistry, and etc..

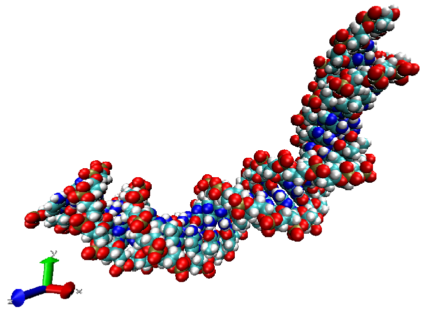




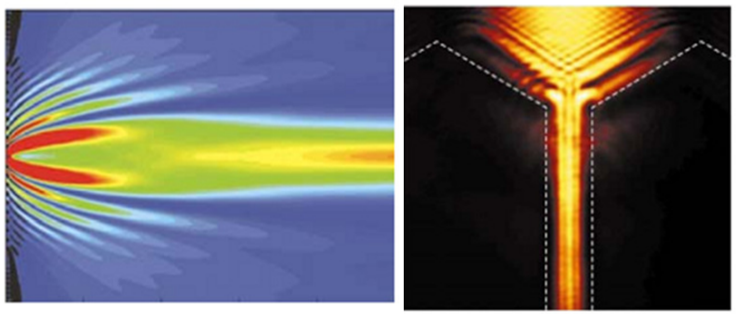


Interface Problems: Two examples

- Molecules in ionic solution:
  Poisson-Boltzmann Equation



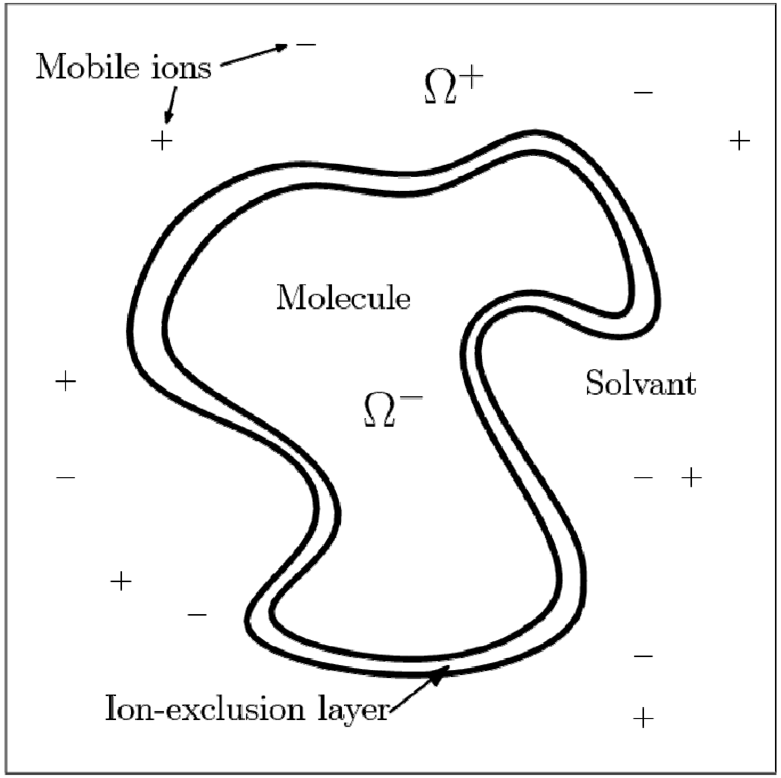
- Surface plasmon:
  Maxwell's Equations



quoted from the article: Nature, vol. 424, p. 824, 2003.

Molecules in ionic solution

- A continuum model for computing the electrostatic potential in an ionic solution.
- Based on Gauss' law and Boltzmann distribution law.



Poisson-Boltzmann Equation

$$\nabla \cdot (\varepsilon(\mathbf{r}) \nabla \psi(\mathbf{r})) = \underbrace{-\sum_i c_i z_i q \lambda(\mathbf{r}) \exp\left(\frac{-z_i q \psi(\mathbf{r})}{k_B T}\right)}_{\text{ions}} \underbrace{- \sum_j z_j q \delta(\mathbf{r} - \mathbf{r}_j)}_{\text{molecules}}$$

- $\mathbf{r}$: location
- ε : dielectric coefficient
- ψ : electrostatic potential (unknown)
- c_i : concentration of the i-th ion at a distance of infinity
- z_i, z_j : the number of charges of the i-th ion, j-th point charge
- q : charge of a proton
- k_B : Boltzmann constant
- T : temperature
- λ : accessibility to the ions in the solution. 1 in the solution.
- δ : delta function

Linearized Poisson-Boltzmann Equation

$$\nabla\cdot(\varepsilon(\mathbf{r})\nabla\psi(\mathbf{r})) = -\sum_i c_i z_i q \lambda(\mathbf{r}) \exp\left(\frac{-z_i q \psi(\mathbf{r})}{k_B T}\right) - \sum_j z_j q \delta(\mathbf{r}-\mathbf{r}_j)$$

- Debye-Hückel approximation: when $z_i q \psi << k_B T$

sufficiently low concentrations of ions

$$\exp\left(\frac{-z_i q \psi(\mathbf{r})}{k_B T}\right) \approx 1 - \frac{z_i q \psi(\mathbf{r})}{k_B T}$$

- Electro-neutrality: $\sum_i c_i z_i q \lambda(\mathbf{r}) = 0$

$$\nabla\cdot(\varepsilon(\mathbf{r})\nabla\psi(\mathbf{r})) = \left(\sum_i \frac{c_i z_i^2 q^2}{k_B T}\lambda(\mathbf{r})\right)\psi(\mathbf{r}) - \sum_j z_j q \delta(\mathbf{r}-\mathbf{r}_j)$$

Model problem

- Governing equation:

$$-\nabla\cdot(\varepsilon(\mathbf{r})\nabla u(\mathbf{r}))+Ku(\mathbf{r})=f$$

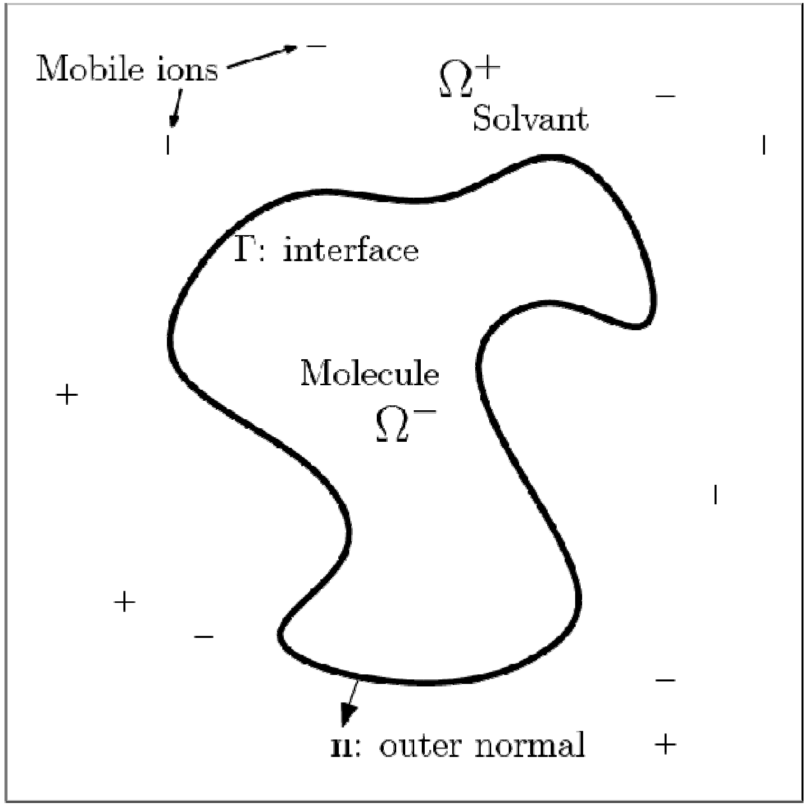
- Dielectric coefficient:

$$\varepsilon(\mathbf{r})=\begin{cases}\varepsilon^-, \mathbf{r}\in\Omega^-\\ \varepsilon^+, \mathbf{r}\in\Omega^+\end{cases}$$

- Interface conditions:

$$[u]_\Gamma=0, [\varepsilon\nabla u\cdot\mathbf{n}]_\Gamma=0$$

- No ion-exclusion layer



Some approaches

- Body-fitting approaches
  - W. Wang, A jump condition capturing finite difference scheme for elliptic interface problems
- Finite element approaches
  - Z. Li, T. Lin, X. Wu, New Cartesian grid methods for interface problems using the finite element formulation
  - J. Huang, J. Zou, A mortar element method for elliptic problems with discontinuous coefficients
- Finite difference approaches
  - A. Tornberg, B. Engquist, Regularization techniques for numerical approximation of PDEs with singularities
  - C. Peskin, The immersed boundary method
  - R. Leveque, Z. Li, The immersed interface method for elliptic equations with discontinuous coefficients and singular sources
  - Y. Zhou, S. Zhao, M. Feig, G. Wei, High order matched interface and boundary method for elliptic equations with discontinuous coefficients and singular sources

What are the problems?

- Regularization techniques: simple but they are only first-order accurate.

- Immersed interface method: The discretization may not exist even the maximum principal preserving scheme is used.

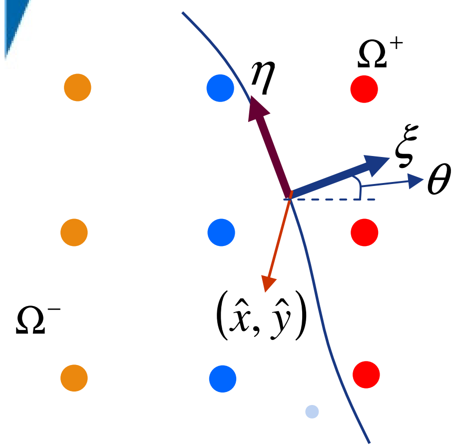
- High order matched interface and boundary method: The stencil is large. It is not suitable for complex interfaces.

Immersed interface method (2D)

- Second order Taylor expansion at an interface point with a local coordinate (ξ, η). (12 unknowns)

$$\begin{cases} \xi &= (x-\hat{x})\cos\theta + (y-\hat{y})\sin\theta \\ \eta &= -(x-\hat{x})\sin\theta + (y-\hat{y})\cos\theta \end{cases}$$

- Rewrite the derivatives in one side

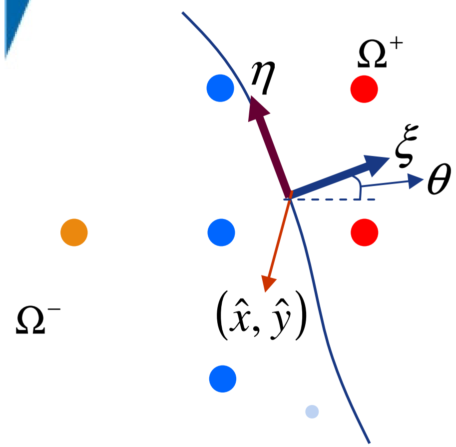


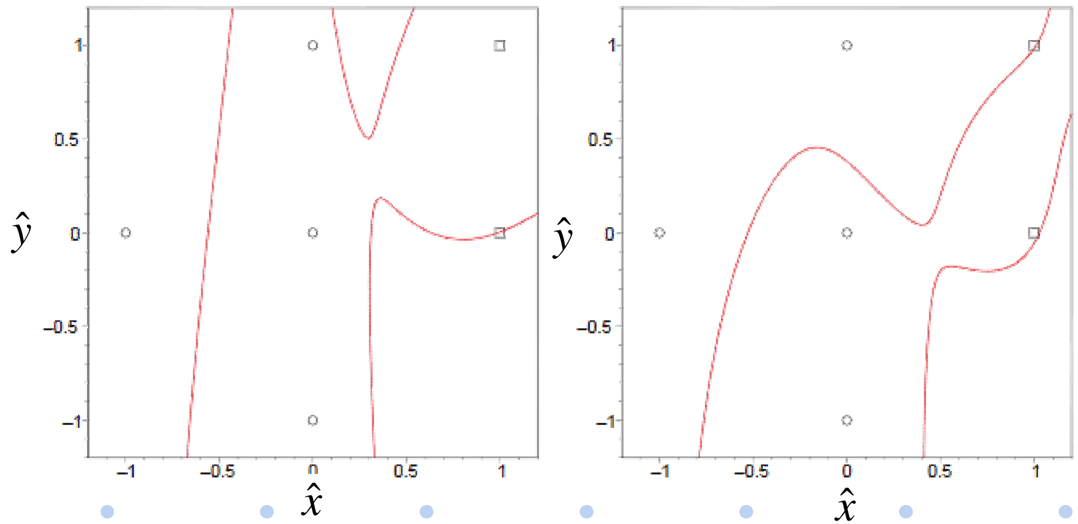
$$\begin{bmatrix} u^+ \\ u^+_\xi \\ u^+_\eta \\ u^+_{\xi\xi} \\ u^+_{\eta\eta} \\ u^+_{\xi\eta} \end{bmatrix} = \boldsymbol{R} \begin{bmatrix} u^- \\ u^-_\xi \\ u^-_\eta \\ u^-_{\xi\xi} \\ u^-_{\eta\eta} \\ u^-_{\xi\eta} \end{bmatrix} + \begin{bmatrix} \tau \\ \sigma/\varepsilon^+ \\ \tau_\eta \\ [f]/\varepsilon^+ - \tau_{\eta\eta} \\ \tau_{\eta\eta} \\ \sigma_\eta/\varepsilon^+ \end{bmatrix} \quad \boldsymbol{R} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & \rho & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & (\rho-1)\kappa & 0 & \rho & (\rho-1) & 0 \\ 0 & (1-\rho)\kappa & 0 & 0 & 1 & 0 \\ 0 & 0 & (1-\rho)\kappa & 0 & 0 & \rho \end{bmatrix}$$

$\tau = [u], \sigma = [\varepsilon \nabla u \cdot \mathbf{n}], \rho = \dfrac{\varepsilon^+}{\varepsilon^-}$, κ is the curvature at the interface point.

Immersed interface method (2D)

- With 6 grid values, the immersed interface method solve a 6x6 matrix to make the truncation error of $u_{xx} + u_{yy}$ to be $O(h)$. However, the matrix may not be solvable in some cases.

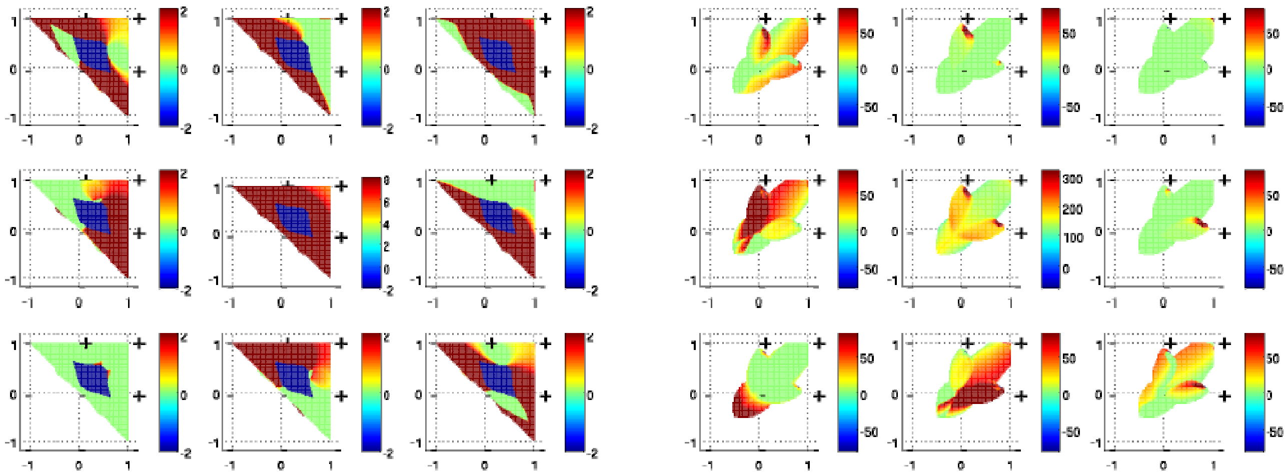




(a) $\rho = 1/40,\ \kappa = 2,\ \theta = \pi/6$ (b) $\rho = 40,\ \kappa = 2,\ \theta = \pi/6$

Immersed interface method (2D)

- Maximum principle preserving scheme: They use 9 grid values to find better coefficients. However, they need to solve a linear programming problem and the coefficients are not feasible in some cases.



(a) $\rho = 1/40,\ \kappa = 2,\ \theta = \pi/4$ (b) $\rho = 40,\ \kappa = 2,\ \theta = \pi/4$

Our approach: coupling interface method

- Finite difference approach on Cartesian grid.
- Dimension-by-dimension approach.
- The information of each dimension is coupled by the interface conditions.
- Advantages:
  - Accuracy: second-order in maximum norm.
  - Simplicity: smaller size of stencil, easy to program.
  - Robustness: capable to handle complex interfaces.
  - Speed: linear computational complexity

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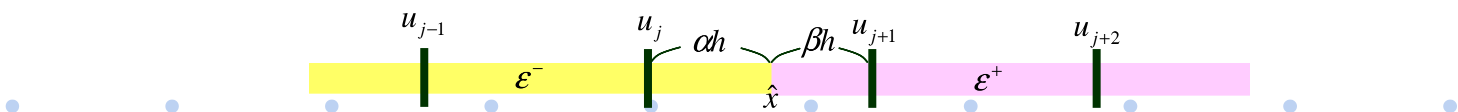
Coupling Interface Method (CIM2): 1D

- Governing equation: $-\varepsilon u'' = f$
- Suppose the interface is located in $[x_j, x_{j+1})$
- Standard finite difference method on interior points.

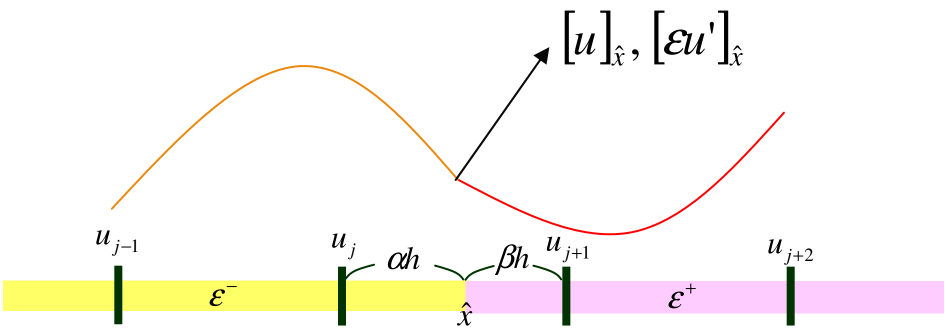
$$
\begin{aligned}
u''(x_i) &= \lim_{h\to 0}\frac{1}{h^2}\left(u(x_i-h)-2u(x_i)+u(x_i+h)\right)\\
&= \frac{1}{h^2}\left(u(x_i-h)-2u(x_i)+u(x_i+h)\right)+O\left(h^2\right)\\
&\approx \frac{1}{h^2}\left(u_{i-1}-2u_i+u_{i+1}\right) \quad \text{when } i\neq j,\ j+1
\end{aligned}
$$



Coupling Interface Method (CIM2): 1D

- Quadratic approximations on both side of the interface.

$$u(x)=\begin{cases} u_j+\dfrac{(u_j-u_{j-1})}{h}(x-x_j)+\dfrac{1}{2}u_j''(x-x_j)(x-x_{j-1})+O(h^3),\ x<\hat{x} \\ u_{j+1}+\dfrac{(u_{j+2}-u_{j+1})}{h}(x-x_{j+1})+\dfrac{1}{2}u_{j+1}''(x-x_{j+1})(x-x_{j+2})+O(h^3),\ x>\hat{x} \end{cases}$$



Coupling Interface Method (CIM2): 1D

$$u(x)=\begin{cases} u_j+\dfrac{(u_j-u_{j-1})}{h}(x-x_j)+\dfrac{1}{2}u_j''(x-x_j)(x-x_{j-1})+O(h^3), & x<\hat{x} \\ u_{j+1}+\dfrac{(u_{j+2}-u_{j+1})}{h}(x-x_{j+1})+\dfrac{1}{2}u_{j+1}''(x-x_{j+1})(x-x_{j+2})+O(h^3), & x>\hat{x} \end{cases}$$

- A linear system of the second order derivatives are given by two interface conditions:

$$\begin{cases} [u]_{\hat{x}}=u(\hat{x}^+)-u(\hat{x}^-) \\ [\varepsilon u']_{\hat{x}}=\varepsilon^+u'(\hat{x}^+)-\varepsilon^-u'(\hat{x}^-) \end{cases}$$

$$\begin{cases} \dfrac{1}{2}(\alpha+\alpha^2)u_j''-\dfrac{1}{2}(\beta+\beta^2)u_{j+1}''=\dfrac{1}{h^2}\left(\alpha u_{j-1}-(1+\alpha)u_j+(1+\beta)u_{j+1}-\beta u_{j+2}-[u]_{\hat{x}}\right)+O(h) \\ \left(\dfrac{1}{2}+\alpha\right)\varepsilon^-u_j''+\left(\dfrac{1}{2}+\beta\right)\varepsilon^+u_{j+1}''=\dfrac{1}{h^2}\left(\varepsilon^-u_{j-1}-\varepsilon^-u_j-\varepsilon^+u_{j+1}+\varepsilon^+u_{j+2}-h[\varepsilon u']_{\hat{x}}\right)+O(h) \end{cases}$$

Coupling Interface Method (CIM2): 1D

- The second order derivatives can be approximated by the linear combination of four grid values and two interface conditions.

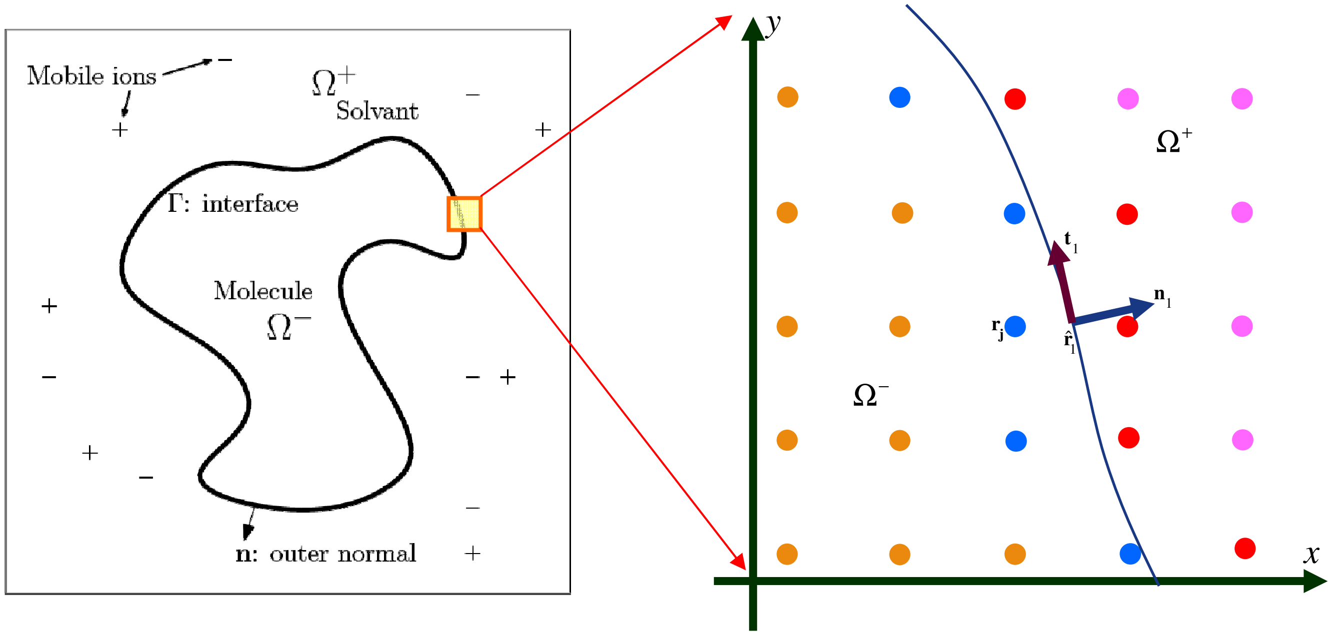
$$
\begin{cases}
\frac{1}{2}(\alpha+\alpha^2)u''_j - \frac{1}{2}(\beta+\beta^2)u''_{j+1} = \frac{1}{h^2}\left(\alpha u_{j-1} - (1+\alpha)u_j + (1+\beta)u_{j+1} - \beta u_{j+2} - [u]_{\hat{x}}\right) + O(h) \\
\left(\frac{1}{2}+\alpha\right)\varepsilon^- u''_j + \left(\frac{1}{2}+\beta\right)\varepsilon^+ u''_{j+1} = \frac{1}{h^2}\left(\varepsilon^- u_{j-1} - \varepsilon^- u_j - \varepsilon^+ u_{j+1} + \varepsilon^+ u_{j+2} - h[\varepsilon u']_{\hat{x}}\right) + O(h)
\end{cases}
$$

The determinant is positive and bounded when ε is positive

$$
\begin{cases}
u''_j = \frac{1}{h^2}\left(c_{j,-1}u_{j-1} + c_{j,0}u_j + c_{j,1}u_{j+1} + c_{j,2}u_{j+2} + \tau_j[u]_{\hat{x}} + \sigma_j h[\varepsilon u']_{\hat{x}}\right) + O(h) \\
\quad = \frac{1}{h^2}\left(\mathcal{L}_j(u_{j-1}, u_j, u_{j+1}, u_{j+2}) + \tau_j[u]_{\hat{x}} + \sigma_j h[\varepsilon u']_{\hat{x}}\right) + O(h) \\
u''_{j+1} = \frac{1}{h^2}\left(c_{j+1,-1}u_{j-1} + c_{j+1,0}u_j + c_{j+1,1}u_{j+1} + c_{j+1,2}u_{j+2} + \tau_{j+1}[u]_{\hat{x}} + \sigma_{j+1} h[\varepsilon u']_{\hat{x}}\right) + O(h) \\
\quad = \frac{1}{h^2}\left(\mathcal{L}_{j+1}(u_{j-1}, u_j, u_{j+1}, u_{j+2}) + \tau_{j+1}[u]_{\hat{x}} + \sigma_{j+1} h[\varepsilon u']_{\hat{x}}\right) + O(h)
\end{cases}
$$

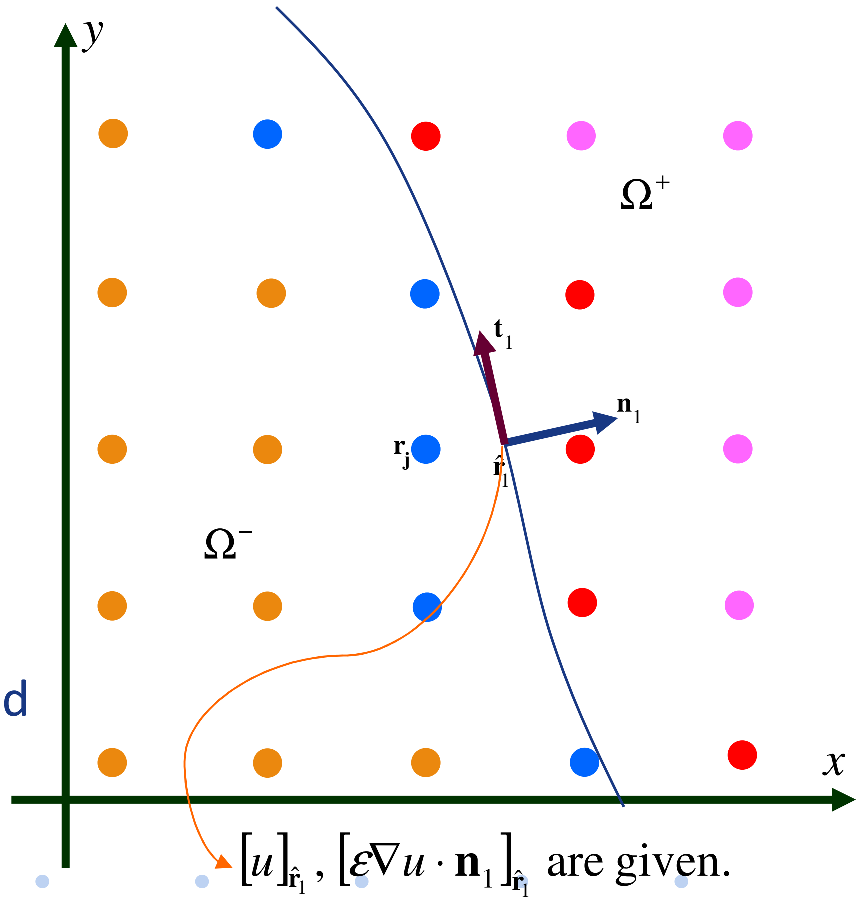
Coupling Interface Method (CIM2): 2D

- Governing equation: $-\varepsilon\left(\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}\right)=f$



Coupling Interface Method (CIM2): 2D

- Interior points (orange and pink disks): standard finite difference method.
- On-front points (blue and red disks): Coupling interface method.
- Interface conditions at the intersection of grid lines and the interface are needed.



Coupling Interface Method (CIM2): 2D

- Dimension-by-dimension approach

$$\frac{\partial^2 u}{\partial x^2}(\mathbf{r_j}) = \frac{1}{h^2}\left(\mathcal{L}_{\mathbf{j},1}\left(u_{i-1,j},u_{i,j},u_{i+1,j},u_{i+2,j}\right) + \tau_1[u]_{\hat{\mathbf{r}}_1} + \sigma_1 h\left[\varepsilon\frac{\partial u}{\partial x}\right]_{\hat{\mathbf{r}}_1}\right) + O(h)$$

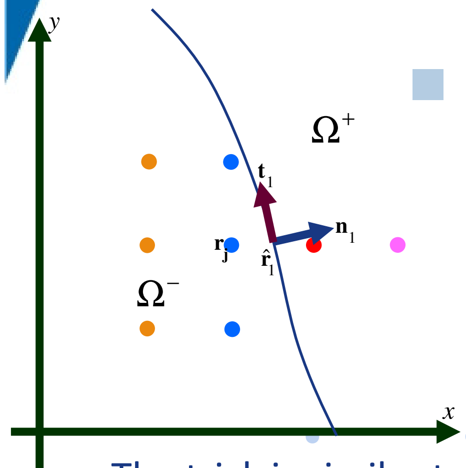
- Decomposition of the interface condition

$$\left[\varepsilon\frac{\partial u}{\partial x}\right]_{\hat{\mathbf{r}}_1} = [\varepsilon\nabla u\cdot\mathbf{n}_1]_{\hat{\mathbf{r}}_1}(\mathbf{n}_1\cdot\mathbf{e}_1) + \left(\varepsilon^+[\nabla u\cdot\mathbf{t}_1]_{\hat{\mathbf{r}}_1} + [\varepsilon]_{\hat{\mathbf{r}}_1}\nabla u^-(\hat{\mathbf{r}}_1)\cdot\mathbf{t}_1\right)(\mathbf{t}_1\cdot\mathbf{e}_1)$$

It can be derived from [u]

- Approximation of one-side gradient

$$\nabla u(\hat{\mathbf{r}}_1) = \begin{bmatrix} \frac{1}{h}\left(u_{i,j}-u_{i-1,j}\right) + \left(\frac{1}{2}+\alpha\right)h\frac{\partial^2 u}{\partial x^2}(\mathbf{r_j}) + O(h^2) \\ \frac{1}{2h}\left((1+\alpha)\left(u_{i,j+1}-u_{i,j-1}\right) - \alpha\left(u_{i-1,j+1}-u_{i-1,j-1}\right)\right) + O(h^2) \end{bmatrix}$$



The trick is similar to $\int e^x \sin x = e^x \sin x - \int e^x \cos x = e^x \sin x - e^x \cos x - \int e^x \sin x$

Coupling Interface Method (CIM2): 2D

- We get a equation for the second order partial derivative for x:

Positive and bounded when ε is positive

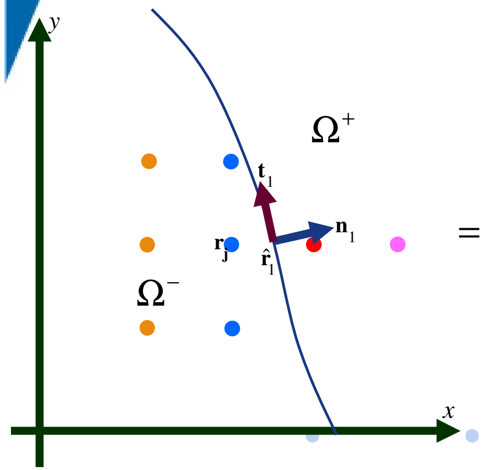
$$\left(1-\left(\frac{1}{2}+\alpha_1\right)\sigma_1[\varepsilon]_{\hat{\mathbf{r}}_1}(\mathbf{t}_1\cdot\mathbf{e}_1)^2\right)\frac{\partial^2 u}{\partial x^2}(\mathbf{r}_\mathbf{j})$$

$$=\frac{1}{h^2}\left(\mathcal{L}_{\mathbf{j},1}\left(u_{i-1,j},u_{i,j},u_{i+1,j},u_{i+2,j}\right)\right)+$$

$$\frac{1}{h^2}\sigma_1(\mathbf{t}_1\cdot\mathbf{e}_1)\left((u_{i,j}-u_{i-1,j})(\mathbf{t}_1\cdot\mathbf{e}_1)+\frac{1}{2}\left((1+\alpha)(u_{i,j+1}-u_{i,j-1})-\alpha(u_{i-1,j+1}-u_{i-1,j-1})\right)(\mathbf{t}_1\cdot\mathbf{e}_1)\right)+$$

$$\frac{1}{h^2}\left(\tau_1[u]_{\hat{\mathbf{r}}_1}+\sigma_1 h\left([\varepsilon\nabla u\cdot\mathbf{n}_1](\mathbf{n}_1\cdot\mathbf{e}_1)+\varepsilon^+[\nabla u\cdot\mathbf{t}_1](\mathbf{t}_1\cdot\mathbf{e}_1)\right)\right)+O(h)$$

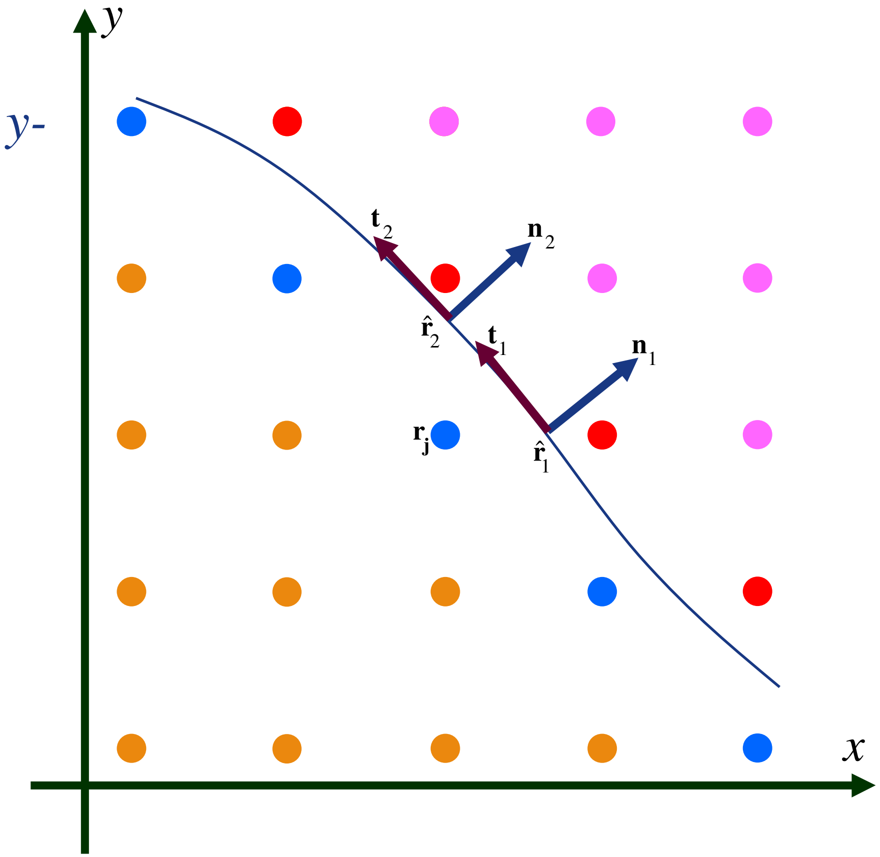
$$=\frac{1}{h^2}\left(\mathcal{L}_{\mathbf{j},1}u+\mathcal{T}_{\mathbf{j},1}u+\mathcal{J}_{\mathbf{j},1}\right)+O(h)$$



$$\frac{\partial^2 u}{\partial y^2}(\mathbf{r}_\mathbf{j})=\frac{1}{h^2}\left(u_{i,j-1}-2u_{i,j}+u_{i,j+1}\right)+O(h^2)$$

Coupling Interface Method (CIM2): 2D

- A complicated case: there are intersections in x- and y-directions.



Coupling Interface Method (CIM2): 2D

- Dimension-by-dimension approach

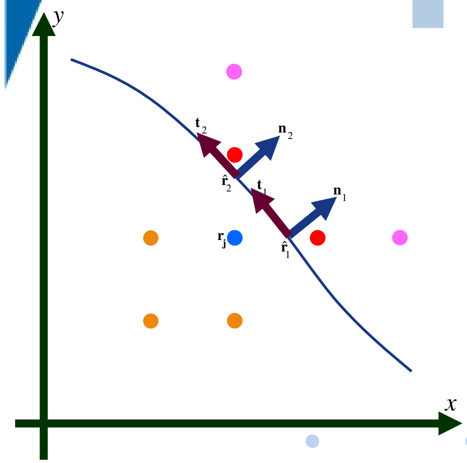
$$\frac{\partial^2 u}{\partial x^2}(\mathbf{r_j}) = \frac{1}{h^2}\left(\mathcal{L}_{\mathbf{j},1}\left(u_{i-1,j}, u_{i,j}, u_{i+1,j}, u_{i+2,j}\right) + \tau_1 [u]_{\hat{\mathbf{r}}_1} + \sigma_1 h \left[\varepsilon \frac{\partial u}{\partial x}\right]_{\hat{\mathbf{r}}_1}\right) + O(h)$$

$$\frac{\partial^2 u}{\partial y^2}(\mathbf{r_j}) = \frac{1}{h^2}\left(\mathcal{L}_{\mathbf{j},2}\left(u_{i,j-1}, u_{i,j}, u_{i,j+1}, u_{i,j+2}\right) + \tau_2 [u]_{\hat{\mathbf{r}}_2} + \sigma_2 h \left[\varepsilon \frac{\partial u}{\partial y}\right]_{\hat{\mathbf{r}}_2}\right) + O(h)$$

- Decomposition of the interface conditions

$$\left[\varepsilon \frac{\partial u}{\partial x}\right]_{\hat{\mathbf{r}}_1} = [\varepsilon \nabla u \cdot \mathbf{n}_1]_{\hat{\mathbf{r}}_1}(\mathbf{n}_1 \cdot \mathbf{e}_1) + \left(\varepsilon^+ [\nabla u \cdot \mathbf{t}_1]_{\hat{\mathbf{r}}_1} + [\varepsilon]_{\hat{\mathbf{r}}_1} \nabla u^-(\hat{\mathbf{r}}_1) \cdot \mathbf{t}_1\right)(\mathbf{t}_1 \cdot \mathbf{e}_1)$$

$$\left[\varepsilon \frac{\partial u}{\partial y}\right]_{\hat{\mathbf{r}}_2} = [\varepsilon \nabla u \cdot \mathbf{n}_2]_{\hat{\mathbf{r}}_2}(\mathbf{n}_2 \cdot \mathbf{e}_2) + \left(\varepsilon^+ [\nabla u \cdot \mathbf{t}_2]_{\hat{\mathbf{r}}_2} + [\varepsilon]_{\hat{\mathbf{r}}_2} \nabla u^-(\hat{\mathbf{r}}_2) \cdot \mathbf{t}_2\right)(\mathbf{t}_2 \cdot \mathbf{e}_2)$$



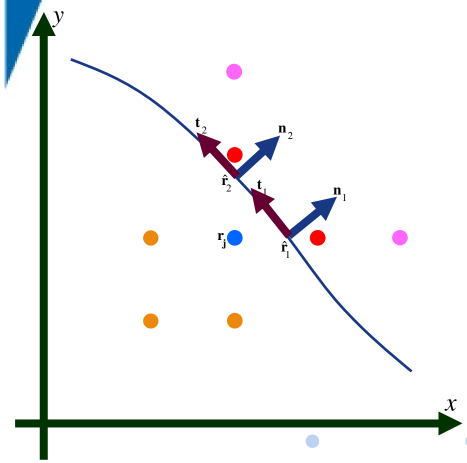
Coupling Interface Method (CIM2): 2D

- One-side gradients and cross derivative

$$\nabla u(\hat{\mathbf{r}}_1)=\begin{bmatrix}\frac{1}{h}\left(u_{i,j}-u_{i-1,j}\right)+\left(\frac{1}{2}+\alpha_1\right)h\frac{\partial^2 u}{\partial x^2}(\mathbf{r_j})+O\left(h^2\right)\\ \frac{1}{h}\left(u_{i,j}-u_{i,j-1}\right)+\frac{1}{2}h\frac{\partial^2 u}{\partial y^2}(\mathbf{r_j})+\alpha_1 h\frac{\partial^2 u}{\partial x\partial y}(\mathbf{r_j})+O\left(h^2\right)\end{bmatrix}$$

$$\nabla u(\hat{\mathbf{r}}_2)=\begin{bmatrix}\frac{1}{h}\left(u_{i,j}-u_{i-1,j}\right)+\frac{1}{2}h\frac{\partial^2 u}{\partial x^2}(\mathbf{r_j})+\alpha_2 h\frac{\partial^2 u}{\partial x\partial y}(\mathbf{r_j})O\left(h^2\right)\\ \frac{1}{h}\left(u_{i,j}-u_{i,j-1}\right)+\left(\frac{1}{2}+\alpha_2\right)h\frac{\partial^2 u}{\partial y^2}(\mathbf{r_j})+O\left(h^2\right)\end{bmatrix}$$

$$\frac{\partial^2 u}{\partial x\partial y}(\mathbf{r_j})=\frac{1}{h^2}\left(u_{i,j}-u_{i-1,j}-u_{i,j-1}+u_{i-1,j-1}\right)+O(h)$$



Coupling Interface Method (CIM2): 2D

- A coupling system for principal second order derivatives:

$$\begin{bmatrix} 1-\left(\frac{1}{2}+\alpha_1\right)\sigma_1[\varepsilon]_{\hat{\mathbf{r}}_1}(\mathbf{t}_1\cdot\mathbf{e}_1)^2 & -\frac{1}{2}\sigma_1[\varepsilon]_{\hat{\mathbf{r}}_1}(\mathbf{t}_1\cdot\mathbf{e}_1)(\mathbf{t}_1\cdot\mathbf{e}_2) \\ -\frac{1}{2}\sigma_2[\varepsilon]_{\hat{\mathbf{r}}_2}(\mathbf{t}_2\cdot\mathbf{e}_1)(\mathbf{t}_2\cdot\mathbf{e}_2) & 1-\left(\frac{1}{2}+\alpha_2\right)\sigma_2[\varepsilon]_{\hat{\mathbf{r}}_2}(\mathbf{t}_2\cdot\mathbf{e}_2)^2 \end{bmatrix} \begin{bmatrix} \frac{\partial^2 u}{\partial x^2}(\mathbf{r}_\mathbf{j}) \\ \frac{\partial^2 u}{\partial x^2}(\mathbf{r}_\mathbf{j}) \end{bmatrix}$$

$$= \frac{1}{h^2}\begin{bmatrix} (\mathcal{L}_{\mathbf{j},1}+\mathcal{T}_{\mathbf{j},1})u+\mathcal{J}_{\mathbf{j},1} \\ (\mathcal{L}_{\mathbf{j},2}+\mathcal{T}_{\mathbf{j},2})u+\mathcal{J}_{\mathbf{j},2} \end{bmatrix} + \begin{bmatrix} O(h) \\ O(h) \end{bmatrix}$$

The determinant is positive and bounded when ε is positive and mesh size is fine enough. ($\kappa h < C$)

CIM2: d dimensions

- Dimension-by-dimension approach

$$\frac{\partial^2 u}{\partial x_k^2}(\mathbf{r_j}) = \frac{1}{h^2}\mathcal{L}_{\mathbf{j},k}\left(u_{\mathbf{j}-\mathbf{e}_k}, u_{\mathbf{j}}, u_{\mathbf{j}+\mathbf{e}_k}, u_{\mathbf{j}+2\mathbf{e}_k}\right) + \tau_k [u]_{\hat{\mathbf{r}}_k} + \sigma_k [\varepsilon \nabla u \cdot \mathbf{e}_k]_{\hat{\mathbf{r}}_k}$$

- Project the interface condition on the normal and the selected tangential directions:

$$[\varepsilon \nabla u \cdot \mathbf{e}_k]_{\hat{\mathbf{r}}_k} = [\varepsilon \nabla u \cdot \mathbf{n}_k]_{\hat{\mathbf{r}}_k} \mathbf{n}_k \cdot \mathbf{e}_k + \left(\varepsilon^+ [\nabla u \cdot \mathbf{t}_k]_{\hat{\mathbf{r}}_k} + [\varepsilon]_{\hat{\mathbf{r}}_k} \nabla u^-_{\hat{\mathbf{r}}_k} \cdot \mathbf{t}_k\right) \mathbf{t}_k \cdot \mathbf{e}_k$$

- The one side gradient is approximated by the grid values and the second order derivatives (principal and cross):

$$\nabla u^-_{\hat{\mathbf{r}}_k} = \frac{1}{h}\left[u_{\mathbf{j}} - u_{\mathbf{j}-\mathbf{e}_k} + \frac{h^2}{2}\frac{\partial^2 u}{\partial x_k^2}(\mathbf{r_j}) + \alpha_k \boxed{\frac{\partial^2 u}{\partial x_k \partial x_\ell}(\mathbf{r_j})}\right]_{\ell=1}^{d}$$

Approximated by near-by grid values

A coupled system for principal derivatives

- A coupled system for principal second order derivatives

$$\mathbf{M}\left[\frac{\partial^2 u}{\partial x_k^2}(\mathbf{r}_\mathbf{j})\right]_{k=1}^{d} = \frac{1}{h^2}\left[\left(\mathcal{L}_{\mathbf{j},k} + \mathcal{T}_{\mathbf{j},k}\right)\mathbf{u} + \mathcal{J}_{\mathbf{j},k}\right]_{k=1}^{d}$$

- where
  - $\mathbf{M}_{k,\ell} = \delta_{k,\ell} - \sigma_k [\varepsilon]_{\hat{\mathbf{r}}_k}\left(\frac{1}{2} + \alpha_k \delta_{k,\ell}\right)(\mathbf{t}_k \cdot \mathbf{e}_k)(\mathbf{t}_k \cdot \mathbf{e}_\ell)$
  - $\mathcal{T}_{\mathbf{j},k}$: collection of grid values in the second and third steps.
  - $\mathcal{J}_{\mathbf{j},k}$: collection of the terms of interface conditions.

Determinant of M is positive and bounded when ε is positive and the mesh size is fine enough.

Comparisons with other methods (2D)

- The ratio of the dielectric coefficient is 1000

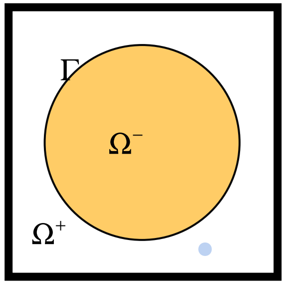
1:1000

N	CIM2 CPU	CIM2 $\|\nabla u - \nabla u_e\|_{\infty,\Gamma}$	CIM2 $\|u - u_e\|_\infty$	DIIM $\|u - u_e\|_\infty$	MIIM $\|u - u_e\|_\infty$
32	0.04	6.841×10^{-3}	2.732×10^{-4}	2.083×10^{-4}	5.136×10^{-4}
64	0.19	1.920×10^{-3}	3.875×10^{-5}	5.296×10^{-5}	8.235×10^{-5}
128	1.03	5.156×10^{-4}	5.337×10^{-6}	1.330×10^{-5}	1.869×10^{-5}
256	4.84	1.345×10^{-4}	7.241×10^{-7}	3.330×10^{-6}	4.026×10^{-6}
512	22.52	3.463×10^{-5}	9.891×10^{-8}	–	9.430×10^{-7}

1:0.001

N	CIM2 CPU	CIM2 $\|\nabla u - \nabla u_e\|_{\infty,\Gamma}$	CIM2 $\|u - u_e\|_\infty$	DIIM $\|u - u_e\|_\infty$	MIIM $\|u - u_e\|_\infty$
32	0.03	8.030×10^{0}	4.278×10^{-1}	4.971×10^{0}	9.346×10^{0}
64	0.18	1.829×10^{0}	1.260×10^{-1}	1.176×10^{0}	2.006×10^{0}
128	1.03	4.658×10^{-1}	3.773×10^{-2}	2.900×10^{-1}	5.808×10^{-1}
256	5.3	1.254×10^{-1}	1.365×10^{-2}	7.086×10^{-2}	1.374×10^{-1}
512	23.48	4.141×10^{-2}	2.446×10^{-3}	–	3.580×10^{-2}

$O(N^2)$ $O(h^2)$ $O(h^2)$



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Comparisons with other methods (2D)

- The ratio of the dielectric coefficient is 10

1:10

N	CPU	CIM2 $\|\nabla u - \nabla u_e\|_{\infty,\Gamma}$	CIM2 $\|u - u_e\|_\infty$	DIIM $\|u - u_e\|_\infty$	EJIIM $\|u - u_e\|_\infty$	MIIM $\|u - u_e\|_\infty$
20	0.00	1.557×10^{-2}	1.259×10^{-3}	5.378×10^{-4}	7.6×10^{-4}	–
40	0.02	4.714×10^{-3}	2.565×10^{-4}	1.378×10^{-4}	2.4×10^{-4}	4.864×10^{-4}
80	0.17	1.305×10^{-3}	5.215×10^{-5}	3.470×10^{-5}	7.9×10^{-5}	1.448×10^{-4}
160	0.74	3.462×10^{-4}	1.142×10^{-5}	8.704×10^{-6}	2.2×10^{-5}	3.012×10^{-5}
320	3.65	8.948×10^{-5}	2.725×10^{-6}	2.177×10^{-6}	5.3×10^{-6}	8.226×10^{-6}
640	15.86	2.276×10^{-5}	6.740×10^{-7}	–	–	2.060×10^{-6}

1:10

n	CPU	CIM $\|\nabla u - \nabla u_e\|_{\infty,\Gamma}$	CIM $\|u - u_e\|_\infty$	MIB $\|u - u_e\|_\infty$	IIM $\|u - u_e\|_\infty$
20	0.01	1.471×10^{-3}	3.158×10^{-4}	2.852×10^{-4}	2.167×10^{-3}
40	0.04	3.087×10^{-4}	7.622×10^{-5}	7.707×10^{-5}	5.000×10^{-4}
80	0.16	9.474×10^{-5}	2.036×10^{-5}	2.069×10^{-5}	1.131×10^{-4}
160	0.83	2.001×10^{-5}	4.973×10^{-6}	5.131×10^{-6}	2.748×10^{-5}
320	4.14	7.054×10^{-6}	1.329×10^{-6}	1.257×10^{-6}	6.781×10^{-6}

Comparisons with other methods (3D)

- The ratio of the dielectric coefficient is 1, 10, 1000

1:1

	CIM2				MIIM, 27 points	
N	CPU	$\|\nabla u - \nabla u_e\|_{\infty,\Gamma}$	$\|u_a - u_e\|_\infty / \|u_e\|_\infty$	Order	$\|u_a - u_e\|_\infty / \|u_e\|_\infty$	Order
26	1.52	1.005×10^{-2}	1.822×10^{-4}		1.247×10^{-3}	
52	20.5	3.685×10^{-3}	4.153×10^{-5}	2.133	3.979×10^{-3}	1.648
104	212	9.729×10^{-4}	9.529×10^{-6}	2.124	9.592×10^{-4}	2.052
208	2355	2.540×10^{-4}	2.230×10^{-6}	2.095	–	–

1:10

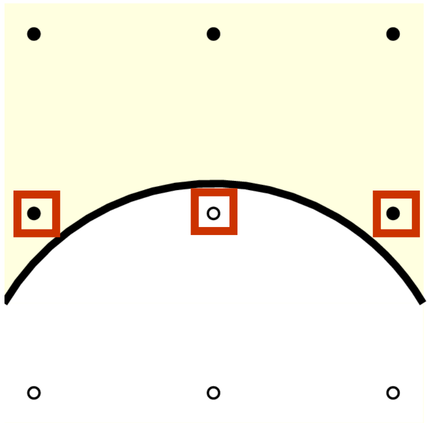
	CIM2				MIIM, 27 points	
N	CPU	$\|\nabla u - \nabla u_e\|_{\infty,\Gamma}$	$\|u_a - u_e\|_\infty / \|u_e\|_\infty$	Order	$\|u_a - u_e\|_\infty / \|u_e\|_\infty$	Order
26	1.45	7.174×10^{-3}	4.332×10^{-4}		1.525×10^{-3}	
52	19.14	2.693×10^{-3}	9.240×10^{-5}	2.229	5.240×10^{-4}	1.541
104	161	7.401×10^{-4}	1.636×10^{-5}	2.498	1.010×10^{-4}	2.375
208	1867	1.979×10^{-4}	3.330×10^{-6}	2.297	–	–

1:1000

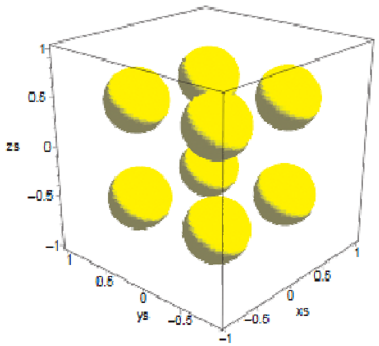
	CIM2				MIIM, 27 points	
N	CPU	$\|\nabla u - \nabla u_e\|_{\infty,\Gamma}$	$\|u_a - u_e\|_\infty / \|u_e\|_\infty$	Order	$\|u_a - u_e\|_\infty / \|u_e\|_\infty$	Order
26	1.48	6.825×10^{-3}	9.133×10^{-4}		3.845×10^{-3}	
52	24.54	2.594×10^{-3}	2.466×10^{-4}	1.889	1.111×10^{-3}	1.649
104	209	7.183×10^{-4}	3.447×10^{-5}	2.839	1.605×10^{-4}	2.791
208	3299	1.925×10^{-4}	4.727×10^{-6}	2.866	–	–

Complex interface

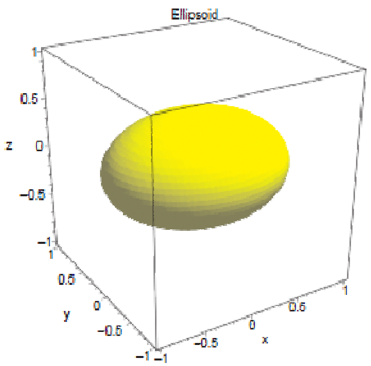
- If the interface is complex, CIM2 may not be applicable at some points.
- Exceptional points are those points that CIM2 cannot be applied. ➔ First order approximations (CIM1) of u at those exceptional points are used.
- Due to the number of the exceptional points are O(1) in practice, second order convergence of the solution can be maintained.



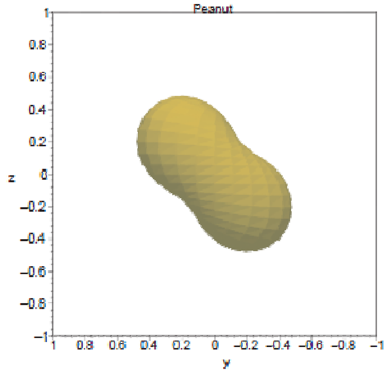
Complex interfaces



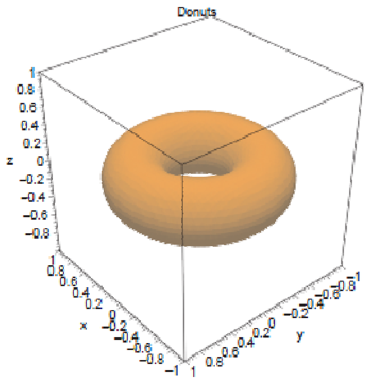
(a) 8 balls



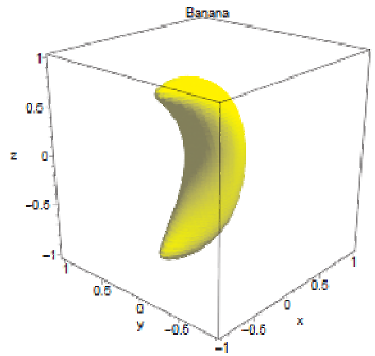
(b) Ellipsoid



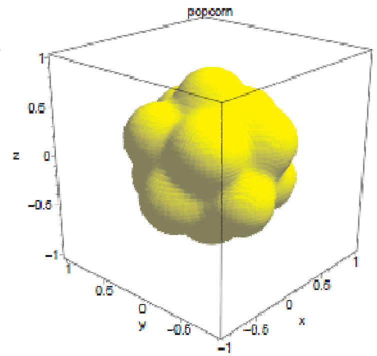
(c) Peanut



(d) Donut

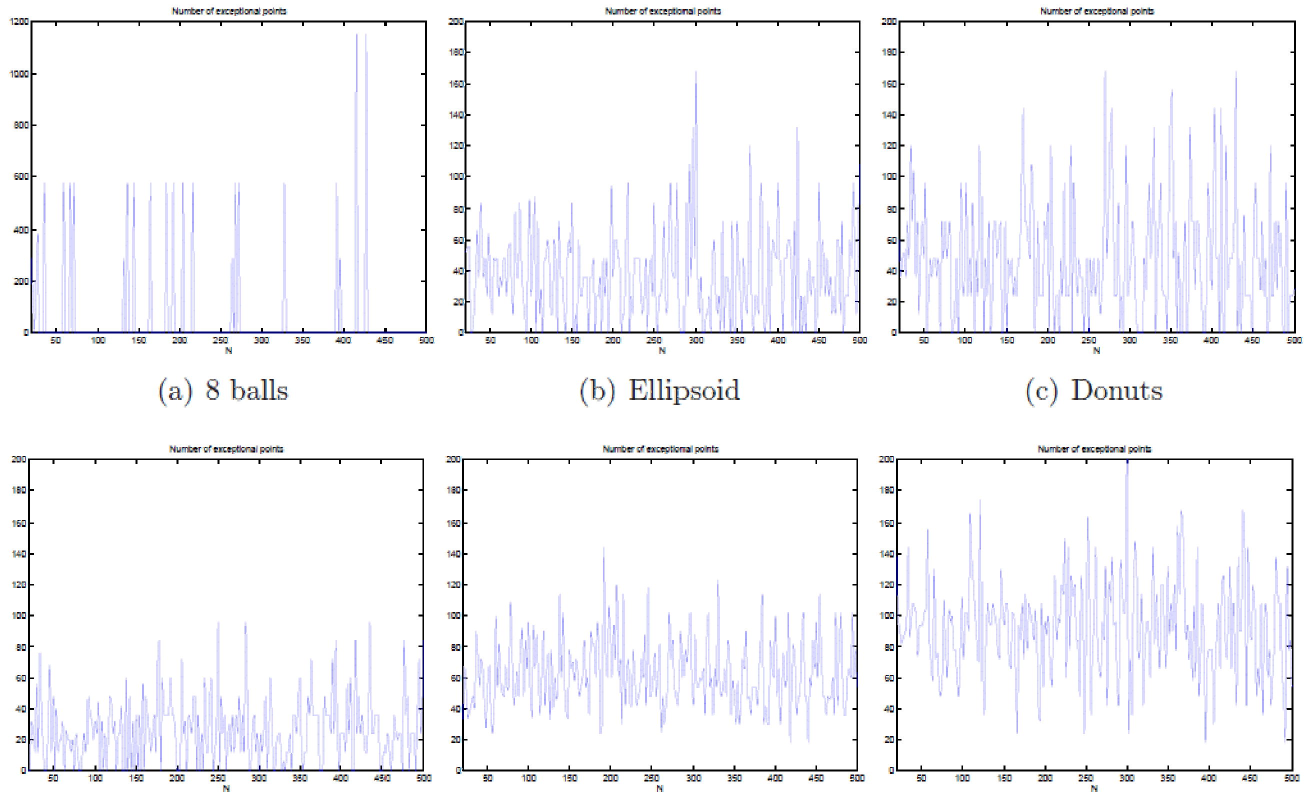


(e) Banana



(f) Popcorn

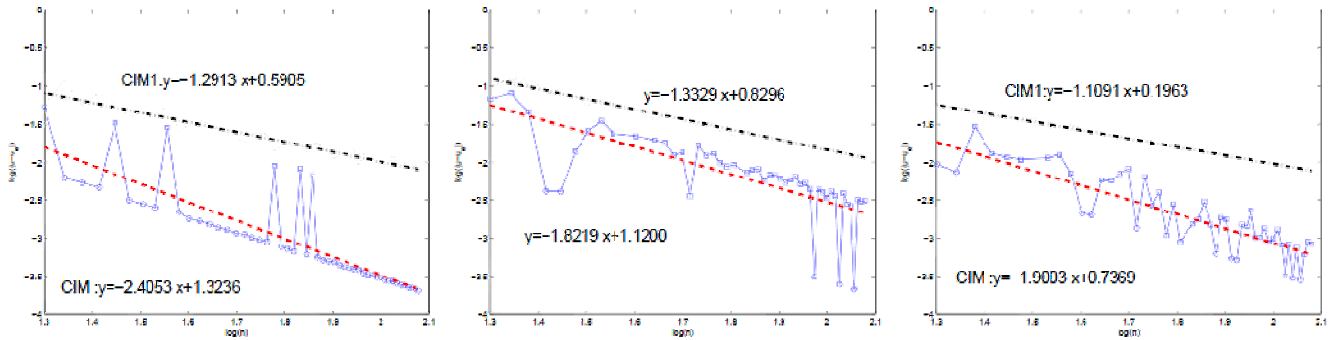
Number of exceptional points



(a) 8 balls (b) Ellipsoid (c) Donuts

(d) Peanut (e) Banana (f) Popcorn

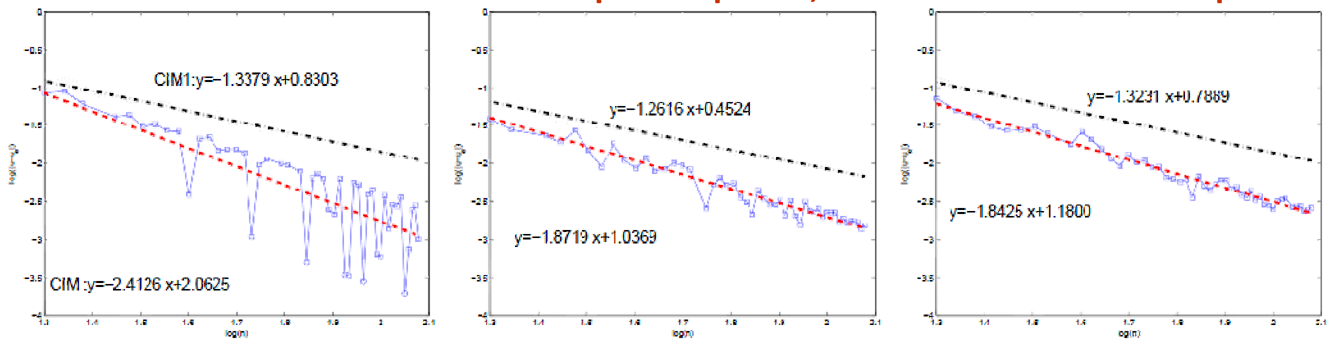
Convergence, with CIM1 and CIM2



(a) 8 balls (b) Ellipsoid (c) Peanut

Black: CIM1

Red: CIM1 at exceptional points, CIM2 at normal on-front points



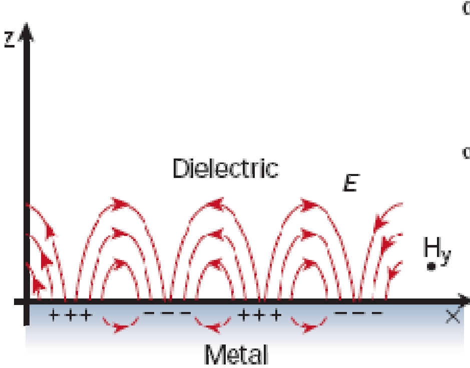
(d) Donut (e) Banana (f) Popcorn

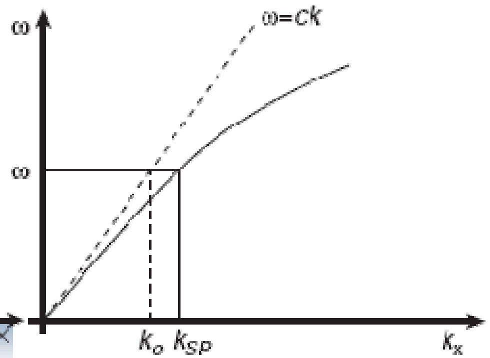
Outline

- Introduction of Interface problems
- Coupling Interface Method for elliptic interface problem
- Coupling Interface Method for wave-guide modes of surface plasmon
- Concluding Remarks

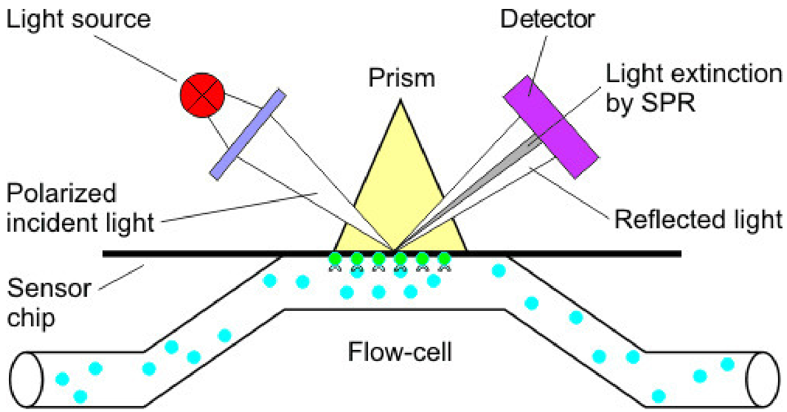
Surface plasmon

- Electromagnetic wave propagating along the interface between two different materials (dielectric and metal)





- Applications: magneto-optic data storage, microscopy, solar cells, sensors for detecting biological molecules, and plasmonic crystals



http://www.fz-juelich.de/isb/isb-1/protein-protein_interaction

CIM for wave-guide modes of SP

Wave-guide modes

- Suppose the waveguide is homogeneous in the z direction

$$\mathbf{E}(x,y,z,t)=(E_x,E_y,E_z)e^{i(k_z z-\omega t)}$$

$$\mathbf{H}(x,y,z,t)=(H_x,H_y,H_z)e^{i(k_z z-\omega t)}$$

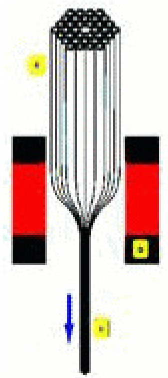
- Maxwell's equations

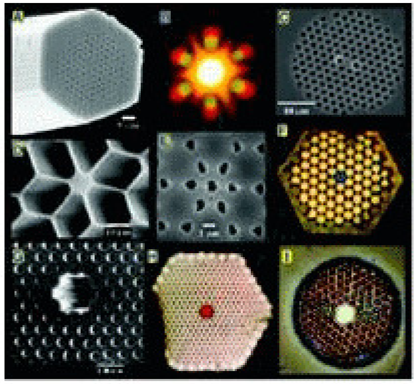
$$\nabla\cdot\mathbf{D}=\rho$$

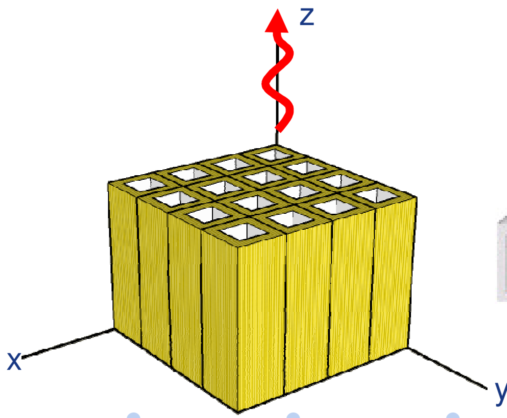
$$\nabla\cdot\mathbf{B}=0$$

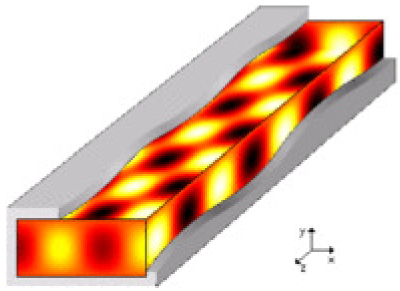
$$\nabla\times\mathbf{E}=-\frac{\partial\mathbf{B}}{\partial t}$$

$$\nabla\times\mathbf{H}=\mathbf{J}+\frac{\partial\mathbf{D}}{\partial t}$$









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Assumptions

- We assume that no charges and no currents.

$$\rho = 0, \mathbf{J} = 0$$

- Constitutive relations: isotropic and linear material.

$$\mathbf{D} = \varepsilon \mathbf{E}, \mathbf{B} = \mu \mathbf{H}$$

- Permittivity ε and permeability μ do not depend on the location in each material but may depend on the frequency.

Governing equations for z-component

- z-component: in x-y plane

$$\nabla_2 = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}\right)$$

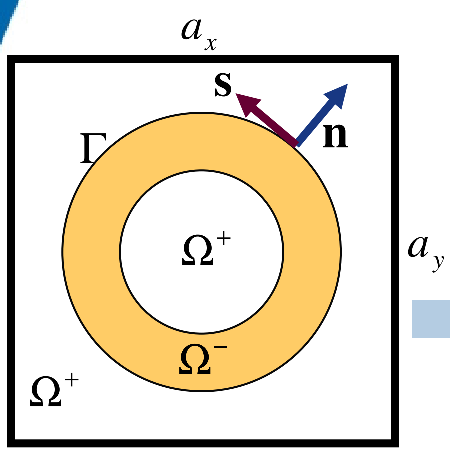
$$\nabla_2 \cdot \left(\frac{\omega\varepsilon\nabla_2 E_z}{\omega^2\varepsilon\mu - k_z^2}\right) + \nabla_2 \times \left(\frac{k_z \nabla_2 H_z}{\omega^2\varepsilon\mu - k_z^2}\right) = \omega\varepsilon E_z$$

$$\nabla_2 \cdot \left(\frac{\omega\mu\nabla_2 H_z}{\omega^2\varepsilon\mu - k_z^2}\right) - \nabla_2 \times \left(\frac{k_z \nabla_2 E_z}{\omega^2\varepsilon\mu - k_z^2}\right) = \omega\mu H_z$$

- Interface conditions: $[E_z]_\Gamma = 0, [H_z]_\Gamma = 0$

$$\left[\frac{\omega\varepsilon}{\omega^2\varepsilon\mu - k_z^2}\nabla_2 E_z \cdot \mathbf{n}\right]_\Gamma = -\left[\frac{k_z}{\omega^2\varepsilon\mu - k_z^2}\nabla_2 H_z \cdot \mathbf{s}\right]_\Gamma$$

$$\left[\frac{\omega\varepsilon}{\omega^2\varepsilon\mu - k_z^2}\nabla_2 H_z \cdot \mathbf{n}\right]_\Gamma = \left[\frac{k_z}{\omega^2\varepsilon\mu - k_z^2}\nabla_2 E_z \cdot \mathbf{s}\right]_\Gamma$$



- Boundary conditions: $E_z(x + a_x, y + a_y) = e^{i(k_x x + k_y y)} E_z$

$$H_z(x + a_x, y + a_y) = e^{i(k_x x + k_y y)} H_z$$

Eigenvalue problem

- Simple eigenvalue problem?

$$\left(\nabla_2^2 + \omega^2 \varepsilon\mu\right)E_z = k_z^2 E_z$$
$$\left(\nabla_2^2 + \omega^2 \varepsilon\mu\right)H_z = k_z^2 H_z$$

- With complicated interface conditions: the eigenvalue involves in the interface conditions.

$$\left[\frac{\omega\varepsilon}{\omega^2\varepsilon\mu - k_z^2}\nabla_2 E_z \cdot \mathbf{n}\right] + \left[\frac{k_z}{\omega^2\varepsilon\mu - k_z^2}\nabla_2 H_z \cdot \mathbf{s}\right] = 0$$
$$\left[\frac{\omega\varepsilon}{\omega^2\varepsilon\mu - k_z^2}\nabla_2 H_z \cdot \mathbf{n}\right] - \left[\frac{k_z}{\omega^2\varepsilon\mu - k_z^2}\nabla_2 E_z \cdot \mathbf{s}\right] = 0$$

Some approaches

- Plane wave expansion: most common used
  - Search in the frequency such that the zero-determinant of the matrix occurs for a given wave number.
- Finite difference time domain method
  - Calculate the dipole spectrum for each wave number and its resonance peaks gives frequencies after enough cycles.
- Multiple-scattering method
  - Solve a non-linear eigenvalue problem and search for a minimum of a cost function

They are not direct approaches.

Augmented Coupling Interface Method

- Direct approach:
  - Gives (all) wave number for a given frequency without searching.

- Integrate with interfacial operator approach:
  - Reduce the original problem to a quadratic eigenvalue problem by introducing an interfacial variable.

    Solve the problem with complicated interface conditions

- Adaptive-order strategy:
  - Interpolating polynomials of different orders on different sides of interfaces are used to avoid the singularity of the local linear system. It also enables us to handle complex interfaces.

    Solve the problem with sign-changed coefficients

Interfacial operator approach

$$\left[\frac{\omega\varepsilon}{\omega^2\varepsilon\mu-k_z^2}\nabla_2 E_z\cdot\mathbf{n}\right]_\Gamma+\left[\frac{k_z}{\omega^2\varepsilon\mu-k_z^2}\nabla_2 H_z\cdot\mathbf{s}\right]_\Gamma=0$$

$$\left[\frac{\omega\varepsilon}{\omega^2\varepsilon\mu-k_z^2}\nabla_2 H_z\cdot\mathbf{n}\right]_\Gamma-\left[\frac{k_z}{\omega^2\varepsilon\mu-k_z^2}\nabla_2 E_z\cdot\mathbf{s}\right]_\Gamma=0$$

- Re-arrange the above interface conditions to the following form:

$$\Lambda\left(\left[\frac{1}{\mu}\nabla E_z\cdot\mathbf{n}\right]_\Gamma+\frac{k_z}{\omega}\left[\frac{1}{\varepsilon\mu}\nabla H_z\cdot\mathbf{s}\right]_\Gamma\right)=k_z^2\left[\varepsilon\nabla E_z\cdot\mathbf{n}\right]_\Gamma:=k_z^2 J_E$$

$$\Lambda\left(\left[\frac{1}{\varepsilon}\nabla H_z\cdot\mathbf{n}\right]_\Gamma-\frac{k_z}{\omega}\left[\frac{1}{\varepsilon\mu}\nabla E_z\cdot\mathbf{s}\right]_\Gamma\right)=k_z^2\left[\mu\nabla H_z\cdot\mathbf{n}\right]_\Gamma:=k_z^2 J_H$$

  - where $\Lambda=\omega^2\varepsilon^+\varepsilon^-\mu^+\mu^-$
  - LHS: interfacial operator
  - interfacial variable: J_E, J_H

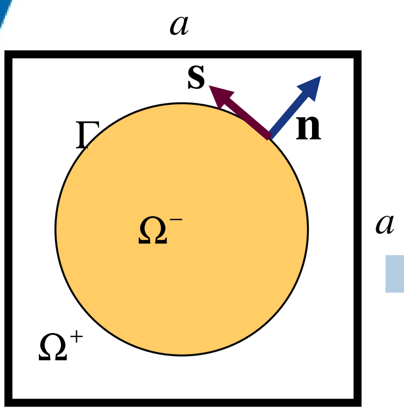
Simplified equations

- Governing equation:

$$\left(\nabla_2^2 + \omega^2 \varepsilon\mu\right)E = k^2 E$$
$$\left(\nabla_2^2 + \omega^2 \varepsilon\mu\right)H = k^2 H$$

- Interface conditions: $[E]_\Gamma = [H]_\Gamma = 0$

$$\Lambda\left(\left[\frac{1}{\mu}\nabla E\cdot\mathbf{n}\right]_\Gamma + \frac{k}{\omega}\left[\frac{1}{\varepsilon\mu}\nabla H\cdot\mathbf{s}\right]_\Gamma\right) = k^2\left[\varepsilon\nabla E\cdot\mathbf{n}\right]_\Gamma$$
$$\Lambda\left(\left[\frac{1}{\varepsilon}\nabla H\cdot\mathbf{n}\right]_\Gamma - \frac{k}{\omega}\left[\frac{1}{\varepsilon\mu}\nabla E\cdot\mathbf{s}\right]_\Gamma\right) = k^2\left[\mu\nabla H\cdot\mathbf{n}\right]_\Gamma$$



- Boundary conditions:

$$E(x+a, y+a) = e^{i(k_x x + k_y y)}E$$
$$H(x+a, y+a) = e^{i(k_x x + k_y y)}H$$

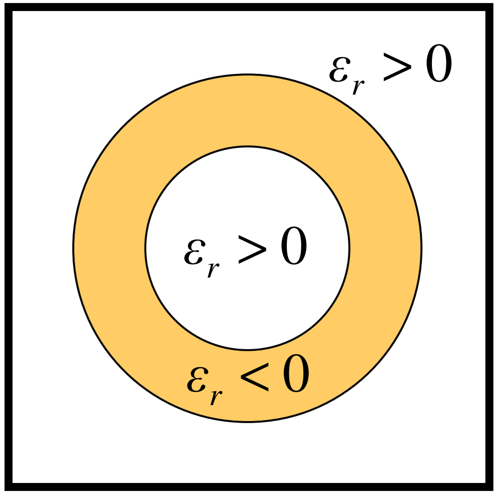
We still have the problem: sign-changed coefficient: ε

Different signs in dielectric and metal!

- Permittivity of metal : Drude model.
  ω_p : plasma frequency;
  ω_τ : electron collision rate.

$$\varepsilon_r = 1 - \frac{\omega_p^2}{\omega(\omega + i\omega_\tau)}$$

- When $\omega < \omega_p$, the permittivity of metal is negative. (That is why metal can be a good mirror).



One dimension

- E and H are decoupled:

TM modes

$$E''+\omega^2\varepsilon\mu E = k^2 E$$

$$[E]_\Gamma = 0,\ \Lambda\left[\frac{1}{\mu}E'\right]_\Gamma = k^2[\varepsilon E']_\Gamma$$

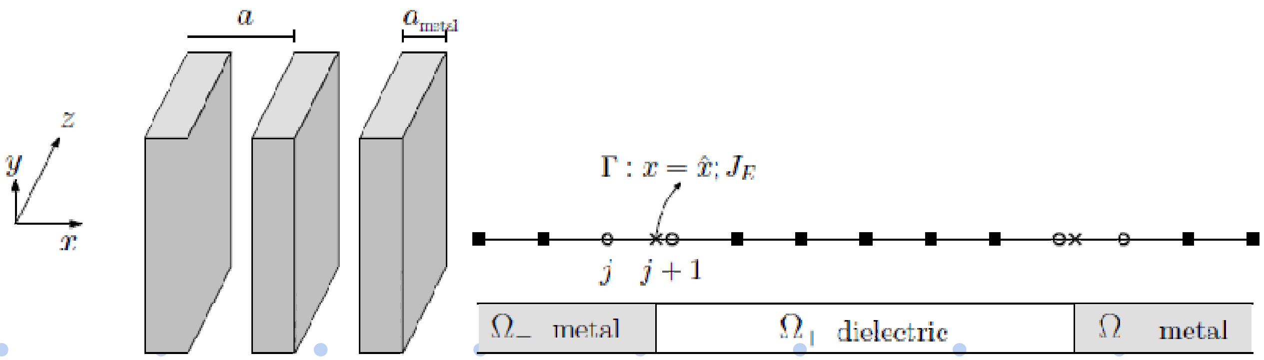
$$E(a) = e^{ik_x a}E(0)$$

TE modes

$$H''+\omega^2\varepsilon\mu H = k^2 H$$

$$[H]_\Gamma = 0,\ \Lambda\left[\frac{1}{\varepsilon}H'\right]_\Gamma = k^2[\mu H']_\Gamma$$

$$H(a) = e^{ik_x a}H(0)$$



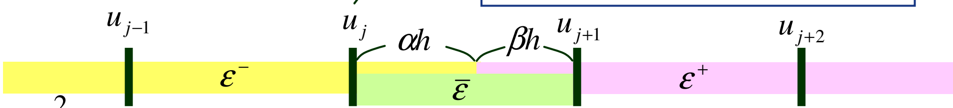
(a) Layer structure (b) Discretization

What is the problem in computation?

- Traditional numerical methods, for example, using harmonic mean of ε as a new coefficient, possibly fail when ε changes its sign.

Numerical approximation:

$$\varepsilon u_j'' = \frac{\varepsilon^- u_{j-1} - (\varepsilon^- + \bar{\varepsilon}) u_j + \bar{\varepsilon} u_{j+1}}{h^2}$$



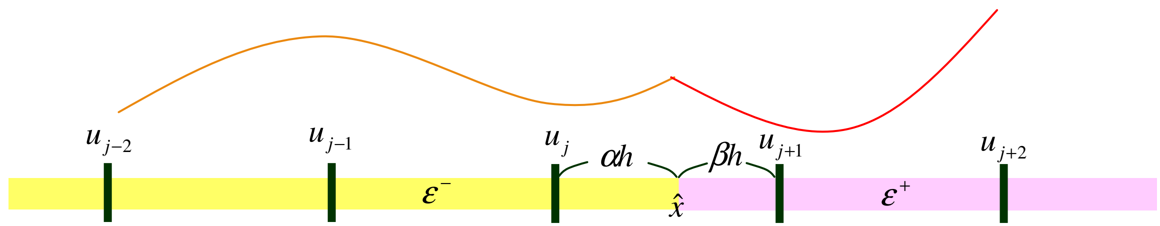
$$\omega = \frac{1}{2}\omega_p,\ \omega_\tau = 0 \Rightarrow \varepsilon_r = 1 - \frac{\omega_p^2}{\omega(\omega + i\omega_\tau)} = -3 = \varepsilon^- \quad \bar{\varepsilon} = \frac{\varepsilon^+\varepsilon^-}{\alpha\varepsilon^+ + \beta\varepsilon^-}$$

Maybe zero if $\varepsilon^-\varepsilon^+ < 0$!

$$\text{if } \varepsilon^+ = 1,\ \alpha = \frac{3}{4} \Rightarrow \alpha\varepsilon^+ + \beta\varepsilon^- = 0 \Rightarrow \bar{\varepsilon} = \infty!$$

Solution: adaptive order strategy

- One dimension:
  - Different order approximation on different sides of the interface.
  - Left: order p; right: order q.
  - These two polynomials are solved by using grid values u_{j-p+1} to u_{j+q} and two jump conditions $[u] = [\varepsilon u'] = 0$.



$$p = 3, q = 2$$

Determinant when solving polynomials

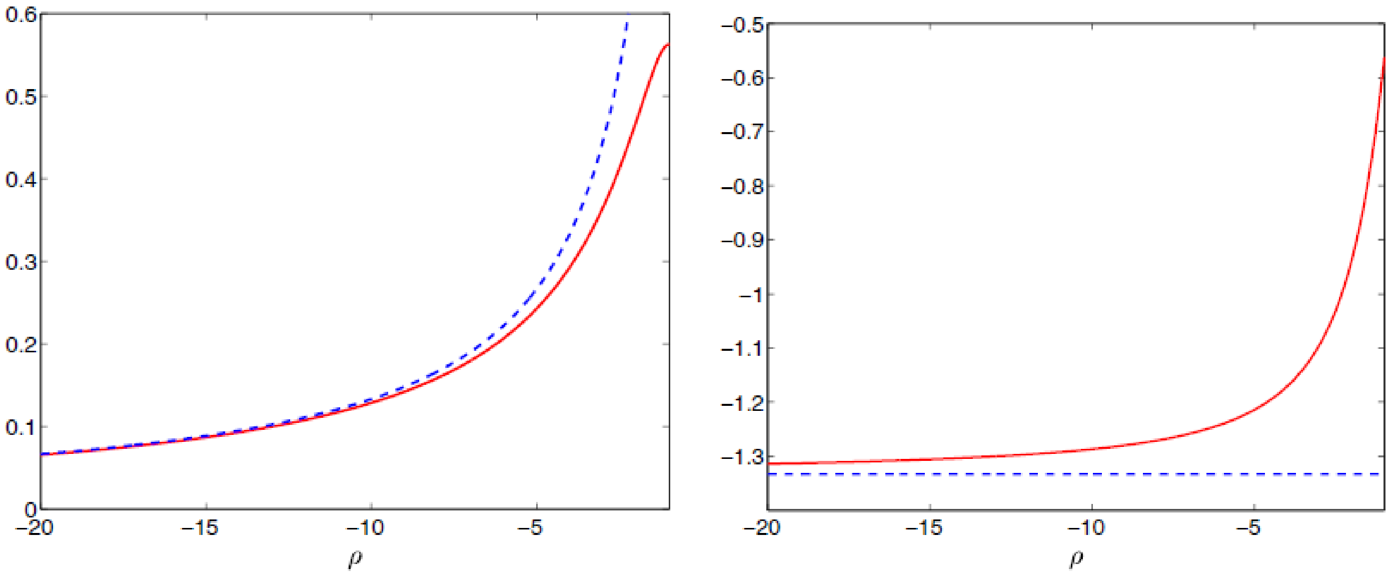
	p	q	The determinant $D_{p,q}$ of the linear system
CIM1➔	1	1	$\varepsilon^- \beta + \varepsilon^+ \alpha$
	2	1	$\varepsilon^- \beta(1+2\alpha) + \varepsilon^+ \alpha(1+\alpha)$
	1	2	$\varepsilon^- \beta(1+\beta) + \varepsilon^+ \alpha(1+2\beta)$
CIM2➔	2	2	$\varepsilon^- \beta(1+\beta)(1+2\alpha) + \varepsilon^+ \alpha(1+\alpha)(1+2\beta)$
	3	2	$\varepsilon^- \beta(1+\beta)(3\alpha^2+6\alpha+2) + \varepsilon^+ \alpha(1+\alpha)(2+\alpha)(1+2\beta)$
	2	3	$\varepsilon^- \beta(1+\beta)(2+\beta)(1+2\alpha) + \varepsilon^+ \alpha(1+\alpha)(3\beta^2+6\beta+2)$

When $\varepsilon^- \varepsilon^+ < 0$, the determinant would be zero!!

Root of zero determinant

- Normalized determinant: $f_{p,q}\left(\alpha, \rho = \frac{\varepsilon^{+}}{\varepsilon^{-}}\right) = \frac{D_{p,q}}{\varepsilon^{-}}$
  - Example: $f_{2,2}(\alpha,\rho) = (1-\alpha)(2-\alpha)(1+2\alpha) + \rho\alpha(1+\alpha)(3-2\alpha)$
- Root of zero determinant: $\alpha_{p,q}(\rho)$: $f_{p,q}(\alpha_{p,q}(\rho),\rho) = 0$
- We claim: $f_{p+1,q}(\alpha_{p,q}(\rho),\rho) \neq 0,\ f_{p,q+1}(\alpha_{p,q}(\rho),\rho) \neq 0$

Proof when p = q = 2



(a) $f_{3,2}(\alpha_{2,2}(\rho),\rho)$ (b) $f_{2,3}(\alpha_{2,2}(\rho),\rho)$

- Asymptotic behavior:

$$f_{3,2}(\alpha_{2,2}(\rho),\rho) \approx -\frac{4}{3}\rho^{-1}, \quad \boxed{f_{2,3}(\alpha_{2,2}(\rho),\rho) \approx -\frac{4}{3},} \quad \text{for} \quad \rho \ll -1.$$

Adaptive order strategy

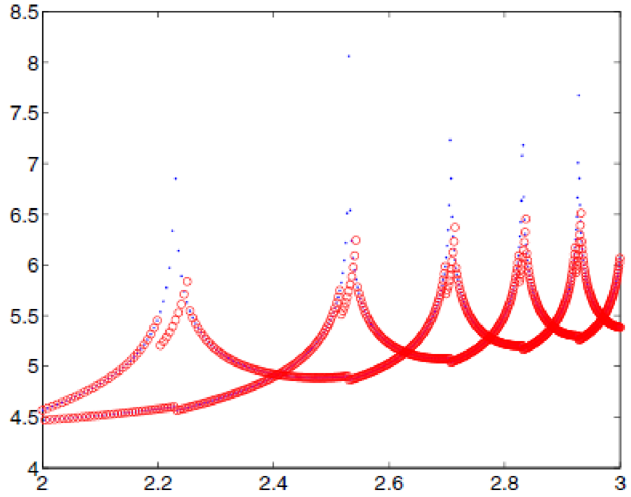
- Choose the orders p and q to approximate u on different sides of the interface.

- If the determinant is smaller than a prescribed tolerance, then the order in the region with larger absolute value of ε is increased by 1.

Solve the problem with sign-changed coefficients

Condition number

- The log-log plot of the scaled condition number versus the number of meshes.
- The tolerance: 0.15.
- The condition number is under controlled.



Numerical Results

Two dimensions:

- Dimension-by-dimension approach: adaptive-order approximation on both sides of the interface.
- Project the interface condition on the normal and tangential directions.
- The one side gradient is approximated by the grid values and second order derivatives (principal and cross).
- It will deduce a coupling system of principal second order derivatives. Adaptive order strategy is also used when the determinant of the coupling system is almost zero.

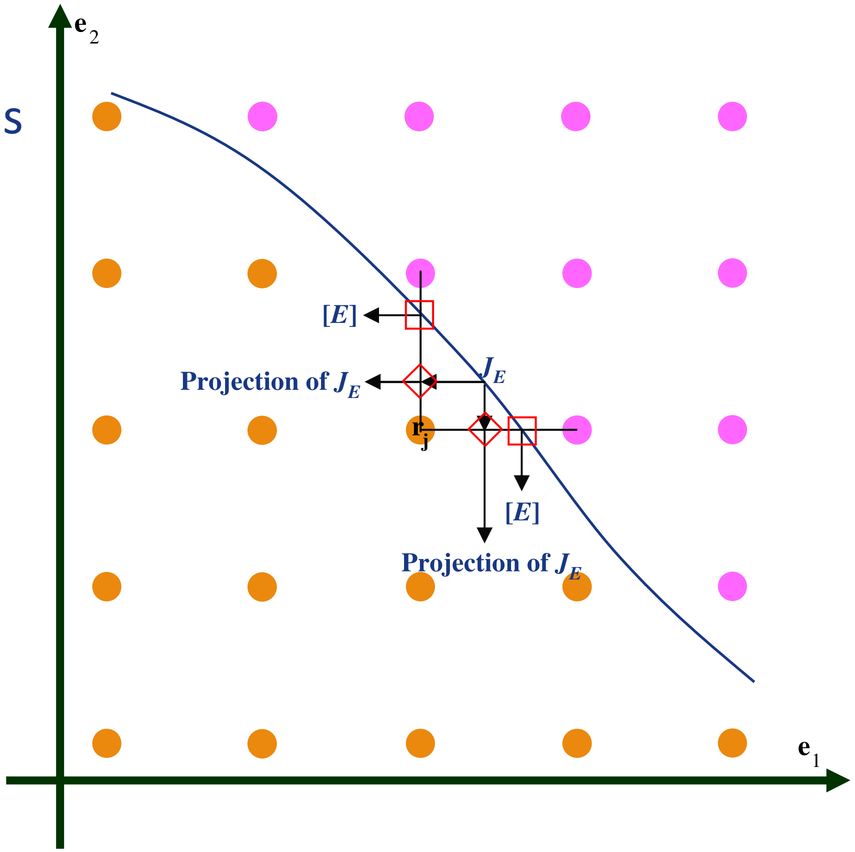
Other problem

- The location of the introduced interfacial variable:
  - CIM use the jump conditions at the intersection of the interface and the grid lines. However, they cannot be too closed otherwise they will be dependent.

- We need to locate them uniformly on the interface.

Solution for the problem

- We project the jump condition J_E to the grid lines by Taylor expansion.
- Different locations of different jump conditions are used in the dimension-by-dimension approach.
- The remaining terms are approximated by nearby grid values.



The modifications

- Suppose the interfacial variable is located at $(x_i + \xi h,\, y_j + \eta h)$, then
  - The projection is

$$\left[\varepsilon\frac{\partial E}{\partial x}\right]_{(x_i+\xi h, y_j)} = \left[\varepsilon\frac{\partial E}{\partial x}\right]_{\hat{\mathbf{r}}_\ell} - \eta h\left[\varepsilon\frac{\partial^2 E}{\partial x \partial y}\right]_{\hat{\mathbf{r}}_\ell} + O(h^2).$$

  - The dimension-by-dimension approaches

$$\frac{\partial^2 E_{i,j}}{\partial x^2} = \frac{1}{h^2}\mathcal{L}_x(E_{i-p_1+1:i+q_1,j}) + \frac{\sigma_1}{h}\left(\left[\varepsilon\frac{\partial E}{\partial x}\right]_{\hat{\mathbf{r}}_\ell} - \eta h\left[\varepsilon\frac{\partial^2 E}{\partial x\partial y}\right]_{\hat{\mathbf{r}}_\ell}\right) + O(h),$$

$$\frac{\partial^2 E_{i,j}}{\partial y^2} = \frac{1}{h^2}\mathcal{L}_y(E_{i,j-p_2+1:j+q_2}) + \frac{\sigma_2}{h}\left(\left[\varepsilon\frac{\partial E}{\partial y}\right]_{\hat{\mathbf{r}}_\ell} - \xi h\left[\varepsilon\frac{\partial^2 E}{\partial x\partial y}\right]_{\hat{\mathbf{r}}_\ell}\right) + O(h)$$

  - The one side gradient

$$\nabla E(\hat{\mathbf{r}}_\ell^-) = \begin{bmatrix} \frac{1}{h}(E_{i,j} - E_{i-1,j}) + (\frac{1}{2}+\xi)h\frac{\partial^2 E_{i,j}}{\partial x^2} + \eta h\frac{\partial^2 E_{i,j}}{\partial x\partial y} \\ \frac{1}{h}(E_{i,j} - E_{i,j-1}) + (\frac{1}{2}+\eta)h\frac{\partial^2 E_{i,j}}{\partial y^2} + \xi h\frac{\partial^2 E_{i,j}}{\partial x\partial y} \end{bmatrix} + O(h^2).$$

The approximation of interfacial operator

$$\Lambda\left(\left[\frac{1}{\mu}\nabla E_z\cdot\mathbf{n}\right]+\frac{k_z}{\omega}\left[\frac{1}{\varepsilon\mu}\nabla H_z\cdot\mathbf{t}\right]\right)=k_z^2\left[\varepsilon\nabla E_z\cdot\mathbf{n}\right]:=k_z^2 J_E$$

$$\Lambda\left(\left[\frac{1}{\varepsilon}\nabla H_z\cdot\mathbf{n}\right]-\frac{k_z}{\omega}\left[\frac{1}{\varepsilon\mu}\nabla E_z\cdot\mathbf{t}\right]\right)=k_z^2\left[\mu\nabla H_z\cdot\mathbf{n}\right]:=k_z^2 J_H$$

- The interfacial operators are approximated by the interfacial variables and the one-side gradient

$$\left[\frac{1}{\mu}\nabla E\cdot\hat{\mathbf{n}}\right]_{\hat{\mathbf{r}}_\ell} = \frac{1}{\varepsilon_+\mu_+}J_{E,\ell}+\frac{\varepsilon_-\mu_- - \varepsilon_+\mu_+}{\varepsilon_+\mu_+\mu_-}\nabla E(\hat{\mathbf{r}}_\ell^-)\cdot\hat{\mathbf{n}},$$

$$\left[\frac{1}{\varepsilon\mu}\nabla H\cdot\hat{\mathbf{t}}\right]_{\hat{\mathbf{r}}_\ell} = \frac{\varepsilon_-\mu_- - \varepsilon_+\mu_+}{\varepsilon_+\varepsilon_-\mu_+\mu_-}\nabla H(\hat{\mathbf{r}}_\ell^-)\cdot\hat{\mathbf{t}},$$

A quadratic eigenvalue problem

- Finally, we arrive at

$$\mathbf{A}_{\text{mix}}\mathbf{U}_{\text{mix}} + k\mathbf{B}_{\text{mix}}\mathbf{U}_{\text{mix}} = k^2\mathbf{U}_{\text{mix}}$$

  - where $\mathbf{U}_{\text{mix}} = [E_{1:N,1:N}, H_{1:N,1:N}, J_{E,1:N_J}, J_{H,1:N_J}]^T$

- We solve this quadratic eigenvalue problem by doubling the matrix

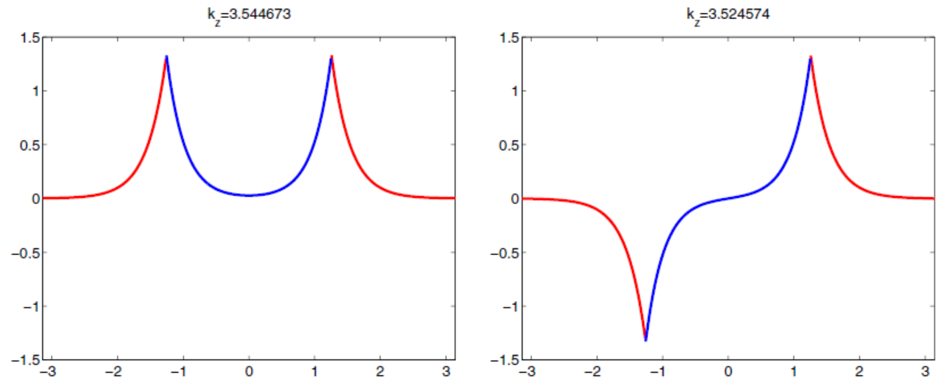
$$\begin{bmatrix} \mathbf{0} & \mathbf{I} \\ \mathbf{A} & \mathbf{B} \end{bmatrix} \begin{bmatrix} \mathbf{U}_{\text{mix}} \\ k\mathbf{U}_{\text{mix}} \end{bmatrix} = k \begin{bmatrix} \mathbf{U}_{\text{mix}} \\ k\mathbf{U}_{\text{mix}} \end{bmatrix}$$

Numerical results

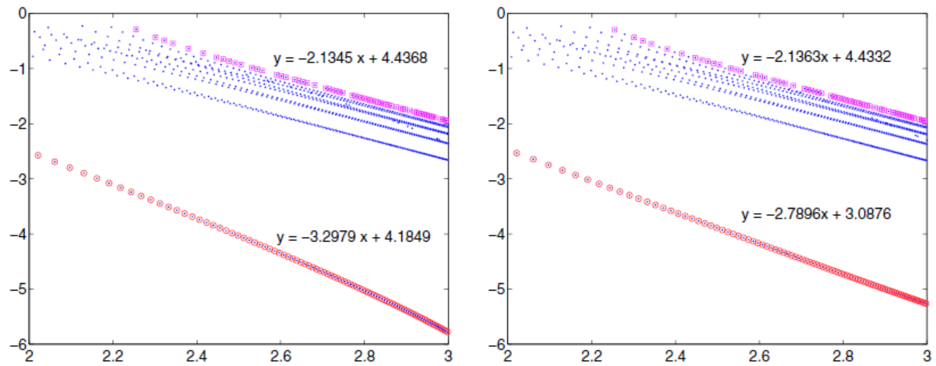
- One dimensional test.
- Band structure of a layer structure.
- Two dimensional test with exact solution.
- Two dimensional test without exact solution.
- Band structure of two dimensional strutures

One dimensional test

- The dimensionless frequency is 0.7.
- $\Omega = [-\pi, \pi]$. The filling ratio is 40%, i.e., the interfaces are located at $-2\pi/5$ and $2\pi/5$.
- The convergence of worst cases is second order.
- Due to the symmetry, the convergence of the best cases is about third order.



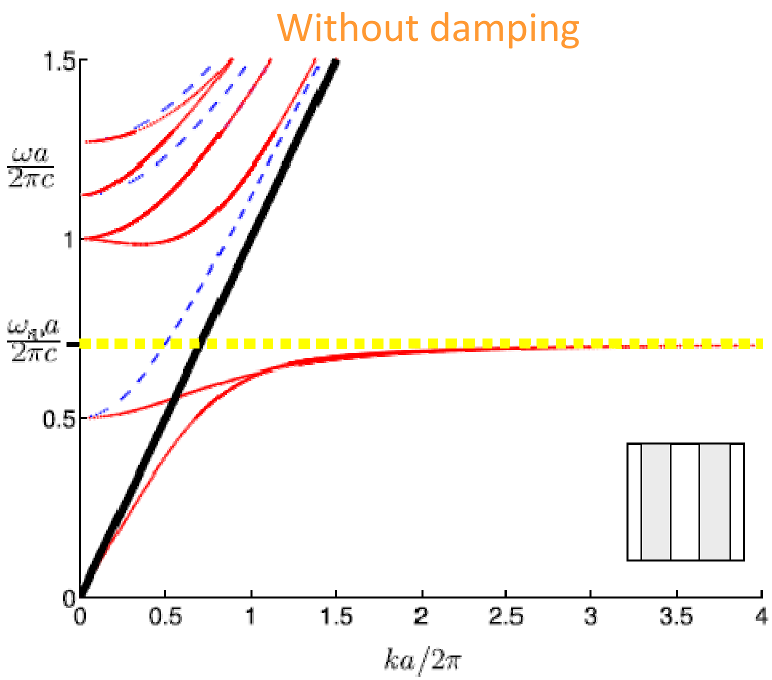
(a) symmetric eigenmode (b) anti-symmetric eigenmode

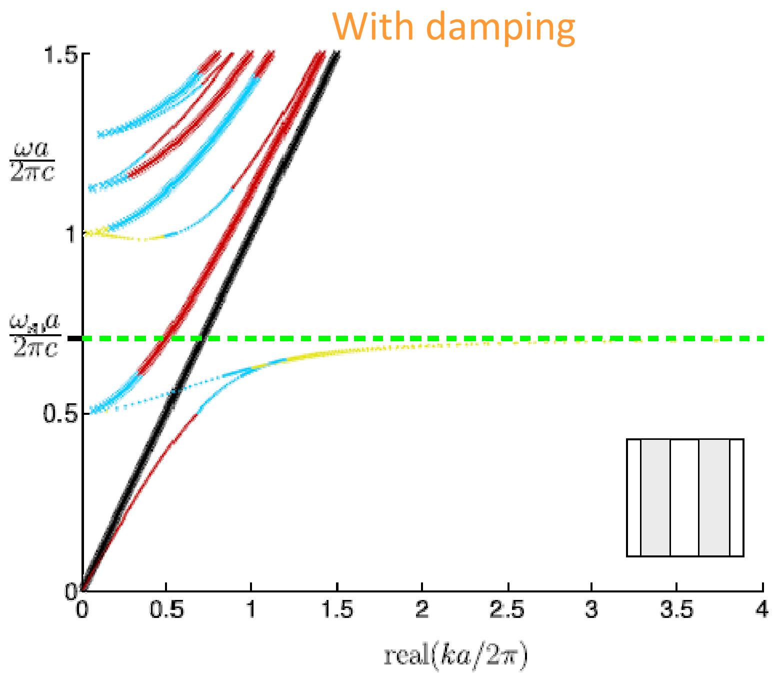


(a) error of symmetric eigenvalue (b) error of anti-symmetric eigenvalue

One dimensional result

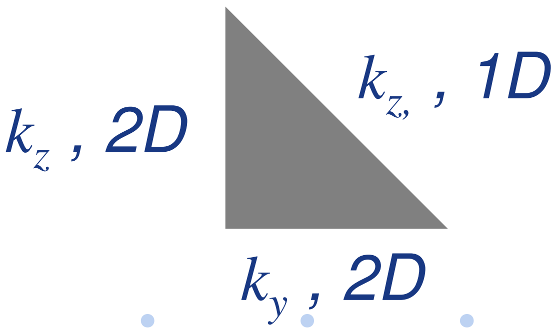
- Band structure of a layer structure



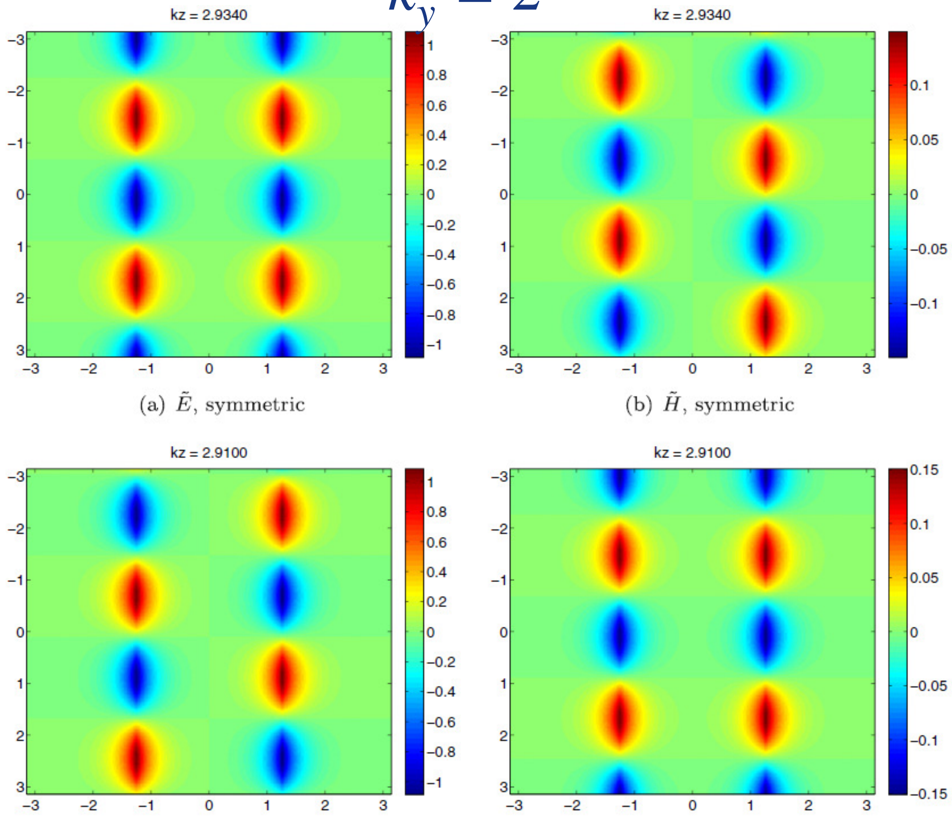


Two dimensional test with exact solution

- The exact solution can be found from the one dimensional case. The wave vector k_z changes with different Bloch wave vector k_y.



$k_y = 2$



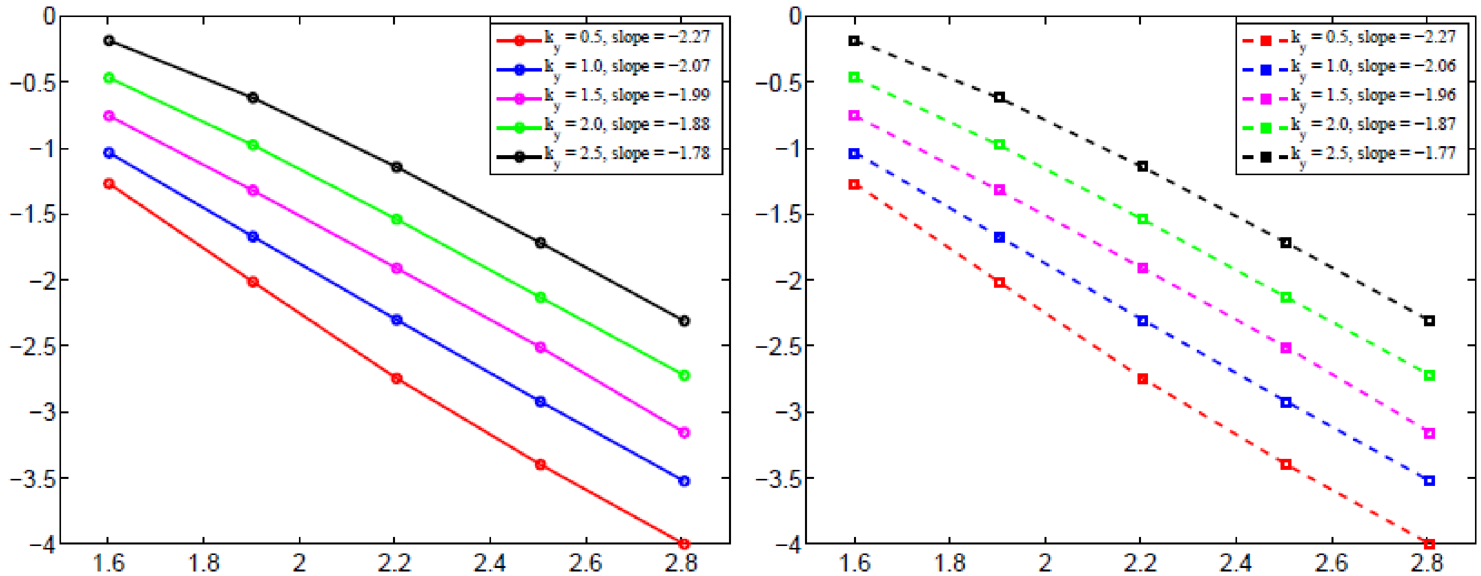
(a) $\tilde{E}$, symmetric (b) $\tilde{H}$, symmetric

(c) $\tilde{E}$, antisymmetric (d) $\tilde{H}$, antisymmetric

CIM for wave-guide modes of SP

Two dimensional test with exact solution

- The convergence slightly decreases when the oscillatory along the interface (k_y) increases.

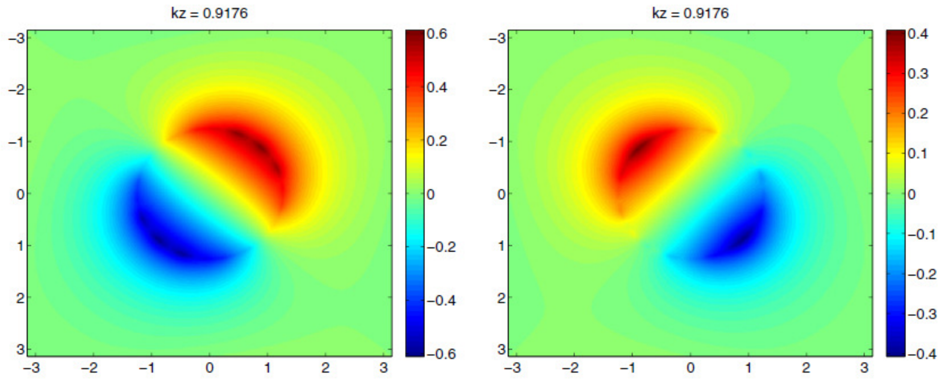


(a) error of symmetric eigenmode (b) error of anti-symmetric eigenmode

CIM for wave-guide modes of SP

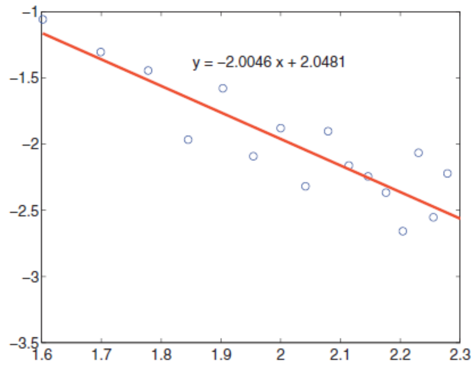
Two dimensional test without exact solution

- No analytical solution is available.



(a) $\tilde{E}$ (b) $\tilde{H}$

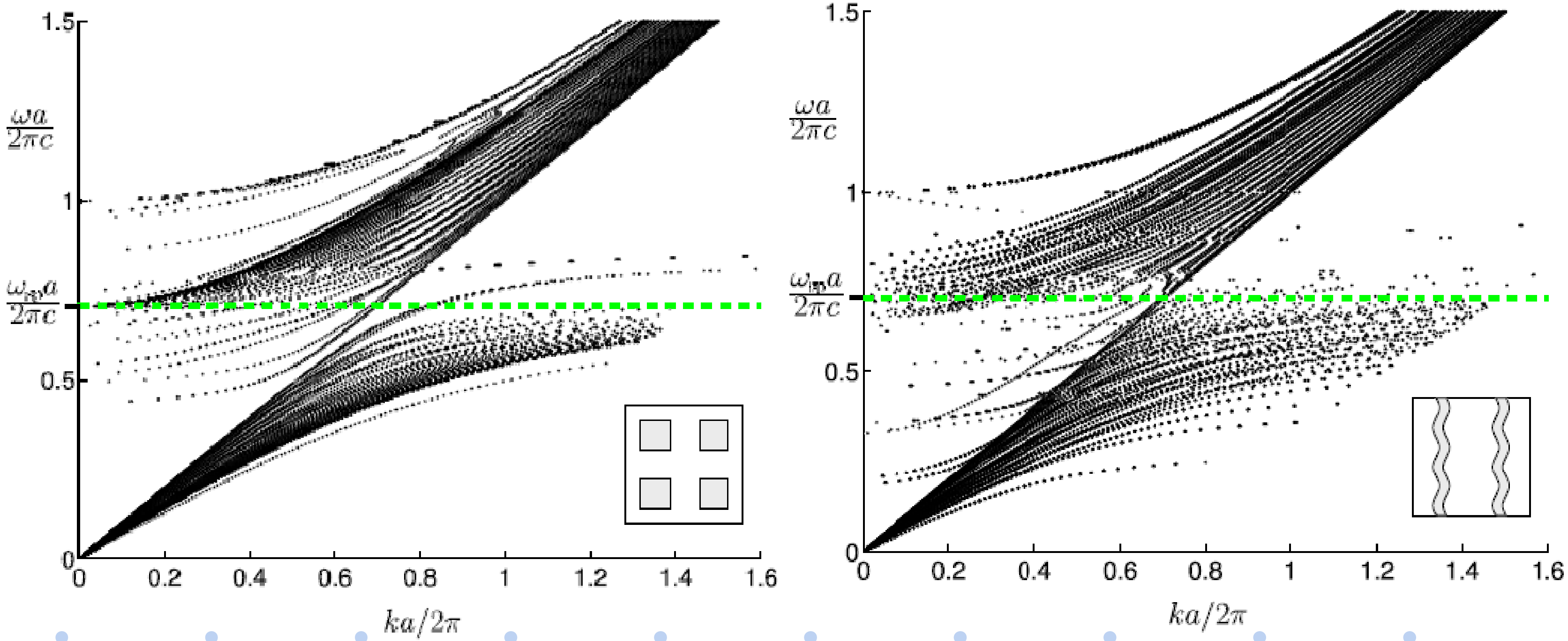
- We use a fine grid result (640 $\times$ 640) as our referenced solution for comparison.



(a) Convergence result

Two dimensional result

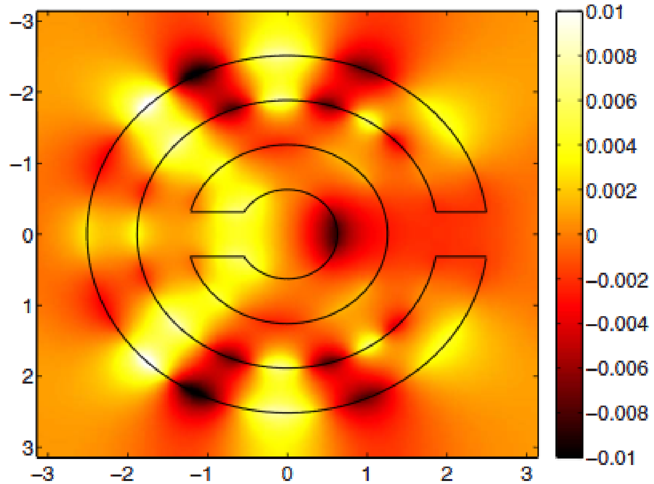
- Band structures of box and wavy structures (2D, periodic)



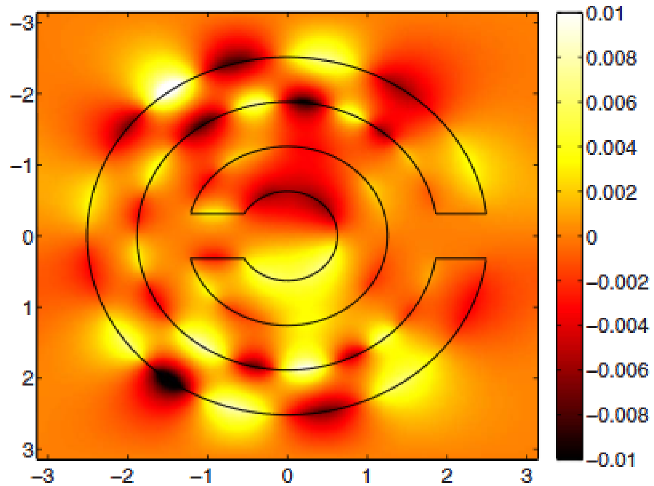
CIM for wave-guide modes of SP

Two dimensional result

- Eigenmode for a split-ring structure. It is widely used in metamaterial with negative refractive index.



(a) E



(b) H

- Introduction of Interface problems
- Coupling Interface Method for elliptic interface problem
- Coupling Interface Method for wave-guide modes of surface plasmon
- Concluding Remarks

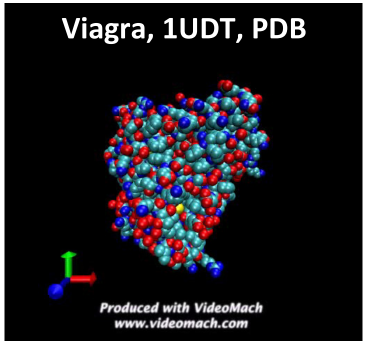
Concluding remarks

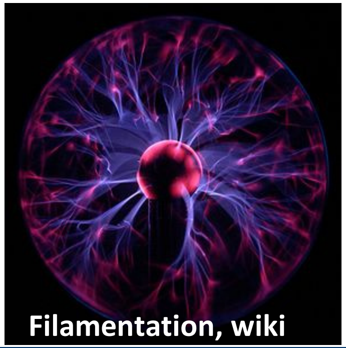
- Coupling interface method has its potential for interface problems:
  - It is simple to program.
  - Second order accurate for the solution.
  - It can handle complex interfaces.
  - Computational complexity is linear.

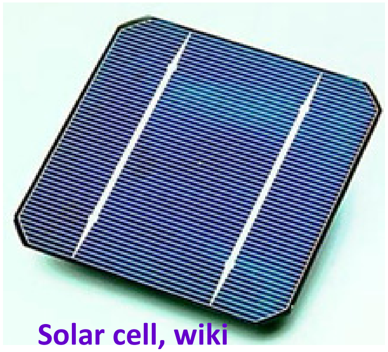
- It is the first direct approach for wave-guide mode of surface plasmon.

Future works

- Non-linear Poisson-Boltzmann Equation
  - Drug design, molecular dynamics, surface potential calculations
- Anisotropic materials
  - Chemical anisotropic filter, medical ultrasound imaging, MEMS
- Moving interface problems
  - Stefan problem, Debris flow, red blood cells in blood
- Band gap optimization (2D and 3D).
  - Light filter, solar cell







Thank you for your attention