

弱形式離散化スキーム逐次伝達法を用いた 散乱問題の数値解析手法の提案

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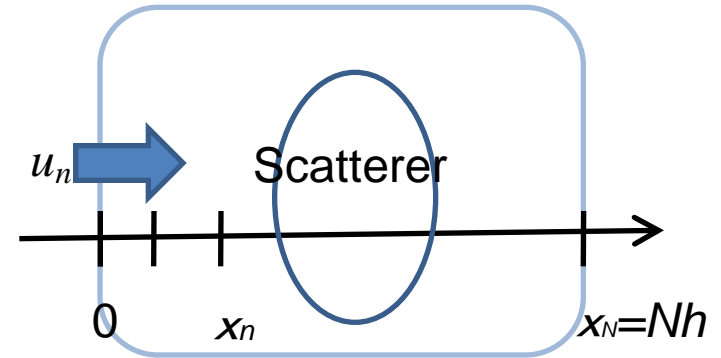
2) 苫小牧高専



離散化 (Numerov法)

■ 2階微分方程式

$$u''(x) + v(x) u(x) = 0$$



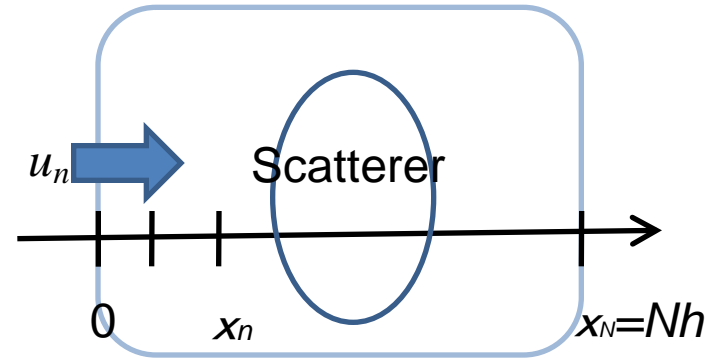
■ 2階差分

$$\begin{aligned} u(x+h) - 2u(x) + u(x-h) &= 2\frac{h^2}{2!}u''(x) + 2\frac{h^4}{4!}u''''(x) + \dots \\ &= -\frac{h^2}{12}v(+xh)u(x+h) - \frac{5h^2}{6}v(x)u(x) + \frac{h^2}{12}v(x-h)u(x-h) \\ &\quad + o(h^6) \end{aligned}$$

離散化 (Numerov法)

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■ 2階差分

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■ 2階差分方程式

$$a_n u(x_{n+1}) + b_n u(x_n) + c_n u(x_{n-1}) = 0$$

$$a_n = 1 + \frac{h^2}{12}v(x_{n+1}), \quad b_n = -2 + \frac{5h^2}{6}v(x_n), \quad c_n = 1 + \frac{h^2}{12}v(x_{n-1})$$

伝達行列 S_n とRTM(逐次伝達法)

■ 伝達行列 (Stepping Matrix) S_n

$$u(x_{n+1}) = S_n u(x_n)$$

$$u(x_{n-1}) = (S_{n-1})^{-1} u(x_n)$$

$$c_n u(x_{n-1}) + b_n u(x_n) + a_n u(x_{n+1}) = 0$$

$$c_n (S_{n-1})^{-1} + b_n + a_n S_n = 0$$

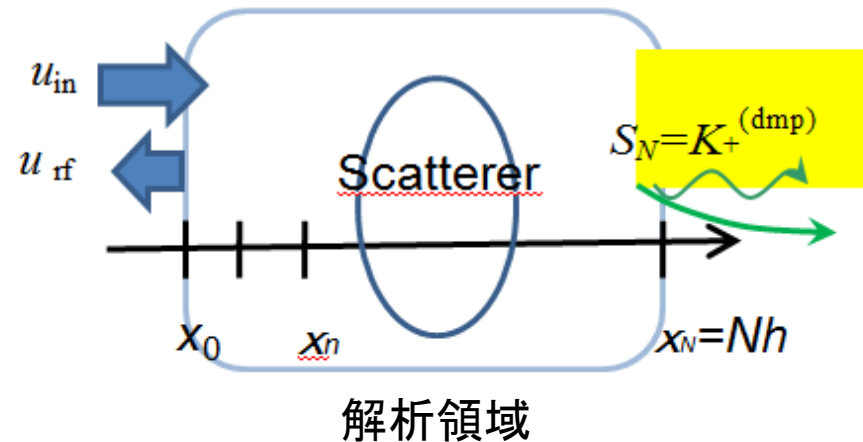
$$S_{n-1} = -(b_n + a_n S_n)^{-1} c_n$$

漸化式

■ RTM-整合ポット境界条件

$$S_N = K_+^{(\text{dmp})}$$

ABC(吸収境界条件)



逐次伝達法(RTM)と散乱問題

- 分子軌道や電子伝導の解析法として始まる：
RTM(逐次伝達法 Recursive Transfer Method)
⇒ 局在波の抽出が可能(RTM整合ポート境界条件)
- RTMの適用範囲を拡大：
 - ・空間次元や微分階数の多様さに対応⇒ 弱形式離散化
- Fano効果が現れる共鳴現象に適用：
⇒ 周波数に虚数成分

屈曲変位の共変性を分離した運動表現

$u(x,y)$ 弾性平板の面に垂直な変位

$$\Delta_0 u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}$$

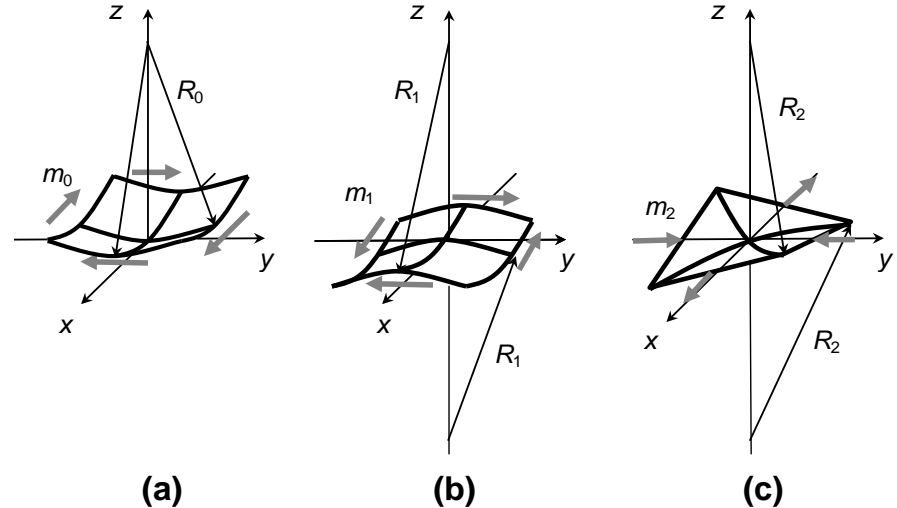
$$\Delta_1 u = \frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u}{\partial y^2},$$

$$\Delta_2 u = 2 \frac{\partial^2 u}{\partial x \partial y}$$

座標軸の回転角度 θ

$$\Delta_0 u \rightarrow \Delta_0 u$$

$$\begin{bmatrix} \Delta_1 u \\ \Delta_2 u \end{bmatrix} \rightarrow \begin{bmatrix} \cos 2\theta & \sin 2\theta \\ -\sin 2\theta & \cos 2\theta \end{bmatrix} \begin{bmatrix} \Delta_1 u \\ \Delta_2 u \end{bmatrix}$$



エネルギー表現

ポテンシャル $U[u] = \frac{1}{2} [D_0(\Delta_0 u)^2 + D_1(\Delta_1 u)^2 + D_2(\Delta_2 u)^2]$

運動エネルギー $K[u] = \frac{\omega^2 b \rho}{2} u^2$

共変な表現

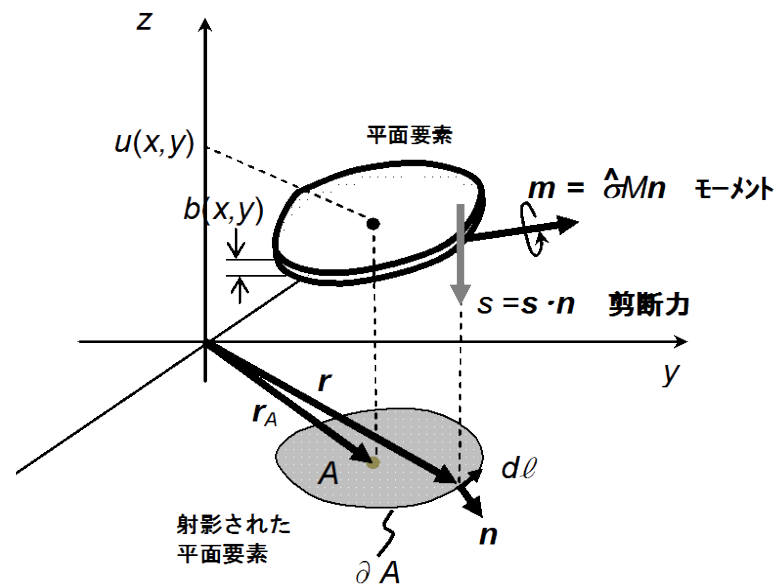
平板のスティフネス定数

$$D_0(x,y) = \frac{Eb^3}{24(1-\nu)} \quad D_1(x,y) = D_2(x,y) = \frac{Eb^3}{24(1+\nu)}$$

屈曲振動の弱形式表現

停留値問題 $w(x,y)$ テスト関数

$$F[w,u] = \int_S \{ \Delta_0 w D_0 \Delta_0 + \Delta_1 w D_1 \Delta_1 u + \Delta_2 w D_2 \Delta_2 u - w \omega^2 \rho b u \} dS$$



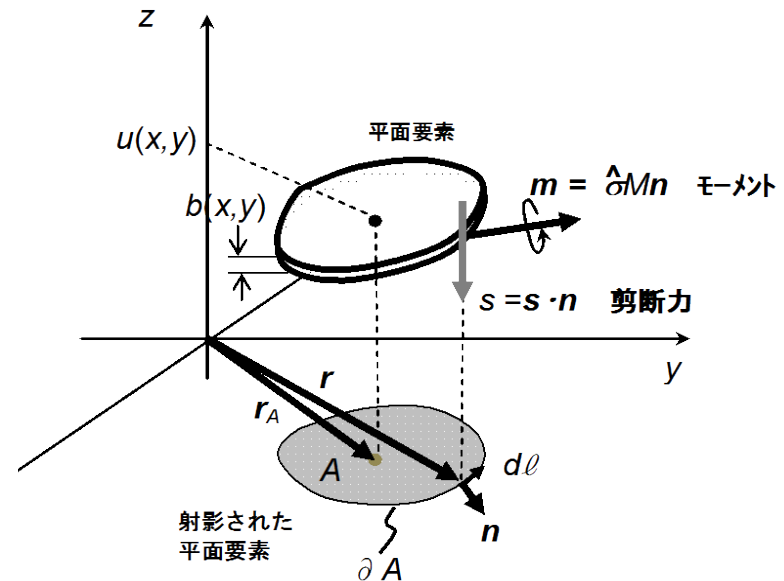
屈曲振動の弱形式表現

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$$= \int_S w [\Delta_0 (D_0 \Delta_0) + \Delta_1 (D_1 \Delta_1 u) + \Delta_2 (D_2 \Delta_2 u) - \omega^2 \rho b u] dS$$

$$+ \int_{\partial S} \mathbf{n} \cdot [w \mathbf{s} - M \nabla w] d\ell$$



屈曲振動の弱形式表現

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$$+ \int_{\partial S} \mathbf{n} \cdot [w \mathbf{s} - M \nabla w] d\ell$$

$$\Rightarrow 0 \quad (\nabla w)$$

重調和方程式の拡張

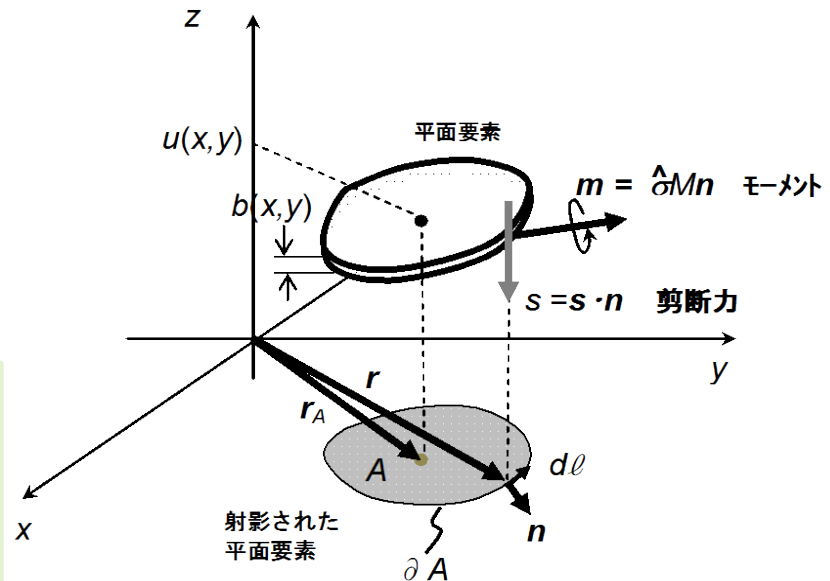
運動方程式

$$\Delta_0 (D_0 \Delta_0 u) + \Delta_1 (D_1 \Delta_1 u) + \Delta_2 (D_2 \Delta_2 u) - \omega^2 \rho b u = 0$$

エネルギー流束

$$\mathbf{J} = \dot{u} \mathbf{s} - M \nabla \dot{u}$$

$$= \sum_{r=0}^2 D_r [\dot{u} (\Delta_r^2 u) - (\Delta_r \dot{u}) (\Delta_r u)]$$



共変な表現

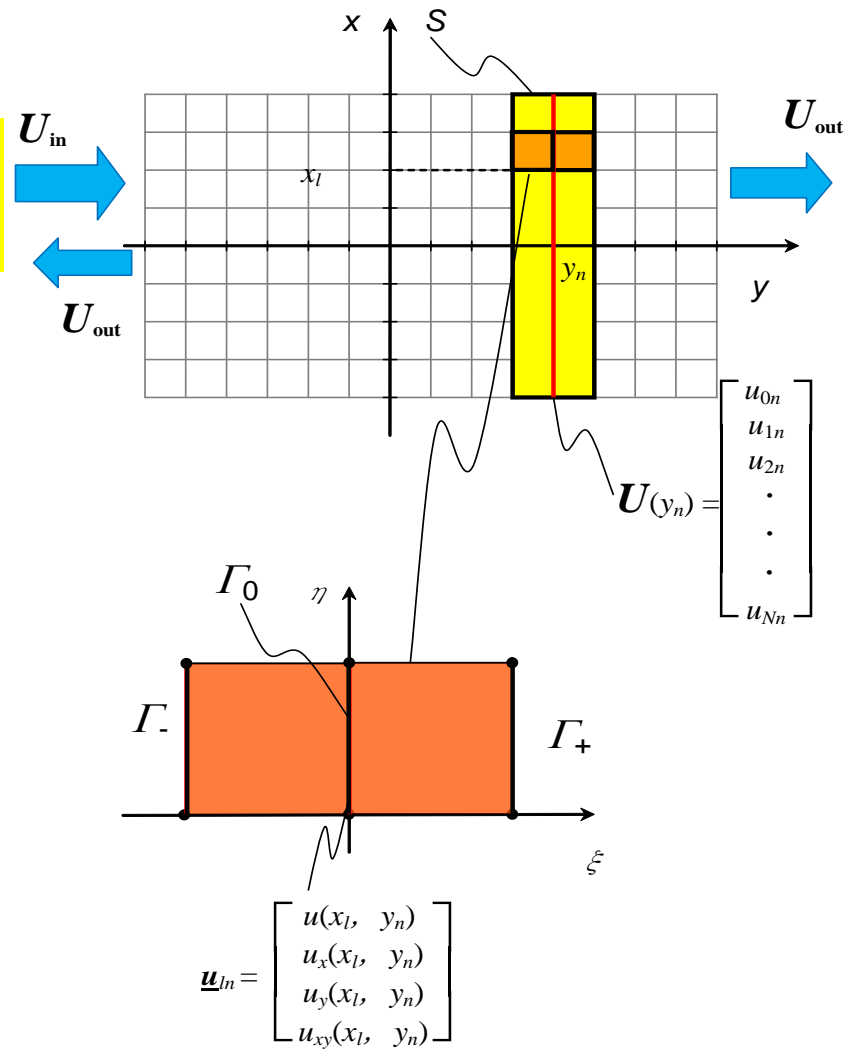
弱形式離散化 = 境界要素での解の接続 =

$$F_{S_+ + S_-}[w, u] = \int_{S'_+ + S'_-} \{\text{eq. of motion}\} dS$$

$$+ \int_{\Gamma_0} dl [w(s_- - s_+) - (M_- - M_+) \nabla w]$$

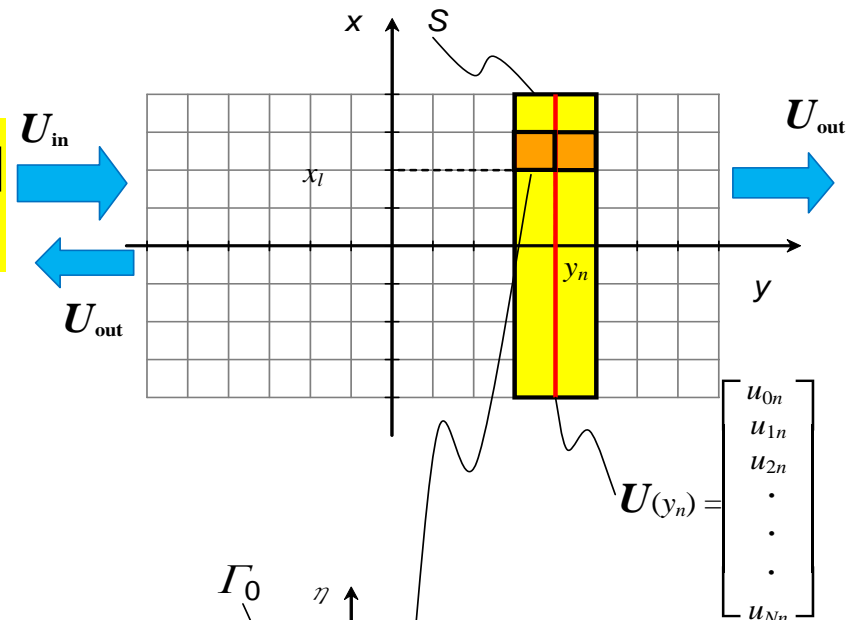
$$+ \int_{\partial S - \Gamma_0} dl [w s - M \nabla w]$$

$$\Rightarrow 0 \quad (\forall w)$$



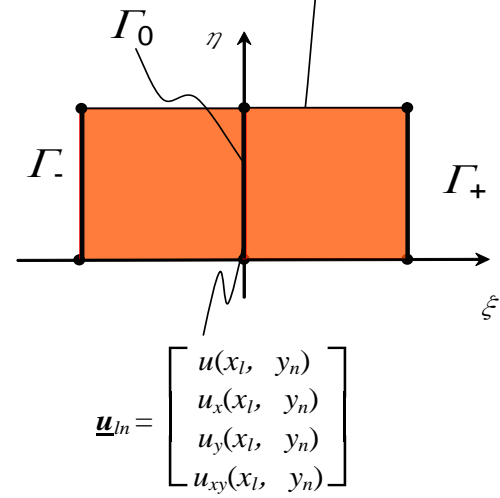
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 &+ \int_{\partial S - \Gamma_0} dl [w s - M \nabla w] \\
 &\Rightarrow 0 \quad (\forall w)
 \end{aligned}$$



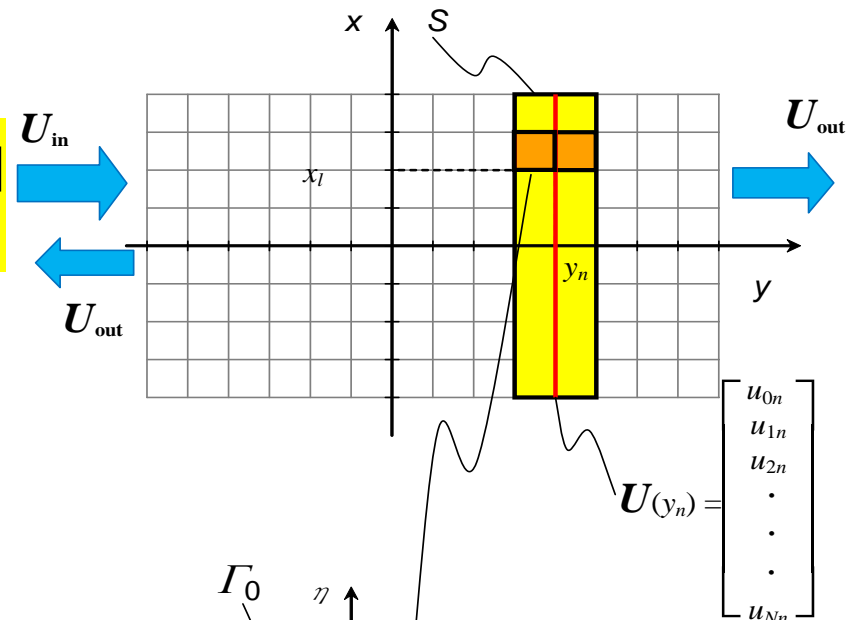
■ Γ_0 上で $w, \nabla w$ が任意 **力学的な条件**

$s_- = s_+$	剪断力が連続
$M_- = M_+$	モーメントが連続



弱形式離散化 = 境界要素での解の接続 =

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 &+ \int_{\Gamma_0} dl [w(s_- - s_+) - (M_- - M_+) \nabla w] \\
 &+ \int_{\partial S - \Gamma_0} dl [w s - M \nabla w] \\
 &\Rightarrow 0 \quad (\forall w)
 \end{aligned}$$

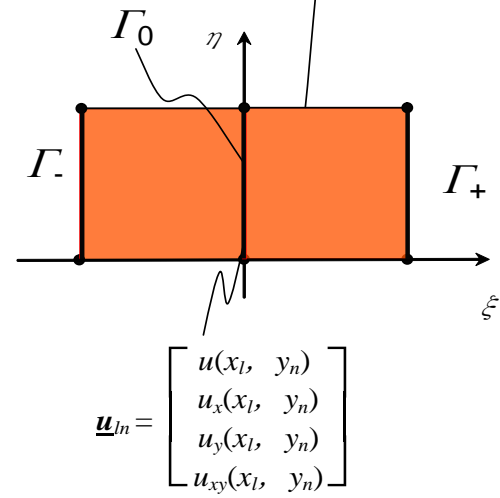


■ Γ_0 上で $w, \nabla w$ が任意 **力学的な条件**

$$\begin{aligned}
 s_- = s_+ & \quad \text{剪断力が連続} \\
 M_- = M_+ & \quad \text{モーメントが連続}
 \end{aligned}$$

■ Γ_{\pm} 上で $w = \nabla w = 0$ **境界条件の多様さ**

$$\begin{aligned}
 s, M \text{ を別途設定可能} \\
 \Rightarrow \text{RTM-整合ポート境界条件}
 \end{aligned}$$



要素内補間による差分方程式の導出(その1)

■ 補間関数

$$u(x,y) = \sum_{p=1}^4 [L_0^{(p)}(x,y)u(P_p) + L_1^{(p)}(x,y)u_x(P_p) + L_2^{(p)}(x,y)u_y(P_p) + L_3^{(p)}(x,y)u_{xy}(P_p)]$$

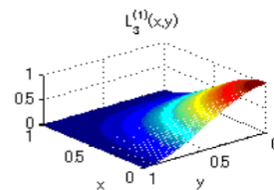
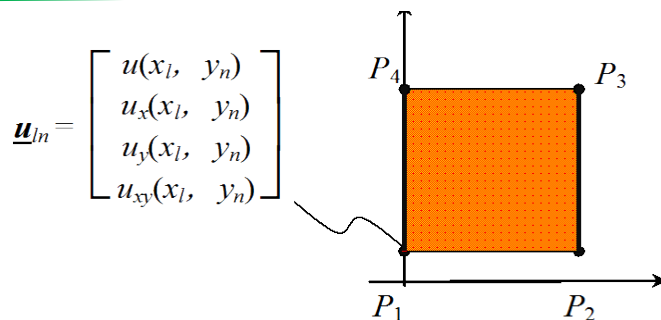
$L_0^{(p)}(x,y)$ 6 次の代数多項式

$u(P_p)$ 節点 P_p での関数値

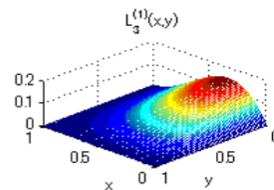
$u_x(P_p)$ 節点 P_p での導関数値(偏微分).

$u_y(P_p), \dots$

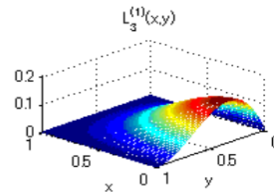
$u_{xy}(P_p) \dots$



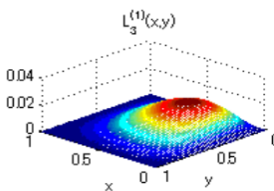
$$L_0^1(x,y) = (2*x + 1)*(x - 1)^2*(2*y + 1)*(y - 1)^2$$



$$L_1^1(x,y) = (2*x + 1)*(x - 1)^2*(2*y + 1)*(y - 1)^2$$



$$L_2^1(x,y) = (2*x + 1)*(x - 1)^2*(2*y + 1)*(y - 1)^2$$



$$L_3^1(x,y) = (2*x + 1)*(x - 1)^2*(2*y + 1)*(y - 1)^2$$

要素内補間による差分方程式の導出(その2)

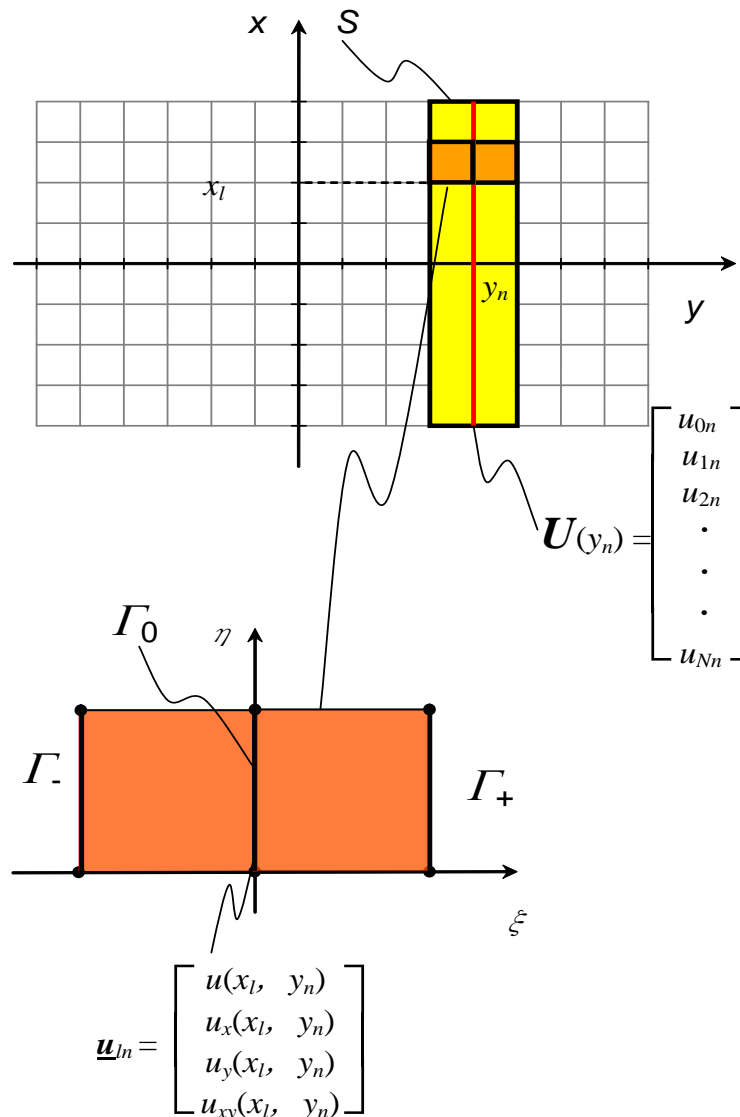
■補間関数

$$u(x,y) = \sum_{p=1}^4 [L_0^{(p)}(x,y)u(P_p) + L_1^{(p)}(x,y)u_x(P_p) + L_2^{(p)}(x,y)u_y(P_p) + L_3^{(p)}(x,y)u_{xy}(P_p)]$$

$L_0^{(p)}(x,y)$ 6次の代数多項式
 $u(P_p)$ 節点 P_p での関数値
 $u_x(P_p)$ 節点 P_p での導関数値(偏微分).
 $u_y(P_p), \dots$
 $u_{xy}(P_p) \dots$

■2階の差分方程式

$$a_n U(y_{n+1}) + b_n U(y_n) + c_n U(y_{n-1}) = 0$$



RTM整合ポート境界条件

■ 入出力ポートにおける伝達定数

$$c_{\text{port}}\mathbf{u}(y_{n-1}) + b_{\text{port}}\mathbf{u}(y_n) + a_{\text{port}}\mathbf{u}(y_{n+1}) = 0$$

$$\mathbf{u}(y_{n+1}) = e^{\eta h} \mathbf{u}(y_n)$$

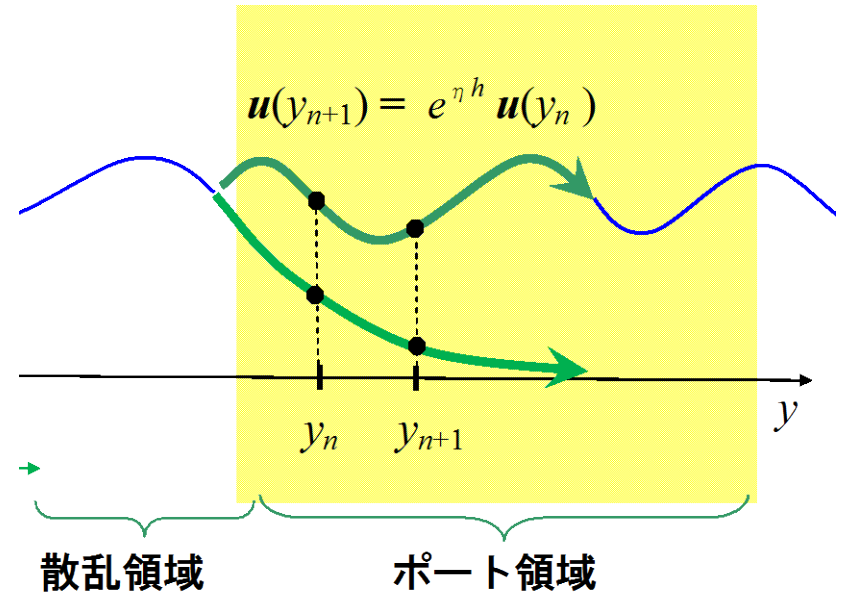
■ 固有値問題への帰着

$$\begin{bmatrix} c_{\text{port}} & b_{\text{port}} \\ 0 & I \end{bmatrix} \begin{bmatrix} \mathbf{u}(y_{n-1}) \\ \mathbf{u}(y_n) \end{bmatrix} = e^{\eta h} \begin{bmatrix} 0 & a_{\text{port}} \\ -I & 0 \end{bmatrix} \begin{bmatrix} \mathbf{u}(y_{n-1}) \\ \mathbf{u}(y_n) \end{bmatrix}$$

$$\eta = \begin{cases} \pm ik & \text{(進行波)} \\ \pm \gamma & \text{(減衰/増大波)} \end{cases}$$

■ 伝達行列 (Stepping matrices)

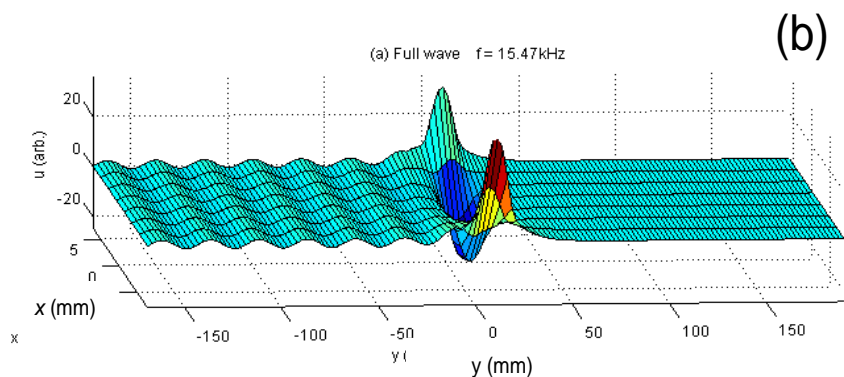
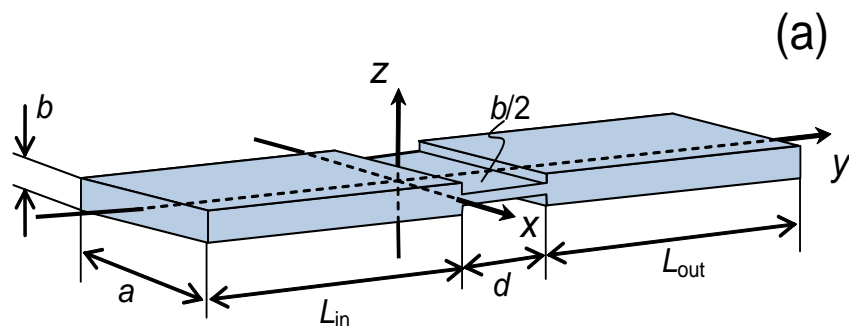
$$K_{\pm}^{(\text{dmp/grw})} = V \begin{bmatrix} e^{\pm ikh} & 0 \\ \cdot & \cdot \\ 0 & e^{\pm \gamma h} \end{bmatrix} V^{-1}$$



■ RTM 整合ポート境界条件

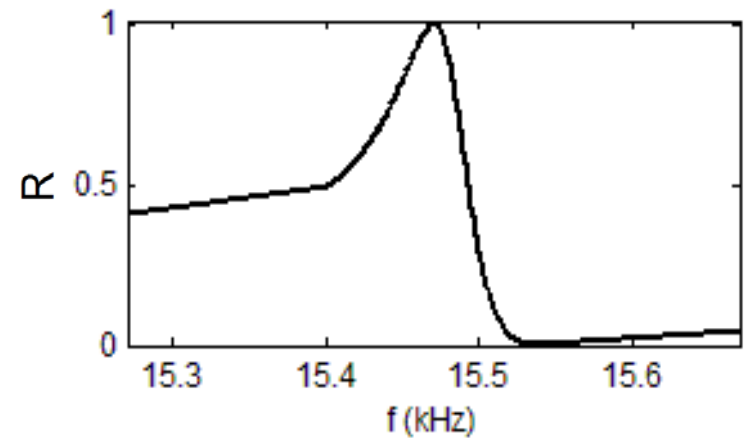
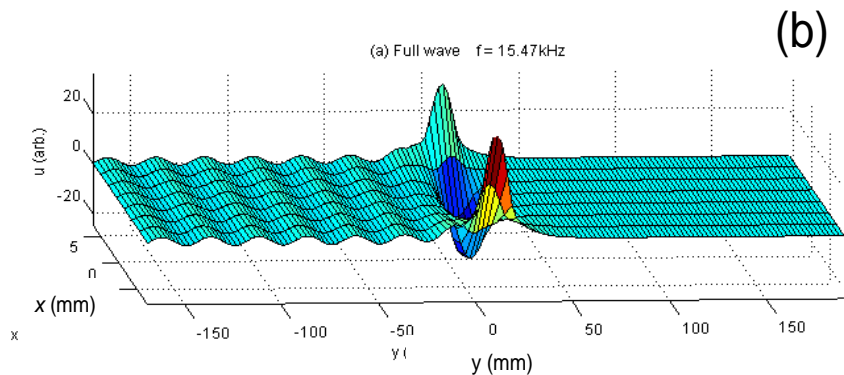
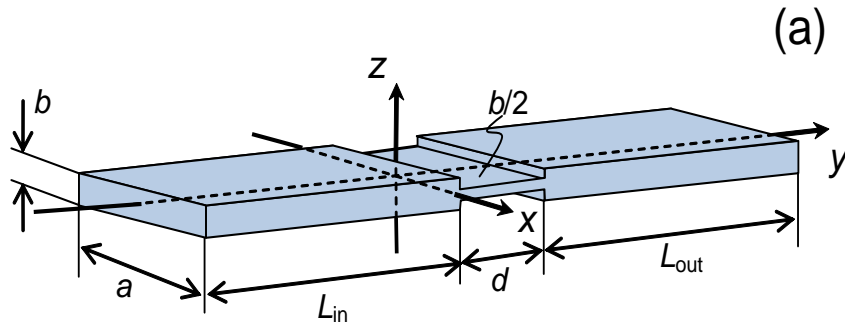
$$S_N = K_+^{(\text{dmp})} \quad S_0 = K_-^{(\text{grw})}$$

弾性平板におけるFano効果 = 共鳴反射 =



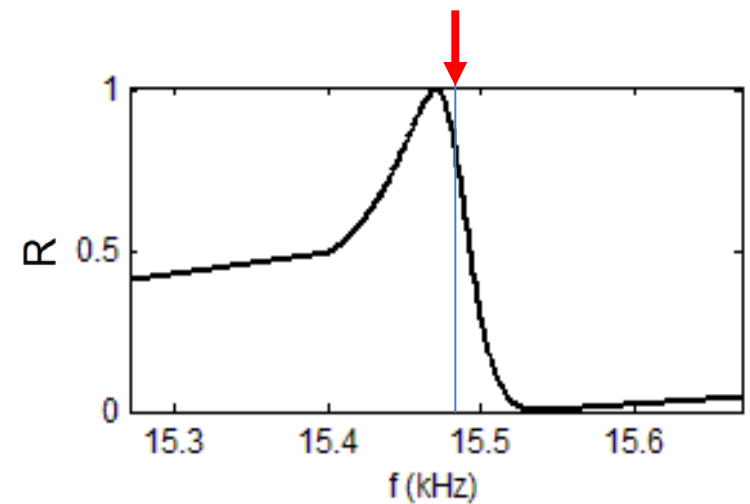
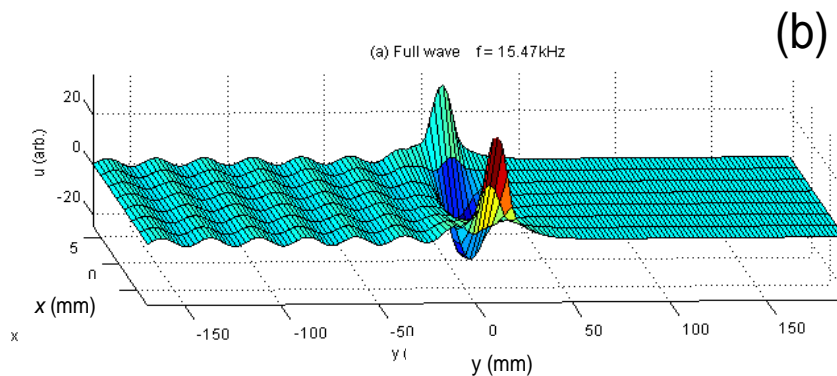
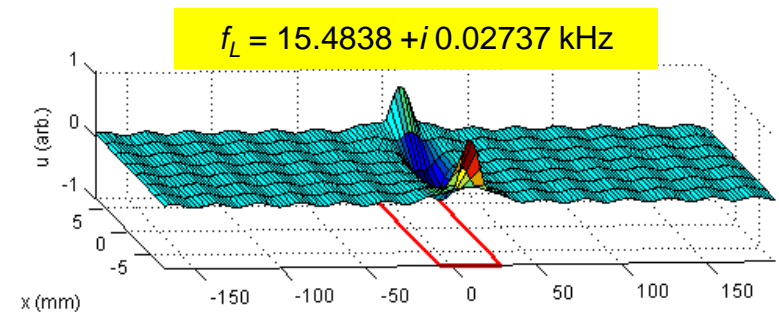
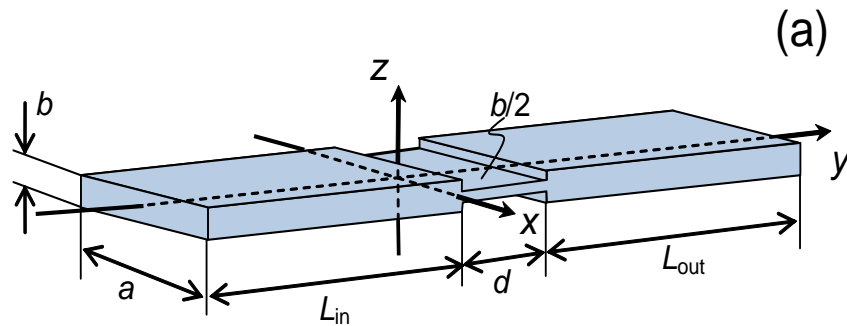
$d = 20\text{mm}$ $a = 16\text{mm}$ $b = 1\text{mm}$
 $Z_{in} = -80\text{mm}$ $N_x = 15$ ($h_x = 1.067$)
 $Z_{out} = 28\text{mm}$ $N_y = 30$ ($h_y = 1.200$)

弾性平板におけるFano効果 = 共鳴反射 =



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複素周波数をもつ擬似局在波



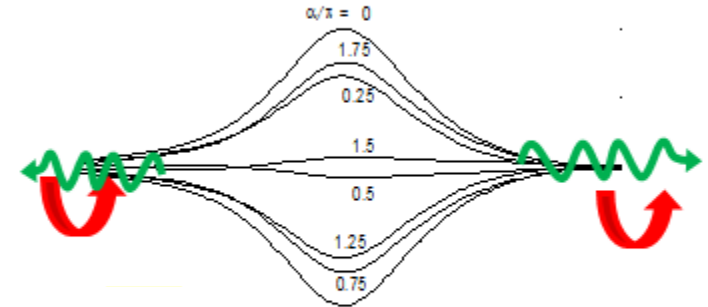
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局在波/擬似局在波の抽出

■RTM 整合ポット境界条件

$$u(y_{N+1}) = K_+^{(\text{dmp})} u(y_N)$$

$$u(y_{-1}) = \left(K_-^{(\text{grw})} \right)^{-1} u(y_0)$$



■大域的な連立次方程式 $u(y_n)$

$$c_0 u(y_{-1}) + b_0 u(y_0) + a_0 u(y_1) = 0, \quad (n=0)$$

$$c_n u(y_{n+1}) + b_n u(y_n) + a_n u(y_{n-1}) = 0, \quad (n=1, 2, \dots, N-1)$$

$$c_N u(y_{N-1}) + b_N u(y_N) + a_N u(y_{N+1}) = 0. \quad (n=N)$$

■仮固有値 ω_0^2 と固有値 ω_L^2 の逐次代入法による一致

$$\omega_L^2 b(x,y) \rho \Rightarrow (\omega_0^2 - \omega_L^2) b(x,y) \rho + \omega_L^2 b(x,y) \rho$$

$$c_n \Rightarrow c_n^{(1)} + \omega_L^2 c_n^{(2)}, \quad b_n \Rightarrow b_n^{(1)} + \omega_L^2 b_n^{(2)}, \quad a_n \Rightarrow a_n^{(1)} + \omega_L^2 a_n^{(2)}.$$

単極 $f_L (= \omega_L/2\pi)$ による共鳴曲線の近似モデル

S行列と位相シフト, および単極モデル

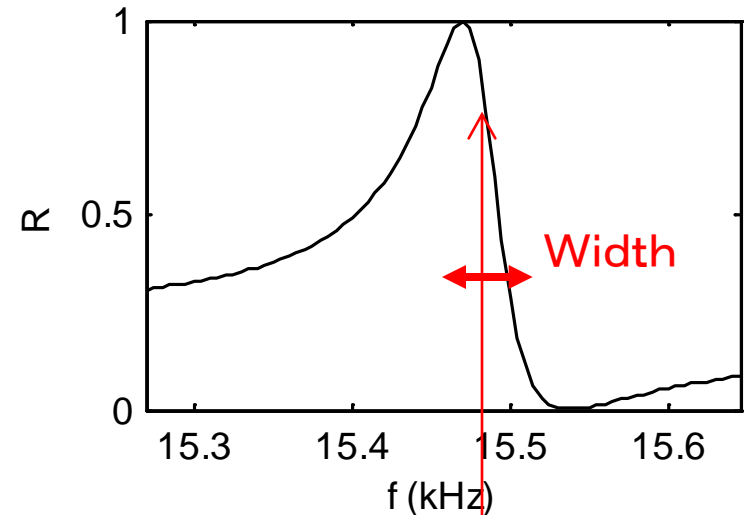
$$S(k) = \begin{bmatrix} r(f) & t'(f) \\ t(f) & r'(f) \end{bmatrix}$$

$$\begin{aligned} \det S(f) &= e^{i2\delta(f)} \\ &\approx e^{i2\delta_{bg}(f)} \frac{f-f_L^*}{f-f_L} \end{aligned}$$

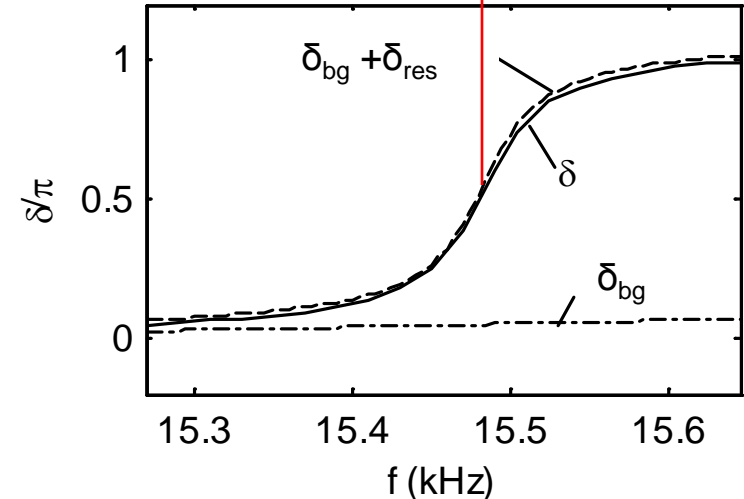
位相シフトの分離

$$\delta(f) \approx \delta_{bg}(f) + \delta_{res}(f)$$

$$\begin{aligned} \delta_{res}(f) &= \frac{1}{2i} \log \frac{f-f_L^*}{f-f_L} \\ &= \cot^{-1} \frac{f - \text{Re}[f_L]}{\text{Im}[f_L]} \end{aligned}$$



$$f_L = 15.483 - 0.027i \text{ kHz}$$



まとめ

- RTMの弱形式離散化スキームの提案
弱形式表現が可能なシステムへ適用範囲が拡大
- RTM整合ポート境界条件(RTM-consistent PBC)
ポート境界で全モードを接続
エネルギーを保存しつつ無反射
- 局在波/擬似局在波の抽出法
複素周波数の単極モデル
Fano効果の解析に有効
- 重調和方程式を拡張
テンソル基底を用いた屈曲波の定式化と流束の定義
4階の微分方程式の共変的な表現

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加藤初弘, 加藤初儀,

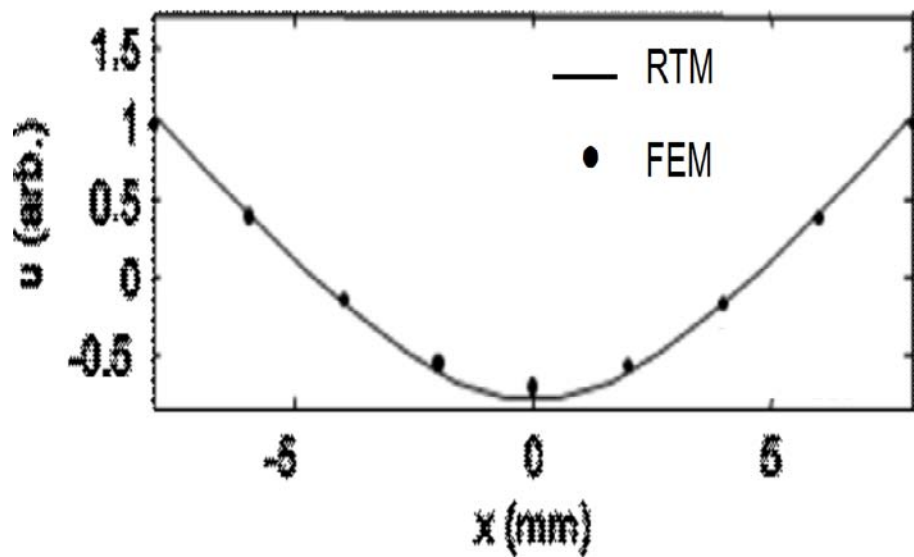
「逐次伝達法のための弱形式離散化スキームとその離散化誤差」,
日本応用数理学会 論文誌, vol.25, no.1, pp. 31-46, (March 2015).



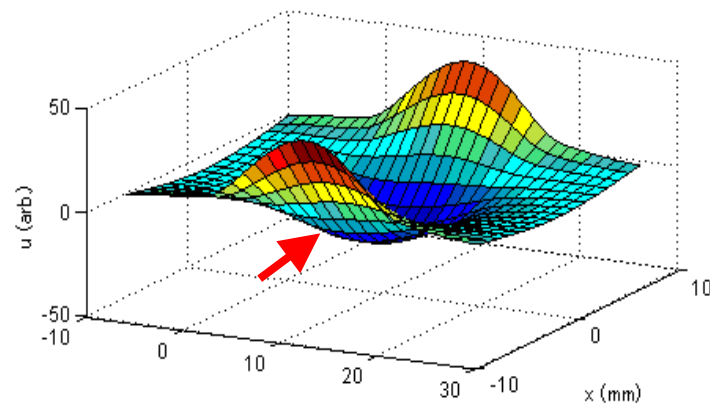
An RTMとFEMの比較

RTM with RTM-consistent PBC

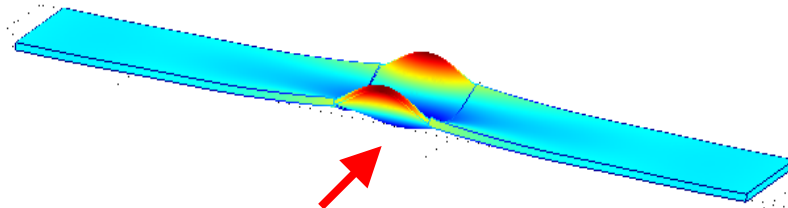
$$f_L = 15.4838 + i0.02737 \text{ kHz}$$



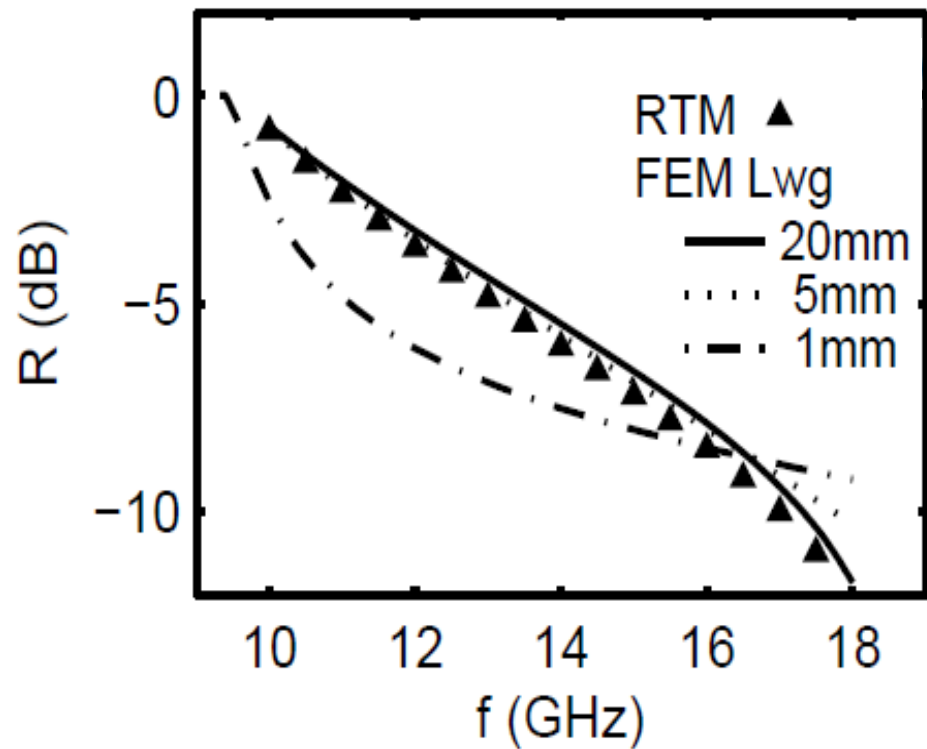
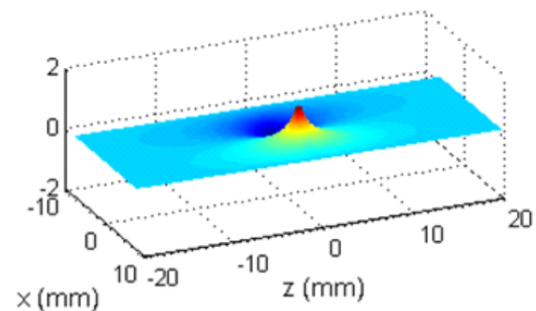
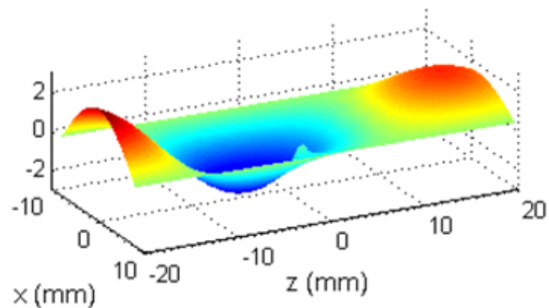
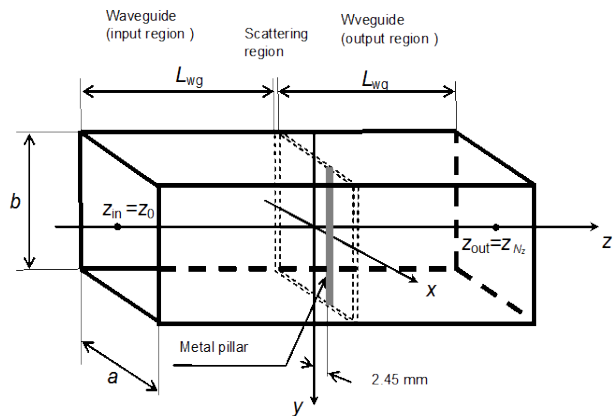
3%の不一致



FEM with free BC



解析境界に達する局在波の裾による影響



Neumann型境界条件における高階微分の欠落

■ 単一モード状態

$$u = a_0 X_0$$

$$\frac{\partial u}{\partial y} = ik_0 a_0 X_0$$

$$\frac{\partial u}{\partial y} = ik_0 u$$

■ 複数モード状態

$$u = a_0 X_0 + a_1 X_1 + a_2 X_2$$

$$\frac{\partial u}{\partial y} = ik_0 a_0 X_0 + ik_1 a_1 X_1 + ik_2 a_2 X_2,$$

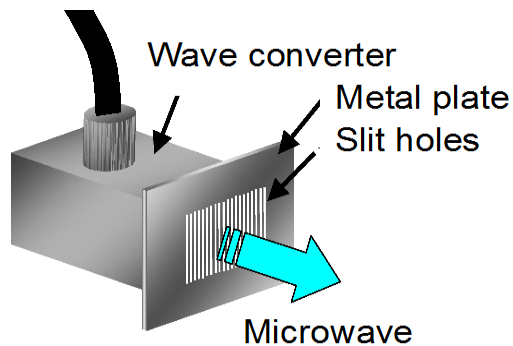
$$\frac{\partial^2 u}{\partial y^2} = (ik_0)^2 a_0 X_0 + (ik_1)^2 a_1 X_1 + (ik_2)^2 a_2 X_2,$$

$$\frac{\partial^3 u}{\partial y^3} = (ik_0)^3 a_0 X_0 + (ik_1)^3 a_1 X_1 + (ik_2)^3 a_2 X_2, .$$

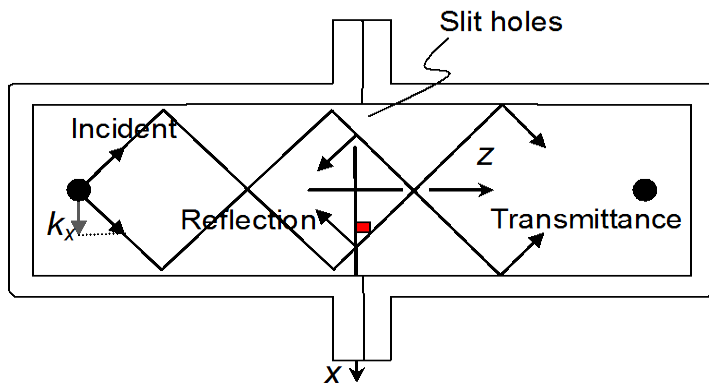
$$\begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} X_0 & X_1 & X_2 \\ (ik_0)^2 X_0 & (ik_1)^2 X_1 & (ik_2)^2 X_2 \\ (ik_0)^3 X_0 & (ik_1)^3 X_1 & (ik_2)^3 X_2 \end{bmatrix}^{-1} \begin{bmatrix} u \\ \frac{\partial^2 u}{\partial y^2} \\ \frac{\partial^3 u}{\partial y^3} \end{bmatrix} .$$

$$\frac{\partial u}{\partial y} = [ik_0 X_0 \quad ik_1 X_1 \quad ik_2 X_2] \begin{bmatrix} X_0 & X_1 & X_2 \\ (ik_0)^2 X_0 & (ik_1)^2 X_1 & (ik_2)^2 X_2 \\ (ik_0)^3 X_0 & (ik_1)^3 X_1 & (ik_2)^3 X_2 \end{bmatrix}^{-1} \begin{bmatrix} u \\ \frac{\partial^2 u}{\partial y^2} \\ \frac{\partial^3 u}{\partial y^3} \end{bmatrix} .$$

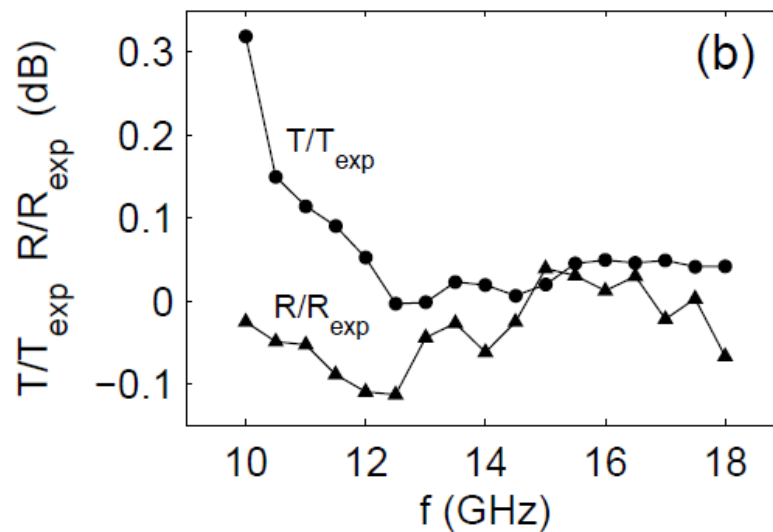
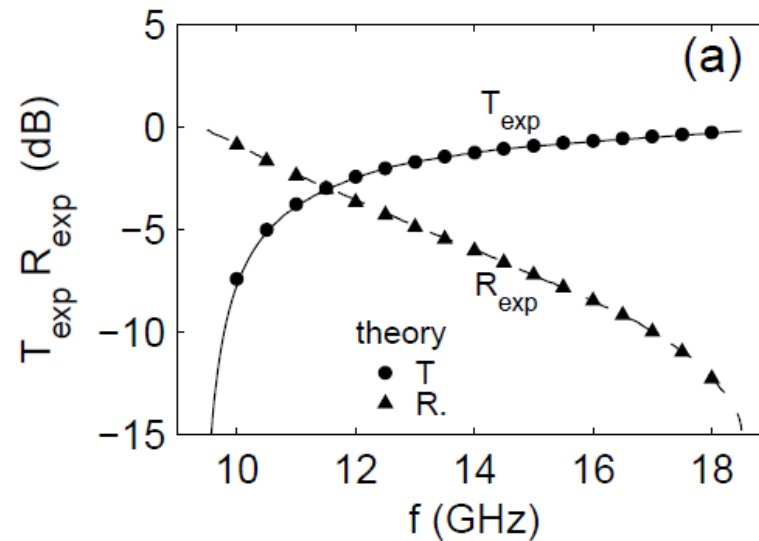
RTM confirmed by experiment



(a)



(b)



誤差の離散化幅 h -依存

1次元シュエディンガー方程式

$$u''(x) + [\varepsilon - \text{sech}^2(x)] u(x) = 0$$

ε 入射エネルギー

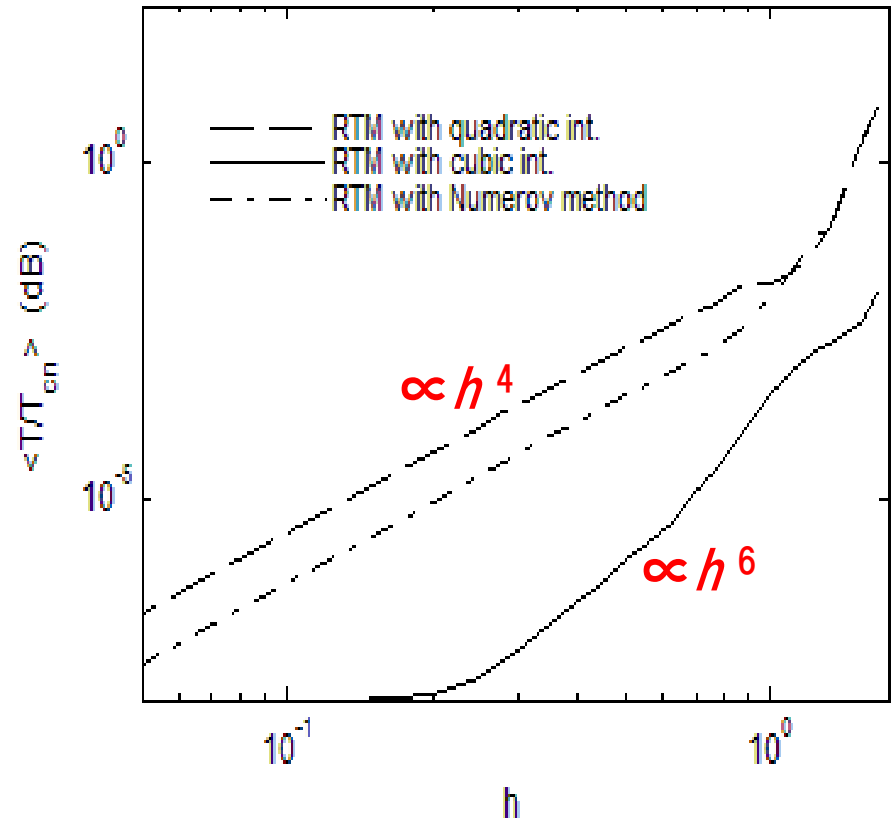
$\text{sech}^2(x)$ 散乱ポテンシャル

連続システムでの透過率

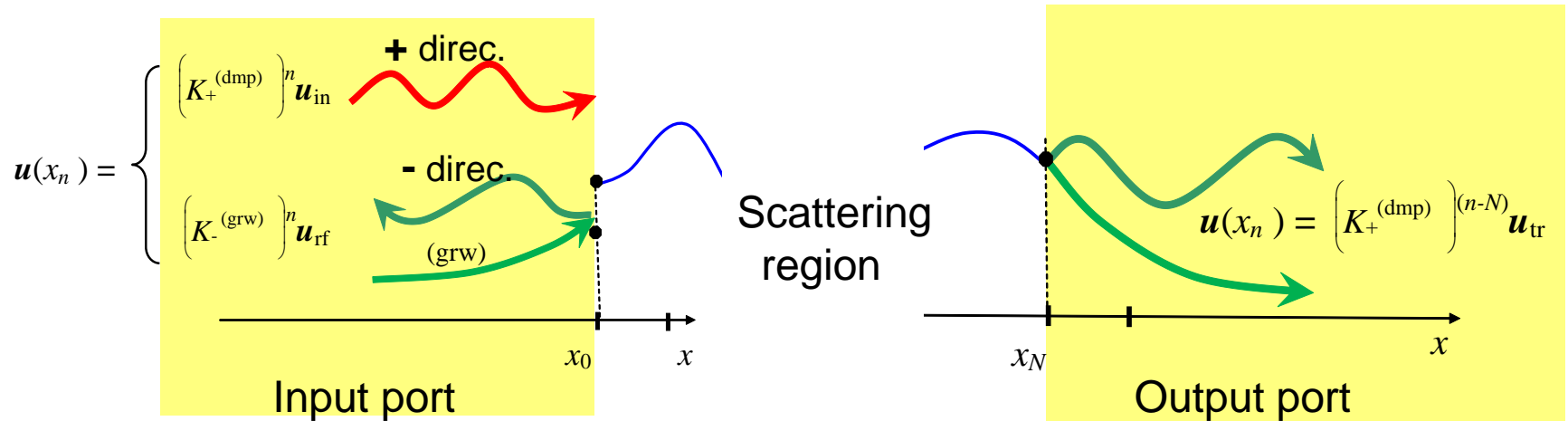
$$T_{\text{cn}} = \frac{\sinh^2(\pi\sqrt{\varepsilon})}{\sinh^2(\pi\sqrt{\varepsilon}) + \cosh^2(\pi\sqrt{3}/2)}$$

$\langle T/T_{\text{cn}} \rangle$ 相対誤差の総乗平均
($0.1 < \varepsilon < 2.8$)

h T_{cn} = 空間の離散化幅



Discretized wave expression in port regions



■ Waves in Ports

$$u(x_n) = \begin{cases} K_+^{(\text{dmp})}{}^n u_{\text{in}} + K_-^{(\text{grw})}{}^n u_{\text{rf}} & \text{input port} \\ K_+^{(\text{dmp})}{}^{(n-N)} u_{\text{tr}} & \text{output port} \end{cases}$$

■ Expressions for wave connections

$$u(x_1) = K_+^{(\text{dmp})} u_{\text{in}} + K_-^{(\text{grw})} u_{\text{rf}} \quad \text{at } x = x_1$$

$$u(x_{n+1}) = K_+^{(\text{dmp})} u(x_n) \quad \text{at } x_n > x_N$$

Reflection and transmission coefficients by RTM

■ Connection at x_1

$$K_+^{(\text{dmp})} \mathbf{u}_{\text{in}} + K_-^{(\text{grw})} \mathbf{u}_{\text{rf}} = S_0 (\mathbf{u}_{\text{in}} + \mathbf{u}_{\text{rf}})$$

Reflection field

$$\mathbf{u}_{\text{rf}} = -(S_0 - K_-^{(\text{grw})})^{-1} (S_0 - K_+^{(\text{dmp})}) \mathbf{u}_{\text{in}}$$

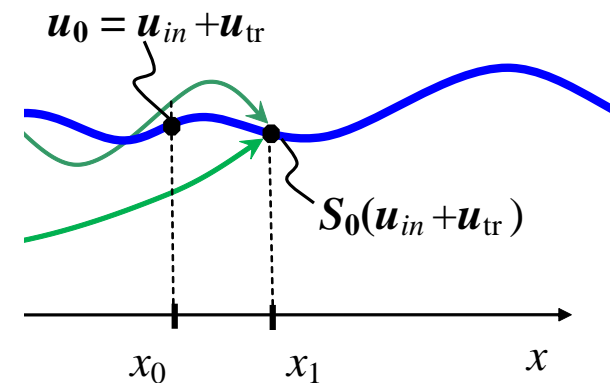
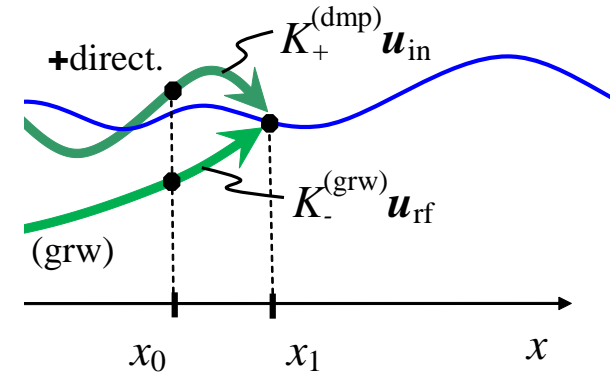
$$r = \mathbf{e}_1 \cdot \mathbf{u}_{\text{rf}} \quad \text{Reflection coefficient}$$

Transmission field

$$\mathbf{u}_{\text{tr}} = S_{N-1} \cdots S_2 S_1 S_0 (\mathbf{u}_{\text{in}} + \mathbf{u}_{\text{rf}})$$

$$t = \mathbf{e}_1 \cdot \mathbf{u}_{\text{tr}} \quad \text{Transmission coefficient}$$

$$\mathbf{e}_1 = [1 \ 0]^T \quad \text{Unit vector}$$



RTM 整合ポート境界条件 ～並進対称な入出力ポート～

$$a_{\text{port}}U(y_{n+1}) + b_{\text{port}}U(y_n) + a_{\text{port}}U(y_{n-1}) = 0$$

$$U(y_{n+1}) = KU(y_n), U(y_{n-1}) = K^{-1}U(y_n)$$

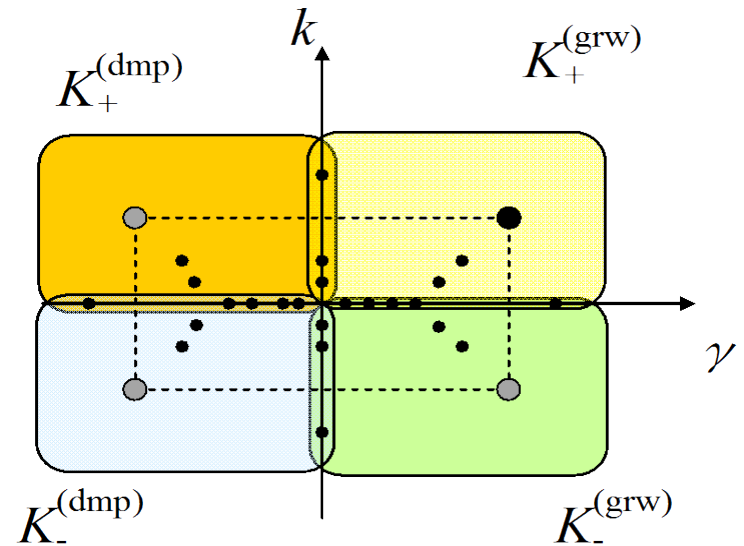
$$K = e^{Hh_y}$$

$$\Rightarrow H = \frac{1}{h_y} \cosh^{-1} \left(\frac{-1}{2} a_{\text{port}}^{-1} b_{\text{port}} \right)$$

$$K = T^{-1} \begin{bmatrix} e^{\eta_0 h_y} & & & & \\ & e^{\eta_1 h_y} & & & \\ & & e^{\eta_2 h_y} & & \\ & & & \cdot & \\ & & & & \cdot \\ & & & & & e^{\eta_{N_x} h_y} \end{bmatrix} T$$

時間・空間反転対称性

$$\eta_p = \pm \gamma_p \pm ik_p \quad (p=0,1,2,\dots,N_x)$$



境界の外部に接続

$$U_{\text{tr}}(y_{N_y+1}) = K_+^{(\text{dmp})} U_{\text{tr}}(y_{N_y})$$

$$U_{\text{in}}(y_0) = K_+^{(\text{grw})} U_{\text{in}}(y_{-1})$$

$$U_{\text{rf}}(y_0) = K_-^{(\text{grw})} U_{\text{rf}}(y_{-1})$$

Extraction of quasi-localized wave (2/2)

■ Actual k_L^2 as eigenvalue and wave shape as eigenvector

$$\begin{bmatrix} c_0^{(1)} (K_+^{(\text{grw})})^{-1} + b_0^{(1)} & a_0^{(1)} & 0 & \dots & 0 & 0 \\ c_1^{(1)} & b_1^{(1)} & a_1^{(1)} & & & \\ 0 & c_2^{(1)} & b_2^{(1)} & a_2^{(1)} & & \\ & & \ddots & \ddots & & \\ 0 & 0 & \dots & & c_N^{(1)} & b_N^{(1)} + a_N^{(1)} (K_+^{(\text{dmp})}) \end{bmatrix} \begin{bmatrix} u(x_0) \\ u(x_1) \\ u(x_2) \\ \vdots \\ \vdots \\ u(x_N) \end{bmatrix} = k_L^2 \begin{bmatrix} c_0^{(2)} (K_+^{(\text{grw})})^{-1} + b_0^{(2)} & a_0^{(2)} & 0 & \dots & 0 & 0 \\ c_1^{(2)} & b_1^{(2)} & a_1^{(2)} & & & \\ 0 & c_2^{(2)} & b_2^{(2)} & a_2^{(2)} & & \\ & & \ddots & \ddots & & \\ 0 & 0 & \dots & & 2 c_N^{(2)} & b_N^{(2)} + a_N^{(2)} (K_+^{(\text{dmp})}) \end{bmatrix} \begin{bmatrix} u(x_0) \\ u(x_1) \\ u(x_2) \\ \vdots \\ \vdots \\ u(x_N) \end{bmatrix}$$

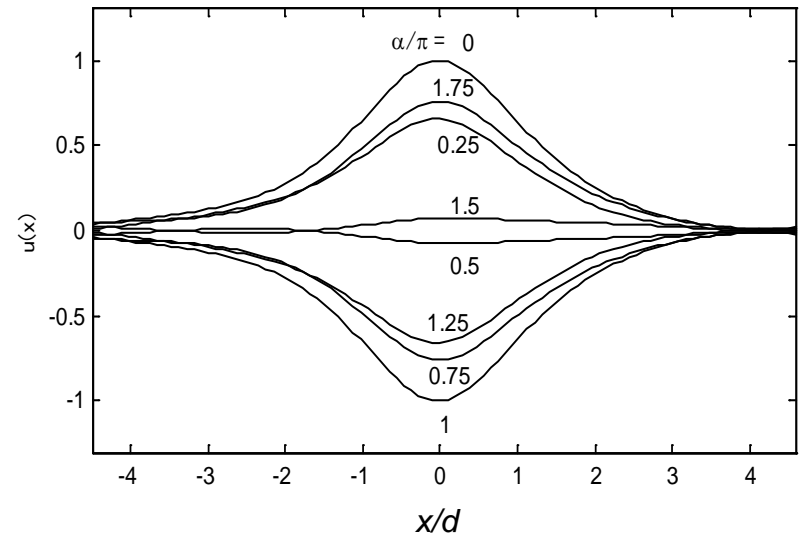
Consistency by iterative use

$$k_0 \rightarrow K_+^{(\text{dmp})}, K_-^{(\text{grw})} \rightarrow k_L$$

Eleven times iterations

$$\left| \frac{k_L^{(p+1)} - k_L^{(p)}}{k_L^{(p)}} \right| < 10^{-5}$$

$$k_L d = 0.99766 + i 0.00062$$





要素内補間による差分方程式の導出(その1b)

■ 補間関数

$$u(x,y) = \sum_{p=1}^4 [L_0^{(p)}(x,y)u(P_p) + L_1^{(p)}(x,y)u_x(P_p) + L_2^{(p)}(x,y)u_y(P_p) + L_3^{(p)}(x,y)u_{xy}(P_p)]$$

- $L_0^{(p)}(x,y)$ 6 次の代数多項式
- $u(P_p)$ 節点 P_p での関数値
- $u_x(P_p)$ 節点 P_p での導関数値(偏微分).
- $u_y(P_p), \dots$
- $u_{xy}(P_p) \dots$

流束保存条件

$$\int_S \nabla \cdot \mathbf{J} \, dS = 0$$

$$\nabla \cdot \mathbf{J} = \sum_{r=0}^2 D_r [w(\Delta_r^2 u) - (\Delta_r w)(\Delta_r u)]$$

