Design of Nano-Photonic devices

Achim Schädle

Zuse Institute Berlin

DFG Research Center MATHEON
Mathematics for key technologies

2/22/2008

Application Area D:

Circuits simulation and opto-electronic devices

- Circuits simulation
- Modelling of active optical devices
- Simulation of passive optical devices
- Chip design verification

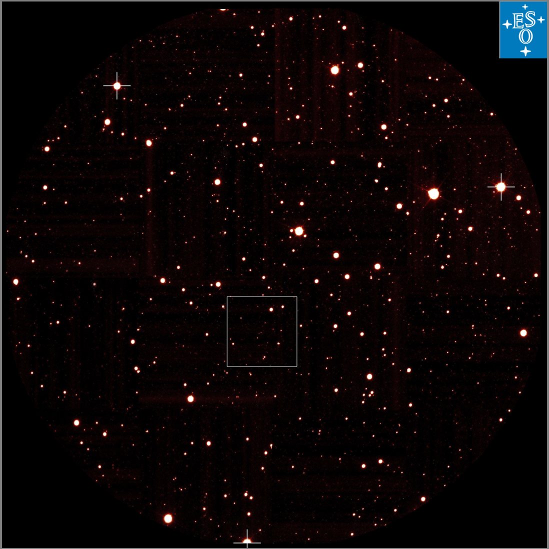
Projects: D9, D15

Heads: P. Deuflhard, F. Schmidt
Staff: B. Kettner, T. Pollok, A. Schädle

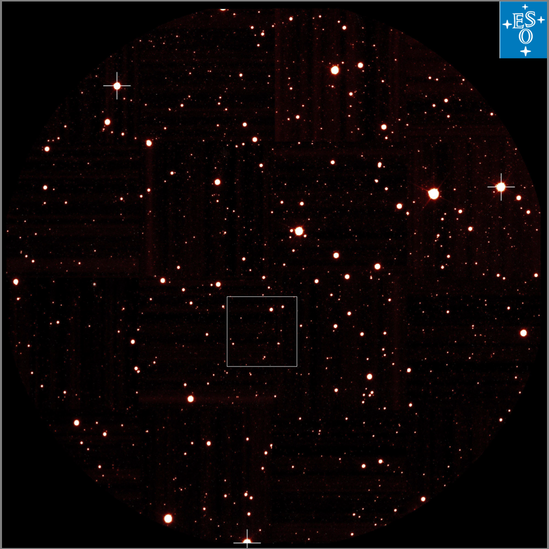
Computation of electromagnetic fields in three space dimensions.

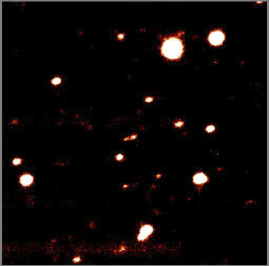
Wavelength of light: $\lambda = 100 - 1000\mathrm{nm}$
Structure size: $10 - 100\mathrm{nm} = 10 - 100 \cdot 10^{-9} m$

- Photonic crystals
- Photonic crystal fibres
- Metamaterials
- Lithography masks
- Photonic cavities



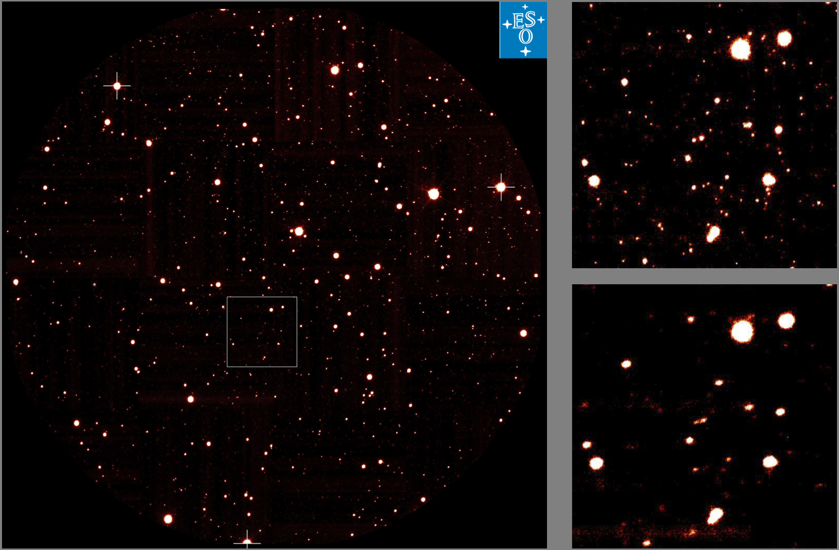
Omega Centauri, European Southern Observatory (ESO)





Omega Centauri, European Southern Observatory (ESO)

Adaptive optics



Omega Centauri, European Southern Observatory (ESO)


ESO
Photograph: Y. Beletsky

Guide a laser beam to the telescope

- Transport very high energy at $\lambda = 589.2nm$
- Reduce radiation loos

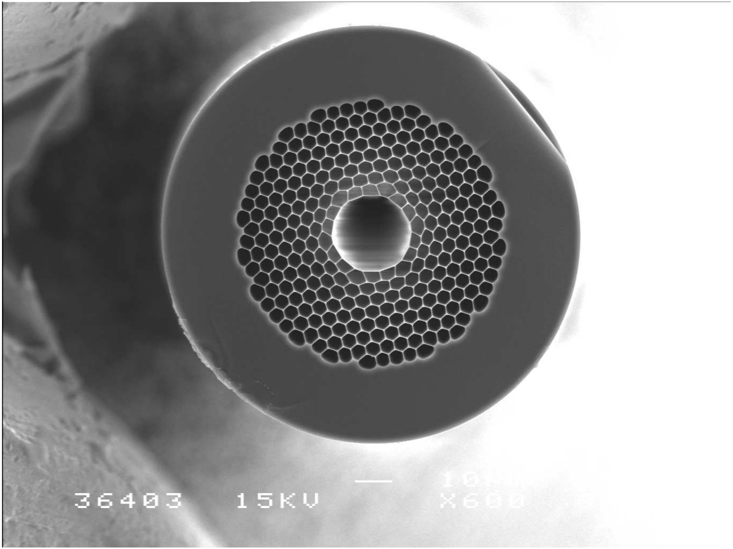


Image courtesy: Crystal Fibre A/S, Denmark.

$$\mathbf{H}(r,t) = \exp(i\omega t)\mathbf{H}(r)$$

Time harmonic Maxwell's equations

$$\nabla \times \epsilon(r)^{-1}\nabla \times \mathbf{H}(r) + \mu(r)\omega^2\mathbf{H}(r) = 0$$

+ boundary conditions + divergence condition

$$\mathbf{H}(r,t) = \exp(i\omega t)\mathbf{H}(r)$$

Time harmonic Maxwell's equations

$$\nabla \times \epsilon(r)^{-1}\nabla \times \mathbf{H}(r) + \mu(r)\omega^2\mathbf{H}(r) = 0$$

+ boundary conditions + divergence condition

Propagating mode

$$\mathbf{H}(r) = \mathbf{H}(x,y,z) = \exp(ik_z z)\mathbf{H}(x,y)$$

$$\mathbf{H}(x,y) = \begin{bmatrix} H_x(x,y) \\ H_y(x,y) \\ H_z(x,y) \end{bmatrix} = \begin{bmatrix} \mathbf{H}_\perp \\ H_z \end{bmatrix}$$

Trick: $\tilde{H}_z = k_z H_z$

$$\begin{bmatrix} \mathrm{P}\nabla_\perp \epsilon^{-1} \nabla_\perp \cdot \mathrm{P} - \omega^2 \mu & -i\mathrm{P}\epsilon^{-1}\mathrm{P}\nabla_\perp \\ 0 & \nabla_\perp \cdot \mathrm{P}\epsilon^{-1}\mathrm{P}\nabla_\perp - \omega^2\mu \end{bmatrix} \begin{bmatrix} \mathbf{H}_\perp \\ \tilde{H}_z \end{bmatrix}$$

$$= k_z^2 \begin{bmatrix} \mathrm{P}\epsilon^{-1}\mathrm{P} & 0 \\ i\nabla_\perp \cdot \mathrm{P}\epsilon^{-1}\mathrm{P} & 0 \end{bmatrix} \begin{bmatrix} \mathbf{H}_\perp \\ \tilde{H}_z \end{bmatrix}$$

with $\mathrm{P} = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}, \nabla_\perp = \begin{bmatrix} \partial_x \\ \partial_y \end{bmatrix}$

General eigenvalue problem for k_z with singular B

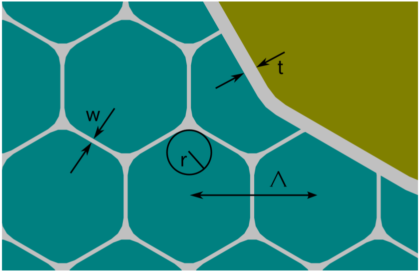
$$A \begin{bmatrix} \mathbf{H}_\perp \\ \tilde{H}_z \end{bmatrix} = k_z^2 \, B \begin{bmatrix} \mathbf{H}_\perp \\ \tilde{H}_z \end{bmatrix},$$

General eigenvalue problem for k_z with singular B

$$A \begin{bmatrix} \mathbf{H}_\perp \\ \tilde{H}_z \end{bmatrix} = k_z^2 \, B \begin{bmatrix} \mathbf{H}_\perp \\ \tilde{H}_z \end{bmatrix},$$

$\Im(k_z) \propto$ energy flux across boundary

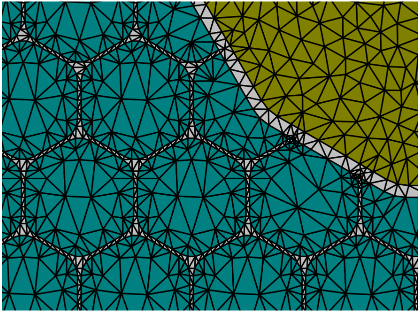
- High order curl conforming finite elements
- Adaptive grid refinement
- Transparent boundary conditions (PML, Pole condition)

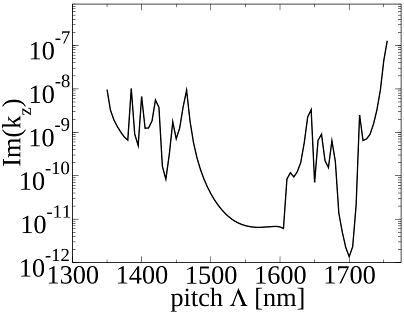


Geometry cut out

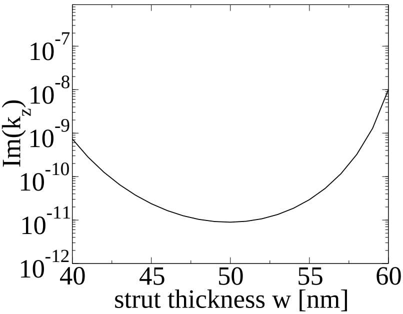
Parameters to be optimized

Finite element grid

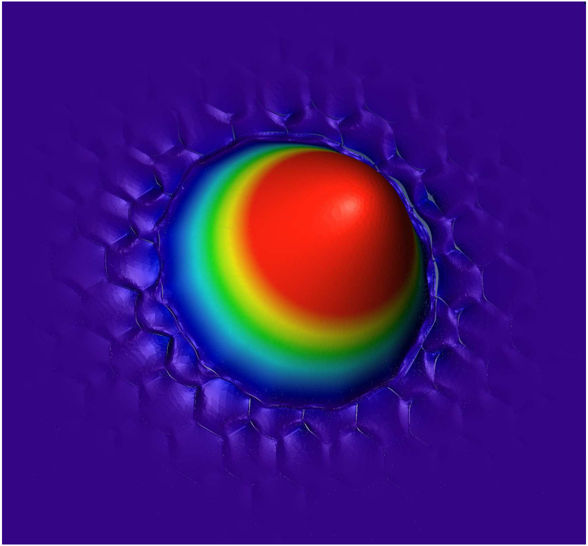




Im(k_z)
10^-7
10^-8
10^-9
10^-10
10^-11
10^-12
1300
1400
1500
1600
1700
pitch Λ [nm]



Im(k_z)
10^-7
10^-8
10^-9
10^-10
10^-11
10^-12
40
45
50
55
60
strut thickness w [nm]



Intensity of the field

2D scalar case (Helmholtz equation)

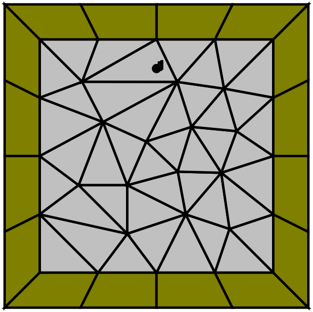
$$\Delta u(x,y) + k^2(x,y)u(x,y) = f, \quad (x,y) \in \mathbb{R}^2$$

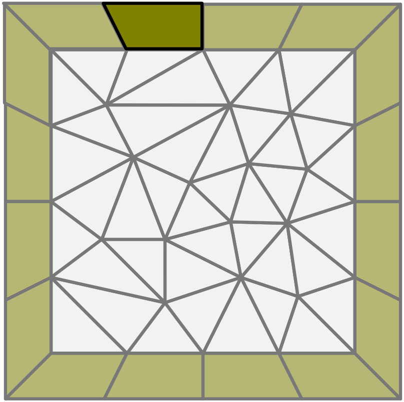
$$\lim_{|r|\to\infty} \sqrt{r}\left(\partial_r u - iku\right) = 0\,, \qquad r = \frac{(x,y)}{||(x,y)||}$$

2D scalar case (Helmholtz equation)

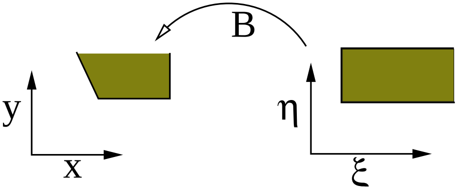
$$\Delta u(x,y) + k^2(x,y)u(x,y) = f\,, \quad (x,y) \in \mathbb{R}^2$$

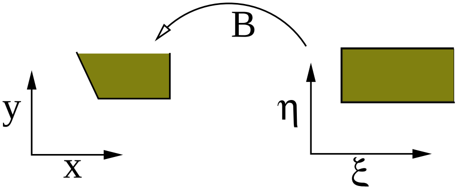
$$\lim_{|r|\to\infty} \sqrt{r}\left(\partial_r u - iku\right) = 0\,, \qquad r = \frac{(x,y)}{||(x,y)||}$$





Transformation unit rectangle





$$J_B = \begin{pmatrix} 1 & 0 \\ \eta b - a & h_\eta + \xi b \end{pmatrix} \;; \quad |J_B| = h_\eta + \xi b$$

$$\int_{prism} \nabla u(x,y) \cdot \nabla \phi(x,y) dx\, dy =$$

$$\int_0^1 \int_0^\infty \left(J_B^{-T} \nabla_{\xi,\eta} \tilde{u}(\xi,\eta) \right) \cdot J_B^{-T} \nabla_{\xi,\eta} \tilde{\phi}(\xi,\eta) |J_B| d\xi\, d\eta$$

Exponential test function

$$\int_{prism} \nabla u(x,y) \cdot \nabla \phi(x,y) dx\, dy =$$

$$\int_0^1 \int_0^\infty \left(J_B^{-T} \nabla_{\xi,\eta} u(\xi,\eta) \right) \cdot J_B^{-T} \nabla_{\xi,\eta} \phi(\xi,\eta) |J_B| d\xi\, d\eta$$

$$\phi(\xi,\eta) = \phi(\eta) \exp(-s\xi)$$

$$\int_{prism} \nabla u(x,y) \cdot \nabla \phi(x,y) dx\, dy =$$

$$\int_0^1 \int_0^\infty \left(J_B^{-T} \nabla_{\xi,\eta} u(\xi,\eta) \right) \cdot J_B^{-T} \nabla_{\xi,\eta} \phi(\xi,\eta) |J_B| d\xi\, d\eta$$

$$\phi(\xi,\eta) = \phi(\eta) \exp(-s\xi)$$

Laplace transform of u in distance variable ξ

$$U(\eta,s) = \int_0^\infty u(\eta,\xi) \exp(-s\xi) d\xi$$

Transformed equation

$$\int_0^\infty \left(J_B^{-T} \nabla_{\xi,\eta} u(\xi,\eta) \right) \cdot J_B^{-T} \nabla_{\xi,\eta} \phi(\xi,\eta) |J_B| d\xi$$

$$= \int_0^\infty (h_\eta + \xi b) \partial_\xi \phi \partial_\xi u$$

$$-(\eta b - a) \partial_\eta \phi \partial_\xi u$$

$$-(\eta b - a) \partial_\xi \phi \partial_\eta u$$

$$+\frac{1 + (\eta b - a)^2}{(h_\eta + \xi b)} \partial_\eta \phi \partial_\eta u d\xi$$

$$\int_0^\infty \left(J_B^{-T}\nabla_{\xi,\eta}u(\xi,\eta)\right)\cdot J_B^{-T}\nabla_{\xi,\eta}\phi(\xi,\eta)|J_B|d\xi$$

$$= \int_0^\infty (h_\eta + \xi b)\partial_\xi\phi\partial_\xi u \qquad = h_\eta s(sU(s,\eta) - u|_{\xi=0})$$

$$-(\eta b - a)\partial_\eta\phi\partial_\xi u$$

$$-(\eta b - a)\partial_\xi\phi\partial_\eta u$$

$$+\frac{1+(\eta b - a)^2}{(h_\eta + \xi b)}\partial_\eta\phi\partial_\eta u d\xi$$

$$\int_0^\infty \left(J_B^{-T} \nabla_{\xi,\eta} u(\xi,\eta) \right) \cdot J_B^{-T} \nabla_{\xi,\eta} \phi(\xi,\eta) |J_B| d\xi$$

$$= \int_0^\infty (h_\eta + \xi b) \partial_\xi \phi \partial_\xi u \qquad = h_\eta s(sU(s,\eta) - u|_{\xi=0}) \quad bs(-U(s,\eta) - s\partial_s U(s,\eta))$$

$$-(\eta b - a)\partial_\eta \phi \partial_\xi u$$

$$-(\eta b - a)\partial_\xi \phi \partial_\eta u$$

$$+\frac{1 + (\eta b - a)^2}{(h_\eta + \xi b)} \partial_\eta \phi \partial_\eta u d\xi$$

$$\int_0^\infty \left(J_B^{-T}\nabla_{\xi,\eta}u(\xi,\eta)\right)\cdot J_B^{-T}\nabla_{\xi,\eta}\phi(\xi,\eta)|J_B|d\xi$$

$$= \int_0^\infty (h_\eta + \xi b)\partial_\xi\phi\partial_\xi u$$

$$-(\eta b - a)\partial_\eta\phi\partial_\xi u$$

$$-(\eta b - a)\partial_\xi\phi\partial_\eta u$$

$$+\frac{1 + (\eta b - a)^2}{(h_\eta + \xi b)}\partial_\eta\phi\partial_\eta u d\xi$$

$$= h_\eta s(sU(s,\eta) - u|_{\xi=0})$$

$$bs(-U(s,\eta) - s\partial_s U(s,\eta))$$

$$-(\eta b - a)\partial_\eta\phi(sU(s,\eta) - u|_{\xi=0})$$

$$\int_0^\infty \Big(J_B^{-T}\nabla_{\xi,\eta}u(\xi,\eta)\Big)\cdot J_B^{-T}\nabla_{\xi,\eta}\phi(\xi,\eta)|J_B|d\xi$$

$$= \int_0^\infty (h_\eta + \xi b)\partial_\xi\phi\partial_\xi u$$

$$-(\eta b - a)\partial_\eta\phi\partial_\xi u$$

$$-(\eta b - a)\partial_\xi\phi\partial_\eta u$$

$$+\frac{1+(\eta b - a)^2}{(h_\eta + \xi b)}\partial_\eta\phi\partial_\eta u d\xi$$

$$= h_\eta s(sU(s,\eta) - u|_{\xi=0})$$

$$bs(-U(s,\eta) - s\partial_s U(s,\eta))$$

$$-(\eta b - a)\partial_\eta\phi(sU(s,\eta) - u|_{\xi=0})$$

$$-(\eta b - a)\partial_\eta sU(s,\eta)$$

$$\int_0^\infty \left(J_B^{-T} \nabla_{\xi,\eta} u(\xi,\eta) \right) \cdot J_B^{-T} \nabla_{\xi,\eta} \phi(\xi,\eta) |J_B| d\xi$$

$$\begin{aligned}
= \int_0^\infty & (h_\eta + \xi b) \partial_\xi \phi \partial_\xi u \\
& -(\eta b - a) \partial_\eta \phi \partial_\xi u \\
& -(\eta b - a) \partial_\xi \phi \partial_\eta u \\
& + \frac{1 + (\eta b - a)^2}{(h_\eta + \xi b)} \partial_\eta \phi \partial_\eta u \, d\xi
\end{aligned}$$

$$\begin{aligned}
= & h_\eta s(sU(s,\eta) - u|_{\xi=0}) \\
& bs(-U(s,\eta) - s\partial_s U(s,\eta)) \\
& -(\eta b - a)\partial_\eta \phi (sU(s,\eta) - u|_{\xi=0}) \\
& -(\eta b - a)\partial_\eta s U(s,\eta) \\
& + \partial_\eta \phi \partial_\eta I(U(s,\eta))
\end{aligned}$$

A function $u(x, \eta)$ satisfies the Pole Condition if for all η the Lapalcetransform $U(s, \eta)$ of $u(\cdot, \eta)$ has a holomorphic extension to the lower complex halfplane H.

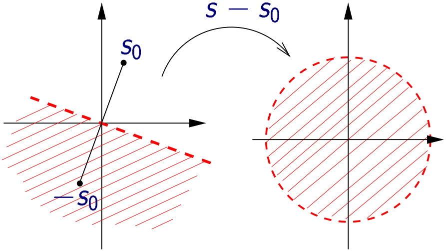
Theorem (Schmidt, Hohage, Zschiedrich 1998):

The Pole condition is equivalent to the Sommerfeld radiation condition:

$$\lim_{|r|\to\infty} \sqrt{r}\left(\partial_r u - iku\right) = 0$$

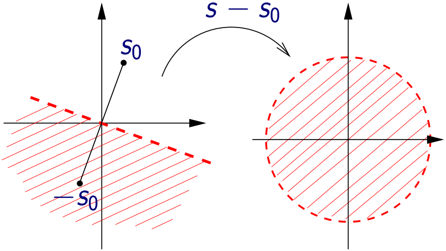
A Möbius tranform maps the half plane H onto the interior of the unit circle.

$$\tilde{s} = \frac{s + s_0}{s - s_0}$$



A Möbius tranform maps the half plane H onto the interior of the unit circle.

$$\tilde{s} = \frac{s + s_0}{s - s_0}$$

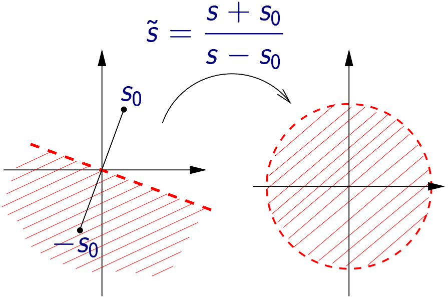


We have

$$\lim_{s \to \infty} sU(s) = u(0)$$

$$\lim_{\tilde{s} \to 1} s_0 \frac{\tilde{s} + 1}{\tilde{s} - 1} U(\tilde{s}) = u(0)$$

A Möbius tranform maps the half plane H onto the interior of the unit circle.



We have

$$\lim_{s\to\infty} sU(s) = u(0)$$

$$\lim_{\tilde{s}\to 1} s_0 \frac{\tilde{s}+1}{\tilde{s}-1} U(\tilde{s}) = u(0)$$

In the variable $\tilde{s}$, U is expanded into a power series.

$$U(\tilde{s}) = (\tilde{s}-1)\left(\frac{u(0)}{2s_0} + (\tilde{s}-1)\sum_{n\geq 0} a_n \tilde{s}^{\,n}\right)$$

Equations for the a_n

$$s(sU(s)-u_0) \leftrightarrow s_0^2 \begin{bmatrix} \frac{1}{2s_0} & 1 & & & \\ \frac{1}{2s_0} & 2 & 1 & & \\ & 1 & 2 & 1 & \\ & & & & \\ & & & 1 & 1 \end{bmatrix} \begin{bmatrix} u|_{\xi=0} \\ a_0 \\ a_1 \\ \\ a_N \end{bmatrix}$$

$$s\partial_s(sU(s)) \leftrightarrow s_0 \begin{bmatrix} -\frac{1}{2s_0} & 0 & 1/2 & & \\ 0 & -1 & 0 & 1 & \\ \frac{1}{2s_0} & 0 & -2 & 0 & 3/2 \\ & & & & \\ & & \frac{n-1}{2} & \frac{-n}{2} & \frac{1-2n}{2} \end{bmatrix} \begin{bmatrix} u|_{\xi=0} \\ a_0 \\ a_1 \\ \\ a_N \end{bmatrix}$$

$$sU(s) - u_0 \leftrightarrow s_0 \begin{bmatrix} -\frac{1}{2s_0} & -1 & & & \\ \frac{1}{2s_0} & 0 & -1 & & \\ & 1 & 0 & -1 & \\ & & & & \\ & & & 1 & -1 \end{bmatrix} \begin{bmatrix} u|_{\xi=0} \\ a_0 \\ a_1 \\ \\ a_N \end{bmatrix}$$

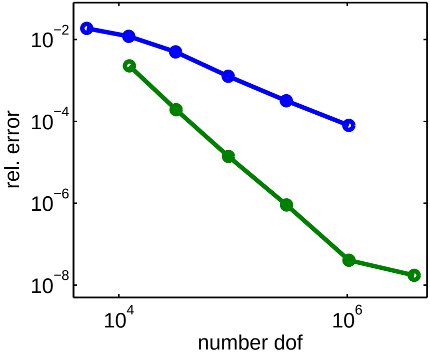
$$sU(s) \leftrightarrow s_0 \begin{bmatrix} \frac{1}{2s_0} & -1 & & & \\ \frac{1}{2s_0} & 0 & -1 & & \\ & 1 & 0 & -1 & \\ & & & & \\ & & & 1 & -1 \end{bmatrix} \begin{bmatrix} u|_{\xi=0} \\ a_0 \\ a_1 \\ \\ a_N \end{bmatrix}$$

$$\int_0^\infty \frac{1}{c+b\xi} u(\xi) \exp(-\xi s) d\xi = \left(b\partial_s + c\right)^{-1} U(s)$$

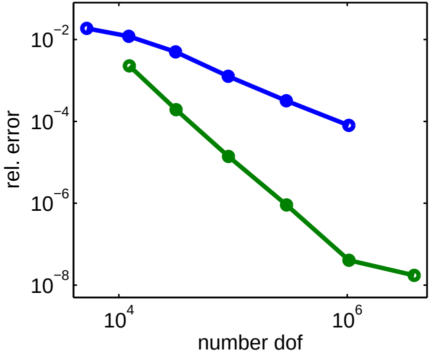
$\dots$

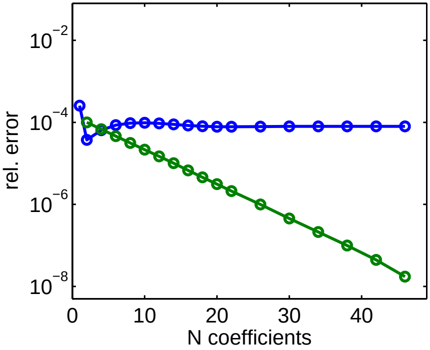
Infinite element of size $N+2$

Convergence



Convergence





- Extension to time-dependent problems
- Regularity of the exterior Helmholtz problem
- Is $\exp(-\xi s)$ “dense” ?
- Convergence theory