Ongoing developments for variational forms: coupled problems, parallelization

Xavier Claeys Axel Fourmont Frédéric Hecht Pierre Jolivet Pierre Marchand Jacques Morice Pierre-Henri Tournier

FreeFEM Days, 14th Edition

December 8, 2022

Outline

- vectorial BEM equation: Maxwell
- 2 Composite FE Spaces
- 3 Examples:
- FEM-BEM coupling example
- Parallelization

Quick recap on the Boundary Element Method

Model problem

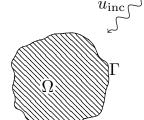
Volume form of the problem:

$$\begin{cases} -\Delta u - k^2 u = 0 & \text{in } \mathbb{R}^3 \backslash \Omega \\ \\ u = -u_{\text{inc}} & \text{on } \Gamma \\ \\ + \text{ radiation condition} \end{cases}$$

Green kernel: $\mathcal{G}(\mathbf{x}) = \exp(\imath k |\mathbf{x}|)/(4\pi |\mathbf{x}|)$

Single Layer Potential $SL: \forall q \in H^{-1/2}(\Gamma)$,

$$SL(q)(x) = \int_{\Gamma} \mathcal{G}(x - y)q(y)d\sigma(y), \quad \forall x \in \mathbb{R}^3 \setminus \Gamma$$



SL produces solutions of the PDE which satisfy the necessary conditions at infinity (here the Helmholtz equation and the Sommerfeld radiation condition)

$$\implies$$
 look for $p \in H^{-1/2}(\Gamma)$ such that $SL(p)(x) = u(x)$ with $u = -u_{inc}$ on Γ

A variational formulation of the integral equation can be obtained by imposing the Dirichlet condition in a weak manner: find $p:\Gamma \to \mathbb{C}$ such that

$$\int_{\Gamma \times \Gamma} \frac{\exp(\imath k |\mathbf{x} - \mathbf{y}|)}{4\pi |\mathbf{x} - \mathbf{y}|} p(\mathbf{y}) q(\mathbf{x}) d\sigma(\mathbf{x}, \mathbf{y}) = -\int_{\Gamma} u_{\text{inc}}(\mathbf{x}) q(\mathbf{x}) d\sigma(\mathbf{x}) \quad \forall q : \Gamma \to \mathbb{C}$$

Quick recap on the Boundary Element Method BEMTool library

BEMTool is a general purpose BEM library written by Xavier Claeys (LJLL). It is written in C++ and handles:

- Laplace, Yukawa, Helmholtz, Maxwell
- both in 2D and in 3D
- 1D, 2D and 3D triangulations (not necessarily flat)
- \mathbb{P}_k -Lagrange k = 0, 1, 2 and surface \mathbb{RT}_0

BEMTool is interfaced with FreeFEM.

It is available on GitHub () https://github.com/xclaeys/BemTool

Hierarchical matrices

Hierarchical block structure, Low-rank approximation

Let $\mathbf{B} \in \mathbb{C}^{N \times N}$ be a dense BEM matrix

quadratic cost in storage and complexity of the matrix-vector product

Low-rank approximation ?

BEM matrices do not have fast decreasing singular values,

BUT near the diagonal : near-field interactions

away from the diagonal : far-field \Longrightarrow Green function very regularizing

Idea: build a hierarchical representation of the blocks of the matrix identify and compress admissible blocks using low-rank approximation

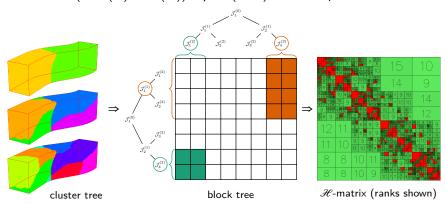
 \Rightarrow Build a low-rank approximation $\mathbf{B} \approx \sum_{j=1}^{r} \mathbf{u}_{j} \mathbf{v}_{j}^{T}$ (\sim approx. truncated SVD) for each admissible block \mathbf{B} , using e.g. Partially pivoted Adaptive Cross Approximation, which needs only 2r rows/columns

Hierarchical matrices

Summary

- build a hierarchical, geometric clustering of the degrees of freedom
- traverse the block tree recursively
- geometric admissibility condition:

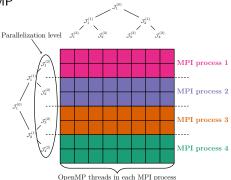
 $\max(\operatorname{diam}(X),\operatorname{diam}(Y)) \leq \eta \operatorname{dist}(X,Y) \implies \operatorname{compress the block}$



Hierarchical matrices

Htool library

- C++ library available on GitHub
 https://github.com/PierreMarchand20/htool
 by Pierre Marchand and P.-H. T.
- interfaces with BEMTool for BEM kernels
- Parallel assembly, \mathcal{H} -matrix/vector and \mathcal{H} -matrix/matrix products using MPI and OpenMP



BEM variational forms in FreeFEM

Define the type of operator

$$-\Delta u - k^2 u = 0, \quad k \in \mathbb{C}$$

k = 0	Laplace
$k \in \mathbb{R}_+^*$	Helmholtz
$k \in i\mathbb{R}_+^*$	Yukawa

Operators

BemKernel Ker("SL", k=2*pi);

"SL"	Single Layer
"DL"	Double Layer
"HS"	Hyper Singular
"TDL"	Transpose Double Layer

NEW Maxwell EFIE:

 $k \in \mathbb{R}_+^*$ and surface \mathbb{RT}_0 space (RT0S)

Potentials

BemPotential Pot("SL", k=2*pi);

"SL"	Single Layer
"DL"	Double Layer

BEM variational forms in FreeFEM

Define the problem

• Bilinear form on 3D surface mesh :

```
BemKernel Ker("SL", k=2*pi);
varf vbem(u,v) = int2dx2d(ThS)(ThS)(BEM(Ker,u,v));
or directly:
varf vbem(u,v) =
int2dx2d(ThS)(ThS)(BEM(BemKernel("SL",k=2*pi),u,v));
```

Bilinear form on 2D curve mesh :

```
varf vbem(u,v) = intldxld(ThL)(ThL)(BEM(Ker,u,v));
```

Assemble the HMatrix with BEMTool and Htool :

```
load "bem"
HMatrix<complex> H = vbem(Uh,Uh);
```

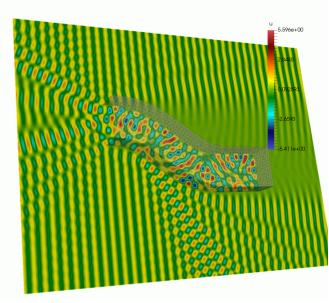
BEM variational forms in FreeFEM

Solve the problem

```
fespace Uh (ThS, P1);
Uh < complex > p, b;
HMatrix < complex > H=vbem (Uh, Uh); // assemble the HMatrix
varf vrhs(u,v) = int2d(ThS)(finc*v);
b[] = vrhs(0,Uh):// assemble the right-hand side
Solve the linear system with GMRES, with Jacobi preconditioner:
p[] = H^-1*b[];
Reconstruct the solution on an output mesh using the Potential:
varf vpot(u,v) = int2d(ThS) (POT(BemPotential("SL", k=2*pi),u,v));
meshS ThOut = square3(50,50);
fespace UhOut (ThOut, P1);
UhOut < complex > u;
HMatrix<complex> HP = vpot(Uh, UhOut);
// reconstruct the field on every node of ThOut:
u[] = HP*p[]; // p is the BEM solution
plot(u);
```

Plane wave scattering by the COBRA cavity

- P1, 10 points per wavelength
- 33K dofs
- Dirichlet B.C.
- First kind formulation
- 94.4% compression
- two-level DD precond, coarse mesh w/ 3.3 p.p. wavelength (3.7K dofs)
- assembly: 29.5s on 192 cores
 - -
- 7 gmres it (0.5s)
- radiation: 6.8s



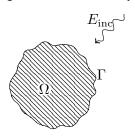
vectorial BEM equation: Maxwell

volumic equation

Time-harmonic Maxwell's equations

Scattered field of a perfect electric conductor (PEC) object. The scattered fields \boldsymbol{E} and \boldsymbol{H} for an homogeneous medium verify:

$$\begin{aligned} \operatorname{curl} & \boldsymbol{E} + \imath \omega \mu_0 \boldsymbol{H} = 0, & \operatorname{in} \mathscr{R}^3 \backslash \Omega \\ & \operatorname{curl} & \boldsymbol{H} + \imath \omega \varepsilon_0 \boldsymbol{E} = 0, & \operatorname{in} \mathscr{R}^3 \backslash \Omega \\ & \boldsymbol{E} \wedge \boldsymbol{n} = -\boldsymbol{E}_{inc} \wedge \boldsymbol{n}, & \operatorname{on} \Gamma \\ & \lim_{r \to +\infty} r \left\| \sqrt{\varepsilon_0} \boldsymbol{E} - \sqrt{\mu_0} \boldsymbol{H} \nabla \frac{\boldsymbol{r}}{|\boldsymbol{r}|} \right\| = 0. \end{aligned}$$



Time convention: $\exp(\imath \omega t)$.

We introduce the total magnetic trace:

$$\mathbf{j} = \iota \kappa Z_0 \mathbf{n} \wedge (H + H_{\text{inc}}).$$

vectorial BEM equation: Maxwell

EFIE equation: BEMTool

The total magnetic trace:

$$\mathbf{j} = \iota \kappa Z_0 \mathbf{n} \wedge (H + H_{\text{inc}})$$

Electric field integral equation (EFIE)

$$\int_{\Gamma \times \Gamma} \mathcal{G}_{\kappa}(\mathbf{x} - \mathbf{y}) (\mathbf{j}(\mathbf{x}) \cdot \mathbf{v}(\mathbf{y}) - \kappa^{-2} \operatorname{div}_{\Gamma} \mathbf{j}(\mathbf{x}) \operatorname{div}_{\Gamma} \mathbf{v}(\mathbf{y})) \, d\sigma(\mathbf{x}) \, d\sigma(\mathbf{y})$$

$$= -\int_{\Gamma} \mathbf{E}_{inc}(\mathbf{x}) \cdot \mathbf{v}(\mathbf{x}) \, d\sigma(\mathbf{x})$$

Green kernel: $\mathscr{G}_{\kappa}(x) = \exp(\imath \kappa |x|)/(4\imath \pi |x|)$

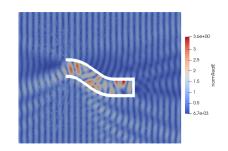
The scattered field \boldsymbol{E} is obtained with the Stratton-Chu Formula:

$$\boldsymbol{E}(\boldsymbol{y}) = \int_{\Gamma} \mathcal{G}_{\kappa}(|\boldsymbol{y} - \boldsymbol{x}|) \boldsymbol{j}(\boldsymbol{x}) d\sigma(\boldsymbol{x}) + \frac{1}{\kappa^2} \nabla_{\boldsymbol{y}} \left(\int_{\Gamma} \mathcal{G}_{\kappa}(|\boldsymbol{y} - \boldsymbol{x}|) \operatorname{div}_{\Gamma} \boldsymbol{j}(\boldsymbol{x}) \, d\sigma(\boldsymbol{x}) \right).$$

vectorial BEM equation: Maxwell

Cobracavity

- Thickness arround the cavity.
- f = 5Ghz Hz, RT0, 21204 dofs
- PFC material
- FFIF:
- assembly: 426 s
- 84 % compression
- Block Jacobi preconditioner, 8 mpi.
- solution *j*: 2743 gmres it (410s)
- potentiel E: 44 s
- total time 881s



Definition and example 1/2

- FE space is defined with a Finite element (P1, P2, ...) and a mesh.
- Vectorial FE Space :

```
fespace Xh(Th,[P2,P2,P1]); // depends on one mesh
fespace XhPeriodic(Th,[P2,P2,P1],periodic=[[1,x],[3,x]]);
XhPeriodic [u1,u2,p]; // periodic for all components
```

Definition of composite FE space :

$$X_h = U_h^1\big(T_h^1, FE_1\big) \times U_h^2\big(T_h^2, FE_2\big) \cdots \times U_h^n\big(T_h^n, FE_n\big),$$

where T_h^i and T_h^j can be different meshes ($\times =$ cartesian product).

• Rewritting Vectorial FE space:

```
fespace Uh1(Th,P2);
fespace Uh2(Th,P2,periodic=[[1,x],[3,x]]);
fespace Ph(Th,P1);

fespace Xh(<Uh1,Uh2,Ph>); // Xh = Uh1 × Uh2 × Ph
```

Definition and example 2/2

Definition of composite FE space:

$$X_h = U_h^1(T_h^1, FE_1) \times U_h^2(T_h^2, FE_2) \cdots U_h^n(T_h^n, FE_n),$$

where T_h^i and T_h^j can be different meshes (x = cartesian product).

• Rewritting Vectorial FE space:

```
fespace Uh1(Th,P2);
fespace Uh2(Th,P2,periodic=[[1,x],[3,x]]);
fespace Ph(Th,P1);

fespace Xh(< Uh1,Uh2,Ph> ); // Xh = Uh1 × Uh2 × Ph
```

FEM-BEM coupling:

```
fespace Xfem(Th,P1); // Th is a 2d volumic mesh
fespace Xbem(ThL,P1); // ThL is a curve mesh (meshL)
fespace Xh(<Xfem,Xbem>); // Xh = Xfem x Xbem
```

problem/solve keyword

Current way of defining a problem:

Limitations:

- All FE spaces are defined on the *same* mesh (Th1=Th2···=Th4).
- Uh1 and Vh1 (resp. Uh2 and Vh2) are the same FE space.
- same = computer memory
- ⇒ Rewrite of problem/solve function in the kernel with composite FE space to bypass these limitations.

Remark limitations

- In the current, we can bypass this limitations by using the keyword varf.
- Mixed variational form: Uh1=Vh1, Uh2=Vh2 are different FE spaces.

```
// definition of the FE spaces
fespace Uh1(Th1,P2);
fespace Uh2(Th2,P1); // Th1 and Th2 are different mesh
// definition of FE functions
Uh1 u1, v1;
Uh2 u2.v2;
\mathbf{varf} \quad \text{vfA11} (u1, v1) = \mathbf{int2d} (Th1) \left( \mathbf{dx} (u1) * \mathbf{dx} (v1) + \mathbf{dy} (u1) * \mathbf{dy} (v1) \right)
+ int2d(Th1) ( f1*v1) + on (1,u1=0);
matrix A11 = vfA11(Uh1,Uh1); // Interaction between Uh1 and Uh1
matrix A21 = vfA21(Uh1,Uh2); // Interaction between Uh1 and Uh2
matrix A12 = vfA12(Uh2,Uh1); // Interaction between Uh2 and Uh1
matrix A22 = vfA22(Uh2,Uh2); // Interaction between Uh2 and Uh2
matrix A = [[A11,A12], [A21,A22]]; // global matrix
real[int] rhs = [rhs1,rhs2]; // where real[int] rhs1=vfA11(0,Vh1);
real[int] sol = A^-1*rhs; // solution of the system
```

Limitations:

- A variational form for each block of the system for mixed variationnal form.
- \Rightarrow The goal of composite FE space is to write one varf in this case.

problem/solve keyword

New formulation with composite FE spaces:

```
// definition of the FE spaces
  fespace Uh(Th1, [P2, P2]);
  fespace Ph(Th2,P1);
  // definition of FE functions
  Uh [u1.u2];
  Uh [v1, v2];
  Ph p;
  Ph q;
// use angle bracket "<" ">" for composite
// "[" "]" defined a FE function
  problem myCompositePB(\langle [u1,u2],[p] \rangle,\langle [v1,v2],[q] \rangle) = ...
  myCompositePB;
  plot([u1,u2]); // u1 and u2 contains the solution of the
      problem
```

- allows for different meshes, and even different mesh types (mesh, meshS, meshL, ...)
- Uh1 and Vh1 (resp. Uh2 and Vh2) are the same FE space for the moment.

Thermic contact

Consider the following thermic contact problem:

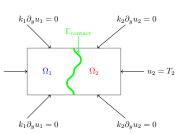
$$\begin{cases} \nabla \big(\,k_i\,\nabla u_i\,\big) = f_i & \text{in}\Omega_i,\\ k_i\nabla u_i\cdot \textbf{\textit{n}} = 0, \text{on upper and lower boundary of}\,\Omega_i, & k_1\partial_y u_1 = 0\\ u_1 = T_1\,\text{for}\,x = 0,\\ u_2 = T_2\,\text{for}\,x = L. &\\ & \Gamma_{\text{contact}} \text{ is the boundary between the two} & u_1 = T_1 \end{cases}$$

domains:

$$k_1 \nabla u_1 . n_1 = -k_2 \nabla u_2 . n_2$$
 in Γ_{contact} .

- hypothesis on the Thermal flux in the contact boundary: $k_1 \nabla u_1 . n_1 = c (u_2 - u_1)$
- variational form:

$$\forall (v_1, v_2), \begin{cases} \int_{\Omega_1} k_1 \nabla u_1 . \nabla v_1 dX + c \int_{\Gamma_{\text{contact}}} (u_1 - u_2) v_1 d\sigma(X) = 0, \\ \int_{\Omega_2} k_2 \nabla u_2 . \nabla v_2 dX + c \int_{\Gamma_{\text{contact}}} (u_2 - u_1) v_2 d\sigma(X) = 0. \end{cases}$$



Thermic contact

variational form:

$$\forall (v_1, v_2), \begin{cases} \int_{\Omega_1} k_1 \nabla u_1 . \nabla v_1 dX + c \int_{\Gamma_{contact}} (u_1 - u_2) v_1 d\sigma(X) = 0, \\ \int_{\Omega_2} k_2 \nabla u_2 . \nabla v_2 dX + c \int_{\Gamma_{contact}} (u_2 - u_1) v_2 d\sigma(X) = 0. \end{cases}$$

```
fespace Vh1(Th1,P1); // definition of FE space
fespace Vh2(Th2,P1);
Vh1 u1, v2; // definition of the FE function
Vh2 u2, v2;
// use angle bracket "<" ">" for composite
problem compositeThermic(<[u1],[u2]>,<[v1],[v2]>) =
int2d (Th1) (k1*dx(u1)*dx(v1) + k1*dy(u1)*dy(v1))
+ int2d (Th2) (k2*dx (u2) *dx (v2) + k2*dy (u2) *dy (v2))
+ intld(Th1,10,mortar=1)(c*(u1-u2)*v1)
+ intld(Th2,10,mortar=1) (c*(u2-u1)*v2)
+ on (3, u1=T0)
+ on (4, u2=T1);
compositeThermic;
// u1 and u2 contains the solution of the problem
```

Thermic contact

conclusion for problem/solve:

- FE space composite allow to avoid penalization in Ω_2 for u_1 .
- FE space composite allow to used non conformal mesh for Ω_1 and Ω_2 .
 - \Rightarrow The only relation between Ω_1 and Ω_2 is due to the coupled interface problem.
- FEspace composite allow to have different kind of physics in different domain.
- \Rightarrow Point (2) and (3) are true also for varf.

Stokes example

Consider the following Stokes problem:

$$\begin{cases} -\Delta u + \nabla p = f & \text{in } \Omega \\ -\text{div} u = 0 & \text{in } \Omega \end{cases}$$
$$u = u_D & \text{on } \Gamma_D$$

The variationnal form is given by:

$$\forall (v, q), \begin{cases} \int_{\Omega} \nabla u . \nabla v \, dX - \int_{\Omega} p div(v) dX = \int_{\Omega} f \cdot v \, dX, \\ -\int_{\Omega} div(u) q dX - \int_{\Omega} \epsilon p \, q = 0. \end{cases}$$

- (u,p) are solution $\Rightarrow (u,p+C)$ is also a solution.
- stabilized term (blue term) allow to have only one solution $\epsilon = 1e 10$.

Stokes example

variational form:

$$\forall (v, q), \begin{cases} \int_{\Omega} \nabla u . \nabla v \, dX - \int_{\Omega} p div(v) \, dX = \int_{\Omega} f \cdot v \, dX, \\ - \int_{\Omega} div(u) q dX - \int_{\Omega} \epsilon p \, q = 0. \end{cases}$$

- stabilized term (blue term) allow to have only one solution $\epsilon = 1e 10$.
- The choice of the fespace for u and p must be chosen carefully (LBB condition)

$$\forall u \in U_h$$
, $\sup_{p \in P_h} \frac{\int_{\Omega} \nabla p.v dX}{\|p\|_{P_h}} \ge \beta \|u\|_{U_h}$

- $T_h^u = T_h^p$ and P1(u)-P1(p) FE doesn't work.
- $T_h^u = T_h^p$ and P2-P1 FE (Taylor-Hood Element)

Stokes Example : driven cavity

- The driven cavity is a standard test. It is a box full of liquid with its lid moving horizontally at speed one.
- upper boundary u = (1,0) and otherwise u = (0,0).
- we have also added a hole inside with zero velocity at the boundary.

```
composite_stokes_cavite_entrainee.edp
```

Conclusion:

Composite FE space allow to use different mesh for the same domain.

Stokes Example: periodic in one direction.

$$\begin{cases} -\Delta u + \nabla p = f & \text{in } \Omega \\ -\text{div} u = 0 & \text{in } \Omega \end{cases}$$

- In this test, we suppose that we know the solution:
- $u = (\sin(x) * \cos(y), -\cos(x) * \sin(y))$
- p = 2 * cos(x) * cos(y)
- f = (0, -4 * cos(x) * sin(y))

composite_stokes_periodic_problem.edp

Conclusion:

Composite FE space allow to use a periodic condition in one direction.

Model problem

Consider the following Helmholtz problem:

$$\begin{cases} -\Delta u - n(\mathbf{x})k^2 u = f & \text{in } \Omega_{\text{int}} \\ -\Delta u_{\text{ext}} - n_{\text{ext}}k^2 u_{\text{ext}} = 0 & \text{in } \Omega_{\text{ext}} \\ u = u_{\text{ext}} & \text{on } \Gamma \\ \nabla u \cdot \mathbf{n} = \nabla u_{\text{ext}} \cdot \mathbf{n} & \text{on } \Gamma \\ + \text{ radiation condition} \end{cases}$$

Variational form in Ω_{int} : $\forall v$,

$$\int_{\Omega_{int}} \nabla u \nabla v - \int_{\Omega_{int}} n k^2 u v - \int_{\Gamma} \nabla u \cdot \boldsymbol{n} v = \int_{\Omega_{int}} f v$$

Bielak-MacCamy formulation

$$\int_{\Omega_{int}} \nabla u \nabla v - \int_{\Omega_{int}} n k^2 u v - \int_{\Gamma} \nabla u_{\text{ext}} \cdot \boldsymbol{n} v = \int_{\Omega_{int}} f v$$

Bielak-MacCamy indirect coupling: find ansatz ϕ s.t. $u_{\text{ext}} = SL(\phi)$ in Ω_{ext}

We have

$$\begin{cases} \gamma_D(u) = \gamma_D(u_{\text{ext}}) &= \gamma_D \circ SL(\phi) \\ \nabla u \cdot \boldsymbol{n} = \nabla u_{\text{ext}} \cdot \boldsymbol{n} &= -\gamma_N \circ SL(\phi) \end{cases}$$

with γ_D and γ_N the Dirichlet and Neumann trace operators.

Thus, the coupled problem is: find (u,ϕ) such that $\forall (v,\psi)$

$$\begin{cases} \int_{\Omega_{\rm int}} \nabla u \nabla v - \int_{\Omega_{\rm int}} n k^2 u v + \int_{\Gamma} \gamma_N \circ SL(\phi) v = \int_{\Omega_{\rm int}} f v \\ \int_{\Gamma} \gamma_D(u) \psi - \int_{\Gamma} \gamma_D \circ SL(\phi) \psi = 0 \end{cases}$$

Bielak-MacCamy formulation

$$\begin{cases} \int_{\Omega_{\rm int}} \nabla u \nabla v - \int_{\Omega_{\rm int}} n k^2 u v + \int_{\Gamma} \gamma_N \circ SL(\phi) v = \int_{\Omega_{\rm int}} f v \\ \int_{\Gamma} \gamma_D(u) \psi - \int_{\Gamma} \gamma_D \circ SL(\phi) \psi = 0 \end{cases}$$

In the current version of Freefem, no mixed formulation in FreeFEM: assemble blocks separately

⇒ With Composite FE spaces: only one coupled variational form

```
varf Lenses([uf,ub],[vf,vb]) =
  int2d(Th)((-k^2*uf*vf+Grad(uf)'*Grad(vf))) // Fem
+ int1dx1d(ThL)(ThL)(BEM(-1*BemKernel("SL",k=k),ub,vb)) // -SL
+ int1d(ThL)(uf*vb) // Mass
+ int1d(ThL)(0.5*ub*vf) + int1dx1d(ThL)(ThL)(BEM(BemKernel("TDL",k=k),ub,vf)); // TDL
```

Note: the bilinear form associated to the transpose double layer operator is

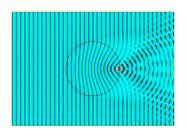
$$a_{K'}(\phi, v) = \frac{1}{2} \int_{\Gamma} \phi v + \int_{\Gamma} K'(\phi) v := \int_{\Gamma} (\gamma_N \circ SL)(\phi) v$$

Application: gradient index lenses

Wave focusing and bending using gradient index lenses

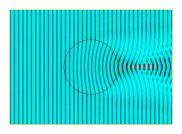
Maxwell's fish-eye lens (1854)

$$n(r) = \frac{2}{1 + \left(\frac{r}{R}\right)^2}$$



Luneburg lens (1944)

$$n(r) = \sqrt{2 - \left(\frac{r}{R}\right)^2}$$



Helmholtz-2d-FEM-BEM-coupling-MUMPS.edp

Variational form

Helmholtz-2d-FEM-BEM-coupling-MUMPS.edp

- 35 lines for the definition of the matrix and the rhs.
- Matrix system is

```
\begin{pmatrix} F & TDL \\ mass & -SL \end{pmatrix} \begin{pmatrix} u_{\text{fem}} \\ u_{\text{hem}} \end{pmatrix} = \begin{pmatrix} F_{\text{rhs}} \\ 0 \end{pmatrix} \quad \text{wheresol} = \begin{pmatrix} u_{\text{fem}} \\ u_{\text{hem}} \end{pmatrix}.
fespace Uh(Th,P1); // Th is a 2d volumic mesh
fespace UhL(ThL,P1); // ThL is a meshL
fespace CUh (<Uh, UhL>); // CUh = Uh × UhL
varf Lenses([ufem,ubem],[vfem,vbem]) =
int2d(Th) ((-ind*k^2*ufem*vfem+Grad(ufem)'*Grad(vfem))) // F
+ intldxld(ThL)(ThL)(BEM(BemKernel("TDL", k=k), ubem, vfem)) // TDL
        + int1d(ThL)(0.5*ubem*vfem) // TDL
+ intld(ThL)(ufem*vbem) // mass
+ intldxld(ThL)(ThL)(BEM(-1*BemKernel("SL", k=k), ubem, vbem)) // -SL
+ int2d(Th)(finc*vfem) + on(waveguide,ufem=0); // RHS
matrix<complex> A = Lenses(CUh, CUh);
complex[int] rhs = Lenses(0,CUh);
```

Variational form

```
fespace Uh(Th,P1); // Th is a 2d volumic mesh
fespace UhL(ThL,P1); // ThL is a meshL
fespace CUh(<Uh,UhL>); // CUh = Uh × UhL
...
varf Lenses([ufem,ubem],[vfem,vbem]) = ...
matrix<complex> A = Lenses(CUh,CUh);
complex[int] rhs = Lenses(0,CUh);
complex[int] sol = A^-1*rhs;
```

• In the version in development, FE function of composite FE space is not defined:

```
CUh [ufem, ubem]; // compile error
```

As $CUh = Uh \times UhL$, we have $sol = \begin{pmatrix} u_{\text{fem}} \\ u_{\text{bem}} \end{pmatrix}$.

Uh<complex> ufem; // ufem
UhL<complex> ubem; // ubem
// method 1: extract solution
ufem[] = sol(0:(Uh.ndof)-1); // extract ufem
ubem[] = sol(Uh.ndof:(sol.n-1)); // extract ubem
// method 2: dispatch solution
[ufem[], ubem[]] = sol;

Ultimate Dream Goal:

run any sequential script in parallel on N processes \Rightarrow same result, fully distributed data structures (completely hidden to the user), speedup of N

What we are working on for now:

- Hide the parallelization of the assembly and solution steps (main bottlenecks) as mush as possible
- \blacksquare Generalize the matrix format, using PETSc for now ; useful for handling composite operators stemming from coupled problems (e.g. sparse + $\mathscr{H}-\text{matrices}$ for FEM-BEM)

or

Parallel assembly and MUMPS distributed solver

Hide parallel assembly, give distributed matrix to MUMPS:

```
load "MUMPS"
solve pb(u,v,solver=sparsesolver,master=-1) = int3d(
   Th) (Grad(u)'*Grad(v)) - int3d(Th)(f*v) + on(1, u=2);
load "MUMPS"
varf pb(u,v) = int3d(Th)(Grad(u)'*Grad(v)) +int3d(Th
   ) (f*v) + on(1, u=2);
matrix A = pb(Uh,Uh,solver=sparsesolver,master=-1);
real[int] rhs = pb(0,Uh);
u[] = A^{-1} * rhs;
```

PETSc matrices

Also works with composite FE spaces for coupled problems, e.g. FEM-BEM lenses:

```
load "MUMPS"
varf Lenses([ufem, ubem], [vfem, vbem]) =
int2d(Th) ((-ind*k^2*ufem*vfem+Grad(ufem)'*Grad(vfem))) // F
+ intldxld(ThL)(ThL)(BEM(BemKernel("TDL", k=k), ubem, vfem)) // TDL
      + int1d(ThL)(0.5*ubem*vfem) // TDL
+ int1d(ThL)(u1*v2) // mass
+ intldxld(ThL)(ThL)(BEM(-1*BemKernel("SL", k=k), ubem, vbem)) // -SL
+ int2d(Th)(finc*vfem) + on(waveguide.ufem=0); // RHS
matrix < complex > A = Lenses (CUh, CUh, solver = sparsesolver, master = -1);
complex[int] rhs = Lenses(0,CUh);
complex[int] sol = A^-1*rhs;
BUT for now, densifies the compressed BEM blocks (\mathcal{H}-
matrices)
⇒ use PETSc instead, construct a distributed nested Mat.
each block has its own matrix type
```

PETSc preconditioners

We can then take advantage of the wide range of available solvers in PETSc. In particular, we can easily use *fieldsplit* preconditioners for coupled problems, each variable naturally defining its own *field*:

```
load "PETSc-complex"
varf Lenses([ufem, ubem], [vfem, vbem]) =
int2d(Th) ((-ind*k^2*ufem*vfem+Grad(ufem)'*Grad(vfem))) // F
+ intldxld(ThL)(ThL)(BEM(BemKernel("TDL", k=k), ubem, vfem)) // TDL
      + intld(ThL)(0.5*ubem*vfem) // TDL
+ intld(ThL)(u1*v2) // mass
+ intldxld(ThL)(ThL)(BEM(-1*BemKernel("SL", k=k), ubem, vbem)) // -SL
+ int2d(Th)(finc*vfem) + on(waveguide, ufem=0); // RHS
Mat < complex > A = Lenses (CUh, CUh);
set (A, sparams="-ksp_view_-ksp_monitor_-ksp_type_fgmres")
-ksp_view_final_residual.-ksp_gmres_restart, 200, -pc_type, fieldsplit,
    -fieldsplit_0_pc_type_asm_-fieldsplit_0_sub_pc_type_lu
-fieldsplit 0 ksp type amres -fieldsplit 1 ksp type amres
-fieldsplit 1 ksp max it 20");
complex[int] rhs = Lenses(0,CUh);
complex[int] sol = A^-1*rhs;
```

Current/Future developments

• use PETSc as a solver directly in problem/solve:

```
solve pb(u, v, solver=petsc, sparams="...");
```

- C++ implementation of Domain Decomposition macros (macro_ddm.idp) to hide difficulties to the user ⇒ will be able to use DD solvers such as GenEO transparently
- developments in Htool: *H*-LU factorization, more compression techniques (Block ACA, HCA, randomized SVD, ...)