FEM-BEM coupling in FEniCS and BEMpp for high-intensity focused ultrasound

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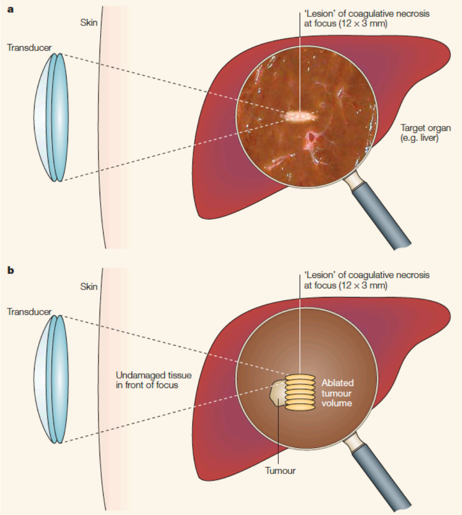
Outline

1. What is high-intensity ultrasound?
2. Mathematical model
3. Computational challenges
4. Why FEM-BEM?
5. FEniCS and BEMpp software for wave problems
6. Summary and outlook

What is high-intensity focused ultrasound (HIFU)?

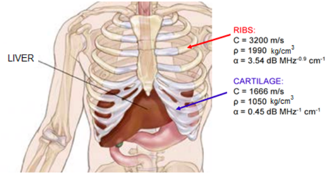
- Promising **non-invasive** treatment modality for tumor ablation in the abdomen
- At the beam focus, **temperature rises to about 80°C**, sufficient for instantaneous cell death.
- Unlike radiotherapy, **HIFU is not tumour-specific** and so a wide variety of tumour types may be targeted.
- **The treatment can be repeated** as there is no upper limit of tissue tolerance to ultrasound exposure.

What is high-intensity focused ultrasound (HIFU)?

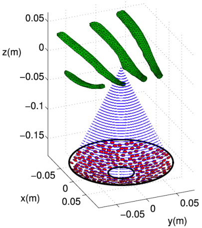


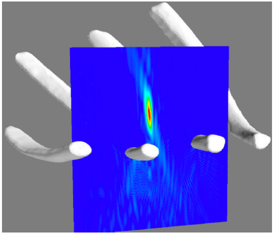
J. E. Kennedy, *High-intensity focused ultrasound in the treatment of solid tumours*, Nature Reviews (2005)

Why are HIFU simulations required?



- In the abdomen, there are ribs and organs of different densities.
- Scattering can lead to heating at non-target regions.
- Wish to optimize transducer array in the presence of ribs to minimize treatment time.
- Physical experiments are expensive/unethical.

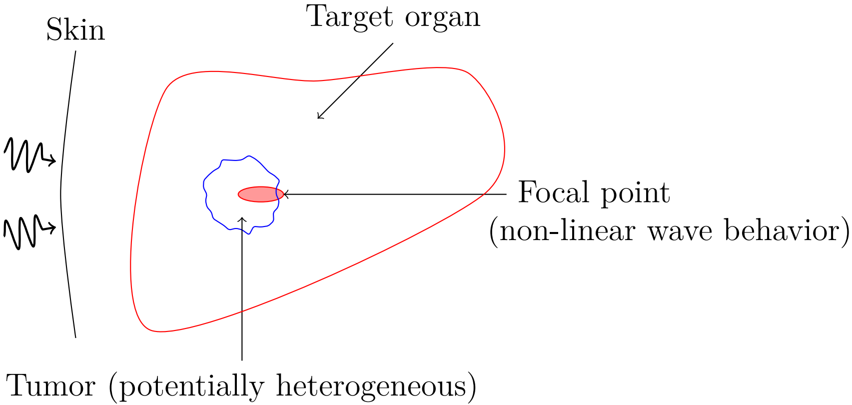




T. Betcke et al., *Computationally efficient boundary element methods for high-frequency Helmholtz problems in unbounded domains*, Modern Solvers for Helmholtz Problems (2017)

Problem details

- Time-harmonic source with wavelength 1.5mm (1MHz)
- Tumor < 10cm
- Total simulation domain up to 20cm



Computational challenges for HIFU

- **High frequency**: computation domain is potentially hundred of wavelengths in each dimension.
  - Memory
  - Preconditioning
  - Dispersion and pollution
- Near focal point non-linearities play an important role.
- Medical practitioners desire simulation times < 1 minute!
- (Generating appropriate computational meshes from CT or MR scans)

Linear wave equation

$$\boxed{\nabla^2 p - \frac{1}{c_0^2}\frac{\partial^2 p}{\partial t^2} = 0}$$

Non-linear (Westervelt) equation

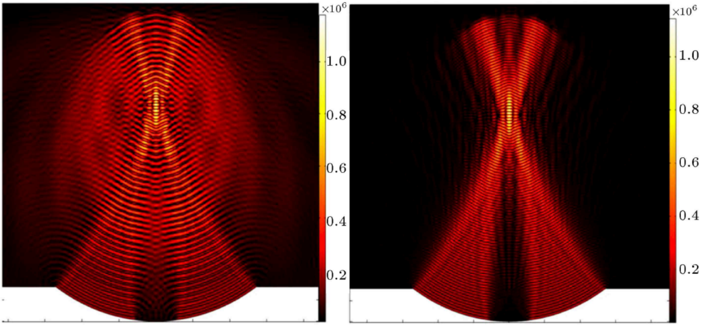
$$\boxed{\nabla^2 p - \frac{1}{c_0^2}\frac{\partial^2 p}{\partial t^2} + \frac{\delta}{c_0^4}\frac{\partial^3 p}{\partial t^3} = -\frac{\beta}{\rho c_0^4}\frac{\partial^2 p^2}{\partial t^2},}$$

where δ is diffusivity of sound and β is nonlinearity parameter.

Solve in conjunction with bioheat equation $\rightarrow$ tissue temperatures.

KZK equation also popular although relies on strong assumption.

Linear vs. non-linear



- Solving the Westervelt equation provides stronger focusing
- Far from focal point, linear wave equation is accurate
- Motivates using FEM near target region and BEM outside

S. Haddadi and M. T. Ahmadian, *Analysis of nonlinear acoustic wave propagation in HIFU treatment using the Westervelt equation*, Scientifica Iranica B (2018)

FEM/BEM

Finite elements

- − Discretize the entire domain
- + Sparse matrices
- − Truncate domain artificially (PML)
- + Easily generalized
- − Dispersion errors

Boundary elements

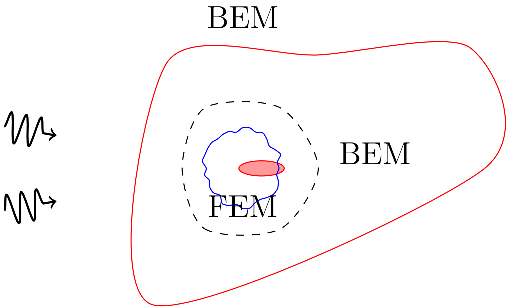
- + Discretize only boundaries
- − Dense matrices
- + Truncate domain analytically
- − Require Green's rep.
- + Dispersion free

Boundary elements are *potentially* much more efficient for wave problems in piecewise homogeneous domains.

Finite elements are appropriate for non-linear inhomogeneous media.

Desire best of both worlds...

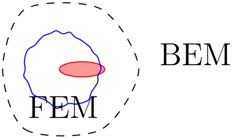
FEM-BEM coupling



FEM-BEM coupling

Field in FEM region: $u \approx \sum_i U_i \phi_i$

Normal derivative of field on boundary: $\frac{\partial u}{\partial n} \approx \sum_j V_j \psi_j$



FEM equation: $\mathbf{A}\mathbf{u} + \mathbf{B}\mathbf{v} = \mathbf{b}_{\text{FEM}}$

BEM equation: $\mathbf{C}\mathbf{u} + \mathbf{D}\mathbf{v} = \mathbf{b}_{\text{BEM}}$

Coupled system:

$$\begin{bmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{C} & \mathbf{D} \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ \mathbf{v} \end{bmatrix} = \begin{bmatrix} \mathbf{b}_{\text{FEM}} \\ \mathbf{b}_{\text{BEM}} \end{bmatrix}$$

See Matthew Scroggs on YouTube for more detail.

Frequency domain vs. time domain

Frequency domain

Ultrasound transducers are typically time-harmonic ($e^{-i\omega t}$).

Then Westervelt becomes a sequence of Helmholtz equations for harmonics:

$$\begin{aligned}(\nabla^2 + k^2)p_1 &= 0,\\ (\nabla^2 + 4k^2)p_2 &= \frac{2\beta k^2}{\rho c_0^2}p_1^2,\\ (\nabla^2 + 9k^2)p_3 &= \frac{9\beta k^2}{\rho c_0^2}p_1 p_2,\\ &\vdots\end{aligned}$$

- Relatively straightforward to implement.
- But how many harmonics to consider is not known a priori.
- High harmonic problems can be extremely expensive.

Frequency domain vs. time domain

Time domain

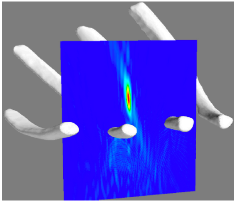
Employ **convolution-quadrature** techniques for FEM-BEM, such as those developed by F.-J. Sayas, M. Hassell, L. Banjai, J. M. Melenk, and others.

Laplace transform and solve set of modified Helmholtz problems

***Potentially* much more accurate and efficient, though yet to be tested for challenging high-frequency 3D problems.**

Project goals

Build on preceding BEM-only work by UCL team.



Explore algorithms of mathematical interest and practical utility

- Time-domain or frequency domain
- FEM or FEM-BEM
- Implicit or explicit
- Control dispersion with high p

Make everything open-source!

FEniCS and BEMpp

FEniCS

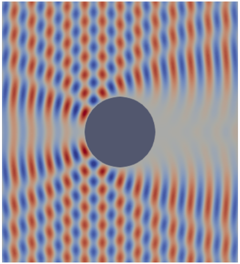
- open-source platform for solving PDEs
- quickly translate mathematical models into efficient FE code
- high-level Python and C++ interfaces
- development version, FEniCS-X, includes complex number support - particularly useful for time-harmonic wave problems
- 1D to 3D support

BEMpp

- open-source platform for solving BIE formulations of Laplace, Helmholtz, Maxwell
- high-level Python interface
- 3D only

FEniCS-X example

$$
\boxed{\begin{aligned}
(\nabla^2 + k^2)u &= 0 \text{ in } \Omega,\\
u &= 0 \text{ on } \Gamma,\\
\frac{\partial u^s}{\partial n} - iku^s &= 0 \text{ on } \partial\Omega,\\
u^s &= u - u^i.
\end{aligned}}
$$



Variational problem: Find $u \in V$ such that

$$a(u,v) = L(v) \quad \forall v \in \tilde{V},$$

where

$$
\begin{aligned}
a(u,v) &= \int_\Omega \nabla u \nabla \overline{v} \mathrm{d}x - k^2 \int_\Omega u\overline{v}\mathrm{d}x - ik\int_{\partial\Omega} u\overline{v}\mathrm{d}s,\\
L(v) &= \int_{\partial\Omega} \left(\frac{\partial u^i}{\partial n} - iku^i\right)\overline{v}\mathrm{d}s.
\end{aligned}
$$

FEniCS-X example

$$a(u, v) = L(v) \quad \forall v \in \tilde{V},$$

where

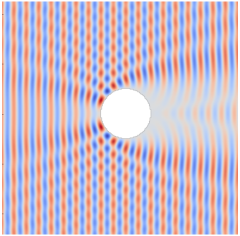
$$a(u, v) = \int_\Omega \nabla u \nabla \overline{v} \mathrm{d}x - k^2 \int_\Omega u \overline{v} \mathrm{d}x - ik \int_{\partial\Omega} u \overline{v} \mathrm{d}s,$$

$$L(v) = \int_{\partial\Omega} \left(\frac{\partial u^i}{\partial n} - iku^i \right) \overline{v} \mathrm{d}s.$$

```
# Define function space
V = FunctionSpace(mesh, ("Lagrange", 2))

# Define variational problem
u = TrialFunction(V)
v = TestFunction(V)
a = inner(grad(u), grad(v)) * dx - k**2 * inner(u, v) * dx - \
1j * k * inner(u, v) * ds
L = inner(dot(grad(ui), n) - 1j * k * ui), v) * ds

# Compute solution
u = Function(V)
solve(a == L, u, bc)
```

BEMpp example

$$\begin{aligned}(\nabla^2 + k^2)u &= 0 \text{ in } \Omega,\\ u &= 0 \text{ on } \Gamma,\\ \frac{\partial u^s}{\partial r} - iku^s &= o(r^{-1}) \text{ as } r \to \infty,\\ u^s &= u - u^i.\end{aligned}$$



Green's representation formula gives

$$u(x) = u^i(x) - \int_\Gamma G(x,y)\frac{\partial u}{\partial n}(y)\mathrm{d}y, \quad x \in \Omega.$$

Taking $x \to \Gamma$ yields the single-layer boundary integral equation:

$$\int_\Gamma G(x,y)\frac{\partial u}{\partial n}(y)\mathrm{d}y = u^i(x), \quad x \in \Gamma.$$

BEMpp example

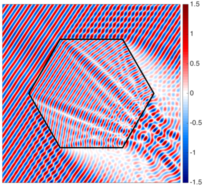
$$\int_\Gamma G(x,y)\frac{\partial u}{\partial n}(y)\mathrm{d}y = u^i(x), \quad x \in \Gamma.$$

```
# Define function space
V = bempp.api.function_space(grid, "DP", 0)

# Initialize boundary integral operator
slp = bempp.api.operators.boundary.helmholtz.single_layer(V, V, V, k)

# Define right-hand side
def plane_wave(x):
    return np.exp(1j * k * x[0])
rhs = bempp.api.GridFunction(V, fun=plane_wave)

# Compute solution using GMRES
from bempp.api.linalg import gmres
neumann_fun, info = gmres(slp, rhs, tol=1E-5)
```

Solve a 3D scattering problem in a few lines of easy code!

FEM-BEM

$$\boxed{\begin{aligned}(\nabla^2 + (nk)^2)u &= 0 \text{ in } \Omega,\\ (\nabla^2 + k^2)u &= 0 \text{ in } \mathbb{R}^3\backslash\Omega,\\ \frac{\partial u^s}{\partial r} - iku^s &= o(r^{-1}) \text{ as } r \to \infty,\end{aligned}}$$



Weak form for FEM:

$$\int_\Omega \nabla u \nabla \overline{v} \mathrm{d}x - k^2 \int_\Omega n^2 u \overline{v} \mathrm{d}x - \int_{\partial\Omega} \frac{\partial u}{\partial n} \overline{v} \mathrm{d}s = 0$$

BIE for BEM:

$$\left(\frac{1}{2}I - D\right) u + S\frac{\partial u}{\partial n} = u^{\text{inc}}.$$

$$\begin{bmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{C} & \mathbf{D} \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ \mathbf{v} \end{bmatrix} = \begin{bmatrix} \mathbf{0} \\ u^{\text{inc}} \end{bmatrix}$$

```python
# Define variational problem
u = dolfin.TrialFunction(fenics_space), v = dolfin.TestFunction(fenics_space)
A = FenicsOperator(inner(grad(u), grad(v)) * dx - k**2 * n**2 inner(u, v) * dx)

# Import boundary integral operators
id_op = bempp.api.operators.boundary.sparse.identity(
    trace_space, bempp_space, bempp_space)
mass = bempp.api.operators.boundary.sparse.identity(
    bempp_space, bempp_space, trace_space)
dlp = bempp.api.operators.boundary.helmholtz.double_layer(
    trace_space, bempp_space, bempp_space, k)
slp = bempp.api.operators.boundary.helmholtz.single_layer(
    bempp_space, bempp_space, bempp_space, k)

blocks[0][1] = A.weak_form()
blocks[0][1] = -trace_matrix.T * mass.weak_form().sparse_operator
blocks[1][0] = (.5 * id - dlp).weak_form() * trace_op
blocks[1][1] = slp.weak_form()

# Define right-hand side
rhs_bem = u_inc.projections(bempp_space)
rhs = np.concatenate([np.zeros(mesh.num_vertices()), rhs_bem])

# Compute solution using GMRES
from bempp.api.linalg import gmres
soln, info = gmres(blocks, rhs, tol=1E-5)
```

Summary

- Practical HIFU simulations are extremely challenging
- BEM has shown promise for linear wave simulations
- Non-linearities are important to consider near focal region
- Coupling to FEM generalizes BEM-only simulations
- Numerous techniques to explore, the most effective is still unclear
- Powerful FEniCS and BEMpp software tools are ideal for developing new frequency- and time-domain wave simulation algorithms