LENR: Toward a Small Form Factor Sonoluminescence Reactor

FEA SIMULATION GUIDE



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Design History:

3/31/25 - v0.1.0, Initial Draft – Suspect there are still simulation issues, since we are not achieving a standing wave at either 40kHz or 60kHz, and 60 should have an antinode (red area) in the middle. Higher frequencies attempted too with no visible standing wave in the bulk water sphere.

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SCOPE

This working document details the methods necessary for accurate simulation of reactor horn geometries using open-source tools after the initial CAD generation. The workflow will be in order of operations:

CAD >> Gmsh (meshing) >> Elmer (Helmholtz FEA) >> ParaView (Visualization)

Process 1.1: Simulation order

Downloads

This workflow was done on a Windows x64 PC. All downloads were for this OS.

Gmsh:

https://gmsh.info/

Elmer:

https://www.elmerfem.org/blog/binaries/

https://sourceforge.net/projects/elmerfem/

ParaView:

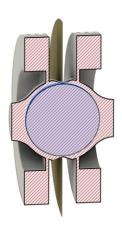
https://www.paraview.org/

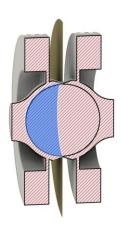
kHz to Radians Converter:

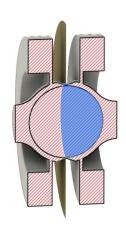
https://www.xconvert.com/unit-converter/kilohertz-to-radians-per-second/?measure=frequency&value=60

3D CAD MODEL

To have an accurate simulation, there are boundary conditions that must happen during the application of the Helmholtz equation. For example, the driven horn volume (aluminum) must touch the bulk media (water) without any gap in the mesh. To do this, we'll need to develop a simplified geometrically accurate model of our reactor as one solid volume, split with surfaces designed to represent our boundaries. This can be done on the 'surfaces' workflow of Autodesk Fusion after the 3D solid has been created in the 'solid' workflow tab.







Full Spherical Volume

Left Hemisphere

Right Hemisphere

Workflow: Surface >> Modify >> Split Body

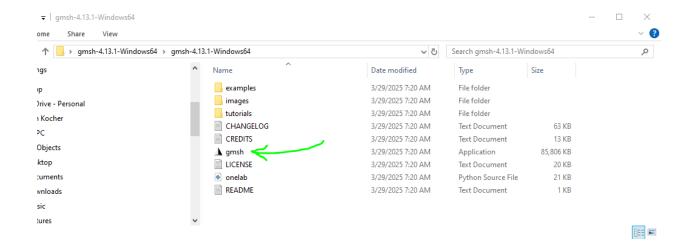
Export to STEP

Once the file is split correctly, export to a STEP file format. This will later be used by Gmsh and OpenCascade to create a suitable mesh for Elmer.

NOTE: It is ok to have separate bodies and surfaces in the 3D model.

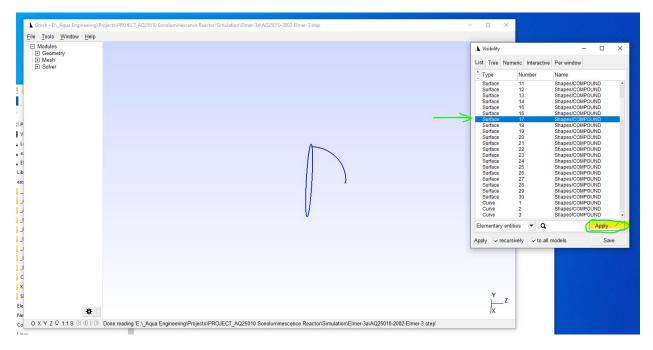
Gmsh

Gmsh is a free utility that will create a suitable mesh from the STEP file we just created. The program lives in a folder, and there is no installation process when you download it:

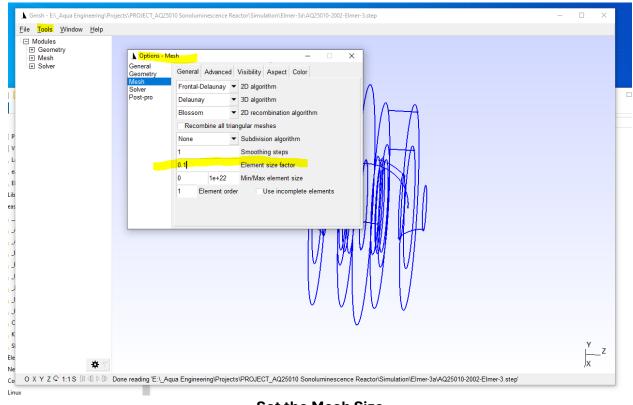


NOTE: Heads up - When you click on a text string in the left hand outline window, it will execute an action! For example, we'll be clicking on "3D", and that is the action that will mesh the STEP file with the given settings.

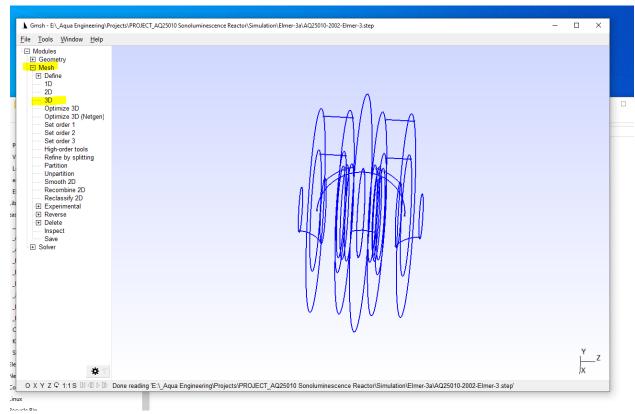
The first thing we need to do is document what the names of the surfaces are. One way to do this at a beginner level is to use the visibility tab and "apply" as a hack to see boundary surface names. These names will be used later in Elmer and will not change during the mesh and export process.



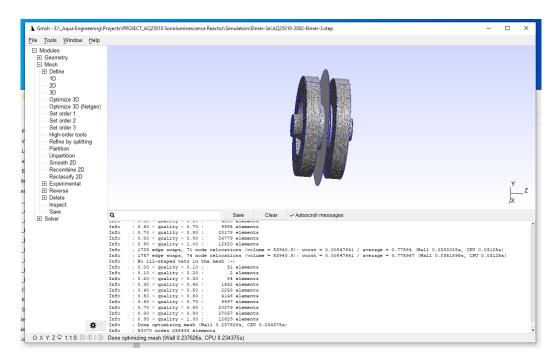
Document the Relevant Surface Names



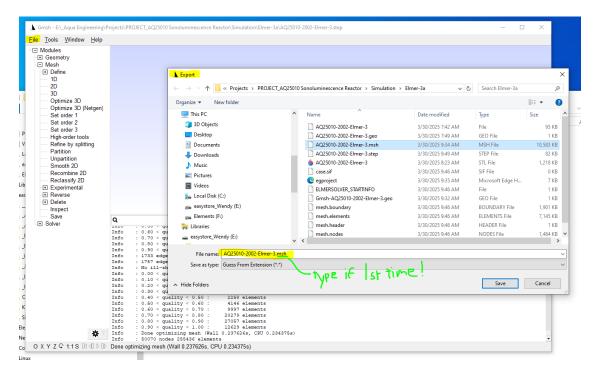
Set the Mesh Size



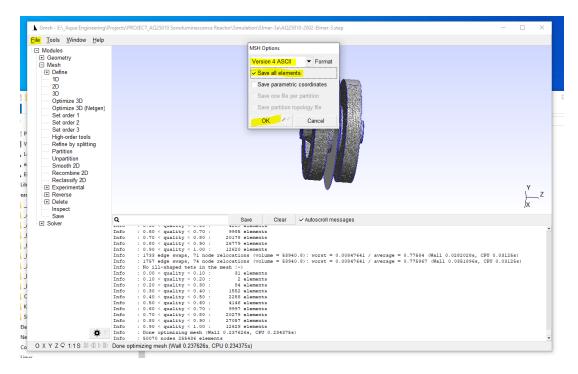
Execute The 3D Mesh



Example Mesh Result

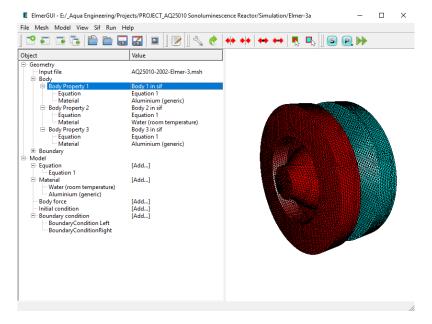


Export the Mesh - Type Extension on Name!!



Export the Mesh as v4 ASCII, Save All Elements

ElmerGUI



ElmerGUI is free software we'll use to run an acoustic Helmholtz FEA simulation. For those unfamiliar with this process, essentially this is a frequency-domain analysis of standing waves that requires no animation or time duration. There will be a bunch of differential equations that require configuration before they can be run. The diff eq's will have to converge for the simulation to work. Once the basic simulation is successful, details and fine tuning can be iterated. It is suggested that we do not overcomplicate the details on the first pass; or else the process will be infinitely complex. We will configure the simulation for the following main aspects:

Configure the Elmer Geometry and Model

- Input File (Our .msh file AQ25010-2002-Elmer-3.msh)
- Bodies
 - Left Hemisphere
 - o Bulk Water Volume
 - Right Hemisphere
- Equation (in this case it's the Helmholtz equation)
 - Helmholtz Equation
 - Active
 - Angular Frequency:
 - 251327.4 (40 kHz)
 - 276991.1 (60 kHz)
 - Pick one of these or run others

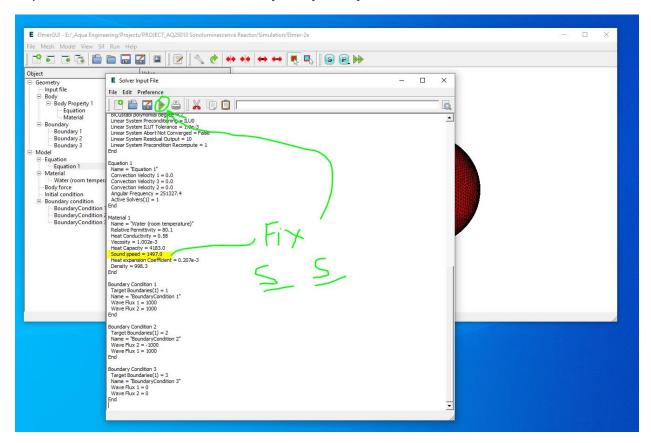
- Convection
 - Convection Velocity 1 = 0.0
 - Convection Velocity 2 = 0.0
 - Convection Velocity 3 = 0.0
- Apply to Bodies
 - Body Property 1
 - Body Property 2
 - Body Property 3
- Materials:
 - Water (room temperature) from library
 - Density 998.3
 - Heat Capacity: 4183.0
 - Heat Expansion Coeff.: 0.207e-3
 - Apply to Body Property 2
 - Aluminum (generic) from library
 - Density: 2700.0
 - Heat Capacity: 897.0
 - Heat Expansion Coeff.: 23.1e-6
 - Apply to Body Property 1
 - Apply to Body Property 2
- Boundary conditions:
 - Boundary Condition Left
 - Flux conditions
 - Real Part of the flux: 10000
 - Imag part of the flux: 0
 - Apply to boundaries:
 - Boundary 2 (Change for your specific case)
 - Boundary Condition Right
 - Flux conditions
 - Real part of the flux: 10000
 - Imag part of the flux:-10000
 - Apply to Boundaries:
 - Boundary 27

SIF >> Generate

Run this command to generate the SIF file. This file contains all of the parameters of the simulation and interestingly, can be used by a Python script to sweep values for those who

want to experiment at an advanced level. The python program would define a variable for some or all of the values in the SIF, and Elmer would be called from a command line utility.

WARNING: There is a quirk in this process, where the "Sound Speed" is not correctly capitalized. You must do this manually every time you create the SIF.



Fix the SIF, Then Save and Run

Example SIF file:

Header
CHECK KEYWORDS Warn
Mesh DB "." "."
Include Path ""
Results Directory ""
End

Simulation

Max Output Level = 5
Coordinate System = Cartesian
Coordinate Mapping(3) = 1 2 3
Simulation Type = Steady state
Steady State Max Iterations = 1
Output Intervals(1) = 1
Solver Input File = case.sif
Post File = case.vtu
End

Constants

Gravity(4) = 0 -1 0 9.82 Stefan Boltzmann = 5.670374419e-08 Permittivity of Vacuum = 8.85418781e-12 Permeability of Vacuum = 1.25663706e-6 Boltzmann Constant = 1.380649e-23 Unit Charge = 1.6021766e-19 End

Body 1

Target Bodies(1) = 1 Name = "Body Property 1" Equation = 1 Material = 2 End

Body 2

Target Bodies(1) = 2 Name = "Body Property 2" Equation = 1 Material = 1 End

Body 3

Target Bodies(1) = 3
Name = "Body Property 3"
Equation = 1
Material = 2
End

Solver 1

Equation = Helmholtz Equation

Procedure = "HelmholtzSolve" "HelmholtzSolver"

Variable = -dofs 2 Pressure Wave

Exec Solver = Always

Stabilize = True

Optimize Bandwidth = True

Steady State Convergence Tolerance = 1.0e-5

Nonlinear System Convergence Tolerance = 1.0e-7

Nonlinear System Max Iterations = 20

Nonlinear System Newton After Iterations = 3

Nonlinear System Newton After Tolerance = 1.0e-3

Nonlinear System Relaxation Factor = 1

Linear System Solver = Iterative

Linear System Iterative Method = BiCGStab

Linear System Max Iterations = 500

Linear System Convergence Tolerance = 1.0e-10

BiCGstabl polynomial degree = 2

Linear System Preconditioning = ILU0

Linear System ILUT Tolerance = 1.0e-3

Linear System Abort Not Converged = False

Linear System Residual Output = 10

Linear System Precondition Recompute = 1

End

Equation 1

Name = "Equation 1"

Angular Frequency = 251327.4

Convection Velocity 2 = 0.0

Convection Velocity 3 = 0.0

Convection Velocity 1 = 0.0

Active Solvers(1) = 1

End

Material 1

Name = "Water (room temperature)"

Relative Permittivity = 80.1

Heat expansion Coefficient = 0.207e-3

Heat Conductivity = 0.58

Viscosity = 1.002e-3

Sound damping = 0.01

Heat Capacity = 4183.0

Density = 998.3 Sound Speed = 1497.0 End

Material 2
Name = "Aluminium (generic)"
Poisson ratio = 0.35
Density = 2700.0
Heat expansion Coefficient = 23.1e-6
Heat Capacity = 897.0
Youngs modulus = 70.0e9
Sound Speed = 5000.0
Heat Conductivity = 237.0
End

Boundary Condition 1
Target Boundaries(1) = 2
Name = "BoundaryCondition Left"
Wave Flux 2 = 0
Wave Flux 1 = 10000
End

Boundary Condition 4
Target Boundaries(1) = 27
Name = "BoundaryConditionRight"
Wave Flux 2 = -10000
Wave Flux 1 = 10000
End

ParaView

Once we have run the SIF and our Helmholtz FEA has converged successfully, there will be an output file created with a .vtu extension. We need to open this with ParaView and configure a bunch of stuff to visualize the waveform.

WARNING: This process is a game of finding correct orders of magnitude and a using a careful workflow in the Pipeline Browser. Most of our focus is on combining the real and

imaginary waveforms "pressure wave 1" and "pressure wave 2" into "result" and being extra careful not to get lost in a cycle of auto rescaling that wipes out our images. As such, it is strongly recommended to SAVE STATE (file >> save state) every time a change is made. This way, as you find your wave images, you can build on progress and avoid an endless cycle of searching for the proper data window.

Open the .vtu File in ParaView

Navigate to your simulation directory and open the .vtu file with ParaView.

Add a Calculator Filter

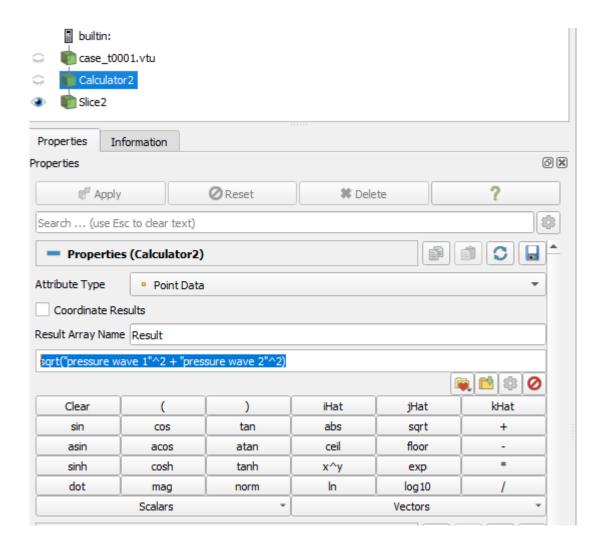
Add a calculator filter to the case_t0001.vtu. You must click on this line in the Pipeline Browser.

WARNING: ParaView treats these Pipeline Browser entries as pipelines, meaning stuff is downstream from other stuff and dependent on upstream entries! This may seem obvious after you use it a few times.

Add the calculator to recover the magnitude waveform from the real and imaginary waveforms.

Filters >> Common >> Calculator

Equation: sqrt("pressure wave 1"^2 + "pressure wave 2"^2)

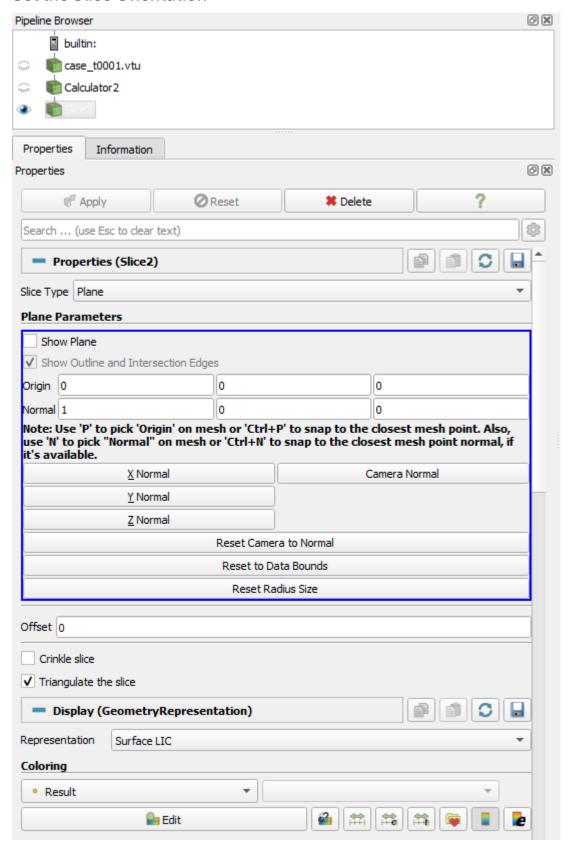


Add a Slice Filter

Add a slice filter so you can visualize a section of the standing waveform across both hemispheres and the center region.

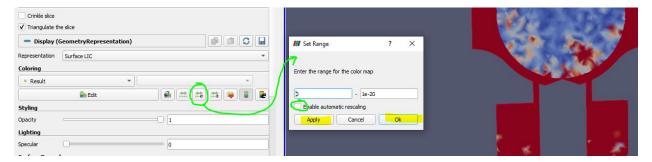
Filters >> Common >> Slice

Set the Slice Orientation



Set the Colorization Data Range

This is where you might spend most of your time testing, iterating, analyzing, and adjusting so you can interpret the waveform. Fine color details can be easily lost in a range that's an order of magnitude off and the resulting images saturated beyond value.



Reload Files Regularly

Pipeline Browser>>.vtu file>>Right Click>>Reload Files

Iteration Loop between Elmer and ParaView

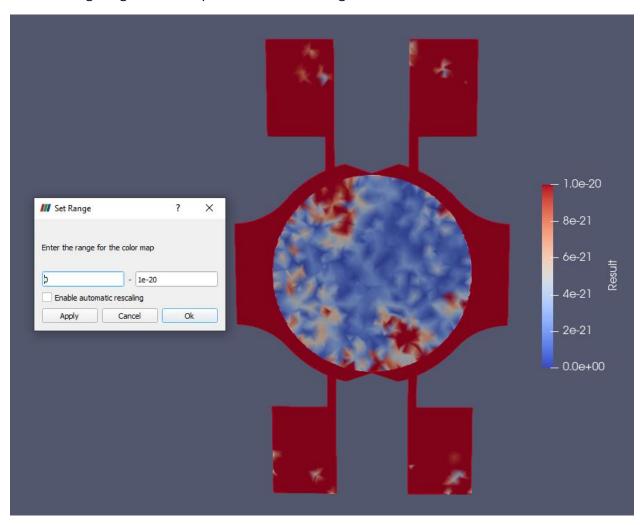
As of this writing, Elmer was unable to directly open ParaView, even though the option exists in Elmer. So we'll manually open and update the vtu file in ParaView every time we run a new simulation.

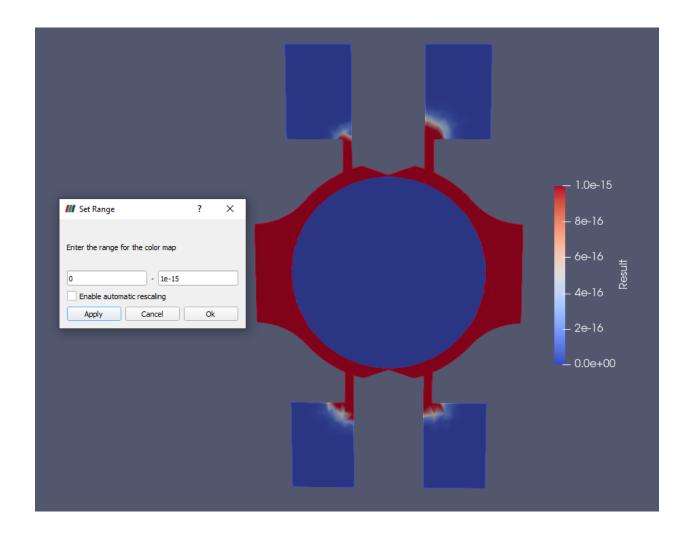
Here is the general workflow to iterate the simulation quickly:

- Set values and configuration in Elmer
- Elmer>>SIF>>Generate>> Edit Sound Speed for correct case>> Save and Run
- Pipeline Browser>> Right click on the .vtu file>>Reload Files
- Pipeline Browser>>Slice2>>Coloring>>Rescale to Custom Range>>Adjust manually
- Screen shot and save your image with a name that makes sense
- File>>Save State>>Rename as needed to save critical data ranges and colorizations you wish to reproduce later when you adjust the Helmholtz values. This ensures you don't chase your tail on a fresh auto-scaled data-desert.

Example Images

The following images are examples from these settings for reference.





Issues and Gotchas Summary

The following were the most painful beginner issues and gotchas:

- 3D model not having a solid volume with split plane regions going into the mesh step
- Gmsh saving the mesh requires typing the .msh extension the first time, even though there's a dropdown showing that it will be (should be) in .msh format.
- Elmer avoid directly driving the wrong surfaces in boundary conditions (BCs). Original pitfall was to assign left drive surface 2 BC (left piezo), surface 14 BC (bulk water sphere), and surface 27 BC (right piezo). This would inject direct energy into the water sphere when what we need is energy transmitted from the left and right aluminum bulkhead horns via

- their driving surfaces (the flats on each side). It was easier to get a waveform by doing this incorrectly, but it's not a real life scenario.
- ParaView Finding a valid data range in a vast sea of orders of magnitude was challenging. A good workflow is to adjust the Coloring>>Set Range fields manually, without automatic rescaling, to avoid chasing your tail when doing tight iteration.

License:

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