Factors for validation of measurement-based simulations

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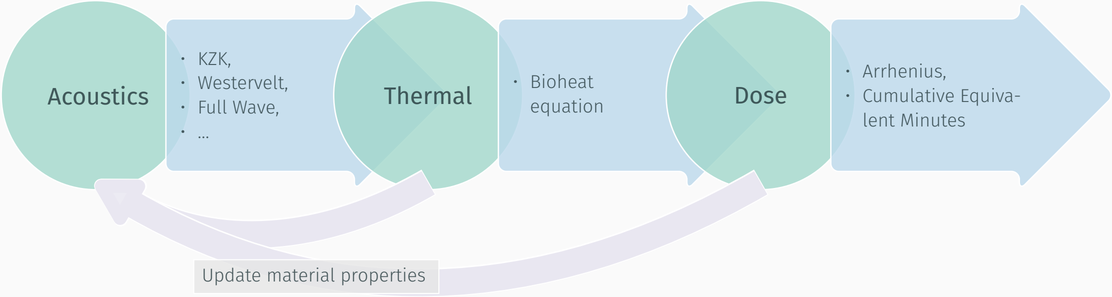
A Simulation Process



Acoustics

- KZK,
- Westervelt,
- Full Wave,
- ...

Thermal

- Bioheat equation

Dose

- Arrhenius,
- Cumulative Equivalent Minutes

Update material properties

- The acoustic equations may be an order of magnitude more computationally expensive than the thermal equations, which may be an order of magnitude more computationally expensive than the dose equations.

Why Simulations? Why Measurement-based Simulations?

Advantages

- Measurements enable transducer performance to be assessed
- Ability to predict pressures in regions where it is not possible to make measurements, for example due to inaccessibility or damaging or hostile exposure conditions
- Interrogate entire field without the need to scan everywhere
- Devices may not be well characterised by analytical formulations
- With a set of measurements, now able to simulate through a variety of different materials

Disadvantages

- Measurements require expensive equipment and some experience
- Simulations can be computationally expensive
- Limited applications with regard to electronic steering etc

What Should be Measured?

Ultrasound can be used to deliver acoustic, mechanical or thermal effects and the measurands may be based on this.

"All models are wrong, but some are useful."

Furthermore, it is difficult to decouple the governing equations and the solution methods.

Choice of model may be influenced by computational resources available.

Governing Equations

Acoustic equations may contain three features, i.e. for a homogeneous KZK-type equation

$$\frac{\partial p}{\partial t} = \underbrace{\frac{c_0}{2}\int_{-\infty}^{t} \nabla^2 p \, \mathrm{d}\tau}_{\text{Diffraction}} + \underbrace{\frac{2}{c_0^3}\mathcal{L}\left[p; \alpha_0, \eta\right]}_{\text{Attenuation}} + \underbrace{\frac{\beta}{2\rho c_0^3}\frac{\partial p^2}{\partial t}}_{\text{Nonlinearity}}$$

- Diffraction: the property of a wave to spread as it propagates
- Attenuation: the absorption of the wave by the medium
- Nonlinearity: the change in the waveform as it propagates

The equations can be propagated forward or backwards in space and time.

Which Governing Equation and Which Numerical Scheme?

An appropriate choice of governing equation and numerical scheme can be formulated based on consideration of three factors:

1. Duration: time or frequency domain?
2. Nonlinearity: linear or nonlinear wave propagation?
3. Homogeneity of source and domain: can dimension of system be reduced?

Broadly, each choice influences the next. Also the more complex, the more difficult to perform both simulations and measurements.

Additionally, the implementation of perfectly matched layers is dependent on the governing equation [1].

Duration

This determines whether it is appropriate to work in the time or the frequency domain.

- Short, pulsed waves should be handled in the time domain
- Longer pulsed waves comprising of many hundreds cycles can be handled in the frequency domain

Typically time for a time-domain solver to reach a steady state is dependent on boundary conditions and the presence of multiple reflections from scatterers: in many cases this can be thousands of cycles. Care may be needed to handle numerical dispersion in this situation when using finite-difference time domain methods.

Intensity

This determines whether it is appropriate to compute linear or nonlinear wave propagation

IEC 62556 defines a local distortion parameter, σ, determining quasi-linear regimes, $\sigma < 0.5$

- If in the time domain, the number of time steps needs to adequately resolve the highest harmonic.
- If in the frequency domain, the number of harmonics computed may need to be determined before computing.

If a shock forms care is needed in measurements to ensure that the bandwidth of the measurement device can record the high frequency components.

Furthermore, information is lost at a shock front, so that back propagation through a shock can not recover pre-shock measurements.

Homogeneity of Source and Domain

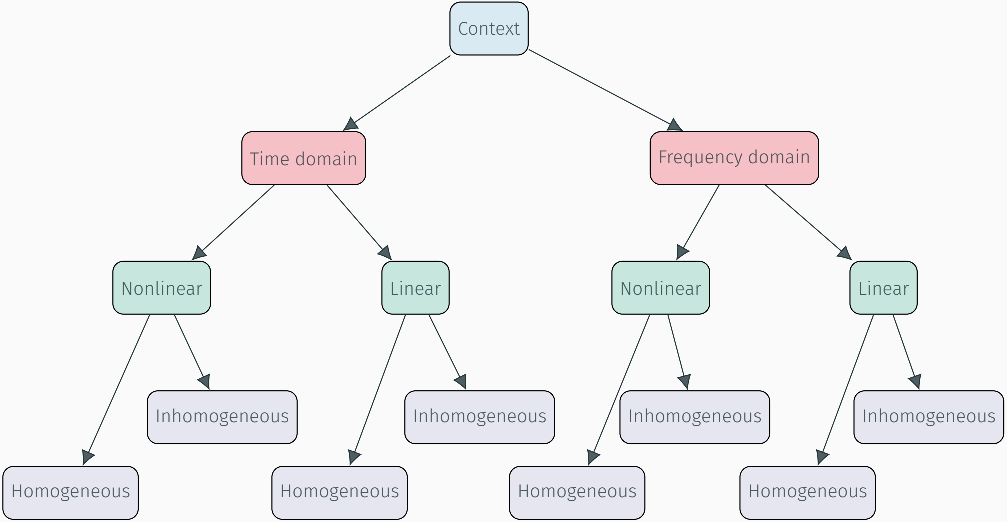
For complex media, exhibiting power-law attenuation, both duration and intensity influence the choice of attenuation operator:

- (time domain) distribution of relaxation processes [2]
- (pseudo-spectral spatial marching) fractional time-derivative [3]
- (pseudo-spectral time stepping) fractional Laplacian [4]

The duration and the intensity also determines the magnitude of the thermal field and any changes in material properties [5].

Paraxial approximation assumes essentially one-way propagation, but limits off-axis accuracy [6].

A Proposed Decision Tree



Scan Planes

- What is the required spacing between points, what is the size of the active element of the hydrophone and are spatial averaging corrections [7] required?
- Does the scan plane capture the complete acoustic field? Measuring pressure or velocity fields?
- If required, when is a steady state reached? Require a tone-burst which is of sufficient length to capture contributions from all of the transducer as well as avoiding ramp-up, but sufficiently short to not be effected by reflected signal, standing-waves, or electrical pick-up etc contaminating measurements.
- Is acquisition plane in linear regime?
- Ensure alignment of scan plane is known, so that measurement points can be related to computation points
- Ensure temperature of water is known (and stable)

Scan Planes

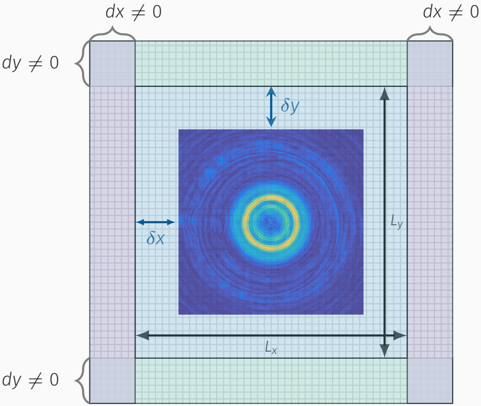


Figure 1: Schematic diagram of measurement (magnitude) data in computational domain and perfectly matched layers. Data can be padded and windowed.

Domain Size

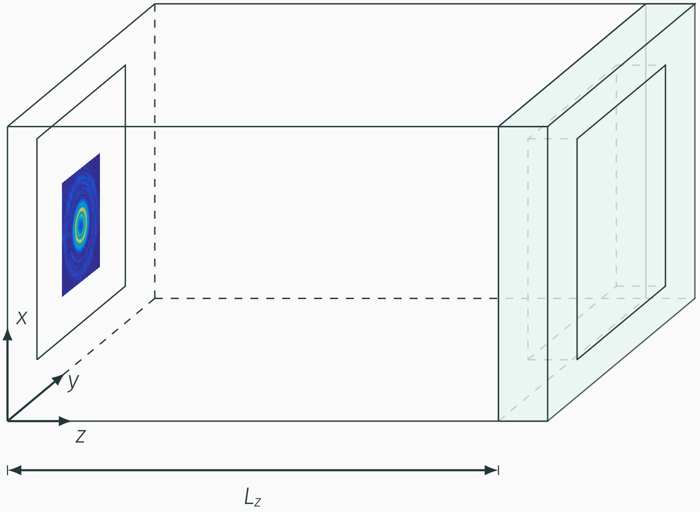


Figure: The axial distance, including a perfectly matched layer at the back to suppress spurious reflections.

Data Quality

Simple projections using Rayleigh integral methods can identify issues with alignment or coverage of scan plan etc.

The spectrum of the eigenvalues of the holography matrix suggests the data is low-rank.

Matrix completion techniques [8] can be used to:

- Identify outliers in the data
- Recover incomplete data

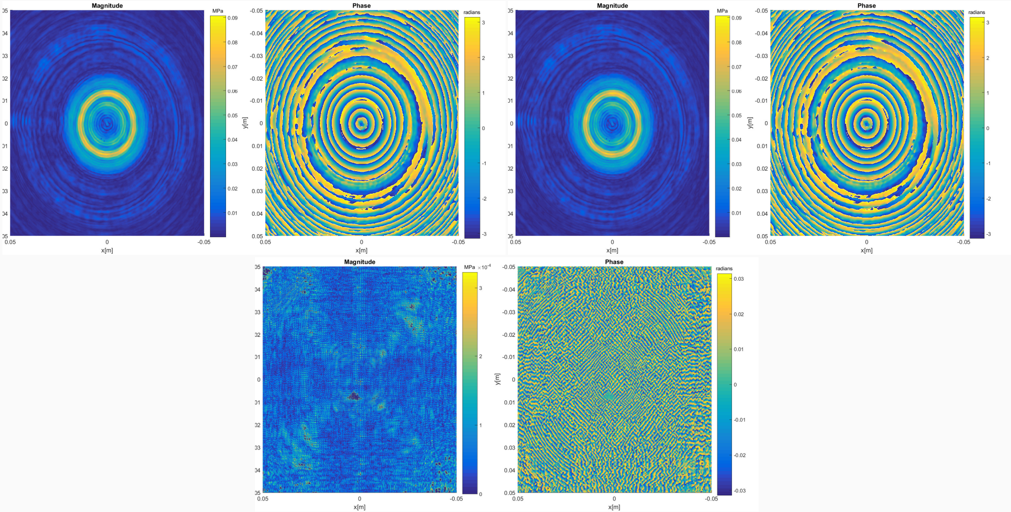


Figure 2: Measurement, reconstructed and errors from, which are from data with 70% of measurement data acquired.

Thermal Equations

The standard bioheat equation [9]

$$\rho c_v \frac{\partial T}{\partial t} = \nabla \left(\kappa \cdot \nabla T \right) + \underbrace{\nu \left(T - T_{\infty} \right)}_{\text{bulk perfusion}} + q$$

Computational domain is typically smaller than acoustic field and spatial and temporal scales larger: impose Dirichlet conditions on down-sampled grid. Furthermore, heat equation spreads, with losses of fine-scale detail in comparison to acoustic field.

In the absence of shocks [10] and cavitation [11], the heat source, q, is proportional to $\nabla \cdot \langle \boldsymbol{v} p \rangle$ or, assuming particle velocity is in phase with the pressure, plane-wave approximation p^2.

In the presence of shocks, an additional source term, independent of absorption, proportional to the cube of the shock height must be included.

Dose Equations

Two formulations for the damage, Ω,

- Arrhenuis component models, based on chemical kinetic models. For example, the first-order rate equation

$$@1[E_a][r]^{k_d}[E_d] \quad \text{leads to} \quad \Omega = \int_0^t A e^{-E_a/(R\bar{T})} \mathrm{d}s$$

- Cumulative equivalent minutes, typically threshold value of an isothermal dose value of 240 min at 43°

$$\Omega = \int_0^t R^{\bar{T}(\mathbf{x},t) - \bar{T}_{\mathrm{ref}}} \mathrm{d}s \quad \text{with} \quad \bar{T}_{\mathrm{ref}} = 43^{\circ} \quad \text{and} \quad R = \begin{cases} 0.25 & \text{for} \quad T < 43^{\circ} \\ 0.5 & \text{for} \quad T \geq 43^{\circ} \end{cases}$$

Updating Equations

- Material properties will change with temperature, changing all fields. However, there is large additional computational cost through updating changes in material properties in the computational of deformation fields and, if in frequency domain, through the re-computation of the acoustic field.

What can change:

- Changes in material properties due to deformation this is dependent on both temperature and dose, experimental data exists for three component Arrhenius model [12]
- Changes in material properties with temperature [5]
- Changes in material state, i.e. due to boiling, which significantly alter some properties such as density [13]

- Furthermore, the rate at which material properties should be updated must be ascertained through a sensitivity study.

Acoustic Measurements

There are a large range of potential uncertainties [14] in measurements

- Calibration uncertainty
- Directional response of hydrophone
- Bandwidth limitations for highly nonlinear waves
- Spatial averaging
- Complex-frequency response of hydrophone
- Alignment
- Changes in speed of sound due to temperature variations

Optical methods can also be used to rapidly interrogate acoustic fields in optically transparent materials [15]

Thermal and Dosimetric Measurements

Due to differing spatial and temporal scales, as well as the blurring effect of heat equation, validating temperature measurements is less precise, but with additional sources of uncertainties.

- Need to account for viscous heating artefacts in most thermocouples [16]

Comparing predicted dose fields requires accurate segmentation and registration of ablated volume and the computation of Dice or overlap scores.

Summary & Discussion

- Validation and verification requires combined consideration of governing equation and numerical scheme and is dependent on the context, i.e. is the desired outcome thermal or mechanical damage etc.

- There are uncertainties in both the measurement-based simulations and validation measurements: to date there is little rigorous uncertainty quantification of the full process [17]

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