k-Wave short course – Part 1
Model equations

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Codes and slides available from:
http://www.k-wave.org/downloads/isna2022.zip

What we will cover today

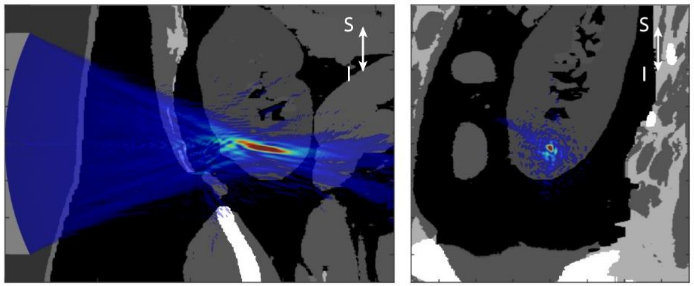
1. Model equations (20 mins)
   – Introduction to the acoustic equations used in k-Wave
2. Numerical methods (45 mins)
   – Derivation of the k-space model used in k-Wave
3. Introduction to k-Wave (15 mins)
   – Overview of k-Wave code structure and syntax

BREAK

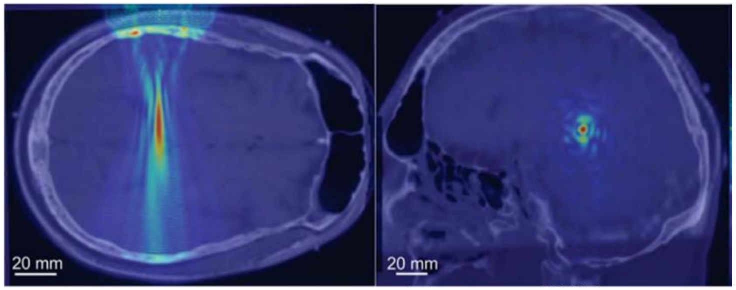
4. Modelling sources (45 mins)
   – Bandlimited interpolant, source scaling, off-grid source
5. Accuracy and convergence (45 mins)
   – Factors affecting accuracy, including staircasing and dispersion, plus C++ codes and experimental validation

Some applications of k-Wave

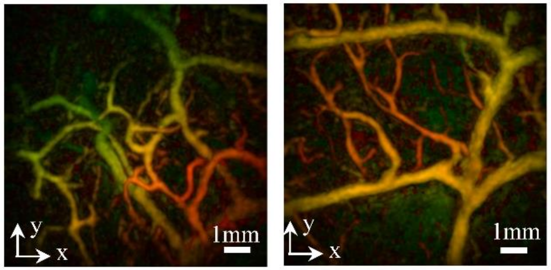
focused ultrasound surgery



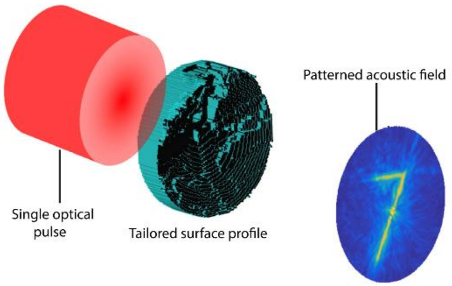
ultrasonic deep brain stimulation



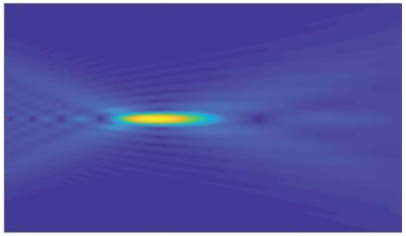
photoacoustic tomography



novel ultrasound sources



source characterisation



What makes a good model?

captures the physics,
easy to solve

1 governing equations

2 numerical methods

stable, accurate,
efficient, convergent

3 computer code

fast, reliable, scalable, well documented,
easy to use, regulatory compliant

4 model inputs

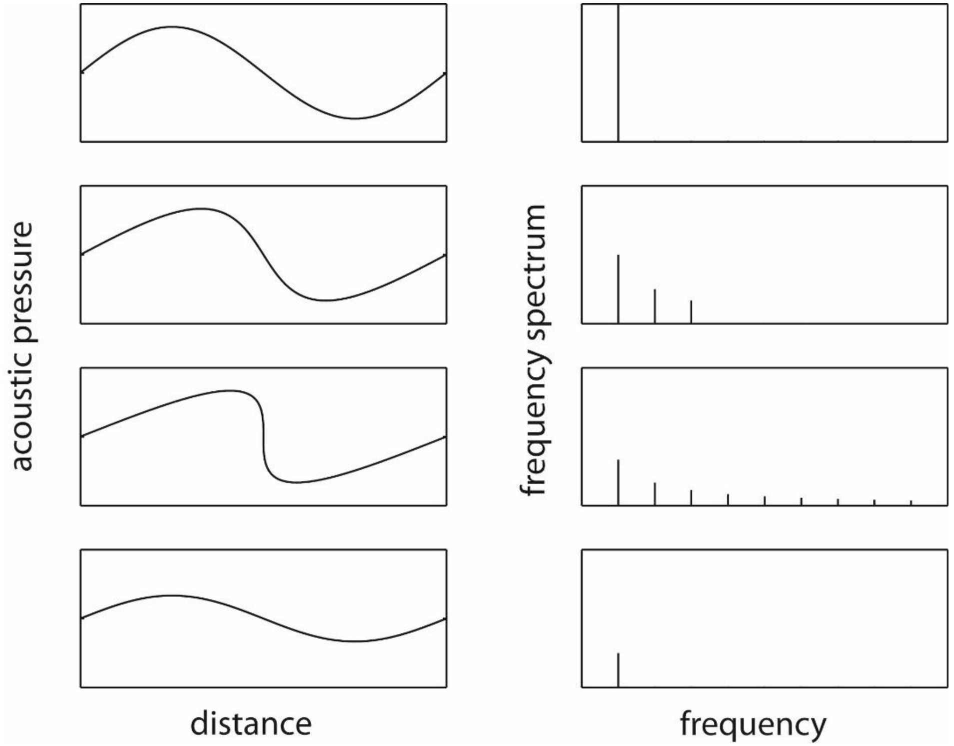
physical, easy to measure

5 validation

convergence tests,
canonical solutions,
experimental data

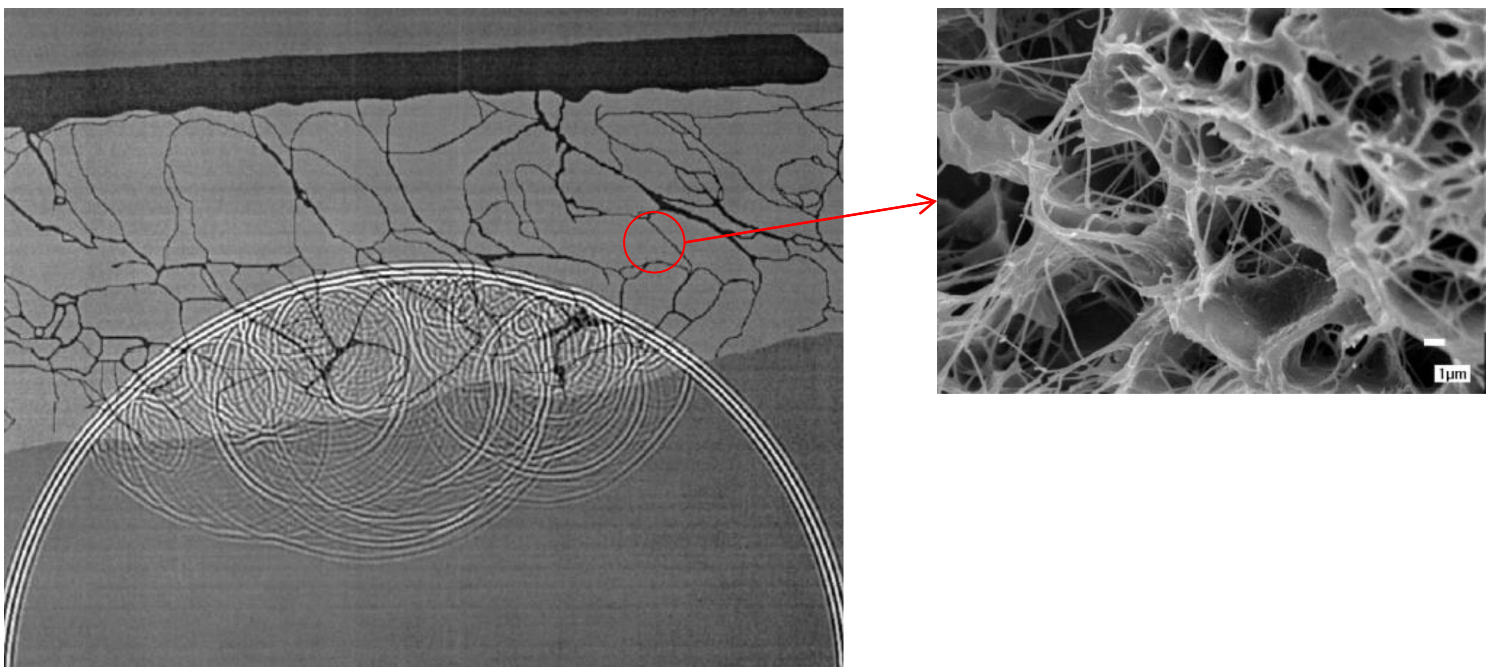
Simulating ultrasound waves in tissue

- To model ultrasound in tissue, we need to consider:
  - The wave propagation can be nonlinear



Simulating ultrasound waves in tissue

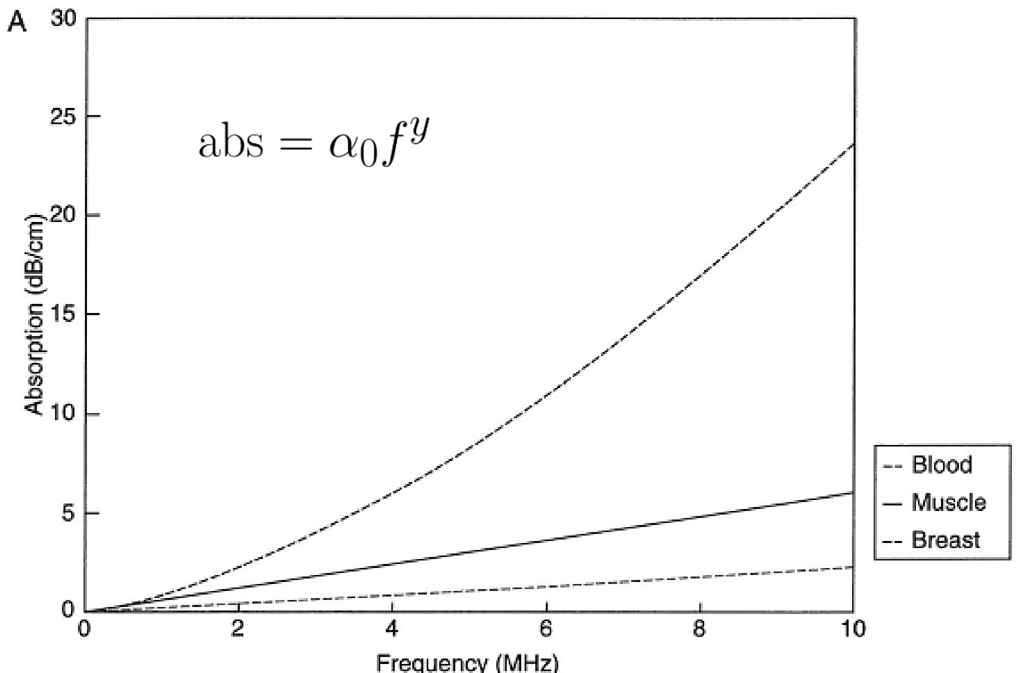
- To model ultrasound in tissue, we need to consider:
  - The wave propagation can be nonlinear
  - The acoustic medium is heterogeneous (fluid media)



M. Tabei *et al.*, “Simulation of ultrasonic focus aberration and correction…” *J. Acoust. Soc. Am.* **113**(2), (2003)

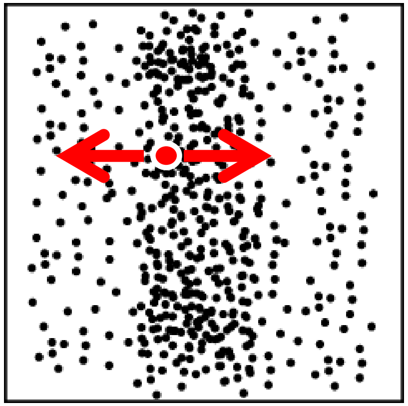
Simulating ultrasound waves in tissue

- To model ultrasound in tissue, we need to consider:
  - The wave propagation can be nonlinear
  - The acoustic medium is heterogeneous
  - The acoustic medium is absorbing



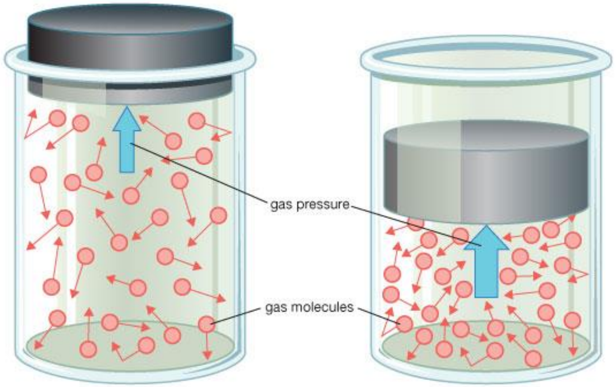
T. Szabo, Diagnostic Ultrasound Imaging, Elsevier (2004)

Acoustic variables



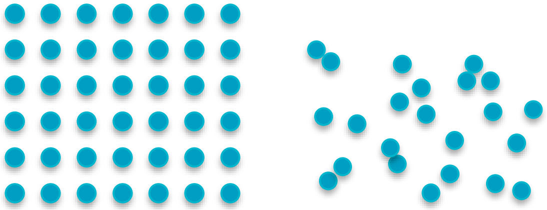
particle velocity: fluctuation of particles about mean position [m], [m.s^{-1}]

$\mathbf{u}$



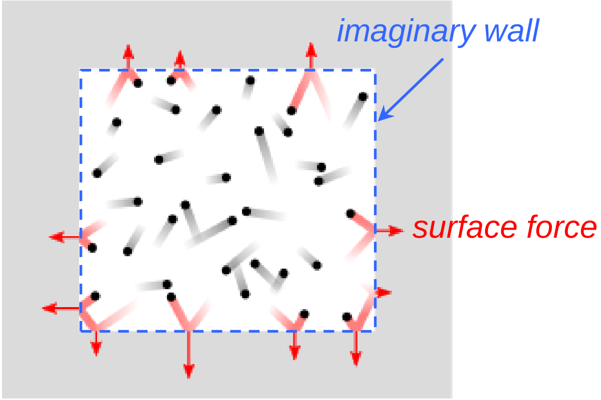
density: mass per unit volume [kg.m^{-3}]

$\hat{\rho}$



entropy: measure of disorder [K]

s

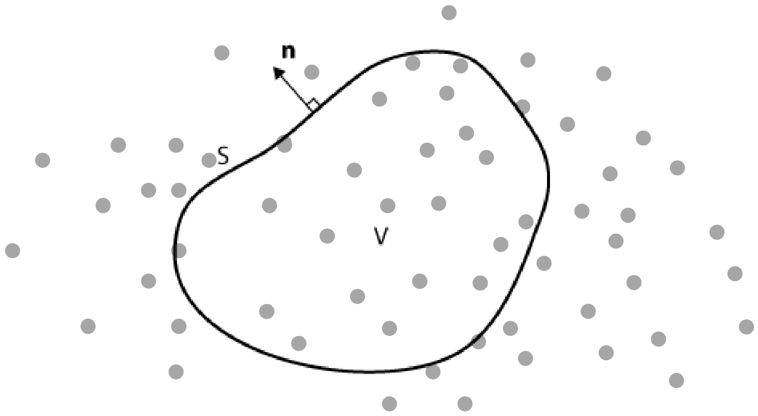


pressure: force per unit area [Pa = N.m^{-2}]

$\hat{p}$

Mass conservation

Consider a fixed volume in a flowing fluid



Mass conservation: the rate of change of mass in V is equal to the net rate of mass flow into V

$$\frac{d}{dt}\int_V \hat{\rho}\, dV = -\int_S \hat{\rho}\mathbf{u}\cdot\mathbf{n}\, dS$$

$\hat{\rho}$ mass density

$\mathbf{u}$ particle velocity

Mass conservation

The volume is not time dependent, so the LHS becomes

$$\frac{d}{dt}\int_V \hat{\rho} dV = \int_V \frac{\partial \hat{\rho}}{\partial t} dV$$

Using Gauss' divergence theorem on the RHS gives

$$-\int_S \hat{\rho}\mathbf{u}\cdot\mathbf{n} dS = -\int_V \nabla\cdot(\hat{\rho}\mathbf{u})\, dV$$

Recombining these gives the volume integral equation

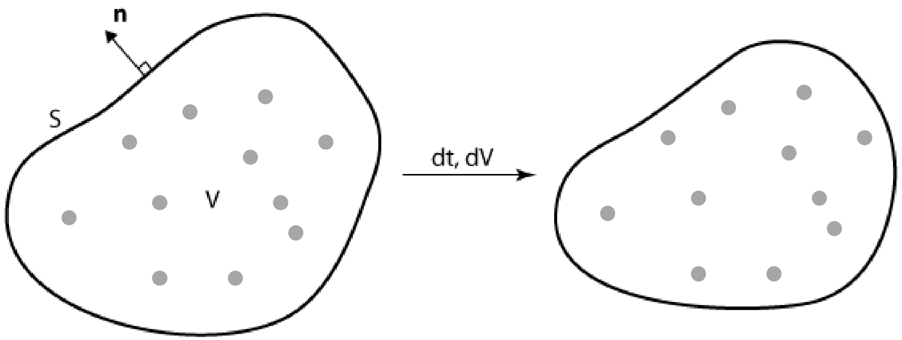
$$\int_V \left(\frac{\partial \hat{\rho}}{\partial t} + \nabla\cdot(\hat{\rho}\mathbf{u})\right) dV = 0$$

but as the volume is arbitrary the integrand must be zero:

$$\boxed{\frac{\partial \hat{\rho}}{\partial t} + \nabla\cdot(\hat{\rho}\mathbf{u}) = 0}$$

Momentum conservation

Consider a material element moving with the fluid



Momentum conservation: the rate of change of momentum of the element is equal to the net force on it

$$\frac{d}{dt}\int_{V(t)} \hat{\rho}\mathbf{u}\, dV = -\int_{S(t)} \hat{p}\mathbf{n} dS$$

$\hat{p}$ pressure

Momentum conservation

LHS: The volume is moving, but the density of each of the individual fluid particles within it remains constant, so:

$$\frac{d}{dt}\int_{V(t)} \hat{\rho}\mathbf{u}\,dV = \int_{V(t)} \hat{\rho}\left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u}\cdot\nabla)\,\mathbf{u}\right)\,dV$$

RHS: Using Gauss' divergence theorem gives

$$-\int_{S(t)} \hat{p}\mathbf{n}dS = -\int_{V(t)} \nabla\hat{p}\,dV$$

Noting $(\mathbf{u}\cdot\nabla)\,\mathbf{u} = \frac{1}{2}\nabla|\mathbf{u}|^2 = \frac{1}{2}\nabla u^2$ and recombining gives

$$\int_{V(t)} \left(\hat{\rho}\frac{\partial \mathbf{u}}{\partial t} + \tfrac{1}{2}\hat{\rho}\nabla u^2 + \nabla\hat{p}\right)\,dV = 0$$

$$\boxed{\hat{\rho}\frac{\partial \mathbf{u}}{\partial t} + \tfrac{1}{2}\hat{\rho}\nabla u^2 + \nabla\hat{p} = 0}$$

Introducing the acoustic variables

The total variables can be divided into ambient and acoustic parts:

$$\hat{\rho}(\mathbf{x},t) = \rho_0(\mathbf{x}) + \rho(\mathbf{x},t)$$
$$\hat{p}(\mathbf{x},t) = P_0 + p(\mathbf{x},t) \text{ etc.}$$

Assuming no bulk flow and retaining only terms up to second order in the acoustic variables, gives

$$\frac{\partial \hat{\rho}}{\partial t} + \nabla \cdot (\hat{\rho}\mathbf{u}) = 0 \qquad \rightarrow \qquad \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho_0 \mathbf{u}) = -\nabla \cdot (\rho \mathbf{u})$$

$$\hat{\rho}\frac{\partial \mathbf{u}}{\partial t} + \nabla \hat{p} + \tfrac{1}{2}\hat{\rho}\nabla u^2 = 0 \qquad \rightarrow \qquad \rho_0 \frac{\partial \mathbf{u}}{\partial t} + \nabla p = -\rho \frac{\partial \mathbf{u}}{\partial t} - \tfrac{1}{2}\rho_0 \nabla u^2$$

Nonlinearity

It is convenient to rewrite the nonlinear terms as functions of the acoustic Lagrangian density

$$\mathcal{L} = \frac{1}{2}\rho_0 u^2 - \frac{p^2}{2\rho_0 c_0^2}$$

After some algebra, the conservation equations become

$$\rho_0 \frac{\partial \mathbf{u}}{\partial t} + \nabla p = -\nabla \mathcal{L}$$

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho_0 \mathbf{u}) = \frac{1}{c_0^2}\frac{\partial \mathcal{L}}{\partial t} - 2\rho \nabla \cdot \mathbf{u}$$

When cumulative nonlinear effects dominate local effects, the contributions from the Lagrangian can be neglected.

First two model equations

The conservation equations, in acoustic form, are now

$$\rho_0 \frac{\partial \mathbf{u}}{\partial t} + \nabla p = 0$$

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho_0 \mathbf{u}) = -2\rho \nabla \cdot \mathbf{u}$$

Two equations, three unknowns. Need another equation.

Acoustic equation of state

The acoustic pressure can be written in general as a function of any two other thermodynamic variables, eg.

$$p = p(\rho, s) \qquad s \quad \text{specific entropy}$$

The first few terms of a Maclaurin series expansion are

$$p = \left.\frac{\partial p}{\partial \rho}\right|_s \rho + \frac{1}{2}\left.\frac{\partial^2 p}{\partial \rho^2}\right|_s \rho^2 \ldots + \left.\frac{\partial p}{\partial s}\right|_\rho s \ldots$$

Using the thermodynamic relations

$$A = \rho_0 \left.\frac{\partial p}{\partial \rho}\right|_s \equiv \rho_0 c_0^2 \qquad B = \rho_0^2 \left.\frac{\partial^2 p}{\partial \rho^2}\right|_s$$

results in…

Acoustic equation of state

…the acoustic equation of state

$$p = c_0^2 \left(\rho + \frac{1}{2} \frac{B}{A} \frac{\rho^2}{\rho_0} \right) + \left. \frac{\partial p}{\partial s} \right|_{\rho} s$$

where B/A is the acoustic nonlinearity parameter.

The loss term is replaced by a phenomenological term

$$p = c_0^2 \left(\rho + \frac{1}{2} \frac{B}{A} \frac{\rho^2}{\rho_0} - \mathrm{L}\rho \right)$$

where the operator L is chosen to give the observed absorption behaviour

Acoustic equation of state

Adiabatic equation of state

$$\mathrm{L} = 0 \qquad\qquad p = c_0^2 \rho$$

acoustic pressure and density are in phase – no absorption

Stokes equation of state (viscous losses)

$$\mathrm{L} = \tau \frac{\partial}{\partial t} \qquad\qquad p = c_0^2 \left(1 + \tau \frac{\partial}{\partial t}\right) \rho$$

change in density is delayed but absorption is proportional to f^2

Caputo's equation of state (fractional Kelvin-Voigt)

$$\mathrm{L} = \tau \frac{\partial^{y-1}}{\partial t^{y-1}} \qquad\qquad p = c_0^2 \left(1 + \tau \frac{\partial^{y-1}}{\partial t^{y-1}}\right) \rho$$

gives f^y *but operator is non-local in time (memory intensive to compute with)*

Acoustic equation of state

- k-Wave uses a *fractional Laplacian* equation of state

$$\mathrm{L} = \underbrace{\tau \frac{\partial}{\partial t} \left(-\nabla^2\right)^{\frac{y}{2}-1}}_{\text{absorption}} + \underbrace{\eta \left(-\nabla^2\right)^{\frac{y+1}{2}-1}}_{\text{dispersion}}$$

  – both τ, η are functions of the absorption coefficient

- Operator is non-local in space rather than time
- For spectral methods, spatial gradient calculations are already global, so this operator is efficient to compute

Model equations

- k-Wave solves the following system of equations

$$\frac{\partial \mathbf{u}}{\partial t} = -\frac{1}{\rho_0} \nabla p$$

momentum conservation

$$\frac{\partial \rho}{\partial t} = -\left(2\rho + \rho_0\right) \nabla \cdot \mathbf{u}$$

mass conservation

$$p = c_0^2 \left(\rho + \frac{1}{2} \frac{B}{A} \frac{\rho^2}{\rho_0} - \mathrm{L} \rho \right)$$

pressure-density relation

$$\mathrm{L} = \tau \frac{\partial}{\partial t} \left(-\nabla^2\right)^{\frac{y}{2}-1} + \eta \left(-\nabla^2\right)^{\frac{y+1}{2}-1}$$

absorption term

- The acoustic variables are circled. The other letters represent material properties.

Generalised Westervelt equation

- The system of equations can be collapsed into a single second order wave equation

$$\nabla^2 p - \frac{1}{c_0^2}\frac{\partial^2 p}{\partial t^2} - \frac{1}{\rho_0}\nabla\rho_0 \cdot \nabla p + \frac{\beta}{\rho_0 c_0^4}\frac{\partial^2 p^2}{\partial t^2} - \mathrm{L}\nabla^2 p = 0$$

where the coefficient of nonlinearity is given by

$$\beta \equiv 1 + \frac{1}{2}\frac{B}{A}$$

- This wave equation has a similar form to the well-known Westervelt equation

Summary

- k-Wave solves a system of three coupled equations
  - mass conservation
  - momentum conservation
  - acoustic equation of state
- Heterogeneous sound speed and density can be modelled
- Cumulative nonlinearities are included
- Absorption is modelled using a fractional Laplacian term