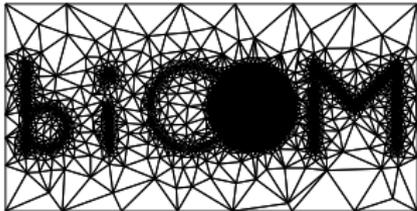


# Acoustic Localisation of Coronary Artery Disease

Simon Shaw

[people.brunel.ac.uk/~icsrsss](http://people.brunel.ac.uk/~icsrsss)



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# Contents

- [▶ jump](#) Viscoelasticity and wave equations
- [▶ jump](#) Acoustic Localisation of Coronary Artery Disease (CAD)
- [▶ jump](#) High Order (in time) Space-Time FEM

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# Viscoelasticity

## PDE's with memory

## Main themes

- Viscoelastic materials exhibit memory

## Details

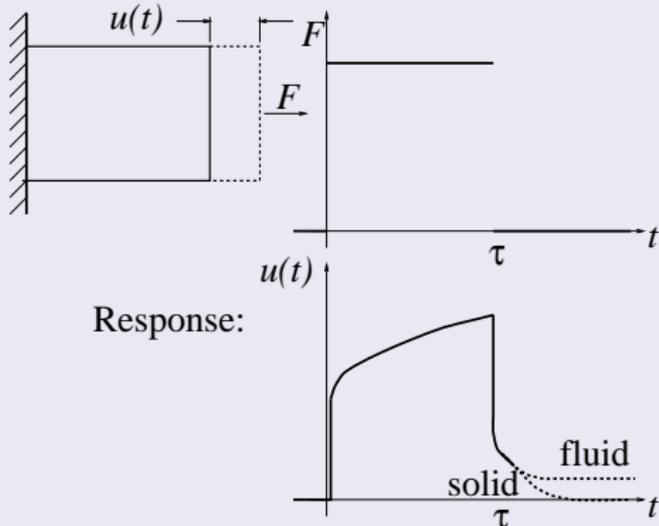
### Application areas:

- damping (polymers)
- structures (concrete)
- porous media (geomechanics)
- electromagnetics (Debye media)
- non-Fickian diffusion
- soft tissue biomechanics

## Main themes

- Viscoelastic materials exhibit **memory**
- **which manifests as:**
  - **creep**

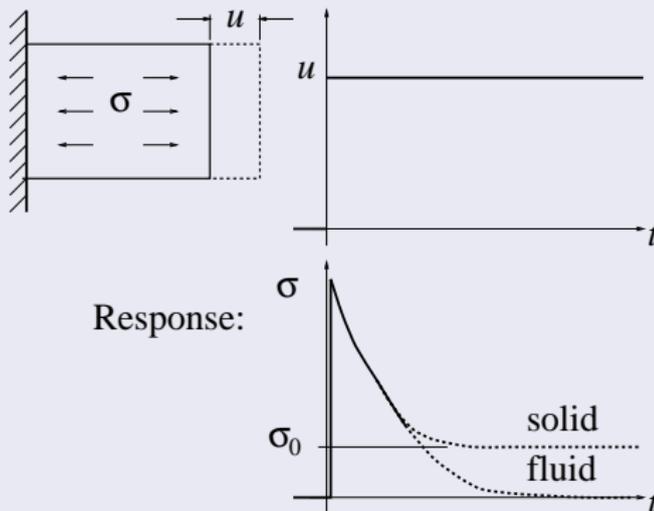
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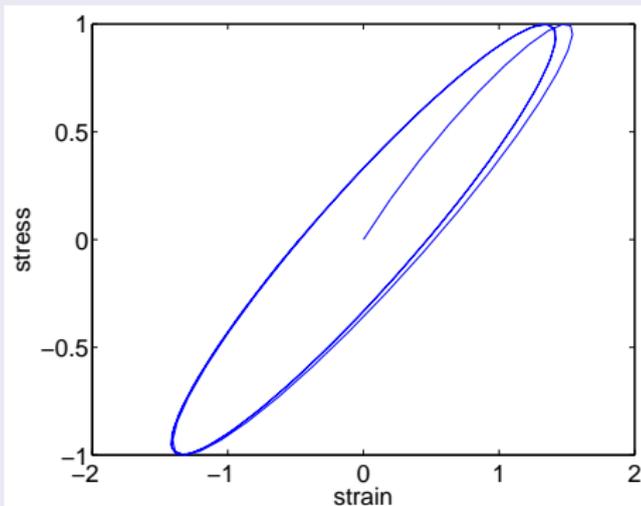
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## Main themes

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  - **hysteresis**

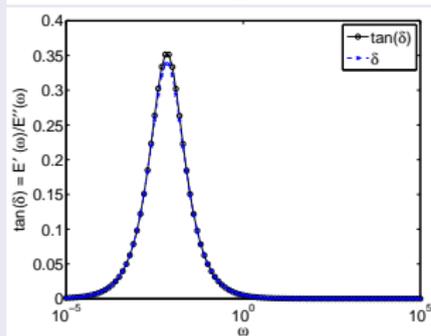
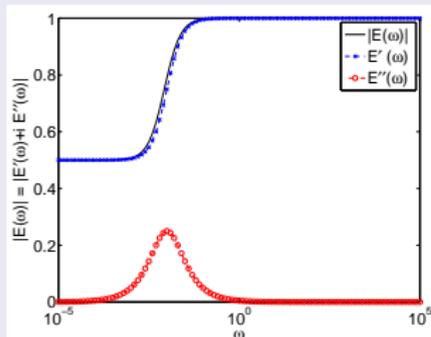
## Details



## Main themes

- Viscoelastic materials exhibit **memory**
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  - **hysteresis**
  - **frequency dependence**

## Details



## Main themes

- Viscoelastic materials exhibit **memory**
- which manifests as:
  - **creep**
  - **relaxation**
  - **hysteresis**
  - **frequency dependence**
- Typically described by **partial differential equations** with either
  - **internal variables**
  - or **memory**

## Details

$$u_{tt} - \nabla^2 u = f - \nabla \cdot \sigma$$

$$\sigma_t + \gamma \sigma = \mu \nabla u$$

$$u_{tt} - \nabla^2 u = f - \int_0^t b(t-s) \nabla^2 u(s) ds$$

$$\text{Prony: } b(t) = \sum_i b_i e^{-t/\tau_i}$$

or weakly singular:  $t^p$

or fractional calculus

**nonlinearity, e.g.  $\gamma \leftarrow \gamma(u)$**

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**nonlinearity, e.g.  $\gamma \leftarrow \gamma(u)$**

**Analysis can exploit the fading memory: an example...**

# Maxwell's equations — dispersive dielectrics

$$\begin{aligned}\nabla \times \mathbf{E} + \dot{\mathbf{B}} &= \mathbf{0} & \nabla \cdot \mathbf{B} &= 0 \\ \nabla \times \mathbf{H} - \dot{\mathbf{D}} &= \mathbf{J} & \nabla \cdot \mathbf{D} &= \rho\end{aligned}$$

What has this got to do with viscoelasticity? Dispersion...

# Maxwell's equations — dispersive dielectrics

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What has this got to do with viscoelasticity? Dispersion...

$\mathbf{B} = \mu\mathbf{H}$  but dielectric polarization is not **instantaneous**...

Debye:  $\mathbf{D} = \varepsilon_0(1 + \chi)\mathbf{E} + \mathbf{P}$  with  $\tau\dot{\mathbf{P}} + \mathbf{P} = (\varepsilon_s - \varepsilon_\infty)\varepsilon_0\mathbf{E}$

with  $\mathbf{P}(0) = \mathbf{0}$  and the  $\varepsilon$ 's known. Hence, we can use either of...

$$(\varepsilon_0\varepsilon_\infty)^{-1}\mathbf{D} = \mathbf{E} + \dot{\psi} * \mathbf{E} \quad \text{or} \quad \varepsilon_0\varepsilon_\infty\mathbf{E} = \mathbf{D} + \dot{\varphi} * \mathbf{D}$$

which is **viscoelasticity**! Exploit related results...

# Example of *a priori* control. No Gronwall!

Find  $\mathbf{D}$  such that: 
$$\ddot{\mathbf{D}} + \nabla \times \mu^{-1} \nabla \times \mathbf{E} + \sigma \dot{\mathbf{E}} = -\mathbf{J}_a,$$

where 
$$\varepsilon \dot{\mathbf{E}}(t) = \dot{\mathbf{D}}(t) + \varphi'(t) \mathbf{D}(0) - \int_0^t \varphi_s(t-s) \dot{\mathbf{D}}(s) ds.$$

## Theorem

With  $\mathbf{G}(t) = -\mathbf{J}_a(t) - \sigma \varepsilon^{-1} \varphi'(t) \mathbf{D}(0)$  known and if  $\sigma > 0$  we have,

$$\begin{aligned} \mu \varepsilon \|\dot{\mathbf{D}}(t)\|_0^2 + \check{\varphi} \|\nabla \times \mathbf{D}(t)\|_0^2 + \mu \sigma \check{\varphi} \|\dot{\mathbf{D}}\|_{L_2(0,t;L_2(\Omega))}^2 \\ \leq \mu \varepsilon \|\dot{\mathbf{D}}(0)\|_0^2 + \|\nabla \times \mathbf{D}(0)\|_0^2 + \frac{\mu \varepsilon^2}{\sigma \check{\varphi}} \|\mathbf{G}\|_{L_2(0,t;L_2(\Omega))}^2. \end{aligned}$$

*Remark: similar results are possible if  $\sigma = 0$ .*

Using also Rivera & Menzala's lemma (Quart. Appl. Math., LVII, 1999)

## Example: a discrete abstract wave equation

Relaxation (fading memory) expressed through internal variable rate equations: find  $\mathbf{u}: I \rightarrow V$  such that,

$$(\rho \ddot{\mathbf{u}}(t), \mathbf{v}) + a(\mathbf{u}(t), \mathbf{v}) + b(\dot{\mathbf{u}}(t), \mathbf{v}) = \langle L(t), \mathbf{v} \rangle + \sum_{q=1}^{N_\varphi} a(\mathbf{u}_q^*(t), \mathbf{v}) \quad \forall \mathbf{v} \in V,$$

$$a(\tau_q \dot{\mathbf{u}}_q^*(t) + \mathbf{u}_q^*(t), \mathbf{v}) = a(\varphi_q \mathbf{u}(t), \mathbf{v}) \quad \text{for } q = 1, \dots, N_\varphi, \quad \forall \mathbf{v} \in V.$$

And its DG-in-time approximation: find  $(U, W) \approx (u, \dot{u})$  such that

$$(\rho \dot{W}, \vartheta)_n + (\rho [W]_{n-1}, \vartheta_{n-1}^+) + a((U, \vartheta))_n + b((W, \vartheta))_n - \sum_{q=1}^{N_\varphi} a((Z_q, \vartheta))_n = \langle L, \vartheta \rangle_n$$

$$a((\dot{U} - W, \zeta))_n + a([U]_{n-1}, \zeta_{n-1}^+) = 0,$$

$$\text{for } q = 1, \dots, N_\varphi \quad a((\tau_q \dot{Z}_q + Z_q - \varphi_q U, \xi_q))_n + a(\tau_q [Z_q]_{n-1}, \xi_{q,n-1}^+) = 0,$$

for all test functions  $\theta, \zeta, \xi_1, \dots \in \mathbb{P}_r(I_n; V^h)$ .

# Sharp discrete stability

The discrete scheme. . .

$$\langle \varrho \dot{W}, \vartheta \rangle_n + \langle \varrho [W]_{n-1}, \vartheta_{n-1}^+ \rangle + a((U, \vartheta))_n + b(W, \vartheta)_n - \sum_{q=1}^{N_\varphi} a((Z_q, \vartheta))_n = \langle L, \vartheta \rangle_n$$

$$a((\dot{U} - W, \zeta))_n + a([U]_{n-1}, \zeta_{n-1}^+) = 0,$$

$$\text{for } q = 1, \dots, N_\varphi \quad a((\tau_q \dot{Z}_q + Z_q - \varphi_q U, \xi_q))_n + a(\tau_q [Z_q]_{n-1}, \xi_{q,n-1}^+) = 0,$$

satisfies, for each time  $t_m$ ,

$$\begin{aligned} & \|\varrho^{1/2} W_m^-\|_0^2 + \|\varphi_0^{1/2} U_m^-\|_V^2 + \sum_{q=1}^{N_\varphi} \left\| \frac{Z_{q,m}^- - \varphi_q U_m^-}{\sqrt{\varphi_q}} \right\|_V^2 + 2 \int_0^{t_m} \left( \sum_{q=1}^{N_\varphi} \left\| \frac{Z_q - \varphi_q U}{\sqrt{\tau_q \varphi_q}} \right\|_V^2 + b(W, W) \right) dt \\ & + \sum_{n=1}^m \left( \sum_{q=1}^{N_\varphi} \left\| \left[ \frac{Z_q - \varphi_q U}{\sqrt{\varphi_q}} \right]_{n-1} \right\|_V^2 + \|\varrho^{1/2} [W]_{n-1}\|_0^2 + \|\varphi_0^{1/2} [U]_{n-1}\|_V^2 \right) \\ & = 2 \int_0^{t_m} \langle L, W \rangle dt + \|\varrho^{1/2} W_0^-\|_0^2 + \|\varphi_0^{1/2} U_0^-\|_V^2. \end{aligned}$$

Leads to **Non-Gronwall** discrete stability. (Error bounds?)

# Coronary Artery Disease

[◀ back](#)

# Coronary Artery Disease

[◀ back](#)

# Coronary Artery Disease (CAD)



- In the UK in 2010 CAD caused over 14% of all deaths (80,568/561,666).
  - About 95% in people aged 55+ yrs.
- €7.5 billion — approx 2009 cost. . .
  - €2 billion — healthcare (*per capita* €32)
  - €3.5 billion — lost productivity
  - €2 billion — informal patient care
- An expensive killer — huge tax burden.
- Poor diet & ageing population will exacerbate problem.

**Source:** *Tables 6.2, 6.3, Coronary Heart Disease Statistics. A compendium of health statistics. 2012 ed. British Heart Foundation. ISBN 978-1-899088-12-6*

## What is Coronary Artery Disease?

- Lipids & calcium deposits form **atheromatous plaques** between endothelium and artery wall
- Stenosis grows and reduces artery calibre.
- **Vulnerable plaque** suddenly ruptures — causes clot
- *Myocardial Ischaemia/Infarction*: a 'heart attack'



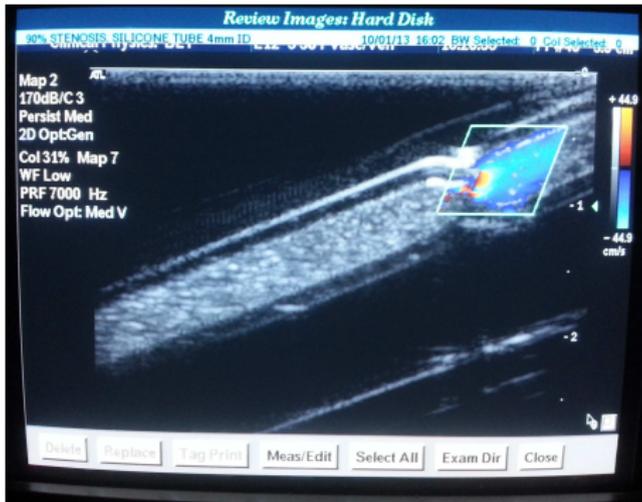
## What can mathematics offer?

- **biotissue** highly viscoelastic and hysteretic
- acoustic shear waves caused by **stenotic wake disturbance** travel at frequency-dependent speed
- 150–750 Hz signals detectable at chest surface
- Exploit this for **non-invasive computational diagnosis** of **arterial stenosis** via inverse problem
- Challenging and ambitious: **at a very early stage**...

## Coronary Artery Disease (CAD)

# Localised disturbance: illustrative experiment. . .

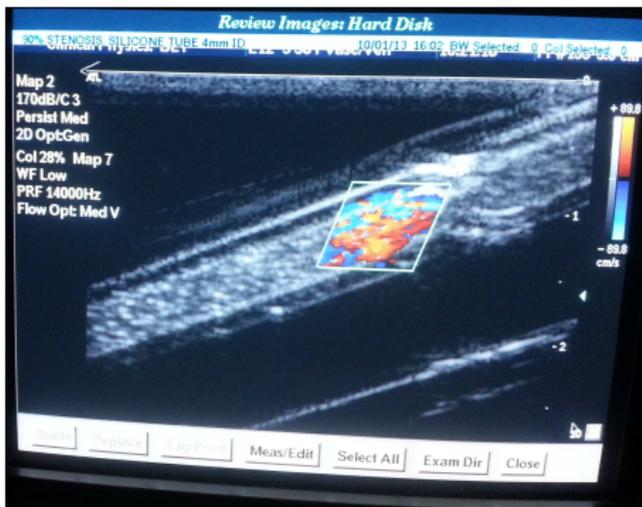
Blood mimicking fluid pumped through artificially stenosed tube constrained within a TMM block (blue, forward; red, reversed).



## Coronary Artery Disease (CAD)

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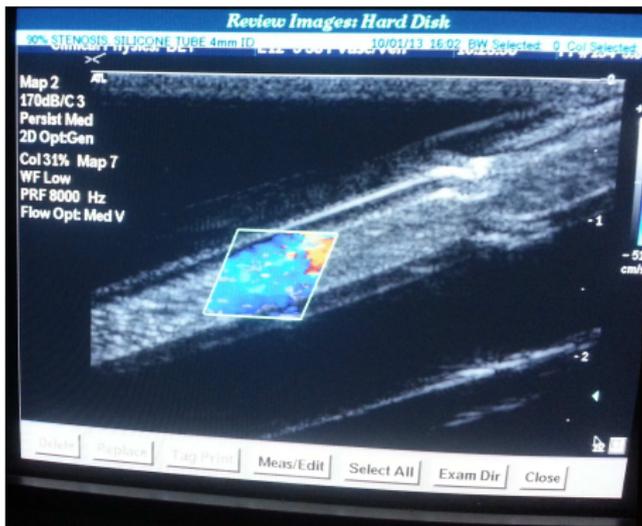
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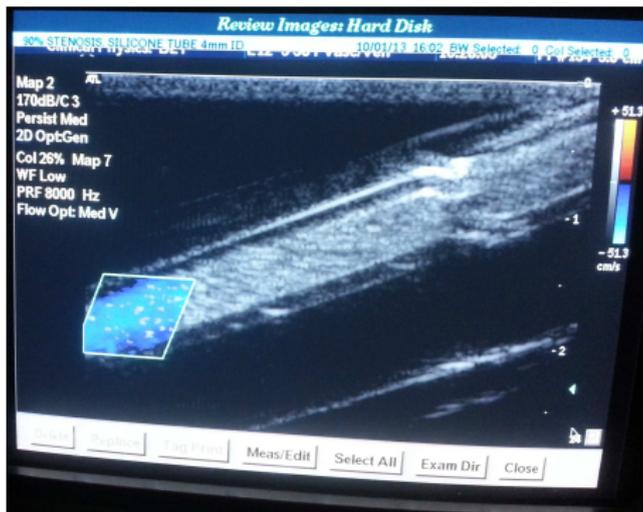
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Semmlow and Rahalkar, *Ann. Rev. Biomed. Eng.* 2007 9:449–69Acoustic Detection of  
Coronary Artery DiseaseJohn Semmlow<sup>1</sup> and Ketaki Rahalkar<sup>2</sup><sup>1</sup>Robert Wood Johnson Medical School, Rutgers University, Piscataway,  
New Jersey 08854; email: Semmlow@biomed.rutgers.edu<sup>2</sup>Department of Biomedical Engineering, Rutgers University, Piscataway,  
New Jersey 08854; email: kctaki\_kholkute@yahoo.com*Annu. Rev. Biomed. Eng.* 2007. 9:449–69First published online as a Review in Advance on  
April 10, 2007The *Annual Review of Biomedical Engineering* is  
online at [bioeng.annualreviews.org](http://bioeng.annualreviews.org)This article's doi:  
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1523-9829/07/0815-0449\$20.00

**Key Words**phonocardiography, heart sounds, coronary stenosis, coronary  
bruits, signal processing, cardiac microphones**Abstract**

Coronary artery disease (CAD) occurs when the arteries to the heart (the coronary arteries) become blocked by deposition of plaque, depriving the heart of oxygen-bearing blood. This disease is arguably the most important fatal disease in industrialized countries, causing one-third to one-half of all deaths in persons between the ages of 35 and 64 in the United States. Despite the fact that early detection of CAD allows for successful and cost-effective treatment of the disease,

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## Coronary Artery Disease

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*Annu. Rev. Biomed. Eng.* 2007. 9:449–69

First published online as a Review in Advance on April 10, 2007

The *Annual Review of Biomedical Engineering* is online at [bioeng.annualreviews.org](http://bioeng.annualreviews.org)

This article's doi:  
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Key Finding...

no other approach ... promises  
to be as inexpensive,  
simple... and risk free

# What can computational mathematics offer?

## Scoping/Feasibility Project: Methods and Aims

- Use the signature chest surface signal for **screening and diagnosis**. (Expected range  $\sim 150$  Hz — 750 Hz.)
- *In vitro* biomechanics:
  - Characterize tissue mimicking agarose gel.
  - Build gel chest phantoms with controllable ‘stenoses’.
  - Use a fluid loaded model to create shear waves.
- Computational Mathematics:
  - Material characterization through inverse problem data-fitting.
  - Simulations of wave transit through mimicked chest.
  - Stenosis localization through inverse solver.

**EVENTUAL AIM**  
**noninvasive screening & diagnosis**

# Acoustic Localisation of CAD

[◀ back](#)

## EPSRC

Engineering and Physical Sciences  
Research Council

Acoustic Localisation of  
Coronary Artery Stenosis

Brunel: EP/H011072/1

Queen Mary: EP/H011285/1

April 2010 — March 2014

## Speculative Research

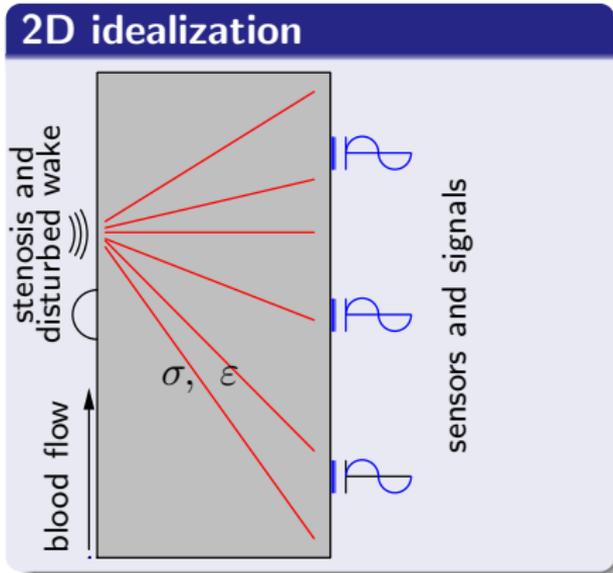
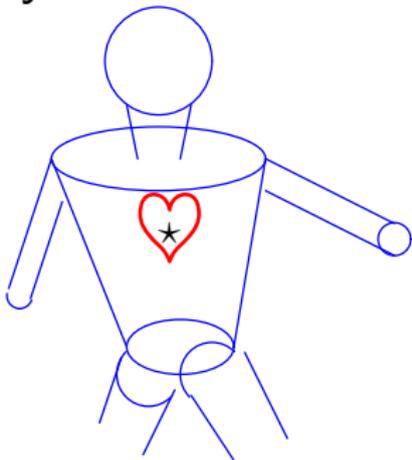
Multidisciplinary/international:

- **Blizard (Queen Mary)**: chest phantom construction and experiments
- **CRSC (North Carolina State)**: identification and inverse problem
- **BICOM (Brunel)**: FE models & computation of direct problem

People: C Kruse, JR Whiteman, SE Greenwald, MJ Birch, MP Brewin, J Reeves, HT Banks, ZR Kenz, S Hu, B Kehra, E Cantor, D Mehta, I Ganeswaren, S Shaw

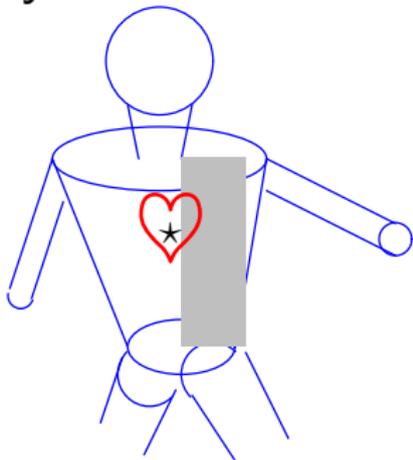
# Schematics - first steps

The reality...

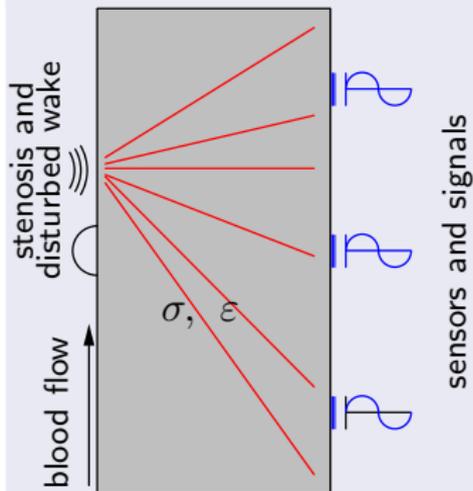


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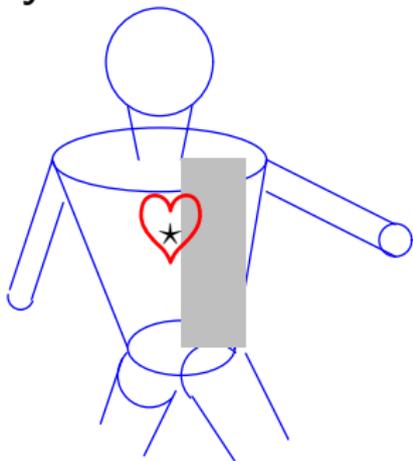


## 2D idealization



# Schematics - first steps

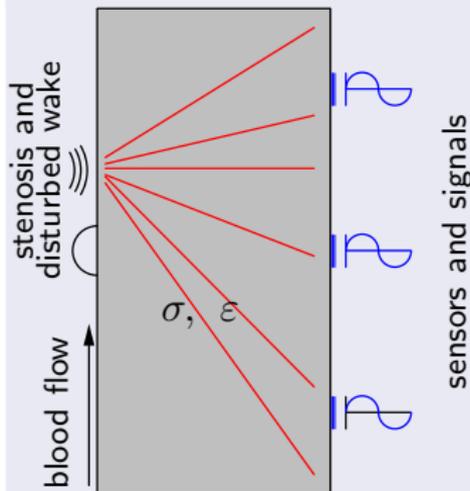
The reality...



2D is computationally tractable  
at this **early stage**

Proof of Concept: Agar Gel  
Chest Phantom

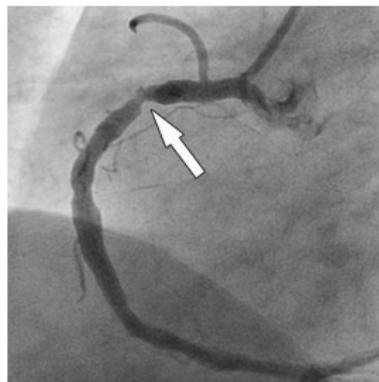
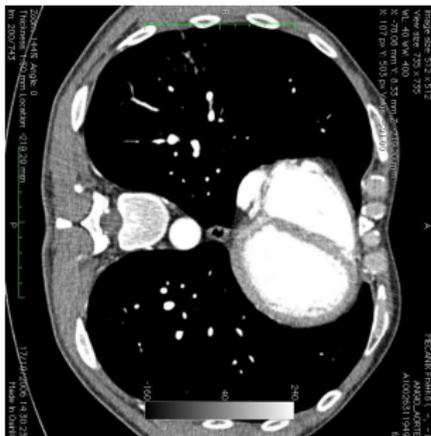
2D idealization



# Length scales of interest

Vertical chest cross section.

10cm (approx)



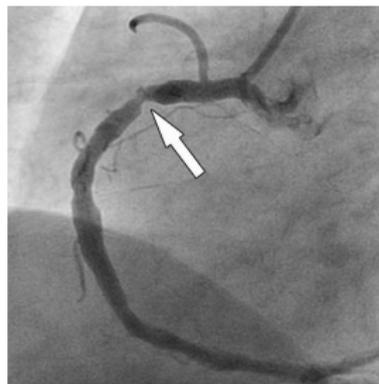
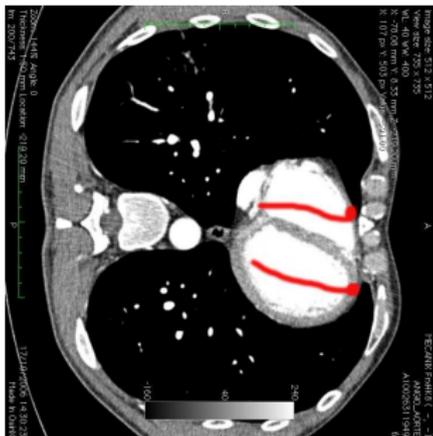
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Figure 4b from Baumüller S, Leschka S, Desbiolles L, et al. Dual-source versus 64-section CT coronary angiography at lower heart rates: comparison of accuracy and radiation dose. *Radiology* 2009;253:56-64. (c) RSNA 2009

# Length scales of interest

Vertical chest cross section.

10cm (approx)

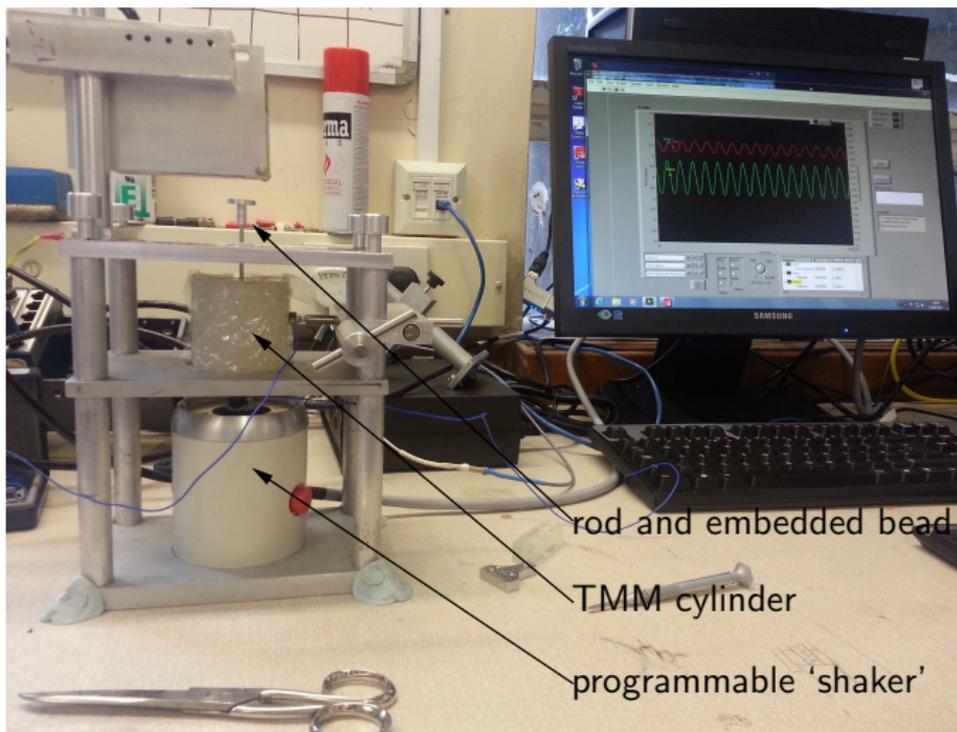


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Figure 4b from Baumüller S, Leschka S, Desbiolles L, et al. Dual-source versus 64-section CT coronary angiography at lower heart rates: comparison of accuracy and radiation dose. *Radiology* 2009;253:56-64. (c) RSNA 2009

## Acoustic Localisation of CAD

## The initial 2D rig – small scale at first



# The mathematical model — classical linear viscodynamics

$$\rho \dot{\mathbf{w}} - \nabla \cdot \underline{\boldsymbol{\sigma}} = \rho \mathbf{f} \quad + \text{initial and boundary data,}$$

with  $\mathbf{w} = \dot{\mathbf{u}}$  and constitutive relationship,

$$\underline{\boldsymbol{\sigma}}(t) = \underbrace{\underline{\mathbf{C}} \underline{\boldsymbol{\varepsilon}}(\mathbf{w}(t))}_{\text{Voigt}} + \underbrace{\underline{\mathbf{D}} \underline{\boldsymbol{\varepsilon}}(\mathbf{u}(t))}_{\text{Hooke}} + \underbrace{\underline{\mathbf{D}} \int_0^t \varphi'(t-s) \underline{\boldsymbol{\varepsilon}}(\mathbf{u}(s)) ds}_{\text{Maxwell/Zener}}$$

or internal variables for the Maxwell/Zener term,

$$\mathbf{z}_q(t) := \int_0^t \frac{\varphi_q}{\tau_q} e^{-(t-s)/\tau_q} \mathbf{u}(s) ds$$

**Linearity!!!!** Why? Justifiable? If not then is there any chance? ...

# Current status [◀ back](#)

Using the gel cylinder pictured earlier and the three outputs. . .

## Assumptions

- For tensors  $\underline{C}$  and  $\underline{D}$  we take as a constitutive law,

$$\underline{\sigma}(t) = \underbrace{\underline{C}\underline{\epsilon}(\dot{\mathbf{u}}(t))}_{\text{Voigt}} + \underbrace{\underline{D}\underline{\epsilon}(\mathbf{u}(t))}_{\text{Hooke}} + \underbrace{\underline{D} \int_0^t \varphi'(t-s)\underline{\epsilon}(\mathbf{u}(s)) ds}_{\text{Maxwell/Zener}}$$

- We assume perfect knowledge of material data by experiments (QMUL/BLT) & inverse problems (CRSC):  
 $E_0 = 229,389 \text{ Pa}$ ,  $\nu = 0.44$ ,  $E_1 = 55,284 \text{ Pa} \cdot \text{s}$ ,  
 $G_1 = 3.51 \text{ Pa} \cdot \text{s}$ ,  $\varphi(t) = 1$  and  $\rho = 1010 \text{ kg/m}^3$  on the meridian domain:  $(0.175, 2.7) \text{ cm} \times (0, 5.1) \text{ cm}$ .
- We allow **additive/multiplicative Gaussian noise** on the signals.

# Current progress on the localisation problem

Use: gel cylinder, embedded vibrator and three surface outputs. . .

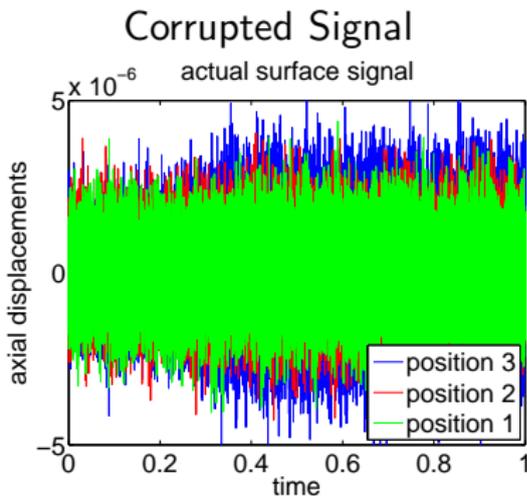
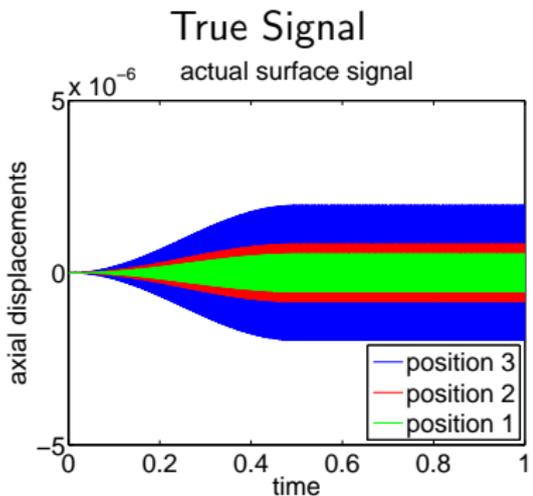
## Algorithm

- A ramped-up sinusoidal 500 Hz axial-displacement source is placed at a known position  $\bar{z}$  in the central bore.
- The forward solver computes the axial displacement surface signal at heights 13 mm, 26 mm and 39 mm.
- These 'truth' data are 'banked' and may or may not be deliberately corrupted with additive noise: **noisy truth = truth +  $N_L \times \epsilon$**  for  $N_L$  a noise level amplitude and  $\epsilon \sim N(0, 1)$ . (Or with multiplicative noise.)
- The position of the source  $\bar{z}$  is now 'forgotten'.
- `matlab's fminsearch` iteratively estimates  $\bar{z}$  given only the (noisy) truth and the forward solve outputs

Forward solver: Bicubic Galerkin finite elements were used on a  $25 \times 51$  element mesh and with 24,000 Crank-Nicolson time steps for  $0 \leq t \leq 1$  s.

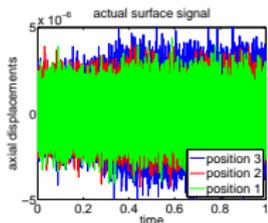
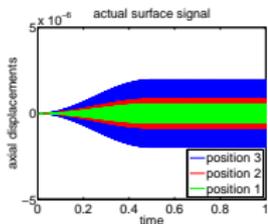
# Some results for a 500 Hz source signal.

Assume perfect knowledge of material constants.  
 Examples of a 'true' signal and a corrupted version: additive Gaussian noise, amplitude  $10^{-6}$ .

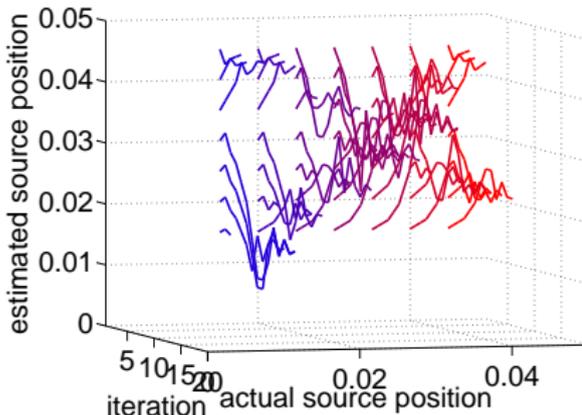


Current Status

Example: 500 Hz with  $10^{-6}$  noise

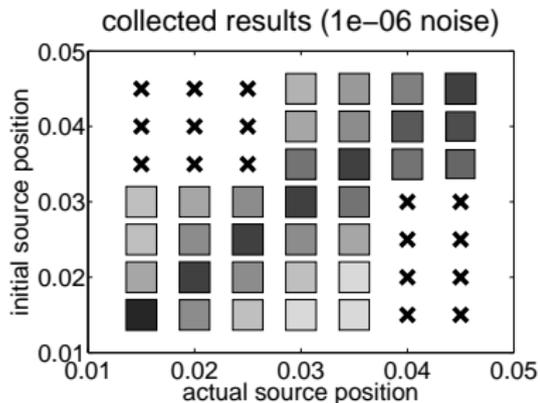


collected results: noise level =  $1.0e-06$



Well posed-ness seems to follow from a good starting value.  
Some **robustness** in the presence of significant measurement noise.

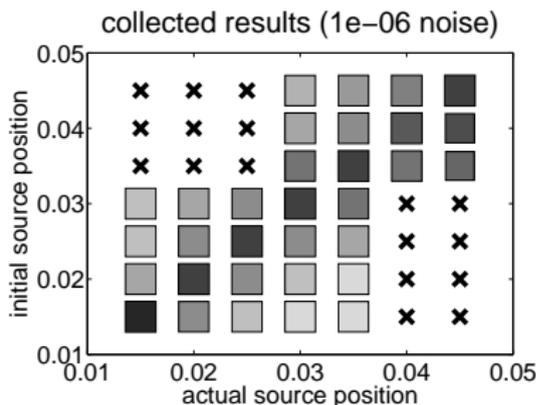
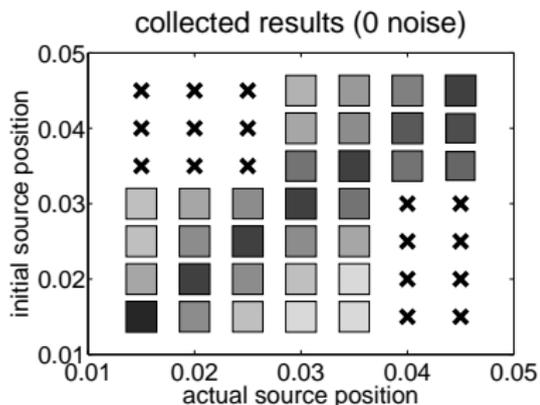
# Summary: 500 Hz with $10^{-6}$ noise



Well posed-ness seems to follow from a good starting value.  
Some **robustness** in the presence of significant measurement noise.

Current Status

# Comparison: 500 Hz no noise (left) $10^{-6}$ noise (right)



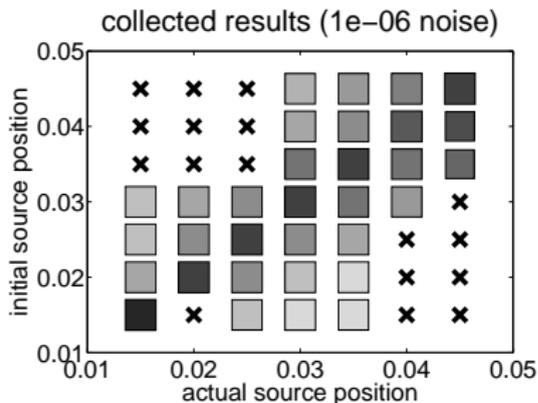
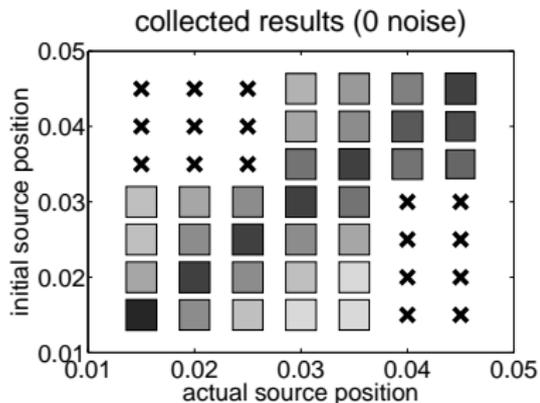
Square indicate success: darker shades mean fewer iterations.

Crosses represent failure.

Current Status

# Comparison: 500 Hz

hi-fi and noiseless (left), lo-fi with  $10^{-6}$  noise (right)



Left:  $25 \times 51$  mesh of bicubics, 24000 time steps

Right:  $25 \times 51$  mesh of bilinears, 12000 time steps

# The story so far, and what comes next

[◀ back](#)

- Little change of performance with lo-fi forward solves and very significant additive and multiplicative Gaussian signal-noise.
- Reasonably good initial guesses lead to correct localisation: **end effects seem a problem.**
- Each localization problem needs about 12 hours: need parallelism, further optimized code, . . .
- **Next step is to build and simulate a 3D virtual chest with phantom ribs, lungs, heart, arteries, skin and fat.**

[Next Steps](#)

# High Order DG-in-time FEM

[◀ back](#)

# High Order Space-Time FEM for Wave Equations

[◀ back](#)

# Space-Time Finite Elements

High order numerical schemes are known for . . .

- smaller dispersion error in wave propagation problems
- better work/accuracy ratios

We've developed **temporally high order time-diagonalised space-time finite element** codes for elasto- and visco-dynamics.

We use continuous **spectral** (i.e. Galerkin with Gauss-Lobatto) FEM in space and **discontinuous Galerkin** in time. [▶ jump](#)

We can compute easily using fifth-degree space-time polynomial approximations.

Hi-Fi solutions are not necessarily important for inverse solvers but speed/parallelism is . . .

Discretize a wave equation in time with DGFEM: for each  $n = 1, 2, \dots, N$  in turn, find  $(U, W)|_{I_n} \in \mathbb{P}_r(I_n; V) \times \mathbb{P}_r(I_n; V)$  such that

$$\begin{aligned} & \int_{I_n} (\dot{W}(t), \vartheta(t)) + a(U(t), \vartheta(t)) dt + (\llbracket W \rrbracket_{n-1}, \vartheta_{n-1}^+) + a(\llbracket U \rrbracket_{n-1}, \zeta_{n-1}^+) \\ & + \int_{I_n} a(\dot{U}(t), \zeta(t)) - a(W(t), \zeta(t)) dt = \int_{I_n} \langle L(t), \vartheta(t) \rangle dt \\ & \quad \forall \vartheta \in \mathbb{P}_r(I_n; V) \quad \text{and} \quad \forall \zeta \in \mathbb{P}_r(I_n; V), \end{aligned}$$

with IC's:  $U_0^- := \check{u}$  and  $W_0^- := \check{w}$ ; and  $\mathbb{P}_r(I_n; X)$  the space of polynomials of degree  $r$  on the time interval  $I_n$  with coefficients in the target space  $X$ . Note that  $r$  could be  $n$ -dependent.

Diagonalize following: [Werder, Gerdes, Schötzau and Schwab, CMAME 2001; 190:6685—6708.](#)

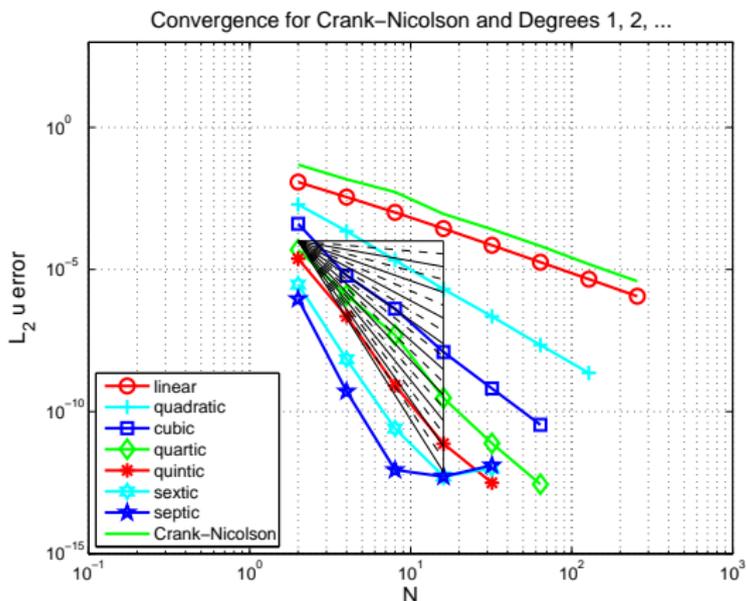
... then gives the decoupled form,

$$\begin{aligned} 2\lambda_i(Y_i, \vartheta) + k_n a(Z_i, \vartheta) &= 2F_i(\vartheta), \\ a(2\lambda_i Z_i - k_n Y_i, \vartheta) &= 2\beta_i a(U_{n-1}^-, \vartheta) \end{aligned}$$

for  $i = 0, 1, 2, \dots, r =$  the temporal polynomial degree.

This **complex symmetric** system requires just **one matrix solve for each pair**  $(Y_i, Z_i)$  and  $(U, W)$  are recovered from them.

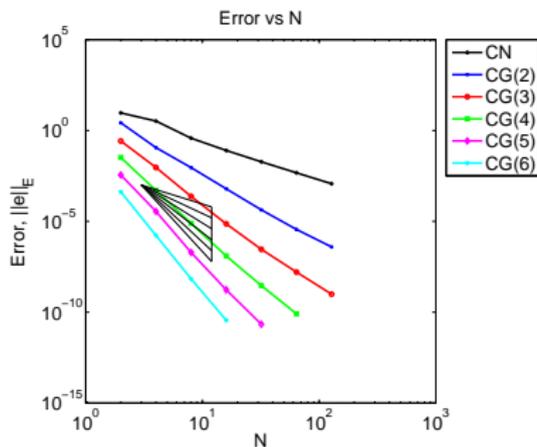
In IJNME 2014, 98:131156 (DOI: 10.1002/nme.4631), we showed that **expected convergence rates are obtained for temporal polynomial degrees up to seven**.



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◀ back

# Spectral FE for CG-in-time heat equation



Using Gauss-Lobatto for time integration. . .

In SISC, 36:B1B13 (DOI: 10.1137/130914589), we showed that **expected convergence rates are obtained for temporal polynomial degrees up to six.**

# Lots to do/test

This is to some extent empirical. Unclear how it deals with

- variable coefficients
- nonlinearities
- dispersion error
- singularities

But it is suited to the coming many-core era. . .

And one can imagine several variant schemes.

# BRUNEL MAFELAP 2016

The **fifteenth** conference on  
**The Mathematics of Finite Elements and  
Applications 2016**

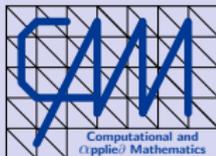
14 - 17 June 2016

Over 330 participants in 2013.

Mini-Symposia proposals welcomed.

**registration is open.**

A last thought



$$\nabla^2 \phi = 0 \quad \text{Bil}(f, v)_B = (f, v)_B \quad \forall v \in H \quad z \leftarrow z^2 + c \quad \nabla \times \vec{E} + \vec{B} = 0$$

$$u_t + u \cdot \nabla u = \frac{1}{\rho} \nabla p + \mu \nabla^2 u \quad \frac{\partial C}{\partial t} + \frac{\sigma^2 S^2}{2} \frac{\partial^2 C}{\partial S^2} + r S \frac{\partial C}{\partial S} = r C \quad \ddot{u} = c^2 \nabla^2 u$$

$$Y_t = e^{-r(T-t)} \mathbb{E}_Q(X | \mathcal{F}_t) \quad x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} \quad -\sigma_{i,j} = f_i \quad (uv)' = uv' + u'v$$

$$\varepsilon(u) := \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \quad Av = \lambda v \quad i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar}{2m} \nabla^2 \psi + V\psi$$

$$a(u, v) = f(v) \quad \forall v \in \dot{H}^1(\Omega) \quad \phi(y) = \psi(y) + \int_{\Omega} \kappa(y-x) z(x) \phi(x) dx$$

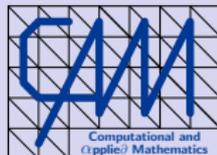
$$\frac{dy}{dx} = \frac{dy}{du} \frac{du}{dv} \frac{dv}{dx} \quad \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right) \quad \frac{\partial u}{\partial t} - \nabla^2 u = 0$$

$$\nabla \times H - \dot{D} = J \quad \frac{dS}{S} = \mu dt + \sigma dX \quad f(z_0) = \frac{1}{2\pi i} \int_{\gamma} \frac{f(z)}{z - z_0} dz$$

$$G = \left( \frac{\partial}{\partial x} \frac{\partial}{\partial y} \right) \dots$$



## A last thought



$$\nabla^2 \phi = 0 \quad \mathbb{H}(f, v)_{\mathbb{H}} = (f, v)_{\mathbb{H}} \quad \forall v \in \mathbb{H} \quad z \mapsto z^2 + c \quad \nabla \times \mathbf{E} + \mathbf{B} = 0$$

*The difference between theory and practice in practice  
is greater than  
the difference between theory and practice in theory*  
Yogi Berra, Albert Einstein, . . .

Barts Health NHS Trust

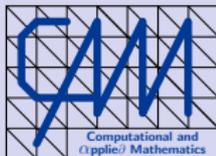
$$\nabla \times \mathbf{H} - \dot{\mathbf{D}} = \mathbf{J} \quad \frac{dS}{S} = \mu dt + \sigma dX \quad f(z_0) = \frac{1}{2\pi i} \int_{\gamma} \frac{f(z)}{z - z_0} dz$$

$$\mathbf{G} = \left( a \frac{\partial}{\partial x} \right) \left( \frac{dv}{dx} - u \frac{dv}{dx} \right) \quad v^2$$

Center for Research in Scientific Computation  
at North Carolina State University



A last thought



$$\nabla^2 \phi = 0 \quad \mathbb{H}(f, v)_H = (f, v)_H \quad \forall v \in H \quad z \mapsto z^2 + c \quad \nabla \times \mathbf{E} + \dot{\mathbf{B}} = 0$$

*The difference between theory and practice in practice  
is greater than  
the difference between theory and practice in theory*  
Yogi Berra, Albert Einstein, . . .

**THANK YOU FOR LISTENING**

$$\nabla \times \mathbf{H} - \dot{\mathbf{D}} = \mathbf{J} \quad \frac{dS}{S} = \mu dt + \sigma dX \quad f(z_0) = \frac{1}{2\pi i} \int_{\gamma} \frac{f(z)}{z - z_0} dz$$

$$\mathbf{G} = \begin{pmatrix} a & \frac{\partial}{\partial x} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial x} \end{pmatrix} \quad \frac{dv}{dx} - u \frac{dv}{dx} \quad v^2$$



# Appendix — time permitting

# Time Diagonalisation [◀ back](#)

Consider a generic wave equation in weak form: find  $u: L_2(0, T) \rightarrow V$  such that

$$\int_{I_n} (\dot{w}(t), v(t)) + a(u(t), v(t)) dt = \int_{I_n} \langle L(t), v(t) \rangle dt \quad \forall v \in L_2(0, T; V).$$

where:  $I_n = (t_{n-1}, t_n)$ ,  $w = \dot{u}$ ,  $V$  is a Hilbert space,  $a: V \times V \rightarrow \mathbb{R}$  a symmetric bilinear form and  $L: L_2(0, T) \rightarrow V'$  a time dependent linear form containing body loads and boundary tractions.

Discretize in time using Discontinuous Galerkin finite elements. . .

Discretize in time with DGFEM: for each  $n = 1, 2, \dots, N$  in turn, find  $(U, W)|_{I_n} \in \mathbb{P}_r(I_n; V) \times \mathbb{P}_r(I_n; V)$  such that

$$\begin{aligned} & \int_{I_n} (\dot{W}(t), \vartheta(t)) + a(U(t), \vartheta(t)) dt + (\llbracket W \rrbracket_{n-1}, \vartheta_{n-1}^+) + a(\llbracket U \rrbracket_{n-1}, \zeta_{n-1}^+) \\ & + \int_{I_n} a(\dot{U}(t), \zeta(t)) - a(W(t), \zeta(t)) dt = \int_{I_n} \langle L(t), \vartheta(t) \rangle dt \\ & \quad \forall \vartheta \in \mathbb{P}_r(I_n; V) \quad \text{and} \quad \forall \zeta \in \mathbb{P}_r(I_n; V), \end{aligned}$$

with the understanding that the initial conditions are  $U_0^- := \check{u}$  and  $W_0^- := \check{w}$ . Here, for each  $n$ , we use  $\mathbb{P}_r(I_n; X)$  to denote the space of polynomials of degree  $r$  on the time interval  $I_n$  with coefficients in the target space  $X$ . Note that  $r$  could be  $n$ -dependent.

Diagonalize following: [Werder, Gerdes, Schötzau and Schwab, CMAME 2001; 190:6685—6708.](#)

$$\begin{aligned}
 & \int_{I_n} (\dot{W}(t), \vartheta(t)) + a(U(t), \vartheta(t)) dt + (\llbracket W \rrbracket_{n-1}, \vartheta_{n-1}^+) + a(\llbracket U \rrbracket_{n-1}, \zeta_{n-1}^+) \\
 & + \int_{I_n} a(\dot{U}(t), \zeta(t)) - a(W(t), \zeta(t)) dt = \int_{I_n} \langle L(t), \vartheta(t) \rangle dt \\
 & \quad \forall \vartheta \in \mathbb{P}_r(I_n; V) \quad \text{and} \quad \forall \zeta \in \mathbb{P}_r(I_n; V),
 \end{aligned}$$

Let  $\{\phi_i : i = 0, 1, \dots, r\}$  be a basis for  $\mathbb{P}_r(I_n)$  and introduce the ansatz forms of the approximations to  $u$  and  $w$  on  $I_n$  as,

$$U(t)|_{I_n} = \sum_{j=0}^r \phi_j(t) U_j \quad \text{and} \quad W(t)|_{I_n} = \sum_{j=0}^r \phi_j(t) W_j$$

where  $\{U_0, U_1, \dots\}, \{W_0, W_1, \dots\} \subseteq V$ . **Replacing each of  $\vartheta(t)$  and  $\zeta(t)$  with  $\phi_i(t)\vartheta$  for  $\phi_i \in \mathbb{P}_r(I_n)$  and  $\vartheta \in V$  we obtain...**

$$\sum_{j=0}^r \int_{I_n} \dot{\phi}_j(t) \phi_i(t) (W_j, \vartheta) + \phi_j(t) \phi_i(t) a(U_j, \vartheta) dt$$

$$+ \sum_{j=0}^r \phi_{j,n-1}^+ \phi_{i,n-1}^+ (W_j, \vartheta) = \int_{I_n} \phi_i(t) \langle L(t), \vartheta \rangle dt + \phi_{i,n-1}^+ (W_{n-1}^-, \vartheta)$$

and,

$$\sum_{j=0}^r \int_{I_n} \dot{\phi}_j(t) \phi_i(t) a(U_j, \vartheta) - \phi_j(t) \phi_i(t) a(W_j, \vartheta) dt$$

$$+ \sum_{j=0}^r \phi_{j,n-1}^+ \phi_{i,n-1}^+ a(U_j, \vartheta) = \phi_{i,n-1}^+ a(U_{n-1}^-, \vartheta)$$

where each holds for all  $\vartheta \in V$  and for each  $i \in \{0, 1, \dots, r\}$ .

Define matrices via,

$$\mathbf{A}_{ij} := \int_{I_n} \dot{\phi}_j(t)\phi_i(t) dt + \phi_{j,n-1}^+ \phi_{i,n-1}^+ \quad \text{and} \quad \mathbf{M}_{ij} := \int_{I_n} \phi_j(t)\phi_i(t) dt,$$

where  $i$  indexes the rows. Choosing basis functions as the image under the linear map from  $[-1, 1]$  to  $I_n$  of the normalized Legendre polynomials gives  $2M = k_n I$  — **diagonal!**

$\mathbf{A}$  is diagonalizable over  $\mathbb{C}$  for all polynomial degrees of practical interest ( $r \leq 100$ ). Ref: Werder *et al.* CMAME 2001; 190:6685—6708.

In fact:  $\mathbf{D} = \mathbf{Q}^{-1}\mathbf{A}\mathbf{Q} = \lceil \lambda_0 \cdots \lambda_r \rceil$  where  $\lceil \cdots \rceil$  indicates a diagonal matrix of pairwise complex conjugate eigenvalues and where  $\mathbf{Q}$  has complex entries.

Using the summation convention our system is:

$$A_{ij}(W_j, \vartheta) + \delta_{ij} \frac{k_n}{2} a(U_j, \vartheta) = F_i(\vartheta),$$

$$A_{ij}a(U_j, \vartheta) - \delta_{ij} \frac{k_n}{2} a(W_j, \vartheta) = G_i(\vartheta),$$

where  $F_i$  and  $G_i$  contain known data.

Let  $\{Y_q\}$  and  $\{Z_q\}$  uniquely solve  $W_j = Q_{jq}Y_q$  and  $U_j = Q_{jq}Z_q$ :

$$A_{ij}Q_{jq}(Y_q, \vartheta) + \delta_{ij} \frac{k_n}{2} Q_{jq}a(Z_q, \vartheta) = F_i(\vartheta),$$

$$A_{ij}Q_{jq}a(Z_q, \vartheta) - \delta_{ij} \frac{k_n}{2} Q_{jq}a(Y_q, \vartheta) = G_i(\vartheta),$$

Premultiply with  $R = Q^{-1}$ , noting that,

$$R_{pi}A_{ij}Q_{jq} = \delta_{pq}\lambda_p \text{ and } R_{pi}\delta_{ij}Q_{jq} = \delta_{pq},$$

and setting  $F_i(\vartheta) := R_{ip}F_p(\vartheta)$  and  $G_i(\vartheta) := R_{ip}G_p(\vartheta) \dots$

... then gives the decoupled form,

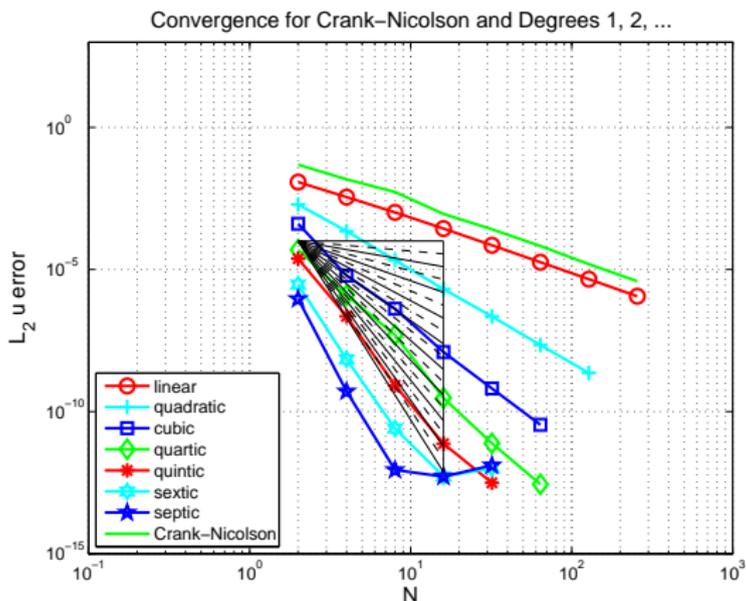
$$\begin{aligned}2\lambda_i(Y_i, \vartheta) + k_n a(Z_i, \vartheta) &= 2F_i(\vartheta), \\2\lambda_i a(Z_i, \vartheta) - k_n a(Y_i, \vartheta) &= 2G_i(\vartheta)\end{aligned}$$

for  $i = 0, 1, 2, \dots, r$  = the temporal polynomial degree.

This **complex symmetric** system requires just one matrix solve.

In IJNME 2014, 98:131156 (DOI: 10.1002/nme.4631), we showed that **expected convergence rates are obtained for temporal polynomial degrees up to seven**.

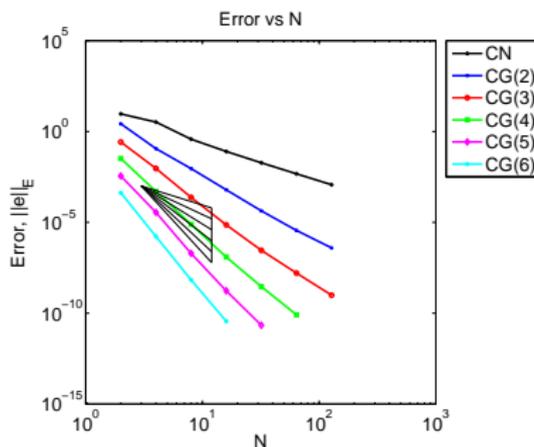
◀ back



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[← back](#)

## Spectral FE for CG-in-time heat equation



Using Gauss-Lobatto for time integration. . .

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[← back](#)